Condensed Matter Many-Body Physics and Field Theory II (TMP-TA 4)

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Winter term 2022/23

Date: February 7, 2023

Organization

- Lectures: In-person teaching, start on Oct. 17, 2022.
  - Mondays: 14:20 - 15:05 and 15:10 - 15:55 (Theresienstr. 37, A449)
  - Tuesdays: 12:00 - 12:45 and 12:50 - 13:35 (Theresienstr. 41, C111)
- Tutorial sessions: Benedikt Schneider (Schneider.Benedikt@physik.uni-muenchen.de), start on Oct. 25, 2022.
  - Tuesdays: 16:15 - 18:00 (Theresienstr. 37, A450)
  - Weekly homework will be assigned in the Monday lecture and collected one week later at the start of the lecture. The homework will be graded according to a coarse grading scheme with 0, 1 or 2 points per problem. In the tutorial session, the homework will be handed back and the solutions will be discussed.
  - A bonus on the final grade (1.3→1.0, 1.7→1.3, 2.0→1.7 etc.) will be granted to candidates who (i) earned at least 50% of all available homework points and (ii) presented at least one homework problem at the board in the tutorial session.
- Exam (9 ETCS): Tuesday Feb 14, 2023; 12:00 - 14:00 in room C111, closed book exam but one double-sided sheet of notes allowed, no electronic devices allowed, 120 minutes.
- Website including lecture notes:
  Website: https://www2.physik.uni-muenchen.de/lehre/vorlesungen/wise_22_23/TVI_TMP-TA4/index.html
- Hint: If you electronically annotate the PDF of the lecture notes, the program "PDF arranger" (for linux) allows you to merge the newly added sections with your annotated pages.

Prerequisites

- Quantum Mechanics, Solid State Theory, Statistical Physics
- Condensed Matter Many-Body Physics and Field Theory I (TMP - TA 3)
  (basics of quantum field theory, correlation functions, functional integral, generating functionals, perturbation theory)

Contents (short)

Contents

Literature

[Altland] Alexander Altland and Ben Simons, *Condensed Matter Field Theory*, Cambridge University Press, 2nd Ed. →I-IV

[Auerbach] Assa Auerbach, *Interacting Electrons and Quantum Magnetism*, Springer →IV

[Cardy] John Cardy, *Scaling and Renormalization in Statistical Physics*, Cambridge Lecture Notes in Phys. →I

[Kamenev] Alex Kamenev, *Field Theory of Non-Equilibrium Systems*, Cambridge University Press →III

[Kopietz] Peter Kopietz, Lorenz Bartosch, Florian Schütz, *Introduction to the Functional Renormalization Group*, Lecture Notes in Phys. →I,II

Part I
Critical phenomena and renormalization group

1 Phase transitions, universality and the scaling hypothesis

Aims:

- Get familiar with phase transitions in classical or quantum systems
- Phenomenology: Power laws, critical exponents, universality
- Link phenomenology to scaling hypothesis

1.1 Classification of phase transitions

- Consider macroscopic (quantum) system with Hamiltonian H in contact with heat bath (temperature T) and particle reservoir (at chemical potential μ). The grand canonical partition function is

$$\mathcal{Z}(T,\mu) = \mathrm{Tr}\left[e^{-(H-\mu N)/T}\right] \tag{1}$$

  where N is the number operator and the trace is over Fock-space with any number of particles. In the thermodynamic limit with volume $V \to \infty$ while $n = \langle N \rangle / V = const.$, we expect that the free energy is extensive,

$$F = -T \log\left[\mathcal{Z}(T,\mu)\right] = V f(T,\mu) \tag{2}$$

- We can add more coupling constants like magnetic field h, doping p etc.. In general, with k coupling constants $g_{1,2,3...,k}$, we have to consider $f(g_1, g_2, ..., g_k)$.
- In the k-dimensional coupling space, $f(g_1, g_2, ..., g_k)$ is almost everywhere analytic (locally described by convergent power series, $f(g) = a_0 + a_1(g - g_0) + a_2(g - g_0)^2 + ...$).
- Phases: Domains in coupling space where f is analytic. Phases can often be described by one or more **order parameters**, that are only non-vanishing in a particular phase.
- Phase transitions: Points, lines or other manifolds with dimension $< k$ so that f exhibits some kind of non-analyticity.
- Note: Non-analyticity of $f(g_1, g_2, ..., g_k)$ can only come from infinite summation in Tr..., so infinite systems are required.
- Classification of phase transition:
  - First order (discontinuous): There is at least one $i \in 1, ..., k$ so that at the phase boundary $\partial f / \partial g_i$ is discontinuous.
  - Second order (continuous): For all $i \in 1, ..., k$, the derivative $\partial f / \partial g_i$ is continuous.
- Quantum phase transitions:
  - Occur at $T = 0$ if some non-thermal control parameter (e.g. B-field) is varied
  - Driven by quantum fluctuations, not thermal fluctuation.
  - Same classification as above, for more details see Sec. 3.

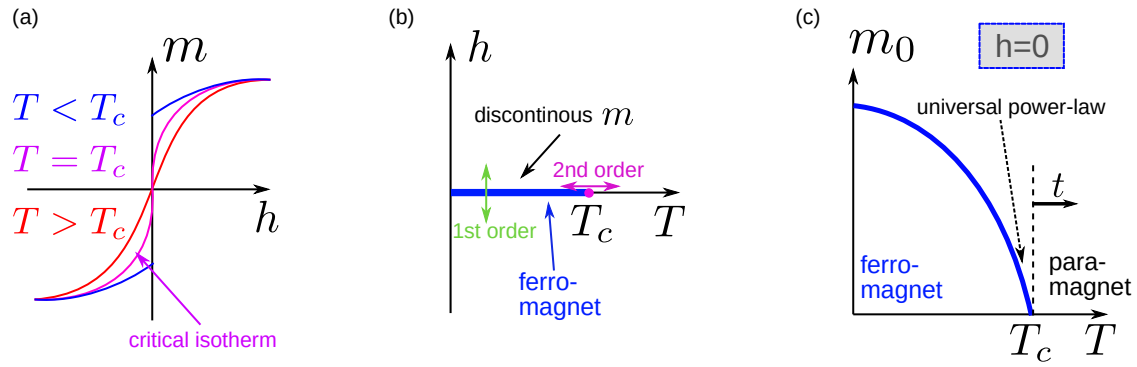


Figure 1: Sketches of the magnetization of a classical Ising model for dimension $D \geq 2$.

1.2 Example: Paramagnet-Ferromagnet transition

- Consider $g_1 = T$ and $g_2 = h$ (magnetic field), for concreteness think about the nearest neighbor classical Ising model in D-dimensions ($s_i = \pm 1$, the sum is over nearest neighbors)

$$H = -J \sum_{\langle ij \rangle} s_i s_j - h \sum_i s_i, \tag{3}$$

  At $h = 0$, we have a $\mathbb{Z}_2$ symmetry for H under $s_i \to -s_i$ for all i.

- The partition function for the Ising model is known exactly for D=1 (see Ex. 1.1) and for D=2 at $h = 0$ [Onsager,1944] (see Ex. 1.3 for a calculation of T_c for the square-lattice case)

- Magnetization per site can be calculated from free energy

$$m(T,h) = -\frac{\partial f(T,h)}{\partial h} = \lim_{V\to\infty} \frac{1}{V} \sum_i \langle s_i \rangle . \tag{4}$$

  and plot it as a function of h with T as a parameter (Fig. 1a). If we are in $D \geq 2$, there is a critical temperature $T = T_c > 0$ below which we find a discontinuity at $h = 0$ (Fig. 1b). Tuning h across this discontinuity, m jumps, so that we have a 1st order phase transition.

- Next, we focus on the limit of vanishing field,

$$m_0 \equiv -\lim_{h\to 0^+} \frac{\partial f(T,h)}{\partial h} = \lim_{h\to 0} \lim_{V\to\infty} \frac{1}{V} \left\langle \sum_i s_i \right\rangle \tag{5}$$

  (note the order of limits) and find a result as in Fig. 1c. We say that m_0 is the **order parameter** which vanishes on one side of the phase transition point.

- **Spontaneous symmetry breaking**: The state has smaller symmetry than the Hamiltonian. This occurs because under the $\mathbb{Z}_2$-symmetry, we would have $m_0 \to -m_0$.

- Critical exponent: Slightly below the critical temperature $T \lesssim T_c$, we can fit the measured magnetization to $m_0 \propto (T_c - T)^\beta$ (for $T \leq T_c$).
  The dimensionless number $\beta > 0$ is a critical exponent (do not confuse it with inverse temperature).

- Universality: β depends only on dimensionality and symmetries of the model, see table below.
  - Symmetry groups encoded by names [Ising = $\mathbb{Z}_2$, Heisenberg = $O(3)$ for continuous rotation of a classical spin]
  - Understanding of universality is one main achievement of the RG.

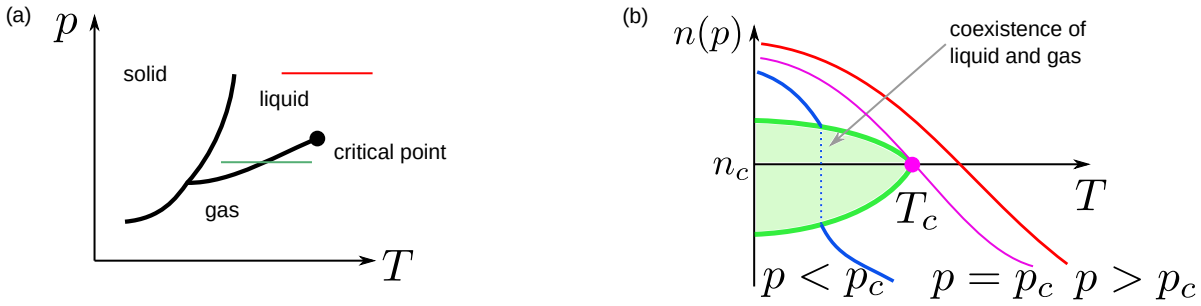


Figure 2: (a) Phase diagram of a simple fluid in the temperature pressure plane. (b) Curves of constant pressure in the temperature-density plane. The green region for $T < T_c$ is the coexistence region for liquid and gas.

– Note: The dimensionful quantity T_c is *not universal*.

	Ising ($\mathbb{Z}_2$ sym.)		Heisenberg ($O(3)$-sym.)
	D=2	D=3	D=3
β	$1/8 = 0.125$	0.327	0.36
ν	1	0.63	0.7
η	$1/4 = 0.25$	0.0364	0.027

- Examples for different members of 3D-Ising universality class (same β):
  - Uni-axial ferromagnet in 3D (see above, control T, h, observable: m)
  - Simple fluid (Fig. 2). Control T, p, observable: density $n = -\partial f/\partial\mu$. Focus on gas-liquid transition.
    * Gas and liquid have same symmetry
    * Difference to magnet: $\int d\mathbf{r} n(\mathbf{r}) = const.$, leads to coexistence of gas and liquid at 1st order line.
    * Exponent β defined via shape of green coexistence curves: $n_{liquid} - n_{gas} \propto (T_c - T)^\beta$
    * Where is the $\mathbb{Z}_2$ symmetry? Lattice gas approximation, correspondence $s_i = +1 \hat{=}$occupied site and $-1 \hat{=}$empty site $\rightarrow$ Ising model, emergent $\mathbb{Z}_2$ symmetry close to critical point.

- Other thermodynamic observables with their respective critical exponents (historical notation). Definition of "reduced temperature": $t \equiv (T - T_c)/T_c$.

magnetization at $h = 0$	specific heat
$m(t) = -\frac{\partial f}{\partial h}\|_{h=0} \propto \|t\|^\beta$ $(t < 0)$	$C(t) = T_c^{-1} \frac{\partial^2 f}{\partial t^2}\|_{h=0} \propto \|t\|^{-\alpha}$
magnetic susceptibility	critical $(t = 0)$ isotherm
$\chi(t) = \frac{\partial^2 f}{\partial h^2}\|_{h=0} \propto \|t\|^{-\gamma}$	$m(t = 0, h) = -\frac{\partial f}{\partial h}\|_{t=0} \propto \|h\|^{1/\delta} \mathrm{sgn}(h)$

1.3 Correlation function, anomalous dimension and correlation length exponent

- Split local magnetization into average and fluctuating part,

$$s(\mathbf{r}) = m + \delta s(\mathbf{r}) \tag{6}$$

where

$$m = \langle s(\mathbf{r}) \rangle = \frac{\mathrm{Tr}\left[s(\mathbf{r}) e^{-(H-\mu N)/T}\right]}{\mathrm{Tr}\left[e^{-(H-\mu N)/T}\right]} \tag{7}$$

and $\langle \delta s(\mathbf{r}) \rangle = 0$.

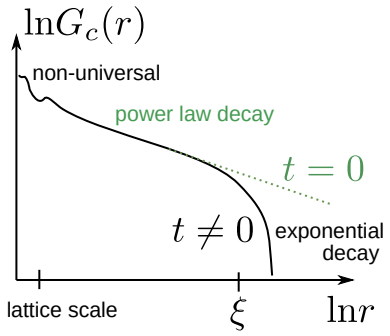


Figure 3: Connected correlation function in real-space close to a phase transition point with regions of power-law and exponential decay.

- Correlation function covers spatial correlations of local order parameter with non-decaying contribution subtracted ("connected" correlation function):

$$G(\mathbf{r}) = \langle \delta s(\mathbf{r}) \delta s(0) \rangle = \langle s(\mathbf{r}) s(0) \rangle - m^2 \tag{8}$$

  Hallmark of approaching continuous phase transition: Microscopic degrees of freedom become increasingly correlated over larger length scales and behave as a single entity.

- Large-r behavior of correlation function defines two other critical exponents (Fig. 3):

$$G(r \to \infty) \propto \begin{cases} 1/r^{D-2+\eta} & : t = 0 \\ e^{-r/\xi}/\sqrt{\xi^{D-3} r^{D-1}} & : t \neq 0 \end{cases} \tag{9}$$

  The values of η, ν for some universality classes are given in the above table.

- At criticality $t = 0$:
  - There is **no characteristic length** scale in the decay of $G(r)$
  - $G(r)$ decays with a power-law, defines universal **anomalous dimension** $\eta > 0$
  - Later: $\eta = 0$ characterizes critical points with non-interacting critical fluctuations ("Gaussian approximation")

- Away from criticality $t \neq 0$:
  - Correlations are characterized by finite **emergent** correlation length ξ

$$\boxed{\xi \propto |t|^{-\nu}} \tag{10}$$

    where ν is the universal **correlation length exponent**.
  - ξ is length scale for exponential decay, $G(r) \propto e^{-r/\xi}$.
  - Exponential decay sets in beyond $r \sim \xi$.
  - For $r \ll \xi$, find power-law decay as in the critical case (Fig. 3).

1.4 Scaling hypothesis

- Experimental finding: Critical exponents $\alpha, \beta, \gamma, \delta, \nu, \eta$ are not independent.
  They can be computed from two numbers y_t and y_h characteristic for each universality class:

$\alpha = 2 - D/y_t$	$\beta = (D - y_h)/y_t$	$\gamma = (2y_h - D)/y_t$	$\delta = y_h/(D - y_h)$	$\nu = 1/y_t$	$\eta = D + 2 - 2y_h$

- This can be understood from a **scaling hypothesis** for the free energy and the correlation function.

- The scaling hypothesis was postulated in the 1960s by Widom and Kadanoff and was later justified via the RG.

Scaling hypothesis for free energy

- Assume that close to the critical point, we have a regular and singular part of the free energy $f(t,h) = f_{sing}(t,h) + f_{reg}(t,h)$. The singular part contains the non-analyticity.
- Scaling hypothesis (for singular part) with an *arbitrary* dimensionless scale factor b takes the form of homogeneity relation:

$$\boxed{f_{\text{sing}}(t,h) = b^{-D} f_{\text{sing}}\left(b^{y_t} t, b^{y_h} h\right)} \tag{11}$$

- Finding $\beta = \beta(y_t, y_h)$ (magnetization at zero field): Since b was arbitrary, let $b^{y_t} = 1/|t|$ and thus $b = |t|^{-1/y_t}$.

$$f_{\text{sing}}(t,h) = |t|^{D/y_t} \underbrace{f_{\text{sing}}\left(\pm 1, \frac{h}{|t|^{y_h/y_t}}\right)}_{\equiv \Phi_{\pm}\left(\frac{h}{|t|^{y_h/y_t}}\right)} \tag{12}$$

  Assume that around the phase transition, derivatives of $f(t,h)$ are dominated by its singular part ("$\simeq$" signs):

$$m(t,h) \simeq -\frac{\partial f_{\text{sing}}}{\partial h} = |t|^{(D-y_h)/y_t} \Phi'_{\pm}\left(\frac{h}{|t|^{y_h/y_t}}\right) \tag{13}$$

  We can let $h = 0$ and read off $\beta = (D - y_h)/y_t$ as in the table above. In a similar manner one can find α and γ.
- Finding $\delta = \delta(y_t, y_h)$ (critical isotherm): We need to let $t \to 0$ in Eq. (13). To find something finite, we request that $\Phi'_{\pm}(x) \sim x^{D/y_h - 1}$. Then $m(t=0,h) \propto h^{D/y_h - 1}$ and we can read off $\delta = y_h/(D - y_h)$.

Scaling hypothesis for correlation function

- To relate $\{\nu, \eta\}$ to $\{y_t, y_h\}$, we conjecture a scaling hypothesis for the singular part of the correlation function

$$\boxed{G_{\text{sing}}(r;t,h) = b^{-2(D-y_h)} G_{\text{sing}}\left(r/b; b^{y_t} t, b^{y_h} h\right)} \tag{14}$$

  and put again $b^{y_t} = 1/|t|$. We also set $h = 0$:

$$G_{\text{sing}}(r;t,h=0) = |t|^{2(D-y_h)/y_t} \underbrace{G_{\text{sing}}\left(r|t|^{1/y_t}; \pm 1, 0\right)}_{\equiv \Psi_{\pm}\left(r|t|^{1/y_t}; \pm 1, 0\right)} \tag{15}$$

- For $|t| \neq 0$, expect $G_{\text{sing}}(r) \propto e^{-r/\xi}$ which yields $\xi \propto |t|^{-1/y_t}$ and thus the expression $\nu = 1/y_t$ follows.
- For $|t| = 0$, to get a finite (non-zero) $G_{\text{sing}}(r; t=0, h=0)$, we request:

$$\Psi_{\pm}\left(r|t|^{1/y_t}; \pm 1, 0\right) \propto \left(r|t|^{1/y_t}\right)^{-2(D-y_h)} \tag{16}$$

  We compare to Eq. 9, we read off $D - 2 + \eta = 2(D - y_h)$ from which the expression in the table follows.
- Remark: Scaling hypothesis yields experimentally testable...
  - scaling relations, e.g.

$$2 - \alpha = 2\beta + \gamma = \beta(\delta + 1) \tag{17}$$

  - hyperscaling relations (relating power-laws for thermodynamic observables with the $G(r)$-exponents)

$$2 - \alpha = D\nu$$
$$\gamma = (2 - \eta)\nu$$

Dynamical critical exponent

- For time-dependent $G(r,\tau)$, the correlation time τ_c is the decay time of order-parameter fluctuations. It relates to the correlation length via a power law:

$$\tau_c \propto \xi^z \propto |t|^{-\nu z} \tag{18}$$

- z is the **dynamical critical exponent**, it controls the relative speed of divergence of the temporal and spatial correlation length.
- **Critical slowing down**: Order parameter fluctuations decay slower and slower as one gets closer and closer to the critical point.
  See Ex. 1.2 for an application involving z.

Exercises

Exercise 1.1. Classical Ising model in 1D: Exact solution

Consider the nearest-neighbor classical Ising model of Eq. (3) on a ring of N sites (in $D = 1$ dimensions) with periodic boundary conditions.

1. Show that the partition function can be written as $\mathcal{Z} = \mathrm{Tr}\left[\mathbf{T}^N\right]$ with the *transfer matrix* given by

$$\mathbf{T} = \begin{pmatrix} e^{(J+h)/T} & e^{-J/T} \\ e^{-J/T} & e^{(J-h)/T} \end{pmatrix} \tag{19}$$

2. Using the eigenvalues of $\mathbf{T}$, show that in the thermodynamic limit ($N \to \infty$) the free energy per spin reads

$$f(h,T) = -J - T\ln\left[\cosh(h/T) + \sqrt{\sinh^2(h/T) + e^{-4J/T}}\right]. \tag{20}$$

   Show that one can approximate

$$f(h,T) = \begin{cases} -J - Te^{-2J/T} & : h = 0, \\ -J - |h| - Te^{-4J/T}e^{-2|h|/T} & : h \neq 0, \end{cases} \tag{21}$$

   if $T \ll J$ or $T \ll J, |h|$, respectively. Argue that there is a critical line at $(T = 0, h)$ but no phase transition at any finite temperature.

3. Roughly sketch the magnetization per spin $m(T,h) = -\frac{\partial f}{\partial h}$ as a function of h for various T (no new calculation needed).

4. Confirm that the spin-spin correlation function can be expressed as

$$\langle s_j s_1\rangle = \frac{1}{\mathcal{Z}}\mathrm{Tr}\left[\mathbf{S}\mathbf{T}^{j-1}\mathbf{S}\mathbf{T}^{N-j+1}\right], \text{ with } \mathbf{S} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{22}$$

   Confirm that for $N \to \infty$, we have $\langle s_j s_1\rangle = \langle s_1\rangle^2 + c\left(\lambda^-/\lambda^+\right)^{j-1}$ where c is a constant independent of j that does not need to be determined. Set $h = 0$ and find the correlation length ξ as a function of T by matching $G_j = \langle s_j s_1\rangle - \langle s_1\rangle^2 \propto e^{-r/\xi}$. *Hint: There is no need to compute the eigenvectors of* $\mathbf{T}$ *explicitly.*

Exercise 1.2. Kibble-Zurek mechanism

Let a continuous phase transition with control parameter t be equipped with universal critical exponents ν, z as defined above. In contrast to the discussion for the equilibrium case above, the control parameter is now varied in time τ from the disordered ($t > 0$) towards the ordered ($t < 0$) side following the linearized approximation

$$t(\tau) \propto -\lambda\tau \tag{23}$$

so that the equilibrium critical value $t = 0$ is crossed at $\tau = 0$. It can be expected that instead of a spatially homogeneous order parameter, the driving at finite velocity λ results in a random configuration of ordered domains of finite size l.

1. Argue that the time-evolution of the system can be divided in three stages where the dynamics is essentially adiabatic far away from $\tau = 0$ for $|t| > \tilde{t}$ and frozen otherwise. Show that

$$\tilde{t} \propto \lambda^{1/(1+\nu z)}. \tag{24}$$

2. Show that the typical domain size l depends on the driving velocity λ as

$$l \propto \lambda^{-\nu/(1+\nu z)}. \tag{25}$$

The remarkable prediction of Eq. 25 connects *static* critical exponents z, ν to the observable l measured in a *dynamic* protocol. It can be used in experiment, see e.g. [Ebadi et al., Nature **595**, 227 (2021)] around Fig. 3 for a recent example involving a quantum phase transition of the 2+1 dimensional Ising universality class.

Exercise 1.3. Classical Ising model in 2D: Critical temperature from duality

Consider the nearest-neighbor Ising model (3) at vanishing magnetic field $h = 0$ for a square lattice in D=2 with periodic boundary conditions and N sites. The goal is to find the critical temperature T_c from a duality argument. To simplify notation, set $K = J/T$.

1. High-temperature expansion: Show that the partition function can be written as

$$\mathcal{Z} = \sum_{\{s_i\}=\pm 1} \prod_{n.n.} e^{K s_i s_j} = (\cosh K)^{N_b} \sum_{\{s_i\}=\pm 1} \prod_{\langle i,j \rangle} (1 + s_i s_j v) = 2^N (\cosh K)^{N_b} \sum_r n(r) v^r \tag{26}$$

where $N_b = N/2$ is the number of bonds and $v = \tanh K$. If a bond in the expansion is denoted by a black line as in Fig. 4(a), argue that only closed graphs as in (c) contribute to the partition function. The number of closed graphs with r bonds is $n(r)$. In what sense does Eq. (26) represent a high-temperature expansion?

2. Low-temperature expansion: Starting from the ferromagnetic ground state, show that the partition function can be written as

$$\mathcal{Z} = e^{K N_b} \sum_r m(r) e^{-2Kr} \tag{27}$$

with $m(r)$ the number of distinct ways to arrange r unsatisfied bonds $\langle i, j \rangle$ with $s_i s_j = -1$ on the lattice.

3. Consider the dual lattice "D" with lattice points (blue $\star$) at the crossings of dashed lines that cut orthogonally through the midpoints of bonds of the original lattice, see Fig. 4(e) and argue that $m(r) = n_D(r)$ and $n(r) = m_D(r)$. Use this to show the following relation between partition functions on the original and dual lattice,

$$\mathcal{Z}(K) = 2^{-N_D} e^{K N_b} (\cosh K^\star)^{-N_{D,b}} \mathcal{Z}_D(K^\star) \tag{28}$$

where the couplings are related by $e^{-2K} = \tanh K^\star \equiv v^\star$.

4. Use the fact that the dual lattice of the square lattice is again a square lattice and the assumption that there is only a single critical temperature T_c to conclude $\sinh 2K_c^\star = 1$.

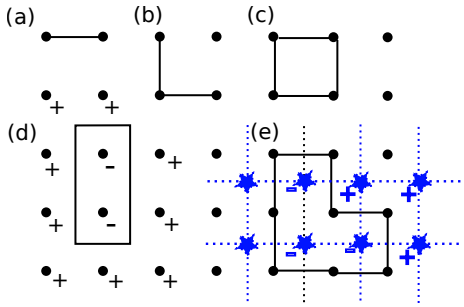


Figure 4: Duality for Ising model on D=2 square lattice: Graphs with r=1,2,3 bonds are shown in (a),(b),(c) and a domain wall around 2 minority spins is shown in (d). Panel (e) shows that domain walls correspond to closed graphs on the dual (blue-starred) lattice.

2 Mean-field theory and Gaussian approximation

Aims:

- Simple microscopic description of phase transitions
- Mean-field theory (MFT): Neglect fluctuations
- Gaussian approximation: Include fluctuations which are exactly tractable

2.1 Mean-field theory

- Recall D-dimensional nearest-neighbor Ising model, Eq. (3), $H = -J\sum_{\langle ij\rangle} s_i s_j - h\sum_i s_i$. Set $\beta \equiv 1/T$ (don't confuse with critical exponent!).
- (Thermal-) fluctuation: More than one most likely configuration $\{s_i\}$ contributes to the partition function

$$\mathcal{Z} = \sum_{\{s_i\}=\pm 1} e^{-\beta H[\{s_i\}]} \tag{29}$$

- Idea: Split s_i into average value $m \in \mathbb{R}$ and **fluctuation**, see Eq. (6):

$$s_i = \underbrace{\langle s_i \rangle}_{m} + \delta s_i \tag{30}$$

- Mean-field approximation: Neglect terms in H quadratic in the fluctuation:

$$s_i s_j = (m+\delta s_i)(m+\delta s_j) = m^2 + m(\delta s_i + \delta s_j) + \delta s_i \delta s_j \simeq m^2 + m(\delta s_i + \delta s_j) = -m^2 + m(s_i + s_j) \tag{31}$$

and obtain (with $\sum_{\langle ij\rangle}$ counting bonds!)

$$H_{MF} = \frac{NzJ}{2} m^2 - \sum_i (h + zJm)\, s_i$$

$$z = \text{coordination number, N} = \#\text{sites}$$

- Partition function in mean-field approximation:

$$\begin{aligned}
\mathcal{Z}_{MF}(T,h;m) &= \sum_{\{s_i\}=\pm 1} e^{-\beta H_{MF}} && (32)\\
&= \sum_{\{s_i\}=\pm 1} e^{-\beta \frac{NzJ}{2} m^2 + \sum_i \beta(h+zJm)s_i} && (33)\\
&= e^{-\beta \frac{NzJ}{2} m^2} \prod_i \left[\sum_{s_i=\pm 1} e^{\beta(h+zJm)s_i} \right] && (34)\\
&= e^{-\beta \frac{NzJ}{2} m^2} \left\{ 2\cosh\left[\beta(h+zJm)\right] \right\}^N && (35)\\
&= e^{-\beta N \mathcal{L}_{MF}(T,h;m)} && (36)
\end{aligned}$$

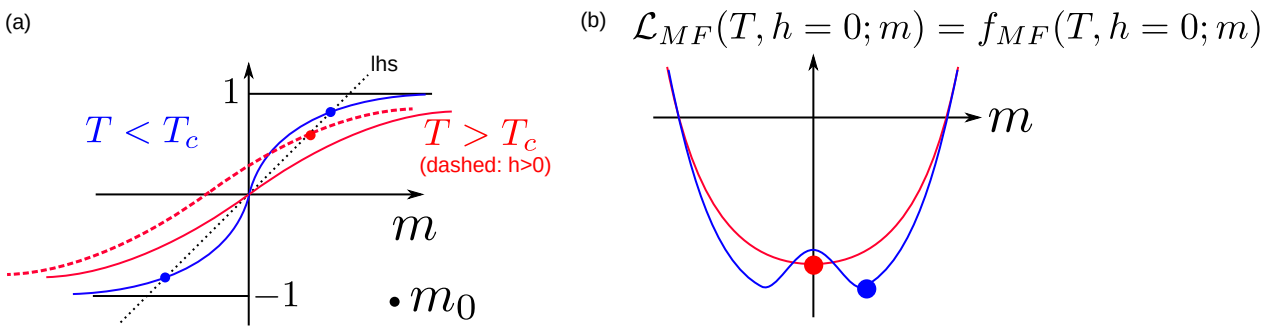


Figure 5: Mean-field approximation for the Ising model. Panel (a) shows the graphical solution of Eq. (39) and panel (b) the Landau function above (red) and below (blue) the critical temperature.

Note: m is yet to be determined! With the approximation the sum of exponentials factorizes and one obtains the partition function of a single spin in an effective field $h_{eff} = h + zJm$.

- **Landau-function:**

$$\mathcal{L}_{MF}(T, h; m) = \frac{zJ}{2} m^2 - T \ln\left[2 \cosh\left[\beta\left(h + zJm\right)\right]\right] \tag{37}$$

determines the probability density $e^{-\beta N \mathcal{L}_{MF}(T,h;m)}$ to observe order parameter m.

- MFT-prediction for physically realized value of m (denoted by m_0): The *most probable* value. $\Rightarrow$ Find minimum of $\mathcal{L}_{MF}(T, h; m)$.

$$\frac{\partial \mathcal{L}_{MF}(T, h; m)}{\partial m}|_{m=m_0} \stackrel{!}{=} 0 \tag{38}$$

which defines $m_0(T, h)$ and leads to

$$\boxed{m_0 \stackrel{!}{=} \tanh\left[\beta\left(h + zJm_0\right)\right]} \tag{39}$$

- Free energy density: Once m_0 is determined as a function of T, h, we find:

$$f_{MF}(T, h) = \mathcal{L}_{MF}\left(T, h; m_0\left(T, h\right)\right) \tag{40}$$

- Remarks:
  - For $h \neq 0$, there is always at least one non-trivial solution, see Fig. 5a. If there are two solutions (for $T < T_c$ and, possibly, $h \neq 0$), one has to find the one with the smaller $\mathcal{L}_{MF}(T, h; m_0)$.
  - First-order phase transition: For $T < T_c$ and changing h across 0, the minimum m_0 jumps discontinously. This corresponds to a first-order phase transition.
  - Eq. (39) can also be found directly from the self-consistency equation

$$\begin{aligned} m_0 &= \frac{1}{\mathcal{Z}_{MF}(T, h; m_0)} \sum_{\{s_i\}=\pm 1} s_j e^{-\beta H_{MF}} \\ &= \frac{1}{\sum_{s_j=\pm 1} e^{\beta(h+zJm_0)s_j}} \sum_{s_j=\pm 1} s_j e^{\beta(h+zJm_0)s_j} \end{aligned}$$

  - Before m_0 is determined, $\mathcal{L}_{MF}(T, h; m)$ is not a proper free energy as it contains magnetization m which is not a control parameter like T or h. In particular, in some situations the global minimum of $\mathcal{L}_{MF}(T, h; m)$ with respect to m can be different from the local minimum which yields the correct condition (39).

Mean-field critical temperature

- Set $h = 0$ to find critical temperature: Compare the slopes on the left and the right-hand-side of Eq. (39). Obtain two non-zero m_0-solutions below a critical temperature

$$T_{c,MF} \equiv zJ. \tag{41}$$

- Example: Hyper-cubic lattice in D-dimensions: $z = 2D \rightarrow T^D_{c,MF} = 2DJ$.
  Compare to exact results: For D=1, $T_c^{D=1} = 0$; for D=2, $T_c^{D=2} = 2.269J$ (which derives from $\sinh(2J/T_c) = 1$, see Ex. 1.3). For $D \geq 3$, Monte-Carlo simulations are required.

D	1	2	3	4	5	6	7
$T_c^D/T^D_{c,MF}$	0	0.57	0.752	0.835	0.878	0.903	0.919

- General rule:
  - The lower D, the more important are fluctuations that disorder the system and thus reduce T_c.
  - In large D, fluctuations tend to average out.

Mean-field thermodynamic critical exponents

- For temperatures $T \simeq T_{c,MF}$, the minimum of $\mathcal{L}_{MF}(T, h; m)$ is close to $m = 0$. Expand Landau-function in m (see Fig. 5b):

$$\mathcal{L}_{MF}(T, h; m) = f + \frac{r}{2}m^2 + \frac{u}{4!}m^4 - hm + ... \tag{42}$$

  with $(\ln[2\cosh x] = \ln 2 + \frac{x^2}{2} - \frac{x^4}{12} + \mathcal{O}(x^6))$

$$f = -T\ln 2 \tag{43}$$
$$r = \frac{T_{c,MF}}{T}(T - T_{c,MF}) \simeq T - T_{c,MF} \tag{44}$$
$$u = 2T(T_{c,MF}/T)^4 \simeq 2T_{c,MF} \tag{45}$$

- Find m_0 from $\frac{\partial \mathcal{L}_{MF}(T,h;m)}{\partial m}|_{m=m_0} \stackrel{!}{=} 0$ and neglect higher order terms (...):

$$rm_0 + \frac{u}{6}m_0^3 = h \tag{46}$$

- Read off critical exponents in MFT:
  - Mean-field exponents are independent of dimension D.
  - We find, e.g. $\beta_{MF} = 1/2$ far from the exact results $\beta^{Ising}_{D=2} = 0.125$ or $\beta^{Ising}_{D=3} = 0.327$.

Ising mean-field critical exponents			
α	β	γ	δ
0 (C jumps)	1/2	1	3

- Remark: Critical exponents ν, η are defined via $G(r)$. These cannot be described in MFT if a spatially homogeneous order parameter is assumed.

2.2 Continuum φ^4-field theory for the Ising model

Heuristic derivation of continuum field theory

- Heuristic steps to continuum field theory (detail in Ex. 2.1):
  - Consider again

$$\mathcal{Z} = \sum_{\{s_i=\pm 1\}} \exp\left[-\beta H\right] = \sum_{\{s_i=\pm 1\}} \exp\left[\beta J \sum_{\langle ij\rangle} s_i s_j + \beta h \sum_i s_i\right] \tag{47}$$

  - Smooth discrete spins $s_i = \pm 1$ over a region $V_{\mathbf{r}}$ of volume $[1/\Lambda_0]^D$ to obtain the field $\varphi(\mathbf{r})$ instead of the spins.
  - The field φ and space coordinate $\mathbf{r}$ are now **continuous**. This is beneficial for subsequent approximations.
  - Motivation: We could not do the sum $\sum_{\{s_i=\pm 1\}} e^{-cs_i s_j}$, but we know how to do Gaussian integrals over N-component real field, $(2\pi)^{-N/2}\int_{-\infty}^{+\infty} d\boldsymbol{\varphi} e^{-\frac{1}{2}\boldsymbol{\varphi}^T M \boldsymbol{\varphi}} = 1/\sqrt{\det M}$.
- **Functional integral** (c.f. field-theory I): Integrate over probability $e^{-S_{\Lambda_0}[\varphi(\mathbf{r})]}$ of $\varphi(\mathbf{r})$ configurations in the thermodynamic ensemble:

$$\mathcal{Z} = \int \mathcal{D}\left[\varphi\right] e^{-S_{\Lambda_0}[\varphi]} \tag{48}$$

- Expand $S_{\Lambda_0}\left[\varphi\right]$: Close to the critical point, $\varphi(\mathbf{r}) \sim m$ is small and fluctuations are smooth.
- Obtain the **Ginzburg-Landau-Wilson action** (form can be guessed by symmetry):

$$\begin{aligned} S_{\Lambda_0}\left[\varphi\right] &= \int d^D\mathbf{r}\left[f_0 - h_0\varphi(\mathbf{r}) + \frac{r_0}{2}\varphi^2(\mathbf{r}) + \frac{c_0}{2}\left[\nabla\varphi(\mathbf{r})\right]^2 + \frac{u_0}{4!}\varphi^4(\mathbf{r})\right] && (49)\\ &\overset{(FT)}{=} V f_0 - h_0\varphi(\mathbf{k}=0) + \frac{1}{2}\int_{\mathbf{k}}\left[r_0 + c_0 k^2\right]\varphi(-\mathbf{k})\varphi(\mathbf{k}) && (50)\\ &+ \frac{u_0}{4!}\int_{\mathbf{k}_{1,2,3,4}} (2\pi)^D \delta\left(\mathbf{k}_1 + ... + \mathbf{k}_4\right)\varphi(\mathbf{k}_1)\varphi(\mathbf{k}_2)\varphi(\mathbf{k}_3)\varphi(\mathbf{k}_4) \end{aligned}$$

  with (see Ex. 2.1, a = lattice-constant of hyper-cubic lattice)

$$\begin{aligned} f_0 &\equiv -a^{-D}\ln 2 && (51)\\ h_0 &\equiv \beta h a^{-1-D/2} && (52)\\ r_0 &\equiv \frac{T - T_c}{a^2 T_c} && (53)\\ c_0 &\equiv 1/(2D) && (54)\\ u_0 &\equiv 2a^{D-4} && (55) \end{aligned}$$

- Remarks:
  - There should be a cut-off at the momentum integrals at $k \leq \Lambda_0$.
    Reason: No information on the spin fluctuations below coarse graining length scale $1/\Lambda_0$.
  - Conventions used: $\varphi(\mathbf{r}) \equiv \int_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}\varphi(\mathbf{k})$ and $\frac{1}{V}\sum_{\mathbf{k}} \to (2\pi)^{-D}\int_{-\infty}^{+\infty} d^D\mathbf{k} \equiv \int_{\mathbf{k}}$
  - Dimension of the fields $[\varphi(\mathbf{k})] = [a]^{1+D/2}$ and $[\varphi(\mathbf{r})] = [a]^{1-D/2}$.
  - Identity $\int_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} = \delta(\mathbf{r})$ is only strictly correct for $\Lambda_0 \to \infty$.

Recovering mean-field theory

- Use the **saddle point approximation** which approximates $\varphi(\mathbf{r}) \to \bar{\varphi}$ (homogeneous field):

$$\mathcal{Z} \simeq \int_{-\infty}^{+\infty} \frac{d\bar{\varphi}}{\sqrt{2\pi}} e^{-S_{\Lambda_0}[\bar{\varphi}]} = \int_{-\infty}^{+\infty} \frac{d\bar{\varphi}}{\sqrt{2\pi}} \exp\left[-V\left(f_0 + \frac{r_0}{2}\bar{\varphi}^2 + \frac{u_0}{4!}\bar{\varphi}^4 - h_0\bar{\varphi}\right)\right] \tag{56}$$

- In the limit $V \to \infty$, the integrand is strongly peaked. Let $\bar{\varphi}$ attain its most probable value $\bar{\varphi}_0$:

$$0 \overset{!}{=} \frac{\partial S_{\Lambda_0}[\bar{\varphi}]}{\partial \bar{\varphi}}|_{\bar{\varphi}=\bar{\varphi}_0} = r_0\bar{\varphi}_0 + \frac{u_0}{6}\bar{\varphi}_0^3 - h_0 = 0 \tag{57}$$

  This is the same as the MF equation (42) if we identify (proportionality factors will be worked out in the exercise)

$$\bar{\varphi} \propto m \tag{58}$$
$$r_0, u_0, h_0 \propto r, u, h \tag{59}$$

- Relation between the Landau function and the saddle-point action:

$$S_{\Lambda_0}[\bar{\varphi} \propto m] = \beta N \mathcal{L}_{MF}(T, h; m) \tag{60}$$

- Conclusion:
  MFT = Saddle-point approximation for functional integral representation where spatial fluctuations of order parameter are ignored.

2.3 Gaussian approximation

Truncating the action

- Split $\varphi(\mathbf{r})$ in homogeneous part and fluctuation (c.f. idea of MFT, but still exact):

$$\varphi(\mathbf{r}) = \bar{\varphi}_0 + \delta\varphi(\mathbf{r})$$
$$\varphi(\mathbf{k}) = (2\pi)^D \delta(\mathbf{k})\bar{\varphi}_0 + \delta\varphi(\mathbf{k})$$

- In MFT above, we discarded the quadratic order fluctuation terms $\delta s_i \delta s_j$ **in Hamiltonian** because we had no way to compute them.
  Now: **Keep $\delta\varphi(\mathbf{k})\delta\varphi(-\mathbf{k})$ in action**, can now be evaluated using Gaussian functional integral.

- Assume $h_0 = 0$ (such that $r_0\bar{\varphi}_0 + \frac{u_0}{6}\bar{\varphi}_0^3 = 0$).
  Obtain the Gaussian approximation of the φ^4-action Eq. (49):

$$S_{\Lambda_0}[\bar{\varphi}_0 + \delta\varphi] = V\left[f_0 + \frac{r_0}{2}\bar{\varphi}_0^2 + \frac{u_0}{4!}\bar{\varphi}_0^4\right] + \underbrace{\left[r_0\bar{\varphi}_0 + 4\frac{u_0}{4!}\bar{\varphi}_0^3\right]}_{\to 0}\delta\varphi(\mathbf{k}=0)$$
$$+ \frac{1}{2}\int_{\mathbf{k}}\left[r_0 + c_0k^2 + \frac{4\cdot 3}{2}\cdot 2\frac{u_0}{4!}\bar{\varphi}_0^2\right]\delta\varphi(\mathbf{k})\delta\varphi(-\mathbf{k})$$

  The factor $\frac{4\cdot 3}{2}$ stems from choosing two out of the four fields in the interaction term.

- Substitute the saddle point value $\bar{\varphi}_0^2 = 0$ or $\bar{\varphi}_0^2 = -6r_0/u_0$ for $r_0 \gtrless 0$:

$$S_{\Lambda_0}[\varphi] = \begin{cases} V f_0 + \frac{1}{2}\int_{\mathbf{k}}\left[r_0 + c_0k^2\right]\delta\varphi(\mathbf{k})\delta\varphi(-\mathbf{k}) & : T > T_c \\ V\left[f_0 - \frac{3}{2}\frac{r_0^2}{u_0}\right] + \frac{1}{2}\int_{\mathbf{k}}\left[-2r_0 + c_0k^2\right]\delta\varphi(\mathbf{k})\delta\varphi(-\mathbf{k}) & : T < T_c \end{cases} \tag{61}$$

Thermodynamics in Gaussian approximation

- β, γ, δ: Related to the homogeneous part of the magnetization, $\bar{\varphi}_0^2$
  This is the same in the Gaussian approximation as in the MFT $\rightarrow$ exponents do not change.
- α: (Heat-capacity exponent) Need to calculate $\mathcal{Z} = \int \mathcal{D}[\varphi]\, e^{-S_{\Lambda_0}[\varphi]}$ using a Gaussian integral (see Ch. 2.3.3 in [Kopietz]). Result:

$$\alpha = \begin{cases} 2 - D/2 & : D < 4 \\ 0 & : D \geq 4 \end{cases} \tag{62}$$

Correlation function in Gaussian approximation: η, ν

- Gaussian approximation: Have access to spatial order parameter spatial fluctuations (beyond MFT):

$$\varphi(\mathbf{r}) = \bar{\varphi}_0 + \delta\varphi(\mathbf{r}) \tag{63}$$

- We find [with $\varphi(\mathbf{r}) \equiv \int_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}\varphi(\mathbf{k})$]

$$G(\mathbf{r}) = \langle \delta\varphi(\mathbf{r})\delta\varphi(0)\rangle = \int_{\mathbf{k},\mathbf{k}'} e^{i\mathbf{k}\cdot\mathbf{r}} \underbrace{\langle \delta\varphi(\mathbf{k})\delta\varphi(\mathbf{k}')\rangle}_{(2\pi)^D\delta(\mathbf{k}+\mathbf{k}')G(\mathbf{k})} = \int_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} G(\mathbf{k}) \tag{64}$$

- From last semester (quadratic field theory with complex field - where is the inverse propagator?), we know:

$$G_0(\mathbf{k}) = \frac{1}{c_0}\frac{1}{\xi^{-2} + k^2} \tag{65}$$

  The subscript 0 stands for "Gaussian approximation" and we defined

$$c_0\xi^{-2} \equiv \begin{cases} r_0 & : T > T_c, \\ -2r_0 & : T < T_c. \end{cases} \tag{66}$$

- In Ex. 2.2 we find the FT in Eq. (64)

$$G_0(\mathbf{r}) = \frac{1}{c_0}\int_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}\frac{1}{\xi^{-2}+k^2} \overset{D\geq 2}{\sim} \begin{cases} 1/r^{D-2} & r \ll \xi \\ e^{-r/\xi}/\sqrt{\xi^{D-3}r^{D-1}} & r \gg \xi \end{cases} \tag{67}$$

  which confirms our postulate in Eq. (9).

- Read off ν from the definition of ξ (recall $r_0 \sim t$) and η from the power-law in $G(\mathbf{r})$ at the critical point at which $\xi = \infty$:

$$\boxed{\nu = 1/2,\ \eta = 0} \tag{68}$$

Validity of Gaussian approximation

- Q: Is Gaussian approximation correct for critical exponents at least for large D?
  ($T_{c,MF}$ improves with increasing D but is never exact in mean-field unless $D \rightarrow \infty$.)
- Assess error of neglecting quartic term $\propto u_0$ in the full Ginzburg-Landau-Wilson action Eq. (50):

$$S_{\Lambda_0}[\varphi] = Vf_0 + \frac{1}{2}\int_{\mathbf{k}}\left[r_0 + c_0k^2\right]\varphi(-\mathbf{k})\varphi(\mathbf{k}) + \frac{u_0}{4!}\int_{\mathbf{k}_{1,2,3,4}} (2\pi)^D\delta\left(\mathbf{k}_1 + ... + \mathbf{k}_4\right)\varphi(\mathbf{k}_1)\varphi(\mathbf{k}_2)\varphi(\mathbf{k}_3)\varphi(\mathbf{k}_4) \tag{69}$$

- Move to $T \gtrsim T_c$ so that $r_0 = c_0/\xi^2$ (ξ is the correlation length in Gaussian approximation).

- Rewrite $S_{\Lambda_0}[\varphi]$ with dimensionless momenta $\tilde{\mathbf{k}} = \mathbf{k}\xi$ and dimensionless fields $\tilde{\varphi}(\tilde{\mathbf{k}}) \equiv \sqrt{c_0/\xi^{2+D}}\varphi(\mathbf{k}\xi)$. We obtain

$$S_{\Lambda_0}[\varphi] = V f_0 + \frac{1}{2}\int_{\tilde{\mathbf{k}}} \underbrace{\left[1+\tilde{k}^2\right]}_{\simeq 1 \text{ for small } k} \tilde{\varphi}(-\tilde{\mathbf{k}})\tilde{\varphi}(\tilde{\mathbf{k}}) + \frac{1}{4!}\left(\frac{u_0\xi^{4-D}}{c_0^2}\right)\int_{\tilde{\mathbf{k}}_{1,2,3,4}} (2\pi)^D \delta\left(\tilde{\mathbf{k}}_1 + ... + \tilde{\mathbf{k}}_4\right)\tilde{\varphi}(\tilde{\mathbf{k}}_1)\tilde{\varphi}(\tilde{\mathbf{k}}_2)\tilde{\varphi}(\tilde{\mathbf{k}}_3)\tilde{\varphi}(\tilde{\mathbf{k}}_4) \tag{70}$$

- Relative strength of quartic part:

$$\tilde{u}_0 = u_0\xi^{4-D}/c_0^2. \tag{71}$$

- For $D < 4$: Regardless of how small u_0, if $\xi \propto |t|^{-\nu}$ diverges as $t \to 0$, the relative strength of the quartic part diverges. $\to$ Gaussian approximation to critical exponents (defined in the limit $t \to 0$) is *not* reliable.
- Critical dimensions:
  - Upper critical dimension D_{up}: For $D > D_{up}$, the critical exponents of the Gaussian approximation are exact.
  - Lower critical dimension D_{low}: The largest dimension where one has $T_c = 0$.
- Ising model: $D_{low} = 1$, $D_{up} = 4$.

Exercises

Exercise 2.1. Derivation of continuum φ^4-field theory for Ising model

In this exercise, you formally derive the continuum field theory Eq. (50) starting from the partition function Eq. (47).

1. Use the identity

$$e^{\frac{1}{2}\mathbf{s}^T[\mathbf{A}^{-1}]\mathbf{s}} = \sqrt{\det\mathbf{A}}\int \mathcal{D}[x]\, e^{-\frac{1}{2}\mathbf{x}^T\mathbf{A}\mathbf{x}+\mathbf{x}^T\mathbf{s}} \tag{72}$$

to rewrite the J-part of the partition function. Here, $\mathbf{x}$ and $\mathbf{s}$ are real vectors with N entries x_i and s_i, respectively and $\int\mathcal{D}[x] \equiv \Pi_{i=1}^N \int_{-\infty}^{+\infty} dx_i/\sqrt{2\pi}$ and $\mathbf{A}$ is a real, symmetric and positive-definite $N\times N$ matrix with entries a_{ij}. Show that

$$\mathcal{Z} = \frac{1}{\sqrt{\det\tilde{\mathbf{J}}}}\int\mathcal{D}[x]\exp\left[-\frac{1}{2}\mathbf{x}^T\tilde{\mathbf{J}}^{-1}\mathbf{x} + \sum_{i=1}^N \ln\left[2\cosh\left(x_i+\beta h\right)\right]\right] \equiv \frac{1}{\sqrt{\det\tilde{\mathbf{J}}}}\int\mathcal{D}[x]\, e^{-\tilde{S}[\mathbf{x}]} \tag{73}$$

where $\tilde{J}_{ij} = \beta J_{ij}$. Convince yourself that the average of x_i is a re-scaled version of the s_i, $\langle\mathbf{x}\rangle_{\tilde{S}} = \tilde{\mathbf{J}}\langle\mathbf{s}\rangle$. Define $\boldsymbol{\varphi} \equiv \tilde{\mathbf{J}}^{-1}\mathbf{x}$ which can be interpreted as a spatially fluctuating order parameter as $\langle\varphi_i\rangle_{\tilde{S}} = \langle s_i\rangle = m$. Confirm:

$$\mathcal{Z} = \sqrt{\det\tilde{\mathbf{J}}}\int\mathcal{D}[\varphi]\exp\left[-\frac{1}{2}\boldsymbol{\varphi}^T\tilde{\mathbf{J}}\boldsymbol{\varphi} + \sum_{i=1}^N \ln\left[2\cosh\left(\left[\tilde{\mathbf{J}}\boldsymbol{\varphi}\right]_i + \beta h\right)\right]\right] \equiv \sqrt{\det\tilde{\mathbf{J}}}\int\mathcal{D}[\varphi]\, e^{-S[\varphi]} \tag{74}$$

2. Assume a hyper-cubic lattice in D-dimensions where $T_c = 2DJ$ and the lattice constant is a. Close to the critical point $T \simeq T_c$, the integral is dominated by configurations where φ_i is small. Expand $S[\varphi]$ accordingly neglecting terms of order $\mathcal{O}(\varphi_i^6)$ and assume small fields h. Use the Fourier-transform $\varphi_j = \frac{1}{N}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}_j}\varphi_{\mathbf{k}}$ with $\sum_j e^{i\mathbf{k}\cdot\mathbf{r}_j} = N\delta_{\mathbf{k},0}$ and $J_{\mathbf{k}} = \sum_j e^{-i\mathbf{k}\cdot\mathbf{r}_j}J(\mathbf{r}_j)$ where $J(\mathbf{r}_i - \mathbf{r}_j) = J_{ij}$ is the translational invariant coupling. You should obtain

$$S[\varphi] = -N\ln 2 - \beta^2 h J_{\mathbf{k}=0}\varphi_{\mathbf{k}=0} + \frac{\beta}{2}\frac{1}{N}\sum_{\mathbf{k}} J_{\mathbf{k}}\left(1-\beta J_{-\mathbf{k}}\right)\varphi_{-\mathbf{k}}\varphi_{\mathbf{k}}$$
$$+ \frac{\beta^4}{12}\frac{1}{N^3}\sum_{\mathbf{k}_{1,2,3,4}} \delta_{\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3+\mathbf{k}_4,0} J_{\mathbf{k}_1}J_{\mathbf{k}_2}J_{\mathbf{k}_3}J_{\mathbf{k}_4}\varphi_{\mathbf{k}_1}\varphi_{\mathbf{k}_2}\varphi_{\mathbf{k}_3}\varphi_{\mathbf{k}_4} + \mathcal{O}\left(\varphi_i^6, h^2, h\varphi_i^3\right)$$

3. For the situation above, long-wavelength (small k) contributions will dominate. Expand $J_{\mathbf{k}}$ to leading non-trivial order k^2 and then take the limit of infinite volume $N \equiv V/a^D \to \infty$. In this case use

$$\frac{1}{V}\sum_{\mathbf{k}} \to (2\pi)^{-D} \int_{-\infty}^{+\infty} d^D\mathbf{k} \equiv \int_{\mathbf{k}},$$
$$V\delta_{\mathbf{k},\mathbf{k}'} \to (2\pi)^D \, \delta\left(\mathbf{k}-\mathbf{k}'\right)$$

and re-scale the fields as $a^{1+D/2}\varphi_{\mathbf{k}} \equiv \varphi(\mathbf{k})$. Up to a unimportant shift to f_0, you should recover Eq. (50) with the given values for h_0, r_0, c_0 and u_0.

Comment: In step 1, you might wonder if the matrix $\mathbf{A}$ is positive-definite for realistic systems - it usually is not, consider a simple nearest neighbor chain with its $\cos(ak)$ dispersion, i.e. with eigenvectors of both signs. The above derivation can still be applied if we restrict to spin configurations $\mathbf{s}$ varying smoothly, i.e. with a maximal wavevector Λ_0, ensuring a positive-definite $\mathbf{A}$ in this subspace. That is the technical origin of the cutoff Λ_0 mentioned in the lecture.

Exercise 2.2. Fourier transformation of model propagator

Find the D-dimensional Fourier transform $G_0(\mathbf{r}) = \int_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} G_0(\mathbf{k})$ for

$$G_0(\mathbf{k}) = \frac{1}{\xi^{-2}+k^2} \tag{75}$$

assuming $D > 2$ and approximate the integral for the two regimes $r \ll \xi$ and $r \gg \xi$. You should express your result using $K_D \equiv \Omega_D/(2\pi)^D$ where $\Omega_D \equiv 2\pi^{D/2}/\Gamma(D/2)$ is the surface area of a unit-sphere in D-dimensional space (Can you show this?).

3 Quantum phase transitions

Aims:

- What is different from classical phase transitions when quantum mechanics is involved?

3.1 Overview

- Quantum phase transitions (QPT) are driven by quantum fluctuations.
- Quantum fluctuations are generated by non-commuting parts of the Hamiltonian that compete in minimizing ground-state energy.
- QPT are controlled by a non-thermal control parameter r.
- QPT only occur at $T = 0$ (see below).
- Paradigmatic example: Transversal magnetic field in easy-axis Ising ferromagnet (Lithium holmium fluoride, $LiHoF_4$, $D = 3$ cubic lattice), approximation of physics using the transverse-field Ising model (TFIM, also called "quantum Ising model"):

$$\hat{H}_{TFIM} = -J \sum_{\langle i,j \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z - \Gamma \sum_i \hat{\sigma}_i^x \tag{76}$$

  Control parameter: $r = \Gamma/J$. The two non-commuting terms in $\hat{H}_{TFIM}$ compete between ferromagnetic state $|\uparrow\uparrow ... \uparrow\rangle$ (or $|\downarrow\downarrow ... \downarrow\rangle$) and paramagnetic state $|\rightarrow\rightarrow\rangle$.
  (Mean-field analysis in $\Gamma - T$-plane: Ex. 3.1)

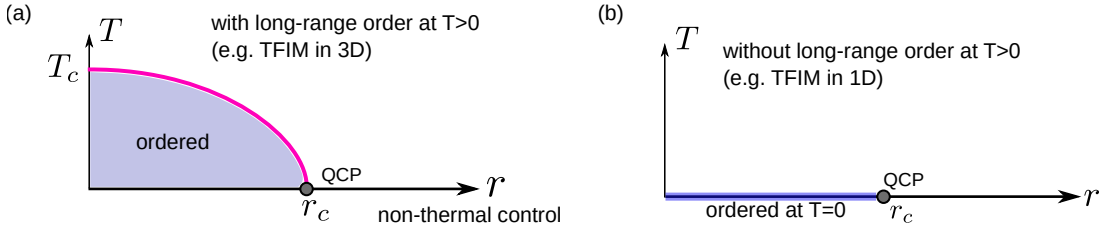


Figure 6: Generic phase diagram for quantum system showing QPT like the TFIM.

- QPT classification (similar to thermal phase transitions):
  - first order (simple ground-state level crossing)
  - second order ("continuous", with diverging length- and time scale).
- Further examples for QPT:
  - Anderson localization: Electrons in disordered, non-interacting $D = 3$ systems can undergo a transition between insulator (localized wavefunction at $E = E_F$) and metal (delocalized). Reason: Quantum interference of scattered waves.
    Control parameter: Disorder strength or Fermi energy E_F.
  - Quantum Hall effect: Transition between quantum Hall plateaus $\sigma_{xy} = ne^2/h$.
    Control parameter: Magnetic field or Fermi energy E_F.
  - Mott-Hubbard transition: Interacting electrons can transit between itinerant (metal) phase and a localized phase.
    Control parameter: Interaction strength (tuned by pressure, doping,...).

3.2 Quantum-to-classical mapping

Classical kinetic energy does *not* drive phase transition:

- Typical classical Hamiltonian: Kinetic part depends only on momenta p, potential part only on positions q:

$$H(p,q) = H_{kin}(p) + H_{pot}(q) \tag{77}$$

- Classical partition function: A high-dimensional phase-space integral, which factorizes:

$$\mathcal{Z}_C = \int dpdq \, \exp\left[-\beta H(p,q)\right] = \underbrace{\int dp \, \exp\left[-\beta H_{kin}(p)\right]}_{\to f_{reg}} \int dq \exp\left[-\beta H_{pot}(q)\right] \tag{78}$$

- If $H_{kin}(p) \sim p^2$ as usual, kinetic contribution to $\mathcal{Z}_C$ is just a product of independent Gaussian integrals. It cannot produce singularity in free energy f and is thus regular.

- Conclusion: Phase transition must originate from the q-(configuration) integral (c.f. Ising model indeed lacks kinetic part).

Quantum case

- No factorization in path integral: if $\left[\hat{H}_{kin}, \hat{H}_{pot}\right] \neq 0$, then:

$$e^{\hat{H}_{kin}+\hat{H}_{pot}} \neq e^{\hat{H}_{kin}} e^{\hat{H}_{pot}} \tag{79}$$

- Feynman's trick to compute path integral: Use Trotter formula and insert suitable basis, e.g. from bosonic/fermionic coherent states (see Cond-Mat-Field-theory I lecture)

$$\begin{aligned}
\mathcal{Z}_Q &= \mathrm{Tr} e^{-\beta\hat{H}} \\
&= \mathrm{Tr} \lim_{N\to\infty} \left[e^{-\beta\hat{H}/N}\right]^N \\
[\Delta\tau = \beta/N] &= \mathrm{Tr} \lim_{\Delta\tau\to 0} \left[e^{-\Delta\tau\hat{H}}\right]^{\beta/\Delta\tau} \\
&= \int D\left[q(\mathbf{r},\tau)\right] \exp\left[-S(q)\right]
\end{aligned}$$

  Observation: $q(\mathbf{r},\tau)$ is $D+1$-dimensional with $\mathbf{r}$ in D-dim space and one extra imaginary-time coordinate $\tau \in [0,\beta]$.

  – Example 1: Single Ising spin in transverse magnetic field $\hat{H} = -\tilde{h}\hat{\sigma}^z - \Gamma\hat{\sigma}^x$ (0-D quantum model)

$$\mathcal{Z}_Q \simeq \mathrm{Tr}\left[e^{-\beta\hat{H}/N}\right]^N \simeq \mathrm{Tr}\left[1 + \Delta\tau\tilde{h}\hat{\sigma}^z + \Delta\tau\Gamma\hat{\sigma}^x\right]^N = \mathrm{Tr}\begin{pmatrix} 1+\Delta\tau\tilde{h} & \Delta\tau\Gamma \\ \Delta\tau\Gamma & 1-\Delta\tau\tilde{h} \end{pmatrix}^N \tag{80}$$

  The matrix can be expressed as the transfer matrix of the 1D *classical* Ising model in a longitudinal magnetic field, c.f. Ex. 1.1.

$$\mathbf{T} = \begin{pmatrix} e^{\beta_c(J+h)} & e^{-\beta_c J} \\ e^{-\beta_c J} & e^{\beta_c(J-h)} \end{pmatrix} \tag{81}$$

  – Example 2: Interacting fermions

$$\begin{aligned}
&S\left[\bar{\psi},\psi\right] \\
&= \int_0^\beta d\tau \left[\sum_{ij} \bar{\psi}(\mathbf{r}_i,\tau)\left[\partial_\tau\delta_{ij} + h_{ij}\right]\psi(\mathbf{r}_j,\tau) + \sum_{ijkl} V_{ijkl}\bar{\psi}(\mathbf{r}_i,\tau+\eta)\bar{\psi}(\mathbf{r}_j,\tau+\eta)\psi(\mathbf{r}_k,\tau)\psi(\mathbf{r}_l,\tau)\right]
\end{aligned}$$

– Example 3: Partition function of TFIM in Eq. (76) maps to partition function of anisotropic classical 2D Ising model, see Ex. 3.2.
Thus expect generalized Landau-Ginzburg-Wilson action Eq. (49) for order parameter φ.

$$S[\varphi] = \int d^D\mathbf{r} \int_0^\beta d\tau \left[f_0 + \frac{r_0}{2}\varphi^2 + \frac{c_0}{2}\left[\nabla_{\mathbf{r}}\varphi\right]^2 + \frac{u_0}{4!}\varphi^4 - h_0\varphi + \frac{c_1}{2}\left[\partial_\tau\varphi\right]^2 \right] \tag{82}$$

- Zero temperature limit: $T \to 0 \Leftrightarrow \beta \to \infty$
  - Extension of imaginary-time integration becomes infinite.
  - *Quantum* partition function $\mathcal{Z}_Q$ is equivalent to $D+1$-dimensional *classical* partition function $\mathcal{Z}_C$ in infinite $D+1$-dimensional space.
  - Conclusion: QPT in D-space dimensions is equivalent to a classical (thermal) phase transition in $D+1$ space dimension. (e.g. "The QPT is in the 2+1D Ising universality class.")

Remarks on quantum-to-classical mapping

- Role of temperature T:
  - Classical: T just multiplies coupling constants to become dimensionless, e.g.: Ising model $J/T \equiv K$.
  - Quantum: T controls length of τ-dimension in path-integral expression for partition function.
- After mapping: Classical $D+1$-dimensional system may be unusual, e.g. anisotropic between $\mathbf{r}$- and τ-direction.
- Critical exponents for D-dim quantum systems may already be known from $D+1$-classical systems.
- Dynamics of quantum system: Requires analytic continuation $G(\tau) \to G(t = i\tau)$
  - ok for scaling arguments and power-laws
  - spoils precise mapping of dynamic time-dependent quantities
- If resulting action $S[q]$ becomes negative or complex, it cannot be interpreted as a classical action. [Sign-problem!]

3.3 Scaling around continuous QPT

Scaling at $T = 0$

- Dynamical critical exponent z: Require $z \neq 1$ for possible anisotropic scaling in $D+1$ dimensional space, $\mathbf{r} \to b\mathbf{r}$, $\tau \to b^z\tau$. This also means for the correlation lengths:

$$\xi \sim |r - r_c|^{-\nu},$$
$$\xi_\tau \sim \xi^z \sim |r - r_c|^{-z\nu}.$$

- Scaling hypothesis for free energy. Extend Eq. (11), $f_{\text{sing}}(t) = b^{-D} f_{\text{sing}}(b^{y_t} t)$, for quantum case:

$$f_{\text{sing}}(r - r_c) \quad = \quad b^{-(D+z)} f_{\text{sing}}\left(b^{y_r}\left[r - r_c\right]\right)$$

- From scaling hypothesis, repeat derivation of scaling form of observable O (= thermodynamic quantity, correlation function,...):

$$O(r - r_c, k, \omega_n) = \xi^{d_O} O(k\xi,\, \omega_n\xi_\tau) \tag{83}$$

where k is momentum and ω_n is a Matsubara frequency (=momentum along τ-axis).

- Remarks:

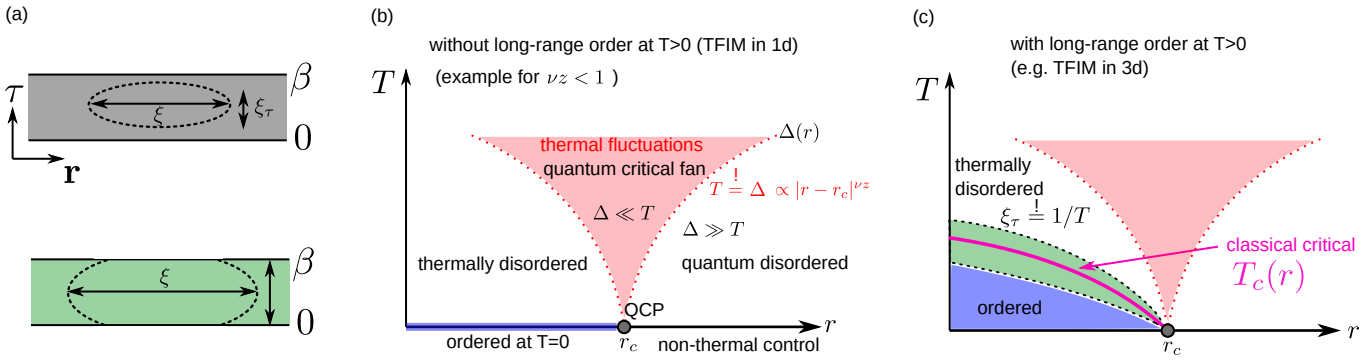


Figure 7: Finite temperature phase diagrams in the presence of a quantum critical point.

- $d_O = d_O(D, z, y_r, ...)$ is scaling dimension that depends on O. For correlation function $O \to G$, we had $d_G = 2 - \eta$.
- Interpretation: Close to criticality, there is no other length scale than ξ, no other time-scale than ξ_τ. These scales have to control the k- and ω_n-dependence.
- Scaling form also holds for real frequencies, $i\omega_n \to \omega + i0$.

Effect of $T > 0$ and phase diagram in $r - T-$plane

- For $T > 0$, the τ-direction becomes finite, $\tau \in [0, \beta]$: "Slab"-geometry with and infinite extent in $\mathbf{r}$ (see Fig. 7a).
- Consequence of slab-geometry for phase-diagram:
  1. Absence of ordered phase in D dimensions (Fig. 7b), order for $r < r_c$ only in $D + 1$ dimensions, i.e. at $T = 0$ where $\beta = \infty$.
  2. Phase transition in D-dimensional *classical universality class* (Fig. 7c).
     Expect r-dependent critical temperature $T_c(r)$. Crossover to classical behavior when $\xi_\tau \stackrel{!}{=} \beta$ (green region).
- Consequence for scaling of observables:
  - Appearance of characteristic energy scale $L_\tau = \beta$, characteristic length scale $L_\tau^{1/z}$.
  - Competition of $L_\tau = \beta$ with imaginary-time correlation length $\xi_\tau \sim |r - r_c|^{-z\nu}$ of infinite system (see Fig. 7a).
- Formal description: "Finite-size scaling" (see Sec. 4)

$$f_{\text{sing}}(r - r_c, T) \quad = \quad b^{-(D+z)} f_{\text{sing}}\left(b^{y_r}[r - r_c], T b^z\right)$$

- This yields scaling forms like in Eq. (83), but expressed in terms of L_τ:

$$O(r - r_c, k, \omega, T) = L_\tau^{d_O/z} O\left(k L_\tau^{1/z}, \omega L_\tau, L_\tau/\xi_\tau\right) \tag{84}$$

- *Quantum critical fan* (red region in Fig. 7b,c):
  - Region above QCP for which last argument in Eq. (84) is negligible:

$$L_\tau/\xi_\tau \sim |r - r_c|^{\nu z}/T \ll 1 \tag{85}$$

    Shape depends on $\nu z \gtrless 1$.

– Simplified scaling form independent of $r - r_c$ but dependent on $y_r, z, ...$:

$$O(k, \omega, T) = L_\tau^{d_O/z} O\left(kL_\tau^{1/z}, \omega L_\tau\right) \tag{86}$$

– Predicted scaling collapse of experimental or numerical data, e.g. for uniform ($k = 0$) susceptibilities $\chi(\omega, T)$. Note: No fine-tuning to $r = r_c$ needed!

- Interpretation of quantum critical fan:
  - At $T = 0$ temporal fluctuation time-scale goes like $\tau_c \sim \xi_\tau \sim \xi^z$, c.f. Eq. (18).
  - Quantum mechanics: Relate τ_c to fluctuation energy scale or gap $\Delta = \hbar/\tau_c \propto \xi^{-z} \propto |r - r_c|^{\nu z}$ with power $\nu z > 0$.
  - $T > 0$: Will system notice gap? Depends on $T \lessgtr \Delta$.
  - Quantum critical fan: System does not notice gap, $\Delta \ll T$ [equivalent to condition (85)].
  - Physics in fan is dominated by thermal excitations of the quantum critical ground state.

Exercises

Exercise 3.1. Mean-field theory for quantum spin-1/2 transverse field Ising model (TFIM)

In this exercise, we perform a mean-field analysis for the (quantum!) TFIM of Eq. (76). We work on the hyper-cubic lattice with coupling $J \equiv 1$ to the $z = 2D$ nearest neighbors.

1. Derive the mean-field Hamiltonian $\hat{H}_{MF}$ of the TFIM, use $\hat{\sigma}_i^z = m^z + \delta\hat{\sigma}_i^z$ where $m^z = \langle\hat{\sigma}_i^z\rangle$ and neglect terms quadratic in $\delta\hat{\sigma}_i^z$. Find the partition function $\mathcal{Z}_{MF}$ and the self-consistency condition for possible non-trivial $m^z(\Gamma, T)$:
$$\tanh\left(\beta z\sqrt{[m^z]^2 + (\Gamma/z)^2}\right) = \sqrt{[m^z]^2 + (\Gamma/z)^2} \tag{87}$$

2. Solve the self-consistency condition for the special cases (i) $\Gamma = 0$ and (ii) $T = 0$. For $T = 0$, calculate m^z explicitly, sketch $m^z(\Gamma, T = 0)$ and determine the value for the critical exponent in $m^z \propto (\Gamma_c - \Gamma)^{\beta_\Gamma}$.

3. Use your results from the previous part and suitable expansions close to the critical points on the T- and Γ-axis to sketch the phase boundary in the $\Gamma - T-$plane.
[Hint: To see how the phase boundary (Γ_c, T_c) emerges from the critical point $(0, T_c[\Gamma = 0])$ found above, set $(\Gamma_c, T_c) = (0 + \delta\Gamma_c, T_c[\Gamma = 0] + \delta T_c)$ and assume small $\delta\Gamma_c, \delta T_c$. Do the same close to $(\Gamma_c[T = 0], 0)$.]
What kind of phase transitions (quantum/classical) would you expect in an exact (non mean-field) treatment? Why is the mean-field phase diagram even qualitatively *incorrect* for the TFIM in $D = 1$?

Exercise 3.2. Transverse field Ising model in 1D (I): Mapping to 2D classical system

Consider the 1D TFIM in Eq. (76) in one spatial dimension (1D) with $J = 1$ and L_x sites

$$\hat{H} = -\sum_i \hat{\sigma}_i^z\hat{\sigma}_{i+1}^z - \Gamma\sum_i \hat{\sigma}_i^x \tag{88}$$

and assume periodic boundary conditions (ring geometry). In this exercise, we show the equivalence of the quantum partition function $\mathcal{Z}_{1D,q} = \mathrm{Tr}_{1D} e^{-\beta_q \hat{H}}$ for low enough $T_q = 1/\beta_q$ and the partition function of a 2D classical Ising model (without magnetic field, with anisotropic coupling constants $K_x = J_x\beta_c$, $K_y = J_y\beta_c$),

$$\mathcal{Z}_{2\mathrm{D,c}} = \mathrm{Tr}_{2\mathrm{D}} e^{K_x\sum_{i,j}\sigma_{i,j}\sigma_{i+1,j} + K_y\sum_{i,j}\sigma_{i,j}\sigma_{i,j+1}}. \tag{89}$$

In the last expression, $\sigma_{i,j} = \pm 1$ denotes the value of the classical spin at position (i, j). Our strategy is to start from $\mathcal{Z}_{2D,c}$ and leverage the transfer matrix approach to $\mathcal{Z}_{1D,c}$ to 2D.

1. Express $e^{K_x \sum_i \sigma_i \tilde{\sigma}_{i+1}}$ and $e^{K_y \sum_i \tilde{\sigma}_i \sigma_i}$ as matrix elements of two operators O_x, O_y in the 2^{L_x}-dimensional Hilbert space of a spin-1/2 chain spanned by the basis $|\sigma_1, \sigma_2, ..., \sigma_{L_x}\rangle$, $\{\sigma_i\}_{i=1,...,L_x} = \pm 1$. Use these results to show

$$\mathcal{Z}_{\mathrm{2D,c}} = (2\sinh[2K_y])^{L_y L_x/2} \mathrm{Tr}_{\mathrm{1D}} \left(\left[e^{K_x \sum_i \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z} e^{\sum_i \bar{K}_y \hat{\sigma}_i^x} \right]^{L_y} \right) \tag{90}$$

   where $\tanh \bar{K}_y \equiv e^{-2K_y}$.

2. Use the Trotter-formula $\mathcal{Z}_{\mathrm{1D,q}} \simeq \mathrm{Tr}_{\mathrm{1D}} \left[e^{-\beta_q \hat{H}/L_y} \right]^{L_y}$ for L_y large enough to establish the mapping between $\mathcal{Z}_{1D,q}$ and an anisotropic $\mathcal{Z}_{2D,c}$. Use the mapping to argue that $\hat{H}$ has a (quantum) critical point only in limit $L_x \to \infty$ and $T_q \to 0$.

3. It is known that anisotropy in the 2D classical Ising model does not change the critical exponents. In generalization of the result of Ex. 1.3, the critical temperature is given implicitly by $\sinh(2K_x)\sinh(2K_y) = 1$. Use this to find the exact critical transverse field Γ_c. By which factor does the mean-field solution of Ex. 3.1 overestimate the exact Γ_c?

Exercise 3.3. Transverse field Ising model in 1D (II): Exact eigenenergies

Here we are interested in finding the exact eigenenergies of the 1D TFIM in Eq. 88. We will find the gap Δ as a function of Γ and confirm the value of Γ_c found in Ex. 3.2

1. Consider the Jordan-Wigner transformation in 1D that maps spin-1/2 to fermionic operators $c_i, c_i^\dagger$:

$$\begin{aligned} \hat{\sigma}_i^x &= \left(1 - 2c_i^\dagger c_i\right) \\ \hat{\sigma}_i^z &= -\prod_{j<i} \left(1 - 2c_j^\dagger c_j\right) \left(c_i + c_i^\dagger\right) \end{aligned}$$

   Confirm that this mapping indeed fulfills the spin algebra by computing $\hat{\sigma}_i^\alpha \hat{\sigma}_{i'}^\beta$ for $\alpha, \beta = \{x, z\}$, $i = i'$ and $i \neq i'$.

2. Insert the Jordan-Wigner transformation in the 1D TFIM Hamiltonian and use a Fourier-transformation $c_k = \frac{1}{\sqrt{L_x}} \sum_j c_j e^{-ikj}$ to obtain

$$\hat{H} = \sum_k \left(2\left[\Gamma - \cos k\right] c_k^\dagger c_k + i \sin k \left[c_{-k}^\dagger c_k^\dagger + c_{-k} c_k \right] - \Gamma \right) \tag{91}$$

3. Solve this c-particle number non-conserving Hamiltonian using a Bogoliubov transformation, $c_k = u_k \gamma_k + i v_k \gamma_{-k}^\dagger$ where $\gamma_k^{(\dagger)}$ again fulfill fermionic anti-commutation relations if u_k, v_k are real numbers satisfying $u_k^2 + v_k^2 = 1$, $u_{-k} = u_k$ and $v_{-k} = -v_k$. They can be parameterized by an angle, $u_k = \cos(\theta_k/2)$ and $v_k = \sin(\theta_k/2)$. Find (k-dependent!) θ_k such that

$$\hat{H} = \sum_k E_k \gamma_k^\dagger \gamma_k + const. \tag{92}$$

   and obtain the single-particle energy $E_k = 2\sqrt{1 - 2\Gamma \cos k + \Gamma^2}$. What is the critical value of Γ at which E_k becomes gapless (at which k?).

4 Wilsonian renormalization group

Aims:

- Renormalization group (RG) = Set of ideas, not one coherent theory.
  Requires experience for application ($\rightarrow$ examples and exercises).
- Study interacting systems, but *beyond* perturbation theory.
- Connect physics at different energy scales (high to low energy / short to large length)
- Provides simplified effective models valid for each scale.
  Example for hierarchy of length scales: Lattice spacing $a \ll$ correlation length $\xi \ll$ system size L.
- Obtain justification for scaling hypothesis and thus for universality of critical exponents.
- Approximate calculation of critical exponents for ϕ^4-theory (beyond Gaussian approximation, using $\epsilon \equiv 4 - D \ll 1$ expansion and perturbative arguments in u_0).
- Deeper understanding of phase diagrams and emergent scales [i.e. Kondo temperature T_K].
- Here: Only condensed matter application (skip high-energy physics viewpoint).

4.1 Basic RG idea

- Partition function as path integral over field Φ (bosonic/fermionic/mixed), coupling constants $\mathbf{g} = (g_1, g_2, g_3, ...)$. (E.g. Ex. 2.1 for the derivation of ϕ^4-theory from Ising model):

$$\mathcal{Z}(\mathbf{g}) = \int \mathcal{D}[\Phi]\, e^{-S_{\Lambda_0}[\Phi,\mathbf{g}]} \tag{93}$$

- RG-Idea: Integration over Φ in Eq. (93) in iterative fashion.
  - Organize such that we move towards low-energy / long-distance effective theory (start integrating large energy scales).
  - Need simplifying assumptions for generic case.
- Two steps:

1. **Mode elimination:**
   For momentum-shell RG in Fig. 8a (other incarnations - see below):
   Define "shell" of high-energy modes close to the UV cutoff Λ_0, e.g. in k-space $k \in (\Lambda, \Lambda_0]$ with

$$\Lambda = \Lambda_0/b, \quad b > 1. \tag{94}$$

   Those are the high-energy (fast, ">") modes that should be integrated out:

$$\Phi(\mathbf{k}) = \underbrace{\Theta(\Lambda - k)\Phi(\mathbf{k})}_{\Phi^<} + \underbrace{\Theta(k - \Lambda)\Phi(\mathbf{k})}_{\Phi^>} \tag{95}$$

   and define

$$\mathcal{Z} = \int \mathcal{D}[\Phi^<] \int \mathcal{D}[\Phi^>]\, e^{-S[\Phi^< + \Phi^>, \mathbf{g}]} = \int \mathcal{D}[\Phi^<] e^{-S^<_\Lambda[\Phi^<, \mathbf{g}^<]} \tag{96}$$

   Remark:

   (a) Integration in the last step can only be carried out approximately in practice.

   (b) Set of coupling constants $\mathbf{g}$ is usually enlarged and must be truncated.

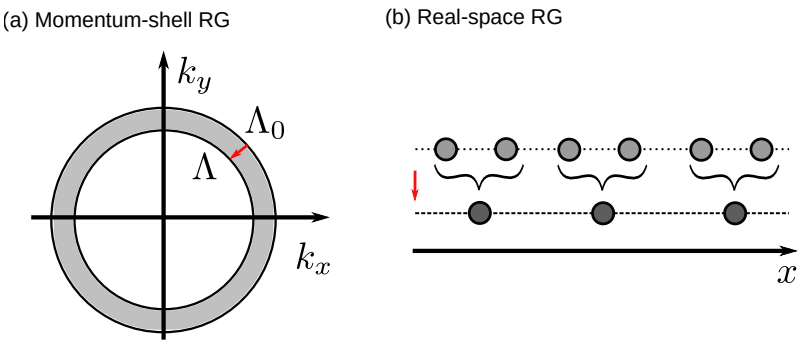


Figure 8: Different incarnations of the RG mode-elimination step.

2. **Rescaling:**
   Re-scale momenta and fields such that $S^<_\Lambda[\Phi^<, \mathrm{g}^<]$ has the same form as S_{Λ_0}.
   In momentum-shell RG: Stretch momenta from $k \in [0, \Lambda]$ to $k' \in [0, \Lambda_0]$:

$$\begin{aligned} \mathbf{k} &\to \mathbf{k}' = b\mathbf{k} \\ \Phi^<(\mathbf{k}) &\to \Phi'(\mathbf{k}') = \zeta_b^{-1}\Phi^<(\mathbf{k}'/b) \end{aligned}$$

   Arrive at action $S'_{\Lambda_0}[\Phi', \mathbf{g}']$. Read off the RG-trafo of coupling constants:

$$\boxed{\mathbf{g}' = \mathcal{R}(b; \mathbf{g})} \tag{97}$$

   Remark: For quantum system, also eliminate (large) Matsubara frequencies $i\omega$, re-scale with possibly *different* factor:

$$i\omega \to i\omega' = i\omega b^z \tag{98}$$

- Remark: RG-trafo $\mathcal{R}$ is semi-group [associativity holds $(a \cdot (b \cdot c) = (a \cdot b) \cdot c)$, but no inverse]:
  - Associativity: Can combine RG steps for b and b' to $b'' = b'b$. This yields

$$\mathbf{g}'' = \mathcal{R}(b'; \underbrace{\mathcal{R}(b; \mathbf{g})}_{\mathbf{g}'}) = \mathcal{R}(b'b; \mathbf{g}) \tag{99}$$

  - No inverse: Due to truncation of coupling space. This means that different microscopic models can give rise to same long-wavelength properties.

- Iterating the RG transformation:

$$\mathbf{g}^{(n)} = \mathcal{R}(b; \mathbf{g}^{(n-1)}) = \mathcal{R}(b^n; \mathbf{g}) \tag{100}$$

- In limit $n \to \infty$, it holds $\Lambda = \Lambda_0/b^n \overset{n\to\infty}{\to} 0$. We then have integrated out all degrees of freedom and obtain $\mathcal{Z}$.
  Note: As the RG cannot be carried out exactly, this is usually not what it is used for in practice.

- Incarnations of mode-elimination step:
  1. Momentum-shell RG (Wilson), as outlined above. Requires translation invariant systems. See Sec. 4.4.
  2. Real-space RG (Migdal-Kadanoff): For spin systems, eliminate certain lattice sites by partial traces over Hilbert space. See Sec. 4.2 for clean 1D system, and Ex. 4.2 for disordered 1D system. Hard to generalize to $D = 2, 3, ...$
  3. Numerical RG (Wilson): For impurity models (interacting site + non-interacting bath), numerical implementation, for some "poor-man" version, see Sec. 4.5.
  4. Functional RG (Wegner, Wetterich): Formally exact version of momentum-shell RG (1), go from the level of coupling parameters $g_i^{(n)}$ to correlation functions $G_\Lambda(K_1, K_2, ...)$ or vertex functions $\Gamma_\Lambda(K_1, K_2, ...)$ which depend smoothly on cutoff Λ. See part II.

4.2 Example: Real-space RG for Ising model in 1D

- Recall 1D classical Ising model

$$H = -J\sum_{i=1}^{N} s_i s_{i+1} - h\sum_{i=1}^{N} s_i - E_0 \tag{101}$$

where E_0 is an energy offset and the number of sites N is assumed to be even.

- Recall transfer matrix solution (Ex. 1.1) for partition function:

$$\mathcal{Z}_N\left(\tilde{f}, g, \tilde{h}\right) = \sum_{\{s_i\}=\pm 1} e^{-\beta H} = \mathrm{Tr}\left[T^N\right]$$

$$T = e^{\tilde{f}} \begin{pmatrix} e^{g+\tilde{h}} & e^{-g} \\ e^{-g} & e^{g-\tilde{h}} \end{pmatrix}$$

and $g = \beta J$, $\tilde{h} = h\beta$, $\tilde{f} = \beta E_0/N$.

RG step

- Mode elimination step (Fig. 8b): Carry out trace $\sum_{\{s_i\}} = \sum_{\{s_{i\,even}\}}\sum_{\{s_{i\,odd}\}}$ only for *even* sites i:

$$\mathcal{Z}_{N'}\left(\tilde{f}', g', \tilde{h}'\right) = \mathrm{Tr}\left[\left(T'\right)^{N'}\right] \tag{102}$$

with $N' = N/2$ and

$$T' \equiv T^2 = e^{2\tilde{f}} \begin{pmatrix} e^{2g+2\tilde{h}} + e^{-2g} & e^{\tilde{h}} + e^{-\tilde{h}} \\ e^{\tilde{h}} + e^{-\tilde{h}} & e^{2g-2\tilde{h}} + e^{-2g} \end{pmatrix}. \tag{103}$$

- Important observation: $\mathcal{Z}$ after mode elimination has same form as the initial $\mathcal{Z}$, but for lattice of lattice constant $a' = 2a$ and for only $N' = N/2$ sites.

- We want to write T' using the form of T with parameters $\{\tilde{f}', g', \tilde{h}'\}$:

$$T' \stackrel{!}{=} e^{\tilde{f}'} \begin{pmatrix} e^{g'+\tilde{h}'} & e^{-g'} \\ e^{-g'} & e^{g'-\tilde{h}'} \end{pmatrix} \tag{104}$$

- Relation between primed and unprimed parameters (short calculation):

$$\tilde{f}' = 2\tilde{f} + \frac{1}{4}\ln\left[16\cosh^2\left(\tilde{h}\right)\cosh\left(2g+\tilde{h}\right)\cosh\left(2g-\tilde{h}\right)\right]$$

$$g' = \frac{1}{4}\ln\left[\frac{\cosh\left(2g+\tilde{h}\right)\cosh\left(2g-\tilde{h}\right)}{\cosh^2\left(\tilde{h}\right)}\right]$$

$$\tilde{h}' = \tilde{h} + \frac{1}{2}\ln\left[\frac{\cosh\left(2g+\tilde{h}\right)}{\cosh\left(2g-\tilde{h}\right)}\right]$$

Remarks:

  - Existence of exact relations are peculiar to $D = 1$. For $D = 2, 3, ...$ new couplings would be generated.
  - The above equations already contain rescaling step. Indeed, the contribution $2\tilde{f}$ on the rhs of $\tilde{f}'$ comes from the reduced number of sites $N' = N/2$. However, no field (spin) rescaling was needed ($\zeta_b = 1$).

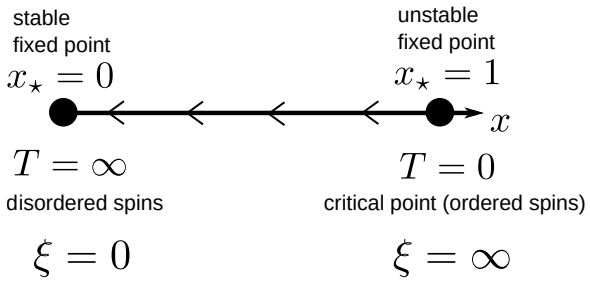


Figure 9: RG flow of the dimensionless coupling $x = \tanh(J/T)$ for the Ising model in 1D.

- Consider special case $\tilde{h} = 0$ ($\to \tilde{h}' = 0$):

$$\begin{aligned} \tilde{f}' &= 2\tilde{f} + \ln\left[2\sqrt{\cosh(2g)}\right] \\ g' &= \ln\left[\sqrt{\cosh(2g)}\right] \end{aligned}$$

  For the g' equation, we exponentiate $e^{g'} = \sqrt{\cosh(2g)}$ and find with

$$e^{g'} \pm e^{-g'} = \sqrt{\cosh(2g)}\left(1 \pm \frac{1}{\cosh(2g)}\right) \tag{105}$$

  that

$$\tanh g' = \frac{1 + \frac{1}{\cosh(2g)}}{1 - \frac{1}{\cosh(2g)}} \tag{106}$$

  We use $\cosh(2g) = 2\cosh^2(g) - 1 = 2\sinh^2(g) + 1$ to finally obtain (similar for $\tilde{f}'$):

$$\boxed{\tanh g' = \tanh^2 g} \tag{107}$$

$$\boxed{\tilde{f}' = 2\tilde{f} + \ln[2\cosh(g)] + \ln\left[\frac{\cosh(g)}{\cosh(g')}\right]} \tag{108}$$

Iteration and fixed points

- Recall the definition of $g = J/T$ with T the temperature. Define $x_n \equiv \tanh g^{(n)} \in [0, 1]$.
  RG step in terms of x_n, see also Fig. 9:

$$\boxed{x_{n+1} = x_n^2} \tag{109}$$

- *Fixed point:* Configuration $x_\star$ that does not change under the action of the RG, here Eq. (109).
  - Fixed point at $x_\star = 0$ is stable (corresponds to $T_\star = \infty$, disordered spins, $\xi = 0$)
  - Fixed point at $x_\star = 1$ is unstable ($T_\star = 0$, ordered spins, $\xi = \infty$)
- Stable / unstable fixed point: Perturbation away from fixed point is reduced / increased under the action of the RG transformation.
- One may interpret either the coupling constant T or J as changing under RG:
  If we choose T:
  - T stays at $T = 0$ at the unstable fixed point.
  - $T > 0$ increases under the flow to reach the stable fixed point $T = \infty$.

Correlation length ξ

- Correlation length defined via the long-distance tail of correlation function $G(\mathbf{r}_i - \mathbf{r}_j)$.
- We can chose $\mathbf{r}_{i,j}$ from the non-decimated sites. We show that site-decimation does not affect the correlation function ($\tilde{H} = \beta H$):

$$\begin{aligned} G(\mathbf{r}_i - \mathbf{r}_j) &= \frac{\sum_{s_1,s_2,s_3,\ldots,s_N} \delta s_i \delta s_j e^{-\tilde{H}(s_1,s_2,s_3\ldots,s_N)}}{\sum_{s_1,s_2,s_3,\ldots,s_N} e^{-\tilde{H}(s_1,s_2,s_3\ldots,s_N)}} \\ &= \frac{\sum_{s_1,s_3,\ldots,s_{N-1}} \delta s_i \delta s_j \sum_{s_2,s_4,\ldots,s_N} e^{-\tilde{H}(s_1,s_2,s_3\ldots,s_N)}}{\sum_{s_1,s_3,\ldots,s_{N-1}} \underbrace{\sum_{s_2,s_4,\ldots,s_N} e^{-\tilde{H}(s_1,s_2,s_3\ldots,s_N)}}_{e^{-\tilde{H}'(s_1,s_3,\ldots,s_{N-1})}}} \\ &= \frac{\sum_{s_1,s_3,\ldots,s_{N-1}} \delta s_i \delta s_j e^{-\tilde{H}'(s_1,s_3,\ldots,s_{N-1})}}{\sum_{s_1,s_3,\ldots,s_{N-1}} e^{-\tilde{H}'(s_1,s_3,\ldots,s_{N-1})}} \end{aligned}$$

- Correlation length is defined in units of lattice constant a. The lattice constant *does change* under RG step.
  After the decimation, $\mathbf{r}_i, \mathbf{r}_j$ have moved closer together:

$$\xi' \equiv \xi(x') \overset{above}{=} \xi(x)/2. \tag{110}$$

  On the other hand, we have $x' = x^2$ from the RG transformation. This leads to

$$\xi(x^2) = \xi(x)/2 \tag{111}$$

- The equation has the solution

$$\xi(x) = -\frac{a_0}{\ln(x)} \tag{112}$$

  where a_0 is arbitrary length scale, it can be taken to physical (initial) lattice constant a.
- The result $\xi \sim -1/\log(\tanh[J/T])$ has already been found via the transfer matrix method in Ex. 1.1.
- Use Eq. (112) to obtain correlation length at low temperature: Use $g = J/T \gg 1$ in:

$$x = \tanh g \simeq 1 - 2e^{-2g} \tag{113}$$

  and then obtain from Eq. (112)

$$\xi \simeq \frac{a}{2} e^{2J/T} \tag{114}$$

- The correlation length is finite for any $T > 0$ and the 1D Ising chain is disordered.

Infinitesimal form of RG recursion and beta-function

- Above, we eliminated every 2nd spin, corresponding to rescaling factor $b = 2$.
  We can equally well work with $b = 3, 4, \ldots$ to get

$$\tanh g' = \tanh^b g \tag{115}$$

$$\tilde{f}' = b\tilde{f} + (b-1)\ln[2\cosh(g)] + \ln\left[\frac{\cosh(g)}{\cosh(g')}\right] \tag{116}$$

- Analytically continue for arbitrary real b (which is a natural choice for momentum shell-RG):

$$\boxed{b \equiv e^l = 1 + l + \mathcal{O}(l^2)} \tag{117}$$

  Set $g' \equiv g_l$ with $g_0 = g$ and likewise for $x_l = \tanh g_l$.

- For $l \to 0$, write the RG iteration for x_l in form of a differential equation:

$$\begin{aligned} x_l = x_0^b &= \exp\left(\ln x_0^b\right) = \exp\left(e^l \ln x_0\right) \\ &\simeq \exp\left([1+l]\ln x_0\right) = \exp\left(\ln x_0\right)\exp\left(l \ln x_0\right) = x_0\left(1 + l \ln x_0\right) \\ \frac{x_l - x_0}{l} &= x_0 \ln x_0 + \mathcal{O}(l) \end{aligned}$$

  or, taking the limit $l \to 0$,

$$\boxed{\partial_l x \equiv \frac{\partial x}{\partial l} \equiv \beta(x) = x \ln x} \tag{118}$$

  also known as the *beta-function* for x.

- Fixed points of the RG flow are zeros of the beta-function, $\beta(x_\star) \stackrel{!}{=} 0$.

- Infinitesimal form for RG transformation of free energy per site from Eq. (116) (short calculation):

$$\begin{aligned} \partial_l \tilde{f}_l &= \tilde{f} + \ln\left[2\cosh\left(g_l\right)\right] + \partial_l \ln\left[\frac{\cosh\left(g_0\right)}{\cosh\left(g_l\right)}\right]|_{l=0} \\ &= 1\times\tilde{f} + \ln\left[2\cosh\left(g_l\right)\right] - \sinh^2\left(g_l\right)\ln\left(\tanh g_l\right) \end{aligned}$$

- *Canonical dimension* D_g of coupling constant g (from rescaling step, also called "engineering dimension"): Flow equations for coupling constant g of dimension $1/(\text{length})^{D_g}$ start out with

$$\partial_l g = D_g g + ... \tag{119}$$

  Example: For free-energy flow of the D-dimensional Ising model, we have that $\tilde{f}$ has units of $1/(\text{length})^D$, thus $D_{\tilde{f}} = D$ and

$$\partial_l \tilde{f} = D\tilde{f} + ... \tag{120}$$

4.3 General properties of RG flows

Fixed points and critical surface

- Recall RG transformation:
  - for general couplings $\mathbf{g} = \{g_1, g_2, ...\}$: $\mathbf{g}' = \mathcal{R}(b > 1; \mathbf{g})$, see Eq. (97)
  - for correlation length $\xi(\mathbf{g}') = \xi(\mathbf{g})/b$, see Eq. (110)

- A *fixed point* $\mathbf{g}^\star = \{g_1^\star, g_2^\star, ...\}$ fulfills

$$\begin{aligned} \mathbf{g}^\star &= \mathcal{R}(b; \mathbf{g}^\star) \\ \xi\left(\mathbf{g}^\star\right) &= \xi\left(\mathbf{g}^\star\right)/b \end{aligned}$$

- Classification of fixed points according to the two possible solutions for $\xi\left(\mathbf{g}^\star\right)$:
  - *Trivial* fixed point: $\xi\left(\mathbf{g}^\star\right) = 0$
  - *Critical* fixed point: $\xi\left(\mathbf{g}^\star\right) = \infty$

- Example: Square-lattice Ising model (2D) RG flow in Fig. 10 (projected onto $\beta J - \beta J'$ plane), see Ex. 4.1:
  - Three f.p. (two trivial f.p.: disordered $T = \infty$ and ordered at $T = 0$, one critical f.p. with $\xi = \infty$)
  - Each f.p. (trivial and critical) has its own *basin of attraction* (points flowing into f.p.).
  - Basin of attraction for trivial f.p. = phases

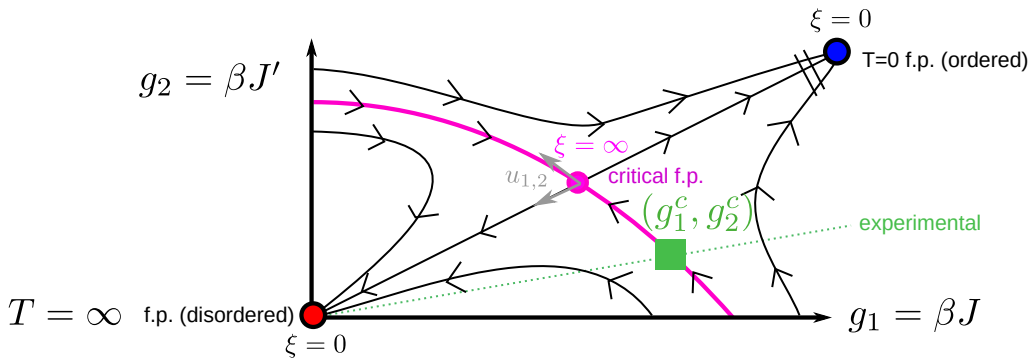


Figure 10: RG-flow of the 2D Ising model, projected in the plane of nearest and next-nearest neighbor couplings J,J'.

- Basin of attraction for critical f.p. = critical surface (critical manifold), has also $\xi = \infty$.
  Reason: $\xi(\mathbf{g}) = b\xi\left(\mathbf{g}^{(1)}\right) = b^2\xi\left(\mathbf{g}^{(2)}\right) = ... = b^n\xi\left(\mathbf{g}^{(n)}\right)$ and for $\mathbf{g}$ on the critical line, we have $\mathbf{g}^{(n)} \underset{n\to\infty}{\to} \mathbf{g}^\star$ for which $\xi(\mathbf{g}^\star) = \infty$. Thus $\xi(\mathbf{g}) = \infty$.
- For start close to critical line, flow is almost towards the critical fixed point where it lingers and is very slow.
  $\to$ Reason to study vicinity of the critical f.p. (next).
- Careful: Critical fixed point (•) is not the same as critical point (■, on critical surface).

Local RG flow close to fixed point

- Linearized flow close to a fixed point $\mathbf{g}^\star$:

$$\delta\mathbf{g}' = \mathbf{g}' - \mathbf{g}^\star = \mathcal{R}(b;\mathbf{g}) - \mathcal{R}(b;\mathbf{g}^\star) \equiv \mathbf{R}(b;\mathbf{g}^\star)\cdot\delta\mathbf{g} \tag{121}$$

  where the derivative-matrix $\mathbf{R}$ has elements

$$R_{ij}(b;\mathbf{g}^\star) \equiv \frac{\partial\mathcal{R}_i(b;\mathbf{g})}{\partial g_j}|_{\mathbf{g}=\mathbf{g}^\star} \tag{122}$$

- $\mathbf{R}$ is a square matrix (but not necessarily symmetric).
  Find the *left* eigenvectors $\mathbf{v}_\alpha^T$ and eigenvalues λ_α,

$$\mathbf{v}_\alpha^T\cdot\mathbf{R}(b;\mathbf{g}^\star) = \mathbf{v}_\alpha^T\cdot\lambda_\alpha \tag{123}$$

  The $\left\{\mathbf{v}_\alpha^T\right\}$ do not need to be all linearly independent, but let us assume they are (matrix is not defective).

- We project the coupling vector $\delta\mathbf{g}$ onto the $\mathbf{v}_\alpha^T$ and obtain the *scaling variables* (see gray arrows in Fig. 10):

$$u_\alpha \equiv \mathbf{v}_\alpha^T\cdot\delta\mathbf{g} = \sum_i v_{\alpha,i}\cdot\delta g_i \tag{124}$$

  The RG transformation doesn't mix different u_α:

$$u'_\alpha = \lambda_\alpha u_\alpha \tag{125}$$

- b-dependence: From the associativity of RG trafo, we have

$$\mathbf{R}(b;\mathbf{g}^\star)\cdot\mathbf{R}(b';\mathbf{g}^\star) = \mathbf{R}(bb';\mathbf{g}^\star) = \mathbf{R}(b';\mathbf{g}^\star)\cdot\mathbf{R}(b;\mathbf{g}^\star) \tag{126}$$

  - Eigenvectors: Commuting matrices have the same eigenvectors $\to$ $\mathbf{v}_\alpha^T$ are independent of b.

– Eigenvalues: Must satisfy $\lambda_\alpha(b)\lambda_\alpha(b') \stackrel{!}{=} \lambda_\alpha(bb')$, thus

$$\lambda_\alpha(b) = b^{y_\alpha} \tag{127}$$

where the *RG eigenvalue* y_α does not depend on b.

- Consequence: RG trafo for the scaling variables u_α around the fixed point $u_\alpha^\star = 0$ for any $b = e^l$:

$$\boxed{u'_\alpha = b^{y_\alpha} u_\alpha, \quad \partial_l u_\alpha = y_\alpha u_\alpha} \tag{128}$$

Warning: Due to the linearization in $\delta\mathbf{g}$ for the derivation of $\mathbf{R}$ in Eq. (121), there are corrections of order $\mathcal{O}(u_\alpha^2)$.

Classification of couplings u_α

- Assume $y_\alpha \in \mathbb{R}$ (case $y_\alpha \notin \mathbb{R}$ possible but rare):
- Distinguish three cases:
  - $y_\alpha > 0$: *Relevant* coupling, $|u_\alpha| \neq 0$ grows exponentially under RG
  - $y_\alpha < 0$: *Irrelevant* coupling, $|u_\alpha| \neq 0$ decreases exponentially under RG
  - $y_\alpha = 0$: *Marginal* coupling.
    Go to higher order in flow equation $\partial_l u_\alpha = 0u_\alpha + \#u_\alpha^2 + ...$ to decide if the coupling u_α is *marginally relevant* or *marginally irrelevant*.

Justification of scaling hypothesis for free energy f

- Consider critical fixed point with two *relevant* scaling variables: $t \sim (T - T_c)/T_c$, $h \propto$ magnetic field (c.f. Ising model).
- RG flow equations (close to fixed point):

$$\partial_l t = y_t t, \ \partial_l h = y_h h \tag{129}$$

or

$$t' = b^{y_t} t, \ h' = b^{y_h} h \tag{130}$$

with $y_t > 0$ and $y_h > 0$. (We will compute $y_{t,h}$ approximately in Sec. 4.4 using φ^4-theory.)

- Recall: RG preserves the partition function

$$\mathcal{Z}_N(t,h) = \mathcal{Z}_{N/b^D}\left(t' = b^{y_t} t, h' = b^{y_h} h\right) \tag{131}$$

with N or N/b^D lattice sites, respectively.

- For the free energy density, we find

$$f(t,h) = -\frac{T}{N} \ln \mathcal{Z}_N(t,h) = -\frac{T}{N} \ln \mathcal{Z}_{N/b^D}(t',h') = \frac{1}{b^D} \cdot \frac{-T}{N/b^D} \ln \mathcal{Z}_{N/b^D}(t',h') \tag{132}$$

and we read off:

$$\boxed{f_{\text{sing}}(t,h) = b^{-D} \cdot f_{\text{sing}}\left(t' = b^{y_t} t, h' = b^{y_h} h\right)} \tag{133}$$

- Restriction to singular part ("sing.") is caused by the neglect of
  - higher-order contributions to flow of t, h
  - marginal or irrelevant couplings (see also Ex. 4.5)
- We confirmed the scaling hypothesis from Eq. (11). Insight:
  Critical exponents (i.e. $\nu = 1/y_t$) are related to the linearized RG flow close to the critical fixed point and its eigenvalues.
- Origin of universality:
  The y_α are properties *of the fixed point*. They do *not* depend on the initial couplings $\mathbf{g}$ which will vary with the physical system.

Scaling hypothesis for correlation function $G(\mathbf{r})$

- Use definition of correlation function in momentum space $(2\pi)^D \delta(\mathbf{k}_1+\mathbf{k}_2) G(\mathbf{k}_1) = \langle \delta\varphi(\mathbf{k}_1)\delta\varphi(\mathbf{k}_2)\rangle$. Assume $k_{1,2} < \Lambda_0/b$ and employ the RG step $\delta\varphi(\mathbf{k}) = \zeta_b \delta\varphi'(\mathbf{k}')$, $\mathbf{k} = \mathbf{k}'/b$:

$$\begin{aligned}
(2\pi)^D \delta(\mathbf{k}_1+\mathbf{k}_2) G(\mathbf{k}_1;\mathbf{g}) &= \langle \delta\varphi(\mathbf{k}_1)\delta\varphi(\mathbf{k}_2)\rangle_{\mathbf{g}} \\
&= \mathcal{Z}^{-1} \int \mathcal{D}[\varphi] e^{-S[\varphi;\mathbf{g}]} \delta\varphi(\mathbf{k}_1)\,\delta\varphi(\mathbf{k}_2) \\
&= \zeta_b^2 \mathcal{Z}^{-1} \int \mathcal{D}[\varphi'] e^{-S[\varphi';\mathbf{g}']} \delta\varphi'(\mathbf{k}_1')\,\delta\varphi'(\mathbf{k}_2') \\
&= \zeta_b^2 (2\pi)^D \delta(\mathbf{k}_1'+\mathbf{k}_2') G(\mathbf{k}_1';\mathbf{g}') \\
\left\{\delta(b\mathbf{k}) = b^{-D}\delta(\mathbf{k})\right\} &= \zeta_b^2 b^{-D} (2\pi)^D \delta(\mathbf{k}_1+\mathbf{k}_2) G(b\mathbf{k}_1;\mathbf{g}')
\end{aligned}$$

  By comparison, we find

$$G(\mathbf{k};\mathbf{g}) = \zeta_b^2 b^{-D} G(b\mathbf{k};\mathbf{g}') \tag{134}$$

- Convention: Parameterization

$$\zeta_b \equiv b^{1+D/2}\sqrt{Z_b} \tag{135}$$

  so that

$$G(\mathbf{k};\mathbf{g}) = b^2 Z_b G(b\mathbf{k};\mathbf{g}') \tag{136}$$

  Using $b = e^l$, define $Z_l = Z_{b=e^l}$. Flow equation for Z_l parameterized as:

$$\boxed{\partial_l Z_l \equiv -\eta_l Z_l}. \tag{137}$$

  Suppose $\lim\limits_{l\to\infty} \eta_l = \eta$, then $Z_l = e^{-\eta l} = b^{-\eta}$ and for large enough l,

$$G(\mathbf{k};\mathbf{g}) = b^{2-\eta} G(b\mathbf{k};\mathbf{g}')\,. \tag{138}$$

  At a fixed point $\mathbf{g} = \mathbf{g}' = \mathbf{g}^\star$, this equation enforces the power-law form:

$$\boxed{G(\mathbf{k}) = |\mathbf{k}|^{-2+\eta}} \tag{139}$$

- Conclusion: This confirms the postulated (real-space) power-law form in Eq. (9). The anomalous dimension η is connected to the microscopic RG via field rescaling factor ζ_b.

- Example: Ising model / ϕ^4-theory.
  Relation between y_h and ζ_b: Consider field-term $\propto \varphi(\mathbf{k}=0)$ from the effective action

$$h\varphi(\mathbf{k}=0) = h'\varphi'(\mathbf{k}'=0) = h'\zeta_b^{-1}\varphi(\mathbf{k}=0) \tag{140}$$

  Compare the pre-factors of $\varphi(\mathbf{k}=0)$. Read off $h' = \zeta_b h$, compare to $h' = b^{y_h} h$. Find

$$\zeta_b = b^{y_h} \tag{141}$$

  Insert in Eq. (134). Consider only relevant couplings $\mathbf{g} = (t,h)$ (singular part only):

$$\boxed{G_{\text{sing}}(\mathbf{k};t,h) = b^{-D} b^{2y_h} G_{\text{sing}}(b\mathbf{k};b^{y_t}t,b^{y_h}h)} \tag{142}$$

  which is the Fourier-transformation of the scaling hypothesis in Eq. (14).

4.4 Example: RG of ϕ^4-theory and Wilson-Fisher fixed point

RG flow equations

- Recall ϕ^4-theory (Ginzburg-Landau-Wilson action) from Eq. (50).
  Set magnetic field to zero, assume high-temperature regime $r_0 > 0$:

$$S_{\Lambda_0}[\varphi] = V f_0 + \frac{1}{2}\int_{\mathbf{k}}^{\Lambda_0}\left[r_0 + c_0 k^2\right]\varphi(-\mathbf{k})\varphi(\mathbf{k}) + \frac{u_0}{4!}\int_{\mathbf{k}_{1,2,3,4}}^{\Lambda_0}(2\pi)^D\delta\left(\mathbf{k}_1 + ... + \mathbf{k}_4\right)\varphi(\mathbf{k}_1)\varphi(\mathbf{k}_2)\varphi(\mathbf{k}_3)\varphi(\mathbf{k}_4) \tag{143}$$

- Implement mode elimination step with cutoff $\Lambda = \Lambda_0/b < \Lambda_0$: $\varphi(\mathbf{k}) = \underbrace{\Theta(\Lambda - k)\varphi(\mathbf{k})}_{\varphi^<} + \underbrace{\Theta(k-\Lambda)\varphi(\mathbf{k})}_{\varphi^>}$,
  yields three contributions:

$$S_{\Lambda_0}[\varphi] = S_\Lambda[\varphi^<] + S_{\Lambda,\Lambda_0}[\varphi^>] + S_{mix}[\varphi^<,\varphi^>] \tag{144}$$

  - "Smaller part": $S_\Lambda[\varphi^<]$ is like $S_{\Lambda_0}[\varphi]$ but with $\int_{\mathbf{k}}^{\Lambda_0}\varphi(\mathbf{k})... \to \int_{\mathbf{k}}^{\Lambda}\varphi^<(\mathbf{k})....$
  - "Larger part": $S_{\Lambda,\Lambda_0}[\varphi^>]$ is similar with $\int_{\mathbf{k}}^{\Lambda_0}\varphi(\mathbf{k})... \to \int_{|\mathbf{k}|>\Lambda}^{\Lambda_0}\varphi^>(\mathbf{k})...$
  - "Mixing term": Of order u_0. Possibilities of picking two $\varphi^<$-fields out of the four φ fields $\binom{4}{2} = 6$:

$$\begin{aligned} S_{mix}[\varphi^<,\varphi^>] = 6\times\frac{u_0}{4!}\int_{\mathbf{k}_{1,2}}^{\Lambda}\int_{|\mathbf{k}_{3,4}|>\Lambda}^{\Lambda_0}(2\pi)^D\delta\left(\mathbf{k}_1 + ... + \mathbf{k}_4\right)\varphi^<(\mathbf{k}_1)\varphi^<(\mathbf{k}_2)\varphi^>(\mathbf{k}_3)\varphi^>(\mathbf{k}_4) \\ + "\varphi^<\left(\varphi^>\right)^3" + "\left(\varphi^<\right)^3\varphi^>" \end{aligned}$$

- Integrate over $\varphi^>$ to get new effective action:

$$e^{-S_\Lambda[\varphi^<,f^<,r^<,c^<,u^<]} = e^{-S_\Lambda[\varphi^<,f_0,r_0,c_0,u_0]}\int\mathcal{D}[\varphi^>]\,e^{-S_{\Lambda,\Lambda_0}[\varphi^>]-S_{mix}[\varphi^<,\varphi^>]} \tag{145}$$

  or

$$S_\Lambda[\varphi^<,f^<,r^<,c^<,u^<] \;=\; S_\Lambda[\varphi^<,f_0,r_0,c_0,u_0] - \ln\left[\int\mathcal{D}[\varphi^>]\,e^{-S_{\Lambda,\Lambda_0}[\varphi^>]-S_{mix}[\varphi^<,\varphi^>]}\right] \tag{146}$$

  Expand the ln in powers of u_0:

$$\begin{aligned} -\ln[...] &= \underbrace{-\ln\left[\int\mathcal{D}[\varphi^>]\,e^{-S_{\Lambda,\Lambda_0}[\varphi^>]}\right]}_{\varphi^<-independent} - \ln\left[\frac{\int\mathcal{D}[\varphi^>]\,e^{-S_{\Lambda,\Lambda_0}[\varphi^>]-S_{mix}[\varphi^<,\varphi^>]}}{\int\mathcal{D}[\varphi^>]\,e^{-S_{\Lambda,\Lambda_0}[\varphi^>]}}\right] \\ &= f^< - f_0 - \ln\left[\frac{\int\mathcal{D}[\varphi^>]\,e^{-S_{\Lambda,\Lambda_0}[\varphi^>]}\left(1 - S_{mix}[\varphi^<,\varphi^>] + \frac{1}{2}S^2_{mix}[\varphi^<,\varphi^>] + \mathcal{O}(u_0^3)\right)}{\int\mathcal{D}[\varphi^>]\,e^{-S_{\Lambda,\Lambda_0}[\varphi^>]}}\right] \\ &\simeq f^< - f_0 - \ln\left[1 - \underbrace{\frac{\int\mathcal{D}[\varphi^>]\,e^{-S_{\Lambda,\Lambda_0}[\varphi^>]}S_{mix}[\varphi^<,\varphi^>]}{\int\mathcal{D}[\varphi^>]\,e^{-S_{\Lambda,\Lambda_0}[\varphi^>]}}}_{\sim\boxed{u_0\varphi^{<2}}+u_0^2\varphi^{<2}+...} + \underbrace{\frac{\int\mathcal{D}[\varphi^>]\,e^{-S_{\Lambda,\Lambda_0}[\varphi^>]}\frac{1}{2}S^2_{mix}[\varphi^<,\varphi^>]}{\int\mathcal{D}[\varphi^>]\,e^{-S_{\Lambda,\Lambda_0}[\varphi^>]}}}_{\sim\boxed{u_0^2\varphi^{<4}}+u_0^2\varphi^{<2}+u_0^2\varphi^{<6}+...}\right] \end{aligned}$$

- Consider leading-in-u_0 corrections to quadratic/quartic parts of $S_\Lambda[\varphi^<,f^<,r^<,c^<,u^<]$: Need to keep [boxed] terms of order $u_0\varphi^{<2}$ and $u_0^2\varphi^{<4}$. The higher-order in u_0-terms, which also come also $\varphi^<\left(\varphi^>\right)^3$, are discarded.

- Hence we can replace the expectation values with respect to the interacting action $S_{\Lambda,\Lambda_0}[\varphi^>]$ by expectation values with respect to its Gaussian part, $S^0_{\Lambda,\Lambda_0}[\varphi^>] = \frac{1}{2}\int_{|\mathbf{k}|>\Lambda}^{\Lambda_0}[r_0 + c_0 k^2]\,\varphi^>(-\mathbf{k})\varphi^>(\mathbf{k})$.
Notation:

$$\langle\cdots\rangle_{0,>} \equiv \frac{\int\mathcal{D}[\varphi^>]\,e^{-S^0_{\Lambda,\Lambda_0}[\varphi^>]}\cdots}{\int\mathcal{D}[\varphi^>]\,e^{-S^0_{\Lambda,\Lambda_0}[\varphi^>]}}. \tag{147}$$

We then have

$$\begin{aligned}
-\ln[...] &\simeq f^< - f_0 - \ln\left[1 - \langle S_{mix}[\varphi^<,\varphi^>]\rangle_{0,>} + \frac{1}{2}\left\langle S^2_{mix}[\varphi^<,\varphi^>]\right\rangle_{0,>}\right] \\
\left\{\ln[1+x]\simeq x - x^2/2\right\} &\simeq f^< - f_0 + \langle S_{mix}[\varphi^<,\varphi^>]\rangle_{0,>} - \frac{1}{2}\left[\left\langle S^2_{mix}[\varphi^<,\varphi^>]\right\rangle_{0,>} - \langle S_{mix}[\varphi^<,\varphi^>]\rangle^2_{0,>}\right]
\end{aligned}$$

- In light of Eq. (146), we compare the parts of order $(\varphi^<)^2$ [terms $\sim\varphi^<$ or $\sim(\varphi^<)^3$ vanish] and read off

$$\begin{aligned}
\frac{1}{2}\left(r^< + c^< k^2\right) &= \frac{1}{2}\left(r_0 + c_0 k^2\right) + \langle S_{mix}[\varphi^<,\varphi^>]\rangle_{0,>}\,|^{\varphi^<-\text{amputated}} \\
&= \frac{1}{2}\left(r_0 + c_0 k^2\right) + 6\frac{u_0}{4!}\int_{|\mathbf{q}|>\Lambda}^{\Lambda_0}\underbrace{\langle\varphi^>(\mathbf{q})\varphi^>(-\mathbf{q})\rangle_{0,>}}_{1/(r_0+c_0q^2)}
\end{aligned}$$

After comparison of both sides, we find

$$\boxed{c^< = c_0} \tag{148}$$

$$\boxed{r^< = r_0 + \frac{u_0}{2}\int_\Lambda^{\Lambda_0}\frac{d^Dq}{(2\pi)^D}\frac{1}{r_0+c_0q^2} \simeq r_0 + u_0\frac{K_D\Lambda_0^{D-1}(\Lambda_0-\Lambda)}{2(r_0+c_0\Lambda_0^2)}} \tag{149}$$

In the above, $K_D \equiv \Omega_D/(2\pi)^D$ where $\Omega_D \equiv 2\pi^{D/2}/\Gamma(D/2)$ is the surface area of a unit-sphere in D-dimensional space (c.f. Ex. 2.2).

- For the new interaction constant $u^<$, we consider the $u_0^2\varphi^{<4}$ contribution on the rhs of $-\ln[...] = ...$

$$\begin{aligned}
&-\frac{1}{2}\left[\left\langle S^2_{mix}[\varphi^<,\varphi^>]\right\rangle_{0,>} - \langle S_{mix}[\varphi^<,\varphi^>]\rangle^2_{0,>}\right] \\
= \;& -\frac{1}{2} < 6\frac{u_0}{4!}\int_{\mathbf{k}_{1,2}}^{\Lambda}\int_{|\mathbf{k}_{3,4}|>\Lambda}^{\Lambda_0}(2\pi)^D\delta(\mathbf{k}_1+...+\mathbf{k}_4)\,\varphi^<(\mathbf{k}_1)\varphi^<(\mathbf{k}_2)\varphi^>(\mathbf{k}_3)\varphi^>(\mathbf{k}_4) \\
\times\; & 6\frac{u_0}{4!}\int_{\mathbf{q}_{1,2}}^{\Lambda}\int_{|\mathbf{q}_{3,4}|>\Lambda}^{\Lambda_0}(2\pi)^D\delta(\mathbf{q}_1+...+\mathbf{q}_4)\,\varphi^<(\mathbf{q}_1)\varphi^<(\mathbf{q}_2)\varphi^>(\mathbf{q}_3)\varphi^>(\mathbf{q}_4) >^{con.}_{0,>} \\
= \;& -\frac{1}{2}2\left(6\frac{u_0}{4!}\right)^2\int_{\mathbf{k}_{1,2}}^{\Lambda}\int_{|\mathbf{k}_{3,4}|>\Lambda}^{\Lambda_0}(2\pi)^D\delta(\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3+\mathbf{k}_4)\int_{\mathbf{q}_{1,2}}^{\Lambda}\int_{|\mathbf{q}_{3,4}|>\Lambda}^{\Lambda_0}(2\pi)^D\delta(\mathbf{q}_1+\mathbf{q}_2+\mathbf{q}_3+\mathbf{q}_4) \\
& \times\varphi^<(\mathbf{q}_1)\varphi^<(\mathbf{k}_1)\varphi^<(\mathbf{q}_2)\varphi^<(\mathbf{k}_2)\,\langle\varphi^>(\mathbf{k}_3)\varphi^>(\mathbf{q}_3)\rangle_{0,>}\,\langle\varphi^>(\mathbf{k}_4)\varphi^>(\mathbf{q}_4)\rangle_{0,>}
\end{aligned}$$

where the factor 2 comes from the Wick-theorem with the two choices of pairing $\mathbf{k}_3 = -\mathbf{q}_{3,4}$.

- We use $\langle\varphi^>(\mathbf{k})\varphi^>(\mathbf{q})\rangle_{0,>} = (2\pi)^D\,\delta(\mathbf{k}+\mathbf{q})\,G_0(\mathbf{k})$ with $G_0(\mathbf{k}) = 1/(r_0+c_0k^2)$ and carefully consider all the δ-functions:

$$\begin{aligned}
... &= \int_{\mathbf{k}_{1,2}}^{\Lambda}\int_{\mathbf{q}_{1,2}}^{\Lambda}(2\pi)^D\delta(\mathbf{q}_1+\mathbf{q}_2+\mathbf{k}_1+\mathbf{k}_2)\,\varphi^<(\mathbf{q}_1)\varphi^<(\mathbf{k}_1)\varphi^<(\mathbf{q}_2)\varphi^<(\mathbf{k}_2) \\
&\times\; -2\frac{1}{2}\left(6\frac{u_0}{4!}\right)^2\int_{|\mathbf{k}_{3,4}|>\Lambda}^{\Lambda_0}(2\pi)^D\delta(\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3+\mathbf{k}_4)\,\frac{1}{(r_0+c_0k_3^2)(r_0+c_0k_4^2)}
\end{aligned}$$

The last line depends on $\mathbf{k}_1+\mathbf{k}_2$. To get a momentum independent interaction strength, we approximate $\mathbf{k}_{1,2} = 0$ which is plausible because they are "smaller" momenta. We get

$$\boxed{u^< = u_0 - \underbrace{4!2\frac{1}{2}\left(6\frac{u_0}{4!}\right)^2}_{\frac{3}{2}u_0^2}\int_\Lambda^{\Lambda_0}\frac{d^Dk}{(2\pi)^D}\frac{1}{(r_0+c_0k^2)^2} \simeq u_0 - \frac{3}{2}u_0^2\frac{K_D\Lambda_0^{D-1}(\Lambda_0-\Lambda)}{(r_0+c_0\Lambda_0^2)^2}} \tag{150}$$

- Remarks:
  - The approximate expressions for $r^<, c^<, u^<$ only involve a single momentum integral, this corresponds to just one loop in the corresponding Feynman diagrams ($\rightarrow$ "one-loop approximation").
  - Formally, terms describing a momentum dependence of a vertex $u(\mathbf{k}_{1,2,3}) = u^{(0)} + u^{(1)}k_1 + ...$ are less relevant than $u^{(0)}$ because $[u^{(1)}] = [u^{(0)}] \times [length]$ under rescaling they have a smaller engineering dimension than $u^{(0)}$. This justifies working with coupling constants (instead of coupling functions).

- Rescaling step (from $r^<, u^<$ to r', u'): Use $\mathbf{k} = b^{-1}\mathbf{k}'$ and $\varphi^<(\mathbf{k}'/b = \mathbf{k}) = \zeta_b \varphi'(\mathbf{k}')$:

$$\begin{aligned}
\frac{1}{2}\int_{\mathbf{k}}^{\Lambda} \left[r^< + c^< k^2\right] \varphi^<(-\mathbf{k})\varphi^<(\mathbf{k}) &= \frac{1}{2}\int_{\mathbf{k}'}^{\Lambda_0} \zeta_b^2 b^{-D} \left[r^< + c^< b^{-2}k'^2\right] \varphi'(-\mathbf{k}')\varphi'(\mathbf{k}') \\
\frac{u_0^<}{4!}\int_{\mathbf{k}_{1,2,3,4}}^{\Lambda} (2\pi)^D \delta\left(\mathbf{k}_1 + ... + \mathbf{k}_4\right) \varphi^<(\mathbf{k}_1)...\varphi^<(\mathbf{k}_4) &= \frac{u_0^<}{4!}\int_{\mathbf{k}'_{1,2,3,4}}^{\Lambda_0} \zeta_b^4 b^{-4D}(2\pi)^D b^D \delta(\mathbf{k}'_1 + ... + \mathbf{k}'_4) \varphi'(\mathbf{k}'_1)...\varphi'(\mathbf{k}_4)
\end{aligned}$$

  Want to keep the prefactor of the k^2-term invariant, this requires $\zeta_b = b^{1+D/2}$. We then get

$$\begin{aligned}
r' &= b^2 r^< \\
u' &= b^{4-D} u^<
\end{aligned}$$

  We change to $b = e^l$ and find with $\Lambda = \Lambda_0 e^{-l}$:

$$\begin{aligned}
r' &= e^{2l}\left[r_0 + u_0 \frac{K_D \Lambda_0^{D-1}\left(\Lambda_0 - \Lambda_0 e^{-l}\right)}{2(r_0 + c_0\Lambda_0^2)}\right] \\
&= r_0 + 2l r_0 + u_0 \frac{K_D \Lambda_0^D l}{2(r_0 + c_0\Lambda_0^2)} + \mathcal{O}(l^2) \\
\partial_l r_l &= 2r_l + \frac{u_l}{2}\frac{K_D\Lambda_0^D}{r_l + c_0\Lambda_0^2}
\end{aligned}$$

  and likewise

$$\partial_l u_l = (4-D)u_l - \frac{3}{2}u_l^2 \frac{K_D \Lambda_0^D}{(r_l + c_0\Lambda_0^2)^2} \tag{151}$$

- Clean up by defining dimensionless couplings:

$$\bar{r}_l \equiv r_l \frac{1}{c_0\Lambda_0^2}, \qquad \bar{u}_l \equiv u_l \frac{K_D}{c_0^2 \Lambda_0^{4-D}} \tag{152}$$

  in terms of which

$$\boxed{\partial_l \bar{r}_l = 2\bar{r}_l + \frac{1}{2}\frac{\bar{u}_l}{\bar{r}_l + 1}} \qquad \boxed{\partial_l \bar{u}_l = (4-D)\bar{u}_l - \frac{3}{2}\frac{\bar{u}_l^2}{(\bar{r}_l + 1)^2}} \tag{153}$$

Wilson-Fisher fixed point for $D > 4$

- Analyze the flow given by Eq. (153) above, see Fig. 11 for flow diagrams at $D = 4.5$, $D = 3.8$ and $D = 3$.
  - For $D > 4$, we only have the Gaussian critical fixed point, $(\bar{u}_\star, \bar{r}_\star) = (0, 0)$. ($\rightarrow D_{up} = 4$)
  - For $D < 4$, the Gaussian fixed point becomes unstable for $\bar{u} > 0$:
    Wilson-Fisher f.p. controls the universality of the phase transition. $\rightarrow$ Gaussian approximation breaks down.

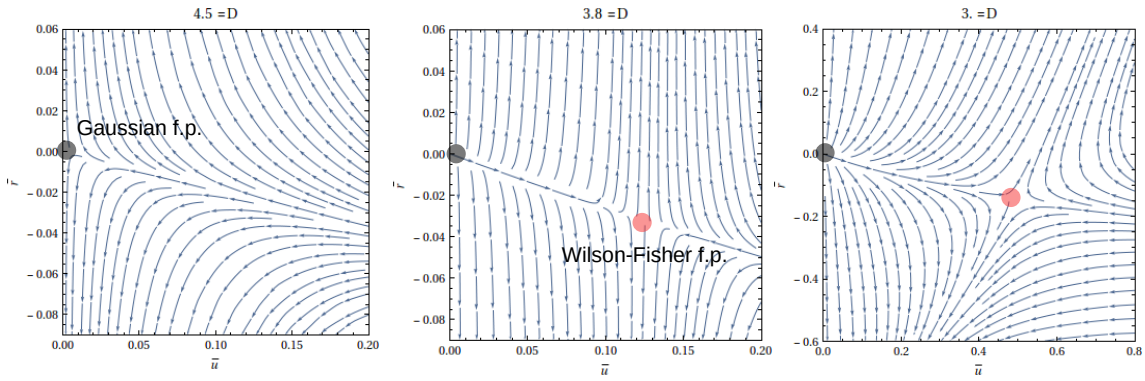


Figure 11: RG flow of the ϕ^4-theory according to Eq. (153) for different dimensions around $D_{up} = 4$: Left $D = 4.5$, middle $D = 3.8$, right $D = 3$.

Critical exponents in $D < 4$: $\epsilon-$expansion

- We are interested in the physical case $D = 3$.
  Q: Can we linearize the flow around the Wilson-Fisher fixed point and find critical exponents?
  This would not be reliable, because the flow equations are approximate and only valid to order u_l^2.
- A more consistent way is to set $\epsilon = D_{up} - D = 4 - D > 0$: The Wilson-Fisher fixed point conditions are

$$0 = 2\bar{r}_\star + \frac{1}{2}\frac{\bar{u}_\star}{\bar{r}_\star + 1},$$
$$0 = \epsilon\bar{u}_\star - \frac{3}{2}\frac{\bar{u}_\star^2}{(\bar{r}_\star + 1)^2}.$$

  Without the $\mathcal{O}(\bar{u}_\star^3)$ terms, we can only solve for $\bar{r}_\star, \bar{u}_\star$ reliably up to $\mathcal{O}(\varepsilon)$:

$$\bar{u}_\star = \frac{2}{3}\epsilon + \mathcal{O}(\epsilon^2)$$
$$\bar{r}_\star = -\epsilon/6 + \mathcal{O}(\epsilon^2)$$

- The linearized flow equations around the Wilson-Fisher fixed point ($\delta\bar{r}_l \equiv \bar{r}_l - \bar{r}_\star$, $\delta\bar{u}_l \equiv \bar{u}_l - \bar{u}_\star$) are

$$\partial_l \begin{pmatrix} \delta\bar{r}_l \\ \delta\bar{u}_l \end{pmatrix} = \begin{pmatrix} 2 - \frac{\epsilon}{3} & \frac{1}{2} + \frac{\epsilon}{12} \\ 0 & -\epsilon \end{pmatrix} \begin{pmatrix} \delta\bar{r}_l \\ \delta\bar{u}_l \end{pmatrix} \tag{154}$$

  One can find the left eigenvectors and eigenvalues (up to order $\mathcal{O}(\varepsilon)$):

$$\mathbf{v}_1^T = (0, 1), \qquad y_1 = -\epsilon = D - 4 < 0\,(irrelevant.)$$
$$\mathbf{v}_2^T = (1, \frac{1 - \epsilon/6}{4}), \qquad y_2 = 2 - \frac{\epsilon}{3} > 0\,(relevant.)$$

- The irrelevant scaling variable is $\mathbf{v}_1^T \cdot \begin{pmatrix} \delta\bar{r}_l \\ \delta\bar{u}_l \end{pmatrix} = \delta\bar{u}_l$, the relevant scaling variable is $\mathbf{v}_2^T \cdot \begin{pmatrix} \delta\bar{r}_l \\ \delta\bar{u}_l \end{pmatrix} = \delta\bar{r}_l + \frac{1-\epsilon/6}{4}\delta\bar{u}_l \equiv t_l$.
- According to Sec. 4.3, we find

$$\boxed{\nu \equiv \frac{1}{y_2} = \frac{1}{2} + \frac{\epsilon}{12} + \mathcal{O}(\epsilon^2)} \tag{155}$$

- Remark:
  - Recall MFT / Gaussian fixed point: $\nu_{\varepsilon=0} = 0.5$. The above formula tells us how ν changes as we lower D below $D = 4$.
  - One can set $\epsilon \to 1$ at the end of this calculation, which yields $\nu_{1-\text{loop}} = 0.58$ and the exact value is $\nu_{ex} \simeq 0.63$. Systematic improvement to order $\mathcal{O}(\epsilon^2)$ is possible in a two-loop calculation (way more complicated!).

4.5 Example: Kondo-Effect and poor-man's scaling

Phenomenology and Single Impurity Anderson Model

- Consider metals with *magnetic* impurities, e.g. Fe in Cu or Mn in Ag.
- Magnetic impurity: Localized moment (spin S=1/2) that gives Curie-Weiss contribution to magnetic susceptibility, $\chi_{\text{imp.}} \simeq \frac{C}{T+\Theta}$ for large T, $T \gg \Theta > 0$.
- Experimental observation: The electrical resistance ρ over temperature has a minimum (Fig. 12a).
- Unusual, since well-known mechanisms would lead to further decaying or constant resistance as $T \to 0$:
  - electron-electron scattering $\rho \sim T^2$
  - electron-phonon scattering $\rho \sim T^5$
  - non-magnetic impurity scattering $\rho \sim const.$
- Single-impurity Anderson model (SIAM): Host metal of non-interacting (Fermi liquid quasiparticles, set Fermi energy $\varepsilon_F = 0$) with localized d-level impurity state $c_{d\sigma}$ (degenerate for impurity spin $\uparrow, \downarrow$) and hybridization to s-level itinerant electron $c_{\mathbf{k}\sigma}$:

$$H = \underbrace{\sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}}_{\equiv H_0} + \sum_\sigma \varepsilon_d c^\dagger_{d\sigma} c_{d\sigma} + U n_{d,\uparrow} n_{d,\downarrow} + \sum_{\mathbf{k},\sigma} V_{\mathbf{k}} c^\dagger_{d\sigma} c_{\mathbf{k}\sigma} + h.c., \tag{156}$$

  where $n_{d,\sigma} = c^\dagger_{d,\sigma} c_{d,\sigma}$.
- Atomic limit: $V_{\mathbf{k}} \to 0$. Four impurity eigenstates (see Fig. 12a, inset): Empty level $E = 0$, single occupation (2x) $E = \varepsilon_d$, double occupation $E = \varepsilon_d + U$.
- Enforce single occupation to obtain local moment (and thus Curie-Weiss law): $\varepsilon_d < 0 < \varepsilon_d + U$. Then it is energetically favorable to add one electron to impurity level, but not a second.

Schrieffer-Wolff transformation: From SIAM to Kondo model

- Q: What happens if $V_{\mathbf{k}}$ is switched on? Depends on ratio $V_{\mathbf{k}}/\Delta E$ where $\Delta E = \varepsilon_d$ or $U + \varepsilon_d$ denote energetical distance to empty or doubly occupied state.
- Assume $V_{\mathbf{k}}/\Delta E$ small, derive effective Hamiltonian H_{eff} for single occupation $n_d = n_{d\uparrow} + n_{d\downarrow} = 1$, $n_d = 0, 2$ are taken into account as virtual states in perturbation theory.
- Start with Schrödinger equation $H\psi = E\psi$, multiply with projection operators $P_n (= P_n^\dagger = P_n^2)$ which project to $n_d = 0, 1, 2$:

$$P_0 = (1 - n_{d,\uparrow})(1 - n_{d,\downarrow}), \quad P_1 = (1 - n_{d,\uparrow}) n_{d,\downarrow} + \{\uparrow \leftrightarrow \downarrow\}, \quad P_2 = n_{d,\uparrow} n_{d,\downarrow}, \tag{157}$$

  and define $\psi_n \equiv P_n \psi$ and $H_{nn'} \equiv P_n H P_{n'} = H^\dagger_{n'n}$.

$$\begin{pmatrix} H_{00} & H_{01} & H_{02} \\ H_{10} & H_{11} & H_{12} \\ H_{20} & H_{21} & H_{22} \end{pmatrix} \begin{pmatrix} \psi_0 \\ \psi_1 \\ \psi_2 \end{pmatrix} = E \begin{pmatrix} \psi_0 \\ \psi_1 \\ \psi_2 \end{pmatrix} \tag{158}$$

- Block-Hamiltonians:

$$H_{10} = \sum_{\mathbf{k},\sigma} V_{\mathbf{k}} c^\dagger_{d\sigma} (1 - n_{d,\bar{\sigma}}) c_{\mathbf{k}\sigma}$$
$$H_{21} = \sum_{\mathbf{k},\sigma} V_{\mathbf{k}} c^\dagger_{d\sigma} n_{d\bar{\sigma}} c_{\mathbf{k}\sigma}$$
$$H_{02} = 0$$

- Effective Hamiltonian for ψ_1: Eliminate ψ_0 and ψ_2 from Eq. (158) (still exact equation for energies E)

$$E\psi_1 = \left[H_{11} + H_{12}\left(E - H_{22}\right)^{-1} H_{21} + H_{10}\left(E - H_{00}\right)^{-1} H_{01}\right]\psi_1 \tag{159}$$

and the term [...], computed to order $(V/\Delta E)^2$ and then E-independent, is the effective Hamiltonian H_{eff}.

- First term: $H_{11} = (H_0 + \varepsilon_d)\, P_1$ and we drop the constant ε_d.
- Second term: Use $H_{22} = (H_0 + 2\varepsilon_d + U)\, P_2$,

$$H_{12}\left(E - H_{22}\right)^{-1} H_{21} = \sum_{\mathbf{k},\sigma}\sum_{\mathbf{k}',\sigma'} V^{\star}_{\mathbf{k}'} c^{\dagger}_{\mathbf{k}'\sigma'} n_{d\bar{\sigma}'} c_{d\sigma'} \left(E - H_0 - 2\varepsilon_d - U\right)^{-1} V_{\mathbf{k}} c^{\dagger}_{d\sigma} n_{d\bar{\sigma}} c_{\mathbf{k}\sigma} \tag{160}$$

- Use from $[E - H_0, c_{\mathbf{q}\sigma}] = \varepsilon_{\mathbf{q}} c_{\mathbf{q}\sigma}$ that $c_{\mathbf{q}\sigma}\frac{1}{E-H_0} = \frac{1}{E-H_0-\varepsilon_{\mathbf{q}}} c_{\mathbf{q}\sigma}$ (and $c^{\dagger}_{\mathbf{q}\sigma}\frac{1}{E-H_0} = \frac{1}{E-H_0+\varepsilon_{\mathbf{q}}} c^{\dagger}_{\mathbf{q}\sigma}$).
- Move all operators to the right, obtain

$$H_{12}\left(E - H_{22}\right)^{-1} H_{21} \;=\; \sum_{\mathbf{k},\sigma}\sum_{\mathbf{k}',\sigma'} V^{\star}_{\mathbf{k}'} V_{\mathbf{k}} \underbrace{\left(E - H_0 + \varepsilon_{\mathbf{k}'} - 2\varepsilon_d - U\right)^{-1}}_{\frac{-1}{U+\varepsilon_d-\varepsilon_{\mathbf{k}'}}\left(1-\frac{E-H_0-\varepsilon_d}{U+\varepsilon_d-\varepsilon_{\mathbf{k}'}}\right)^{-1}} c^{\dagger}_{\mathbf{k}'\sigma'} c_{\mathbf{k}\sigma} n_{d\bar{\sigma}'} c_{d\sigma'} c^{\dagger}_{d\sigma} n_{d\bar{\sigma}}$$

and we drop the small second term in parenthesis as we assume E is close to the ground-state energy of $H_0 + \varepsilon_d$ in the regime of interest.

- In $n_d = 1$ subspace: Define $\mathbf{S} = \frac{1}{2}\sum_{\sigma} c^{\dagger}_{d\sigma}\boldsymbol{\tau}_{\sigma\sigma'} c_{d\sigma'}$ with $\boldsymbol{\tau}$ the vector of Pauli matrices, then $S^z = \frac{1}{2}\left(n_{d\uparrow} - n_{d\downarrow}\right)$ and $S^{+} = S^x + iS^y = c^{\dagger}_{d\uparrow} c_{d\downarrow}$.
- Set $\sigma = \uparrow, \sigma' = \downarrow$ and find

$$H_{12}\left(E - H_{22}\right)^{-1} H_{21}|_{\sigma=\uparrow,\sigma'=\downarrow} \simeq \sum_{\mathbf{k},\mathbf{k}'} \frac{V^{\star}_{\mathbf{k}'} V_{\mathbf{k}}}{U + \varepsilon_d - \varepsilon_{\mathbf{k}'}} c^{\dagger}_{\mathbf{k}'\downarrow} c_{\mathbf{k}\uparrow} S^{+} \tag{161}$$

and similar with $S^{+} \to S^{-}$ for $\sigma = \downarrow, \sigma' = \uparrow$. The contributions from $H_{10}\left(E - H_{00}\right)^{-1} H_{01}$ to H_{eff} is similar, but with $1/(U + \varepsilon_d - \varepsilon_{\mathbf{k}'}) \to 1/(\varepsilon_{\mathbf{k}} - \varepsilon_d)$.

- As we want to find a low-energy effective Hamiltonian, we assume the relevant $\mathbf{k}$ to be close to the Fermi surface and $|\varepsilon_{\mathbf{k}}|$ much smaller than ΔE. We assume that $V_{\mathbf{k}}$ does not strongly depend on $\mathbf{k}$ at the Fermi surface. Then the exchange interaction is anti-ferromagnetic.

$$J = |V|^2\left(\frac{1}{U + \varepsilon_d} + \frac{1}{-\varepsilon_d}\right) = |V|^2 \frac{U}{(U + \varepsilon_d)\,(-\varepsilon_d)} > 0 \tag{162}$$

- For equal spins $\sigma = \sigma'$, we get a term $JS^z\left(c^{\dagger}_{\mathbf{k}'\uparrow} c_{\mathbf{k}\uparrow} - c^{\dagger}_{\mathbf{k}'\downarrow} c_{\mathbf{k}\downarrow}\right)$ and a potential scattering term $\sum_{\mathbf{k},\mathbf{k}'} K_{\mathbf{k},\mathbf{k}'} c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k}',\sigma}$.
- The potential scattering term $\propto K_{\mathbf{k},\mathbf{k}'}$ does not dependent on the local spin S and does not flip the bath spins. We drop it in the following (it could be removed by re-defining $c_{\mathbf{k},\sigma}$).
- We obtain an isotropic Heisenberg interaction between impurity spin S and the local spin of the c-electrons, $\mathbf{S}_c(\mathbf{r} = 0) = \sum_{\mathbf{k},\mathbf{k}'} \frac{1}{2}\sum_{\sigma} c^{\dagger}_{\mathbf{k}\sigma}\boldsymbol{\tau}_{\sigma\sigma'} c_{\mathbf{k}'\sigma'}$.

$$\boxed{H_{\text{eff}} \simeq H_0 + \sum_{\mathbf{k},\mathbf{k}'} J\left(S^{+} c^{\dagger}_{\mathbf{k}',\downarrow} c_{\mathbf{k}\uparrow} + S^{-} c^{\dagger}_{\mathbf{k}\uparrow} c_{\mathbf{k}',\downarrow} + S^z\left[c^{\dagger}_{\mathbf{k}'\uparrow} c_{\mathbf{k}\uparrow} - c^{\dagger}_{\mathbf{k}'\downarrow} c_{\mathbf{k}\downarrow}\right]\right) = H_0 + 2J\mathbf{S}\cdot\mathbf{S}_c(\mathbf{r} = 0) \equiv H_K} \tag{163}$$

which is also known as the Kondo model.

- Remarks:

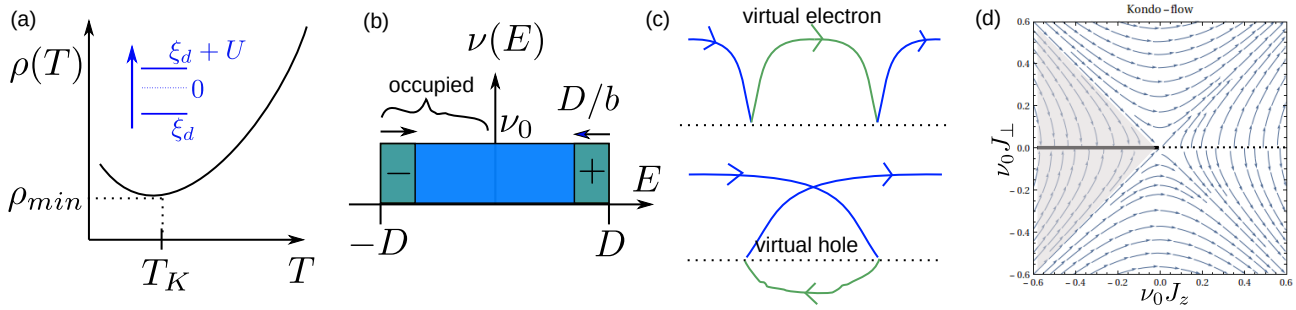


Figure 12: Kondo problem: (a) Typical resistance versus temperature curve for metals with magnetic impurities. (b) Flat density of states assumed for host system with bandwidth $2D$. (c) Diagrams for virtual electron or virtual hole excitations. (d) Poor man's scaling: Flow diagram in the $\nu_0 J_z$-$\nu_0 J_\perp$-plane.

- Kondo model also known as "s-d model" (since d-shell electrons form impurity and itinerant electrons come from s-shells)
- in the last step, note: $S^+ S_c^-(\mathbf{r}=0) + h.c. = 2S^x S_c^x(\mathbf{r}=0) + 2S^y S_c^y(\mathbf{r}=0)$
- [Schrieffer and Wolff, Phys. Rev. 149(2) 491 (1966)] originally used a unitary transformation to obtain the same result, $H_{\text{eff}} = e^S H e^{-S}$
- there is also a path-integral version of this transformation: [Zamani et al 2016 New J. Phys. 18 063024]

Perturbation theory for Kondo model

- Assumption: Box-shaped density of states with bandwidth $2D$ (per spin, with units [1/energy]), $\nu(E) \equiv \sum_{\mathbf{k}} \delta(E - \varepsilon_{\mathbf{k}}) \equiv \nu_0$ for $|E| \leq D$ (Fig. 12b).
- Perturbation theory for resistivity ρ for small $J\nu_0$ [Kondo,1964]:

$$\rho = \rho_0 \left(1 - 4J\nu_0 \ln(T/D) + ...\right) \tag{164}$$

  - explains increase of $\rho(T)$ for $T/D \ll 1$ when $\ln(T/D) < 0$
  - identifies a temperature at which perturbation theory breaks down (second term $\mathcal{O}(1)$): $T_K \sim D \exp\left(-\frac{1}{\#\nu_0 J}\right)$
- Beyond perturbation theory: Wilson solved the problem using **numerical RG** (NRG): Below the *crossover* temperature T_K, the impurity **S** forms a singlet with the c-electrons. This bound state is decoupled from remaining c-electrons but leads to enhanced scattering.

Anderson's "Poor-man's" scaling

- Here: Derive T_K using RG based on Hamiltonian. We will see that there is no critical fixed point, but a "run-away-flow". We will see how to extract the "crossover temperature" T_K from the flow equations.
- Generalize to anisotropic Kondo model:

$$H = H_0 + J_\perp \sum_{\mathbf{k},\mathbf{k}'} \left(c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}'\downarrow} S^- + c_{\mathbf{k}\downarrow}^\dagger c_{\mathbf{k}'\uparrow} S^+\right) + J_z \sum_{\mathbf{k},\mathbf{k}'} \left(c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}'\uparrow} - c_{\mathbf{k}\downarrow}^\dagger c_{\mathbf{k}'\downarrow}\right) S^z \tag{165}$$

- Plan for RG (Fig. 12b):
  - Ground state of H_0 is filled Fermi sea up to $E = 0$.
  - $\left|\psi_{-/+}\right\rangle$: highly excited states with energy $\geq D/b$ with at least one hole/electron in the lower/upper band-edge $D/b < |\varepsilon_{\mathbf{k}}| < D$

  - Integrate out $\left|\psi_{-/+}\right\rangle$ (take them into account as virtual states in perturbation theory) $\rightarrow$ flow of $J_{z,\perp}$

- Comparison: Schrieffer-Wolff transformation vs Poor-man's scaling
  - integrating out discrete level vs continuum of excitations
  - well defined perturbation theory vs divergent perturbation theory (for $T/D \rightarrow 0$)
  - plain perturbation theory with bare parameters vs continuous modification of coupling $J(b)$ with feedback

- Formal setup of perturbation theory: Divide Hilbert-space into $\left|\psi_{-/+}\right\rangle$-like states and the rest $|\psi_0\rangle$,

$$H|\psi\rangle = \begin{pmatrix} H_{--} & H_{-0} & \simeq 0 \\ H_{0-} & H_{00} & H_{0+} \\ \simeq 0 & H_{+0} & H_{++} \end{pmatrix} \begin{pmatrix} |\psi_-\rangle \\ |\psi_0\rangle \\ |\psi_+\rangle \end{pmatrix}, \tag{166}$$

- The sectors are coupled by scattering off the impurity, thus the off-diagonal terms are $\sim J$.

- Write Schrödinger equation for $|\psi_0\rangle$-states:

$$(H_{00} + \underbrace{H_{0+}\frac{1}{E-H_{++}}H_{+0}}_{\text{virtual electron}} + \underbrace{H_{0-}\frac{1}{E-H_{--}}H_{-0}}_{\text{virtual hole}})|\psi_0\rangle = E|\psi_0\rangle \tag{167}$$

- Because $H_{0+} \sim J$, we can neglect J that appear in $H_{00,--,++}$ in the denominators and approximate them with $1/(E-H_0)$ with H_0 the non-interacting Hamiltonian.

- For the second and third term, we have 8 different processes each: S^zS^z, S^+S^-, S^zS^+, S^zS^- and the flipped orders.

- $S^zS^z = 1/4$ processes: Focus on the *virtual electron* term with H_{+0} involving $c^\dagger_{\mathbf{q}_+\sigma}c_{\mathbf{q}_0\sigma}$ with $\mathbf{q}_+$ at energy $\simeq D$ of the *upper* band edge and arbitrary $\mathbf{q}_0$.

$$\begin{aligned} H_{0+}\frac{1}{E-H_0}H_{+0}|\psi_0\rangle &= J_z^2(S^z)^2 \sum_{\mathbf{k}_0,\mathbf{k}_+,\mathbf{q}_0,\mathbf{q}_+} \left(c^\dagger_{\mathbf{k}_0\uparrow}c_{\mathbf{k}_+\uparrow} - c^\dagger_{\mathbf{k}_0\downarrow}c_{\mathbf{k}_+\downarrow}\right)\frac{1}{E-H_0}\left(c^\dagger_{\mathbf{q}_+\uparrow}c_{\mathbf{q}_0\uparrow} - c^\dagger_{\mathbf{q}_+\downarrow}c_{\mathbf{q}_0\downarrow}\right)|\psi_0\rangle \\ &= J_z^2(S^z)^2 \sum_{\mathbf{k}_0,\mathbf{k}_+,\mathbf{q}_0,\mathbf{q}_+} \frac{1}{E-H_0-D+\varepsilon_{\mathbf{k}_0}}\left(c^\dagger_{\mathbf{k}_0\uparrow}c_{\mathbf{k}_+\uparrow} - c^\dagger_{\mathbf{k}_0\downarrow}c_{\mathbf{k}_+\downarrow}\right)\left(c^\dagger_{\mathbf{q}_+\uparrow}c_{\mathbf{q}_0\uparrow} - c^\dagger_{\mathbf{q}_+\downarrow}c_{\mathbf{q}_0\downarrow}\right)|\psi_0\rangle \end{aligned}$$

- Strategy: Use $c_{\mathbf{k}_+\sigma}|\psi_0\rangle = 0$ since $|\psi_0\rangle$ does not contain any excited electrons in the upper band-edge:

$$\begin{aligned} &\left(c^\dagger_{\mathbf{k}_0\uparrow}c_{\mathbf{k}_+\uparrow} - c^\dagger_{\mathbf{k}_0\downarrow}c_{\mathbf{k}_+\downarrow}\right)\left(c^\dagger_{\mathbf{q}_+\uparrow}c_{\mathbf{q}_0\uparrow} - c^\dagger_{\mathbf{q}_+\downarrow}c_{\mathbf{q}_0\downarrow}\right)|\psi_0\rangle \\ =&(c^\dagger_{\mathbf{k}_0\uparrow}\underbrace{c_{\mathbf{k}_+\uparrow}c^\dagger_{\mathbf{q}_+\uparrow}}_{\rightarrow\delta_{\mathbf{k}_+,\mathbf{q}_+}}c_{\mathbf{q}_0\uparrow} + c^\dagger_{\mathbf{k}_0\downarrow}\underbrace{c_{\mathbf{k}_+\downarrow}c^\dagger_{\mathbf{q}_+\downarrow}}_{\rightarrow\delta_{\mathbf{k}_+,\mathbf{q}_+}}c_{\mathbf{q}_0\downarrow})|\psi_0\rangle \end{aligned}$$

  and use $\sum_{\mathbf{k}_+} = \int_{D/b}^{D}\nu_0 dE = \nu_0 D(1-1/b)$.

$$\begin{aligned} H_{0+}\frac{1}{E-H_0}H_{+0}|\psi_0\rangle &= \frac{J_z^2}{4}\nu_0 D(1-1/b)\sum_{\mathbf{k}_0,\mathbf{q}_0}\frac{1}{E-H_0-D+\varepsilon_{\mathbf{k}_0}}\left(c^\dagger_{\mathbf{k}_0\uparrow}c_{\mathbf{q}_0\uparrow} + c^\dagger_{\mathbf{k}_0\downarrow}c_{\mathbf{q}_0\downarrow}\right)|\psi_0\rangle \\ &= \frac{J_z^2}{4}\nu_0 D(1-1/b)\sum_{\mathbf{k}_0,\mathbf{q}_0}\left(\sum_\sigma c^\dagger_{\mathbf{k}_0\sigma}c_{\mathbf{q}_0\sigma}\right)\frac{1}{E-H_0-D+\varepsilon_{\mathbf{q}_0}}|\psi_0\rangle \end{aligned}$$

The corresponding process for the *virtual hole* $c_{\mathbf{q}-\sigma}$ excitations follows as

$$\begin{aligned} H_{0-}\frac{1}{E-H_0}H_{-0}\left|\psi_0\right\rangle &= J_z^2\left(S^z\right)^2\sum_{\mathbf{k}_0,\mathbf{k}_+,\mathbf{q}_0,\mathbf{q}_+}\left(c^\dagger_{\mathbf{k}_-\uparrow}c_{\mathbf{k}_0\uparrow}-c^\dagger_{\mathbf{k}_-\downarrow}c_{\mathbf{k}_0\downarrow}\right)\frac{1}{E-H_0}\left(c^\dagger_{\mathbf{q}_0\uparrow}c_{\mathbf{q}_-\uparrow}-c^\dagger_{\mathbf{q}_0\downarrow}c_{\mathbf{q}_-\downarrow}\right)\left|\psi_0\right\rangle \\ &= \frac{J_z^2}{4}\nu_0 D\left(1-1/b\right)\sum_{\mathbf{k}_0,\mathbf{q}_0}\left(\sum_\sigma c_{\mathbf{k}_0\sigma}c^\dagger_{\mathbf{q}_0\sigma}\right)\frac{1}{E-H_0-D-\varepsilon_{\mathbf{q}_0}}\left|\psi_0\right\rangle \end{aligned}$$

- Assume $E\simeq E_0$ where E_0 is the g.s. energy of H_0 $\rightarrow$ approximate all denominators by $1/(-D)$.
- Result: Virtual S^zS^z-processes lead to non-magnetic scattering (does not depend on the spin of the scattered). This is what an ordinary impurity potential would do. $\rightarrow$ Neglect these terms, since also absent in initial Hamiltonian.
- $S^-S^+=1/2-S_z$ and $S^+S^-=1/2+S_z$ processes: Create *virtual electron* $c^\dagger_{\mathbf{q}+\sigma}$

$$\begin{aligned} H_{0+}\frac{1}{E-H_0}H_{+0}\left|\psi_0\right\rangle &\simeq \frac{1}{-D}J_\perp^2\sum_{\mathbf{k},\mathbf{q}_+,\mathbf{q}'}\left(c^\dagger_{\mathbf{k}\uparrow}c_{\mathbf{q}_+\downarrow}S^-+c^\dagger_{\mathbf{k}\downarrow}c_{\mathbf{q}_+\uparrow}S^+\right)\left(c^\dagger_{\mathbf{q}_+\uparrow}c_{\mathbf{q}'\downarrow}S^-+c^\dagger_{\mathbf{q}_+\downarrow}c_{\mathbf{q}'\uparrow}S^+\right)\left|\psi_0\right\rangle \\ &= \frac{1}{-D}J_\perp^2\nu_0 D\left(1-1/b\right)\sum_{\mathbf{k},\mathbf{q}'}\left(c^\dagger_{\mathbf{k}\uparrow}c_{\mathbf{q}'\uparrow}\underbrace{S^-S^+}_{1/2-S_z}+c^\dagger_{\mathbf{k}\downarrow}c_{\mathbf{q}'\downarrow}\underbrace{S^+S^-}_{1/2+S_z}\right)\left|\psi_0\right\rangle \\ &= \frac{1}{D}J_\perp^2\nu_0 D\left(1-1/b\right)S_z\sum_{\mathbf{k},\mathbf{q}'}\left(c^\dagger_{\mathbf{k}\uparrow}c_{\mathbf{q}'\uparrow}-c^\dagger_{\mathbf{k}\downarrow}c_{\mathbf{q}'\downarrow}\right)\left|\psi_0\right\rangle+\left(pot.\,scatt.-from\,1/2-terms\right) \end{aligned}$$

and we do the same for the *virtual hole* $c_{\mathbf{q}-\sigma}$:

$$\begin{aligned} H_{0-}\frac{1}{E-H_0}H_{-0}\left|\psi_0\right\rangle &\simeq \frac{1}{-D}J_\perp^2\sum_{\mathbf{k},\mathbf{q}_-,\mathbf{q}}\left(c^\dagger_{\mathbf{q}_-\uparrow}c_{\mathbf{k}\downarrow}S^-+c^\dagger_{\mathbf{q}_-\downarrow}c_{\mathbf{k}\uparrow}S^+\right)\left(c^\dagger_{\mathbf{q}\uparrow}c_{\mathbf{q}_-\downarrow}S^-+c^\dagger_{\mathbf{q}\downarrow}c_{\mathbf{q}_-\uparrow}S^+\right)\left|\psi_0\right\rangle \\ &= \frac{1}{-D}J_\perp^2\nu_0 D\left(1-1/b\right)\sum_{\mathbf{k},\mathbf{q}}\left(c_{\mathbf{k}\downarrow}c^\dagger_{\mathbf{q}\downarrow}S^-S^+ + c_{\mathbf{k}\uparrow}c^\dagger_{\mathbf{q}\uparrow}S^+S^-\right)\left|\psi_0\right\rangle \\ &= \frac{1}{D}J_\perp^2\nu_0 D\left(1-1/b\right)S_z\sum_{\mathbf{k},\mathbf{q}}\left(c^\dagger_{\mathbf{q}\uparrow}c_{\mathbf{k}\uparrow}-c^\dagger_{\mathbf{q}\downarrow}c_{\mathbf{k}\downarrow}\right)\left|\psi_0\right\rangle+\left(pot.\,scatt.\right) \end{aligned}$$

which is the same as in the virtual electron term.

- In summary: We read off for the effective S_z-term:

$$J_z(b)=J_z+2\nu_0 J_\perp^2\left(1-1/b\right) \tag{168}$$

- Remaining processes ($S^zS^+=S^+/2$, ...) analogously lead to:

$$J_\perp(b)=J_\perp+2\nu_0 J_\perp J_z\left(1-1/b\right) \tag{169}$$

- No need for re-scaling, as the Hamiltonian stays in its initial form and D does not appear explicitly. Understand $J_{z,\perp}(b)$ as the result of iterative application of perturbation theory, integrating out bath electrons with $|\varepsilon_{\mathbf{k}}|\in[D/b,D]$.
- The dimensionless quantity which should be small for the equations above to be trusted is $J_{z,\perp}\nu_0$. Use infinitesimal b (via $b=e^l$) to write flow:

$$\boxed{\partial_l\left(J_z\nu_0\right)=2\left(J_\perp\nu_0\right)^2,\quad \partial_l\left(J_\perp\nu_0\right)=2\left(J_\perp\nu_0\right)\left(J_z\nu_0\right)} \tag{170}$$

Interpretation of flow and Kondo scale

- The flow diagram is shown in Fig. 12(d). There is a line of fixed points at $J_\perp = 0$.
- Observations: $(J_z\nu_0)^2 - (J_\perp\nu_0)^2 = const.$ Follows from $\partial_l(...) = 0$.
- $J_z\nu_0$ never decreases, since $\partial_l (J_z\nu_0) \geq 0$. Have a line of stable fixed points $(J_z\nu_0, 0)$ for $J_z \leq 0$ with basin of attraction $|J_\perp| \leq |J_z|$ (gray).
- The isotropic *ferromagnetic* Kondo model $J_z = J_\perp \equiv J < 0$ is asymptotically free (flows to $J = 0$).
- All other initial conditions with $J_\perp \neq 0$ flow to strong coupling and the flow equations break down ("runaway flow"). At which scale does that happen?
- Specialize to isotropic Heisenberg coupling $J_\perp = J_z \equiv J$ with $0 < \nu_0 J \ll 1$. Find the Kondo scale $D_l \equiv T_K$ where strong coupling is reached.
  Integrate the flow
  $$\frac{d(\nu_0 J)}{(\nu_0 J)^2} = 2dl \;\rightarrow\; \frac{1}{J_l\nu_0} - \frac{1}{J\nu_0} = 2l = 2\ln\left(\frac{D}{D_l}\right) \tag{171}$$
  The flow has to terminate at $D_l \equiv T_K$ when the dimensionless running coupling constant $J_l\nu_0$ becomes $\mathcal{O}(1)$.
  $$\underbrace{\left(\frac{1}{J_l\nu_0}\right)}_{\mathcal{O}(1)} - \underbrace{\left(\frac{1}{J\nu_0}\right)}_{\gg 1} = 2\ln\left(\frac{D}{T_K}\right) \tag{172}$$
  We neglect the left term and obtain $\frac{1}{J\nu_0} \simeq 2\ln\left(\frac{D}{T_K}\right)$ or
  $$\boxed{T_K \simeq D\exp\left(-\frac{1}{2J\nu_0}\right)} \tag{173}$$
- Note: This result does *not* depend on the exact value $\mathcal{O}(1)$ where we stopped the flow.

4.6 Example: Fermi-Liquid theory – RG with a Fermi surface

[Polchinski, arxiv hep-the/9210046 (1999)] and [Shankar, Rev. Mod. Phys. 66, 129 (1994)]

- Question: Real metals have (strong) Coulomb interactions.
  Why is the model of non-interacting electrons still working so well?
- Answer by Lev Landau (1956): Landau's Fermi liquid theory.
  Main idea: Most important excitations of metals (with dispersion $\varepsilon_\mathbf{k}$) are particle-hole pairs close to the Fermi surface $\varepsilon_\mathbf{k} = \mu$, see Fig. 13(a).
- At low enough energies, these excitations behave like non-interacting particles/holes. They carry charge $\pm e$ and spin $S = 1/2$ and can be described as free Fermi gas.
  Some parameters differ from bare electrons, i.e. effective mass $m^\star \gtrsim m_0$.
- Here: RG perspective.

Model

- Modeling:
  $$H_0 = \sum_{\mathbf{k},\sigma} (\varepsilon_\mathbf{k} - \mu)\, c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \tag{174}$$
  assume $\varepsilon_\mathbf{k} = k^2/(2m)$ and k_F the radius of Fermi surface defined by $\varepsilon_\mathbf{k} \stackrel{!}{=} \mu$ in $D = 2, 3$.
  Remark: Parabolic dispersion could approximate band-bottom of nearest-neighbor hopping on hypercubic lattice, $\varepsilon_\mathbf{k} = -t\sum_{\mu=1}^{D} \cos k_\mu \simeq -Dt + \frac{t}{2}k^2$.

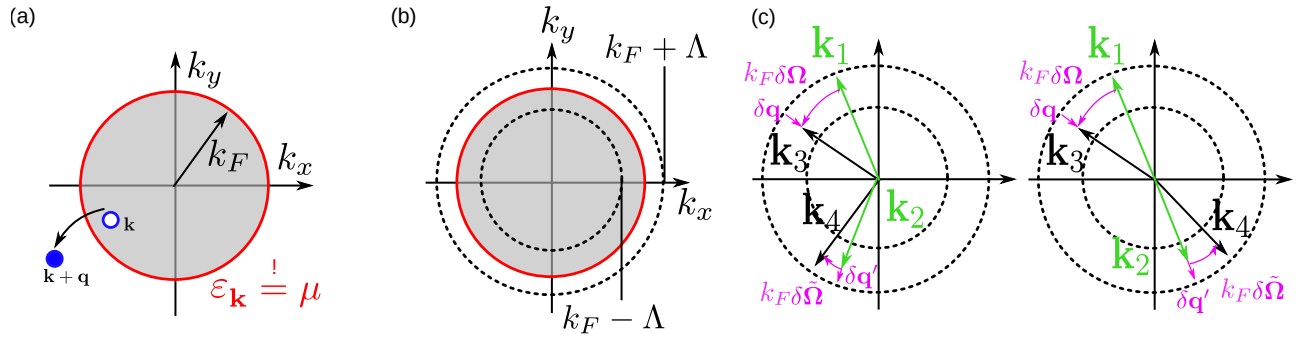


Figure 13: Landau's Fermi liquid theory: (a) Definition of Fermi sea (gray) and Fermi surface (red). (b) Scaling towards Fermi surface. (c) Wave-vectors at a 2-particle scattering process (before application of the momentum conserving δ-function), in the generic case (left) and for vanishing initial momentum $\mathbf{k}_1 = -\mathbf{k}_2$ (right).

- Consider excitation from $\mathbf{k}$ with $k \simeq k_F$ to wave-vector $\mathbf{k}+\mathbf{q}$ with $q \ll k_F$:

$$\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}} = \frac{(\mathbf{k}+\mathbf{q})^2}{2m} - \frac{k^2}{2m} = \frac{\mathbf{k}}{m}\cdot\mathbf{q} + \mathcal{O}(q^2) \simeq \mathbf{v}_F \cdot \mathbf{q} \tag{175}$$

  where $\mathbf{v}_F = \partial_{\mathbf{k}}\varepsilon_{\mathbf{k}}|_{k=k_F}$ is the Fermi velocity (linear approximation).

- RG: Want to integrate out high-energy excitations successively and take into account their effect on low energy degrees of freedom.

- Problem: Low energy modes don't live at $\mathbf{k} = 0$, but at the Fermi surface $k = k_F \rightarrow$ need to scale towards k_F, see Fig. 13(b).

Gaussian action

- Gaussian imaginary time action with $\Omega \equiv (\theta, \phi)$ the angular coordinate.

$$S_0 = \int d\tau \int d\Omega \int_{-\Lambda}^{+\Lambda} \frac{dq}{2\pi} \bar{\psi}\left(\tau, q, \Omega\right)\left[\partial_\tau + v_F q\right]\psi\left(\tau, q, \Omega\right) \tag{176}$$

  This is a collection of independent one-dimensional theories parameterized by $\Omega = (\theta, \phi)$.
  If the curvature for the Fermi surface is taken into account, the theories are coupled $\rightarrow$ irrelevant perturbation.

- RG for S_0: Integration over $\psi(q)$ with $q \in \pm(\Lambda/b, \Lambda)$, decouples from integration over $\psi(q)$ with $|q| \leq \Lambda/b$, thus only need to consider re-scaling step. Want to keep v_F fixed, we find

$$\begin{aligned}
\Omega &\rightarrow \Omega \\
q &\rightarrow q' = qb \\
\tau &\rightarrow \tau' = \tau/b \\
\psi &\rightarrow \psi' = b^{-1/2}\psi
\end{aligned}$$

  which indeed reproduces S_0:

$$\begin{aligned}
S_0 &= \int d\tau \int d\Omega \int_{-\Lambda/b}^{+\Lambda/b} \frac{dq}{2\pi} \bar{\psi}\left(\tau, q, \Omega\right)\left[\partial_\tau + v_F q\right]\psi\left(\tau, q, \Omega\right) \\
&\rightarrow b \int d\tau' \int d\Omega \int_{-\Lambda}^{+\Lambda} b^{-1}\frac{dq'}{2\pi} b^{1/2}\bar{\psi}'\left(\tau', q', \Omega'\right) b^{-1}\left[\partial_{\tau'} + v_F q'\right] b^{1/2}\psi'\left(\tau', q', \Omega'\right) \\
&= S_0
\end{aligned}$$

- Strategy: Write down perturbations to S_0, apply the above re-scalings, and then decide if they are relevant, marginal, or irrelevant.
- Example: Deformations of Fermi surface $m(\Omega)\bar{\psi}\psi$:

$$\int d\tau \int d\Omega \int_{-\Lambda}^{+\Lambda} \frac{dq}{2\pi} m\bar{\psi}\psi \to \int d\tau' \int d\Omega \int_{-\Lambda}^{+\Lambda} \frac{dq'}{2\pi} \underbrace{mb}_{m'=mb^{y_m}} \bar{\psi}'\psi' \tag{177}$$

and we read off $y_m = 1$, so $m(\Omega)$ is relevant.
Can absorb $m(\Omega)$ in definition of dispersion $\varepsilon_{\mathbf{k}}$, need to expand around correct Fermi surface, shape can change under RG.

Interactions - naive approach

- Interaction U couples different Ω. Need to preserve 3d momentum,

$$\mathbf{k}_i = (k_F + q_i)\mathbf{\Omega}_i \tag{178}$$

with $\mathbf{\Omega}_i = \begin{pmatrix} \cos\phi_i \sin\theta_i, & \sin\phi_i \sin\theta_i & \cos\theta_i \end{pmatrix}^T$ vectors on the unit sphere:

$$S_{int} = \int d\tau \prod_{i=1}^{4} \int d\Omega_i \int_{-\Lambda}^{+\Lambda} \frac{dq_i}{2\pi} \bar{\psi}_1\bar{\psi}_2\psi_3\psi_4 U(1,2,3,4)\, \delta^D(\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3 - \mathbf{k}_4) \tag{179}$$

- Rescaling for δ-function: In Eq. (178), the q_i scale to zero, but the k_F stay fixed. Thus

$$\delta^D(\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3 - \mathbf{k}_4) \simeq \frac{1}{k_F}\delta^D(\mathbf{\Omega}_1 + \mathbf{\Omega}_2 - \mathbf{\Omega}_3 - \mathbf{\Omega}_4) \tag{180}$$

and the δ-function does not change under rescaling since $\mathbf{\Omega}_i$ are dimensionless.

- Rescaling of interaction U:

$$S_{int} = \int d\tau' \prod_{i=1}^{4} \int d\Omega_i \int_{-\Lambda}^{+\Lambda} \frac{dq_i'}{2\pi} \bar{\psi}_{1'}'\bar{\psi}_{2'}'\psi_{3'}'\psi_{4'}' b^{1-4+4\times(1/2)} U(1',2',3',4') \frac{1}{k_F}\delta(\mathbf{\Omega}_1 + \mathbf{\Omega}_2 - \mathbf{\Omega}_3 - \mathbf{\Omega}_4) \tag{181}$$

so that $U' = b^{-1}U$ which means

$$y_U = -1 \tag{182}$$

- Result: Electron-electron interactions are irrelevant.
- Strong argument for Fermi-Liquid theory: Interactions become weaker as energy is lowered and nearly free electron gas is good description of conductor at low energy scales.

Interactions revisited

- Fact: Superconductivity is interaction driven phenomenon.
Q: How can we ever get superconductivity if interactions become weaker and weaker at low energy? → What is wrong with our argument?
- Parameterize scattering process $\mathbf{k}_{1,2} \to \mathbf{k}_{3,4}$ with [see Fig. 13(c)]

$$\mathbf{k}_3 = \mathbf{k}_1 + k_F\delta\mathbf{\Omega} + \delta\mathbf{q}$$
$$\mathbf{k}_4 = \mathbf{k}_2 + k_F\delta\tilde{\mathbf{\Omega}} + \delta\tilde{\mathbf{q}}$$

so that

$$\delta^D(\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3 - \mathbf{k}_4) = \delta^D\left(k_F\delta\mathbf{\Omega} + \delta\mathbf{q} + k_F\delta\tilde{\mathbf{\Omega}} + \delta\tilde{\mathbf{q}}\right) \tag{183}$$

- For generic momenta $\mathbf{k}_{1,2,3,4}$, the large momenta $k_F\delta\mathbf{\Omega}$ and $k_F\delta\tilde{\mathbf{\Omega}}$ are linearly independent vectors in D-dimensional space. The above argument around Eq. (180) is valid.

- Consider special case where directions $\mathbf{\Omega}_{1,2}$ of scattering electrons are opposite, $\mathbf{\Omega}_1 \stackrel{!}{=} -\mathbf{\Omega}_2$.
  For a parity-symmetric Fermi surface (with $\varepsilon_{-\mathbf{k}} = \varepsilon_{\mathbf{k}}$): Large variational momenta $k_F\delta\mathbf{\Omega}$ and $k_F\delta\tilde{\mathbf{\Omega}}$ come from the same tangential planes and there remains an explicit δ-function constraint on the $\mathbf{q}$-direction:

$$\delta^D\left(\mathbf{k}_1+\mathbf{k}_2-\mathbf{k}_3-\mathbf{k}_4\right) = \delta^{D-1}\left(k_F\delta\mathbf{\Omega}+k_F\delta\tilde{\mathbf{\Omega}}\right)\delta\left(\delta\mathbf{q}+\delta\tilde{\mathbf{q}}\right) \tag{184}$$

- Now, we get and additional factor b upon rescaling

$$\delta\left(\delta\mathbf{q}+\delta\tilde{\mathbf{q}}\right) = \delta\left(\frac{\delta\mathbf{q}'+\delta\tilde{\mathbf{q}}'}{b}\right) = b\delta\left(\delta\mathbf{q}'+\delta\tilde{\mathbf{q}}'\right) \tag{185}$$

  which yields $y_U = 0$.

- Conclusion: Interactions corresponding to vanishing incoming (and outgoing) momenta

$$U\left(\mathbf{\Omega}_1,-\mathbf{\Omega}_1,\mathbf{\Omega}_3,-\mathbf{\Omega}_3\right) \equiv V\left(\mathbf{\Omega}_1,\mathbf{\Omega}_3\right) \stackrel{rot.\,invariant}{=} V\left(\mathbf{\Omega}_1\cdot\mathbf{\Omega}_3\right) \tag{186}$$

  are marginal under re-scaling!

- Comment:
  - Interpretation: Interactions are generically irrelevant, but special kinematics can change this to marginal.
  - Many Feynman diagrams are irrelevant, unless certain momentum restrictions apply, see e.g. for $\mathbf{p}=\mathbf{p}'$ for the current in Fig. 14(a).
  - In D=1, $k_F\delta\mathbf{\Omega}=0$, so all interaction is always marginal.

- One-loop correction of the marginal interaction in Fig. 14(b) to understand fate of interaction. Expand $V\left(\mathbf{\Omega}_1\cdot\mathbf{\Omega}_3\right)$ to angular momentum channels L. Then find the flow [Shankar, Rev. Mod. Phys. 66, 129 (1994)]:

$$\partial_l V_L = -\frac{1}{4\pi}V_L^2 \tag{187}$$

  so that:
  - Repulsive $V_L > 0$ are marginally irrelevant, $\partial_l|V_L| = -\frac{1}{4\pi}|V_L|^2$. Example: Screened Coulomb interactions.
  - Attractive $V_L < 0$ are marginally relevant, $\partial_l|V_L| = +\frac{1}{4\pi}|V_L|^2$. Example: Effectively attractive interactions from phonons at initial scale.

- Initial attractive interaction leads to superconductivity: Solve flow

$$V_L(l) = \frac{V_L(0)}{1+lV_L(0)/(4\pi)} \tag{188}$$

  diverges at $l_\star = 4\pi/V_L(0)$ or

$$\Lambda_\star = \Lambda e^{-l_\star} = e^{-4\pi/|V_L(0)|} \hat{=} T_c^{BCS} \tag{189}$$

  Comment: Similar in spirit to Kondo temperature T_K which we derived from run-away flow of marginal coupling. But here: Phase transition with broken $U(1)$ symmetry.

- Initial repulsive interaction: It the Fermi liquid stable? Not in general, irrelevant couplings can generate some $V_L < 0$ which then run away.

- Consistent with *Kohn-Luttinger Theorem*: Every Fermi liquid with $\varepsilon_{\mathbf{k}} = \varepsilon_{-\mathbf{k}}$ is unstable towards superconductivity at sufficiently small temperatures.

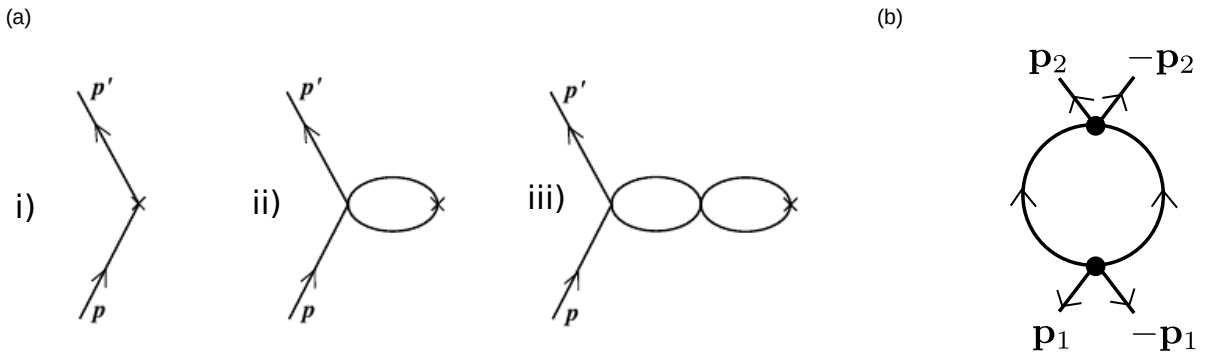


Figure 14: (a) The loop corrections ii),iii) to scattering i) from $\mathbf{p}$ to $\mathbf{p}'$ are generally RG-irrelevant unless $\mathbf{p} = \mathbf{p}'$ when the 4-point interaction becomes marginal. (b) One-loop renormalization of marginal interaction.

4.7 Example: Crossover theory and finite-size scaling

- More realistic systems with more complicated fixed point structure and flow diagram. Make connection to phase diagrams.
- Investigate cross-over behavior where multiple fixed points govern properties of the same system on different lenght scales.

Crossover from explicit symmetry breaking in Heisenberg magnet

- Model O(3)-symmetric Heisenberg magnet [$\mathbf{s}(r) = (s_x(r), s_y(r), s_z(r))$] with single ion uniaxial anisotropy:

$$\beta H = -\frac{1}{2}\sum_{r,r'} K(r-r')\mathbf{s}(r)\cdot\mathbf{s}(r') - D\sum_r s_z(r)^2 \tag{190}$$

- 3 limiting cases:
  - $D = 0$: Heisenberg universality class, Heisenberg fixed point H with relevant thermal $u_{t,H}$ and y'_H for a scaling variable involving D.
  - $D \gg 0$ fixes $\mathbf{s} \parallel s_z$: Ising physics with critical Ising fixed point I with relevant thermal $u_{t,I}$.
  - $D \ll 0$ fixes $\mathbf{s} \perp s_z$: XY physics,with XY fixed point XY with relevant thermal $u_{t,XY}$.
- For general D: Plausible guess of flow diagram projected into $D, K^{-1} \propto T$ plane, see Fig. 15(a). Shape close to H will be found later.
- For small $D \neq 0$ we have either Ising or XY like critical behaviour in crossing from ordered to disordered phase.
- Suppose $D > 0$ but small and vary T (walk on dashed blue line).
  - System at point A: Scaling of $f(t, D)$ (and other observables) determined by H (RG trajectory never sees I)
  - System at point B: Critical behavior determined by I.
- For formal description of case A, consider the scaling equation for $f_{\rm sing}$, Eq. (11) for flow close to H:

$$f_{\rm sing}(t, D) = b^{-d} f_{\rm sing}\left(b^{y_{tH}} t, b^{y'_H} D\right) \tag{191}$$

  Chose b such that $b^{y_{tH}} t = O(1)$ and find scaling form with $\alpha_H = 2 - d/y_{tH}$

$$f_{\rm sing}(t, D) = |t|^{2-\alpha_H}\,\Psi\left(D\,|t|^{-\overbrace{y'_H/y_{tH}}^{\equiv\phi}}\right) \tag{192}$$

  with $\phi = y'_H/y_{tH}$ defined as *cross-over exponent* given in terms of RG eigenvalues at H.

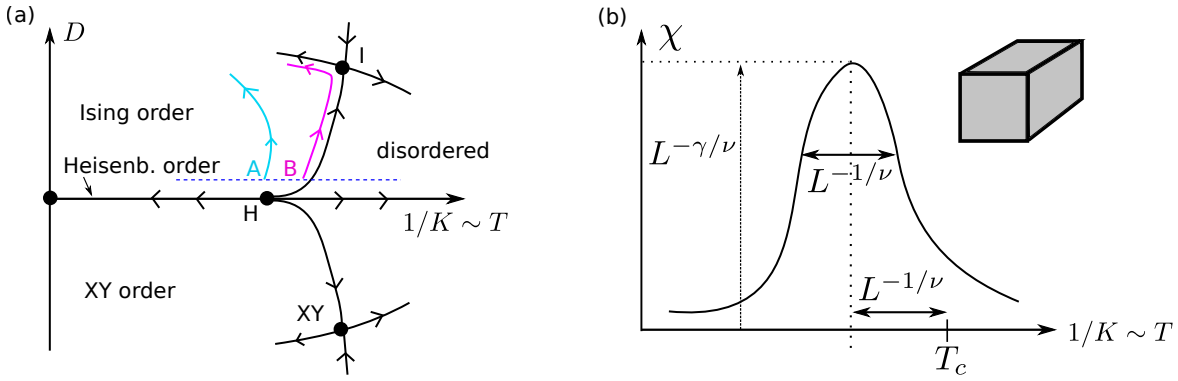


Figure 15: (a) RG flow diagram of anisotropic Heisenberg model, Eq. (190) (b) Finite-size (L) induced changes for the critical susceptibility peak.

- Application: Specific heat $C \propto \partial_t^2 f_s$.
  - For $D = 0$, $C \propto |t|^{-\alpha_H}$ as expected.
  - For $D > 0$, no significant departures from $D = 0$ behavior until $|t|$ so small that $D|t|^{-\phi} \simeq 1$. Define this $|t| = t_X = D^{1/\phi}$ as crossover temperature.
  - For $|t| \ll t_X$ (case B), the I-fp comes into play and we should observe $C \propto |t|^{-\alpha_I}$. Now introduce this behaviour by hand as boundary condition to Ψ!
- Rewrite scaling form of C with new scaling function $\tilde{\Psi}$ designed to carry all the $|t|$ dependence:

$$C \quad \propto \quad |t|^{-\alpha_H} \Psi\left(D\,|t|^{-\phi}\right) = D^{-\alpha_H/\phi} \underbrace{\left(D|t|^{-\phi}\right)^{\alpha_H/\phi} \Psi\left(D\,|t|^{-\phi}\right)}_{\equiv \tilde{\Psi}\left(tD^{-1/\phi}\right)} \tag{193}$$

- We know that for small $|t|$, we must have $C \propto A(D)\,(t - t_c(D))^{-\alpha_I}$ so $\tilde{\Psi}$ must have singularity

$$\tilde{\Psi}\left(tD^{-1/\phi}\right) \propto \tilde{a}\left(tD^{-1/\phi} - \tilde{b}\right)^{-\alpha_I} \tag{194}$$

  with constants $\tilde{a}, \tilde{b}$. We find:

$$C \propto \underbrace{\tilde{a} D^{(\alpha_I - \alpha_H)/\phi}}_{A(D)} \left(t - \tilde{b} D^{1/\phi}\right)^{-\alpha_I} \tag{195}$$

- We read off two dependencies of the $C(t)$-peak on D:
  1. Amplitude $A(D) \propto \tilde{a} D^{(\alpha_I - \alpha_H)/\phi}$, $\alpha_I - \alpha_H > 0$, so Ising peak increases with increasing D.
  2. Shift of critical temperature which gives phase boundary close to H: $t_c \propto D^{1/\phi}$. Since it can be shown that $\phi < 1$, we have form as in Fig. 15.
- Model-independent RG prediction: Amplitude $A(D)$ and shift of critical temperature both related to $\phi = y_H'/y_{tH}$. This could be observed by changing D in experiment.

Crossover due to finite size (finite-size scaling)

- Consider system with isotropic fixed point govering critical behavior, but only a finite piece with linear dimension $L = Na$ (e.g. cube L^3 with N^3 sites, here N is number of sites per direction). Under RG ($a \to ba$, e.g. real-space RG for spin model) but keep L fixed so that

$$\left(N^{-1}\right) \to b\left(N^{-1}\right)^1 \tag{196}$$

- Think of N^{-1} as a relevant scaling variable with eigenvalue $y = 1$, thermodynamic limit is $N^{-1} \to 0$.
- Assume that N^{-1} does not affect the RG equations for the coupling t (ok for short-range interactions), obtain scaling of free energy:

$$f_{\text{sing}}\left(t, h, N^{-1}\right) = b^{-d} f_{\text{sing}}\left(b^{y_t} t, b^{y_h} h, bN^{-1}\right) \tag{197}$$

- Study implications of this for zero field susceptibility, $\chi \propto \partial^2 f_s / \partial h^2$,in Eq. (197) set $b^{y_t} t = O(1)$ we find the scaling form

$$\chi\left(t, N^{-1}\right) \propto |t|^{-\gamma} \phi\left(N^{-1}|t|^{-\nu}\right) = |t|^{-\gamma} \phi\left(\xi/N\right) \tag{198}$$

- Conclusion: Behavior of χ for $N \gg \xi$ resembles thermodynamic limit where $N \to \infty$. When $|t|$ decreases and therefore $\xi \propto t^{-\nu}$ increases things change, crossover at $\xi_X/N = 1$ or $t_X \simeq N^{-1/\nu}$ where finite size effects become pronounced.
- What happens close to the critical temperature $t = 0$ of $N \to \infty$ system? In finite system, there are no thermodynamic singularities, peak in susceptibility must be rounded. Rewrite scaling form such that t only appears in the scaling function (same trick as in Eq. (193)):

$$\boxed{\chi\left(t, N^{-1}\right) \propto N^{\gamma/\nu} \tilde{\psi}\left(tN^{1/\nu}\right)} \tag{199}$$

  where $\tilde{\psi}(x)$ will have a rounded maximum, but not necessarily at $x = 0$. Predictions:
  - Shift of *effective* critical temperature is $\propto N^{1/\nu}$. Origin and sign of the shift:
    Periodic boundary conditions quantize momenta and thus suppress fluctuations, peak is shifted to right.
    Open bounary conditions allow enhanced fluctuations at boundary, peak is shifted to left.
  - Width (over t) of peak scales with $\propto N^{1/\nu}$ ($\tilde{\psi}(x)$ has a certain width, replacing $x \to tN^{1/\nu}$)
  - Height of the peak scales as $N^{\gamma/\nu}$

Exercises

Exercise 4.1. Real-space RG for the Ising model in two dimensions

Consider the nearest-neighbor (n.n.) ferromagnetic (classical) Ising model on a square lattice in two dimensions and in the absence of a magnetic field,

$$-\beta H = \sum_{n.n.} \sum_{\{s_i\}=\pm 1} K s_i s_j, \tag{200}$$

with $K = -\beta J > 0$ and N sites with periodic boundary conditions. This exercise explores the Migdal-Kadanoff real-space RG for this model.

1) Decimation step: Color the sites of the square lattice as a checkerboard and trace over the white sites. Show that the partition function $\mathcal{Z}_N$ can be written exactly in terms of the spins on the $N' = N/2$ black sites, s'_j as

$$\mathcal{Z}_N = e^{N' K'_0} \sum_{\{s'_i\}=\pm 1} \exp\left(K' \sum_{n.n} s'_j s'_k + L' \sum_{n.n.n.} s'_j s'_k + M' \sum_{pl.} s'_j s'_k s'_l s'_m \right) \tag{201}$$

where new couplings for next-nearest neighbors (n.n.n., L') and on plaquettes (pl., M') had to be added.

$$\begin{aligned} K'_0 &= \ln 2 + \frac{1}{2} \ln \cosh 2K + \frac{1}{8} \ln \cosh 4K \\ K' &= \frac{1}{4} \ln \cosh 4K \\ L' &= \frac{1}{8} \ln \cosh 4K \\ M' &= \frac{1}{8} \ln \cosh 4K - \frac{1}{2} \ln \cosh 2K \end{aligned}$$

2) Iteration: To make progress, approximate $M' = 0$ and assume that $K \ll 1$. Assume that the n.n.n. coupling L is present from the beginning and argue that the RG transformation reads

$$K' = L + 2K^2, \quad L' = K^2. \tag{202}$$

Sketch the flow diagram in the $K - L-$plane and find the non-trivial fixed point of (202). Linearize these equations around the fixed point and show that the critical exponent is

$$\nu = \frac{\ln \sqrt{2}}{\ln\left[(2+\sqrt{10})/3\right]} = 0.6385. \tag{203}$$

Discuss reasons for the deviation of this value from the exact result $\nu = 1$.

Exercise 4.2. Real-space RG for disordered Heisenberg chain

This exercise applies the real-space RG to a spin-1/2 Heisenberg chain with disordered anti-ferromagnetic couplings $J_i > 0$ chosen randomly from a (normalized) probability distribution $P(J)$ for each site i:

$$H \quad = \quad \sum_i J_i \mathbf{S}_i \cdot \mathbf{S}_{i+1}. \tag{204}$$

1) Decimation step: Assume strong disorder, meaning a wide distribution $P(J)$. Assume $J_n \equiv \Omega$ to be the largest coupling in the whole chain, with the neighboring couplings likely satisfying $J_{n\pm1} \ll \Omega$. Diagonalize the isolated strongest-bond subsystem $H_n = J_n \mathbf{S}_n \cdot \mathbf{S}_{n+1}$, assume it to be in its ground-state (singlet) and compute the resulting effective coupling between the two neighboring spins, in lowest non-trivial (second) order perturbation theory. You should find again a Heisenberg term, $J^{eff}_{n-1,n+2}\mathbf{S}_{n-1} \cdot \mathbf{S}_{n+2}$, with

$$J^{eff}_{n-1,n+2} = \frac{J_{n-1}J_{n+1}}{2\Omega} \tag{205}$$

which is much smaller than $J_{n\pm1}$. After the decimation step, we have retained again a Heisenberg chain where the largest bond is now what used to be the second-largest in the initial chain. Assuming that this scheme could be continued, draw a schematic of the ground state spin configuration of the physical chain where singlet bonds are indicated by a line. This state is called a random-singlet state.

2) Iteration: Instead of the RG flow of a few coupling constants, we are now seeking to describe the flow of the full distribution function $P_\Omega(J)$. To facilitate the math, introduce

$$\zeta_i \equiv \ln\left(\Omega/J_i\right) \in [0, \infty), \tag{206}$$

neglect the factor 2 in Eq. (205) and define the RG flow parameter to be

$$\Gamma \equiv \ln\left(\Omega_0/\Omega\right) \tag{207}$$

where Ω is the largest bond at the respective RG step and Ω_0 is the largest bond of the initial chain. By eliminating the strongest bonds J_m within $\Omega - d\Omega < J_m < \Omega$, show that the flow equation for $P_\Gamma(\zeta)$ takes the form

$$\frac{\partial P_\Gamma(\zeta)}{\partial \Gamma} = \frac{\partial P_\Gamma(\zeta)}{\partial \zeta} + P_\Gamma(0) \int d\zeta_l \int d\zeta_r P_\Gamma(\zeta_l) P_\Gamma(\zeta_r) \delta(\zeta - \zeta_l - \zeta_r) \tag{208}$$

where an overall rescaling term has been dropped to ensure conservation of the total probability (show this).

3) Solve the flow equation (208) by rewriting it for the distribution function $Q(x)$ of the quantity $x \equiv \zeta/\Gamma$. You should find

$$0 = (x+1)\frac{\partial Q(x)}{\partial x} + Q(x) + Q(0) \int dx_l \int dx_r Q(x_l) Q(x_r) \delta(x - x_l - x_r) \tag{209}$$

Solve this equation for $Q(x)$ by guessing the simple function that retains its form under convolution, the exponential, $Q(x) = e^{-x}$. Show that it corresponds to

$$P_\Omega(J) = \frac{1}{\Gamma(\Omega)\Omega}\left(\frac{\Omega}{J}\right)^{1-1/\Gamma(\Omega)}. \tag{210}$$

Consider the flow of the mean of ζ, $\langle\zeta\rangle$, and argue that our initial strong disorder assumption is better and better fulfilled as we iterate the flow.
It turns out that our solution (210) represents a stable fixed point which is globally attractive and thus universal, i.e. all initial distributions approach it as Γ grows. It is called infinite-randomness fixed point.

4) Physical properties: Show that the density of surviving spins (not locked up in a singlet) as a function of energy scale Ω (or Γ, respectively) is

$$n = n_0/\Gamma^2 \tag{211}$$

where n_0 is the initial spin density. From this, argue that:

- (a) The excitation energy of singlets of length L is $J_L \sim e^{-\sqrt{L}}$. (This "infinite-randomness" scaling is in strong contrast to the usual quantum-critical scaling $E \sim L^{-z}$.)
- (b) The magnetic susceptibility as a function of temperature T is $\chi(T) \sim \frac{n_0}{T \ln^2(\Omega_0/T)}$. You will have to use that the susceptibility of a free spin scales as $\chi_0 \sim 1/T$.

Exercise 4.3. Fixed points

Consider a system with three coupling constants (r, $g_1 \geq 0$ and g_2), which obey the following set of RG flow equations

$$\partial_l r = 2r - 24r(g_1 + g_2) \tag{212}$$
$$\partial_l g_1 = (4-D)g_1 - 8(n+8)g_1^2 - 48 g_1 g_2 \tag{213}$$
$$\partial_l g_2 = (4-D)g_2 - 72 g_2^2 - 96 g_1 g_2 \tag{214}$$

where $n \in \mathbb{N}$ is some parameter and D is the spatial dimension of the system.

1. Determine the set of RG fixed points (hint: there are four of them). Consider the trivial fixed point $r = g_1 = g_2 = 0$. Below which dimension D do the couplings g_1 and g_2 become relevant perturbations to the trivial fixed point?
2. Set $\varepsilon = 4 - D > 0$ to be small ($\varepsilon \ll 1$), linearise the RG flow equations around each fixed point and determine the corresponding RG eigenvalues, *left* eigenvectors and the scaling variables. Which of the fixed points have only one relevant perturbation (=critical fixed points)? These can control the critical properties of a continuous phase transition. Discuss the cases $n > 4$ and $n < 4$ separately.
3. Set $r = 0$ and sketch the flow diagrams in the $(g_1 \geq 0, g_2)$ half-plane for the $n > 4$ and $n < 4$ case. For concreteness, take $n = 5$ and $n = 3$, respectively.
4. Consider the $n > 4$ case and determine the correlation length exponent ν up to order $\mathcal{O}(\varepsilon)$ at the critical fixed point.

Exercise 4.4. One-loop flow equations for the O(N)-symmetric φ^4-theory

Generalize the φ^4-theory for an N-component vector field, $\varphi(\mathbf{k}) \to \boldsymbol{\varphi}(\mathbf{k}) = (\varphi_1(\mathbf{k}), \varphi_2(\mathbf{k}), ..., \varphi_N(\mathbf{k}))$ for $\mathbf{k} \in \mathbb{R}^D$ with the action

$$S[\boldsymbol{\varphi}] = \frac{1}{2}\int_{\mathbf{k}}^{\Lambda_0} [r_0 + c_0 k^2] \sum_{i=1}^{N} |\varphi_i(\mathbf{k})|^2 + \frac{u_0}{4!}\int_{\mathbf{r}} \sum_{i,j=1}^{N} \varphi_i^2(\mathbf{r})\varphi_j^2(\mathbf{r}). \tag{215}$$

1. Show that the action is invariant under $O(N)$ rotations, $\varphi_i \to \sum_{j=1}^{N} M_{ij}\varphi_j$ where M is an orthogonal $N \times N$ matrix.
2. Fourier transform the interaction term to momentum space and perform the RG step in analogy to the $N = 1$ case of the lecture. Show that the flow equations for the dimensionless couplings $\bar{r}, \bar{u}$ take the form

$$\partial_l \bar{r} = 2\bar{r} + \frac{(N+2)\,\bar{u}}{6\,(1+\bar{r})}, \qquad \partial_l \bar{u} = \underbrace{(4-D)}_{\epsilon}\bar{u} - \frac{(N+8)\,\bar{u}^2}{6\,(1+\bar{r})^2} \tag{216}$$

Hint: Coming from the $N = 1$ case, when generalizing to $N > 1$, you only need to worry about combinatorial factors. They can be tracked by using Feynman diagrams with a vertex $j > -- < i$ which carries flavor-indices of the fields. Internal loops representing integrals over larger fields with flavor indices that are not fixed by outer (smaller) fields lead to a factor of N.

3. Repeat the epsilon-expansion analysis for the non-trivial fixed point appearing for $D < 4$ and find the critical exponents to first order in ϵ. Set $D = 3$, $N = 3$ and find an approximation for ν of the three-dimensional Heisenberg universality class governing magnetic phase transitions in classical spin systems with 3-component magnetization vector. The exact value is $\nu = 0.71$.

Exercise 4.5. Irrelevant couplings

This exercise will discuss the effect of irrelevant couplings on physical observables.

1. Consider the RG flow equations for one relevant and one irrelevant coupling,

$$\partial_l u = y_u u + A(u, v)$$
$$\partial_l v = y_v v + B(u, v)$$

where $y_u = 1 > 0$ and $y_v = -1 < 0$ and argue that for small $|u|, |v|$, the functions A, B have the following expansions:

$$A(u, v) = a_1 u^2 + a_2 uv + a_3 v^2 + ...$$
$$B(u, v) = b_1 u^2 + b_2 uv + b_3 v^2 + ...$$

Specialize to $A(u, v) = -uv$ and $B(u, v) = -u^2$ and plot the flow (u_l, v_l) parameterized by $l \in [0, 2]$ in the $u-v$ plane starting from the points $(0.2, 0)$ and $(0.2, 0.3)$. Use a computer program (e.g. MATHEMATICA'S NDSolve) to solve this task. Show numerically that for large enough l, the flow for the initial couplings $(0.2, 0.3)$ can be reproduced by the flow starting from an initial point $(\tilde{u}_0, 0)$ and give the approximate value of $\tilde{u}_0$. This means the effect of a non-zero irrelevant coupling can be absorbed into a redefinition of the initial relevant coupling and we usually don't need to consider the irrelevant couplings in a scaling equation like Eq. (11).

2. The conclusion above does not hold if the scaling functions exhibit a singular dependence on an irrelevant coupling v so that it cannot be set to zero. This is called a *dangerously irrelevant coupling*. A famous example where this happens is the φ^4-theory for $D > 4$, see Eq. (50). As a preparation, consider the Gaussian action without interaction term:

$$S_{\Lambda_0}[\varphi] = -h_0 \varphi(\mathbf{k} = 0) + \frac{1}{2} \int_{\mathbf{k}}^{\Lambda_0} \left[r_0 + c_0 k^2 \right] \varphi(-\mathbf{k}) \varphi(\mathbf{k}) \tag{217}$$

   (a) Integrate out the fields for $\Lambda_0/b < k < \Lambda_0$ (which just adds a field independent term that we don't consider) and re-scale momenta and fields keeping c_0 fixed to derive the RG relations $r' = b^{y_t} r_0$ and $h' = b^{y_h} h_0$ with $y_t = 2$ and $y_h = 1 + D/2$.

   (b) Add an interaction term

$$S^{int}_{\Lambda_0}[\varphi] = \frac{u_0}{4!} \int_{\mathbf{k}_{1,2,3,4}}^{\Lambda_0} (2\pi)^D \delta(\mathbf{k}_1 + ... + \mathbf{k}_4) \varphi(\mathbf{k}_1) \varphi(\mathbf{k}_2) \varphi(\mathbf{k}_3) \varphi(\mathbf{k}_4) \tag{218}$$

   disregard the terms generated by momentum shell integration (they are considered in Sec. 4.4) and do the above rescaling step, you should find $y_u = 4 - D$ so that the interaction u becomes irrelevant for $D > 4$. [Careful: in the toy model of part (1.) above, the irrelevant coupling was called v.] In the following, consider the case $D > 4$.

   (c) Using the standard scaling ansatz for the free energy $f_{\text{sing}}(t, h)$ without irrelevant fields, determine the critical exponent β.

(d) As β in (c) does not agree with the result of the Gaussian approximation, $\beta = 1/2$ (derived without RG) we need to modify the scaling ansatz including the irrelevant coupling u. Argue that the magnetization $m = \frac{1}{V}\langle\varphi(\mathbf{k}=0)\rangle$ has the scaling form

$$m(t,h,u) = b^{y_h - D} m\left(b^{y_t} t, b^{y_h} h, b^{y_u} u\right), \tag{219}$$

set $h = 0$ and derive the scaling relation

$$m(t,0,u) = |t|^{-(y_h - D)/y_t} m\left(\pm 1, 0, |t|^{-y_u/y_t}\, u\right). \tag{220}$$

According to Landau theory, a finite u is needed to get a spontaneous magnetization at $h = 0$ and we cannot set the last argument to zero. Show that Landau theory predicts $m(-1,0,\bar{u}) \propto \bar{u}^{-1/2}$ and use this to derive $\beta = 1/2$.

Exercise 4.6. Kondo impurity in gapless fermionic system

The Kondo impurity described by the Hamiltonian in Eq. (165) can be studied in the case where the density of states (DOS) as a function of energy is not just a constant (ν_0) as in the lecture but given by a power law,

$$\nu(E) \equiv \sum_{\mathbf{k}} \delta\left(E - \xi_{\mathbf{k}}\right) \stackrel{!}{=} \begin{cases} C\,|E|^r & : |E| \le D \\ 0 & : |E| > D \end{cases} \tag{221}$$

with $r \ge 0$ and $\xi_{\mathbf{k}}$ the bandstructure that already included the chemical potential.

1. Consider the case of two-dimensional graphene with $\xi_{\mathbf{k}} = \pm\hbar v|\mathbf{k}|$: What r corresponds to this situation? Here, $\pm$ correspond to conduction and valence band of a single spin-polarized Dirac node.

2. For the isotropic case $J_\perp = J_z = J$ and general r, generalize the poor man's scaling approach from the lecture to find the flow equation for J_l . Combine this with $\nu_l \equiv \nu(De^{-l})$ to obtain the flow equation for the dimensionless parameter $J_l\nu_l$. Draw the RG flow diagram for $J > 0$ and discuss the changes to the $r = 0$ case treated in the lecture.

Part II
Functional Renormalization Group

5 Functional methods

Aims:

- Prepare standard formulation of the fRG.
- Introduce Green functions (correlators) via source-field derivatives of generating functions.
- Essential part of Green functions: Vertex functions.

5.1 Partition function and conventions

- Assume partition function $\mathcal{Z}$ written as unconstrained functional integral:

$$\mathcal{Z} = \int \mathcal{D}[\Phi] \exp[-\underbrace{(S_0[\Phi] + S_1[\Phi])}_{S[\Phi]}] \tag{1}$$

- Treat classical and quantum systems, fermionic and bosonic particles in *one* formalism:
  Superfield $\Phi = (\Phi_{\alpha_1}, \Phi_{\alpha_2}, ...)$ with single-particle multi-index α containing Matsubara frequency or imaginary time, momentum or position, spin, ...
- (Anti-)commutation properties encoded by $\Phi_{\alpha_1}\Phi_{\alpha_2} = \zeta_\alpha \Phi_{\alpha_2}\Phi_{\alpha_1}$, e.g. $\zeta = \pm 1$ for bosons/fermions. Define statistics matrix $\mathbf{Z}$ with $\mathbf{Z}_{\alpha\alpha'} = \delta_{\alpha\alpha'}\zeta_\alpha$.
- Gaussian part in (anti-)symmetrized notation:

$$\boxed{S_0[\Phi] = -\frac{1}{2}\int_\alpha \int_{\alpha'} \Phi_\alpha \left[\mathbf{G}_0^{-1}\right]_{\alpha\alpha'} \Phi_{\alpha'} \equiv -\frac{1}{2}\left(\Phi, \mathbf{G}_0^{-1}\Phi\right)} \tag{2}$$

  Product is defined as $(\Phi, \Psi) \equiv \int_\alpha \Phi_\alpha \Psi_\alpha$. We assume properly (anti-)symmetrized $\mathbf{G}_0$, i.e. in each sector

$$\boxed{\mathbf{Z}\mathbf{G}_0 = \mathbf{G}_0^T} \tag{3}$$

- Examples: (recall that in the $T \to 0$ and infinite volume limit: $\frac{1}{\beta V}\sum_{\omega,\mathbf{k}} \to \int \frac{d\omega}{2\pi} \int \frac{d\mathbf{k}}{(2\pi)^D} \equiv \int_\omega \int_{\mathbf{k}}$)

  1. Classical φ^4-theory: $\{\Phi_\alpha\} \to \{\varphi_{\mathbf{k}}\}$, $\zeta = 1$, $\int_\alpha \to \int_{\mathbf{k}}$,

$$S_0[\varphi] = \frac{1}{2}\int_{\mathbf{k}} \left[r_0 + c_0 k^2\right] \varphi_{-\mathbf{k}}\varphi_{+\mathbf{k}} \tag{4}$$

     leads to

$$\left[\mathbf{G}_0^{-1}\right]_{\mathbf{k}\mathbf{k}'} = -(2\pi)^D \delta^D(\mathbf{k} + \mathbf{k}')\left[r_0 + c_0 k^2\right] \tag{5}$$

  2. Spinless fermions: Need two types of fields, $\{\Phi_\alpha\} \to \left\{\psi_{i\omega,\mathbf{k}}, \bar{\psi}_{i\omega,\mathbf{k}}\right\}$, $\zeta = -1$, abbreviate $K \equiv (i\omega, \mathbf{k})$, $\int_\omega \int_{\mathbf{k}} \equiv \int_K$. We have $\alpha = (\psi, K)$ or $(\bar{\psi}, K)$.
     Recall Fourier-transform of (independent!) Grassmann fields $\bar{\psi}$ and ψ are oppositely defined:

$\psi(\mathbf{k}\omega) = \int_0^\beta d\tau \int d\mathbf{r}\, \psi(\mathbf{r}\tau) e^{-i\mathbf{kr}+i\omega\tau}$, $\bar{\psi}(\mathbf{k}\omega) = \int_0^\beta d\tau \int d\mathbf{r}\, \bar{\psi}(\mathbf{r}\tau) e^{+i\mathbf{kr}-i\omega\tau}$.

$$\begin{aligned} S_0\left[\bar{\psi},\psi\right] &= -\int_K \bar{\psi}_K \underbrace{G_0^{-1}(K)}_{i\omega-\xi_{\mathbf{k}}} \psi_K \\ &= -\frac{1}{2}\int_K \left(\psi_K, \bar{\psi}_K\right) \begin{pmatrix} 0 & \zeta G_0^{-1}(K) \\ G_0^{-1}(K) & 0 \end{pmatrix} \begin{pmatrix} \psi_K \\ \bar{\psi}_K \end{pmatrix} \\ &= -\frac{1}{2}\int_{K,K'} \left(\psi_K, \bar{\psi}_K\right) \underbrace{(2\pi)^{D+1}\delta(\omega-\omega')\delta^D(\mathbf{k}-\mathbf{k}') \begin{pmatrix} 0 & \zeta G_0^{-1}(K) \\ G_0^{-1}(K) & 0 \end{pmatrix}}_{\equiv\left[\mathbf{G}_0^{-1}\right]_{\alpha\alpha'}} \begin{pmatrix} \psi_{K'} \\ \bar{\psi}_{K'} \end{pmatrix} \end{aligned}$$

5.2 Green functions and generating functionals

- *Disconnected n-point Green functions*: (Mind the index-ordering!)

$$G^{(n)}_{\alpha_1\ldots\alpha_n} = \frac{\int \mathcal{D}[\Phi]\, e^{-S[\Phi]}\Phi_{\alpha_n}\ldots\Phi_{\alpha_1}}{\int \mathcal{D}[\Phi]\, e^{-S[\Phi]}} = \langle \Phi_{\alpha_n}\ldots\Phi_{\alpha_1}\rangle \tag{6}$$

- Sourcefield trick: Want to write generating functional

$$G^{(n)}_{\alpha_1\ldots\alpha_n} = \frac{\delta^n \mathcal{G}[J]}{\delta J_{\alpha_n}\ldots\delta J_{\alpha_1}}|_{J=0} \tag{7}$$

  This is achieved by introducing sourcefields J:

$$\mathcal{G}[J] \equiv \frac{\int \mathcal{D}[\Phi]\, e^{-S[\Phi]+(J,\Phi)}}{\underbrace{\int \mathcal{D}[\Phi]\, e^{-S[\Phi]}}_{\mathcal{Z}}} \tag{8}$$

  Remarks:

  - $\mathcal{G}[J=0] = 1$.
  - Sources J are of same type as Φ and are mutually (anti-)commuting, (J,Φ) commute with all other terms in S.
  - $G^{(n)}_{\alpha_1\ldots\alpha_n}$ are fully (anti-)symmetric under index exchange.

- The $G^{(n)}_{\alpha_1\ldots\alpha_n}$ are the expansion coefficients of $\mathcal{G}[J]$ (now the index-ordering matches!)

$$\mathcal{G}[J] = \sum_{n=0}^{\infty} \frac{1}{n!} \int_{\alpha_1\ldots\alpha_n} G^{(n)}_{\alpha_1\ldots\alpha_n} J_{\alpha_1}\ldots J_{\alpha_n} \tag{9}$$

- *Connected Greens functions* do not contain disconnected contributions when Wick theorem is applied to them.
  Define connected generating functional [in $\mathcal{G}[J]$ replace denominator by $\mathcal{Z}_0$ and put natural logarithm in front - Proof: Linked-cluster theorem]

$$\begin{aligned} \mathcal{G}_c[J] &= \ln\left(\frac{\mathcal{Z}}{\mathcal{Z}_0}\mathcal{G}[J]\right) = \ln\left(\frac{\int \mathcal{D}[\Phi]\, e^{-S[\Phi]+(J,\Phi)}}{\int \mathcal{D}[\Phi]\, e^{-S_0[\Phi]}}\right) = \sum_{n=0}^{\infty}\frac{1}{n!}\int_{\alpha_1\ldots\alpha_n} G^{(n)}_{c,\alpha_1\ldots\alpha_n} J_{\alpha_1}\ldots J_{\alpha_n} \qquad (10) \\ G^{(n)}_{c,\alpha_1\ldots\alpha_n} &= \frac{\delta^n \mathcal{G}_c[J]}{\delta J_{\alpha_n}\ldots\delta J_{\alpha_1}}|_{J=0} \end{aligned}$$

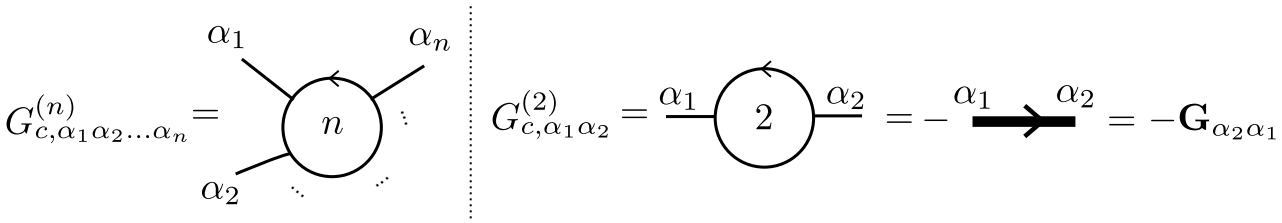


Figure 16: Graphical representation of the connected Green function (left) and its two-point version also called the propagator (right).

- Example: Relation between connected and disconnected GFs

$$\begin{aligned} G^{(0)}_{c} &= \ln\left(\frac{\mathcal{Z}}{\mathcal{Z}_0}\right) \\ G^{(1)}_{c,\alpha_1} &= G^{(1)}_{\alpha_1} = \langle \Phi_{\alpha_1} \rangle \\ G^{(2)}_{c,\alpha_1\alpha_2} &= G^{(2)}_{\alpha_1\alpha_2} - G^{(1)}_{\alpha_1} G^{(1)}_{\alpha_2} = \langle \Phi_{\alpha_2}\Phi_{\alpha_1}\rangle - \langle \Phi_{\alpha_2}\rangle \langle \Phi_{\alpha_1}\rangle \end{aligned}$$

  The first line is equivalent to the interaction correction to the free energy (up to factor T).

- Graphical representation $G^{(n)}_{c,\alpha_1\ldots\alpha_n}$: Empty circle with arrow pointing to α_1-leg, use abbreviated "line" notation for 2-point function.

$\mathcal{G}_c[J]$ for Gaussian theory

- Can find $\mathcal{G}_c[J]$ explicitly for Gaussian theory ($S_1 = 0$):

$$e^{\mathcal{G}_{0c}[J]} = \frac{\int \mathcal{D}[\Phi]\, e^{-\frac{1}{2}\left(\Phi, \mathbf{G}_0^{-1}\Phi\right) + (J,\Phi)}}{\int \mathcal{D}[\Phi]\, e^{-S_0[\Phi]}} \tag{11}$$

  In numerator, shift $\Phi = \Phi' - \mathbf{G}_0^T J$ and obtain

$$-\frac{1}{2}\left(\Phi, \mathbf{G}_0^{-1}\Phi\right) + (J,\Phi) \;=\; -\frac{1}{2}\left(\Phi' - \mathbf{G}_0^T J, \mathbf{G}_0^{-1}\left[\Phi' - \mathbf{G}_0^T J\right]\right) + \left(J, \Phi' - \mathbf{G}_0^T J\right)$$

  clean up and use $\left(\mathbf{G}_0^T\Psi, \Phi\right) = (\Psi, \mathbf{G}_0\Phi)$. The term $\propto \Phi'^2$ cancels with denominator. Comparing the exponents:

$$\mathcal{G}_{0c}[J] = -\frac{1}{2}\left(J, \mathbf{G}_0^T J\right) = -\frac{1}{2}\int_\alpha \int_{\alpha'} [\mathbf{G}_0]_{\alpha\alpha'} J_{\alpha'} J_\alpha \tag{12}$$

  so that

$$\boxed{G^{(2)}_{0c,\alpha'\alpha} = \langle \Phi_\alpha \Phi_{\alpha'}\rangle_0 = \frac{\delta^2 \mathcal{G}_{0c}[J]}{\delta J_\alpha \delta J_{\alpha'}}|_{J=0} \overset{(12)}{=} -[\mathbf{G}_0]_{\alpha\alpha'}} \tag{13}$$

- Definition: Differential operator to generate matrix in superfield space

$$\left[\frac{\delta}{\delta J} \otimes \frac{\delta}{\delta J}\right]_{\alpha\alpha'} \equiv \frac{\delta^2}{\delta J_\alpha \delta J_{\alpha'}} \tag{14}$$

  so that from above

$$\mathbf{G}_0 = -\left(\frac{\delta}{\delta J} \otimes \frac{\delta}{\delta J}\right) \mathcal{G}_{0c}[J]\,|_{J=0} \tag{15}$$

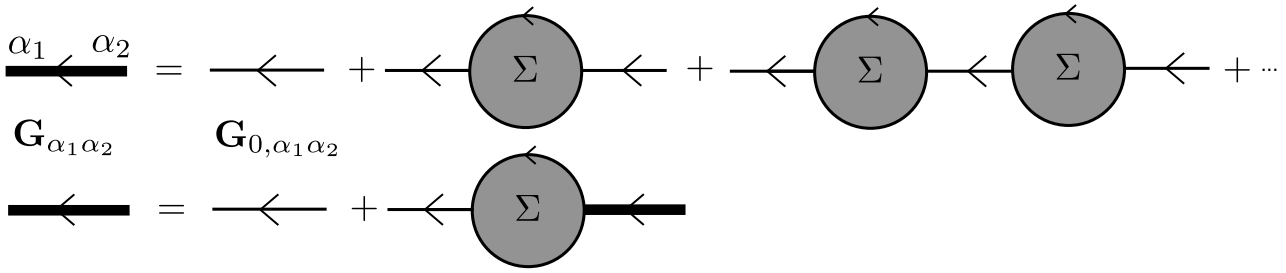


Figure 17: Graphical representation of the Dyson equation.

5.3 Propagator and self-energy

- $G^{(2)}_{c,\alpha\alpha'}$ is called the *propagator* or sometimes simply "Green function" of the theory. Also: "Dressed" or "full" propagator.
- In analogy with the last equation, but for general (not necessarily Gaussian) theory, *define*

$$\mathbf{G} \equiv -\left(\frac{\delta}{\delta J} \otimes \frac{\delta}{\delta J}\right) \mathcal{G}_c\left[J\right]|_{J=0} \tag{16}$$

  and we read off (see right part of Fig. 16)

$$G^{(2)}_{c,\alpha\alpha'} = \langle \Phi_{\alpha'} \Phi_{\alpha} \rangle = -\mathbf{G}_{\alpha'\alpha} \tag{17}$$

- *Self-energy:* Defined as difference between *inverse* Green function and *inverse* Gaussian ("bare") Green function,

$$\boxed{\mathbf{G}^{-1} = \mathbf{G}_0^{-1} - \mathbf{\Sigma}} \tag{18}$$

  and it follows the Dyson equation:

$$\begin{aligned} \mathbf{G} &= \mathbf{G}_0 + \mathbf{G}_0\mathbf{\Sigma}\mathbf{G}_0 + \mathbf{G}_0\mathbf{\Sigma}\mathbf{G}_0\mathbf{\Sigma}\mathbf{G}_0 + ... \\ &= \mathbf{G}_0 + \mathbf{G}_0\mathbf{\Sigma}\mathbf{G} \end{aligned} \tag{19}$$

  With $\mathbf{G}_0$ represented by a thin line, we have the graphical representation in Fig. 17.
- Leveraging perturbation theory: Low-order approximation of $\mathbf{\Sigma}$ generates infinite-order diagrams in $\mathbf{G}$.

5.4 Alternative representation of $\mathcal{G}_c\left[J\right]$ (without $\int \mathcal{D}\left[\Phi\right] ...$)

- Use

$$\left(\Phi_\alpha\right)^n e^{(J,\Phi)} = \left(\frac{\delta}{\delta J_\alpha}\right)^n e^{(J,\Phi)} \tag{20}$$

  to write

$$e^{-S_1[\Phi]+(J,\Phi)} = e^{-S_1\left[\frac{\delta}{\delta J}\right]+(J,\Phi)} \tag{21}$$

- Use this in definition of $\mathcal{G}_c\left[J\right]$, Eq. (10), and pull out $S_1\left[\frac{\delta}{\delta J}\right]$ from the integral

$$e^{\mathcal{G}_c[J]} \equiv \frac{\int \mathcal{D}\left[\Phi\right] e^{-S[\Phi]+(J,\Phi)}}{\int \mathcal{D}\left[\Phi\right] e^{-S_0[\Phi]}} = e^{-S_1\left[\frac{\delta}{\delta J}\right]} \frac{\int \mathcal{D}\left[\Phi\right] e^{-S_0[\Phi]+(J,\Phi)}}{\int \mathcal{D}\left[\Phi\right] e^{-S_0[\Phi]}} = e^{-S_1\left[\frac{\delta}{\delta J}\right]} e^{\mathcal{G}_{0c}[J]} \overset{(12)}{=} e^{-S_1\left[\frac{\delta}{\delta J}\right]} e^{-\frac{1}{2}\left(J,\mathbf{G}_0^T J\right)} \tag{22}$$

5.5 Amputated connected Green function

- Motivation: Later, want to start fRG-flow from $\mathbf{G}_0^{\Lambda=\infty} = 0$, but from (22) have then $\mathcal{G}_c(\mathbf{G}_0 = 0) = 0$. Bad: Generic starting point doesn't know anything about physics of specific model.
- Amputate $\mathbf{G}_0$ from connected Green functions (difference to $\mathcal{G}_c[J]$: now the sources read $\bar{\Phi}$ instead of J and only appear in S_1):

$$\mathcal{G}_{ac}\left[\bar{\Phi}\right] = \ln\left(\frac{\int \mathcal{D}[\Phi]\, e^{-S_0[\Phi]-S_1\left[\Phi+\bar{\Phi}\right]}}{\mathcal{Z}_0}\right) = \sum_{n=0}^{\infty}\frac{1}{n!}\int_{\alpha_1\ldots\alpha_n} G^{(n)}_{ac,\alpha_1\ldots\alpha_n}\,\bar{\Phi}_{\alpha_1}\ldots\bar{\Phi}_{\alpha_n} \tag{23}$$

$$G^{(n)}_{ac,\alpha_1\ldots\alpha_n} = \frac{\delta^n \mathcal{G}_{ac}\left[\bar{\Phi}\right]}{\delta\bar{\Phi}_{\alpha_n}\ldots\delta\bar{\Phi}_{\alpha_1}}|_{\bar{\Phi}=0} \tag{24}$$

- Relation between $\mathcal{G}_{ac}\left[\bar{\Phi}\right]$ and $\mathcal{G}_c[J]$: Use shift of variable in Eq. (23), $\Phi' = \Phi + \bar{\Phi}$,

$$\mathcal{G}_{ac}\left[\bar{\Phi}\right] = \mathcal{G}_c\left[-\left(\mathbf{G}_0^T\right)^{-1}\bar{\Phi}\right] + \frac{1}{2}\left(\bar{\Phi}, \mathbf{G}_0^{-1}\bar{\Phi}\right) \tag{25}$$

  Remarks:
  - Amputation effect obvious from first term.
  - Due to the last term, for a free theory $\mathcal{G}_{0c}[J] = -\frac{1}{2}\left(J, \mathbf{G}_0^T J\right)$ we have $\mathcal{G}_{ac} = 0$.
- Alternative representation of $\mathcal{G}_{ac}\left[\bar{\Phi}\right]$ (similar derivation to the case for $\mathcal{G}_c\left[\bar{\Phi}\right]$)

$$e^{\mathcal{G}_{ac}[\bar{\Phi}]} = e^{-\frac{1}{2}\left(\frac{\delta}{\delta\bar{\Phi}}, \mathbf{G}_0^T\frac{\delta}{\delta\bar{\Phi}}\right)} e^{-S_1[\bar{\Phi}]} \tag{26}$$

5.6 One-line irreducible vertices $\Gamma^{(n)}$ and tree expansion

- Motivation: Connected correlation functions can be sub-divided into "essential" blocks connected by propagators.
  Example: Dyson equation (19) for G where essential block Σ was called self-energy.
- Anticipate similar structure for $G_c^{(n)}$ for $n > 2$.
  Define irreducible vertex $\Gamma^{(m)}_{\alpha_1\alpha_2\ldots\alpha_m}$ (filled circle) as the part of diagrams for $G_c^{(n)}$ $(m \leq n)$ which cannot be separated by cutting a propagator line $G_c^{(2)}$.
- Relation $G_c^{(n)} \leftrightarrow \Gamma^{(m)}_{\alpha_1\alpha_2\ldots\alpha_m}$: *Tree-expansion* (tree diagrams are diagrams without loops). Example for $n = 3, 4$ in Fig. 18.
- $\Gamma^{(m)}_{\alpha_1\alpha_2\ldots\alpha_m}$ ~ true interaction between particles
- Final goal: Write fRG flow equations on the basis of $\Gamma^{(n)}_{\alpha_1\alpha_2\ldots\alpha_n}$.
- Next goal: Find expression for generating functional $\Gamma\left[\bar{\Phi}\right]$ for $\Gamma^{(n)}_{\alpha_1\alpha_2\ldots\alpha_n}$ such that

$$\boxed{\Gamma^{(n)}_{\alpha_1\ldots\alpha_n} = \frac{\delta^n\Gamma\left[\bar{\Phi}\right]}{\delta\bar{\Phi}_{\alpha_n}\ldots\delta\bar{\Phi}_{\alpha_1}}|_{\bar{\Phi}=0} \quad \Leftrightarrow \quad \Gamma\left[\bar{\Phi}\right] = \sum_{n=0}^{\infty}\frac{1}{n!}\int_{\alpha_1\ldots\alpha_n}\Gamma^{(n)}_{\alpha_1\ldots\alpha_n}\,\bar{\Phi}_{\alpha_1}\ldots\bar{\Phi}_{\alpha_n}} \tag{27}$$

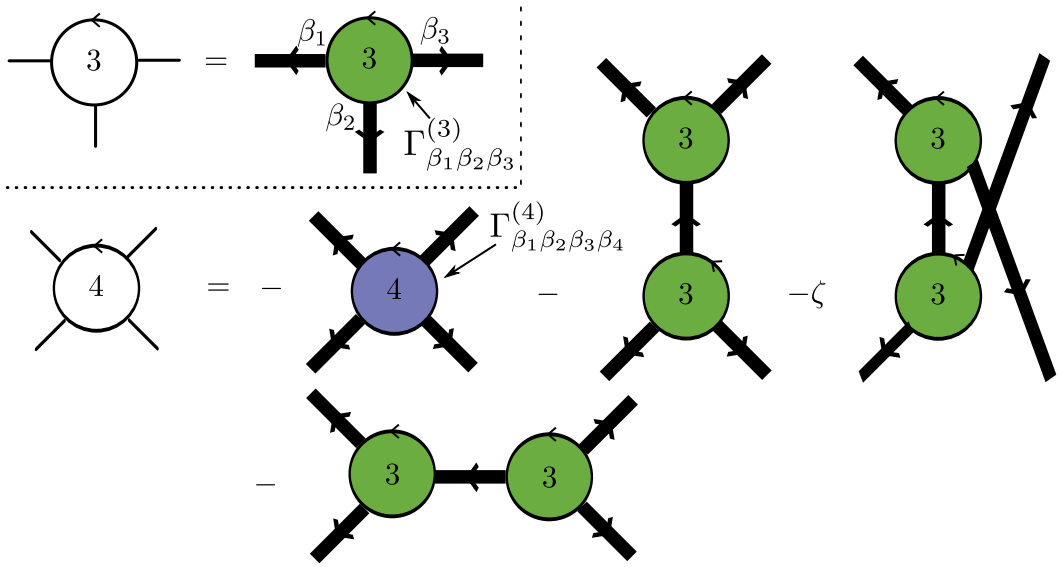


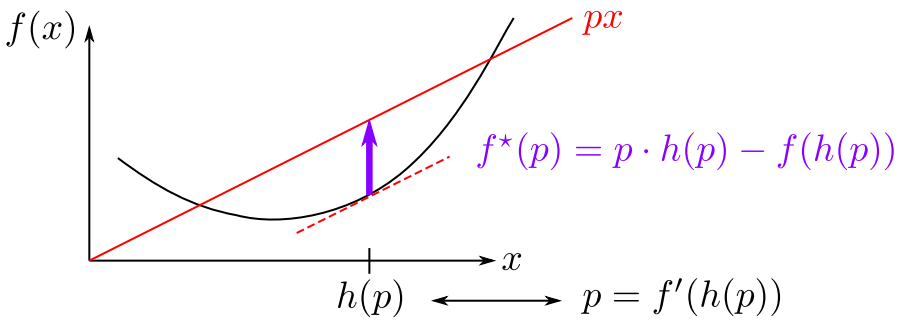
Figure 18: Tree expansion for the 3- and 4-point connected Green functions.

Interlude: Legendre transformation reminder

- Legendre transformation $f^\star$ of convex function $f(x)$ (with $f'' > 0$):

$$f^\star(p) \equiv p \cdot h(p) - f\left(h(p)\right) \tag{28}$$
$$p = f'(h(p)) \tag{29}$$

- From chain rule: $(f^\star)'(p) = h(p) = (f')^{-1}(p)$, i.e. the derivatives of f and $f^\star$ are inverse to each other.
- Graphical construction: Draw $f(x)$ and the linear function px, find the point $x = h$ where the tangent to f has the same slope and call the distance between the curves at that point $f^\star(p)$.



- Legendre transform in thermodynamics (different sign-convention):
  Internal energy U which depends on entropy S, volume V, particle number N (*extensive* variables)

$$U = U(S, V, N) \tag{30}$$
$$dU \equiv TdS - pdV + \mu dN \tag{31}$$

  Relate U to free energy $F(T, V, N)$ which depends on temperature T (T is "slope" of U with respect to S, *intensive* variable)

$$F \equiv -TS + U \tag{32}$$
$$T \equiv dU(S, V, N)/dS \tag{33}$$

  Need to replace all S in F by T. Obtain:

$$dF = -TdS - SdT + dU = -SdT - pdV + \mu dN \tag{34}$$

Generating functional $\Gamma\left[\bar{\Phi}\right]$

- Claim: $\Gamma\left[\bar{\Phi}\right]$ is the *functional* Legendre transform of $\mathcal{G}_c\left[J\right]$

$$\Gamma\left[\bar{\Phi}\right] = \underbrace{\left(J[\bar{\Phi}],\bar{\Phi}\right) - \mathcal{G}_c\left[J[\bar{\Phi}]\right]}_{\equiv \mathcal{L}[\bar{\Phi}]} - S_0\left[\bar{\Phi}\right] \tag{35}$$

$$\bar{\Phi}_\alpha \equiv \frac{\delta \mathcal{G}_c\left[J\right]}{\delta J_\alpha} = \langle \Phi_\alpha \rangle\,|_J \tag{36}$$

  Last contribution $S_0\left[\bar{\Phi}\right] \sim \bar{\Phi}^2$ in Eq. (35) is a convenience convention that "shifts" only $\Gamma^{(2)}_{\alpha_1\alpha_2}$.

- Remarks:
  - In Eq. (35), replace all sources J by the inverted relation Eq. (36). Note that $\bar{\Phi}_\alpha = \langle \Phi_\alpha \rangle\,|_J$ with *non-vanishing* sources.
  - Assume absence of spontaneous symmetry breaking, i.e. as $J \to 0$ one has $\bar{\Phi}_\alpha = \langle \Phi_\alpha \rangle\,|_{J\to 0} = 0$. This can be lifted by using $\bar{\Phi} = \delta\bar{\Phi} + \bar{\Phi}^0$, see [Kopietz].

Three preparations for tree expansion: Relate $\frac{\delta}{\delta\bar{\Phi}} \leftrightarrow \frac{\delta}{\delta J}$.

1. Express J in terms of $\bar{\Phi}$:

$$\frac{\delta \mathcal{L}\left[\bar{\Phi}\right]}{\delta\bar{\Phi}_\alpha} = \frac{\delta\left(J,\bar{\Phi}\right) - \delta\mathcal{G}_c\left[J\right]}{\delta\bar{\Phi}_\alpha} = \zeta_\alpha J_\alpha + \left(\frac{\delta J}{\delta\bar{\Phi}_\alpha},\bar{\Phi}\right) - \int_{\alpha'} \frac{\delta J_{\alpha'}}{\delta\bar{\Phi}_\alpha} \underbrace{\frac{\delta\mathcal{G}_c\left[J\right]}{\delta J_{\alpha'}}}_{\bar{\Phi}_{\alpha'}} = \zeta_\alpha J_\alpha \tag{37}$$

2. Chain-rule: Apply chain-rule to $\delta/\delta\bar{\Phi}_\alpha$ and use (1.):

$$\frac{\delta}{\delta\bar{\Phi}_\alpha} = \int_{\alpha'} \left[\frac{\delta J_{\alpha'}}{\delta\bar{\Phi}_\alpha}\right] \frac{\delta}{\delta J_{\alpha'}} \overset{(1.)}{=} \int_{\alpha'} \left[\frac{\delta^2\mathcal{L}\left[\bar{\Phi}\right]}{\delta\bar{\Phi}_\alpha\delta\bar{\Phi}_{\alpha'}}\zeta_{\alpha'}\right] \frac{\delta}{\delta J_{\alpha'}} \tag{38}$$

   or, in compact notation with $\mathbf{Z}_{\alpha\alpha'} = \delta_{\alpha\alpha'}\zeta_\alpha$,

$$\frac{\delta}{\delta\bar{\Phi}} = \left(\left[\frac{\delta}{\delta\bar{\Phi}} \otimes \frac{\delta}{\delta\bar{\Phi}}\right] \mathcal{L}\left[\bar{\Phi}\right]\right) \mathbf{Z} \frac{\delta}{\delta J} \tag{39}$$

3. Use chain rule for $\frac{\delta}{\delta\bar{\Phi}}$ on $\bar{\Phi} \equiv \frac{\delta\mathcal{G}_c[J]}{\delta J}$ (Eq. 36):

$$\mathbf{1} = \frac{\delta}{\delta\bar{\Phi}}\bar{\Phi} \overset{(36)}{=} \frac{\delta}{\delta\bar{\Phi}}\frac{\delta\mathcal{G}_c\left[J\right]}{\delta J} \overset{(2.)}{=} \left(\left[\frac{\delta}{\delta\bar{\Phi}} \otimes \frac{\delta}{\delta\bar{\Phi}}\right] \mathcal{L}\left[\bar{\Phi}\right]\right) \mathbf{Z} \left(\left[\frac{\delta}{\delta J} \otimes \frac{\delta}{\delta J}\right] \mathcal{G}_c\left[J\right]\right) \tag{40}$$

   or, isolating the J from the $\bar{\Phi}$ terms:

$$\boxed{\left[\frac{\delta}{\delta J} \otimes \frac{\delta}{\delta J}\right] \mathcal{G}_c\left[J\right] = \mathbf{Z}\left(\left[\frac{\delta}{\delta\bar{\Phi}} \otimes \frac{\delta}{\delta\bar{\Phi}}\right] \mathcal{L}\left[\bar{\Phi}\right]\right)^{-1}} \tag{41}$$

Tree expansion

- In identity (41) above, expand both sides in powers of J_α and compare coefficients. For r.h.s. , first expand in powers of $\bar{\Phi}_\alpha$ and then use $\bar{\Phi} \equiv \frac{\delta\mathcal{G}_c[J]}{\delta J}$ to expand in powers of J_α.

- Self energy $\Gamma^{(2)}_{\alpha\alpha'}$: Use

$$\left(\frac{\delta}{\delta J_\alpha}\otimes\frac{\delta}{\delta J_{\alpha'}}\right)\mathcal{G}_c\left[J\right]|_{J=0}\equiv-\mathbf{G}_{\alpha\alpha'}=G^{(2)}_{c,\alpha'\alpha} \tag{42}$$

and get ($J\to 0$ yields $\bar\Phi\to 0$)

$$-\mathbf{Z}\mathbf{G}^{-1}=\left[\frac{\delta}{\delta\bar\Phi}\otimes\frac{\delta}{\delta\bar\Phi}\right]\mathcal{L}\left[\bar\Phi\right]|_{\bar\Phi=0}=\left[\frac{\delta}{\delta\bar\Phi}\otimes\frac{\delta}{\delta\bar\Phi}\right]\left(\Gamma\left[\bar\Phi\right]+S_0\left[\bar\Phi\right]\right)|_{\bar\Phi=0}=\left[\frac{\delta}{\delta\bar\Phi}\otimes\frac{\delta}{\delta\bar\Phi}\right]\Gamma\left[\bar\Phi\right]|_{\bar\Phi=0}-\left[\mathbf{G}_0^{\mathrm{T}}\right]^{-1} \tag{43}$$

and further, using the definition of the self-energy $\mathbf{\Sigma}=\mathbf{G}_0^{-1}-\mathbf{G}^{-1}$,

$$\left[\frac{\delta}{\delta\bar\Phi}\otimes\frac{\delta}{\delta\bar\Phi}\right]\Gamma\left[\bar\Phi\right]|_{\bar\Phi=0}=\mathbf{\Sigma}^{\mathrm{T}} \tag{44}$$

and taking matrix elements

$$\Gamma^{(2)}_{\alpha_1\alpha_2}=\left[\mathbf{\Sigma}\right]_{\alpha_1\alpha_2} \tag{45}$$

- General case $\Gamma^{(m)}$ for $m>2$: Define

$$\mathbf{U}\left[\bar\Phi\right]\equiv\left(\left[\frac{\delta}{\delta\bar\Phi}\otimes\frac{\delta}{\delta\bar\Phi}\right]\Gamma\left[\bar\Phi\right]\right)^{\mathrm{T}}-\underbrace{\left(\left[\frac{\delta}{\delta\bar\Phi}\otimes\frac{\delta}{\delta\bar\Phi}\right]\Gamma\left[\bar\Phi\right]|_{\bar\Phi=0}\right)^{T}}_{\mathbf{\Sigma}}=\sum_{n=1}^{\infty}\frac{1}{n!}\int_{\alpha_1\ldots\alpha_n}\left[\mathbf{\Gamma}^{(n+2)}_{\alpha_1\ldots\alpha_n}\right]\bar\Phi_{\alpha_1}\ldots\bar\Phi_{\alpha_n} \tag{46}$$

with definition of the matrix in superlabel space $\left[\mathbf{\Gamma}^{(n+2)}_{\alpha_1\ldots\alpha_n}\right]_{\alpha\alpha'}\equiv\Gamma^{(n+2)}_{\alpha\alpha'\alpha_1\ldots\alpha_n}$. Note that $\mathbf{U}\left[\bar\Phi=0\right]=0$. Use $\mathcal{L}=\Gamma+S_0$ to get

$$\frac{\delta}{\delta\bar\Phi}\otimes\frac{\delta}{\delta\bar\Phi}\mathcal{L}\left[\bar\Phi\right]=\frac{\delta}{\delta\bar\Phi}\otimes\frac{\delta}{\delta\bar\Phi}\Gamma\left[\bar\Phi\right]-\left[\mathbf{G}_0^{\mathrm{T}}\right]^{-1}=\mathbf{U}^{\mathrm{T}}\left[\bar\Phi\right]+\mathbf{\Sigma}^{\mathrm{T}}-\left[\mathbf{G}_0^{\mathrm{T}}\right]^{-1}=\mathbf{U}^{\mathrm{T}}\left[\bar\Phi\right]-\left[\mathbf{G}^{\mathrm{T}}\right]^{-1} \tag{47}$$

- In order to connect to Eq. (41), we need to expand the inverse of the above

$$\begin{aligned}\left(\frac{\delta}{\delta J}\otimes\frac{\delta}{\delta J}\right)\mathcal{G}_c\left[J\right]&=\mathbf{Z}\left(\frac{\delta}{\delta\bar\Phi}\otimes\frac{\delta}{\delta\bar\Phi}\mathcal{L}\left[\bar\Phi\right]\right)^{-1}=\mathbf{Z}\frac{1}{\mathbf{U}^{\mathrm{T}}\left[\bar\Phi\right]-\left[\mathbf{G}^{\mathrm{T}}\right]^{-1}}\\&=-\mathbf{Z}\mathbf{G}^{\mathrm{T}}\frac{1}{1-\mathbf{U}^{\mathrm{T}}\left[\bar\Phi\right]\mathbf{G}^{\mathrm{T}}}=-\mathbf{G}\sum_{\nu=0}^{\infty}\left[\mathbf{U}^{\mathrm{T}}\left[\bar\Phi\right]\mathbf{G}^{\mathrm{T}}\right]^{\nu}\end{aligned}$$

- Expand in J's (left) and in $\bar\Phi$'s (right). Use definition $\left[\mathbf{G}^{(n+2)}_{c,\alpha_1\ldots\alpha_n}\right]_{\alpha\alpha'}\equiv G^{(n+2)}_{c,\alpha\alpha'\alpha_1\ldots\alpha_n}$. Take the transpose of the matrix structure.

$$\begin{aligned}\sum_{n=0}^{\infty}\frac{1}{n!}\int_{\alpha_1}\ldots\int_{\alpha_n}\mathbf{G}^{(n+2)}_{c,\alpha_1\ldots\alpha_n}J_{\alpha_1}\ldots J_{\alpha_n}\;=\;&-\sum_{\nu=0}^{\infty}\sum_{n_1=1}^{\infty}\ldots\sum_{n_\nu=1}^{\infty}\frac{1}{n_1!\ldots n_\nu!}\int_{\beta_1^1}\ldots\int_{\beta^1_{n_1}}\ldots\int_{\beta_1^\nu}\ldots\int_{\beta^\nu_{n_\nu}}\\&\times\underbrace{\mathbf{G}\left(\mathbf{\Gamma}^{(n_\nu+2)}_{\beta_1^\nu\ldots\beta^\nu_{n_\nu}}\right)\ldots\mathbf{G}\left(\mathbf{\Gamma}^{(n_1+2)}_{\beta_1^1\ldots\beta^1_{n_1}}\right)}_{\times\nu}\mathbf{G}\mathbf{Z}\bar\Phi_{\beta_1^1}\ldots\bar\Phi_{\beta^1_{n_1}}\ldots\bar\Phi_{\beta_1^\nu}\ldots\bar\Phi_{\beta^\nu_{n_\nu}}\end{aligned} \tag{48}$$

- For final comparison of J-coefficients, trade $\bar\Phi$ for J:

$$\bar\Phi_\beta=\frac{\delta\mathcal{G}_c\left[J\right]}{\delta J_\beta}=\sum_{n=0}^{\infty}\frac{1}{n!}\int_{\alpha_1}\ldots\int_{\alpha_n}G^{(n+1)}_{c,\beta\alpha_1\ldots\alpha_n}J_{\alpha_1}\ldots J_{\alpha_n} \tag{49}$$

on the rhs and compare terms with the same powers of sources J_α on both sides.

- Symmetrization:
  - Assume that $G^{(n)}_{c,\alpha_1\ldots\alpha_n}$ (on lhs) and $\Gamma^{(n)}_{\alpha_1\ldots\alpha_n}$ are symmetrized with respect to label exchange. Need to symmetrize rhs.

– Symmetrization operator $\mathcal{S}$:
Consider function $F_{\alpha_1\ldots\alpha_n}$ of n superlabels $\alpha_1..\alpha_{n_1}|\alpha_{n_1+1}...\alpha_{n_1+n_2}|\alpha_{n_1+n_2+1}.....\alpha_n$, grouped into ν groups, $n_1+n_2...+n_\nu=n$ such that $F_{\alpha_1\ldots\alpha_n}$ is already properly symmetrized for exchange of labels *inside* groups.
We get a fully symmetric function from

$$\mathcal{S}_{\alpha_1\ldots\alpha_{n_1};\ldots;\alpha_{n-n_\nu+1}\ldots\alpha_n}\left(F_{\alpha_1\ldots\alpha_n}\right)=\frac{1}{n_1!\cdots n_\nu!}\sum_{P\in S_n}\mathrm{sgn}_\xi\left(P\right)F_{\alpha_{P(1)}\ldots\alpha_{P(n)}}\to n!/(n_1!...n_\nu!)\text{ distinct terms} \tag{50}$$

with $\mathrm{sgn}_\xi\left(P\right)$ defined as follows:

$$\bar{\Phi}_{\alpha_1}...\bar{\Phi}_{\alpha_n}=\mathrm{sgn}_\xi\left(P\right)\bar{\Phi}_{\alpha_{P(1)}}...\bar{\Phi}_{\alpha_{P(n)}}. \tag{51}$$

Example:
If $F_{\alpha_1\alpha_2}$ is not yet symmetrized, we have $\nu=2$ blocks with $n_{1,2}=1$ and $\mathcal{S}_{\alpha_1;\alpha_2}\left(F_{\alpha_1\alpha_2}\right)=F_{\alpha_1\alpha_2}+\mathrm{sgn}_\xi F_{\alpha_2\alpha_1}$.
If $F_{\alpha_1\alpha_2}$ is already symmetrized, we have $\nu=1$ block with $n_1=2$ and then $\mathcal{S}_{\alpha_1\alpha_2}\left(F_{\alpha_1\alpha_2}\right)=F_{\alpha_1\alpha_2}$.

- Full expression for $\mathbf{G}^{(n+2)}_{c,\alpha_1\ldots\alpha_n}$ including symmetrization $\mathcal{S}$ → Ex. 5.2.

Examples

- Case $n=1$ ($\mathbf{G}^{(3)}_c$): Only $\nu=1$, $n_1=1$: Need on rhs $\bar{\Phi}_{\beta_1^1}=\int_{\alpha_1}G^{(n+1)}_{c,\beta_1^1\alpha_1}J_{\alpha_1}+...$ and no symmetrization required

$$\begin{aligned}\mathbf{G}^{(3)}_{c,\alpha_1} &= -\int_{\beta_1^1}\mathbf{G}\cdot\mathbf{\Gamma}^{(3)}_{\beta_1^1}\cdot\mathbf{G}\cdot\mathbf{Z}G^{(2)}_{c,\beta_1^1\alpha_1}\\ &= -\int_{\beta_1}\mathbf{G}\cdot\mathbf{\Gamma}^{(3)}_{\beta_1}\cdot\mathbf{G}\cdot\mathbf{Z}\left[-\mathbf{G}_{\alpha_1\beta_1}\right]\end{aligned}$$

or, using $\mathbf{G}_c\to G_c$ on the left-hand side:

$$\begin{aligned}G^{(3)}_{c,\alpha_2\alpha_3\alpha_1} &= \int_{\beta_1}\left[\mathbf{G}\cdot\mathbf{\Gamma}^{(3)}_{\beta_1}\cdot\mathbf{G}\cdot\mathbf{Z}\right]_{\alpha_2\alpha_3}\mathbf{G}_{\alpha_1\beta_1}\\ &= \int_{\beta_{1,2,3}}\mathbf{G}_{\alpha_2\beta_2}\Gamma^{(3)}_{\beta_2\beta_3\beta_1}\mathbf{G}_{\beta_3\alpha_3}\mathbf{Z}_{\alpha_3\alpha_3}\mathbf{G}_{\alpha_1\beta_1}\end{aligned}$$

Re-label indices on the lhs and some integration variables:

$$\boxed{G^{(3)}_{c,\alpha_1\alpha_2\alpha_3}=\int_{\beta_1,\beta_2,\beta_3}\left[\mathbf{G}\right]_{\alpha_1\beta_1}\left[\mathbf{G}\right]_{\alpha_2\beta_2}\left[\mathbf{G}\right]_{\alpha_3\beta_3}\Gamma^{(3)}_{\beta_1\beta_2\beta_3}} \tag{52}$$

- Case $n=2$ ($\mathbf{G}^{(4)}_c$), assume that $\Gamma^{(3)}=0$ (i.e. fermionic theory): Take $\nu=1$, $n_1=2$, and $\bar{\Phi}_{\beta_1^1}=\int_{\alpha_1}G^{(2)}_{c,\beta_1^1\alpha_1}J_{\alpha_1}$, $\bar{\Phi}_{\beta_2^1}=\int_{\alpha_2}G^{(2)}_{c,\beta_2^1\alpha_2}J_{\alpha_2}$. Need symmetrization on rhs and drop superscript on β:

$$\mathbf{G}^{(4)}_{c,\alpha_1\alpha_2}=-\frac{1}{2}\int_{\beta_{1,2}}\mathbf{G}\mathbf{\Gamma}^{(4)}_{\beta_1\beta_2}\mathbf{G}\cdot\mathbf{Z}\mathcal{S}_{\alpha_1;\alpha_2}\left[G^{(2)}_{c,\beta_1\alpha_1}G^{(2)}_{c,\beta_2\alpha_2}\right] \tag{53}$$

and we insert the matrix structure

$$G^{(4)}_{c,\alpha_3\alpha_4\alpha_1\alpha_2}=-\frac{1}{2}\int_{\beta_{1,2,3,4}}\left[\mathbf{G}\right]_{\alpha_3\beta_3}\Gamma^{(4)}_{\beta_3\beta_4\beta_1\beta_2}\left[\mathbf{G}\right]_{\alpha_4\beta_4}\left[G^{(2)}_{c,\beta_1\alpha_1}G^{(2)}_{c,\beta_2\alpha_2}+\zeta G^{(2)}_{c,\beta_1\alpha_2}G^{(2)}_{c,\beta_2\alpha_1}\right] \tag{54}$$

We can treat the last term in the bracket by re-labeling $\beta_1\leftrightarrow\beta_2$ and then changing the order of these terms in $\Gamma^{(4)}$ back (factor ζ, $\zeta^2=1$). We finish with replacing $G^{(2)}_{c,\beta\alpha}=-\mathbf{G}_{\alpha\beta}$ and some ζ-independent index shuffles

$$\boxed{G^{(4)}_{c,\alpha_1\alpha_2\alpha_3\alpha_4}=-\int_{\beta_{1,2,3,4}}\left[\mathbf{G}\right]_{\alpha_1\beta_1}\left[\mathbf{G}\right]_{\alpha_2\beta_2}\left[\mathbf{G}\right]_{\alpha_3\beta_3}\left[\mathbf{G}\right]_{\alpha_4\beta_4}\Gamma^{(4)}_{\beta_1\beta_2\beta_3\beta_4}.} \tag{55}$$

This reproduces the term with the blue circle in Fig. 18.

- General case for $G^{(4)}_c$ including the 3-point vertices $\Gamma^{(3)}$ → Ex. 5.2.

Exercises

Exercise 5.1. Generating Functions for toy model

This exercise should familiarize you with the concept of generating function(al)s in a simple setting. Consider the classical field theory of an an-harmonic oscillator defined by the action $s(\varphi) = s_0(\varphi) + s_1(\varphi)$ where $\varphi \in \mathbb{R}$ is a single real variable and

$$s_0(\varphi) = -\frac{\varphi^2}{2G_0}, \qquad s_1(\varphi) = \frac{u}{4!}\varphi^4, \tag{56}$$

with $G_0 < 0$ and $u > 0$. The full partition function is given by $Z = \int_{-\infty}^{+\infty} d\varphi e^{-s(\varphi)}$ and the disconnected Green functions are $g^{(n)} = I_n/I_0$ with $I_n = \int_{-\infty}^{+\infty} d\varphi\, \varphi^n e^{-s(\varphi)}$ and $I_0 = Z$.

1. Show that the partition function in Gaussian approximation is given by $Z_0 = \sqrt{2\pi(-G_0)}$. Introduce a source $j \in \mathbb{R}$ and write down the definition of the generating functions (*instead of functionals!*)

   $$g_c(j),\ g_{ac}(\bar{\varphi}),\ \gamma(\bar{\varphi}), \tag{57}$$

   of the connected Green functions, amputated connected Green functions and irreducible vertices, respectively. The latter are denoted by $g_c^{(n)}, g_{ac}^{(n)}, \gamma^{(n)}$ and are related to the generating functions via series expansion, e.g. $g_c(j) = \sum_{n=0}^{\infty} \frac{1}{n!} g_c^{(n)} j^n$. The Legendre transform should be denoted by

   $$\begin{aligned} l(\varphi) &= j(\varphi)\varphi - g_c(j(\varphi)), \\ \varphi &= \partial_j g_c. \end{aligned}$$

   Show explicitly the two relations:

   $$\begin{aligned} g_{ac}(\bar{\varphi}) &= g_c\left(-G_0^{-1}\bar{\varphi}\right) + \bar{\varphi}^2/(2G_0), \\ 1 &= \left(\frac{\partial^2 l}{\partial \varphi^2}\right)\left(\frac{\partial^2 g_c}{\partial j^2}\right). \end{aligned}$$

2. Derive the following relations:

$g_c^{(0)} = \ln[Z/Z_0]$	$g_c^{(2)} = g^{(2)}$	$g_c^{(4)} = g^{(4)} - 3\left[g^{(2)}\right]^2$
$g_{ac}^{(0)} = g_c^{(0)}$	$g_{ac}^{(2)} = G_0^{-2}\left[g_c^{(2)} + G_0\right]$	$g_{ac}^{(4)} = G_0^{-4} g_c^{(4)}$
$l^{(0)} = -g_c^{(0)}$	$l^{(2)} = \left[g_c^{(2)}\right]^{-1}$	$l^{(4)} = -\left[g_c^{(2)}\right]^{-4} g_c^{(4)}$
$\gamma^{(0)} = l^{(0)}$	$\gamma^{(2)} = l^{(2)} + G_0^{-1}$	$\gamma^{(4)} = l^{(4)}$

3. Use the results of part 1.) and 2.) to calculate the irreducible vertices $\gamma^{(0,2,4)}$ perturbatively up to order u^2. First, find Z and $g^{(m)}$ for $m = 1, 2, 3, 4$ in perturbation theory up to order u^2. These results will be needed below in Ex. 7.1 to compare perturbation theory to the fRG for this toy model. You should obtain:

   $$\gamma^{(0)} = \frac{u}{8}G_0^2 - \frac{u^2}{12}G_0^4, \quad \gamma^{(2)} = -\frac{u}{2}G_0 + \frac{5u^2}{12}G_0^3, \quad \gamma^{(4)} = u - \frac{3u^2}{2}G_0^2. \tag{58}$$

Exercise 5.2. General form of tree expansion, full expression for $\Gamma^{(4)}$

1. In the lecture, we have stopped short of writing the complete form of the tree expansion which is free of source terms J_α and $\bar{\Phi}_\alpha$. You should now perform this task which involves somewhat tedious indexing.

Combine Eqns. (48), (49) and (50) to find

$$\begin{aligned}
\mathbf{G}^{(n+2)}_{c,\alpha_1\ldots\alpha_n} &= -\sum_{\nu=0}^{\infty}\sum_{n_1=1}^{\infty}\ldots\sum_{n_\nu=1}^{\infty}\frac{1}{n_1!\ldots n_\nu!}\int_{\beta_1^1}\ldots\int_{\beta_{n_1}^1}\ldots\int_{\beta_1^\nu}\ldots\int_{\beta_{n_\nu}^\nu} \\
&\quad \left(\sum_{m_1^1=1}^{\infty}\ldots\sum_{m_{n_1}^1=1}^{\infty}\right)\ldots\left(\sum_{m_1^\nu=1}^{\infty}\ldots\sum_{m_{n_\nu}^\nu=1}^{\infty}\right)\delta_{n,\sum_{i=1}^{\nu}\sum_{j=1}^{n_i}m_j^i} \\
&\quad \times\ \mathbf{G}\left\{\mathbf{\Gamma}^{(n_\nu+2)}_{\beta_1^\nu\ldots\beta_{n_\nu}^\nu}\mathbf{G}\right\}\ldots\left\{\mathbf{\Gamma}^{(n_1+2)}_{\beta_1^1\ldots\beta_{n_1}^1}\mathbf{G}\right\}\mathbf{Z} \\
&\quad \times\ \mathcal{S}_{\alpha_1\ldots\alpha_{m_1^1};\ldots;\alpha_{n-m_{n_\nu}^\nu+1}\ldots\alpha_n}\left\{G^{(m_1^1+1)}_{c,\beta_1^1\alpha_1\ldots\alpha_{m_1^1}}\ldots G^{(m_{n_\nu}^\nu+1)}_{c,\beta_{n_\nu}^\nu\alpha_n-m_{n_\nu}^\nu+1\ldots\alpha_n}\right\}
\end{aligned}$$

2. Use the above result to derive the complete form of the tree expansion for $G^{(4)}_{c,\alpha_1\alpha_2\alpha_3\alpha_4}$, including the 3-point vertex $\Gamma^{(3)}$ and draw the diagrammatic representation. In the lecture, we have derived the contribution including the four-point vertex $\Gamma^{(4)}$ which you can take from there.

6 Exact fRG flow equations for generating functionals

Aims:

- Implement RG idea in a formally *exact* way, on the level of correlation functions.
- Final goal: fRG flow equation for functional $\Gamma_\Lambda[\bar{\Phi}]$ (Wetterich equation)

6.1 Cutoff procedure

- Idea: Modify the Gaussian propagator

$$\begin{aligned}
\mathbf{G}_0 &\rightarrow \mathbf{G}_{0,\Lambda} \\
S_0[\Phi] &\rightarrow S_{0,\Lambda}[\Phi] = -\frac{1}{2}\left(\Phi, \left[\mathbf{G}_{0,\Lambda}\right]^{-1}\Phi\right)
\end{aligned}$$

- Λ is the boundary between high-energy and low-energy fluctuations.
- Requirements:

$$\mathbf{G}_{0,\Lambda} = \begin{cases}\mathbf{G}_0 & :\Lambda\to 0\\ \mathbf{0} & :\Lambda\to\infty\end{cases} \tag{59}$$

  - For vanishing cutoff ($\Lambda = 0$), recover the original theory.
  - For infinite cutoff ($\Lambda = \infty$), particles do not 'move' and all generating functional are simply known.

- Strategy / workflow:
  - Derive exact differential equations for generating functionals $\mathcal{G}_\Lambda[J], \mathcal{G}_{c,\Lambda}[J], \ldots$ etc. when Λ is varied (fRG flow equations).
  - Find initial conditions for generating functionals at $\Lambda = \infty$.
  - Devise approximation scheme for flow equation and solve [usually on a (super-)computer].
  - Extract physical results at $\Lambda = 0$.

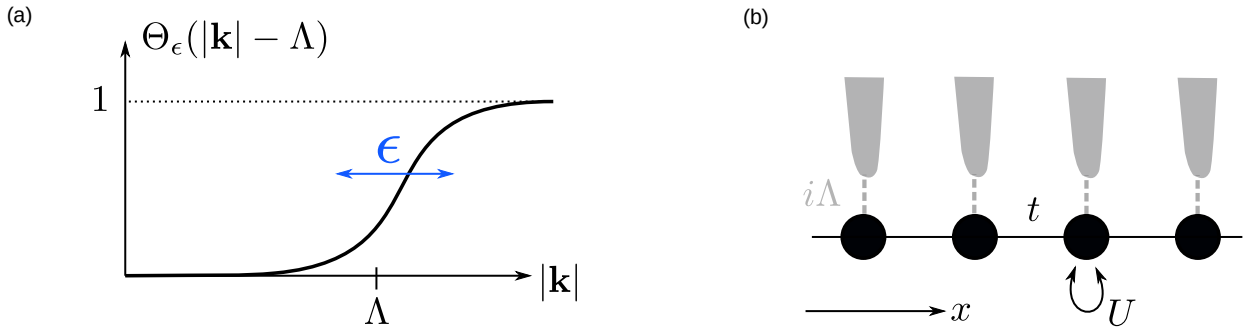


Figure 19: (a) Multiplicative cutoff in momentum space. (b) Sketch of a reservoir cutoff for a one-dimensional system.

Cutoff types and examples

- Multiplicative cutoff: $\mathbf{G}_{0,\Lambda} \equiv \mathbf{\Theta}_\Lambda \mathbf{G}_0$ with boundary condition $\mathbf{\Theta}_{\Lambda=0} = \mathbf{1}$ and $\mathbf{\Theta}_{\Lambda=\infty} = \mathbf{0}$.
- Additive cutoff (regulator): $\mathbf{G}_{0,\Lambda}^{-1} = \mathbf{G}_0^{-1} - \mathbf{R}_\Lambda$ with $|\mathbf{R}_{\Lambda=0}| = 0$ and $|\mathbf{R}_{\Lambda=\infty}| = \infty$.
- Examples:
  - For $\mathbf{G}_0$ diagonal in momentum, can chose $\mathbf{\Theta}_\Lambda = \theta_\epsilon(|\mathbf{k}| - \Lambda)$ where $\theta_\epsilon(x)$ is a step function broadened on a scale ϵ. As Λ lowers, this switches on smaller and smaller momentum modes iteratively, see Fig. 19(a).
  - For quantum systems, can use Matsubara cutoff: $\mathbf{\Theta}_\Lambda = \theta(|\omega_n| - \Lambda)$. This works also for $\mathbf{G}_0$ that are not diagonal in momentum (i.e. disordered systems).
  - Reservoir cutoff: $\mathbf{R}_\Lambda = i\Lambda$, $\mathbf{G}_{0,\Lambda} = \frac{1}{i\omega - H + i\mathrm{sgn}(\omega_n)\Lambda}$, couples a virtual reservoir to the system which is removed as $\Lambda \to 0$. See Fig. 19(b).
  - If $\mathbf{G}_0$ involves several field-types, one can chose different cutoffs for fermions and bosons.
  - Physical flows: Cutoff scheme can vary physical parameter like chemical potential, magnetic field, interaction strength or temperature.
    - Benefit: Each point along the flow corresponds to a physical system.
    - Problem: No RG-like mode elimination.

Morris Lemma

- fRG flow equations will involve Λ-derivative of cutoff function. For sharp cutoffs, $\partial_\Lambda \theta(|\mathbf{k}| - \Lambda) = -\delta(|\mathbf{k}| - \Lambda)$. Convenient: The δ-function cancels loop integrals.
- We might also encounter the ambiguous expression $\delta(x) f(\theta(x))$ where f is a well-behaved function. This is to be interpreted as ($\to$ Ex. 6.1):

$$\delta(x) f(\theta(x)) = \delta(x) \int_0^1 dt\, f(t) \tag{60}$$

Application: $\delta(x)\theta(x) = \delta(x)\frac{1}{2}$.

6.2 Flow of $\mathcal{G}_\Lambda[J]$ (disconnected Green functions)

- The Λ-dependence of all generating functionals arises only from $\mathbf{G}_{0,\Lambda}$.

- Λ-dependent generating functional for disconnected Green functions $\mathcal{G}_\Lambda$:

$$\begin{aligned}\mathcal{G}_\Lambda[J] &= \frac{1}{\mathcal{Z}_\Lambda}\int \mathcal{D}[\Phi]\, e^{-S_{0,\Lambda}[\Phi]-S_1[\Phi]+(J,\Phi)} \\ \mathcal{Z}_\Lambda &= \int \mathcal{D}[\Phi]\, e^{-S_{0,\Lambda}[\Phi]-S_1[\Phi]}\end{aligned}$$

- Differentiate with respect to Λ:

$$\begin{aligned}\partial_\Lambda \mathcal{G}_\Lambda[J] &= \frac{1}{\mathcal{Z}_\Lambda}\int \mathcal{D}[\Phi]\, \frac{1}{2}\underbrace{\left(\Phi, \partial_\Lambda\left[\mathbf{G}_{0,\Lambda}\right]^{-1}\Phi\right)}_{\to\left(\frac{\delta}{\delta J},\left[\partial_\Lambda \mathbf{G}_{0,\Lambda}^{-1}\right]\frac{\delta}{\delta J}\right)} e^{-S_{0,\Lambda}[\Phi]-S_1[\Phi]+(J,\Phi)} - \left(\frac{\partial_\Lambda \mathcal{Z}_\Lambda}{\mathcal{Z}_\Lambda}\right)\mathcal{G}_\Lambda[J] \\ &= \frac{1}{2}\left(\frac{\delta}{\delta J},\left[\partial_\Lambda \mathbf{G}_{0,\Lambda}^{-1}\right]\frac{\delta}{\delta J}\right)\mathcal{G}_\Lambda[J] - \left(\partial_\Lambda \ln \mathcal{Z}_\Lambda\right)\mathcal{G}_\Lambda[J]\end{aligned}$$

- Final result:

$$\partial_\Lambda \mathcal{G}_\Lambda[J] = \frac{1}{2}\mathrm{Tr}\left\{\left[\partial_\Lambda \mathbf{G}_{0,\Lambda}^{-1}\right]\left(\frac{\delta}{\delta J}\otimes\frac{\delta}{\delta J}\mathcal{G}_\Lambda\right)^T\right\} - \left(\partial_\Lambda \ln \mathcal{Z}_\Lambda\right)\mathcal{G}_\Lambda[J]\,. \tag{61}$$

6.3 Flow of $\mathcal{G}_{c,\Lambda}[J]$ (connected Green functions)

- Use definition

$$\mathcal{G}_\Lambda[J] = \frac{\mathcal{Z}_{0,\Lambda}}{\mathcal{Z}_\Lambda} e^{\mathcal{G}_{c,\Lambda}[J]}, \tag{62}$$

take ∂_Λ on both sides,

$$\partial_\Lambda \mathcal{G}_\Lambda = \frac{\mathcal{Z}_{0,\Lambda}}{\mathcal{Z}_\Lambda} e^{\mathcal{G}_{c,\Lambda}[J]}\left[\partial_\Lambda \mathcal{G}_{c,\Lambda} + \partial_\Lambda \ln\left(\frac{\mathcal{Z}_{0,\Lambda}}{\mathcal{Z}_\Lambda}\right)\right] \tag{63}$$

- Solve for $\partial_\Lambda \mathcal{G}_{c,\Lambda}$:

$$\partial_\Lambda \mathcal{G}_{c,\Lambda} = \left(\partial_\Lambda \mathcal{G}_\Lambda\right)\frac{\mathcal{Z}_\Lambda}{\mathcal{Z}_{0,\Lambda}} e^{-\mathcal{G}_{c,\Lambda}[J]} - \partial_\Lambda \ln\left(\frac{\mathcal{Z}_{0,\Lambda}}{\mathcal{Z}_\Lambda}\right) \tag{64}$$

- For $(\partial_\Lambda \mathcal{G}_\Lambda)$, use (61) and re-express all $\mathcal{G}_\Lambda[J]$ by $\mathcal{G}_{c,\Lambda}[J]$: After a straightforward calculation, we obtain

$$\partial_\Lambda \mathcal{G}_{c,\Lambda}[J] = \frac{1}{2}\left(\frac{\delta \mathcal{G}_{c,\Lambda}}{\delta J},\left[\partial_\Lambda \mathbf{G}_{0,\Lambda}^{-1}\right]\frac{\delta \mathcal{G}_{c,\Lambda}}{\delta J}\right) + \frac{1}{2}\mathrm{Tr}\left\{\left[\partial_\Lambda \mathbf{G}_{0,\Lambda}^{-1}\right]^T\left(\frac{\delta}{\delta J}\otimes\frac{\delta}{\delta J}\mathcal{G}_{c,\Lambda}\right)\right\} - \partial_\Lambda \ln\left(\mathcal{Z}_{0,\Lambda}\right) \tag{65}$$

- Initial condition: We saw from Eq. (22) that $\mathcal{G}_{c,\Lambda\to\infty}[J] = 0$.
  This is not convenient, since this initial condition does not contain any information about the system. All physical information has to be generated along the flow. It is better to have an initial condition that corresponds to simple and sensible physical limit.

- Graphical representation (after expansion in correlation functions): Fig. 20, recall $G^{(n)}_{\alpha_1\ldots\alpha_n} = \frac{\delta^n \mathcal{G}[J]}{\delta J_{\alpha_n}\ldots\delta J_{\alpha_1}}|_{J=0}$ and the arrow in the circle points to α_1. The $\partial_\Lambda G^{(n)}$ depends on $G^{(n+1)}$ and $G^{(n+2)}$.

6.4 Flow of $\mathcal{G}_{ac,\Lambda}\left[\bar{\Phi}\right]$ (amputated connected Green functions) - Polchinski Equation

- Initial condition: Recall Eq. (26),

$$e^{\mathcal{G}_{ac}\left[\bar{\Phi}\right]} = e^{-\frac{1}{2}\left(\frac{\delta}{\delta\bar{\Phi}},\mathbf{G}_0^T\frac{\delta}{\delta\bar{\Phi}}\right)} e^{-S_1\left[\bar{\Phi}\right]} \tag{66}$$

and find

$$\lim_{\Lambda\to\infty}\mathcal{G}_{ac,\Lambda}\left[\bar{\Phi}\right] = -S_1\left[\bar{\Phi}\right] \tag{67}$$

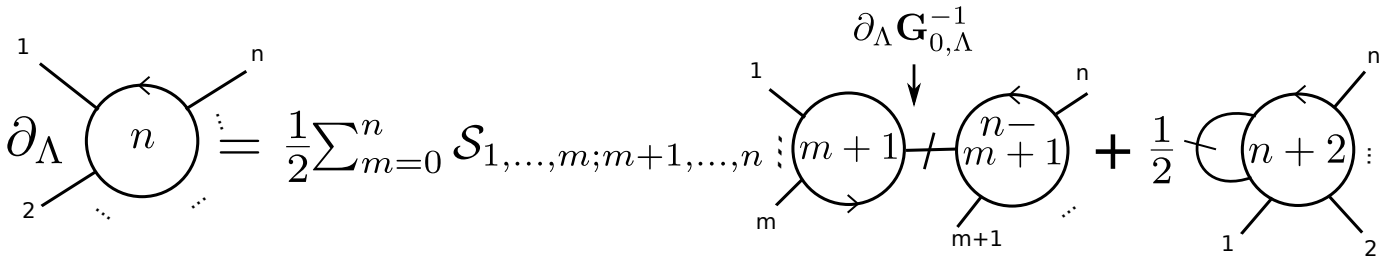


Figure 20: Graphical representation of the flow equation (65) expanded in correlators.

- Flow equation follows from differentiating Eq. (66):

$$\begin{aligned} e^{\mathcal{G}_{ac,\Lambda}}\partial_\Lambda \mathcal{G}_{ac,\Lambda} &= \partial_\Lambda e^{\mathcal{G}_{ac,\Lambda}} \\ &= -\frac{1}{2}\left(\frac{\delta}{\delta\bar{\Phi}}, \left[\partial_\Lambda \mathbf{G}_{0,\Lambda}^T\right]\frac{\delta}{\delta\bar{\Phi}}\right)\underbrace{e^{-\frac{1}{2}\left(\frac{\delta}{\delta\bar{\Phi}}, \mathbf{G}_{0,\Lambda}^T\frac{\delta}{\delta\bar{\Phi}}\right)}e^{-S_1\left[\bar{\Phi}\right]}}_{e^{\mathcal{G}_{ac,\Lambda}}} \\ &= e^{\mathcal{G}_{ac,\Lambda}}\left[-\frac{1}{2}\left(\frac{\delta\mathcal{G}_{ac,\Lambda}}{\delta\bar{\Phi}}, \left[\partial_\Lambda \mathbf{G}_{0,\Lambda}^T\right]\frac{\delta\mathcal{G}_{ac,\Lambda}}{\delta\bar{\Phi}}\right) - \frac{1}{2}\left(\frac{\delta}{\delta\bar{\Phi}}, \left[\partial_\Lambda \mathbf{G}_{0,\Lambda}^T\right]\frac{\delta}{\delta\bar{\Phi}}\right)\mathcal{G}_{ac,\Lambda}\right] \end{aligned}$$

- Compare both sides and find the **Polchinski Equation**, (Polchinski, 1984):

$$\partial_\Lambda \mathcal{G}_{ac,\Lambda} = -\frac{1}{2}\left(\frac{\delta\mathcal{G}_{ac,\Lambda}}{\delta\bar{\Phi}}, \left[\partial_\Lambda \mathbf{G}_{0,\Lambda}^T\right]\frac{\delta\mathcal{G}_{ac,\Lambda}}{\delta\bar{\Phi}}\right) - \frac{1}{2}\mathrm{Tr}\left(\left[\partial_\Lambda \mathbf{G}_{0,\Lambda}^T\right]\left(\frac{\delta}{\delta\bar{\Phi}}\otimes\frac{\delta}{\delta\bar{\Phi}}\mathcal{G}_{ac,\Lambda}\right)^T\right) \tag{68}$$

- Problem: If we expand both sides in correlation functions $G_{ac,\Lambda}$ and use a sharp cutoff, the first term contains δ-function that is not integrated over (no loops, c.f. Fig. 20!).

6.5 Flow of $\Gamma\left[\bar{\Phi}\right]$ (irreducible vertices) - Wetterich Equation

- Augment definition of $\Gamma\left[\bar{\Phi}\right]$ with subscript Λ:

$$\begin{aligned} \Gamma_\Lambda\left[\bar{\Phi}\right] &= \left(J_\Lambda\left[\bar{\Phi}\right], \bar{\Phi}\right) - \mathcal{G}_{c,\Lambda}\left[J_\Lambda\left[\bar{\Phi}\right]\right] + \frac{1}{2}\left(\bar{\Phi}, \left[\mathbf{G}_{0,\Lambda}\right]^{-1}\bar{\Phi}\right) \\ \bar{\Phi} &= \frac{\delta\mathcal{G}_{c,\Lambda}\left[J\right]}{\delta J} \end{aligned} \tag{69}$$

- The arguments $\bar{\Phi}$ do not depend on Λ, but the second equation enforces Λ-dependent $J_\Lambda\left[\bar{\Phi}\right]$.

Initial condition

- We have a simple initial condition:

$$\boxed{\lim_{\Lambda\to\infty}\Gamma_\Lambda\left[\bar{\Phi}\right] = -\lim_{\Lambda\to\infty}\mathcal{G}_{ac,\Lambda}\left[\bar{\Phi}\right] = S_1\left[\bar{\Phi}\right]} \tag{70}$$

- Proof: Start from relation between $\mathcal{G}_c$ and $\mathcal{G}_{ac}$, Eq. (25)

$$\mathcal{G}_{ac,\Lambda}\left[\bar{\Phi}\right] = \mathcal{G}_{c,\Lambda}[\underbrace{-\left(\mathbf{G}_{0,\Lambda}^T\right)^{-1}\bar{\Phi}}_{\equiv J\left[\bar{\Phi}\right]}] + \frac{1}{2}\left(\bar{\Phi}, \mathbf{G}_{0,\Lambda}^{-1}\bar{\Phi}\right) \tag{71}$$

To connect the rhs to Γ, we prepare for the use of the Legendre transform with respect to the $J\left[\bar{\Phi}\right]$:

$$\begin{aligned}
\bar{\Phi}'_\alpha &\equiv \frac{\delta \mathcal{G}_{c,\Lambda}\left[J\right]}{\delta J_\alpha} \\
&= \int_\beta \frac{\delta \bar{\Phi}_\beta}{\delta J_\alpha} \frac{\delta \mathcal{G}_{c,\Lambda}\left[J\right]}{\delta \bar{\Phi}_\beta} \\
&= -\int_\beta \left[\mathbf{G}_{0,\Lambda}^T\right]_{\beta\alpha} \frac{\delta}{\delta \bar{\Phi}_\beta} \left(\mathcal{G}_{ac,\Lambda}\left[\bar{\Phi}\right] - \frac{1}{2}\left(\bar{\Phi}, \left(\mathbf{G}_{0,\Lambda}\right)^{-1}\bar{\Phi}\right)\right) \\
\bar{\Phi}' &= -\mathbf{G}_{0,\Lambda} \frac{\delta \mathcal{G}_{ac,\Lambda}\left[\bar{\Phi}\right]}{\delta \bar{\Phi}} + \bar{\Phi}
\end{aligned}$$

- We write the Legendre transform $\mathcal{G}_{c,\Lambda}\left[J\right] \leftrightarrow \Gamma_\Lambda\left[\bar{\Phi}'\right]$,

$$\mathcal{G}_{c,\Lambda}\left[J\left[\bar{\Phi}'\right]\right] = \left(J\left[\bar{\Phi}'\right], \bar{\Phi}'\right) - \Gamma_\Lambda\left[\bar{\Phi}'\right] + \frac{1}{2}\left(\bar{\Phi}', \left[\mathbf{G}_{0,\Lambda}\right]^{-1}\bar{\Phi}'\right), \tag{72}$$

  and add $\frac{1}{2}\left(\bar{\Phi}, \mathbf{G}_{0,\Lambda}^{-1}\bar{\Phi}\right)$ to find with Eq. (71),

$$\mathcal{G}_{ac,\Lambda}\left[\bar{\Phi}\right] = \left(J, \bar{\Phi}'\right) - \Gamma_\Lambda\left[\bar{\Phi}'\right] + \frac{1}{2}\left(\bar{\Phi}', \mathbf{G}_{0,\Lambda}^{-1}\bar{\Phi}'\right) + \frac{1}{2}\left(\bar{\Phi}, \mathbf{G}_{0,\Lambda}^{-1}\bar{\Phi}\right).$$

- Insert the prepared $\bar{\Phi}'$ to express the right-hand side in $\bar{\Phi}$. After a short calculation, we obtain

$$\mathcal{G}_{ac,\Lambda}\left[\bar{\Phi}\right] = -\Gamma_\Lambda\left[\bar{\Phi} - \mathbf{G}_{0,\Lambda}\frac{\delta \mathcal{G}_{ac,\Lambda}}{\delta \bar{\Phi}}\right] + \frac{1}{2}\left(\frac{\delta \mathcal{G}_{ac,\Lambda}}{\delta \bar{\Phi}}, \mathbf{G}_{0,\Lambda}^T \frac{\delta \mathcal{G}_{ac,\Lambda}}{\delta \bar{\Phi}}\right) \tag{73}$$

  from which the claim follows as $\lim_{\Lambda\to\infty} \mathbf{G}_{0,\Lambda} = 0$.

Flow of $\Gamma_\Lambda\left[\bar{\Phi}\right]$

- The flow for $\Gamma_\Lambda\left[\bar{\Phi}\right]$ follows by taking ∂_Λ of the defining equation (69):

$$\begin{aligned}
\partial_\Lambda \Gamma_\Lambda\left[\bar{\Phi}\right] &= \left(\partial_\Lambda J_\Lambda\left[\bar{\Phi}\right], \bar{\Phi}\right) - \partial_\Lambda\left(\mathcal{G}_{c,\Lambda}\left[J_\Lambda\left[\bar{\Phi}\right]\right]\right) + \frac{1}{2}\left(\bar{\Phi}, \partial_\Lambda\left[\mathbf{G}_{0,\Lambda}\right]^{-1}\bar{\Phi}\right) \\
&= \left(\partial_\Lambda J_\Lambda\left[\bar{\Phi}\right], \bar{\Phi}\right) - (\partial_\Lambda J_\Lambda, \underbrace{\frac{\delta \mathcal{G}_{c,\Lambda}\left[J\right]}{\delta J}}_{\bar{\Phi}}) - \partial_\Lambda \mathcal{G}_{c,\Lambda}\left[J\right]|_{J=J_\Lambda[\bar{\Phi}]} + \frac{1}{2}\left(\bar{\Phi}, \partial_\Lambda\left[\mathbf{G}_{0,\Lambda}\right]^{-1}\bar{\Phi}\right)
\end{aligned}$$

  The first two terms cancel. For the third term we use the flow of the connected functional Eq. (65).

$$\begin{aligned}
\partial_\Lambda \Gamma_\Lambda\left[\bar{\Phi}\right] &= -\frac{1}{2}\left(\frac{\delta \mathcal{G}_{c,\Lambda}}{\delta J}, \left[\partial_\Lambda \mathbf{G}_{0,\Lambda}^{-1}\right]\frac{\delta \mathcal{G}_{c,\Lambda}}{\delta J}\right) - \frac{1}{2}\mathrm{Tr}\left\{\left[\partial_\Lambda \mathbf{G}_{0,\Lambda}^{-1}\right]^T\left(\frac{\delta}{\delta J}\otimes\frac{\delta}{\delta J}\mathcal{G}_{c,\Lambda}\right)\right\} + \partial_\Lambda \ln\left(\mathcal{Z}_{0,\Lambda}\right) \\
&\quad + \frac{1}{2}\left(\bar{\Phi}, \partial_\Lambda {\mathbf{G}_{0,\Lambda}}^{-1}\bar{\Phi}\right)
\end{aligned}$$

  and the brown terms cancel.

- We recall the relation (41) between second functional derivatives of $\mathcal{G}_{c,\Lambda}$, $\mathcal{L}_\Lambda$ and Γ_Λ:

$$\left(\frac{\delta}{\delta J}\otimes\frac{\delta}{\delta J}\mathcal{G}_{c,\Lambda}\right) = \left(\frac{\delta}{\delta \bar{\Phi}}\otimes\frac{\delta}{\delta \bar{\Phi}}\mathcal{L}_\Lambda\left[\bar{\Phi}\right]\right)^{-1} = \left(\frac{\delta}{\delta \bar{\Phi}}\otimes\frac{\delta}{\delta \bar{\Phi}}\Gamma_\Lambda\left[\bar{\Phi}\right] - \left[\mathbf{G}_{0,\Lambda}^T\right]^{-1}\right)^{-1} \tag{74}$$

  and find the exact **Wetterich Equation** (Wetterich, 1993)

$$\boxed{\partial_\Lambda \Gamma_\Lambda\left[\bar{\Phi}\right] = -\frac{1}{2}\mathrm{Tr}\left\{\underbrace{\left[\partial_\Lambda \mathbf{G}_{0,\Lambda}^{-1}\right]}_{-\partial_\Lambda \mathbf{R}_\Lambda}\left(\frac{\delta}{\delta \bar{\Phi}}\otimes\frac{\delta}{\delta \bar{\Phi}}\Gamma_\Lambda\left[\bar{\Phi}\right] - \left[\mathbf{G}_{0,\Lambda}^T\right]^{-1}\right)^{-1}\right\} + \partial_\Lambda \ln\left(\mathcal{Z}_{0,\Lambda}\right)} \tag{75}$$

- Two strategies for approximate solution of Wetterich equation:

  1. Vertex expansion (Sec. 7): Expand both sides in powers of fields $\bar{\Phi}$ and find flow equation for vertices $\Gamma^{(n)}_{\alpha_1 \ldots \alpha_n}$. This is similar to the considerations leading to Fig. 20, but complicated due to the inverse, which together with the trace produces non-trivial loops.
  2. Derivative expansion (Sec. 8): Make ansatz $\Gamma_\Lambda\left[\bar{\Phi}\right] = \int_{\mathbf{r}} U_\Lambda(\rho) + \mathcal{O}(\left[\nabla\bar{\Phi}\right]^2)$ with $\rho = \bar{\Phi}^2$ a scalar. The arbitrary functions $U_\Lambda(\rho)$ fulfill flow equations $\partial_\Lambda U_\Lambda(\rho) = f\left(\Lambda, U_\Lambda^{(\prime,\prime\prime,\ldots)}(\rho), \rho, \ldots\right)$.

Exercises

Exercise 6.1. Morris Lemma

Prove the Morris Lemma (60) by regularizing the unit-step function $\theta(x)$ and Dirac-Delta function $\delta(x)$ by their smooth counterparts $\partial_x \theta_\varepsilon(x) = \delta_\varepsilon(x)$ varying over a scale ε and consider the limiting procedure $\lim_{\varepsilon \to 0}$.

7 Vertex expansion

Aims:

- Strategy 1. to approximately solve exact Wetterich equation
- Expand generating functional $\Gamma_\Lambda\left[\bar{\Phi}\right]$ in vertices $\Gamma^{(n)}_\Lambda$, write flow equations $\partial_\Lambda \Gamma^{(n)}_\Lambda = f\left(\{\Gamma^{(m)}_\Lambda\}_{m \leq n+2}\right)$
- Approximation: Truncation of hierarchy.
- Keep track of momentum- and frequency-dependence of $\Gamma^{(n)}_\Lambda$.
- Quantitative results beyond critical exponents, but usually requires (super-)computers

7.1 Preparations

- Preparation I: From the section on tree expansion, recall Eq. (46). Augment all quantities with subscript Λ:

$$\frac{\delta}{\delta\bar{\Phi}} \otimes \frac{\delta}{\delta\bar{\Phi}} \Gamma_\Lambda\left[\bar{\Phi}\right] - \left[\mathbf{G}^{\mathrm{T}}_{0,\Lambda}\right]^{-1} = \mathbf{U}^{\mathrm{T}}_\Lambda\left[\bar{\Phi}\right] - \left[\mathbf{G}^{\mathrm{T}}_\Lambda\right]^{-1} \tag{76}$$

$$\mathbf{U}_\Lambda\left[\bar{\Phi}\right] = \sum_{n=1}^{\infty} \frac{1}{n!} \int_{\alpha_1 \ldots \alpha_n} \mathbf{\Gamma}^{(n+2)}_{\Lambda, \alpha_1 \ldots \alpha_n} \bar{\Phi}_{\alpha_1} \ldots \bar{\Phi}_{\alpha_n} \tag{77}$$

  The Dyson equation is required to hold for each Λ:

$$[\mathbf{G}_\Lambda]^{-1} = [\mathbf{G}_{0,\Lambda}]^{-1} - \mathbf{\Sigma}_\Lambda \tag{78}$$

- Preparation II: Use $\det A = \exp(\mathrm{tr}[\log A])$ and find

$$\mathcal{Z}_{0,\Lambda} = \int \mathcal{D}[\Phi]\, e^{\frac{1}{2}\Phi_\alpha \left[\mathbf{G}^{-1}_{0,\Lambda}\right]_{\alpha\beta} \Phi_\beta} \propto e^{-\frac{1}{2} Tr\left[\mathbf{Z} ln(-\mathbf{G}^{-1}_{0,\Lambda})\right]} \tag{79}$$

  so that

$$\partial_\Lambda \ln(\mathcal{Z}_{0,\Lambda}) = -\frac{1}{2} \mathrm{Tr}[\underbrace{\mathbf{Z}\mathbf{G}_{0,\Lambda}}_{\mathbf{G}^T_{0,\Lambda}} \left(\partial_\Lambda \mathbf{G}^{-1}_{0,\Lambda}\right)] \tag{80}$$

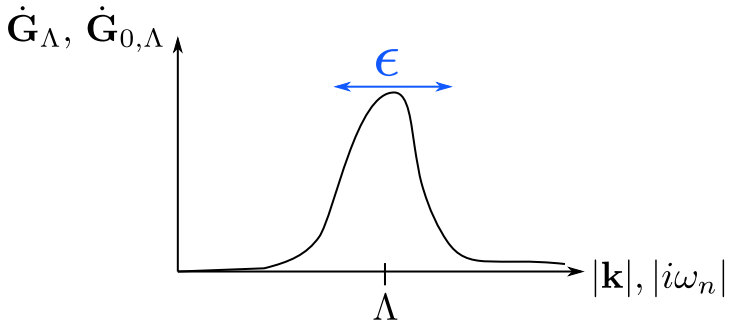


Figure 21: Sketch of the single scale propagator for a multiplicative cutoff in momentum or Matsubara frequency.

- Substitute preparations in Eq. (75) and get

$$\partial_\Lambda \Gamma_\Lambda \left[\bar{\Phi}\right] = -\frac{1}{2}\mathrm{Tr}\left(\left[\partial_\Lambda \mathbf{G}_{0,\Lambda}^{-1}\right]\left\{\left(\mathbf{U}_\Lambda^T\left[\bar{\Phi}\right] - \left[\mathbf{G}_\Lambda^T\right]^{-1}\right)^{-1} + \mathbf{G}_{0,\Lambda}^T\right\}\right) \tag{81}$$

  The term $\{...\}$ can be rewritten as

$$\{...\} = -\mathbf{G}_\Lambda^T\mathbf{U}_\Lambda^T\frac{1}{\mathbf{1}-\mathbf{G}_\Lambda^T\mathbf{U}_\Lambda^T}\mathbf{G}_\Lambda^T - \mathbf{G}_{0,\Lambda}^T\mathbf{\Sigma}_\Lambda^T\frac{1}{\mathbf{1}-\mathbf{G}_{0,\Lambda}^T\mathbf{\Sigma}_\Lambda^T}\mathbf{G}_{0,\Lambda}^T \tag{82}$$

  and we expand the first inverse:

$$\partial_\Lambda \Gamma_\Lambda \left[\bar{\Phi}\right] = -\frac{1}{2}\mathrm{Tr}\left(\dot{\mathbf{G}}_\Lambda\mathbf{U}_\Lambda^T\left[\bar{\Phi}\right]\sum_{\nu=0}^{\infty}\left(\mathbf{G}_\Lambda^T\mathbf{U}_\Lambda^T\left[\bar{\Phi}\right]\right)^\nu + \dot{\mathbf{G}}_{0,\Lambda}\mathbf{\Sigma}_\Lambda^T\frac{1}{\mathbf{1}-\mathbf{G}_{0,\Lambda}^T\mathbf{\Sigma}_\Lambda^T}\right) \tag{83}$$

- In the last equation, we defined the *single-scale propagator,*

$$\dot{\mathbf{G}}_\Lambda \equiv -\mathbf{G}_\Lambda\left[\partial_\Lambda \mathbf{G}_{0,\Lambda}^{-1}\right]\mathbf{G}_\Lambda \overset{\text{Ex.}}{=} \frac{1}{1-\mathbf{G}_{0,\Lambda}\mathbf{\Sigma}_\Lambda}\left[\partial_\Lambda \mathbf{G}_{0,\Lambda}\right]\frac{1}{1-\mathbf{\Sigma}_\Lambda\mathbf{G}_{0,\Lambda}}. \tag{84}$$

  Note that $\dot{\mathbf{G}}_\Lambda \neq \partial_\Lambda \mathbf{G}_\Lambda$, unless for the non-interacting version,

$$\dot{\mathbf{G}}_{0,\Lambda} \equiv -\mathbf{G}_{0,\Lambda}\left[\partial_\Lambda \mathbf{G}_{0,\Lambda}^{-1}\right]\mathbf{G}_{0,\Lambda} = \partial_\Lambda \mathbf{G}_{0,\Lambda}. \tag{85}$$

  For RG-type cutoffs the single-scale propagator has support only close to the (momentum-, frequency-) scale Λ, see Fig. 21.

7.2 Expansion of $\partial_\Lambda \Gamma_\Lambda\left[\bar{\Phi}\right]$ in fields

- Expansion of Eq. (83) in powers of fields: For lhs use,

$$\partial_\Lambda \Gamma_\Lambda\left[\bar{\Phi}\right] = \sum_{n=0}^{\infty}\frac{1}{n!}\int_{\alpha_1\ldots\alpha_n}\partial_\Lambda \Gamma^{(n)}_{\Lambda,\alpha_1\ldots\alpha_n}\bar{\Phi}_{\alpha_1}\ldots\bar{\Phi}_{\alpha_n}, \tag{86}$$

  for rhs use Eq. (77).

- Field independent term $\partial_\Lambda \Gamma_\Lambda^{(0)}$ (second term in the trace): After some small modifications using the cyclic nature of the trace, we have

$$\partial_\Lambda \Gamma_\Lambda^{(0)} = -\frac{1}{2}\mathrm{Tr}\left(\mathbf{Z}\dot{\mathbf{G}}_{0,\Lambda}\mathbf{\Sigma}_\Lambda\frac{1}{1-\mathbf{G}_{0,\Lambda}\mathbf{\Sigma}_\Lambda}\right) \tag{87}$$

  Interpretation: This yields the flow of the interaction-correction to the free energy $F = -T\log\mathcal{Z}$ (up to factor T):

$$F - F_0 = -T\log\left(\mathcal{Z}/\mathcal{Z}_0\right) = -TG_c^{(0)} = T\Gamma^{(0)} \rightarrow \text{link to thermodynamics} \tag{88}$$

- Field-dependent terms $\partial_\Lambda \Gamma^{(n\geq 1)}_{\Lambda,\alpha_1\ldots\alpha_n}$ (first term in the trace): Derivation similar to tree expansion, but simplified by absence of J-sourcefields. Pick the coefficient of $\bar{\Phi}_{\alpha_1}\bar{\Phi}_{\alpha_2}\ldots\bar{\Phi}_{\alpha_n}$ on both sides:

$$\frac{1}{n!}\partial_\Lambda \Gamma^{(n)}_{\Lambda,\alpha_1\ldots\alpha_n} = \\ -\frac{1}{2}\sum_{\nu=1}^{\infty}\sum_{n_{1,2,..,\nu}=1}^{\infty}\frac{\delta_{n,n_1+\ldots+n_\nu}}{n_1!n_2!\ldots n_\nu!}\mathrm{Tr}\left(\dot{\mathbf{G}}_\Lambda \mathbf{\Gamma}^{T(n_1+2)}_{\Lambda,\alpha_1\ldots\alpha_{n_1}}\left[\mathbf{G}^T_\Lambda \mathbf{\Gamma}^{T(n_2+2)}_{\Lambda,\alpha_{n_1+1}\ldots\alpha_{n_2}}\right]\cdots\left[\mathbf{G}^T_\Lambda \mathbf{\Gamma}^{T(n_\nu+2)}_{\Lambda,\alpha_{n-n_\nu+1}\ldots\alpha_n}\right]\right)$$

- We also could have picked a different order of the fields. Sum over all $n!$ permutations of the labels $\alpha_1\ldots\alpha_n$, this leaves $\partial_\Lambda \Gamma^{(n)}_{\Lambda,\alpha_1\ldots\alpha_n}$ on the left and brings the symmetrization operator $\mathcal{S}$ on the right. Also use $\mathrm{Tr}\left(\mathbf{A}^T\right) = \mathrm{Tr}\left(\mathbf{A}\right)$.

$$\partial_\Lambda \Gamma^{(n)}_{\Lambda,\alpha_1\ldots\alpha_n} = -\frac{1}{2}\sum_{\nu=1}^{\infty}\sum_{n_{1,2,..,\nu}=1}^{\infty}\delta_{n,n_1+\ldots+n_\nu}\mathcal{S}_{\alpha_1\ldots\alpha_{n_1};\ldots;\alpha_{n-n_\nu+1}\ldots\alpha_n} \\ \times\mathrm{Tr}\left(\mathbf{Z}\dot{\mathbf{G}}_\Lambda \mathbf{\Gamma}^{(n_\nu+2)}_{\Lambda,\alpha_{n-n_\nu+1}\ldots\alpha_n}\ldots\mathbf{G}_\Lambda \mathbf{\Gamma}^{(n_2+2)}_{\Lambda,\alpha_{n_1+1}\ldots\alpha_{n_2}}\mathbf{G}_\Lambda \mathbf{\Gamma}^{(n_1+2)}_{\Lambda,\alpha_1\ldots\alpha_{n_1}}\right)$$

7.3 Example: Flow of vertices with even number of legs

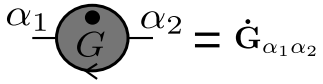
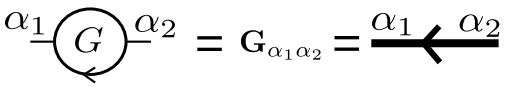
- Assume all vertices with odd number of external legs vanish (e.g. fermionic theory or ϕ^4-theory for $T > T_c$).
- For $n = 2$, have $\nu = 1$ and $n_1 = 2$ ($\nu = 2$ and $n_{1,2} = 1$ would involve $\Gamma^{(3)}$) so that

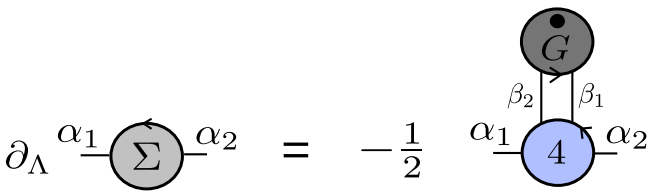
$$\partial_\Lambda \Gamma^{(2)}_{\Lambda,\alpha_1\alpha_2} = \partial_\Lambda\left[\mathbf{\Sigma}_\Lambda\right]_{\alpha_1\alpha_2} = -\frac{1}{2}\mathrm{Tr}\left(\mathbf{Z}\dot{\mathbf{G}}_\Lambda \mathbf{\Gamma}^{(4)}_{\Lambda,\alpha_1\alpha_2}\right) = -\frac{1}{2}\left[\dot{\mathbf{G}}_\Lambda\right]_{\beta_1\beta_2}\Gamma^{(4)}_{\Lambda,\beta_1\beta_2\alpha_1\alpha_2} \tag{89}$$

- For $n = 4$ (effective interaction) we have either $\nu = 1$ ($n_1 = 4$) or $\nu = 2$ ($n_{1,2} = 2$)

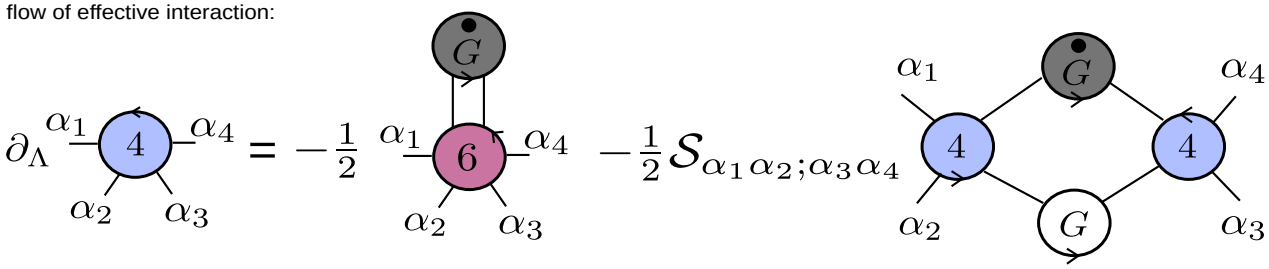
$$\partial_\Lambda \Gamma^{(4)}_{\Lambda,\alpha_1\ldots\alpha_4} = -\frac{1}{2}\mathrm{Tr}\left(\mathbf{Z}\dot{\mathbf{G}}_\Lambda \mathbf{\Gamma}^{(6)}_{\Lambda,\alpha_1\alpha_2\alpha_3\alpha_4} + \mathcal{S}_{\alpha_1\alpha_2;\alpha_3\alpha_4}\left\{\mathbf{Z}\dot{\mathbf{G}}_\Lambda \mathbf{\Gamma}^{(4)}_{\Lambda,\alpha_3\alpha_4}\mathbf{G}_\Lambda \mathbf{\Gamma}^{(4)}_{\Lambda,\alpha_1\alpha_2}\right\}\right)$$

- The $n = 6$ vertex is usually approximated with its initial value (however: Katanin- or 2-loop or multi-loop schemes).

single-scale propagator:  $= \dot{\mathbf{G}}_{\alpha_1\alpha_2}$ full propagator: 

flow of self energy: 

All quantities depend on Λ ! (skipped in diagrammatic notation)

flow of effective interaction: 

7.4 Application: Vertex expansion for φ^4-theory, relation to Wilsonian RG

Aims:

- See vertex expansion at work for non-trivial stat.-mech. field theory
- Recover RG flow equations found for in Wilsonian momentum-shell RG

Preparations

- Single type of bosonic field with momentum index, $\Phi_\alpha \to \varphi_{\mathbf{k}}$, $\zeta = +1$.
- Stay in the disordered phase, zero magnetic field $\to \langle \varphi_{\mathbf{k}=0} \rangle = 0$. For generalization to ordered phase, see [Kopietz], Ch. 8.
- Recall action for φ^4-theory, assign $S_{0,1}$ in non-standard way:

$$S_{\Lambda_0}[\varphi] = \underbrace{\frac{1}{2}\int_{\mathbf{k}} \left[c_0 k^2\right] \varphi(-\mathbf{k})\varphi(\mathbf{k})}_{S_0[\varphi]} + \underbrace{\frac{r_0}{2}\int_{\mathbf{k}} \varphi(-\mathbf{k})\varphi(\mathbf{k}) + \frac{u_0}{4!}\int_{\mathbf{k}_{1,2,3,4}} (2\pi)^D \delta\left(\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3+\mathbf{k}_4\right)\varphi(\mathbf{k}_1)\varphi(\mathbf{k}_2)\varphi(\mathbf{k}_3)\varphi(\mathbf{k}_4)}_{S_1[\varphi]}$$

  Remark on non-standard choice for $S_{0,1}$:
  - reflects flexibility of fRG approach
  - momentum independent self-energy flows starting from r_0 (like in Wilsonian RG)

- Use multiplicative sharp cutoff in momentum space that switches *on* smaller and smaller k:

$$G_{0,\Lambda}(\mathbf{k}) = \frac{\Theta\left(k-\Lambda\right)}{c_0 k^2} \tag{90}$$

  Note: Due to implicit cutoff $k \leq \Lambda_0$ in $S_{\Lambda_0}[\varphi]$, start the flow at $\Lambda = \Lambda_0$ instead of $\Lambda = \infty$.

- Dictionary for convention used in fRG flow equations:

$$\left[\mathbf{G}_{(0,\Lambda)}\right]_{\mathbf{k}\mathbf{k}'} = -(2\pi)^D \delta\left(\mathbf{k}+\mathbf{k}'\right) G_{(0,\Lambda)}(\mathbf{k}) = -\left\langle \varphi_{\mathbf{k}}\varphi_{\mathbf{k}'}\right\rangle \tag{91}$$

$$\left[\dot{\mathbf{G}}_{\Lambda}\right]_{\mathbf{k}\mathbf{k}'} = -(2\pi)^D \delta\left(\mathbf{k}+\mathbf{k}'\right) \dot{G}_{\Lambda}(\mathbf{k}) \tag{92}$$

$$\left[\mathbf{\Sigma}_{\Lambda}\right]_{\mathbf{k}\mathbf{k}'} = +(2\pi)^D \delta\left(\mathbf{k}+\mathbf{k}'\right) \Sigma_{\Lambda}(\mathbf{k}) \tag{93}$$

$$G_{\Lambda}^{-1}(\mathbf{k}) = G_{0,\Lambda}^{-1}(\mathbf{k}) + \Sigma_{\Lambda}(\mathbf{k}) \tag{94}$$

  or

$$G_{\Lambda}(\mathbf{k}) = \frac{1}{G_{0,\Lambda}^{-1}(\mathbf{k}) + \Sigma_{\Lambda}(\mathbf{k})} = \frac{\Theta(k-\Lambda)}{c_0 k^2 + \Theta(k-\Lambda)\Sigma_{\Lambda}(\mathbf{k})} \tag{95}$$

- Single scale propagator:

$$\dot{G}_{\Lambda}(\mathbf{k}) \;=\; \frac{\partial_\Lambda G_{0,\Lambda}(\mathbf{k})}{\left[1+G_{0,\Lambda}(\mathbf{k})\Sigma_{\Lambda}(\mathbf{k})\right]^2} = \frac{-\delta(k-\Lambda)}{c_0 k^2\left[1+\frac{\Theta(k-\Lambda)}{c_0 k^2}\Sigma_{\Lambda}(\mathbf{k})\right]^2} \tag{96}$$

fRG flow equations

- For vertices, in accordance with Eq. (91), we take out a momentum-conserving delta-function out of $\Gamma^{(n)}$ and define
$$\Gamma^{(n)}_{\Lambda,\mathbf{k}_1\ldots\mathbf{k}_n} \equiv (2\pi)^D \delta\left(\mathbf{k}_1 + \ldots + \mathbf{k}_n\right) \Gamma^{(n)}_{\Lambda}\left(\mathbf{k}_1, \ldots, \mathbf{k}_n\right) \tag{97}$$
where $\Gamma^{(n)}_{\Lambda}\left(\mathbf{k}_1, \ldots, \mathbf{k}_n\right)$ only really depends on $n-1$ momenta.

- Recall the general fRG flow equations for vertices, we truncate $\Gamma^{(6)} \stackrel{!}{=} \Gamma^{(6)}_{\Lambda_0} = 0$ and drop all vertices of odd order since we restrict ourselves to the disordered phase.
$$\begin{aligned}
\partial_\Lambda \left[\mathbf{\Sigma}_\Lambda\right]_{\alpha_1\alpha_2} &= -\frac{1}{2}\int_{\beta_{1,2}} \left[\dot{\mathbf{G}}_\Lambda\right]_{\beta_1\beta_2} \Gamma^{(4)}_{\Lambda,\beta_1\beta_2\alpha_1\alpha_2} \\
\partial_\Lambda \Gamma^{(4)}_{\Lambda,\alpha_1\ldots\alpha_4} &= -\frac{1}{2}\mathrm{Tr}\left(\mathcal{S}_{\alpha_1\alpha_2;\alpha_3\alpha_4}\left\{\mathbf{Z}\dot{\mathbf{G}}_\Lambda \mathbf{\Gamma}^{(4)}_{\Lambda,\alpha_3\alpha_4} \mathbf{G}_\Lambda \mathbf{\Gamma}^{(4)}_{\Lambda,\alpha_1\alpha_2}\right\}\right)
\end{aligned}$$

- Insert preparations:
$$\begin{aligned}
\partial_\Lambda \Sigma_\Lambda(\mathbf{k}) &= \frac{1}{2}\int_{\mathbf{k}'} \dot{G}_\Lambda\left(\mathbf{k}'\right) \Gamma^{(4)}_\Lambda\left(\mathbf{k}', -\mathbf{k}', \mathbf{k}, -\mathbf{k}\right) \\
\partial_\Lambda \Gamma^{(4)}_\Lambda\left(\mathbf{k}_{1,2,3,4}\right) &= -\int_{\mathbf{k}} \dot{G}_\Lambda(\mathbf{k}) \\
&\times \left\{\Gamma^{(4)}_\Lambda\left(\mathbf{k}, -\mathbf{k}+\mathbf{k}_1+\mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4\right) G_\Lambda\left(-\mathbf{k}+\mathbf{k}_1+\mathbf{k}_2\right) \Gamma^{(4)}_\Lambda\left(+\mathbf{k}-\mathbf{k}_1-\mathbf{k}_2, -\mathbf{k}, \mathbf{k}_1, \mathbf{k}_2\right)\right. \\
&\left. + \left(\mathbf{k}_2 \leftrightarrow \mathbf{k}_3\right) + \left(\mathbf{k}_2 \leftrightarrow \mathbf{k}_4\right)\right\}
\end{aligned}$$
and the factor of $1/2$ has partially canceled against the symmetrization operator that produces $6!/2!/2!$ terms.

- Initial conditions (momentum independent): $\Sigma_{\Lambda_0} = r_0$ and $\Gamma^{(4)}_{\Lambda_0} = u_0$.

Recovering Wilsonian momentum shell RG

- Outlook: Numerical treatment of full momentum dependence possible, but somewhat involved. Vertex $\Gamma^{(4)}_l$ depends on three D-dimensional momenta. Need to use symmetries, beyond-Mathematica numerics, form-factors and other tricks → Master- & PhD-thesis.

- Here: Assume coupling *constants*, i.e. momentum independence of $\Sigma_\Lambda(\mathbf{k}) \stackrel{!}{=} r_\Lambda$ and $\Gamma^{(4)}_\Lambda\left(\mathbf{k}_{1,2,3,4}\right) \stackrel{!}{=} u_\Lambda$.

- Set momenta to zero at left-hand-side of fRG flow equations.

- Self-energy flow equation:
$$\begin{aligned}
\partial_\Lambda r_\Lambda &= \frac{1}{2}\int_{\mathbf{k}} \dot{G}_\Lambda(\mathbf{k}) \Gamma^{(4)}_\Lambda(\mathbf{k}, -\mathbf{k}, 0, 0) \\
&= \frac{u_\Lambda}{2}\int_{\mathbf{k}} \frac{-\delta(k-\Lambda)}{c_0 k^2\left[1 + \frac{\Theta(k-\Lambda)}{c_0 k^2}\Sigma_\Lambda(\mathbf{k})\right]^2}
\end{aligned}$$
Careful: Integrand requires Morris' lemma (60): We use $\int_0^1 dt[1+tx]^{-2} = -\frac{1}{x[1+tx]}|_{t=0}^{t=1} = \frac{1}{1+x}$ and find
$$\dot{G}_\Lambda(\mathbf{k}) = -\frac{\delta(k-\Lambda)}{c_0 k^2 + \Sigma_\Lambda(k)}. \tag{98}$$
Next, recall the definition of K_D: $\int_{\mathbf{k}} = \frac{1}{(2\pi)^D}\int d^D\mathbf{k} = K_D \int_0^\infty k^{D-1} \cdot dk$. We obtain:
$$\partial_\Lambda r_\Lambda = \frac{-u_\Lambda K_D}{2}\int_0^{\Lambda_0} k^{D-1} \cdot dk \frac{\delta(k-\Lambda)}{c_0 k^2 + \Sigma_\Lambda(k)} = -\frac{u_\Lambda}{2}\frac{K_D \Lambda^{D-1}}{c_0\Lambda^2 + r_\Lambda}$$

- 4-point vertex flow equation:

$$\begin{aligned}
\partial_\Lambda u_\Lambda &= -3u_\Lambda^2 \int_{\mathbf{k}} \dot{G}_\Lambda(\mathbf{k}) G_\Lambda(\mathbf{k}) \\
&= 3u_\Lambda^2 K_D \int_0^{\Lambda_0} dk k^{D-1} \frac{\delta(k-\Lambda)\Theta(k-\Lambda)c_0 k^2}{\left[c_0 k^2 + \Theta(k-\Lambda) r_\Lambda\right]^3} \\
\{\text{Morris}\} &= 3u_\Lambda^2 K_D \int_0^{\Lambda_0} dk k^{D-1} \delta(k-\Lambda) \underbrace{\int_0^1 dt \frac{t c_0 k^2}{\left[c_0 k^2 + t r_\Lambda\right]^3}}_{1/(2\left[c_0 k^2 + r_\Lambda\right]^2)} \\
&= \frac{3K_D}{2} \frac{u_\Lambda^2 \Lambda^{D-1}}{\left[c_0 \Lambda^2 + r_\Lambda\right]^2}
\end{aligned}$$

- Introduce dimensionless quantities as before,

$$\bar{r}_\Lambda = \frac{r_\Lambda}{c_0 \Lambda^2}, \; \bar{u}_\Lambda = K_D \frac{u_\Lambda}{c_0^2 \Lambda^{4-D}}, \tag{99}$$

  and use l in $\Lambda = \Lambda_0 e^{-l}$ such that $\partial_l f_l = -\Lambda \partial_\Lambda f_\Lambda$. Putting things together, we recover the same flow equations as from Wilsonian momentum shell RG in Sec. 4.4

$$\partial_l \bar{r}_l = 2\bar{r}_l + \frac{1}{2}\frac{\bar{u}_l}{1+\bar{r}_l}, \quad \partial_l \bar{u}_l = (4-D)\bar{u}_l - \frac{3}{2}\frac{\bar{u}_l^2}{[1+\bar{r}_l]^2}. \tag{100}$$

- Interpretation: Meaning of $\bar{r}_\Lambda$, $\bar{u}_\Lambda$.
  - Wilsonian RG: Couplings in action S_Λ when high-energy fluctuations with $k \in (\Lambda, \Lambda_0]$ have been integrated out.
  - fRG in vertex expansion: Self-energy and effective interaction vertex defined via correlation functions computed with high-energy fluctuations $k \in (\Lambda, \Lambda_0]$ switched on.

  In both cases the low-energy modes $k \in [0, \Lambda]$ have *not* been used.

7.5 Application: Vertex expansion for spinful fermions

Aims:

- Derive flow equations for fermions, use them in Ex. 7.3 for single-impurity Anderson model (SIAM).

Preparations

- Need two types of fields for creation and annihilation operator, $\{\Phi_\alpha\} \to \left\{\psi_{K\sigma}, \bar{\psi}_{K\sigma}\right\}$, $\zeta = -1$, abbreviate conserved quantities $K \equiv (i\omega, \mathbf{k})$ and $\sigma = \uparrow, \downarrow$ is the spin index.
  In summary: $\alpha = (\psi, K, \sigma)$ or $(\bar{\psi}, K', \sigma')$. Generalize spinless case from the beginning of Sec. 5,

$$\left[\mathbf{G}_0^{-1}\right]_{(\bar{\psi},K',\sigma'),(\psi,K,\sigma)} = \delta_{K,K'} \left(i\omega\delta_{\sigma'\sigma} - H_{K'\sigma';K\sigma}\right) = \left[G_0^{-1}\right]_{K'\sigma';K\sigma} \tag{101}$$

- Full Green function, propagate from $\bar{\psi}_{1'}$ [creation with $1' = (K', \sigma')$] to ψ_1 [annihilation with $1 = (K, \sigma)$]. The overall sign and definition of $G_{11'}$ with $\psi, \bar{\psi}$ not explicitly specified is fermionic **convention**.

$$\boxed{\mathbf{G}_{\psi_1 \bar{\psi}_{1'}} = -\left\langle \psi_1 \bar{\psi}_{1'} \right\rangle \equiv G_{11'}} \tag{102}$$

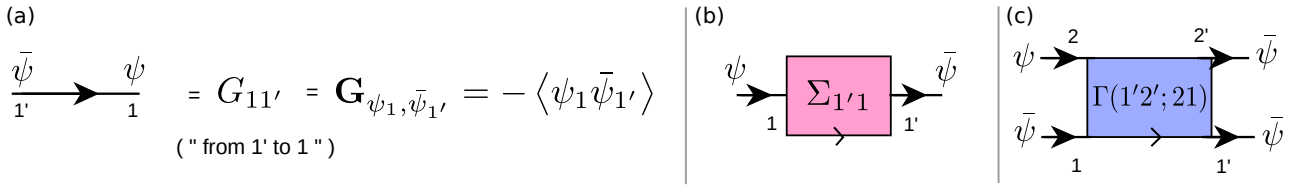


Figure 22: Diagrammatic conventions for fermionic field theories.

- The above points and the inversion rule of a 2x2 off-diagonal matrix require the following assignments (also hold with cutoff Λ):

$$\mathbf{G} = \begin{pmatrix} 0 & \mathbf{G}_{\psi\bar\psi} \\ \mathbf{G}_{\bar\psi\psi} & 0 \end{pmatrix} = \begin{pmatrix} 0 & G \\ \zeta G^T & 0 \end{pmatrix}$$
$$\mathbf{G}^{-1} = \begin{pmatrix} 0 & \zeta\left(G^{-1}\right)^T \\ G^{-1} & 0 \end{pmatrix} = \begin{pmatrix} 0 & \left[\mathbf{G}^{-1}\right]_{\psi\bar\psi} \\ \left[\mathbf{G}^{-1}\right]_{\bar\psi\psi} & 0 \end{pmatrix} = \mathbf{G}_0^{-1} - \mathbf{\Sigma}$$
$$\mathbf{\Sigma} = \begin{pmatrix} 0 & [\mathbf{\Sigma}]_{\psi\bar\psi} \\ [\mathbf{\Sigma}]_{\bar\psi\psi} & 0 \end{pmatrix} \equiv \begin{pmatrix} 0 & \zeta\Sigma^T \\ \Sigma & 0 \end{pmatrix}$$

  and we read off

$$G^{-1} = G_0^{-1} - \Sigma. \tag{103}$$

- The above conventions are summarized in Fig. 22(a,b)

Interaction and initial vertex

- Assume total spin is conserved in bare scattering ($\{\sigma_1,\sigma_2\} \to \{\sigma_1,\sigma_2\}$).

$$S_1[\bar\psi,\psi] = \frac{1}{2}\sum_{\sigma_{1,2}}\int_{K_1'K_2'K_1K_2} U_{\sigma_1\sigma_2}\left(K_1',K_2';K_2,K_1\right)\bar\psi_{K_1'\sigma_1}\bar\psi_{K_2'\sigma_2}\psi_{K_2\sigma_2}\psi_{K_1\sigma_1} \tag{104}$$

  The function U is symmetric under simultaneous exchange within first *and* last index pair.

$$U_{\sigma_1\sigma_2}\left(K_1',K_2';K_2,K_1\right) = U_{\sigma_2\sigma_1}\left(K_2',K_1';K_1,K_2\right) \tag{105}$$

- Do *not* confuse U with the (bare) one-line irreducible vertex $\Gamma^{(4),\Lambda=\infty}_{\alpha_1\alpha_2\alpha_3\alpha_4}$ which is (anti-)symmetric under exchange of *all* of its arguments.

- *Partially* symmetrized vertex (can exchange within first *or* last index pair, separated by ";"):

$$S_1[\bar\psi,\psi] = \frac{1}{(2!)}\int_{K_1'\sigma_1'K_2'\sigma_2'K_1\sigma_1K_2\sigma_2}\Gamma^{(4)}_{\Lambda=\infty}\left(K_1'\sigma_1',K_2'\sigma_2';K_2\sigma_2,K_1\sigma_1\right)\times\bar\psi_{K_1'\sigma_1'}\bar\psi_{K_2'\sigma_2'}\psi_{K_2\sigma_2}\psi_{K_1\sigma_1} \tag{106}$$

$$\Gamma^{(4)}_{\Lambda=\infty}\left(K_1'\sigma_1',K_2'\sigma_2';K_2\sigma_2,K_1\sigma_1\right) = \delta_{\sigma_1'\sigma_1}\delta_{\sigma_2'\sigma_2}U^{(4)}_{\sigma_1\sigma_2}\left(K_1',K_2';K_2,K_1\right) - \delta_{\sigma_1'\sigma_2}\delta_{\sigma_2'\sigma_1}U^{(4)}_{\sigma_1\sigma_2}\left(K_1',K_2';K_1,K_2\right) \tag{107}$$

- Superfield vertex with full (anti-)symmetry:

$$S_1\left[\Phi\right] = \frac{1}{4!}\int_{\alpha_{1,2,3,4}}\Gamma^{(4),\Lambda=\infty}_{\alpha_1\alpha_2\alpha_3\alpha_4}\Phi_{\alpha_1}\Phi_{\alpha_2}\Phi_{\alpha_3}\Phi_{\alpha_4} \tag{108}$$

  which leads to

$$\Gamma^{(4),\Lambda=\infty}_{\alpha_1=(\bar\psi K_1'\sigma_1'),\alpha_2=\left(\bar\psi K_2'\sigma_2'\right),\alpha_3=(\psi K_2\sigma_2),\alpha_4=(\psi K_1\sigma_1)} = \Gamma^{(4)}_{\Lambda=\infty}\left(K_1'\sigma_1',K_2'\sigma_2';K_2\sigma_2,K_1\sigma_1\right) \tag{109}$$

  and $\Gamma^{(4)}_{\alpha_1\alpha_2\alpha_3\alpha_4}$ with other number of $\bar\psi$ and ψ terms vanish. The $1/4! = 1/24$ is related to $1/2!/2! = 1/4$ above by the [4 choose 2] $= 6$ possibilities to pick two $\bar\psi$ and two ψ fields in α-sums.

- Fig. 22(c): In graphical representation of 4-point vertex $\Gamma^{(4)}_{\Lambda=\infty}\left(1',2';2,1\right)$ and self-energy, $\bar\psi$ is outgoing arrow, ψ is in-going arrow. Opposite to Green functions!

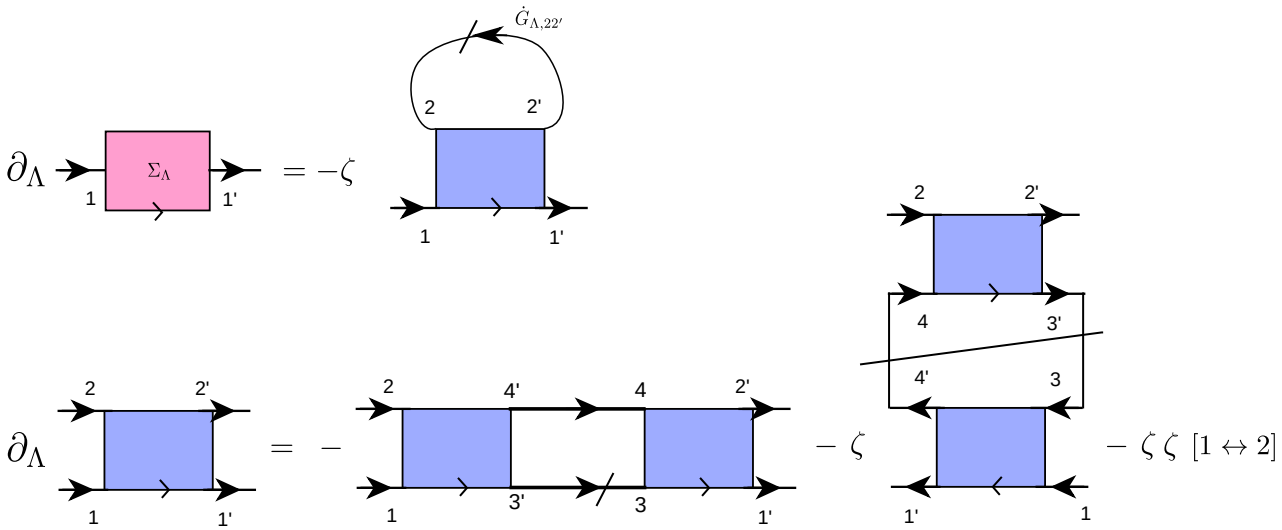


Figure 23: Fermionic fRG flow equations in diagrammatic convention. The last term amounts to exchanging the labels 1 and 2 in the previous diagram and multiplying the statistical factor ζ. The dash over a pair of propagators denotes the application of a "product-rule", $G\dot{G} + \dot{G}G$, see Eq. (113).

Flow equations in $\Gamma^{(4)}$ truncation scheme

- From the general case above, we take the flow equations in terms of fully symmetric Γ:

$$\partial_\Lambda \Gamma^{(2)}_{\Lambda,\alpha_1\alpha_2} = -\frac{1}{2}\left[\dot{\mathbf{G}}_\Lambda\right]_{\beta_1\beta_2} \Gamma^{(4)}_{\Lambda,\beta_1\beta_2\alpha_1\alpha_2} \tag{110}$$

  and

$$\partial_\Lambda \Gamma^{(4)}_{\Lambda,\alpha_1\ldots\alpha_4} = -\zeta\frac{1}{2}\left[\dot{\mathbf{G}}_\Lambda\right]_{\beta_1\beta_2} [\mathbf{G}_\Lambda]_{\beta_3\beta_4}\, \mathcal{S}_{\alpha_1\alpha_2;\alpha_3\alpha_4} \left\{\Gamma^{(4)}_{\Lambda,\beta_2\beta_3\alpha_3\alpha_4} \Gamma^{(4)}_{\Lambda,\beta_4\beta_1\alpha_1\alpha_2}\right\} \tag{111}$$

- Pick $\alpha_1, \alpha_2 = (\bar{\psi}, \underbrace{K_1', \sigma_1'}_{1'}), (\psi, \underbrace{K_2, \sigma_2}_{2}) = \bar{\psi}_{1'}, \psi_1$, and similar for $\Gamma^{(4)}$, $\alpha_1, \alpha_2, \alpha_3, \alpha_4 = \bar{\psi}_{1'}, \bar{\psi}_{2'}, \psi_2, \psi_1$. We obtain (see Fig. 23):
  - For self energy:

$$\begin{aligned}
\partial_\Lambda \Sigma_{\Lambda,1'1} &= \partial_\Lambda \Gamma^{(2)}_{\Lambda,\alpha_1=\bar{\psi}_{1'},\alpha_2=\psi_1} \\
&= -\int_{22'} \frac{1}{2}\left(\left[\dot{\mathbf{G}}_\Lambda\right]_{22'} \Gamma^{(4)}_{\Lambda,22'1'1} + \left[\dot{\mathbf{G}}_\Lambda\right]_{2'2} \Gamma^{(4)}_{\Lambda,2'21'1}\right) \\
&= -\zeta \int_{22'} \left[\dot{\mathbf{G}}_\Lambda\right]_{22'} \Gamma^{(4)}_{\Lambda,1'2'21}
\end{aligned}$$

    and we insert the conventions from above

$$\partial_\Lambda \Sigma_{\Lambda,1'1} = -\zeta \int_{22'} \dot{G}_{\Lambda,22'} \Gamma^{(4)}_\Lambda\,(1'2';21) \tag{112}$$

  - Interaction vertex (see Ex. 7.2 for details):

$$\begin{aligned}
\partial_\Lambda \Gamma^{(4)}_\Lambda\,(1'2';21) = &-\Gamma^{(4)}_\Lambda\,(1'2';43)\left[\dot{G}_{\Lambda,33'} G_{\Lambda,44'}\right] \Gamma^{(4)}_\Lambda\,(3'4';21) \\
&-\zeta\left(\dot{G}_{\Lambda,33'} G_{\Lambda,44'} + \dot{G}_{\Lambda,44'} G_{\Lambda,33'}\right) \Gamma^{(4)}_\Lambda\,(1'4';31)\, \Gamma^{(4)}_\Lambda\,(3'2';24) \\
&-\zeta^2\left(\dot{G}_{\Lambda,33'} G_{\Lambda,44'} + \dot{G}_{\Lambda,44'} G_{\Lambda,33'}\right) \Gamma^{(4)}_\Lambda\,(1'4';32)\, \Gamma^{(4)}_\Lambda\,(3'2';14)
\end{aligned} \tag{113}$$

Exercises

Exercise 7.1. fRG in vertex expansion for toy-model

Consider the toy-model field theory of Ex. 5.1. The goal of this exercise is to derive and solve fRG flow equations for the vertices of this simple model and compare the results with the exact results and perturbative approach.

1. Using the general results from the lecture, write down the flow equations for the generating functions $g_c(j)$, $g_{ac}(\bar{\varphi})$, $\gamma(\bar{\varphi})$.

2. Use the following cutoff procedure $G_0 \to G_{0,\Lambda} = -\Lambda$ where the flow is from $\Lambda = 0$ to $\Lambda = G_0$. Note that this is different from the usual convention where Λ starts at ∞ and end at zero. Expand the flow equations for $\gamma_\Lambda(\bar{\varphi})$ in powers of sources to define the vertices $\gamma_\Lambda^{(n)}$ for $n = 0, 2, 4, 6, 8$ and show explicitly

$$\begin{aligned}
\partial_\Lambda \gamma_\Lambda^{(0)} &= \frac{1}{2}\frac{\gamma_\Lambda^{(2)}}{1+\Lambda\gamma_\Lambda^{(2)}}, \\
\partial_\Lambda \gamma_\Lambda^{(2)} &= \frac{1}{2}\frac{\gamma_\Lambda^{(4)}}{\left[1+\Lambda\gamma_\Lambda^{(2)}\right]^2}, \\
\partial_\Lambda \gamma_\Lambda^{(4)} &= \frac{1}{2}\frac{\gamma_\Lambda^{(6)}}{\left[1+\Lambda\gamma_\Lambda^{(2)}\right]^2} - 3\frac{\Lambda\left[\gamma_\Lambda^{(4)}\right]^2}{\left[1+\Lambda\gamma_\Lambda^{(2)}\right]^3}, \\
\partial_\Lambda \gamma_\Lambda^{(6)} &= 45\frac{\Lambda^2\left[\gamma_\Lambda^{(4)}\right]^3}{\left[1+\Lambda\gamma_\Lambda^{(2)}\right]^4} - 15\frac{\Lambda\gamma_\Lambda^{(4)}\gamma_\Lambda^{(6)}}{\left[1+\Lambda\gamma_\Lambda^{(2)}\right]^3} + \frac{1}{2}\frac{\gamma_\Lambda^{(8)}}{\left[1+\Lambda\gamma_\Lambda^{(2)}\right]^2}.
\end{aligned}$$

3. Find the initial conditions for the quantities in 2) at $\Lambda = 0$. Set $G_0 = -1$ and truncate the above hierarchy of flow equations $\gamma_\Lambda^{(n)}$ for $n > n_c$ equal to their initial values at $\Lambda = 0$. Consider the cases $n_c = 2, 4, 6$. Integrate the set of flow equations numerically (e.g., using Mathematica) from $\Lambda = 0$ to $\Lambda = 1$. Show three plots over $u \in [0, 0.7]$ to compare the fRG results for

$$\gamma^{(0)} = -\ln\left[Z/Z_0\right], \qquad \gamma^{(2)} = \Sigma, \qquad \gamma^{(4)}, \tag{114}$$

to the perturbative result of Ex. 5.1 and to the exact solution (from direct numerical evaluation of the integrals I_n in Ex. 5.1).

Exercise 7.2. Flow of fermionic 4-point vertex

Derive the flow equation (113) for the fermionic 4-point vertex. Start from the general equation (111).

Exercise 7.3. Fermionic fRG for single-impurity Anderson model

The single impurity Anderson model (SIAM) can be used to model a quantum dot (confined region with Hamiltonian H_d with local interaction) with single electronic energy level per spin that is connected to one or more metallic leads l (electrical contacts, Hamiltonian H_l), see Fig. 24(a). The total Hamiltonian with a right and left lead is $H = H_d + H_{l=L} + H_{l=R}$ where

$$H_d = \sum_{\sigma=\uparrow,\downarrow} \varepsilon_\sigma n_\sigma + U\left(n_\uparrow - 1/2\right)\left(n_\downarrow - 1/2\right) - \sum_{l=L,R}\sum_{\sigma=\uparrow,\downarrow} t_l\left(d_\sigma^\dagger c_{1,l,\sigma} + h.c.\right), \quad H_l = -t\sum_\sigma\sum_{m=1}^{\infty}\left(c_{m,l,\sigma}^\dagger c_{m+1,l,\sigma} + h.c.\right). \tag{115}$$

Here, $n_\sigma = d_\sigma^\dagger d_\sigma$ describes the occupation of dot electrons with spin $\sigma = \uparrow, \downarrow$ and in $\uparrow \mathrel{\hat{=}} +1$, $\downarrow \mathrel{\hat{=}} -1$ is understood. The interaction is repulsive, $U > 0$. The singe-particle energy levels $\varepsilon_\sigma = V_g + \sigma h/2$ can be shifted by a gate voltage V_g and split under the influence of a magnetic field h. We assume two leads $l = L, R$ which are coupled from the left and right with hopping strength $t_{l=L,R}$ and lead-internal hopping strength $t > 0$. Consider the case of vanishing temperature where the Matsubara frequencies become continuous.

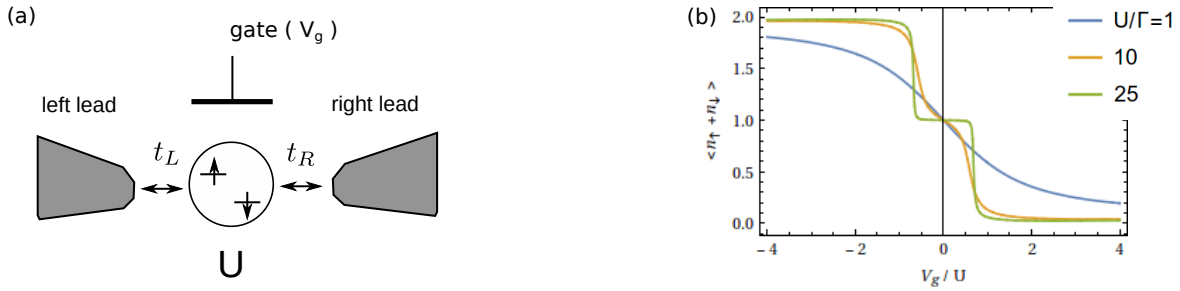


Figure 24: (a) Sketch of the single impurity Anderson model attached to two leads. (b) fRG result for the dot occupation with the approximation $U^\Lambda \stackrel{!}{=} U$.

1. The leads are non-interacting and can be treating exactly, for example by integrating over the Grassman fields $\psi_{m,l,\sigma}(\omega_n)$, $\bar{\psi}_{m,l,\sigma}(\omega_n)$ associated to $c_{m,l,\sigma}$, $c^\dagger_{m,l,\sigma}$ in the path integral formalism. This adds a lead induced self-energy term in the action for the dot electrons. Assume the wide-band limit $|\omega| \ll t$ and show that the bare propagator of the d electron then reads

$$G_{0,\sigma}(i\omega) = [i\omega - (V_g + \sigma h/2) + i\mathrm{sgn}(\omega)\Gamma]^{-1} \tag{116}$$

with $\Gamma = \Gamma_L + \Gamma_R$ and $\Gamma_l \equiv |t_l|^2/t$. Hints: Write down the Matsubara action and integrate over $\psi_{m,l,\sigma}(\omega_n)$, $\bar{\psi}_{m,l,\sigma}(\omega_n)$. As the action containing the Grassman fields $\psi_{m,l,\sigma}(\omega_n)$, $\bar{\psi}_{m,l,\sigma}(\omega_n)$ does not mix lead index, spin or Matsubara frequency, you can simply sum over these quantities at the end of the calculation. It is useful to work with a finite lead of length M, use a Fourier transform $\psi_m(\omega_n) = \frac{1}{\sqrt{M/2}} \sum_{k=0}^{M-1} \sin\left(m\frac{2\pi}{M}k\right) \chi_k(\omega_n)$ and take the limit $M \to \infty$ only at the end.

2. The resulting model only contains a single spinful fermion degree of freedom but is nevertheless physically interesting. Apply the fermionic fRG in vertex expansion by introducing a sharp Matsubara frequency cutoff $G_{0,\Lambda}(i\omega) = \theta(|\omega| - \Lambda)G_0(\omega)$. In a first step, neglect the flow of the four-point vertex, i.e. set $\Gamma^{(4)}_\Lambda(\omega_{1'}\sigma, \omega_{2'}\bar{\sigma}; \omega_2\bar{\sigma}, \omega_1\sigma) \equiv U^\Lambda \stackrel{!}{=} U$ (where $\bar{\sigma} \equiv -\sigma$). From the self-energy fRG flow equation, derive the flow of the effective level position $V^\Lambda_\sigma = V_g + \sigma h/2 + \Sigma^\Lambda_\sigma$ (excluding Γ!):

$$\partial_\Lambda V^\Lambda_\sigma = \frac{U^\Lambda V^\Lambda_\sigma/\pi}{(\Lambda+\Gamma)^2 + \left(V^\Lambda_{\bar{\sigma}}\right)^2}. \tag{117}$$

For the initial condition at large but finite Λ_i, confirm $V^{\Lambda=\Lambda_i}_\sigma = V_g + \sigma h/2$.
Hints: Use Morris' Lemma and confirm $\dot{G}^\Lambda_\sigma(i\omega) = -\delta(|\omega| - \Lambda)/\left(i\omega - \left(V_g + \sigma h/2 + \Sigma^\Lambda_\sigma\right) + i\mathrm{sgn}(\omega)\Gamma\right)$. To prove the initial condition, show that the contribution of the terms $Un_\sigma/2$ to the self-energy vanishes in the first part of the fRG flow from $\Lambda = \infty$ to $\Lambda = \Lambda_i$ where a convergence factor $e^{i\omega\eta}$ coming from the ordering of imaginary time operators in the interaction term has to be considered.

3. Use the flow equation (117) to calculate the dot occupation $\langle n_\uparrow + n_\downarrow \rangle$. Show that the dot occupation can be calculated via $\langle n_\sigma \rangle = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega e^{i\omega\eta} G_\sigma(i\omega) = \frac{1}{2} - \frac{1}{\pi}\int_0^{\omega_0} d\omega \frac{V_\sigma}{[\omega+\Gamma]^2+V_\sigma^2}$ with ω_0 large but finite. Set $\Lambda_i = 100$, $h = 0$, $U/\Gamma = 1, 10$ or 25 and solve the flow equation (117) numerically (e.g. with MATHEMATICA) to obtain $V_\sigma \equiv V^{\Lambda=0}_\sigma$ as a function of V_g/U. Plot the dot occupation $\langle n_\uparrow + n_\downarrow \rangle$ across the dot over $V_g/U \in [-4, 4]$ and discuss your result which should look like in Fig. 24(b).

4. Compute the flow of the four-point vertex assuming that the six-point vertex does not contribute. Use the frequency-independent approximation involving U^Λ from above. You should find

$$\partial_\Lambda U^\Lambda = \frac{2\left(U^\Lambda\right)^2 V^\Lambda_\uparrow V^\Lambda_\downarrow/\pi}{\left[(\Lambda+\Gamma)^2 + \left(V^\Lambda_\uparrow\right)^2\right] \cdot \left[(\Lambda+\Gamma)^2 + \left(V^\Lambda_\downarrow\right)^2\right]}. \tag{118}$$

8 Derivative expansion

Aims:

- $\Gamma_\Lambda[\bar{\Phi}]$ in Wetterich equation: Focus on (homogeneous) field dependence rather than complete $\mathbf{k}, \omega_n$-dependence of $\bar{\Phi}_{\mathbf{k},\omega_n,...}$
- $\rightarrow$ "Non-perturbative renormalization", alternative to vertex-expansion.
- Expansion in orders of $\nabla_{\mathbf{r}}\bar{\Phi}$ (spatial "derivative expansion"), ok for long-wavelength phenomena.
- Most simple ansatz for $\Gamma_\Lambda[\bar{\Phi}]$: Local-potential approximation, yields a single PDE.
- Apply to φ^4-theory, solve PDE numerically, find ν.

8.1 Introduction and preparation

- More convenient for this section: Wetterich's "*Legendre effective action*" is Legendre transform of $\mathcal{G}_{c,\Lambda}[J]$ without any shifts

$$\Gamma_\Lambda^{\mathrm{We}}\left[\bar{\Phi}\right] \equiv \Gamma_\Lambda\left[\bar{\Phi}\right] - \frac{1}{2}\left(\bar{\Phi}, \mathbf{G}_0^{-1}\bar{\Phi}\right) - \ln \mathcal{Z}_{0,\Lambda} \tag{119}$$

- $\Gamma_{\Lambda=0}^{\mathrm{We}}\left[\bar{\Phi}\right]$ differs from $\Gamma_{\Lambda=0}\left[\bar{\Phi}\right]$ in the field-independent term and the second functional derivative which yields the full propagator (and not the irreducible self-energy). Initial condition:

$$\Gamma_{\Lambda\to\Lambda_0}^{\mathrm{We}}\left[\bar{\Phi}\right] = S_{\Lambda_0}\left[\bar{\Phi}\right] = S_{0,\Lambda_0}\left[\bar{\Phi}\right] + S_{1,\Lambda_0}\left[\bar{\Phi}\right] \tag{120}$$

- Flow equation for $\Gamma_\Lambda^{\mathrm{We}}\left[\bar{\Phi}\right]$ (Wetterich equation, use additive regulator $\mathbf{G}_{0,\Lambda}^{-1} = \mathbf{G}_0^{-1} - \mathbf{R}_\Lambda$)

$$\boxed{\partial_\Lambda \Gamma_\Lambda^{\mathrm{We}}\left[\bar{\Phi}\right] = \frac{1}{2}\mathrm{tr}\left\{\left[\partial_\Lambda \mathbf{R}_\Lambda\right]\left(\frac{\delta}{\delta\bar{\Phi}} \otimes \frac{\delta}{\delta\bar{\Phi}}\Gamma_\Lambda^{\mathrm{We}}\left[\bar{\Phi}\right] + \mathbf{Z}\mathbf{R}_\Lambda^{-1}\right)^{-1}\right\}} \tag{121}$$

8.2 Derivative expansion for classical $O(N)$ symmetric φ^4-theory

- Recall $O(N)$ symmetric φ^4-theory with $\boldsymbol{\varphi} = (\varphi_1, \varphi_2, ..., \varphi_N)$ a classical field (c.f. Ex. 4.4).

$$S_{\Lambda_0}[\boldsymbol{\varphi}] = \int d\mathbf{r}\left[\frac{r_0}{2}\boldsymbol{\varphi}^2(\mathbf{r}) + \frac{c_0}{2}\left(\nabla\boldsymbol{\varphi}\right)^2(\mathbf{r}) + \frac{u_0}{4!}\left[\boldsymbol{\varphi}^2(\mathbf{r})\right]^2\right] \tag{122}$$

  We have units $[r_0\boldsymbol{\varphi}^2\Lambda_0^{-D}] = 1$, $[c_0\Lambda_0^{2-D}\boldsymbol{\varphi}^2] = 1$, $[u_0\boldsymbol{\varphi}^4\Lambda_0^{-D}] = 1$.

- Initial condition $\Gamma_{\Lambda_0}^{\mathrm{We}}[\bar{\boldsymbol{\varphi}}] = S_{\Lambda_0}[\bar{\boldsymbol{\varphi}}]$, motivates *ansatz* for flowing $\Gamma_\Lambda^{\mathrm{We}}[\bar{\boldsymbol{\varphi}}]$ that is an expansion in spatial field derivatives. Abbreviate density $\rho(\mathbf{r}) \equiv \bar{\boldsymbol{\varphi}}^2(\mathbf{r})/2$.

$$\boxed{\Gamma_\Lambda^{\mathrm{We}}[\bar{\boldsymbol{\varphi}}] = \int d\mathbf{r}\left[U_\Lambda\left(\rho(\mathbf{r})\right) + \frac{c_0}{2}Z_\Lambda^{-1}\left(\rho(\mathbf{r})\right)\left(\nabla\bar{\boldsymbol{\varphi}}\right)^2(\mathbf{r}) + \frac{c_0}{4}Y_\Lambda\left(\rho(\mathbf{r})\right)\left(\nabla\rho\right)^2(\mathbf{r}) + ...\right]} \tag{123}$$

- First term: Effective potential, scalar function $U_\Lambda(\rho)$ can be obtained from a spatially homogeneous field configuration,

$$U_\Lambda(\rho) = \frac{1}{V}\Gamma_\Lambda^{\mathrm{We}}[\bar{\boldsymbol{\varphi}}]\,|_{\bar{\boldsymbol{\varphi}}(\mathbf{r})=2\sqrt{\rho}\mathbf{e}_1}. \tag{124}$$

- Recall Eq. (37), $\zeta_\alpha J_\alpha = \delta\mathcal{L}\left[\bar{\Phi}\right]/\delta\bar{\Phi}_\alpha$. Thus vacuum expectation value $|\left\langle\boldsymbol{\varphi}\right\rangle_{J\to 0}| = |\bar{\boldsymbol{\varphi}}| = 2\sqrt{\rho_0}$ (magnitude of homogeneous field configuration, spontaneous magnetization) is determined by

$$0 \stackrel{!}{=} \frac{\delta\mathcal{L}_\Lambda[\bar{\boldsymbol{\varphi}}]}{\delta\bar{\boldsymbol{\varphi}}} = \frac{\delta\Gamma_\Lambda^{\mathrm{We}}[\bar{\boldsymbol{\varphi}}]}{\delta\bar{\boldsymbol{\varphi}}} + R_\Lambda(k^2=0)\bar{\boldsymbol{\varphi}}. \tag{125}$$

  For $\Lambda \to 0$, we use $R_{\Lambda\to 0}(k^2) = 0$ and the ansatz (123) to find the condition for ρ_0:

$$U'_\Lambda(\rho_0) \stackrel{!}{=} 0 \tag{126}$$

Flow equation for $U_\Lambda(\rho)$

- Idea: Insert the ansatz (123) in Wetterich equation ($\zeta = 1$), then take uniform field configuration $\bar{\boldsymbol{\varphi}}$.
- Preparation: Recall $\mathrm{tr} = \sum_{\mathbf{k}} \sum_{j=1}^{N}$ and prepare

$$\bar{\varphi}_j(\mathbf{r}) = \sum_{\mathbf{k}} \bar{\varphi}_j(\mathbf{k}) e^{i\mathbf{kr}} \;\rightarrow\; \frac{\delta\bar{\varphi}_j(\mathbf{r})}{\delta\bar{\varphi}_j(\mathbf{k})} = e^{i\mathbf{kr}}, \qquad \frac{\delta\rho(\mathbf{r})}{\delta\bar{\varphi}_j(\mathbf{k})} = \bar{\varphi}_j(\mathbf{r}) e^{i\mathbf{kr}}, \qquad \frac{\delta\nabla\bar{\varphi}_j(\mathbf{r})}{\delta\bar{\varphi}_{j'}(\mathbf{k})} = i\mathbf{k}\delta_{jj'} e^{i\mathbf{kr}}. \tag{127}$$

- Assume regulator to be momentum and flavor diagonal, $[\mathbf{R}_\Lambda]_{\mathbf{k}j,\mathbf{k}'j'} = \delta_{j,j'} V \delta_{\mathbf{k},-\mathbf{k}'} R_\Lambda(k^2)$.
- Prepare term to be inverted $\frac{1}{V}\frac{\delta}{\delta\bar{\varphi}_i(-\mathbf{k})}\frac{\delta}{\delta\bar{\varphi}_i(\mathbf{k})}\Gamma_\Lambda^{\mathrm{We}}[\bar{\boldsymbol{\varphi}}]\,|_{\bar{\boldsymbol{\varphi}}(\mathbf{r})=\bar{\boldsymbol{\varphi}}}$:
  - U-term:

$$\begin{aligned}
\frac{1}{V}\frac{\delta}{\delta\bar{\varphi}_i(-\mathbf{k})}\frac{\delta}{\delta\bar{\varphi}_i(\mathbf{k})}\int d\mathbf{r} U_\Lambda(\rho(\mathbf{r}))\,|_{\bar{\varphi}} &= \frac{1}{V}\int d\mathbf{r}\frac{\delta}{\delta\bar{\varphi}_i(-\mathbf{k})}\frac{\delta\rho(\mathbf{r})}{\delta\bar{\varphi}_i(\mathbf{k})} U'_\Lambda(\rho(\mathbf{r}))\,|_{\bar{\varphi}} \\
&= \frac{1}{V}\int d\mathbf{r}\frac{\delta}{\delta\bar{\varphi}_i(-\mathbf{k})}\bar{\varphi}_i(\mathbf{r}) e^{i\mathbf{kr}} U'_\Lambda(\rho(\mathbf{r}))\,|_{\bar{\varphi}} \\
&= \frac{1}{V}\int d\mathbf{r}\left\{U'_\Lambda(\rho(\mathbf{r})) + \bar{\varphi}_i^2(\mathbf{r}) U''_\Lambda(\rho(\mathbf{r}))\right\}|_{\bar{\varphi}} \\
&= U'_\Lambda(\rho) + \bar{\varphi}_i^2 U''_\Lambda(\rho)
\end{aligned}$$

  - Z-term: Derivatives need to act on gradient terms, otherwise they vanish when setting $\bar{\boldsymbol{\varphi}}(\mathbf{r}) = \bar{\boldsymbol{\varphi}}$.

$$\frac{1}{V}\frac{\delta}{\delta\bar{\varphi}_i(-\mathbf{k})}\frac{\delta}{\delta\bar{\varphi}_i(\mathbf{k})}\int d\mathbf{r}\frac{c_0}{2} Z_\Lambda^{-1}(\rho(\mathbf{r}))\,(\nabla\bar{\boldsymbol{\varphi}})^2(\mathbf{r})|_{\bar{\boldsymbol{\varphi}}(\mathbf{r})=\bar{\boldsymbol{\varphi}}} = c_0 Z_\Lambda^{-1}(\rho)\, k^2 \tag{128}$$

  - Y-term: We use $\nabla\rho(\mathbf{r}) = \sum_j \bar{\varphi}_j(\mathbf{r})\nabla\bar{\varphi}_j(\mathbf{r})$ and again act on the gradient terms,

$$\begin{aligned}
&\frac{1}{V}\frac{\delta}{\delta\bar{\varphi}_i(-\mathbf{k})}\frac{\delta}{\delta\bar{\varphi}_i(\mathbf{k})}\int d\mathbf{r}\frac{c_0}{4} Y_\Lambda(\rho(\mathbf{r}))\underbrace{\left[\sum_j \bar{\varphi}_j(\mathbf{r})\,\nabla\bar{\varphi}_j(\mathbf{r})\right]^2}_{\sum_{j,j'}\bar{\varphi}_j(\mathbf{r})\nabla\bar{\varphi}_j(\mathbf{r})\bar{\varphi}_{j'}(\mathbf{r})\nabla\bar{\varphi}_{j'}(\mathbf{r})}|_{\bar{\varphi}} \\
&= \frac{1}{V}\int d\mathbf{r}\frac{c_0}{2} Y_\Lambda(\rho(\mathbf{r}))\,\bar{\varphi}_i(\mathbf{r})\bar{\varphi}_i(\mathbf{r})k^2|_{\bar{\varphi}} \\
&= \frac{c_0}{2} Y_\Lambda(\rho)\,\bar{\varphi}_i^2 k^2
\end{aligned}$$

- Summary for Wetterich equation:

$$\partial_\Lambda U_\Lambda(\rho) = \frac{1}{2}\underbrace{\frac{1}{V}\sum_{\mathbf{k}}}_{\int_{\mathbf{k}}}\sum_{i=1}^{N}\partial_\Lambda R_\Lambda(k^2)\left[U'_\Lambda(\rho) + \bar{\varphi}_i^2 U''_\Lambda(\rho) + c_0 Z_\Lambda^{-1}(\rho)\,k^2 + \frac{c_0}{2} Y_\Lambda(\rho)\,\bar{\varphi}_i^2 k^2 + R_\Lambda(k^2)\right]^{-1} \tag{129}$$

- The matrix to be inverted is diagonal in flavor and momentum index. We chose a coordinate system in which $\bar{\boldsymbol{\varphi}}$ is aligned along one flavor direction (=longitudinal direction l with $\bar{\varphi}_l^2/2 = \rho$). The remaining $N-1$ transverse directions have $\bar{\varphi}_l = 0$. We obtain

$$\begin{aligned}
\partial_\Lambda U_\Lambda(\rho) &= \frac{K_D}{2}\int_0^\infty k^{D-1} dk\left[\partial_\Lambda R_\Lambda(k^2)\right] \\
&\times \left\{\frac{1}{U'_\Lambda(\rho) + 2\rho U''_\Lambda(\rho) + c_0 Y_\Lambda(\rho)\,\rho k^2 + c_0 Z_\Lambda^{-1}(\rho)\,k^2 + R_\Lambda(k^2)} + \frac{N-1}{U'_\Lambda(\rho) + c_0 Z_\Lambda^{-1}(\rho)\,k^2 + R_\Lambda(k^2)}\right\}
\end{aligned} \tag{130}$$

- Flow equation for $U_\Lambda(\rho)$ is exact, but approximations are again needed to close the equation and find the flow of $Z_\Lambda^{-1}(\rho)$ and $Y_\Lambda(\rho)$.

Local potential approximation (LPA)

- Approximate Y_Λ and Z_Λ^{-1} by their initial values, $Y_\Lambda(\rho) \stackrel{!}{=} 0$ and $Z_\Lambda^{-1}(\rho) \stackrel{!}{=} 1$. This implies $\eta = 0$ which is often reasonable! Only $U_\Lambda(\rho)$ flows according to Eq. (130).
- Initial condition:
$$U_{\Lambda_0}(\rho) = \frac{1}{V} S_{\Lambda_0}[\varphi] = f_0 + r_0\rho + \frac{u_0}{6}\rho^2 \tag{131}$$
Define $\rho_0 \equiv -3r_0/u_0$ which can be tuned by temperature. Also choose $f_0 = u_0\rho_0^2/6$ and find:
$$U_{\Lambda_0}(\rho) = \frac{u_0}{6}(\rho_0 - \rho)^2 \tag{132}$$
so that r_0 is the initial value of the vacuum expectation value $\langle\varphi^2/2\rangle = \rho_0$ which solves $U'_{\Lambda_0}(\rho_0) \stackrel{!}{=} 0$.
- Interpretation: Minimization of $U_{\Lambda_0}(\rho)$ corresponds to mean-field theory ($\rho_0 \sim \bar{\varphi}^2 \sim m^2$). The fRG in local potential approximation takes into account fluctuations scale by scale. The function $U_\Lambda(\rho)$ will change its shape and the minimum will move.
- Litim regulator:
$$R_\Lambda(k^2) = c_0\left(\Lambda^2 - k^2\right)\Theta\left(\Lambda^2 - k^2\right) \tag{133}$$
This leads to inverse propagators independent of k (it subtracts $G_0^{-1}(k) = c_0k^2$) and one has
$$\partial_\Lambda R_\Lambda(k^2) = 2c_0\Lambda\Theta\left(\Lambda^2 - k^2\right) \tag{134}$$
- Insert local potential approximation and regulator in Eq. (130). Use $\frac{K_D}{2}\int_0^\infty k^{D-1}dk\left[2c_0\Lambda\Theta\left(\Lambda^2 - k^2\right)\right] = c_0\Lambda K_D\int_0^\Lambda k^{D-1}dk$:
$$\boxed{\partial_\Lambda U_\Lambda(\rho) = \frac{c_0K_D\Lambda^{D+1}}{D}\left\{\frac{1}{c_0\Lambda^2 + U'_\Lambda(\rho) + 2\rho U''_\Lambda(\rho)} + \frac{N-1}{U'_\Lambda(\rho) + c_0\Lambda^2}\right\}} \tag{135}$$
- This is a partial differential equation (PDE) that usually needs to be solved numerically (e.g. MATHEMATICA).

8.3 Case $N = 1$: φ^4-theory for Ising model in $D = 3$

Numerical solution of flow equation

- Focus on Ising universality class ($N = 1$, only longitudinal direction) in $D = 3$ dimension where $K_3 \equiv 2\pi^{3/2}/\left[\Gamma(3/2)(2\pi)^3\right]$.
- Fix bare interaction strength $u_0 = 0.01c_0^2\Lambda_0$.
- Let $\lambda = \Lambda/\Lambda_0 : 1 \to 0$ and let $u_\lambda(x = \rho/\rho_0) \equiv U_{\Lambda=\lambda\Lambda_0}(\rho)/f_0$ so that $u_{\lambda=1}(x) = (1-x)^2$.
- Flow equation:
$$\partial_\lambda u_\lambda(x) = \frac{12K_3\lambda^4}{0.01^2}\left(\frac{\Lambda_0}{c_0\rho_0}\right)^3\left\{\frac{1}{6\times 0.01^{-2}\frac{\Lambda_0}{c_0\rho_0}\lambda^2 + u'_\lambda(x) + 2xu''_\lambda(x)}\right\} \tag{136}$$
and $\rho_0 = \#\Lambda_0/c_0$ is the tuning parameter. For the numerically obtained flow plotted over $\bar{\varphi}/\bar{\varphi}_0^{MF} = \sqrt{x}$, see Fig. 25.

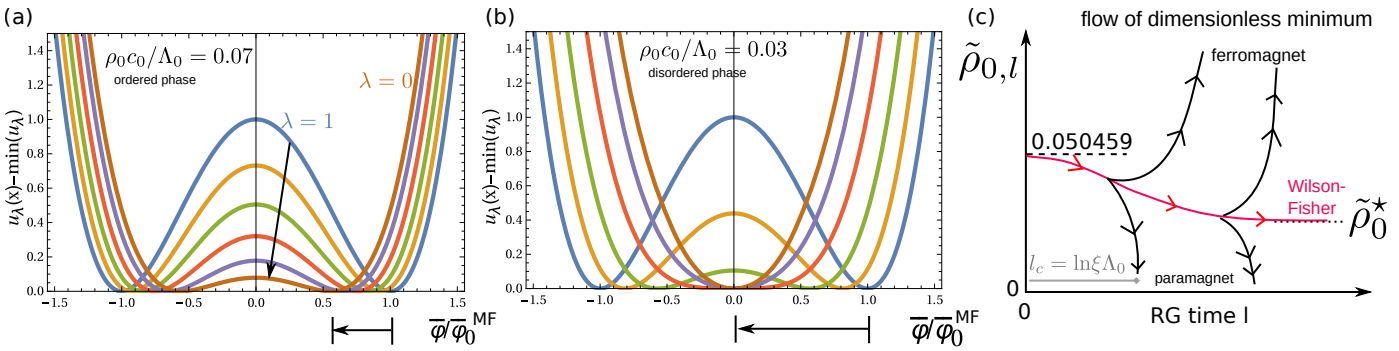


Figure 25: Derivative expansion for φ^4-theory in $D = 3$: (a) Flow of $u_\lambda(x = \sqrt{\bar\varphi/\bar\varphi_0^{MF}})$ reducing the spontaneous magnetization from its mean-field value. (b) Same as in (a), but for smaller mean-field magnetization which corresponds to the disordered phase $\bar\varphi = 0$. (c) Flow of re-scaled position $\tilde\rho_l$ of minimum of $\tilde U_l(\tilde\rho_l)$.

(a) Ordered phase: Start with $\rho_0 = 0.07\Lambda_0/c_0 = \left(\bar\varphi_0^{MF}\right)^2/2$. Flow to $u_{\lambda=0}(x = \sqrt{\bar\varphi/\bar\varphi_0^{MF}})$ that still has minima at finite $\bar\varphi/\bar\varphi_0^{MF} \simeq 0.56$. Interpretation: Fluctuation decrease ordered moment.
Note: If there would be no approximations, we should find $U_{\Lambda=0}(\bar\varphi)$ at the end of the flow to be convex as a function of $\bar\varphi$, i.e. a flat shape in the middle. The convex property is due to the definition of $\Gamma^{\rm We}_{\Lambda=0}[\bar{\boldsymbol\varphi}]$ via a Legendre transform (for $\Lambda \neq 0$, the presence of the regulator R allows non-convex shape).

(b) Disordered phase: Start with $\rho_0 = 0.03\Lambda_0/c_0$ and find flow to $u_{\lambda=0}$ that has single minimum at $\bar\varphi = 0$ which is reached for *finite* λ. The symmetry spontaneously broken by mean-field theory is restored by fluctuations. (Starting with $\rho_0 < 0$ would stay in disordered phase.)

- Right at the critical point, the minimum for $\lambda > 0$ always appears at finite $\bar\varphi$, it takes all fluctuations $\lambda = 0$ to arrive at a minimum at $\bar\varphi = 0$.

Fixed points and critical exponents

- Recall: Non-trivial RG fixed point requires balance of flow driven by canonical dimension (due to dimension of coupling) and one-loop contribution.
Expose canonical dimension by working with dimensionless quantities, e.g. Sec. 7.4.

- Dimensionless LPA: Use $\Lambda = \Lambda_0 e^{-l}$ $(\to \Lambda\partial_\Lambda = -\partial_l)$ and

$$\begin{aligned}
\tilde{\mathbf{k}} &= \mathbf{k}/\Lambda \\
\tilde{\mathbf{r}} &= \mathbf{r}\Lambda \\
\tilde\varphi_i(\tilde{\mathbf{r}}) &= \sqrt{c_0}\Lambda^{(2-D)/2}\bar\varphi(\mathbf{r}) \\
\tilde\rho(\tilde{\mathbf{r}}) &= c_0\Lambda^{2-D}\rho(\mathbf{r}) \\
\tilde U_l(\tilde\rho) &= U_\Lambda(\rho)/\Lambda^D = \tilde f_0 + \frac{\tilde r_l}{2}\tilde\rho^2 + \ldots
\end{aligned}$$

to obtain dimensionless flow equation :

$$\boxed{\partial_l \tilde U_l(\tilde\rho) = \tilde U_l(\tilde\rho)\, D - (D-2)\,\tilde\rho \tilde U_l'(\tilde\rho) - \frac{K_D}{D}\left\{\frac{1}{1+\tilde U_l'(\tilde\rho)+2\tilde\rho\tilde U_\Lambda''(\tilde\rho)} + \frac{N-1}{\tilde U_l'(\tilde\rho)+1}\right\}} \tag{137}$$

- Search for fixed point function $\partial_l \tilde U_l(\tilde\rho) = 0$, it is convenient to rewrite the flow in terms of $\tilde W_l(\tilde\rho) \equiv \tilde U_l'(\tilde\rho)$:

$$\partial_l \tilde W_l(\tilde\rho) = 2\tilde W_l(\tilde\rho) - (D-2)\,\tilde\rho \tilde W_l'(\tilde\rho) + \frac{K_D}{D}\left\{\frac{3\tilde W_\Lambda'(\tilde\rho) + 2\tilde\rho\tilde W_\Lambda''(\tilde\rho)}{\left[1+\tilde W_l(\tilde\rho)+2\tilde\rho\tilde W_\Lambda'(\tilde\rho)\right]^2} + \frac{(N-1)\,\tilde W_l'(\tilde\rho)}{\left[\tilde W_l(\tilde\rho)+1\right]^2}\right\} \tag{138}$$

The location of the running minimum $\tilde{\rho}_{0,l}$ of $\tilde{U}_l(\tilde{\rho})$ is determined by $\tilde{W}_l(\tilde{\rho}_{0,l}) \stackrel{!}{=} 0$.

- Expected fixed point structure (see Fig. 25c):
  - Gaussian fixed point: $\tilde{U}_l(\tilde{\rho}) = \text{const}$ (no interactions and $r_0 = 0$)
  - Ordered/ferromagnetic fixed point: Have finite $\bar{\varphi}_{0,l}$, thus dimensionless $\tilde{\varphi}_{0,l} = \sqrt{c_0}\Lambda^{(2-D)/2}\bar{\varphi}_{0,l} \propto e^{l(D-2)/2}$ diverges.
  - Disordered/paramagnetic fixed point: $\tilde{\varphi}_{0,l}$ vanishes for large l, even if initially finite (c.f. Fig. 25a). This happens at cutoff scale $\Lambda_c \sim 1/\xi$ which should be identified with correlation length.
  - Critical fixed point (Wilson-Fisher fixed point): $\partial_l \tilde{W}_l(\tilde{\rho}) = 0$ and$\tilde{\varphi}_{0,l} \to \tilde{\varphi}_0^\star \neq 0$ for $l \to \infty$.
- Extracting critical exponent ν ($\eta = 0$ by LPA): Fix $\tilde{u}_0$ as above, vary $\tilde{r}_0$ and find $\tilde{\rho}_0^\star = 0.050459$. Go to the paramagnetic side, $\tilde{\rho}_0 \lesssim \tilde{\rho}_0^\star$, "measure" ξ numerically and use $\xi\Lambda_0 \sim |\tilde{r}_0 - \tilde{r}_0^\star|^{-\nu}$ or

$$\ln(\xi\Lambda_0) = -\nu \ln|\tilde{r}_0 - \tilde{r}_0^\star| + const. \tag{139}$$

  For the 3D-Ising case, with Litim regulator and LPA find $\nu_{\text{LPA}} = 0.650$ (very similar to exact $\nu = 0.630$).

8.4 Concluding remarks

- Derivative expansion not applicable for fermions.
  - Reason 1: Recall definition of Grassmann variables $\psi_i\psi_j = -\psi_j\psi_i$ so that $\psi_i^2 = 0$. Thus series expansions only defined up to first order in ψ_i:

$$\Gamma^{\text{We}}[\{\psi_i\}] = \sum_{m_i=0,1} a(m_1, m_2, ..., m_n)\psi_1^{m_1}\psi_2^{m_2}...\psi_n^{m_n} \tag{140}$$

  - Reason 2: To describe Fermi surface, concept of momentum is important.
- For a fermionic system, it can still be useful to define a bosonic order parameter $\phi \sim \bar{\psi}\psi$. Then ϕ might be treated with fRG in derivative expansion.
- Further reading on non-perturbative RG: [Berges et al, Physics Reports 363 (2002) 223]

Part III
Non-equilibrium and Keldysh formalism

9 Quantum dynamics and real-time Green functions

Aims:

- Define various 2-point Green functions and relate them to the Keldysh contour.
- Specialize to equilibrium where spectral density is defined and fluctuation-dissipation theorem holds

9.1 Expectation values

- Quantum expectation value of observable O: $\langle O\rangle = \frac{1}{\mathrm{tr}\rho}\mathrm{tr}[O\rho]$ where ρ is the density matrix (not necessarily normalized) that describes the state of the system and tr... $= \sum_n \langle n|...|n\rangle$ is the sum over matrix elements of a Hilbert space basis $\{|n\rangle\}$.
- So far: Thermal equilibrium (in contact with bath of temperature T):
  - Canonical ensemble $\rho = e^{-\beta H}$
  - Grand canonical ensemble $\rho = e^{-(H-\mu N)\beta}$, with particle number fluctuations, trace is over all particle numbers.
- Non-equilibrium: Not necessarily a bath present, possibly time-dependent Hamiltonian. Assume state is known at $t = t_0 \to -\infty$. For example, $\rho(t_0) = e^{-\beta H}$.

9.2 Dynamics in Schrödinger and Heisenberg picture

- Schrödinger picture: State evolves in time, operators have only explicit time dependence,

$$|\psi(t)\rangle \quad = \quad U(t,t_0)\,|\psi(t_0)\rangle \tag{1}$$

  or for density matrix (von-Neumann equation)

$$\rho(t) = U(t,t_0)\rho_0 U(t_0,t) \tag{2}$$

- Schrödinger equation determines $U(t,t_0)$: From $i\partial_t\,|\psi(t)\rangle = H(t)\,|\psi(t)\rangle$ follows

$$i\partial_t U(t,t_0) = H(t)U(t,t_0). \tag{3}$$

  How to solve for $U(t,t_0)$?

- Preparation: Time ordering operator for general time-dependent operators A, B. Put *later times to the left*:

$$T_t\left[A(t)B(t')\right] = \begin{cases} A(t)B(t') & : t > t' \\ \zeta B(t')A(t) & : t' > t \end{cases} \tag{4}$$

  where ζ encodes the statistics, $\zeta = +1$ for bosons, $\zeta = -1$ for fermions.
  Note: $H = c^\dagger c$ with c fermionic is a bosonic operator.
  Similar: $\tilde{T}_t$ for anti-time-ordering (puts later times to the right).

- Time evolution operator mediates *time evolution from t_0 to t:*

$$\boxed{U(t,t_0) = T_t \exp\left[-i\int_{t_0}^{t} d\tau H(\tau)\right]} \tag{5}$$

The exponent should be interpreted as a power series. The $H(t)$ at different times do not necessarily commute. Due to time-ordering, $H(t)$ always appears on the left.

$$U(t,t_0) = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_{t_0}^{t} dt_1 ... \int_{t_0}^{t} dt_n \, T_t \left(H(t_1) ... H(t_n) \right) \tag{6}$$

- Properties of $U(t,t_0)$:
  - unitarity condition $U^\dagger(t_1,t_2) = U(t_2,t_1)$
  - group properties: $U(t,t) = 1$ and $U(t_3,t_2)U(t_2,t_1) = U(t_3,t_1)$.
  - time-independent Hamiltonian H: $U(t,t_0) = e^{-i(t-t_0)H}$.
- Time evolution of expectation value of operator O:

$$\langle O(t) \rangle = \frac{1}{\mathrm{tr}\rho_0} \mathrm{tr}\left[O U(t,t_0) \rho_0 U(t_0,t) \right] \overset{\text{cycl.}}{=} \frac{1}{\mathrm{tr}\rho_0} \mathrm{tr}\big[\underbrace{U(t_0,t) O U(t,t_0)}_{\equiv O(t) \text{ Heisenberg pic.}} \rho_0 \big] \tag{7}$$

The right-hand side defines the Heisenberg picture, in which operators carry the time-dependence.

9.3 Zoo of real-time Green functions

- Operators A, B:
  - in Heisenberg picture $\rightarrow A(t), B(t')$
  - do not need to be hermitian.
  - with $\zeta = \pm 1$ for bosonic or fermionic operators
- Greater and lesser Green functions [*correlation* functions, do not care about order of times]:

$$G^{>}_{AB}(t,t') = -i \left\langle A(t) B(t') \right\rangle$$
$$G^{<}_{AB}(t,t') = -i\zeta \left\langle B(t') A(t) \right\rangle$$

Note: Unlike in the equilibrium case treated so far, we now generally encounter *two* time arguments, one per operator.

- Retarded and advanced Green functions [expectation values of commutators]:
[with $\theta(0) \equiv 1/2$ and $[A,B]_\zeta \equiv AB - \zeta BA$ is commutator (for $\zeta = 1$, bosons) or anti-commutator (for $\zeta = -1$,fermions)]

$$\begin{aligned} G^R_{AB}(t,t') &\equiv -i\theta(t-t') \left\langle \left[A(t), B(t') \right]_\zeta \right\rangle \\ &= +\theta(t-t') \left(G^{>}_{AB}(t,t') - G^{<}_{AB}(t,t') \right) \end{aligned}$$

$$\begin{aligned} G^A_{AB}(t,t') &\equiv +i\theta(t'-t) \left\langle \left[A(t), B(t') \right]_\zeta \right\rangle \\ &= +\theta(t'-t) \left(G^{<}_{AB}(t,t') - G^{>}_{AB}(t,t') \right) \end{aligned}$$

The retarded $G^R_{AB}(t,t')$ is only non-vanishing for $t - t' \geq 0$, the advanced $G^A_{AB}(t,t')$ for $t - t' \leq 0$.

- Application - Kubo formula: Find change of observable A under perturbation B switched on at time t_0 to order $\mathcal{O}(B)$ ("linear response")

$$\langle A(t) \rangle - \langle A(t_0) \rangle = \int_{-\infty}^{+\infty} dt' G^R_{AB}(t,t') \tag{8}$$

where the right-hand side is calculated for the *unperturbed* system. Thus, retarded (and advanced) Green functions are also called *response* functions.

- Relations at time t, t':

$$\begin{aligned} G^{\lessgtr}_{AB}(t,t') &= -G^{\lessgtr}_{B^\dagger A^\dagger}(t',t)^* \\ G^{>}_{AB}(t,t') &= \zeta G^{<}_{BA}(t',t) \\ G^{A}_{B^\dagger A^\dagger}(t',t) &= G^{R}_{AB}(t,t')^* \\ G^{A}_{BA}(t',t) &= \zeta G^{R}_{AB}(t,t') \end{aligned}$$

  Equal time relations [recall $\theta(0) = 1/2$]:

$$\begin{aligned} G^R_{AB}(t,t) + G^A_{AB}(t,t) &= 0 \\ G^R_{AB}(t,t) - G^A_{AB}(t,t) &= -i\left[A,B\right]_\zeta \end{aligned}$$

- Time ordered Green function [useful for actual calculations]:

$$\begin{aligned} G^T_{A,B}(t,t') &= -i\left\langle T_t A(t) B(t')\right\rangle \\ &= \theta(t-t')G^>_{AB}(t,t') + \theta(t'-t)G^<_{AB}(t,t') \end{aligned}$$

  and anti-time ordered Green function

$$\begin{aligned} G^{\tilde{T}}_{A,B}(t,t') &= -i\left\langle \tilde{T}_t A(t) B(t')\right\rangle \\ &= \theta(t'-t)G^>_{AB}(t,t') + \theta(t-t')G^<_{AB}(t,t') \end{aligned}$$

- Redundancy relation:

$$G^T_{AB}(t,t') + G^{\tilde{T}}_{AB}(t,t') - G^>_{AB}(t,t') - G^<_{AB}(t,t') = 0 \tag{9}$$

- Keldysh Green function (for later):

$$G^K_{AB}(t,t') \equiv G^<_{AB}(t,t') + G^>_{AB}(t,t') \tag{10}$$

  and the above relations imply the "anti-hermitian" property:

$$G^K_{AB}(t,t') = -G^K_{B^\dagger A^\dagger}(t',t)^\star \tag{11}$$

  Parameterization with hermitian matrix F and the hermitian conjugate pair G^R, G^A:

$$\begin{aligned} G^K(t,t') &= \int dt''\left[G^R(t,t'')F(t'',t') - F(t,t'')G^A(t'',t')\right] \\ G^K &= G^R\cdot F - F\cdot G^A \end{aligned}$$

- Temporal Fourier transform for stationary state (or equilibrium) where $G(t,t') \stackrel{!}{=} G(t-t')$:

$$\begin{aligned} G(\omega) &= \int_{-\infty}^{\infty} dt\, e^{i\omega t} G(t) \\ G(t) &= \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\, e^{-i\omega t} G(\omega) \end{aligned}$$

9.4 Green functions in thermal equilibrium and fluctuation-dissipation theorem

- In equilibrium, we can work in single frequency representation.
  All Green functions can be calculated from the *spectral density*:

$$\boxed{A_{AB}(\omega) \equiv i\left(G^R_{AB}(\omega) - G^R_{B^\dagger A^\dagger}(\omega)^\star\right)} \tag{12}$$

- Definition: "Real" and "imaginary" parts of Green function (not the same as for complex numbers unless $A = B^\dagger$, thus denoted by "Gothic" letters).
  Applies for time-ordered, retarded and advanced Green functions:

$$G^{T/R/A} = \Re G^{T/R/A} + i\Im G^{T/R/A} \tag{13}$$

  where

$$\begin{aligned}
\Re G^{T/R/A}_{A,B}(t,t') &\equiv \frac{1}{2}\left(G^{T/R/A}_{A,B}(t,t') + G^{T/R/A}_{B^\dagger,A^\dagger}(t',t)^\star\right), \\
\Im G^{T/R/A}_{A,B}(t,t') &\equiv \frac{1}{2i}\left(G^{T/R/A}_{A,B}(t,t') - G^{T/R/A}_{B^\dagger,A^\dagger}(t',t)^\star\right),
\end{aligned}$$

  or, for stationary states, after Fourier transform,

$$\begin{aligned}
\Re G^{T/R/A}_{A,B}(\omega) &\equiv \frac{1}{2}\left(G^{T/R/A}_{A,B}(\omega) + G^{T/R/A}_{B^\dagger,A^\dagger}(\omega)^\star\right), \\
\Im G^{T/R/A}_{A,B}(\omega) &\equiv \frac{1}{2i}\left(G^{T/R/A}_{A,B}(\omega) - G^{T/R/A}_{B^\dagger,A^\dagger}(\omega)^\star\right).
\end{aligned}$$

  Relations which follow from definitions:

$$\boxed{\Re G^R = \Re G^A = \Re G^T} \tag{14}$$

$$\Im G^R = -\Im G^A = -\frac{1}{2}A \tag{15}$$

- Integral relation for equilibrium: Shift t-integration from real axis to the line $t - i\beta$ (use definition of $\langle ... \rangle$ and $A(t) = e^{-iHt}Ae^{iHt}$)

$$\int dt\, e^{i\omega t}\,\langle A(t)B(0)\rangle = e^{\omega\beta}\int dt\, e^{i\omega t}\,\langle B(0)A(t)\rangle \tag{16}$$

- We derive a relation between $\Im G^{R/A}_{AB}(\omega)$ and $G^>_{AB}(\omega)$:

$$\begin{aligned}
\Im G^R_{AB}(\omega) &= -\Im G^A_{AB}(\omega) \\
&= \frac{1}{2i}\left(G^R_{AB}(\omega) - G^R_{B^\dagger A^\dagger}(\omega)^\star\right) \\
&= \frac{1}{2i}\int_{-\infty}^{\infty} dt\left(e^{i\omega t}G^R_{AB}(t,0) - e^{-i\omega t}\underbrace{G^R_{B^\dagger A^\dagger}(t,0)^\star}_{G^A_{AB}(0,t)}\right) \\
&= \frac{1}{2i}\int_{-\infty}^{\infty} dt\,\left(e^{i\omega t}\theta(t)\left(G^>_{AB}(t,0) - G^<_{AB}(t,0)\right)\right) - e^{-i\omega t}\theta(t)\underbrace{\left(G^<_{AB}(0,t) - G^>_{AB}(0,t)\right)}_{\text{eq.:}G^<_{AB}(-t,0) - G^>_{AB}(-t,0)} \\
(\text{right} : t \to -t) &= \frac{1}{2i}\int_{-\infty}^{\infty} dt\,\left(e^{i\omega t}\theta(t)\left(G^>_{AB}(t,0) - G^<_{AB}(t,0)\right)\right) - e^{i\omega t}\theta(-t)\left(G^<_{AB}(t,0) - G^>_{AB}(t,0)\right) \\
&= \frac{1}{2i}\int_{-\infty}^{\infty} dt\, e^{i\omega t}\left(G^>_{AB}(t,0) - G^<_{AB}(t,0)\right) \\
&= -\frac{1}{2}\int_{-\infty}^{\infty} dt\, e^{i\omega t}\,\langle A(t)B(0) - \zeta B(0)A(t)\rangle \qquad (17) \\
[(16)] &= -\frac{i}{2}\left(1 - \zeta e^{-\omega\beta}\right)G^>_{AB}(\omega) \qquad (18)
\end{aligned}$$

  Similar for time-ordered Green function:

$$\Im G^T_{AB}(\omega) = -\frac{i}{2}\left(1 + \zeta e^{-\omega\beta}\right)G^>_{AB}(\omega)$$

- Combining the last two equations and eliminating $G^>_{AB}(\omega)$, we find a relation between the imaginary parts of retarded, advanced and time-ordered Green functions:

$$\boxed{\Im G^R = -\Im G^A = \frac{1 - \zeta e^{-\beta\omega}}{1 + \zeta e^{-\beta\omega}}\Im G^T(\omega)} \tag{19}$$

- $\Im G^R_{AB}(\omega) = -A_{AB}(\omega)/2$ determines the full $G^R_{AB}(\omega)$: Find full retarded Green function using $\theta(t) = \frac{1}{2\pi i}\int_{-\infty}^{+\infty} d\omega \frac{e^{i\omega t}}{\omega - i\eta}$ and convolution:

$$\begin{aligned} G^R_{A,B}(\omega) &= \int_{-\infty}^{\infty} dt\, e^{i\omega t}\theta(t)\left(G^>_{AB}(t,0) - G^<_{AB}(t,0)\right) \\ &= -\frac{1}{2\pi}\int_{-\infty}^{+\infty} d\omega' \frac{1}{\omega' - \omega - i\eta}\int_{-\infty}^{\infty} dt\, e^{i\omega' t}\left\langle A(t)B(0) - \zeta B(0)A(t)\right\rangle \\ [(17)] &= \frac{1}{\pi}\int_{-\infty}^{+\infty} d\omega' \frac{\Im G^R_{A,B}(\omega')}{\omega' - \omega - i\eta} \\ &= \frac{1}{\pi}\int_{-\infty}^{+\infty} d\omega' \frac{-\frac{1}{2}A_{A,B}(\omega')}{\omega' - \omega - i\eta} \end{aligned}$$

- Similar relations:

$$G^>_{A,B}(\omega) = -\frac{iA_{A,B}(\omega)}{1 - \zeta e^{-\omega\beta}}$$
$$G^<_{A,B}(\omega) = +\frac{iA_{A,B}(\omega)}{1 - \zeta e^{+\omega\beta}}$$

or

$$\boxed{G^K_{AB}(\omega) \equiv G^<_{AB}(\omega) + G^>_{AB}(\omega) = -iA_{AB}(\omega)\frac{e^{\beta\omega} + \zeta}{e^{\beta\omega} - \zeta}} \tag{20}$$

This is the fluctuation-dissipation theorem. It only holds in equilibrium.

  - Fluctuation: Correlation function $G^{\gtrless}$ on the left-hand-side.
  - Dissipation: Imaginary part of the response functions $\Im G^R \sim A$ on the right-hand-side.

9.5 Contour ordered Green function

- Assume the state of a system at $t \to t_0 - \infty$, $\rho(-\infty)$ is known. Recall Eq. (7) for expectation value of operator O:

$$\langle O(t)\rangle = \frac{1}{\mathrm{tr}\rho(t)}\mathrm{tr}\left[U(-\infty,t)OU(t,-\infty)\rho(-\infty)\right]$$

This is shown schematically in Fig. 26(a) in solid lines.

- Extend the time evolution from $-\infty$ to $+\infty$ (top) and back (bottom), see dashed contour also called *Keldysh-contour*. Insert $1 = U(t,+\infty)U(+\infty,t)$ in front of O:

$$\begin{aligned} \langle O(t)\rangle &= \frac{1}{\mathrm{tr}\rho(t)}\mathrm{tr}\left[U(-\infty,t)U(t,+\infty)U(+\infty,t)OU(t,-\infty)\rho(-\infty)\right] \\ &= \frac{1}{\mathrm{tr}\rho(t)}\mathrm{tr}\left[U(-\infty,+\infty)U(+\infty,t)OU(t,-\infty)\rho(-\infty)\right] \end{aligned}$$

Note: Operator O could equally well be inserted on backward branch of contour. Standard choice for later: $O/2$ on both branches.

- Two operators A, B on contour (either on top [+] or bottom branch [-]):
Define contour ordering operator T_c in analogy to time-ordering operator, see gray arrows in Fig. 26(a). This means that time-ordering only matters if two operators are on the same branch. This leads to the 2x2 matrix valued contour-ordered Green function:

$$\boxed{G_{A,B}(t,t') \equiv -i\begin{pmatrix} \langle T_c A_+(t)B_+(t')\rangle & \langle T_c A_+(t)B_-(t')\rangle \\ \langle T_c A_-(t)B_+(t')\rangle & \langle T_c A_-(t)B_-(t')\rangle \end{pmatrix} = \begin{pmatrix} G^T_{A,B}(t,t') & G^<_{A,B}(t,t') \\ G^>_{A,B}(t,t') & G^{\tilde{T}}_{A,B}(t,t') \end{pmatrix}} \tag{21}$$

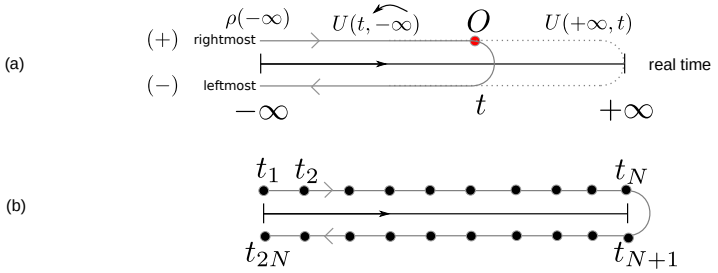


Figure 26: (a) Expectation value $\langle O(t)\rangle$ evaluated on the Keldysh contour c. (b) Time-slice convention for the construction of functional integral representation of partition function.

Exercises

Exercise 9.1. Harmonic oscillator: Green function, spectral density and equation-of-motion technique

The Hamiltonian for a 1D quantum-mechanical oscillator with mass m and frequency ω_0 reads

$$H = \frac{1}{2m}p^2 + \frac{1}{2}m\omega_0^2 x^2 \tag{22}$$

where momentum and position operators satisfy $[p,x]_- = -i$.

1. Introduce the bosonic creation operator $a = x\sqrt{m\omega_0/2} + ip/\sqrt{2m\omega_0}$ and express the Hamiltonian as $H = \omega_0(a^\dagger a + 1/2)$. For the operators $A = a$ and $B = a^\dagger$, find the Heisenberg time-evolution, $a(t)$ and $a^\dagger(t)$. Assuming thermal equilibrium at temperature T, find the greater and lesser Green functions $G^{\gtrless}_{aa^\dagger}$, the retarded and advanced Green function $G^{R/A}_{aa^\dagger}$ and the time ordered Green function $G^{T}_{aa^\dagger}$, both in time and frequency domain. Confirm that the spectral density reads $A_{aa^\dagger} = 2\pi\delta(\omega - \omega_0)$.

2. Use your results in 1.) to find the retarded Green function for the position operator,

$$G^R_{xx}(t) = -\theta(t)\frac{1}{m\omega_0}\sin(\omega_0 t)\,. \tag{23}$$

   Find the same result from the equation-of-motion technique, which does not require a diagonalization of the Hamiltonian: Take the definition of $G^R_{xx}(t)$, apply two t-derivatives and solve the resulting differential equation for $G^R_{xx}(t)$.

Exercise 9.2. Spectral density and tunneling spectroscopy

Consider the equilibrium spectral density $A_{AB}(\omega)$ of Eq. (12) for the case $A = c$, $B = A^\dagger = c^\dagger$ where $c^\dagger$ is a fermionic creation operator. In this exercise, we explore the meaning of $A_{cc^\dagger}(\omega)$ as the energy resolution of a particle created by $c^\dagger$ and discuss an established measurement scheme in the solid state physics context.

1. Show that $A_{cc^\dagger}(\omega)$...
   (a) is normalized $\frac{1}{2\pi}\int_{-\infty}^{+\infty} d\omega A_{cc^\dagger}(\omega) = 1$,
   (b) is real and non-negative (use the Lehmann representation),
   (c) determines the occupation when integrated with the Fermi distribution $n_F(\omega) = \frac{1}{e^{\omega\beta}+1}$, i.e. $\langle c^\dagger c\rangle = \frac{1}{2\pi}\int_{-\infty}^{+\infty} d\omega A_{cc^\dagger}(\omega) n_F(\omega)$.
   (d) is a δ-function for a non-interacting Hamiltonian $H = \varepsilon_0 c^\dagger c$ whereas it broadens if scattering processes remove the particle from its state with rate τ (assume $G^R_{cc^\dagger}(t) = -i\theta(t)e^{-i\varepsilon_0 t}e^{-t/2\tau}$).

2. In solid-state physics, the spectral density can be measured by tunneling spectroscopy. Consider two pieces of metal (described by - *possibly interacting* - Hamiltonians H_A and H_B, respectively) weakly coupled by a tunneling barrier $H_{AB} = \sum_{\nu\mu} T_{\mu\nu} c^\dagger_{A\mu} c_{B\nu} + \text{h.c.}$ with $T_{\mu\nu}$ a small complex tunneling matrix element ($T = T^\dagger$) and Greek letters denoting some basis states of $H_{A,B}$. The total Hamiltonian reads

$H = H_A + H_B + H_{AB}$. The tunnel current through the barrier is given by the rate of change of the charge in metal A (or B), $I = \partial_t Q_A = i[H, Q_A]_-$ where $Q_A = -e\sum_\mu c^\dagger_{A\mu} c_{A\mu}$. Show that

$$I = ie\sum_{\nu\mu}\left(T_{\mu\nu} c^\dagger_{A\mu} c_{B\nu} - T^\star_{\mu\nu} c^\dagger_{B\nu} c_{A\mu}\right) \tag{24}$$

and use the Kubo formula to calculate the (change of) I when the tunneling barrier is added,

$$I(t) = \int_{-\infty}^{+\infty} dt' G^R_{I,H_{AB}}(t,t') \tag{25}$$

where the retarded Green function needs to be calculated with respect to $H_A + H_B$ only. Assume a voltage bias $eV = \mu_A - \mu_B$ between the two metals (i.e. use $H_A \to H_A - \mu_A \sum_\mu c^\dagger_{A\mu} c_{A\mu}$ and analogous for H_B). Show that

$$I = -e\frac{1}{2\pi}\int d\omega \sum_{\nu\mu} |T_{\mu\nu}|^2 A_{c_{A\mu}c^\dagger_{A\mu}}(\omega) A_{c_{B\nu}c^\dagger_{B\nu}}(\omega + eV)\left[n_F(\omega + eV) - n_F(\omega)\right]. \tag{26}$$

Assume that metal B has a spectral density that does not vary strongly with ω, $\sum_\nu |T_{\mu\nu}|^2 A_{c_{B\nu}c^\dagger_{B\nu}}(\omega) \simeq$ const., and we also assumed that $|T_{\mu\nu}|^2$ does not vary strongly with μ. Show that at low temperature, the differential conductance $dI/dV = G(V)$ is proportional to $\sum_\mu A_{c_{A\mu}c^\dagger_{A\mu}}(-eV)$. This underlies the principle of tunneling spectroscopy.

10 Keldysh functional integral

Aims:

- Find functional integral formulation of operator formalism of Sec. 9.

10.1 Generating function $Z[V]$

- Define time-evolution operator on closed time contour c:

$$U_c \equiv U(-\infty, +\infty)\, U(+\infty, -\infty) = 1 \tag{27}$$

- Source-term for observable O: $H(t) \to H^\pm(t) = H(t) \pm OV(t)$ where $V(t)$ is a function and H^+ is applied on forward branch of c, H^- on backward branch. Thus:

$$U_c \to U_c[V] \tag{28}$$

- Generating function (also "partition function")

$$\boxed{Z[V] \equiv \frac{1}{\mathrm{tr}\rho(-\infty)}\mathrm{tr}\left\{U_c[V]\,\rho(-\infty)\right\}} \tag{29}$$

We can compute $\langle O(t)\rangle$ from generating functional as

$$\langle O(t)\rangle = \frac{i}{2}\frac{\delta Z[V]}{\delta V(t)}|_{V=0} \tag{30}$$

Proof:

$$\begin{aligned}
\frac{i}{2}\frac{\delta Z[V]}{\delta V(t)}|_{V=0} &= \frac{i}{2}\frac{1}{\mathrm{tr}\rho(-\infty)}\mathrm{tr}\left\{\frac{\delta}{\delta V(t)} U_c[V]\,\rho(-\infty)\right\}|_{V=0} \\
&= \frac{i}{2}\frac{1}{\mathrm{tr}\rho(-\infty)} \\
&\times \mathrm{tr}\{\frac{\delta U_{-V}(-\infty,+\infty)}{\delta V(t)} U_{+V}(+\infty,-\infty)\rho(-\infty) + U_{-V}(-\infty,+\infty)\frac{\delta U_{+V}(+\infty,-\infty)}{\delta V(t)}\rho(-\infty)\}|_{V=0}
\end{aligned}$$

and use

$$\frac{\delta U_{+V}\left(+\infty,-\infty\right)}{\delta V(t)}|_{V=0}=\frac{\delta}{\delta V(t)}T_t\exp\left[-i\int_{-\infty}^{+\infty}d\tau H(\tau)+OV(\tau)\right]|_{V=0}$$
$$=U\left(+\infty,t\right)\left(-iO\right)U\left(t,-\infty\right)$$

- Remarks:
  - Without source field, partition function is normalized: $Z[V=0]=1$.
  - If source-field is different on the two branches, have $U_c\left[V\right]\neq 1$ and $Z[V]\neq 1$.

10.2 Functional integral representation for $Z[V]$ (Bosons)

Review: Bosonic coherent states

Def. coherent state	$\|\phi\rangle=e^{\sum_{l=1}^{M}\phi_l a_l^\dagger}\|0\rangle,\ \phi_l\in\mathbb{C}$	overlap	$\langle\phi\|\psi\rangle=e^{\sum_l\phi_l^\star\psi_l}$
action of a_l	$a_l\|\phi\rangle=\phi_l\|\phi\rangle$	res. of id.	$1=\int\underbrace{\prod_l\frac{d\phi_l^\star d\phi_l}{\pi}e^{-\sum_l\phi_l^\star\phi_l}}_{d(\phi^\star,\phi)}\|\phi\rangle\langle\phi\|$
action of $a_l^\dagger$	$\langle\phi\|a_l^\dagger=\langle\phi\|\phi_l^\star$	trace	$\mathrm{tr}O=\int d(\phi^\star,\phi)e^{-\sum_l\phi_l^\star\phi_l}\langle\phi\|O\|\phi\rangle$
auxiliary identity	$\left\langle\phi\|c^{a^\dagger a}\|\psi\right\rangle=e^{\phi^\star\psi c},\ c\in\mathbb{C}$		

- Proof of auxiliary identity (does not appear in equilibrium applications): Define

$$f(c)\equiv\left\langle\phi\|c^{a^\dagger a}\|\psi\right\rangle\rightarrow\partial_c f(c)=\left\langle\phi\|a^\dagger a c^{a^\dagger a-1}\|\psi\right\rangle. \tag{31}$$

  Note that for an arbitrary function g, we have

$$ag(a^\dagger a-1)=g(a^\dagger a)a. \tag{32}$$

  This is clear by acting on basis vector $|n\rangle$ which yields $g(n-1)\sqrt{n}\,|n-1\rangle$ on the left and on the right. Then we find

$$\partial_c f(c)=\left\langle\phi\|a^\dagger c^{a^\dagger a}a\|\psi\right\rangle=\phi^\star\psi f(c) \tag{33}$$

  This can be uniquely solved as $f(c)=e^{c\phi^\star\psi}$ since indeed $f(c=1)=\langle\phi|\psi\rangle=e^{\phi^\star\psi}$.

Construction of functional integral representation of Z

- First start without source terms ($V=0$)
- Bosonic Hamiltonian in 2nd quantization with all creation operators left of annihilators ("normal ordered"). The operators fulfill $[a_n,a_m^\dagger]_+=\delta_{nm}$, assume M degrees of freedom $l=1,2,...,M$:

$$H\left(a^\dagger,a\right)=\sum_{l,m}t_{lm}a_l^\dagger a_m+\sum_{l,m,n,o}U_{lmno}a_l^\dagger a_m^\dagger a_n a_o \tag{34}$$

- Take standard steps to coherent state functional integral representation for Z, pay attention to (+) or (-) contour.

1. Use formula for trace
2. Slice closed contour c into $2N-2$ intervals so that $t_1=-\infty=t_{2N}$ and $t_N=+\infty=t_{N+1}$, see Fig. 26(b). We label time-steps by $j=1,2,..,2N$ and use $U_c=U_{-\delta t}...U_{-\delta t}\cdot 1\cdot U_{\delta t}...U_{\delta t}$. Insert resolution of identity operator using bosonic coherent states.

$$
\begin{aligned}
Z &= \frac{1}{\mathrm{tr}\rho}\mathrm{tr}\left\{U_c\rho\right\} \\
(1.) &= \frac{1}{\mathrm{tr}\rho}\int d(\phi^\star_{2N},\phi_{2N})e^{-\sum_l|\phi_{2N,l}|^2}\left\langle\phi_{2N}|U_c\rho|\phi_{2N}\right\rangle \\
(2.) &= \frac{1}{\mathrm{tr}\rho}\int\prod_{j=1}^{2N}d(\phi^\star_j,\phi_j)\left\langle\phi_{2N}|U_{-\delta t}|\phi_{2N-1}\right\rangle\cdots\left\langle\phi_{N+2}|U_{-\delta t}|\phi_{N+1}\right\rangle\underbrace{\left\langle\phi_{N+1}|1|\phi_N\right\rangle}_{=1} \\
&\times \left\langle\phi_N|U_{\delta t}|\phi_{N-1}\right\rangle\cdots\left\langle\phi_2|U_{\delta t}|\phi_1\right\rangle\left\langle\phi_1|\rho|\phi_{2N}\right\rangle\exp\left[-\sum_{j=1}^{2N}\sum_{l=1}^{M}|\phi_{n,l}|^2\right]
\end{aligned}
$$

- Evaluate matrix elements for $\delta t\to 0$ (keep $\delta t\times[2N-2]$ fixed) where we use that H is normal ordered and approximately time-independent on a time-scale δt:

$$
\begin{aligned}
\left\langle\phi_j|U_{\pm\delta t}|\phi_{j-1}\right\rangle &= \left\langle\phi_j|e^{\mp i\delta t H(a_l^\dagger,a_l)}|\phi_{j-1}\right\rangle \\
&= \left\langle\phi_j|1\mp i\delta t H(a_l^\dagger,a_l)+\mathcal{O}(\delta t^2)|\phi_{j-1}\right\rangle \\
&= \left\langle\phi_j|\phi_{j-1}\right\rangle\left[1\mp i\delta t H(\phi^\star_{j,l},\phi_{j-1,l})+\mathcal{O}(\delta t^2)\right] \\
&= e^{\phi^\star_j\phi_{j-1}}\left[e^{\mp i\delta t H(\phi^\star_{j,l},\phi_{j-1,l})}+\mathcal{O}(\delta t^2)\right]
\end{aligned}
$$

  Insert in expression for Z (suppress l and recall $\phi_{N+1}=\phi_N$):

$$
\boxed{Z=\frac{1}{\mathrm{tr}\rho}\int\prod_{j=1}^{2N}d(\phi^\star_j,\phi_j)\exp\left[\sum_{j=2}^{2N}\phi^\star_j\phi_{j-1}-i\delta t\sum_{j=2}^{N}H(\phi^\star_j,\phi_{j-1})+i\delta t\sum_{j=N+2}^{2N}H(\phi^\star_j,\phi_{j-1})-\sum_{j=1}^{2N}|\phi_j|^2\right]\left\langle\phi_1|\rho|\phi_{2N}\right\rangle} \tag{35}
$$

Example: Single non-interacting bosonic mode

- Consider single bosonic mode $H=\omega_0 a^\dagger a$ starting out in equilibrium:

$$
\rho(-\infty)\equiv\rho=e^{-\beta H}=e^{-\beta\omega_0 a^\dagger a} \tag{36}
$$

- Preparations:
  - Normalization: $\mathrm{tr}\rho=\sum_{n=0}^{\infty}e^{-\beta\omega_0 n}=1/(1-e^{-\beta\omega_0})$
  - For last factor in Z, use auxiliary identity from table with $c=e^{-\beta\omega_0}$: $\left\langle\phi_1|e^{-\beta\omega_0 a^\dagger a}|\phi_{2N}\right\rangle=\exp\left(e^{-\beta\omega_0}\phi^\star_1\phi_{2N}\right)$

- Express Z as

$$
Z=\frac{1}{\mathrm{tr}\rho}\int\prod_{j=1}^{2N}d(\phi^\star_j,\phi_j)\exp\left[i\sum_{j,j'=1}^{2N}\phi^\star_j G^{-1}_{jj'}\phi_{j'}\right] \tag{37}
$$

  with the $2N\times 2N$-matrix (here, choose $N=3$ for clarity)

$$
i\left(G^{-1}\right) = \begin{pmatrix}
-1 & 0 & 0 & 0 & 0 & e^{-\beta\omega_0} \\
h_- & -1 & 0 & 0 & 0 & 0 \\
0 & h_- & -1 & 0 & 0 & 0 \\
0 & 0 & 1 & -1 & 0 & 0 \\
0 & 0 & 0 & h_+ & -1 & 0 \\
0 & 0 & 0 & 0 & h_+ & -1
\end{pmatrix} \tag{38}
$$

  where $h_-=1-i\delta t\omega_0$ and $h_+=1+i\delta t\omega_0$ and the $e^{-\beta\omega_0}$ and 1 are the gluing conditions which connect + and - branch.

- Check normalization ($Z = 1$): The functional integral yields $1/\det\left(-iG^{-1}\right)$. Expand the determinant with respect to the top row, use for upper or lower triangular matrix T: $\det T = t_{11}t_{22}...$,

$$\begin{aligned}
\det\left(-iG^{-1}\right) &= \det\left([iG]^{-1}\right) \\
&= (-1)(-1)^{2N-1} - e^{-\beta\omega_0} {h_-}^{N-1} 1 {h_+}^{N-1} \\
&= 1 - e^{-\beta\omega_0} \left(1 - i\delta t\omega_0\right)^{N-1} \left(1 + i\delta t\omega_0\right)^{N-1} \\
&= 1 - e^{-\beta\omega_0} \left(1 + \delta t^2\omega_0^2\right)^{N-1} \\
&= 1 - e^{-\beta\omega_0} \left(1 + (N-1)\frac{\delta t^2\omega_0^2}{N-1}\right)^{N-1} \\
&\simeq 1 - e^{-\beta\omega_0} \underbrace{\exp\left[(N-1)\delta t \times \delta t\omega_0^2\right]}_{\to 1} \\
\{\delta t N = const.\} &\simeq 1 - e^{-\beta\omega_0}
\end{aligned}$$

  This cancels with $1/\mathrm{tr}\rho$, so normalization is confirmed:

$$Z = \frac{1 - e^{-\beta\omega_0}}{1 - e^{-\beta\omega_0}} = 1. \tag{39}$$

Continuum limit (for generic bosons)

- Take continuum limit as $N \to \infty$, $\delta t \to 0$ with $N\delta t = const.$
- For forward branch $\phi_{j=1,2,..,N} \to \phi_+(t)$, $\sum_{j=1}^{N} \delta t \to \int_{-\infty}^{+\infty} dt$, and

$$\phi_j^\star \phi_{j-1} - \phi_j^\star \phi_j = -\delta t \phi_j^\star \frac{\phi_j - \phi_{j-1}}{\delta t} \to -\delta t \phi_+^\star(t) \partial_t \phi_+(t) \tag{40}$$

  Analogous on backward branch.

- Find:

$$Z = \int_{\phi_+(\infty)=\phi_-(\infty)} D\left[\phi_+^\star, \phi_+, \phi_-^\star, \phi_-\right] e^{iS[\phi_+,\phi_-]} \langle \phi_+(-\infty) | \rho | \phi_-(-\infty) \rangle \tag{41}$$

  with

$$\begin{aligned}
S\left[\phi_+, \phi_-\right] &= + \int_{-\infty}^{+\infty} dt \left[\sum_l \phi_{+,l}^\star(t) i\partial_t \phi_{+,l}(t) - H\left[\phi_+^\star(t), \phi_+(t)\right]\right] \\
&\quad - \int_{-\infty}^{+\infty} dt \left[\sum_l \phi_{-,l}^\star(t) i\partial_t \phi_{-,l}(t) - H\left[\phi_-^\star(t), \phi_-(t)\right]\right]
\end{aligned}$$

  and

$$D\left[\phi_+^\star, \phi_+, \phi_-^\star, \phi_-\right] \equiv \frac{1}{\mathrm{tr}\rho} \cdot \lim_{N\to\infty} \int \prod_{j=1}^{2N} d(\phi_j^\star, \phi_j) \tag{42}$$

- Remarks:
  - Keep in mind: Continuum notation is just an abbreviation for discrete form.
  - Compare to equilibrium formalism, $Z = \int D[\phi^\star, \phi] e^{-S[\phi]}$ with $S = \int_0^\beta d\tau \phi^\star(\tau) \partial_\tau \phi(\tau) + H[\phi^\star(\tau), \phi(\tau)]$ and no backward evolution. In Keldysh, we now have *two* copies of the field in real-time for forward and backward branch, with *opposite* signs of the action $(-)$.
  - The field ϕ_+ is coupled to field ϕ_- at the two boundaries, $\phi_+(\infty) = \phi_-(\infty)$ and $\langle \phi_+(-\infty) | \rho | \phi_-(-\infty) \rangle$. In the case of Eq. (38), these correspond to the entries 1, $e^{-\beta\omega_0}$ in the corners of the off-diagonal blocks of $i\left(G^{-1}\right)$.

Green functions (for single bosonic mode)

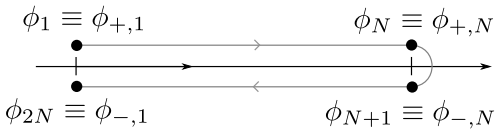
- Find two-point function (no factor of $1/Z$!) at times t, t' corresponding to time slice j, j'. Use Gaussian integral formula:

$$\left\langle T_c a(t) a^\dagger(t') \right\rangle = \left\langle \phi_j \phi^\star_{j'} \right\rangle \equiv \frac{1}{\mathrm{tr}\rho} \int \prod_{k=1}^{2N} d(\phi^\star_k, \phi_k) \phi_j \phi^\star_{j'} \exp\left[i \sum_{k,k'=1}^{2N} \phi^\star_k G^{-1}_{kk'} \phi_{k'} \right] = i G_{jj'} \tag{43}$$

- Back to simple model $H = \omega_0 a^\dagger a$, can invert G^{-1} explicitly ($\rho \equiv e^{-\beta\omega_0}$). Here for $N = 3$ (but generalization to arbitrary N straightforward),

$$iG = \frac{1}{\det(-iG^{-1})} \begin{bmatrix} 1 & \rho h_+^2 h_- & \rho h_+^2 & \rho h_+^2 & \rho h_+ & \rho \\ h_- & 1 & \rho h_+^2 h_- & \rho h_+^2 h_- & \rho h_+ h_- & \rho h_- \\ h_-^2 & h_- & 1 & \rho h_+^2 h_-^2 & \rho h_+ h_-^2 & \rho h_-^2 \\ h_-^2 & h_- & 1 & 1 & \rho h_-^2 h_+ & \rho h_-^2 \\ h_-^2 h_+ & h_- h_+ & h_+ & h_+ & 1 & \rho h_-^2 h_+ \\ h_-^2 h_+^2 & h_- h_+^2 & h_+^2 & h_+^2 & h_+ & 1 \end{bmatrix} \text{ with } \begin{pmatrix} \phi_1 = \phi_{+,1} \\ \vdots \\ \phi_N = \phi_{+,N} \\ \phi_{N+1} = \phi_{-,N} \\ \vdots \\ \phi_{2N} = \phi_{-,1} \end{pmatrix}. \tag{44}$$

For convenience, we re-label the slice-index to indicate the top (+) or bottom (-) part of the contour:



- Compare to Eq. (21), read off four propagators $G^{</>/T/\tilde{T}}$, depending on choice of $\phi_\pm$:

$$\begin{aligned}
iG^<_{jl} &\equiv \left\langle \phi_{+,j} \phi^\star_{-,l} \right\rangle = \frac{e^{-\beta\omega_0} h_+^{l-1} h_-^{j-1}}{\det(-iG^{-1})} \\
iG^>_{jl} &\equiv \left\langle \phi_{-,j} \phi^\star_{+,l} \right\rangle = \frac{h_+^{N-j} h_-^{N-l}}{\det(-iG^{-1})} \\
iG^T_{jl} &\equiv \left\langle \phi_{+,j} \phi^\star_{+,l} \right\rangle = \frac{h_-^{j-l}}{\det(-iG^{-1})} \begin{cases} 1 & : j \geq l \\ e^{-\beta\omega_0} (h_+ h_-)^{N-1} & : j < l \end{cases} \\
iG^{\tilde{T}}_{jl} &\equiv \left\langle \phi_{-,j} \phi^\star_{-,l} \right\rangle = \frac{h_+^{l-j}}{\det(-iG^{-1})} \begin{cases} e^{-\beta\omega_0} (h_+ h_-)^{N-1} & : j > l \\ 1 & : j \leq l \end{cases}
\end{aligned}$$

- Continuum limit, $(h_+ h_-)^N \to 1$ as before. Use $h_\pm^j = \left(1 \pm i \frac{\delta t j}{j} \omega_0\right)^j \to e^{\pm i\omega_0 \delta t j} = e^{\pm i\omega_0 t}$, and $\det(-iG^{-1}) = 1 - e^{-\beta\omega_0}$ and the boson number $n_B = \frac{e^{-\beta\omega_0}}{1-e^{-\beta\omega_0}} = \frac{1}{e^{\beta\omega_0}-1}$

$$\begin{aligned}
iG^<(t,t') &= n_B e^{-i\omega_0(t-t')} \\
iG^>(t,t') &= (n_B + 1) e^{-i\omega_0(t-t')}
\end{aligned}$$

$$G^T(t,t') = \begin{cases} G^>(t,t') & : t \geq t' \\ G^<(t,t') & : t < t' \end{cases} \tag{45}$$

$$G^{\tilde{T}}(t,t') = \begin{cases} G^>(t,t') & : t' \geq t \\ G^<(t,t') & : t' < t \end{cases} \tag{46}$$

Up to the case $t = t'$ (see below), this is in agreement with the result from the operator formalism in Sec. 9.3 and Ex. 9.1.

- Equal times: The last two lines differ from the convention $\theta(0) = 1/2$ put forward in Sec. 9.3! This should not bother us because:
  - What matters for practical calculations in the fulfillment of $G^R(t,t)+G^A(t,t) = G^T(t,t)-G^{\tilde{T}}(t,t) = 0$ and $G^R(t,t) - G^A(t,t) = G^>(t,t) - G^<(t,t) = -i$ (the commutator).
  - The redundancy relation (9) is modified at equal times:

$$G^T(t,t') + G^{\tilde{T}}(t,t') - G^>(t,t') - G^<(t,t') = \begin{cases} 0 & : t \neq t' \\ 1 & : t = t' \end{cases} \tag{47}$$

    The right hand side is a manifold of measure zero in the t-t'-plane and does not bother us further in the next section.

Keldysh rotation (for generic bosons)

- Idea: Take into account the redundancy relation (9) in a simple form. Find retarded, advanced and Keldysh Green functions.
- Define new fields in terms of rotation applied to $\phi_\pm$ (analogous for $\phi^\star_\pm$):

$$\phi_c(t) \equiv \frac{1}{\sqrt{2}}\left(\phi_+(t) + \phi_-(t)\right)$$
$$\phi_q(t) \equiv \frac{1}{\sqrt{2}}\left(\phi_+(t) - \phi_-(t)\right)$$

  The components $\phi_{c,q}$ are called "classical" and "quantum".
- The rotation yields for

$$iG_{\alpha\beta}(t,t') \equiv \left\langle \phi_\alpha(t)\phi^\star_\beta(t')\right\rangle \tag{48}$$

  with $\alpha, \beta \in \{c, q\}$:

$$G = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} G^T & G^< \\ G^> & G^{\tilde{T}} \end{pmatrix}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \begin{pmatrix} G^K(t,t') & G^R(t,t') \\ G^A(t,t') & 0 \end{pmatrix} \tag{49}$$

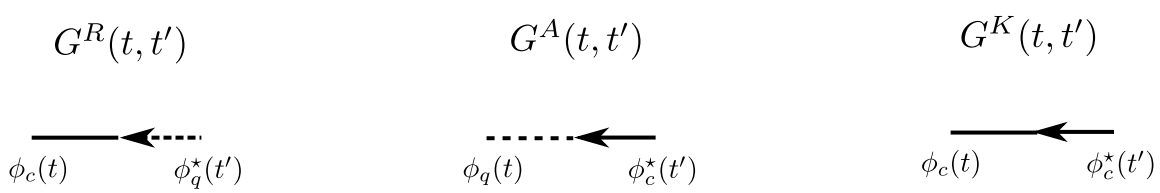
  and we identify the retarded (R), advanced (A) and Keldysh (K) component introduced above in Sec. 9.3. The zero in the bottom right ($\left\langle \phi_q(t)\phi^\star_q(t')\right\rangle = 0$) is the consequence of Eq. (47).
- Example: Single bosonic mode $H_0 = \omega_0 a^\dagger a$ (see Ex. 9.1):

$$G_{aa^\dagger}(t,t') = -ie^{-i\omega_0(t-t')}\begin{pmatrix} 2n_B + 1 & \theta(t-t') \\ -\theta(t'-t) & 0 \end{pmatrix} \tag{50}$$

  and the Fourier-trafo with the important infinitesimal convergence factors η reads:

$$G_{aa^\dagger}(\omega) = \begin{pmatrix} -i2\pi\delta(\omega_0 - \omega)\left[2n_B + 1\right] & \frac{1}{\omega-\omega_0+i\eta} \\ \frac{1}{\omega-\omega_0-i\eta} & 0 \end{pmatrix} \tag{51}$$

- Graphical representation for $-i\left\langle \phi_\alpha(t)\phi^\star_\beta(t')\right\rangle$. Conventions:
  - classical field $\phi_c, \phi^\star_c$: solid line
  - quantum field $\phi_q, \phi^\star_q$: dashed line
  - arrow: from $\phi^\star_\beta(t')$ to $\phi_\alpha(t)$



Keldysh action

- Non-interacting case: Want action $S[\phi_c, \phi_q]$ such that ($\alpha, \beta \in \{c, q\}$)

$$\left\langle \phi_\alpha(t)\phi^\star_\beta(t')\right\rangle = \int D\left[\phi_c, \phi_q\right] \phi_\alpha(t)\phi^\star_\beta(t') e^{iS[\phi_c,\phi_q]} \tag{52}$$

  reproduces Eq. (49). Need

$$\boxed{S[\phi_c, \phi_q] = \int_{-\infty}^{+\infty} dtdt' \left(\phi^\star_c(t), \phi^\star_q(t)\right) \underbrace{\begin{pmatrix} 0 & \left[G^{-1}\right]^A(t,t') \\ \left[G^{-1}\right]^R(t,t') & \left[G^{-1}\right]^K(t,t') \end{pmatrix}}_{\equiv G^{-1}} \begin{pmatrix} \phi_c(t') \\ \phi_q(t') \end{pmatrix}} \tag{53}$$

  with the defining condition for G^{-1}:

$$G^{-1}\cdot G = \begin{pmatrix} 0 & \left[G^{-1}\right]^A \\ \left[G^{-1}\right]^R & \left[G^{-1}\right]^K \end{pmatrix} \cdot \begin{pmatrix} G^K & G^R \\ G^A & 0 \end{pmatrix} = \mathbf{1} \equiv \begin{pmatrix} \delta(t-t') & 0 \\ 0 & \delta(t-t') \end{pmatrix} \tag{54}$$

- Written in components, we have the following relations:

$$\begin{aligned} \left[G^{-1}\right]^A &= \left[G^A\right]^{-1} \\ \left[G^{-1}\right]^R &= \left[G^R\right]^{-1} \\ \left[G^{-1}\right]^K &= -\left[G^{-1}\right]^R \cdot G^K \cdot \left[G^{-1}\right]^A = \left[G^R\right]^{-1}\cdot F - F\cdot\left[G^A\right]^{-1} \end{aligned}$$

  where in the last step, we used $G^K = G^R\cdot F - F\cdot G^A$. Note: $\left[G^{-1}\right]^K \neq \left[G^K\right]^{-1}$.

- Main features of $S[\phi_c, \phi_q]$ (called "causality structure", remains intact even with interactions):
  - $S[\phi_c, \phi_q = 0] = 0 \leftrightarrow c$ - c block of quadratic action vanishes: If $\phi_q = 0$, then $\phi_+ = \phi_-$ and the action on the forward and backward branch is canceled.
  - The $q-c$ and $c-q$ sub-matrices $\left[G^{-1}\right]^A$ and $\left[G^{-1}\right]^R$ of G^{-1} are mutually hermitian conjugated lower and upper triangular matrices in the time-domain. Indeed, in Sec. 9.3 we found for $A = B^\dagger$: $G^A(t',t) = G^R(t,t')^*$
  - The $q-q$ component is anti-hermitian, $G^K(t',t) = -G^K(t,t')^*$. It is responsible for convergence of functional integral and contains information about the distribution function.
    For the single bosonic mode model, we have after a short calculation $\left[G^{-1}\right]^K \propto \eta$, it becomes finite if interactions are added.

External sources

- For the computation of observables, want to include source-fields $Z \to Z[V]$, see Eq. (29). Recall sources should be different on forward and backward branch, assume the following coupling $V_+(t,t')\phi^\star_+(t)\phi_+(t')$ and $V_-(t,t')\phi^\star_-(t)\phi_-(t')$.

- Keldysh-rotation for source fields (like $\phi_\pm \to \phi_{c,q}$ but with extra factor $1/\sqrt{2}$)

$$\begin{aligned} V_c &= \frac{1}{2}\left(V_+ + V_-\right) \\ V_q &= \frac{1}{2}\left(V_+ - V_-\right) \end{aligned}$$

  Note:
  - For $V_q = 0$, we have $V_+ = V_-$ and thus $Z[V_c, V_q = 0] = 1$.

- Keldysh action in continuum:

$$S = \int_{-\infty}^{+\infty} dt dt' \left(\phi_c^\star(t), \phi_q^\star(t)\right) \left[G^{-1}(t,t') - \begin{pmatrix} V_q & V_c \\ V_c & V_q \end{pmatrix}(t,t')\right] \begin{pmatrix} \phi_c(t') \\ \phi_q(t') \end{pmatrix} \tag{55}$$

- Partition function from Gaussian integral

$$Z[V_c, V_q] = \frac{1}{\mathrm{tr}(\rho)} \frac{1}{\det\left(-iG^{-1} + iV\right)} = \frac{1}{\det\left(1 - G \cdot V\right)} = \exp\left(-\mathrm{tr}\ln\left[1 - G \cdot V\right]\right) \tag{56}$$

  where the trace runs over Keldysh-matrix index and time.

Example (single bosonic mode):

- Compute observable

$$\begin{aligned} i\frac{\delta Z[V_c, V_q]}{\delta V_q(t,t')}|_{V_{c,q}=0} &= \left\langle \phi_c^\star(t)\phi_c(t') + \phi_q^\star(t)\phi_q(t') \right\rangle \\ &= \left\langle \phi_+^\star(t)\phi_+(t') + \phi_-^\star(t)\phi_-(t') \right\rangle \end{aligned} \tag{57}$$

  We compute both sides of Eq. (57) separately:

1. Right-hand side: Recall that in the functional integral formalism

$$\left\langle T_t a(t_1) a^\dagger(t_2) \right\rangle = \left\langle \phi_+(t_1)\phi_+^\star(t_2) \right\rangle, \ \left\langle \tilde{T}_t a(t_1) a^\dagger(t_2) \right\rangle = \left\langle \phi_-(t_1)\phi_-^\star(t_2) \right\rangle \tag{58}$$

   and obtain:

$$\begin{aligned} \left\langle \phi_+(t)\phi_+^\star(t') + \phi_-(t)\phi_-^\star(t') \right\rangle &= \left\langle T_t a(t) a^\dagger(t') + \tilde{T}_t a(t) a^\dagger(t') \right\rangle \\ &= iG^T(t,t') + iG^{\tilde{T}}(t,t') \end{aligned}$$

2. Left-hand side:

$$\begin{aligned} i\frac{\delta Z[V_c, V_q]}{\delta V_q(t,t')}|_{V_{c,q}=0} &= i\frac{\delta \exp\left(-\mathrm{tr}\ln\left(1 - G \cdot V\right)\right)}{\delta V_q(t,t')}|_{V_{c,q}=0} \\ &= -i\mathrm{tr}\left[\left(1 - \mathrm{G} \cdot \mathrm{V}\right)^{-1}(-G)\frac{\delta V}{\delta V_q(t,t')}\right]|_{V_{c,q}=0} \\ &= i\mathrm{tr}_2\left[G(t',t)\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\right] \\ &= iG^K(t,t') \end{aligned}$$

   and we now from Sec. 9.3 that both expressions are equal.

Exercises

Exercise 10.1. Driven harmonic oscillator

A quantum harmonic oscillator $H_0 = \omega_0 a^\dagger a$ (with $a, a^\dagger$ bosonic operators) is coupled to a time-dependent driving field $U(t)$ which vanishes for $t \to \pm\infty$,

$$H(t) = H_0 + U(t)\left(a + a^\dagger\right)/\sqrt{2}. \tag{59}$$

This non-interacting but non-equilibrium problem can be treated exactly using the Keldysh formalism. Assume that the oscillator starts out in the ground state at $t \to -\infty$.

1. Upgrade $U(t)$ to a source field $U_\pm(t)$. Note that $U_\pm$ couples differently to the fields ϕ,$\phi^\star$ compared to the source $V_\pm$ used in the lecture. What could be the motivation for the coupling in (59)? Write down the generating functional $Z[U_+, U_-]$ for $H(t)$ in the continuum notation. Perform the Keldysh rotation ($2U_{c/q} = U_+ \pm U_-$) and introduce the (inverse of the) matrix of non-driven harmonic oscillator Green functions

$$G(t,t') = \begin{pmatrix} G^K & G^R \\ G^A & 0 \end{pmatrix}(t,t'). \tag{60}$$

   Evaluate $Z[U_c, U_q]$ by performing the Gaussian integral and show that $Z[U_c, U_q = 0] = 1$.

2. From introductory quantum mechanics, we expect that the periodically driven harmonic oscillator will end up in a coherent state with $\langle a \rangle = \alpha \neq 0$ and $n = \left\langle a^\dagger a \right\rangle = |\alpha|^2$. We want to find α. Compute the functional derivative $i\delta Z\left[U_c, U_q\right]/\delta U_q(t)|_{U_q=0}$ from $Z[U_c, U_q]$ found in part 1.). To which expectation value in terms of the operators $a^{(\dagger)}(t)$ does this correspond? Show that in the limit $t \to \infty$, the coefficient α is given by the Fourier transform of $U_c(t) \equiv U(t)$ (up to an unimportant factor $\sqrt{2}e^{i\varphi}$ with $\varphi \in \mathbb{R}$). Hint: Use the results from (50).

3. Specialize to a periodic driving field with Gaussian envelope, $U(t) = U_0 \cos(\omega t)\, e^{-t^2/(4T^2)}$. Assume T much larger than ω and ω_0. Compute the final occupation number $n = |\alpha|^2$. Which driving frequency ω maximizes n?

11 Interactions and self-energy

11.1 Interactions

- Consider interacting part of bosonic Hamiltonian (now in D-dim real space, contact interaction):

$$H_{int} = g \int d\mathbf{x} a^\dagger(\mathbf{x}) a^\dagger(\mathbf{x}) a(\mathbf{x}) a(\mathbf{x}) \tag{61}$$

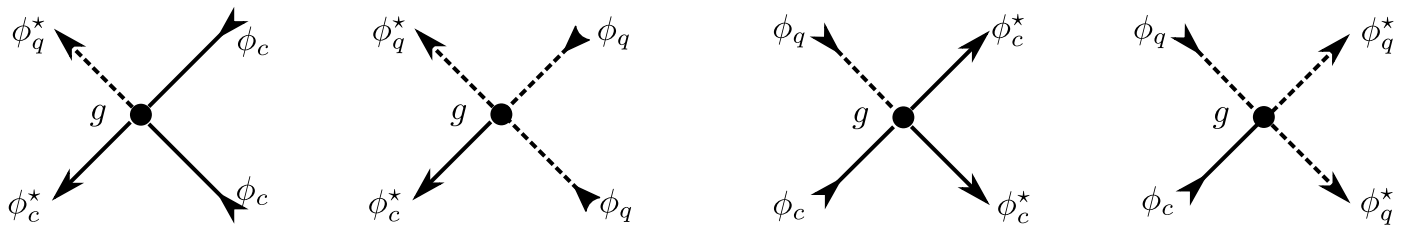
  which yields in terms of the action:

$$\begin{aligned} S_{int} &= -g \int d\mathbf{x} \int_c dt \phi^\star(\mathbf{x},t)\phi^\star(\mathbf{x},t)\phi(\mathbf{x},t)\phi(\mathbf{x},t) \\ &= -g \int d\mathbf{x} \int_{-\infty}^{+\infty} dt \left[\left(\phi_+^\star \phi_+\right)^2 - \left(\phi_-^\star \phi_-\right)^2 \right] \\ (rot.) &= -g \int d\mathbf{x} \int_{-\infty}^{+\infty} dt \left[\phi_c^\star \phi_q^\star \phi_c \phi_c + \phi_c^\star \phi_q^\star \phi_q \phi_q + \phi_c \phi_q \phi_c^\star \phi_c^\star + \phi_c \phi_q \phi_q^\star \phi_q^\star \right] \end{aligned} \tag{62}$$

  Remarks:

  - S_{int} vanishes for $\phi_q = 0$, just like the quadratic action.
  - Diagrammatic notation with the rules defined below Eq. (49) but with arrows pointing to the $\phi^\star$ field (so that Green functions with opposite arrow convention can be attached).

- Interactions maintain normalization ($Z = 1$): Check via perturbation theory to order g and g^2, see Ex. 11.1. Possible reasons are (i) $\left\langle \phi_q^\star \phi_q \right\rangle_0 = 0$, (ii) $\left(G_0^A + G_0^R\right)(t,t) = 0$, or (iii) an integral in the $t_{1,2}$-plane over $G_R(t_2,t_1)G_A(t_2,t_1)$ with incompatible θ-functions.



11.2 Dyson equation

- Although $Z = 1$ is maintained with interactions, the propagators are modified ("dressed"). They are defined as:

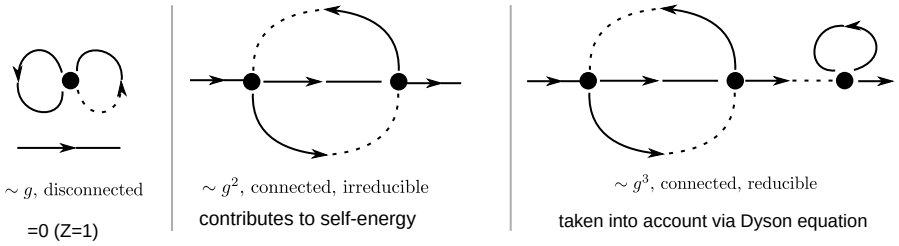
$$G = -i \left\langle \phi_\alpha \phi^\star_\beta \right\rangle = -i \int D[\phi_c, \phi_q] \phi_\alpha \phi^\star_\beta e^{iS_0 + iS_{int}} \tag{63}$$

- Perturbative expansion in g via Wick-theorem generates various diagrams (internal vertices: sum over Keldysh-indices, integrate over space-time coordinates)
  - Disconnected diagrams vanish due to $Z = 1$, they contain $\langle S_{int} \rangle_0 = 0$, $\langle S^2_{int} \rangle_0 = 0$, ...
  - One-line irreducible diagrams contribute to the self-energy Σ (without external legs).
  - One-line reducible diagrams are taken into account via the Dyson equation ("$\cdot$" includes t-integrals!).

$$\begin{aligned} G &= G_0 + G_0 \cdot \Sigma \cdot G_0 + G_0 \cdot \Sigma \cdot G_0 \cdot \Sigma \cdot G_0 + ... \\ &= G_0 + G_0 \cdot \Sigma \cdot G \end{aligned} \tag{64}$$

or

$$G = \left[G_0^{-1} - \Sigma \right]^{-1} \Leftrightarrow \left(G_0^{-1} - \Sigma \right) \cdot G = \mathbf{1} \tag{65}$$



- The matrix self-energy has the same causality structure as G_0^{-1} (similar perturbation theory arguments as for $Z = 1$):

$$\Sigma = \begin{pmatrix} 0 & \Sigma^A \\ \Sigma^R & \Sigma^K \end{pmatrix} \tag{66}$$

The Dyson equation then reads:

$$\begin{pmatrix} 0 & \left(G_0^A\right)^{-1} - \Sigma^A \\ \left(G_0^R\right)^{-1} - \Sigma^R & \left(G_0^{-1}\right)^K - \Sigma^K \end{pmatrix} \cdot \begin{pmatrix} G^K & G^R \\ G^A & 0 \end{pmatrix} = \mathbf{1} \tag{67}$$

Remark: $\left(G_0^{-1}\right)^K = 2i\eta F$ can be omitted if $\Sigma^K \neq 0$.

- Suppose we want to find $\Sigma^{A/R/K}$ from diagrammatic perturbation theory. What are the terminal fields for the diagrams contributing to these self-energies [boxes in Fig. 27]? For the irreducible diagrams appearing in the perturbative expansion of G, we use the second contribution of Eq. (64) together with Eq. (66) and find

$$\begin{pmatrix} G^K & G^R \\ G^A & 0 \end{pmatrix} |_{irr} = \begin{pmatrix} G_0^R \cdot \Sigma^K \cdot G_0^A + G_0^K \cdot \Sigma^A \cdot G_0^A + G_0^R \cdot \Sigma^R \cdot G_0^K & G_0^R \cdot \Sigma^R \cdot G_0^R \\ G_0^A \cdot \Sigma^A \cdot G_0^A & 0 \end{pmatrix} \tag{68}$$

This tells us which diagrams should be accounted for as $\Sigma^{R,A,K}$, see the figure below. In other words, Eq. (66) is to be understood in $\phi^\star - \phi$ space (while G is a matrix in $\phi - \phi^\star$ space). The irreducible Keldysh Green function $G^K|_{irr}$ has also contributions involving $\Sigma^{R,A}$, but we show only the one including Σ^K.

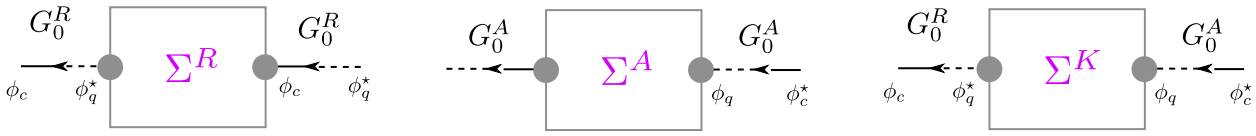


Figure 27: Terminal fields for perturbative expressions of self-energies in Keldysh formalism.

Exercises

Exercise 11.1. Normalization of Keldysh partition function with interactions

Use perturbation theory (up to order g^2) to show that Z is not modified in the presence of interactions described by S_{int} in Eq. (62). Hint: Show explicitly that the two rightmost terms in

$$Z = \int D[\phi_c, \phi_q] e^{iS_0 + iS_{int}} = \left\langle e^{iS_{int}} \right\rangle_0 = 1 + i \left\langle S_{int} \right\rangle_0 - \frac{1}{2} \left\langle S_{int}^2 \right\rangle_0 + ... \tag{69}$$

vanish individually. For the term $\langle S_{int}^2 \rangle_0$, recall that the two interaction vertices can be connected by two or four propagator lines.

12 Kinetic equation

Review: Classical Boltzmann equation

- Definition of classical distribution function $f(\mathbf{x}, t, \mathbf{p}) d\mathbf{x} d\mathbf{p}$ = number of particles in phase-space volume $d\mathbf{x} d\mathbf{p}$.
- From Liouville theorem, under propagation to time $t + dt$, phase space volume preserved under Hamiltonian equation of motion $\dot{\mathbf{x}} \equiv \mathbf{v}(\mathbf{p})$, $\dot{\mathbf{p}} \equiv \mathbf{F}(\mathbf{x}, \mathbf{p})$ (force). Thus $\frac{d}{dt} f(\mathbf{x}, t, \mathbf{p}) = \partial_t f|^{\text{coll}}$ can only change by collisions beyond these equations of motion.
- Apply chain rule on the left-hand-side to find Boltzmann equation: $\frac{d}{dt} f(\mathbf{x}, t, \mathbf{p}) = \{\partial_t + \dot{\mathbf{x}} \cdot \nabla_{\mathbf{x}} + \dot{\mathbf{p}} \cdot \nabla_{\mathbf{p}}\} f$,

$$\{\partial_t + \mathbf{v}(\mathbf{p}) \cdot \nabla_{\mathbf{x}} + \mathbf{F} \cdot \nabla_{\mathbf{p}}\} f = \partial_t f|^{\text{coll}} \tag{70}$$

- Goal: Derive analogous equation from quantum Keldysh formalism.

Solution of Dyson equation

- Assumptions: i) particles with parabolic dispersion, ii) Self-energies $\Sigma^{R/A/K}$ are approximately known, i.e. from perturbation theory.
- Recall from path integral formulation:

$$\left(G_0^{R/A}\right)^{-1} (t\mathbf{x}, t'\mathbf{x}') = \delta(t - t') \delta(\mathbf{x} - \mathbf{x}') \left[i\partial_t + \frac{1}{2m} \nabla_{\mathbf{x}}^2 \pm i\eta - V_c(\mathbf{x}, t) \right] \tag{71}$$

  and abbreviate the space-time arguments $x = (\mathbf{x}, t)$.
- Dyson equation for $G^{R/A} \leftrightarrow \Sigma^{R/A}$ (diagonal components):

$$\int dx'' \left(\left(G_0^{R/A}\right)^{-1} - \Sigma^{R/A} \right) (x, x'') \, G^{R/A}(x'', x') = \delta(x - x') \tag{72}$$

  For $V_c = 0$ (space-time translational invariance) can be solved via Fourier transform of $G^{R/A}(x, x') = G^{R/A}(x - x')$:

$$G^{R/A}(\mathbf{k}, \omega) = \frac{1}{\omega - k^2/(2m) - \Sigma^{R/A}(\mathbf{k}, \omega)} \tag{73}$$

  Observe:

– $\mathrm{Re}\Sigma^R(\mathbf{k},\omega) = \mathrm{Re}\Sigma^A(\mathbf{k},\omega)$ modifies ("renormalizes") the $\omega - \mathbf{k}$ relation (dispersion) of the pole: $\omega \stackrel{!}{=} k^2/(2m) + \mathrm{Re}\Sigma^{R/A}(\mathbf{k},\omega)$.

– $\mathrm{Im}\Sigma^R(\mathbf{k},\omega) = -\mathrm{Im}\Sigma^A(\mathbf{k},\omega)$ has the meaning of an inverse lifetime for the above particle $\mathbf{k}$.

- Dyson equation for off-diagonal component involving G^K:

$$\underbrace{[\left(G_0^R\right)^{-1} - \Sigma^R]}_{(G^R)^{-1}} \cdot \underbrace{G^K}_{G^R\cdot F - F\cdot G^A} = \Sigma^K \cdot G^A \tag{74}$$

  Multiply from the right by $\left(G_0^A\right)^{-1} - \Sigma^A = \left[G^A\right]^{-1}$ and rearrange. Obtain the **quantum kinetic equation** for the matrix $F(x,x')$ ("distribution matrix"):

$$\boxed{F \cdot \left(G_0^A\right)^{-1} - \left(G_0^R\right)^{-1} \cdot F = \Sigma^K - \left(\Sigma^R \cdot F - F \cdot \Sigma^A\right)} \tag{75}$$

- Kinetic equation for $F(x_1,x_2)$ is usually too difficult to solve.
- Simplification: Assume separation of intrinsic and extrinsic time and length scales (e.g. external potential $V_c(\mathbf{x},t)$ smooth compared to wavelength of particle).

Wigner transform

- Tool to approximate convolutions "$\cdot$" as in kinetic equation (75) by algebraic products.
- Wigner transform for general function $A(x_1,x_2)$ that depends on two space-time arguments: Keep center coordinate $(x_1+x_2)/2$, do Fourier trafo with respect to relative coordinate $x_1 - x_2$ only. Use $p = (\mathbf{p},\omega)$ and convention $px = \mathbf{p}\cdot\mathbf{x} - \omega t$ (and $\partial_x\partial_p = \nabla_{\mathbf{x}}\nabla_{\mathbf{p}} - \partial_t\partial_\omega$)

$$\boxed{A(x,p) \equiv \int dx' e^{-ipx'} A\left(x + x'/2, x - x'/2\right)} \tag{76}$$

  and the inverse Wigner transform is

$$A(x_1,x_2) = \sum_p e^{ip(x_1-x_2)} A\left(\frac{x_1+x_2}{2}, p\right). \tag{77}$$

- Wigner transform of function $C = A\cdot B$ which means $C(x_1,x_2) = \int dx_3 A(x_1,x_3)B(x_3,x_2)$ ("convolution"). In Ex. 12.1, one shows the following:
  If for $A(x,p)$ and $B(x,p)$ the dependence on the central coordinate x is slow, one has the following approximation (no "$\cdot$"!)

$$C(x,p) \simeq A(x,p)B(x,p) + \frac{i}{2}\left(\partial_x A(x,p)\partial_p B(x,p) - \partial_p A(x,p)\partial_x B(x,p)\right) \tag{78}$$

  and corrections include higher order x-derivatives $\partial_x^{2,3,4,\cdots}$ which are assumed to be small.

- Prepare Wigner transform of "commutator":

$$[A;B] \equiv A\cdot B - B\cdot A \simeq i\left(\partial_x A(x,p)\partial_p B(x,p) - \partial_p A(x,p)\partial_x B(x,p)\right) \tag{79}$$

  where the notation $[.;.]$ should remind us that we are dealing with "$\cdot$". The rhs is the Poisson bracket $\{A,B\}$ of classical mechanics.

Wigner transform of kinetic equation

- Idea: Apply the Wigner transform on both sides of the kinetic equation (75).
- Left-hand side: We have with the free particle assumption (71) (can drop $\pm i\eta$ terms in this context):

$$\text{lhs} = \left[F; i\partial_t + \frac{1}{2m}\nabla_{\mathbf{x}}^2 - V_c(x)\right] \tag{80}$$

  Last term: Assume $V_c(x)$ to be slow, e.g. $V_c(x) = V_c(x,p)$:

$$[F; -V_c(x)] = -i\Big(\partial_x F \underbrace{\partial_p V_c(x,p)}_{\to 0} - \partial_p F \partial_x V_c(x,p)\Big) = i\partial_x V_c(x)\partial_p F \tag{81}$$

  Other terms: The Wigner transform of the translational invariant derivative operators is $i\partial_t \to \omega$, of $\nabla_{\mathbf{x}}^2 \to -\mathbf{p}^2$. Also use $\partial_x\partial_p = \nabla_{\mathbf{x}}\nabla_{\mathbf{p}} - \partial_t\partial_\omega$:

$$[F; i\partial_t] = i\left(\partial_x F \partial_p \omega - \partial_p F \partial_x \omega\right) = -i\partial_t F$$
$$\left[F; \frac{1}{2m}\nabla_{\mathbf{x}}^2\right] = \frac{-i}{2m}\left(\partial_x F \partial_p \mathbf{p}^2 - \partial_p F \partial_x \mathbf{p}^2\right) = \frac{-i}{m}\mathbf{p}\nabla_{\mathbf{x}} F$$

- Right-hand side: Use $\Sigma^A(x,p) = \left[\Sigma^R(x,p)\right]^\star$:

$$\begin{aligned}
\text{rhs} &= \Sigma^K - \left(\Sigma^R \cdot F - F \cdot \Sigma^A\right) \\
&= \Sigma^K - F\left(\Sigma^R - \Sigma^A\right) - \frac{i}{2}\left(\partial_x \Sigma^R \partial_p F - \partial_p \Sigma^R \partial_x F\right) + \frac{i}{2}\left(\partial_x F \partial_p \Sigma^A - \partial_p F \partial_x \Sigma^A\right) \\
&= \Sigma^K - 2iF\text{Im}\Sigma^R - i\partial_x\left[\text{Re}\Sigma^R\right]\partial_p F + i\partial_p\left[\text{Re}\Sigma^R\right]\partial_x F
\end{aligned}$$

- Final result: Multiply by i, move all derivatives of F on the left-hand side, write out $x = (\mathbf{x}, t)$ and $p = (\mathbf{p}, \omega)$, and define the *effective potential* $\tilde{V}(x,p) \equiv V_c(x) + \text{Re}\Sigma^R(x,p)$:

$$\boxed{\left\{\left(1 - \partial_\omega\left[\text{Re}\Sigma^R\right]\right)\partial_t + \partial_t\tilde{V}(x,p)\partial_\omega + \underbrace{\left(\frac{1}{m}\mathbf{p} + \nabla_{\mathbf{p}}\left[\text{Re}\Sigma^R\right]\right)}_{\to \tilde{\mathbf{v}}_{\mathbf{p}}}\nabla_{\mathbf{x}} - \nabla_{\mathbf{x}}\tilde{V}(x,p)\nabla_{\mathbf{p}}\right\}F = \underbrace{i\Sigma^K + 2F\text{Im}\Sigma^R}_{\text{collision integral } I^{\text{coll}}[F]}} \tag{82}$$

- Remarks on Eq. (82):
  - The left-hand side contains the self-energy enhanced *single-particle dynamics* of F ("kinetic term").
  - The right-hand side is the "collision integral" $I^{\text{coll}}[F]$, it will be caused by interactions or disorder.
  - Can generalize dispersion $\frac{1}{2m}\mathbf{p}^2 \to \omega_{\mathbf{p}}$, leads to $\mathbf{v}_{\mathbf{p}} = \frac{1}{m}\mathbf{p} \to \nabla_{\mathbf{p}}\omega_{\mathbf{p}}$.
  - Consider static situation, such that all $\partial_t \to 0$. The left-hand side is zero for any $F(x,p) = F(\omega)$. The only $F(\omega)$ which also nullifies the right-hand side is the equilibrium solution

$$F^{\text{eq}}(\omega) = 1 + 2n_B(\omega) = \coth\left(\frac{\omega}{2T}\right) \tag{83}$$

Mass-shell approximation

- Shift the energy argument ω of the distribution function F by quasi-particle energy:

$$F(\mathbf{x}, t, \mathbf{p}, \omega) = \tilde{F}(\mathbf{x}, t, \mathbf{p}, \underbrace{\omega - \omega_{\mathbf{p}} - \tilde{V}(x,p)}_{\equiv\tilde{\omega}}) \tag{84}$$

- Express the kinetic equation (82) in terms of $\tilde{F}(\mathbf{x}, t, \mathbf{p}, \tilde{\omega})$. The terms ∂_t, ∂_ω, $\nabla_{\mathbf{x}}$ and $\nabla_{\mathbf{p}}$ acting on F are modified by the chain rule involving $\tilde{V} = V_c + \mathrm{Re}\Sigma^R$ derivatives:

$$\begin{aligned}
\partial_t F &= \partial_t \tilde{F} - \left(\partial_t \tilde{V}\right) \partial_\omega \tilde{F} \\
\partial_\omega F &= \partial_\omega \tilde{F} - \left(\partial_\omega \tilde{V}\right) \partial_\omega \tilde{F} \\
\nabla_{\mathbf{x}} F &= \nabla_{\mathbf{x}} \tilde{F} - \left(\nabla_{\mathbf{x}} \tilde{V}\right) \partial_\omega \tilde{F} \\
\nabla_{\mathbf{p}} F &= \nabla_{\mathbf{p}} \tilde{F} - \left(\nabla_{\mathbf{p}} \omega_{\mathbf{p}} + \nabla_{\mathbf{p}} \tilde{V}\right) \partial_\omega \tilde{F}
\end{aligned}$$

  Use that the external potential V_c (which is a part of $\tilde{V}$) is a "slow" function $\nabla_{\mathbf{p}} V_c(x) = 0$ and $\partial_\omega V_c(x) = 0$, obtain after some straightforward algebra:

$$\boxed{\left\{\left(1 - \partial_\omega \left[\mathrm{Re}\Sigma^R\right]\right) \partial_t + \tilde{\mathbf{v}}_{\mathbf{p}} \nabla_{\mathbf{x}} - \left(\nabla_{\mathbf{x}} \tilde{V}\right) \nabla_{\mathbf{p}}\right\} \tilde{F} = I^{\mathrm{coll}}[\tilde{F}]} \tag{85}$$

  Observation: The derivative $\partial_{\tilde{\omega}}$ is now absent in the kinetic term.

- If $I^{\mathrm{coll}}[\tilde{F}]$ would only depend on ω via $\tilde{\omega}$, we could solve the kinetic equations for each $\tilde{\omega}$ as a parameter. This is generally not the case.

- Quasi-particle approximation:

  - Fact: In $I^{\mathrm{coll}}[\tilde{F}]$, $\tilde{F}$ always multiplies Wigner trafo of $G^R - G^A \sim$ spectral density. We will see this for the disorder application below.
  - The spectral density in the non-interacting limit is $\sim \delta(\omega - \tilde{\omega})$. Not too far from this limit assume the peak in $G^R - G^A$ (of width $1/\tau_{qp}$ where τ_{qp} is quasi-particle lifetime) is much sharper than the $\tilde{\omega}$-dependence of $\tilde{F}$.
  - Hence: For given $\mathbf{p}$, we may focus on

$$\tilde{F}(\mathbf{x}, t, \mathbf{p}, 0) \equiv \tilde{F}(\mathbf{x}, t, \mathbf{p}) \tag{86}$$

    which is the *mass-shell restricted distribution function.*

- Remarks:

  - $\tilde{F}(\mathbf{x}, t, \mathbf{p})$ is a classical object = probability at time t for particle at point $(\mathbf{x}, \mathbf{p})$ in classical phase space.
  - Up to "semi-classical" self–energy effects = tilde-terms $\tilde{Z}^{-1} = 1 - \partial_\omega \left[\mathrm{Re}\Sigma^R\right]|_{\omega=\tilde{\omega}}$ (quasi-particle weight) and $\tilde{V}$, Eq. (85) is equivalent to the classical Boltzmann equation (70).

Example for collision integral: Disorder scattering

- Consider non-interacting bosons in a static disorder potential:

$$H = \sum_{\mathbf{p}} \omega_{\mathbf{p}} a^\dagger_{\mathbf{p}} a_{\mathbf{p}} + \int d\mathbf{x} V(\mathbf{x}) a^\dagger(\mathbf{x}) a(\mathbf{x}) \tag{87}$$

- Assume $V(\mathbf{x})$ comes from randomly placed impurities, $V(\mathbf{x}) = \sum_{j=1}^N v(\mathbf{x} - \mathbf{r}_j)$ where $\mathbf{r}_{1,2,\ldots,N}$ are the N uncorrelated impurity positions.
  Assume $\int d\mathbf{x} v(\mathbf{x}) = 0$, i.e. a potential offset is already taken into account in a shift of dispersion $\omega_{\mathbf{p}}$.

- Disorder average for quantity Q (integrate over all impurity configurations):

$$\overline{Q} \equiv \Pi_{j=1}^N \left[\frac{1}{V} \int d\mathbf{r}_j \, Q\right] \tag{88}$$

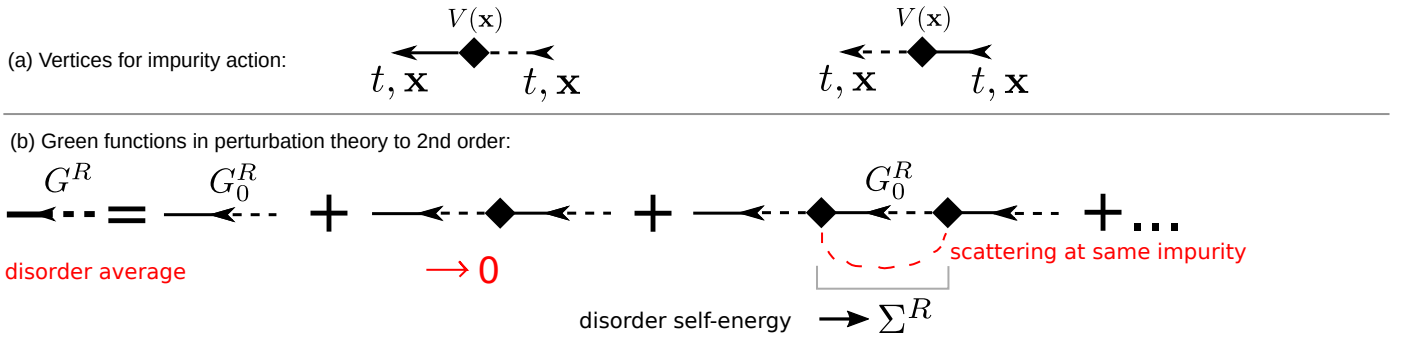


Figure 28: Disordered bosons: (a) Diagrammatic building blocks for impurity scattering. (b) Diagrams for G^R to second order in V.

Application: Averaged disorder correlator:

$$\begin{aligned}\overline{V(\mathbf{x}_1)V(\mathbf{x}_2)} &= \sum_{j=1}^{N}\sum_{j'=1}^{N}\overline{v\left(\mathbf{x}_1-\mathbf{r}_j\right)v\left(\mathbf{x}_2-\mathbf{r}_{j'}\right)} \\ &= \sum_{j=1}^{N}\overline{v\left(\mathbf{x}_1-\mathbf{r}_j\right)v\left(\mathbf{x}_2-\mathbf{r}_j\right)} + \sum_{j\neq j'}\underbrace{\overline{v\left(\mathbf{x}_1-\mathbf{r}_j\right)v\left(\mathbf{x}_2-\mathbf{r}_{j'}\right)}}_{\overline{V}\,\overline{V}=0} \\ (diag.) &= \underbrace{N/V}_{n_i}\int d\mathbf{r}\, v\left(\mathbf{x}_1-\mathbf{r}\right)v\left(\mathbf{x}_2-\mathbf{r}\right) \\ &\equiv K(\mathbf{x}_1-\mathbf{x}_2) \end{aligned} \tag{89}$$

and we used $\overline{V(\mathbf{x})} = \Pi_{j=1}^{N}\frac{1}{V}\int d\mathbf{r}_j \sum_{j=1}^{N} v\left(\mathbf{x}-\mathbf{r}_j\right) = 0$.

- The impurity action for a specific realization is

$$S_V = -\int_{-\infty}^{+\infty} dt \int d\mathbf{x} V\left(\mathbf{x}\right)\left[\underbrace{\phi_c^\star(\mathbf{x},t)\phi_q(\mathbf{x},t)+\phi_q^\star(\mathbf{x},t)\phi_c(\mathbf{x},t)}_{=\phi_+^\star\phi_+-\phi_-^\star\phi_-}\right]$$

and the corresponding diagrammatic building blocks are given in Fig. 28(a).

- Find $G^{R/A/K}$ using perturbation theory to second order. Keep F general as it will be determined from kinetic equation. From Fig. 28(b), we have for example for G^R:

$$\begin{aligned} G^R\left(x_1,x_2\right) = G_0^R\left(x_1-x_2\right) &+ \int dx G_0^R\left(x_1-x\right)V(x)G_0^R\left(x-x_2\right) \\ &+ \int dx \int dx' G_0^R\left(x_1-x\right)V(x)G_0^R\left(x-x'\right)V(x')G_0^R\left(x'-x_2\right) + ... \end{aligned}$$

- Take disorder average, the term $\propto V$ vanishes and for the term $\propto VV$ we use Eq. (89). We recover translational invariance:

$$\overline{G^R}\left(x_1-x_2\right) = G_0^R\left(x_1-x_2\right) + \int dx \int dx' G_0^R\left(x_1-x\right)K(x-x')G_0^R\left(x-x'\right)G_0^R\left(x'-x_2\right) + ...$$

- Introduce self-energy. For the identification of relevant diagram parts, refer to Fig. 27 or $\overline{G^R} = G_0^R + G_0^R\Sigma^R\overline{G^R}$.

$$\Sigma^{R/A/K}\left(x-x'\right) = K(x-x')G_0^{R/A/K}\left(x-x'\right) \tag{90}$$

- For the kinetic equation, we need the Wigner transform of $\Sigma^{R/A/K}(x-x')$. This is simple, because the expression only depends on relative coordinate. Then the Wigner transform is just an ordinary Fourier transform.
- Use "product $\to$ convolution" rule and $K(\mathbf{p}) = n_i v_{\mathbf{p}} v_{-\mathbf{p}} \overset{v(\mathbf{x})\in\mathbb{R}}{=} n_i |v_{\mathbf{p}}|^2$ (Fourier transform of $v(\mathbf{x}) = \sum_{\mathbf{p}} e^{i\mathbf{p}\mathbf{x}} v_{\mathbf{p}}$.)

$$\Sigma^{R/A/K}(x,p) = n_i \sum_{\mathbf{p}'} G_0^{R/A/K}(\mathbf{x},t,\mathbf{p}',\omega) \left|v_{\mathbf{p}-\mathbf{p}'}\right|^2 \tag{91}$$

- Find collision integral $I^{\text{coll}}[\tilde{F}] = i\Sigma^K + 2\tilde{F}\text{Im}\Sigma^R$:
  - $2\tilde{F}\text{Im}\Sigma^R$: Use $G_0^{R,A}(\mathbf{x},t,\mathbf{p},\omega) = G_0^{R,A}(\mathbf{p},\omega) = \frac{1}{\omega-\omega_{\mathbf{p}}\pm i\eta}$ in Eq. (91):

$$2\text{Im}\Sigma^R(x,p) = -i\Sigma^R + i\Sigma^A = -n_i \sum_{\mathbf{p}'} \underbrace{i\left[G_0^R - G_0^A\right](\mathbf{p}',\omega)}_{A_0 = 2\pi\delta(\omega-\omega_{\mathbf{p}'})} \left|v_{\mathbf{p}-\mathbf{p}'}\right|^2 \tag{92}$$

  - $i\Sigma^K$: Use Eq. (91) and insert

$$\begin{aligned} G_0^K(\mathbf{x},t,\mathbf{p}',\omega) &= \left(G_0^R \cdot F - F \cdot G_0^A\right)(\mathbf{x},t,\mathbf{p}',\omega) \\ [\text{lowest order approx.}] &\simeq -ii\left[G_0^R - G_0^A\right](\mathbf{p}',\omega) F(\mathbf{x},t,\mathbf{p}',\omega) \\ &= -i2\pi\delta(\omega-\omega_{\mathbf{p}'}) F(\mathbf{x},t,\mathbf{p}',\omega) \end{aligned}$$

    so that

$$i\Sigma^K = 2\pi n_i \sum_{\mathbf{p}'} \delta(\omega-\omega_{\mathbf{p}'}) \left|v_{\mathbf{p}-\mathbf{p}'}\right|^2 F(\mathbf{x},t,\mathbf{p}',\omega) \tag{93}$$

- Collect terms and work with $\tilde{F}$ at $\tilde{\omega} = 0$ ($\omega \to \omega_{\mathbf{p}}$):

$$\boxed{I^{\text{coll}}\left[\tilde{F}(\mathbf{x},t,\mathbf{p})\right] = -2\pi n_i \sum_{\mathbf{p}'} \delta(\omega_{\mathbf{p}}-\omega_{\mathbf{p}'}) \left|v_{\mathbf{p}-\mathbf{p}'}\right|^2 \left[\tilde{F}(\mathbf{x},t,\mathbf{p}) - \tilde{F}(\mathbf{x},t,\mathbf{p}')\right]} \tag{94}$$

- Interpretation (phase-space classical mechanics + energy conservation):
  - First term: Loss rate proportional to occupation $\tilde{F}(\mathbf{x},t,\mathbf{p})$ due to scattering of particles to other momenta $\mathbf{p}'$.
  - Second term: Gain rate to occupation $\tilde{F}(\mathbf{x},t,\mathbf{p})$ due to particles scattered from other momenta $\mathbf{p}'$.
  - Scattering rates determined by Fermi's golden rule: $W(\mathbf{p},\mathbf{p}') \equiv 2\pi n_i \delta(\omega_{\mathbf{p}}-\omega_{\mathbf{p}'}) \left|\langle\mathbf{p}|v|\mathbf{p}'\rangle\right|^2$.

Exercises

Exercise 12.1. Wigner transform of $C = A \cdot B$

Find the Wigner transform from Eq. (76) for a function $C = A \cdot B$ where the "dot" notation means $C(x_1,x_2) = \int dx_3 A(x_1,x_3) B(x_3,x_2)$. Express your result in terms of the Wigner transforms of A, B. You should find

$$C(x,p) = \sum_{n,m=0}^{\infty} \frac{(+i)^m}{2^m m!} \frac{(-i)^n}{2^n n!} \partial_x^{(m)} \partial_p^{(n)} A(x,p) \, \partial_p^{(m)} \partial_x^{(n)} B(x,p) \tag{95}$$

$$\equiv A(x,p) e^{\frac{i}{2}\left(\overleftarrow{\partial}_x \overrightarrow{\partial}_p - \overleftarrow{\partial}_p \overrightarrow{\partial}_x\right)} B(x,p) \tag{96}$$

where the arrows show the direction of the differentiation. Hints: With appropriate substitutions, first confirm

$$C(x,p) = \int dx_a \int dx_b \sum_{p_{a,b}} e^{ip_b x_a - ip_a x_b} A\left(x + \frac{x_a}{2}, p + p_a\right) B\left(x + \frac{x_b}{2}, p + p_b\right). \tag{97}$$

Expand the p-dependence of A, B and use appropriate x-derivatives of the identity $\sum_p e^{\pm ipx} = \delta(x)$ to replace the $\sum_p e^{\pm ipx} p^n$. Subsequently, evaluate the $x_{a,b}$ integrals.

13 Keldysh for fermions

Grassmann numbers, fermion coherent states

- Consider fermionic Hamiltonian $H\left(\{c_j^\dagger, c_j\}\right)$ with canonical anti-commutation relations $\{c_i, c_j^\dagger\} = \delta_{ij}$.
- Review of Grassmann numbers ψ:
  - mutually anti-commute $\psi\psi' = -\psi'\psi$ and thus $\psi^2 = 0$.
  - function of Grassmann number defined via first two terms in series expansion: $f(\psi) = f_0 + f_1\psi$ (other terms are trivial).
  - integrals are defined as $\int d\psi\, 1 = 0$, $\int d\psi\, \psi = 1$.
  - ψ anti-commutes with fermionic operators, $\{c, \psi\} = \left\{c^\dagger, \psi\right\} = 0$.
  - "bar"-field $\bar{\psi}$ is unrelated to the ψ-field.
- Fermionic coherent states:

coherent state:	$\|\psi\rangle \equiv e^{-\psi c^\dagger}\|0\rangle = (1-\psi c^\dagger)\|0\rangle = \|0\rangle - \psi\|1\rangle$ $\langle\psi\| \equiv \langle 0\| e^{-c\bar{\psi}} = \langle 0\| - \langle 1\|\bar{\psi}$	overlap:	$\langle\psi\|\psi'\rangle = e^{\bar{\psi}\psi'} = 1 + \bar{\psi}\psi'$
		res. of id.	$1 = \int d\bar{\psi}d\psi e^{-\psi\psi}\|\psi\rangle\langle\psi\|$
action of c:	$c\|\psi\rangle = \psi\|\psi\rangle$	trace:	$\mathrm{tr}O = \int d\bar{\psi}d\psi e^{-\bar{\psi}\psi}\langle\psi\|O\|-\psi\rangle$
action of $c^\dagger$:	$\langle\psi\| c^\dagger = \langle\psi\|\bar{\psi}$	Gauss. integral:	$\int \Pi_l d\bar{\psi}_l d\psi_l e^{-\bar{\psi}^T\cdot A\cdot\psi} = \det(A)$

- In $\mathrm{tr}O$, the sign $|-\psi\rangle = |0\rangle + \psi|1\rangle$ comes from the fact that the coherent states contain Grassmann numbers which pick up a sign upon exchange, $\langle n|\psi\rangle\langle\psi|O|n\rangle = \langle\psi|O|n\rangle\langle n|-\psi\rangle$.
- The auxiliary identity $\left\langle\bar{\psi}|x^{c^\dagger c}|\psi\right\rangle = e^{\bar{\psi}\psi x}$ still holds.

Partition function

- Consider single fermionic level, $H = \varepsilon_0 c^\dagger c$. In thermal equilibrium at $t = -\infty$, we have $\rho = e^{-\beta H_0}$ and $\mathrm{tr}\rho = 1 + e^{-\beta\varepsilon_0}$ (no geometric series) and the occupation is $\left\langle c^\dagger c\right\rangle \equiv n_F(\varepsilon_0) = 1/(1+e^{\beta\varepsilon_0})$.
- In definition of Z, add time slices on both branches ($\psi_\pm$) , find in analogy to bosonic case

$$Z = \frac{1}{tr\rho}\int \Pi_{j=1}^{2N} d\bar{\psi}_j d\psi_j \exp\left[i\sum_{j,j'=1}^{2N}\bar{\psi}_j\left(G^{-1}\right)_{jj'}\psi_{j'}\right] \tag{98}$$

with (N=3)

$$i\left(G^{-1}\right)_{jj'} = \begin{pmatrix} -1 & 0 & 0 & 0 & 0 & -e^{-\beta\varepsilon_0} \\ h_- & -1 & 0 & 0 & 0 & 0 \\ 0 & h_- & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 0 & h_+ & -1 & 0 \\ 0 & 0 & 0 & 0 & h_+ & -1 \end{pmatrix} \tag{99}$$

where $h_\pm = 1 \pm i\varepsilon_0\delta t$ and indeed normalization holds, $Z = \frac{\det\left(-iG^{-1}\right)}{tr\rho} \overset{N\to\infty}{=} \frac{1+e^{-\beta\varepsilon_0}}{1+e^{-\beta\varepsilon_0}} = 1$.

- Green functions $G_{c,c^\dagger} \equiv G$ can be read off as in the bosonic case:

$$\begin{aligned}
G^<(t,t') &= +in_F(\varepsilon_0)e^{-i\varepsilon_0(t-t')} \\
G^>(t,t') &= -i\left(1-n_F(\varepsilon_0)\right)e^{-i\varepsilon_0(t-t')} \\
G^T(t,t') &= \theta\left(t-t'\right)G^>(t,t') + \theta\left(t'-t\right)G^<(t,t') = -ie^{-i\varepsilon_0(t-t')}\left[\theta\left(t-t'\right) - n_F(\varepsilon_0)\right] \\
G^{\tilde{T}}(t,t') &= \theta\left(t'-t\right)G^>(t,t') + \theta\left(t-t'\right)G^<(t,t') = -ie^{-i\varepsilon_0(t-t')}\left[\theta\left(t'-t\right) - n_F(\varepsilon_0)\right]
\end{aligned}$$

Keldysh rotation

- Keldysh rotation: Redundancy relation (9) ($G^T + G^{\tilde{T}} - G^> - G^< = 0$) holds also for fermions, take it into account via rotation.
  Careful: Use convention different from bosonic case "Larkin-Ovchinnikov".

$$\psi_{1,2} \equiv \frac{1}{\sqrt{2}} \left(\psi_+ \pm \psi_-\right)$$
$$\bar{\psi}_{1,2} \equiv \frac{1}{\sqrt{2}} \left(\bar{\psi}_+ \mp \bar{\psi}_-\right)$$

  Note that the "classical-quantum" nomenclature is not used: Grassmann variables never have classical meaning.

- Propagators: For $\alpha, \beta \in \{1, 2\}$ we have

$$-i \left\langle \psi_\alpha(t) \bar{\psi}_\beta(t') \right\rangle \equiv G_{\alpha\beta}(t, t') = \begin{pmatrix} G^R & G^K \\ 0 & G^A \end{pmatrix}_{\alpha\beta} (t, t'), \tag{100}$$

  with $G^{R/A}$ now on diagonal. The inverse propagator reads (with convention above, have *same* structure as G)

$$G^{-1} = \begin{pmatrix} \left(G^R\right)^{-1} & \left(G^{-1}\right)^K \\ 0 & \left(G^A\right)^{-1} \end{pmatrix} \tag{101}$$

  With the parametrization $G^K = G^R \cdot F - F \cdot G^A$, find

$$\left(G^{-1}\right)^K = \left(G^R\right)^{-1} \cdot F - F \cdot \left(G^A\right)^{-1} \tag{102}$$

- Single fermionic level in thermal equilibrium

$$G^R(t, t') = -i\theta\left(t - t'\right) e^{-i\varepsilon_0 (t - t')} \overset{FT}{\to} \frac{1}{\omega - \varepsilon_0 + i\eta}$$
$$G^A(t, t') = +i\theta\left(t' - t\right) e^{-i\varepsilon_0 (t - t')} \overset{FT}{\to} \frac{1}{\omega - \varepsilon_0 - i\eta}$$
$$G^K(t, t') = -i\left(1 - 2n_F(\varepsilon_0)\right) e^{-i\varepsilon_0 (t - t')} \overset{FT}{\to} \underbrace{\left(1 - 2n_F(\omega)\right)}_{F(\omega)} \underbrace{\left[-2\pi i \delta\left(\omega - \varepsilon_0\right)\right]}_{G^R(\omega) - G^A(\omega)}$$

  The last identity is the fermionic fluctuation-dissipation theorem.

Exercises

Exercise 13.1. Electron current through interacting region

Consider two metallic leads attached to the left and right (L, R) of an interacting central region where $\{d_n^\dagger\}, \{d_n\}$ form a complete set of orthonormal electron creation and annihilation operators, see Fig. 29. The central region could be a nanostructure like a quantum dot or similar where electrons are confined and screening is weak so that interactions are significant. The leads are approximated as non-interacting with operators $\{c_{k\alpha}^\dagger\}, \{c_{k\alpha}\}$, $k\alpha \in \{L, R\}$ which are characterized by momentum k and channel index α. The latter could be spin or any other single-particle index like a sub-band characterizing the lead states. The Hamiltonian reads

$$H = \sum_{k\alpha \in \{L,R\}} \varepsilon_{k\alpha} c_{k\alpha}^\dagger c_{k\alpha} + H_{int}\left(\{d_n^\dagger\}, \{d_n\}\right) + \sum_{k\alpha \in \{L,R\}} V_{k\alpha,n} c_{k\alpha}^\dagger d_n + V_{k\alpha,n}^\star d_n^\dagger c_{k\alpha}. \tag{103}$$

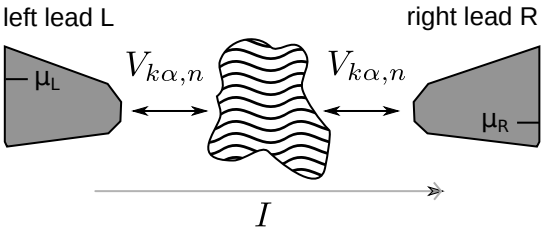


Figure 29: Setup for Ex. 13.1. The electron states belonging to the d_n operators reside in the interacting central region, the $c_{k\alpha}$ operators belong to the leads, $k\alpha \in \{R, L\}$.

We compute the *steady-state* electron current $I_L = I$ between the left lead maintained in equilibrium at chemical potential μ_L and temperature T and the right lead (at μ_R and T). As in Ex. 9.2, we start from

$$\begin{aligned} I_L &= \frac{ie}{\hbar} \sum_{k\alpha\in L} \sum_n V_{k\alpha,n} \left\langle c^\dagger_{k\alpha} d_n \right\rangle - V^\star_{k\alpha,n} \left\langle d^\dagger_n c_{k\alpha} \right\rangle \\ &= \frac{e}{\hbar} \sum_{k\alpha\in L} \sum_n \int \frac{d\omega}{2\pi} V_{k\alpha,n} G^<_{n,k\alpha}(\omega) - V^\star_{k\alpha,n} G^<_{k\alpha,n}(\omega), \end{aligned}$$

where $G^<_{n,k\alpha}(t) = i \left\langle c^\dagger_{k\alpha} d_n(t) \right\rangle$ is the steady-state lesser Green function (note $\zeta = -1$ for fermions). You might want to review Ex. 9.2 to understand similarities and differences between the setups considered and the reason behind the formula for I_L. The goal is to express the current I in terms of appropriate d-electron Green functions $G_{n,m}(\omega)$ in the presence of the leads and the Green functions $G^{(0)}_{\alpha k,\alpha k}$ evaluated for the uncoupled system with $V = 0$. The former are local but hard to compute in general while the latter are trivially known.

1. Consider V as a perturbation and use the (2x2 matrix valued) Dyson equation $G = G^{(0)} + G^{(0)} \cdot \Sigma \cdot G$ to show

$$\begin{aligned} G^<_{k\alpha,n}(\omega) &= \sum_m V_{k\alpha,m} \left[G^{(0),T}_{k\alpha,k\alpha}(\omega) G^<_{m,n}(\omega) - G^{(0),<}_{k\alpha,k\alpha}(\omega) G^{\tilde{T}}_{m,n}(\omega) \right], \\ G^<_{n,k\alpha}(\omega) &= \sum_m V^\star_{k\alpha,m} \left[G^{(0),<}_{k\alpha,k\alpha}(\omega) G^T_{n,m}(\omega) - G^{(0),\tilde{T}}_{k\alpha,k\alpha}(\omega) G^<_{n,m}(\omega) \right]. \end{aligned}$$

   Hint: The self-energy Σ is simple with entries proportional to V. Why?

2. Use the above findings to express the current as

$$I_L = \frac{ie}{\hbar} \sum_{\alpha\in L} \sum_{n,m} \int d\varepsilon\, \rho_\alpha(\varepsilon) V_{\alpha,n}(\varepsilon) V^\star_{\alpha,m}(\varepsilon) \Big\{ n_L(\varepsilon) \left[G^R_{n,m}(\varepsilon) - G^A_{n,m}(\varepsilon) \right] + G^<_{n,m}(\varepsilon) \Big\} \tag{104}$$

   where the retarded and advanced Green functions appear, $V_{\alpha,n}(\varepsilon) = V_{k\alpha,n}$ for $\varepsilon = \varepsilon_{k\alpha}$ and $\rho_\alpha(\varepsilon)$ is the density of lead states in channel α so that $\sum_k \to \int d\varepsilon \rho_\alpha(\varepsilon)$.

3. We could have also chosen the link to the right lead to derive a similar formula for the current $I_R = -I_L$. Symmetrize $I = (I_L - I_R)/2$ and define $\Gamma^L_{m,n}(\varepsilon) = 2\pi\rho_\alpha(\varepsilon) V_{\alpha,n}(\varepsilon) V^\star_{\alpha,m}(\varepsilon)$ to confirm the final result expressed in bold matrix notation for n-indices,

$$I = \frac{ie}{2h} \int d\varepsilon\, \mathrm{tr} \left[\Big(n_L(\varepsilon) \mathbf{\Gamma}^L(\varepsilon) - n_R(\varepsilon) \mathbf{\Gamma}^R(\varepsilon) \Big) \cdot \Big(\mathbf{G}^R(\varepsilon) - \mathbf{G}^A(\varepsilon) \Big) \right] + \mathrm{tr} \left[\Big(\mathbf{\Gamma}^L(\varepsilon) - \mathbf{\Gamma}^R(\varepsilon) \Big) \cdot \mathbf{G}^<(\varepsilon) \right]. \tag{105}$$

   Show that under equilibrium conditions with zero voltage $[n_L(\varepsilon) = n_R(\varepsilon)]$, the current vanishes, $I = 0$.

Part IV
Quantum magnetism

14 Basic concepts

14.1 Magnetic moments

- Circular current I around area A generates magnetic moment $\mathbf{m} = IA\mathbf{e}_A$.
- The magnetic moment determines the energy in magnetic field $\mathbf{B}$, $E = -\mathbf{m}\cdot\mathbf{B}$. Magnetic moments $\mathbf{m}$ minimize their energies when they align parallel with the field $\mathbf{B}$.
- With a macroscopic charged particle (charge Q, mass m) going around the circle in time T we have $I = Q/T$. The angular momentum is $\mathbf{L} = \mathbf{r}\times\mathbf{p}$. It is easy to see that

$$\mathbf{m} = \underbrace{Q/(2m)}_{\gamma}\mathbf{L} \tag{1}$$

  with γ the gyromagnetic ratio.
- Quantum mechanics of moving electrons: Eq. (1) is still valid, $\gamma = -e/(2m_e)$. It is often written as

$$\mathbf{m_L} = -\frac{e}{2m_e}\mathbf{L} = -\mu_B\frac{\mathbf{L}}{\hbar} \tag{2}$$

  with $\mu_B = e\hbar/(2m_e)$ the Bohr magneton.
- Quantum mechanics: Electron spin $\mathbf{S}$ adds to magnetic moment (*intrinsic* to quantum nature of electron, no classical analog),

$$\mathbf{m_S} = -g_e\mu_B\frac{\mathbf{S}}{\hbar} \tag{3}$$

  with Landé-factor g_e from relativistic quantum mechanics including QED correction $\alpha = 1/137$ (fine-structure constant):

$$g_e = 2\left(1 + \frac{\alpha}{2\pi} + \mathcal{O}(\alpha^2)\right) \simeq 2.0023 \tag{4}$$

- From now on: Approximate $g_e = 2$, set $\hbar = 1$.
- Total magnetic moment of electron:

$$\mathbf{m} = \mathbf{m_L} + \mathbf{m_S} = -\mu_B\left(\mathbf{L} + 2\mathbf{S}\right) \tag{5}$$

- Main focus of "Quantum magnetism": Magnetism of spins ($\rightarrow \mathbf{m_S}$), collective behavior of macroscopic number of interacting quantum spins.

14.2 Spin algebra

- Spin operator $\mathbf{S}_i = (S_i^x, S_i^y, S_i^z)$ fulfills angular momentum algebra ($\hbar = 1$),

$$\left[S_i^\alpha, S_j^\beta\right] = i\delta_{ij}\sum_{\gamma=x,y,z}\epsilon^{\alpha\beta\gamma}S_i^\gamma, \tag{6}$$

  where $\epsilon^{\alpha\beta\gamma}$ is the fully antisymmetric tensor with $\epsilon^{xyz} = 1$, $\epsilon^{zyx} = -1$, invariance under cyclic permutations of indices and otherwise vanishing. The rest of this section follows from the spin algebra.
- Spin raising and lowering operators: $S^\pm = S^x \pm iS^y$

- Spin length S: $\mathbf{S}^2 = S^x S^x + S^y S^y + S^z S^z$ commutes with S^α and has eigenvalue $S(S+1)$ with $S = 0, \frac{1}{2}, 1, \frac{3}{2}, ...$ integer or half-integer. Electron has $S = 1/2$, but larger S can arise from addition of multiple electron spin in an ion.
- Spin operators acting on S^z eigenstates $\{|m\rangle\}_{m=-S,-S+1,...,S-1,S}$:

$$\begin{aligned} S^z |m\rangle &= m |m\rangle \\ S^\pm |m\rangle &= \sqrt{S(S+1) - m(m\pm 1)}\, |m \pm 1\rangle \end{aligned}$$

- Example: Spin operators for $S = 1/2$ and $S = 1$.

$S = 1/2$	$S^x = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \frac{1}{2}\sigma^x$	$S^y = \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \frac{1}{2}\sigma^y$	$S^z = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \frac{1}{2}\sigma^z$
$S = 1$	$S^x = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$	$S^y = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}$	$S^z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$

14.3 Single spin thermodynamics

- Single spin in magnetic field B in z-direction with Hamiltonian

$$H = -m_S B = -\left(-2\mu_B S^z\right) B = \underbrace{2\mu_B B}_{\equiv h} S^z = h S^z \tag{7}$$

where we abbreviate $h = 2\mu_B B$.

- Partition function ($k_B = 1$)

$$\mathcal{Z}(h) = \mathrm{Tr} \exp\left[-\beta h S^z\right] \tag{8}$$

Compute the sum using a geometric series

$$\mathcal{Z}(h) = \sum_{m=-S}^{+S} \exp\left[-\beta h m\right] = \exp\left[\beta h S\right] \sum_{m=0}^{+2S} \exp\left[-\beta h\right]^m = \frac{\sinh\left[\beta h (S+1/2)\right]}{\sinh\left[\beta h/2\right]} \tag{9}$$

- Free energy $F = -T \ln \mathcal{Z}$, find magnetization $m^z = -2\mu_B \langle S^z \rangle$ as a function of $\beta h \equiv y$ [**Brillouin function**, Fig. 30(a)]:

$$\begin{aligned} \langle S^z \rangle &= -\partial_h F = \partial_y \ln \frac{\sinh\left[y(S+1/2)\right]}{\sinh\left[y/2\right]}\Big|_{y=\beta h} \\ &= \frac{1}{2}\left\{\coth\left(\frac{y}{2}\right) - (1+2S)\coth\left(\left[S+1/2\right] y\right)\right\} \\ &\overset{S=1/2}{=} -\frac{1}{2}\tanh\left[\frac{y}{2}\right] \end{aligned} \tag{10}$$

- Susceptibility (for $S = 1/2$):

$$\chi = \frac{\partial m^z}{\partial B} = -4\mu_B^2 \partial_h \langle S^z \rangle = \frac{4\mu_B^2}{4T\cosh^2(\beta h/2)} \overset{h=0}{=} \frac{\mu_B^2}{T} \tag{11}$$

This is the famous $\sim 1/T$ **Curie-law** indicative for magnetic insulators with localized *non-interacting* moments. See Fig. 30(b)

- Corrections to Curie law from interactions (phenomenological):
  - FM interaction: $1/\chi \sim T - T_\star$ with $T_\star$ the ordering temperature.
  - AFM interaction: $1/\chi \sim T + \Theta$ with $\Theta > 0$ the Curie-Weiss temperature.

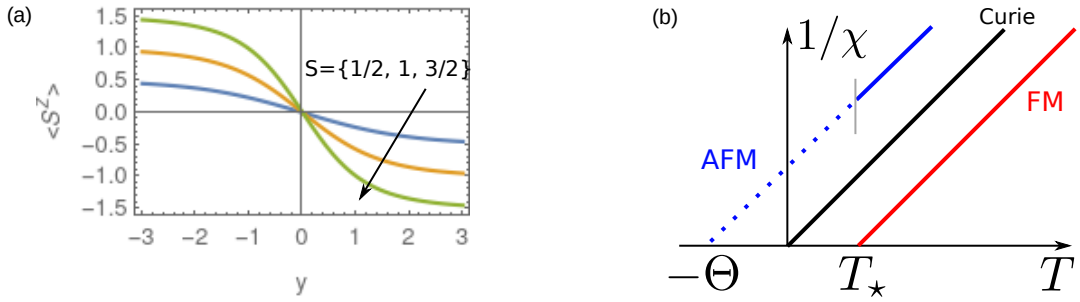


Figure 30: (a) Brillouin function for magnetization of free spin S for various S. (b) Generalized Curie law for paramagnet (black), ferromagnet (red) and anti-ferromagnet (blue).

Exercises

Exercise 14.1. Spin representations in terms of bosons and fermions

Spin operators S_j^α with $\alpha = \{x, y, z\}$ and j a site-index commute on different sites and for the same site fulfill the spin algebra, $\left[S^\alpha, S^\beta\right] = i\epsilon^{\alpha\beta\gamma}S^\gamma$, see Sec. 14.2. The (half-)integer spin length S determines the eigenvalue $S(S+1)$ of $\mathbf{S}^2$. However, for calculations on spin systems it is often desirable to use methods that are well established for bosonic and fermionic operators with their canonical (anti-) commutation relations $\{c_a, c_b^\dagger\} = \delta_{ab}$ and $[b_a, b_b^\dagger] = \delta_{ab}$ where subscript a, b are generic discrete single-particle indices and we denote $n_a = b_a^\dagger b_a$ and $n_a = c_a^\dagger c_a$ for the number operators. This exercise explores two of the most common spin representations.

1) Holstein-Primakoff bosons: This spin representation for arbitrary spin length S is used in spin-wave analysis, see Sec. 16.3. We introduce one boson b_i per site and define

$$\begin{aligned}\tilde{S}_i^+ &= \sqrt{2S - n_i}\, b_i,\\ \tilde{S}_i^- &= b_i^\dagger \sqrt{2S - n_i},\\ \tilde{S}_i^z &= S - n_i.\end{aligned}$$

so that the correspondence between S_i^z eigenvalue m_i and boson number n_i is $m_i = S - n_i$. Show that the spin algebra is fulfilled and check that $\mathbf{S}^2$ evaluates to $S(S+1)$ in the physical subspace defined by $n \leq 2S$. Also show that the operators $\tilde{S}_i^\pm$ do not connect physical and unphysical subspaces.

2) Abrikosov fermions ($S = 1/2$). In this fermionic spin representation $\tilde{S}_i^\alpha = \frac{1}{2}\sum_{a,b\in\{\uparrow,\downarrow\}} c_{ia}^\dagger \sigma_{ab}^\alpha c_{ib}$ where σ^α are the 2x2 Pauli matrices and $a, b \in \{\uparrow, \downarrow\}$. You may assume that the spin algebra is fulfilled (the calculation is straightforward). Show that $\mathbf{S}^2 = \frac{3}{4}P$ with $P = n_\downarrow + n_\uparrow - 2n_\uparrow n_\downarrow$. Show that P is a conserved quantity for any Spin-Hamiltonian $H = H\left(\{\tilde{S}_i^\alpha\}_{i,\alpha}\right)$ written in terms of Abrikosov fermions and that P has eigenvalues $0, 1$. This means the Abrikosov fermion representation for $S = 1/2$ comes with an unphysical spin $S = 0$ subspace.

15 Magnetic interactions

Aims:

- Microscopic interaction mechanisms between electron spins residing on different atoms
- Derive/motivate microscopic models of quantum magnetism (e.g. Heisenberg model)
- Skip: Coulomb exchange for electrons on the same atom (Hunds rules favor ferromagnetic spin alignment)

Dipole-dipole interactions

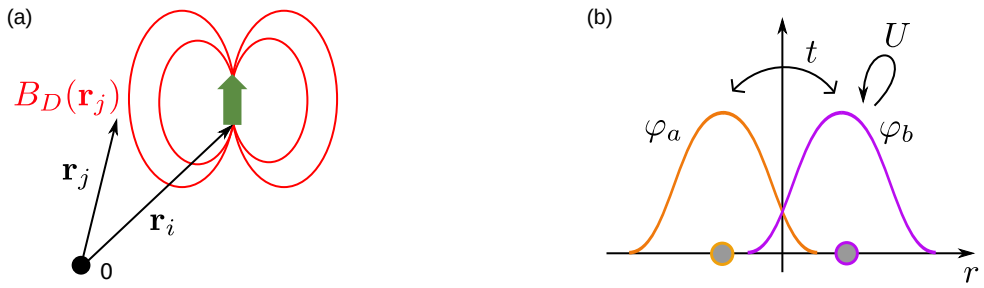


Figure 31: (a) Magnetic field exerted by a magnetic moment. (b) Setup for direct kinetic exchange between two atoms with overlapping wavefunctions $\varphi_{a,b}$.

- Classical magnetic field $\mathbf{B}_D(\mathbf{r}_j)$ exerted by magnetic moment $\mathbf{m}_i$ located at position $\mathbf{r}_i$ (see Fig. 31),

$$\mathbf{B}_D(\mathbf{r}_j) = \frac{\mu_0}{4\pi r_{ij}^5}\left[3(\mathbf{m}_i \cdot \mathbf{r}_{ij})\mathbf{r}_{ij} - r_{ij}^2 \mathbf{m}_i\right] \tag{12}$$

  with $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$.

- Interaction energy

$$E_D = -\mathbf{m}_j \cdot \mathbf{B}_D(\mathbf{r}_j) = \frac{\mu_0}{4\pi r_{ij}^5}\left[r_{ij}^2 \mathbf{m}_i \cdot \mathbf{m}_j - 3(\mathbf{m}_i \cdot \mathbf{r}_{ij})(\mathbf{m}_j \cdot \mathbf{r}_{ij})\right] \tag{13}$$

- In most magnetic materials, dipole-dipole interactions $E_D \sim 0.1K$ cannot explain the observed $J \sim T_\star \sim 100...1000K$ (distances r too large, moments $\mathbf{m}_i$ too small).

- Note: The dipole-dipole interaction is generally anisotropic and long-range (decays as $1/r^3$). The long-range nature has interesting consequences explored in Ex. 16.1.

Kinetic exchange I - Direct exchange

- Consider two spatially separated atoms with single electrons in orbitals φ_a and φ_b, respectively → use 2nd quantization $c_{a\sigma}$, $c_{b\sigma}$ with $\sigma = \{\uparrow, \downarrow\}$.

- Overlap of orbitals → hopping t, two electrons in same orbital on same atom → Hubbard repulsion $U > 0$.

$$H = \sum_\sigma t c_{a\sigma}^\dagger c_{b\sigma} + h.c. + U\left(n_{a\uparrow}n_{a\downarrow} + n_{b\uparrow}n_{b\downarrow}\right) = H_{kin} + H_U \tag{14}$$

  Remark: If generalized to N sites, this is the Hubbard model.

- We now focus on half filling (two electrons in the system). We have $H\left|\uparrow,\uparrow\right\rangle = H\left|\downarrow,\downarrow\right\rangle = 0$. For the remaining states $\{\left|\uparrow,\downarrow\right\rangle, \left|\downarrow,\uparrow\right\rangle, \left|\uparrow\downarrow,0\right\rangle, \left|0,\uparrow\downarrow\right\rangle\}$ we have the Hamiltonian

$$H' = \begin{pmatrix} 0 & 0 & t & t \\ 0 & 0 & -t & -t \\ t & -t & U & 0 \\ t & -t & 0 & U \end{pmatrix} \tag{15}$$

- Perturbation theory in $|t|/U \ll 1$ (degenerate PT, or Schrieffer-Wolff): Effective Hamiltonian in subspace spanned by $\{\left|\uparrow,\downarrow\right\rangle, \left|\downarrow,\uparrow\right\rangle\}$ at energy ~ 0. Find no contribution to first order in t, $H^{(1)} = 0$, but in second order find

$$H^{(2)} = \frac{2t^2}{U}\begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix}. \tag{16}$$

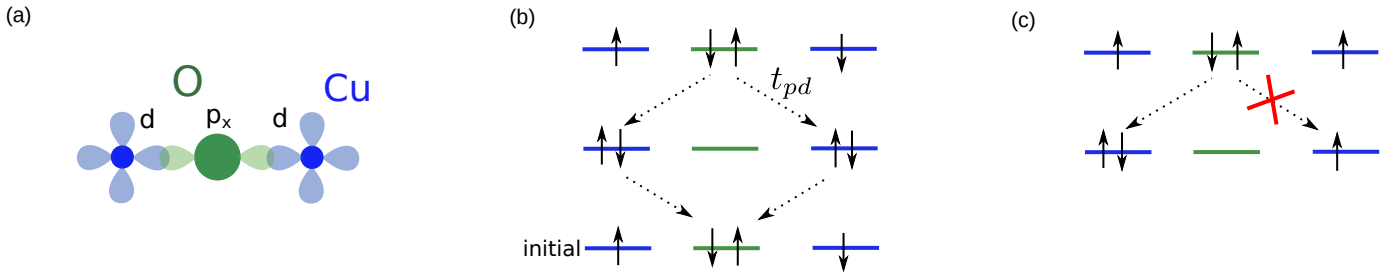


Figure 32: (a) Superexchange for copper oxide. (b) Exchange paths for anti-parallel copper spins exist, but not for parallel copper spins.

- Combine $H^{(2)}$ with the states $|\uparrow,\uparrow\rangle, |\uparrow,\uparrow\rangle$ that were also at energy 0. Find in basis $\{|\uparrow,\uparrow\rangle, |\uparrow,\downarrow\rangle, |\downarrow,\uparrow\rangle, |\downarrow,\downarrow\rangle\}$:

$$H_{eff} = \frac{2t^2}{U}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{17}$$

  Compare to Heisenberg Hamiltonian in the same basis:

$$H = J\left(\mathbf{S}_a \cdot \mathbf{S}_b - \frac{1}{4}\right) = J\left(\frac{1}{2}S_a^+ S_b^- + \frac{1}{2}S_a^- S_b^+ + S_a^z S_b^z - \frac{1}{4}\right) = J\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & -1/2 & 1/2 & 0 \\ 0 & 1/2 & -1/2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{18}$$

  Note: The ground-state is the (total spin)$S_{tot} = 0$ singlet $\psi_s = (|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle)/\sqrt{2}$ at $E_s = -J$ and the other $S_{tot} = 1$ triplet states $(|\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle)/\sqrt{2}$, $|\uparrow,\uparrow\rangle, |\downarrow,\downarrow\rangle$ reside at $E_t = 0$.

- Conclusion:
  - Direct kinetic exchange affects neighboring atoms with singly occupied outermost shells.
  - Quantum tunneling leads to effective AFM Heisenberg Hamiltonian with $J = 4t^2/U > 0$. Generalize for lattice where one can usually focus on nearest-neighbor exchange ($\langle i,j\rangle$) and drop constant:

$$\boxed{H = J\sum_{\langle i,j\rangle} \mathbf{S}_i \cdot \mathbf{S}_j} \tag{19}$$

  - Physical picture: Exchange paths exist for $|\uparrow,\downarrow\rangle, |\downarrow,\uparrow\rangle$ but not for $|\sigma,\sigma\rangle$, $\sigma \in \{\uparrow,\downarrow\}$. Thus anti-parallel spins can lower their energy by H_{kin}, e.g.:

$$\begin{aligned} |\uparrow,\downarrow\rangle &\xrightarrow{H_{kin}} |\downarrow\uparrow,0\rangle \xrightarrow{H_{kin}} |\uparrow,\downarrow\rangle \\ |\sigma,\sigma\rangle &\xrightarrow{H_{kin}} 0 \end{aligned}$$

Kinetic exchange II - Superexchange

- In real materials, the hopping between two magnetic ions often proceeds via a non-magnetic ion in between.
- Example with 180° bond: Copper oxide, CuO_2. See Fig. 32.
  - copper Cu^{2+} has one hole in d-shell ($[Ar]d^9$) and oxygen O^{2-} has a completely filled p-shell (two electrons in p_x-shell).

  - compare exchange paths for anti-parallel spins on Cu to exchange paths for parallel spins (none). This again favors AFM configuration.
  - Detailed calculation: Get again AFM Heisenberg interactions.

- Remark: 90° bonds can lead to weaker FM interactions. Why: Hund's rule for intermediate configuration in p_x and p_y state favors $|\uparrow,\uparrow\rangle$ over $|\uparrow,\downarrow\rangle$.

16 Heisenberg Model

Aims:

- Introduce basic notions around quantum Heisenberg model
- Mean-field theory (recap for FM case, new for AFM case)
- Approximately include quantum fluctuations on top of ordered state by spin-wave theory.
- Assess stability of ordered phase at $T = 0$ and $T > 0$ depending on dimensionality.

16.1 Introduction

- The Heisenberg model is defined as

$$H = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j = J \sum_{\langle ij \rangle} \left(\frac{1}{2} S_i^+ S_j^- + \frac{1}{2} S_i^- S_j^+ + S_i^z S_j^z \right) \tag{20}$$

  where we assume spin $S = 1/2$ and nearest-neighbour couplings.

- Symmetry:
  - Global SU(2) spin rotation, $\mathbf{S}_i \to R^\dagger \mathbf{S}_i R$ for all i with $R = \exp\left(-i\varphi \mathbf{n} \sum_i \mathbf{S}_i\right)$ and unit vector $\mathbf{n} \in \mathbb{R}^3$ defining rotation axis.

- Remarks:
  - Exactly solvable in D=1 (Bethe-Ansatz, 1931)
  - FM case $J < 0$, the exact ground state is known for all D: It is a simple product state, $|0\rangle = \prod_i \otimes |\uparrow\rangle_i$. Note that the terms $S_i^- S_j^+$ act trivially on $|0\rangle$.
  - AFM case $J > 0$, the exact ground state is not known (for D>1). Problem: The staggered state in Fig. 33(a) is not an exact eigenstate of H due to $S_i^+ S_j^- + h.c.$, but it is a good approximation to the true ground state.

- Frustration:
  - For lattices with particular motifs like a triangle in Fig. 33(b), there is not even a staggered state that would be the unique ground-state of the $S_i^z S_j^z$-term (Ising model).
  - Frustration might prevent magnetic order and can give rise to exotic disordered ground states like quantum "spin-liquids".
    Example: Nearest-neighbor $S = 1/2$ AFM Heisenberg model on triangular lattice. The ground-state is magnetically ordered, a few percent of next-nearest-neighbor coupling is needed to melt the order.
  - Remark: If frustration stems from lattice, it is called geometric frustration. Also the coupling-type in the Hamiltonian can result in frustration.

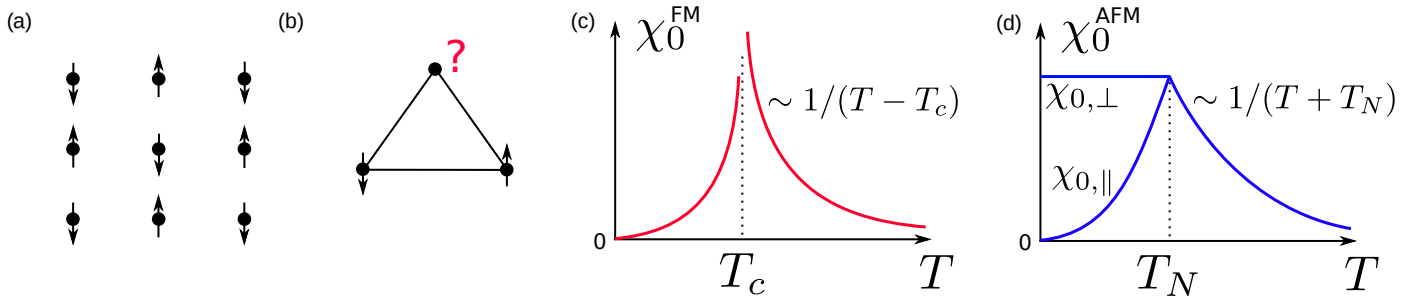


Figure 33: (a) Staggered state on the square lattice. (b) Frustration for an AFM Hamiltonian on a triangle. (c) Mean-field susceptibility for a FM and (d) the same for AFM.

16.2 Mean-field theory (reminder)

- Add magnetic field $\mathbf{B}$ in negative z-direction, $H \to H - h\sum_i S_i^z$ with $h = -2\mu_B B$.
- Mean-field approximation in H:

$$\mathbf{S}_i \cdot \mathbf{S}_j \to \langle \mathbf{S}_i \rangle \cdot \mathbf{S}_j + \mathbf{S}_i \cdot \langle \mathbf{S}_j \rangle - \langle \mathbf{S}_i \rangle \cdot \langle \mathbf{S}_j \rangle \tag{21}$$

  which implies that fluctuations (thermal and quantum) are small, $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle = \langle \mathbf{S}_i \rangle \cdot \langle \mathbf{S}_j \rangle$.
- Recall: Coordination number z, the number of nearest-neighbors. For hypercubic lattices $z = 2D$.

Mean-field approach to FM case ($J < 0$)

- Ansatz $\langle \mathbf{S}_i \rangle = \langle S^z \rangle$ for all i. Up to a constant term, obtain

$$H_{MF} = -\left(Jz\langle S^z\rangle + h\right)\sum_i S_i^z \tag{22}$$

  which is the Hamiltonian of a (independent set of) free spin $S = 1/2$ in a magnetic field (which depends on $\langle S^z\rangle$!). The magnetization has been found in Eq. (10). We obtain the familiar self-consistency equation for $\langle S^z\rangle$:

$$\langle S^z\rangle = \frac{1}{2}\tanh\left(\frac{h + |J|z\langle S^z\rangle}{2T}\right) \tag{23}$$

- Set $h = 0$, obtain critical temperature $T_c = \frac{|J|z}{4}$ and critical exponent $\beta = 1/2$ as in Part I.
- Magnetic susceptibility at zero field (use $m^z = -2N\mu_B\langle S^z\rangle$ and $h = -2\mu_B B$):

$$\chi_0 = \frac{\partial m^z}{\partial B}|_{B=0} = 4N\mu_B^2 \partial_h \langle S^z\rangle|_{h=0} \tag{24}$$

  with

$$\partial_h\langle S^z\rangle|_{h=0} = \frac{1 + |J|z\partial_h\langle S^z\rangle|_{h=0}}{4T}\cosh^{-2}\left(\frac{|J|z\langle S^z\rangle|_{h=0}}{2T}\right) \tag{25}$$

  which can be solved for $\partial_h\langle S^z\rangle|_{h=0}$. We find

$$\chi_0 = N\mu_B^2\frac{1}{T\cosh^2\left(\frac{|J|z\langle S^z\rangle|_{h=0}}{2T}\right) - \frac{|J|z}{4}} \overset{T\geq T_c}{\longrightarrow} \frac{N\mu_B^2}{T - T_c} \tag{26}$$

  which is of the Curie-Weiss form, see Fig. 30(b).
- The susceptibility χ_0 for all T is shown in Fig. 33(c). Below T_c, the susceptibility becomes anisotropic. We so far calculated $\chi_0 = \chi_{0,\parallel}$ with the magnetic field applied parallel to the magnetization $\mathbf{B} \parallel \mathbf{e}_z$.
- The transversal susceptibility $\chi_{0,\perp}$ with $\mathbf{B} \perp \mathbf{e}_z$ diverges as the magnetization can be rotated by an infinitesimal field. This reflects the presence of a gapless Goldstone mode due to broken continous symmetry.

Mean-field approach to AFM case ($J > 0$)

- Split the lattice into sub-lattices A,B. Ansatz $\langle \mathbf{S}_i \rangle = \left\langle S^z_{A,B} \right\rangle$ for $i \in$ sub-lattice A,B.
- Note: The nearest neighbors of i on sub-lattice A are on sub-lattice B. Obtain with $h_{A,B} = -Jz \left\langle S^z_{A,B} \right\rangle$:

$$H_{MF} = -h_A \sum_{i \in B} S^z_i - h_B \sum_{i \in A} S^z_i - h \sum_i S^z_i \tag{27}$$

- Self-consistency equation:

$$\left\langle S^z_{A,B} \right\rangle = \frac{1}{2} \tanh \left(\frac{h - Jz \left\langle S^z_{B,A} \right\rangle}{2T} \right) \tag{28}$$

- Set $h = 0$, obtain $\langle S^z_A \rangle = -\langle S^z_B \rangle = \langle S^z \rangle$ which fulfills the same self-consistency equation as in the FM case. We find the same T_c which is known as the Néel temperature T_N.
- Magnetic susceptibility at zero field:

$$\chi_0 = 2N\mu_B^2 \left(\partial_h \langle S^z_A \rangle + \partial_h \langle S^z_B \rangle \right)|_{h=0} \overset{T \geq T_N}{\longrightarrow} \ldots = N\mu_B^2 \frac{1}{T + T_N} \tag{29}$$

  The susceptibility is shown in Fig. 33(d), it does not diverge and splits below T_N into a constant transversal part $\chi_{0,\perp}$ and a decaying $\chi_{0,\parallel}$.
- Notes:
  - The susceptibility to a hypothetical staggered field (taking opposite values on the two sub-lattices) would diverge.
  - The critical temperatures of an AFM and FM on the same lattice are only the same in MFT, but quantum effects make them differ.

16.3 Spin-wave theory

- Q: What are the excitations of a magnetically ordered Heisenberg system? Naive expectation - spin flip: ↑↑↑↑↑ → ↑↑↓↑↑ would cost energy $\mathcal{O}(J)$.
- This is wrong, the spin-flip excitations are delocalized over the lattice such that they are gapless spin-waves (=magnons).

16.3.1 Spin representation: Holstein-Primakoff bosons (see Ex. 14.1)

- Generalize to arbitrary spin-S, introduce one boson per site, $[b_i, b_j^\dagger] = \delta_{ij}$, $n_i = b_i^\dagger b_i$ and $b_i^\dagger |n_i\rangle = \sqrt{n+1}\,|n_i + 1\rangle$, $b_i |n_i\rangle = \sqrt{n}\,|n_i - 1\rangle$:

$$\begin{aligned} S_i^+ &= \sqrt{2S - n_i}\, b_i \\ S_i^- &= b_i^\dagger \sqrt{2S - n_i} \\ S_i^z &= S - n_i \end{aligned}$$

- The representation fulfills the spin algebra. From the last line, the correspondence between S_i^z quantum number and boson occupation is $m_i = -n_i + S$. What about $n_i > 2S$? Problem: S_i^z has only $2S + 1$ eigenvalues $m_i = -S, -S+1, \ldots, S$ whereas $n_i = 0, 1, 2, \ldots$ has infinite number of eigenvalues. The Hilbert space is too large and we need to restrict to $n_i \leq 2S$.
- The vacuum of bosons $n_i = 0$ for all i corresponds to the fully polarized state ↑↑↑↑ ....
- Note: Holstein-Primakoff bosons single out one direction in spin space. The S^z direction is used to define their vacuum. This is why Holstein-Primakoff bosons are used to describe phases with broken spin rotation symmetry.

16.3.2 Spin-wave theory for ferromagnet ($J < 0$)

- Insert Holstein-Primakoff representation in Heisenberg Hamiltonian

$$\begin{aligned} H &= -|J| \sum_{\langle ij \rangle} \left(\frac{1}{2} S_i^+ S_j^- + \frac{1}{2} S_i^- S_j^+ + S_i^z S_j^z \right) \\ &= -|J| \sum_{\langle ij \rangle} \left(S \sqrt{1 - \frac{n_i}{2S}}\, b_i b_j^\dagger \sqrt{1 - \frac{n_j}{2S}} + b_i^\dagger \sqrt{1 - \frac{n_i}{2S}} \sqrt{1 - \frac{n_j}{2S}} b_j + (S - n_i)(S - n_j) \right) \end{aligned}$$

- Assume that at low T, we are close to the fully polarized ground state state such that $n_i \ll 2S$. This is the case if S is large. Then expand $\sqrt{1 - \frac{n_i}{2S}} = 1 - \frac{n_i}{4S} + O(S^{-2})$ and keep only terms to order $S^{2,1,0}$ and drop terms of order $1/S$ and smaller.

$$\begin{aligned} H &= -|J| S^2 \frac{Nz}{2} + |J| S \sum_{\langle ij \rangle} \left(b_i^\dagger b_i + b_j^\dagger b_j - b_j^\dagger b_i - b_i^\dagger b_j \right) - |J| \sum_{\langle ij \rangle} "b^\dagger b^\dagger b b" + ... \\ &= H_0 + H_1 + H_2 + ... \end{aligned}$$

- Term H_0 contains the classical ground state energy E_0.

- Term $H_1 \propto S$ describes spin-waves. It can be diagonalized with a Fourier transform, $b_i = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\mathbf{R}_i} b_{\mathbf{k}}$. We find

$$\begin{aligned} H_1 &= \frac{|J|S}{N} \sum_{\mathbf{k},\mathbf{k}'} \sum_{\langle ij \rangle} \left(e^{-i(\mathbf{k}-\mathbf{k}')\mathbf{R}_i} + e^{-i(\mathbf{k}-\mathbf{k}')\mathbf{R}_j} - e^{-i\mathbf{k}\mathbf{R}_j} e^{i\mathbf{k}'\mathbf{R}_i} - e^{-i\mathbf{k}\mathbf{R}_i} e^{-i\mathbf{k}'\mathbf{R}_j} \right) b_{\mathbf{k}}^\dagger b_{\mathbf{k}'} \\ &= \sum_{\mathbf{k}} \underbrace{|J|S \sum_{\Delta\mathbf{R}} (1 - \cos[\mathbf{k} \cdot \Delta\mathbf{R}])}_{\equiv \omega_{\mathbf{k}}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}} \end{aligned}$$

  where $\Delta\mathbf{R}$ are the nearest-neighbor vectors and the dispersion $\omega_{\mathbf{k}} = 2|J|S(D - \sum_{\mu=1}^{D} \cos k_\mu)$ describes parabolically dispersing spin-wave excitations (=magnons) that are gapless at $\mathbf{k} = 0$.

- The occurrence of a zero-energy mode follows from Goldstone theorem: Spontaneous breaking of a continous symmetry (here SU(2) spin-rotation) results in a zero-energy "Goldstone" mode.

- Term H_2: Interactions between spin-waves. Hard to treat and sub-leading for large S. Discard.

- Consistency check: Is $n_i \ll 2S$ really true? Check if $\langle S_i^z \rangle$ is close to S.

$$\langle S_i^z \rangle = S - \langle n_i \rangle = S - \frac{1}{N} \sum_{\mathbf{k}} \langle n_{\mathbf{k}} \rangle = S - \frac{1}{(2\pi)^D} \int_{-\pi}^{\pi} d^D\mathbf{k} \frac{1}{e^{\beta\omega_{\mathbf{k}}} - 1} \tag{30}$$

  The integral is dominated at small k where $\omega_{\mathbf{k}} \simeq |J|Sk^2$ is small and can be easily occupied thermally. Extend the k-integral over all space up with a lower boundary set by system size $\Lambda = 2\pi/L$ and approximate the fraction,

$$\langle S_i^z \rangle \simeq S - \frac{\Omega_D}{(2\pi)^D} \int_{\Lambda}^{\infty} k^{D-1} dk \frac{1}{\beta|J|Sk^2} = S - \frac{\Omega_D}{(2\pi)^D \beta|J|S} \int_{\Lambda}^{\infty} k^{D-3} dk. \tag{31}$$

  The integral is yields

$$\int_{\Lambda}^{\infty} k^{D-3} dk \sim \begin{cases} 1/\Lambda & : D = 1 \\ -\ln \Lambda & : D = 2 \\ \text{const.} & : D = 3 \end{cases} \tag{32}$$

  and we are interested in the behavior of the integral as the system size L grows and $\Lambda \to 0$.

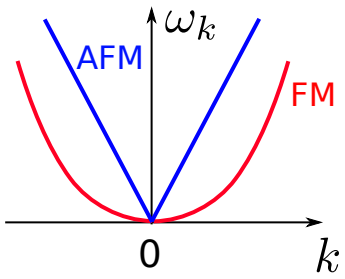


Figure 34: Schematic spin-wave dispersion for nearest-neighbor FM (red) and AFM (blue).

- $D = 1, 2$: The integral diverges for any finite T, the magnetization is not close to S but goes to $-\infty$. Spin wave theory is not valid. Although the result for $\langle S_i^z \rangle$ is unphysical result, we can infer that the magnetic order melts.
  This is in agreement with the [**Mermin-Wagner-Hohenberg theorem**: Continous symmetries cannot be spontaneously broken at $T > 0$ in $D \leq 2$ dimensions with short-range interactions.]
- $D = 3$: Closer inspection of the convergent BZ integral reveals $S - \langle S_i^z \rangle = \frac{\zeta(3/2)}{8} \left(\frac{T}{\pi |J| S} \right)^{3/2} \sim T^{3/2}$ which is small for small enough T. The magnetic order survives finite T.

16.3.3 Spin-wave theory for anti-ferromagnet ($J > 0$)

- We chose the staggered state [Néel state, see Fig. 33(a)] as the reference state.
- Recall: This is *not* an eigenstate for the AFM Heisenberg model → Look out for the effect of quantum fluctuations at $T = 0$.
- Introduce two types of Holstein-Primakoff bosons, one for each sub-lattice. Drop the $\sqrt{\dots}$ factor right away to neglect interactions. The state with $n_{i,a} = 0 = n_{i,b}$ is the Néel state.
  - Sub-lattice A (spin up, a-bosons): $S_i^z = -n_{i,a} + S$, $S_i^+ \simeq a_i$, $S_i^- \simeq a_i^\dagger$.
  - Sub-lattice B (spin down, b-bosons): $S_i^z = +n_{i,b} - S$, $S_i^+ \simeq b_i^\dagger$, $S_i^- \simeq b_i$.
- Insert in spin Hamiltonian:

$$H = -JS^2 \frac{Nz}{2} + JS \sum_{\langle ij \rangle, i \in A, j \in B} \left(a_i^\dagger a_i + b_j^\dagger b_j + a_i b_j + b_j^\dagger a_i^\dagger \right) \tag{33}$$

  and perform Fourier transform $a_i = \frac{1}{\sqrt{N/2}} \sum_{\mathbf{k}} e^{i\mathbf{k}\mathbf{R}_i} a_{\mathbf{k}}$ and $b_i = \frac{1}{\sqrt{N/2}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\mathbf{R}_i} b_{\mathbf{k}}$.
- We obtain

$$H = E_{0,MF} + JSz \sum_{\mathbf{k}} \left(a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + \gamma_{\mathbf{k}} \left[a_{\mathbf{k}} b_{\mathbf{k}} + b_{\mathbf{k}}^\dagger a_{\mathbf{k}}^\dagger \right] \right) \tag{34}$$

  with $\gamma_{\mathbf{k}} = \frac{1}{D} \sum_{\mu=1}^{D} \cos k_\mu$ and $E_{0,MF} = -JS^2 \frac{Nz}{2} = -JS^2 ND$ the mean-field g.s.-energy.
- The latter two terms are anomalous as they do not conserve the boson number. This is analogous to what happens in the *fermionic* BCS mean field theory.
- We apply a canonical Bogoliubov transformation $a, b \to \alpha, \beta$ to get rid of the anomalous terms,

$$\begin{aligned} a_{\mathbf{k}} &= \cosh \theta_{\mathbf{k}} \alpha_{\mathbf{k}} - \sinh \theta_{\mathbf{k}} \beta_{\mathbf{k}}^\dagger \\ b_{\mathbf{k}} &= -\sinh \theta_{\mathbf{k}} \alpha_{\mathbf{k}}^\dagger + \cosh \theta_{\mathbf{k}} \beta_{\mathbf{k}} \end{aligned}$$

  Since the transformation is canonical, the new bosonic operators $\alpha_{\mathbf{k}}$, $\beta_{\mathbf{k}}$ still fulfill the standard bosonic commutation relations.

- We find with $c_{\mathbf{k}} \equiv \cosh\theta_{\mathbf{k}}$, $s_{\mathbf{k}} \equiv \sinh\theta_{\mathbf{k}}$

$$\begin{aligned} H &= E_{0,MF} + JSz\sum_{\mathbf{k}}\left\{2s_{\mathbf{k}}^2 - 2\gamma_{\mathbf{k}}c_{\mathbf{k}}s_{\mathbf{k}}\right\} \\ &+ JSz\sum_{\mathbf{k}}\left\{c_{\mathbf{k}}^2 + s_{\mathbf{k}}^2 - 2\gamma_{\mathbf{k}}s_{\mathbf{k}}c_{\mathbf{k}}\right\}\left(\alpha_{\mathbf{k}}^\dagger\alpha_{\mathbf{k}} + \beta_{\mathbf{k}}^\dagger\beta_{\mathbf{k}}\right) \\ &+ JSz\sum_{\mathbf{k}}\left\{\gamma_{\mathbf{k}}\left(s_{\mathbf{k}}^2 + c_{\mathbf{k}}^2\right) - 2c_{\mathbf{k}}s_{\mathbf{k}}\right\}\left(\alpha_{\mathbf{k}}^\dagger\beta_{\mathbf{k}}^\dagger + \alpha_{\mathbf{k}}\beta_{\mathbf{k}}\right) \end{aligned}$$

  The last line with the anomalous terms vanish if we pick $\theta_{\mathbf{k}}$ such that $\tanh 2\theta_{\mathbf{k}} = \gamma_{\mathbf{k}}$. Then we have after some algebra for hyperbolic functions ($\cosh^{-1} x = \sqrt{1-\tanh^2 x}$)

$$H = E_{0,MF} - JSz\frac{N}{2} + \sum_{\mathbf{k}}\underbrace{JSz\sqrt{1-\gamma_{\mathbf{k}}^2}}_{\equiv\omega_{\mathbf{k}}}\left(\alpha_{\mathbf{k}}^\dagger\alpha_{\mathbf{k}} + \beta_{\mathbf{k}}^\dagger\beta_{\mathbf{k}} + 1\right)$$

- The magnon dispersion close to $k = 0$ is $\omega_k \simeq JSz\sqrt{1-\frac{1}{D^2}\left[D - k^2/2\right]^2} \simeq 2JS\sqrt{D}k$. This vanishes linearly, i.e. with a finite velocity in contrast to the parabolic dispersion for the FM case, see Fig. 34.

Zero temperature (ground state)

- Ground state is the vacuum of α and β-bosons.
- Energy: $E_0 = E_{0,MF} - JSz\frac{N}{2} + \sum_{\mathbf{k}}\omega_{\mathbf{k}}$ can be calculated numerically and is smaller than $E_{0,MF}$. The results are shown in the table. For $S = 1/2$, agreement with Bethe-ansatz (1D) and Quantum Monte Carlo (2D) is surprisingly good.

$T=0$ (g.s.)	$E_0/E_{0,MF}$	$E_0/(NJ)\vert_{S=1/2}$		$m^z(\mathbf{Q})/m^z_{sat}$	$m^z(\mathbf{Q})/m^z_{sat}\vert_{S=1/2}$	
	SWT	SWT	exact	SWT	SWT	exact
$D=1$	$1+0.363/S$	-0.4315	-0.4434	divergent	divergent	0
$D=2$	$1+0.158/S$	-0.658	$-0.669(2)$	$1-0.197/S$	0.607	0.614(12)
$D=3$	$1+0.097/S$	-	-	$1-0.078/S$	-	-

- Staggered magnetization [at wavevector $\mathbf{Q} = (\pi, \pi, ...)$]

$$\begin{aligned} m^z(\mathbf{Q}) &= -2\mu_B\left(\langle S_A^z\rangle - \langle S_B^z\rangle\right) \\ &= -2\mu_B\left(2\langle S_A^z\rangle\right) \\ &= -2\mu_B\left(2S - 2\left\langle a_i^\dagger a_i\right\rangle\right) \\ &= m^z_{sat} + \frac{4\mu_B}{N}\sum_{\mathbf{k}}\left\langle\cosh^2\theta_{\mathbf{k}}\alpha_{\mathbf{k}}^\dagger\alpha_{\mathbf{k}} - \sinh\theta_{\mathbf{k}}\cosh\theta_{\mathbf{k}}\beta_{\mathbf{k}}\alpha_{\mathbf{k}} - \cosh\theta_{\mathbf{k}}\sinh\theta_{\mathbf{k}}\alpha_{\mathbf{k}}^\dagger\beta_{\mathbf{k}}^\dagger + \sinh^2\theta_{\mathbf{k}}\beta_{\mathbf{k}}\beta_{\mathbf{k}}^\dagger\right\rangle \end{aligned}$$

  The two anomalous middle terms vanish and we use $\left\langle\alpha_{\mathbf{k}}^\dagger\alpha_{\mathbf{k}}\right\rangle = n_B(\omega_{\mathbf{k}}) \overset{T=0}{\to} 0$ and $\left\langle\beta_{\mathbf{k}}\beta_{\mathbf{k}}^\dagger\right\rangle = 1 + n_B(\omega_{\mathbf{k}}) \overset{T=0}{\to} 1$. We use $\sinh^2\theta_{\mathbf{k}} = (1/\sqrt{1-\gamma_{\mathbf{k}}^2} - 1)/2$. We find

$$m^z(\mathbf{Q})/m^z_{sat} = 1 - \frac{1}{2S}\frac{1}{(2\pi)^D}\int_{-\pi}^{\pi} d^D\mathbf{k}\left(\frac{1}{\sqrt{1-\gamma_{\mathbf{k}}^2}} - 1\right) \tag{35}$$

  - $D = 2, 3$: The integral converges. See table for numerical value. Néel state is not real ground state of AFM Heisenberg model, the true staggered magnetization (in 2D) is reduced to ~60% of the saturated magnetization.
  - $D = 1$, the integrand $\sim 1/k$ and is thus infrared log-divergent (ground state is disordered by quantum fluctuations). Note the difference to the ordered ground state in the $D = 1$ FM case.

Finite temperature

- As before, we find that staggered magnetization survives thermal fluctuations only in $D = 3$,

$$m^z(\mathbf{Q}, T) \simeq m^z(\mathbf{Q}, T = 0) - \frac{2\sqrt{3}\mu_B}{144}\left(\frac{T}{JS}\right)^2 \tag{36}$$

  which is different from the $\sim T^{3/2}$ law for the FM.

Exercises

Exercise 16.1. Spin-wave theory for FM XY model on 2D square lattice: Nearest-neigbor vs. dipolar coupling Consider the ferromagnetic XY model on a 2D square lattice with lattice constant $a = 1$ for spin length $S = 1/2$,

$$H = -\sum_{i \neq j} J\left(|\mathbf{r}_i - \mathbf{r}_j|\right)\left(S_i^x S_j^x + S_i^y S_j^y\right). \tag{37}$$

Note that each bond is counted twice! We are mostly interested in the long-range coupled case $J^{dip.}(r) = |J|/r^3$ but also consider the nearest-neighbor (n.n.) case, $J^{n.n}(r) = |J|\delta_{r,1}$, for reference. The goal of this exercise is to understand how the long-range model emerges from dipole-dipole coupling and how the long-range nature drastically alters the predictions from spin-wave theory when compared to the n.n. case.

1) Motivation for long-range coupling: Consider magnetic moments $\mathbf{m}_i = (S_i^x, S_i^y, S_i^z)$ on the sites $\mathbf{r}_i$ of a square lattice interacting with dipole-dipole interactions $H_{D,ij} \sim r_{ij}^{-5}[r_{ij}^2 \mathbf{m}_i \cdot \mathbf{m}_j - 3(\mathbf{m}_i \cdot \mathbf{r}_{ij})(\mathbf{m}_j \cdot \mathbf{r}_{ij})]$ and show that the in-plane nature of $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j = r_{ij}(\cos\phi_{ij}, \sin\phi_{ij}, 0)^{\mathrm{T}} \perp \mathbf{e}_z$ simplifies H_D to

$$H_{D,ij} \sim \frac{1}{4r_{ij}^3}\left[-S_i^+ S_j^- - S_i^- S_j^+ + 4S_i^z S_j^z - 3\left(e^{-2i\phi_{ij}} S_i^+ S_j^+ + e^{+2i\phi_{ij}} S_i^- S_j^-\right)\right]. \tag{38}$$

If a *large* Zeeman field $\sim h(S_i^z + S_j^z) = hM_{ij}^z$ is present, the dynamics caused by $H_{D,ij}$ can be restricted to the subspace of the initial M_{ij}^z, say $M_{ij}^z = 0$ and we can drop off-resonant terms. Argue that in this case, the long-range XY-Hamiltonian (37) emerges.

2) Assume a classical ordered state with spins pointing in the negative x-direction. Show that the energy per site in this state in mean-field approximation is $\epsilon_{0,MF} = \frac{E_{0,MF}}{N} = -|J|\frac{\varepsilon_{\mathbf{0}}}{4}$ where the Fourier transform of the coupling is defined as

$$\varepsilon_{\mathbf{k}} \equiv \frac{1}{|J|}\sum_{\mathbf{r}_j \neq 0} e^{i\mathbf{k}\cdot\mathbf{r}} J\left(|\mathbf{r}_j|\right). \tag{39}$$

Note that $\varepsilon_{\mathbf{k}}$ is real-valued, positive and fulfills $\varepsilon_{-\mathbf{k}} = \varepsilon_{\mathbf{k}}$ due to inversion symmetry. Show the following leading-order behaviors for small k around the ordering wavevector $\mathbf{k} = 0$,

$$\varepsilon_{\mathbf{k}} = \varepsilon_{\mathbf{0}} - \begin{cases} c_{n.n.}k^2 + \ldots & (n.n.) \\ c_{dip.}k + \ldots & (dip.) \end{cases} \tag{40}$$

where the positive constants $c_{n.n.}$ and $c_{dip.}$ do not need to be determined.

3) Spin-wave analysis: Adapt the Holstein-Primakoff bosonic representation to the situation that the magnetic order is in the negative x-direction, e.g. $S_i^x = n_i - 1/2$. You can work with $S = 1/2$ and drop the square-root term in $S_i^{y,z}$ right away. Insert in Hamiltonian (37) and use a Fourier transform $a_i = \frac{1}{\sqrt{N}}\sum_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}_i} a_{\mathbf{k}}$ and a Bogoliubov transform

$$\begin{pmatrix} b_{\mathbf{k}} \\ b_{-\mathbf{k}}^\dagger \end{pmatrix} = \begin{pmatrix} u_{\mathbf{k}} & -v_{\mathbf{k}} \\ -v_{\mathbf{k}} & u_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} a_{\mathbf{k}} \\ a_{-\mathbf{k}}^\dagger \end{pmatrix} \tag{41}$$

with $u_{\mathbf{q}}^2 - v_{\mathbf{q}}^2 = 1$ to eliminate anomalous terms $b_{\mathbf{k}}^\dagger b_{-\mathbf{k}}^\dagger$ and $b_{\mathbf{k}} b_{-\mathbf{k}}$. Show that the spin-wave Hamiltonian and dispersion of Goldstone modes from broken $U(1)$ symmetry reads:

$$H = E_{0,MF} + \frac{1}{2}\sum_{\mathbf{k}} E_{\mathbf{k}} + \sum_{\mathbf{k}} E_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}}, \text{ where } E_{\mathbf{k}} = |J|\sqrt{\varepsilon_{\mathbf{0}}\left(\varepsilon_{\mathbf{0}} - \varepsilon_{\mathbf{k}}\right)} \sim \begin{cases} k & : \text{n.n.} \\ \sqrt{k} & : \text{dipolar} \end{cases} \tag{42}$$

4) Compute the spin-wave correction to the classical magnetization $\Delta m^x = \langle S_i^x \rangle + \frac{1}{2} = \left\langle a_i^\dagger a_i \right\rangle = \frac{1}{N} \sum_{\mathbf{k}} \left\langle a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \right\rangle$ and show that

$$\Delta m^x = \frac{1}{N} \sum_{\mathbf{k}} \left(\frac{1}{4} \frac{2\varepsilon_{\mathbf{0}} - \varepsilon_{\mathbf{k}}}{\sqrt{\varepsilon_{\mathbf{0}} \left(\varepsilon_{\mathbf{0}} - \varepsilon_{\mathbf{k}} \right)}} \frac{1}{\tanh \frac{\beta E_{\mathbf{k}}}{2}} - \frac{1}{2} \right). \tag{43}$$

Consider the cases $T = 0$ and small $T > 0$ separately. In which cases (n.n./dip. and $T = 0/T > 0$) does the momentum sum converge? What can you conclude about the ordered or disordered nature of ground- and low-temperature states for the n.n. and dipolar model? Is there a contradiction to the Mermin-Wagner-Hohenberg theorem?

17 Antiferromagnetic Heisenberg chain (D=1)

- We consider the AFM n.n. Heisenberg chain

$$H = J \sum_{i=1}^{N} \mathbf{S}_i \mathbf{S}_{i+1}, \tag{44}$$

  with $J > 0$, N even and periodic boundary conditions, $\mathbf{S}_{N+1} \equiv \mathbf{S}_1$.

- We have seen that AFM interactions in $D = 1$ are special: Even at $T = 0$, staggered magnetization vanishes by quantum fluctuations.

- What are the properties of the ground-state and the excitations? Important: Keep spin-length $S = \frac{1}{2}, 1, \frac{3}{2}, 2, ...$ general as this will matter!

Bipartite lattice

- A lattice with couplings J_{ij} that can be separated into two disjoint sub-lattices A and B where J_{ij} are non-zero only for $i \in A, B \in j$ or $i \in B, j \in A$ is called bipartite.

- Examples for bipartite lattices: Nearest-neighbor (n.n.) coupling on a chain (D=1), the square lattice (D=2) or the cubic lattice (D=3)

- Examples for non-bipartite lattices: Chain with n.n. and next-n.n. coupling (D=1), triangular lattice (D=2) with n.n. coupling.

Marshall's theorem (any D)

- Total spin defined as $\mathbf{S}_{tot} = \sum_i \mathbf{S}_i$. For Heisenberg systems, $[H, \mathbf{S}_{tot}] = 0$, the total spin in each of its three components is conserved.

- Theorem: Consider the Heisenberg model on a bipartite lattice with sub-lattices A and B of equal and *finite* size and $J_{ij} \geq 0$ (AFM) for all $i \in A$, $j \in B$ (or vice versa) and every pair of sites connected by a string of bonds with $J_{kl} \neq 0$: The ground state $|0\rangle$ is (i) non-degenerate and (ii) a singlet of total spin, i.e. $\mathbf{S}_{tot} |0\rangle = 0$.

Remarks:

- Proof can be found in [Auerbach]. Simple check: AFM Heisenberg dimer with g.s. $|0\rangle \propto |\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle$ which is indeed non-degenerate and a singlet.

- The theorem does not uniquely determine the g.s. In general, there are many total spin singlet eigenstates, that are not the ground state.

- The theorem does not contradict a $SU(2)$ symmetric degenerate manifold of ground states allowing for spontaneous symmetry breaking. This happens only for $N \to \infty$.

Lieb-Schulz-Mattis theorem [for Hamiltonian (44)]

- Theorem: For half-integer spin, $S = 1/2, 3/2, ...$ there is an excited eigenstate with energy that approaches the ground-state energy E_0 as $N \to \infty$. (The chain is "gapless".)

Proof:

- Denote the (non-degenerate) ground state of H by $|0\rangle$, define state $|1\rangle = U|0\rangle$ using twist operator $U = \prod_{j=1}^{N} \exp\left[i\frac{2\pi j}{N} S_j^z\right]$ which rotates spins around z-axis by an angle increasing linearly with position j, e.g. $U|\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\rangle \propto |\nwarrow\leftarrow\swarrow\downarrow\searrow\rightarrow\nearrow\uparrow\rangle$. Note: $|1\rangle$ is not necessarily an eigenstate of H.
- Define unitary translation operator T_1, $T_1 \mathbf{S}_j T_1^\dagger = \mathbf{S}_{j+1}$. Since $[H, T_1] = 0$, all eigenstates of H are also eigenstates of the T_1, in particular the g.s., $T_1|0\rangle = e^{ik_0}|0\rangle$ with $k_0 \in [-\pi, \pi)$.
- Overlap $\langle 0|1\rangle$:

$$\langle 0|1\rangle = \langle 0|U|0\rangle = \langle 0|\underbrace{T_1^\dagger T_1}_{=1} U T_1^\dagger T_1|0\rangle = \langle 0|e^{-ik_0} \prod_{j=1}^{N} \exp\left[i\frac{2\pi j}{N} S_{j+1}^z\right] e^{ik_0}|0\rangle. \tag{45}$$

The $e^{\pm ik_0}$ cancel. We split off the contribution $j = N$ from the sum, recall the periodic boundary conditions, $S_{N+1}^z \equiv S_1^z$. Then we shift $j \to j-1$ and note that the $j = 1$ contribution is trivial,

$$\langle 0|1\rangle = \langle 0| \left(\prod_{j=1}^{N} \exp\left[i\frac{2\pi(j-1)}{N} S_j^z\right] \right) \exp\left[i2\pi S_1^z\right]|0\rangle. \tag{46}$$

The parentheses are almost the U operator, up to $\exp\left[-i\frac{2\pi}{N}\sum_{j=1}^{N} S_j^z\right]$ which involves S_{tot}^z. We have

$$\langle 0|1\rangle = \langle 0|U \exp\left[i2\pi S_1^z\right] \exp\left[-i\frac{2\pi}{N} S_{tot}^z\right]|0\rangle. \tag{47}$$

We invoke Marshall's theorem (bipartite, with $N/2$ sub-lattice sites each). Thus $S_{tot}^z|0\rangle = 0$. We are left with $\langle 0|1\rangle = \langle 0|U \exp\left[i2\pi S_1^z\right]|0\rangle$ and note that S_1^z has eigenvalues $m_1^z = -S, -S+1, ..., S$. Thus

$$\exp\left[i2\pi S_1^z\right] = \begin{cases} +1 & : S = 1, 2, 3, ... \\ -1 & : S = 1/2, 3/2, ... \end{cases} \tag{48}$$

We only get a non-trivial result for the half-integer spins:

$$\langle 0|1\rangle = -\langle 0|U|0\rangle = -\langle 0|1\rangle \tag{49}$$

and conclude $\langle 0|1\rangle = 0$, the states are orthogonal!

- Energy expectation value for $|1\rangle$:

$$\begin{aligned}
\langle 1|H|1\rangle &= \left\langle 0|U^\dagger H U|0\right\rangle \\
&= J\sum_{j=1}^{N} \left\langle 0|U^\dagger \left[S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + S_j^z S_{j+1}^z\right] U|0\right\rangle \\
&= J\sum_{j=1}^{N} \langle 0| \\
&\quad + \left(\cos\frac{2\pi j}{N} S_j^x + \sin\frac{2\pi j}{N} S_j^y\right)\left(\cos\frac{2\pi[j+1]}{N} S_{j+1}^x + \sin\frac{2\pi[j+1]}{N} S_{j+1}^y\right) \\
&\quad + \left(\cos\frac{2\pi j}{N} S_j^y - \sin\frac{2\pi j}{N} S_j^x\right)\left(\cos\frac{2\pi[j+1]}{N} S_{j+1}^y - \sin\frac{2\pi[j+1]}{N} S_{j+1}^x\right) \\
&\quad + S_j^z S_{j+1}^z|0\rangle \\
&= J\sum_{j=1}^{N} \langle 0|\cos\frac{2\pi}{N}\left(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y\right) + \sin\frac{2\pi}{N}\left(S_j^x S_{j+1}^y - S_j^y S_{j+1}^x\right) + S_j^z S_{j+1}^z|0\rangle
\end{aligned}$$

The middle parentheses vanish because they go to their negative under a global π-rotation around the $(1,1,0)$ axis in spin space which lets $S_l^{x,y} \to S_l^{y,x}$ but does not affect the singlet $|0\rangle$.

- We finish the proof with a a few inequalities:

$$\langle 1|H|1\rangle = E_0 + J\sum_{j=1}^{N} \langle 0| \underbrace{\left[\cos\frac{2\pi}{N} - 1\right]}_{\leq 0} \left(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y\right)|0\rangle \tag{50}$$

and use $\langle 0|\left(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y\right)|0\rangle \geq -2S^2$. Finally, we use $1-\cos x \leq x^2/2$ and obtain

$$\langle 1|H|1\rangle \leq E_0 + 2JNS^2\left(1-\cos\frac{2\pi}{N}\right) \leq E_0 + 4\pi^2 JS^2/N \tag{51}$$

so that $\langle 1|H|1\rangle - E_0 \overset{N\to\infty}{\longrightarrow} 0$.

- Since $\langle 0|1\rangle = 0$, the state $|1\rangle$ is a superposition of exited eigenstates. If all excitations were gapped, this would lead to a contradiction. Thus at least one excited eigenstate needs to be gapless. Q.E.D.
- Remark: Model (44) with integer $S = 1, 2, 3, ...$ has an excitation gap ("Haldane gap").

Spinon excitations

- Recall Goldstone theorem: Spontaneous broken continous symmetry → gapless excitation.
  Lieb-Schulz-Mattis theorem shows that one does not need spontaneous symmetry breaking to obtain gapless excitations. (The g.s. of the 1D AFM Heisenberg chain is not ordered.)
- The gapless mode in the 1D-AFM Heisenberg model (assume $S = 1/2$) cannot be a magnon, since we have no long-range ordered background. Question: What is it?
- Recall: The g.s. of the 1D-AFM chain is close to a superposition of staggered configurations in all directions ($\langle \mathbf{S}_j\rangle = 0$, no spontaneous breaking of spin-rotation symmetry, power law algebraic correlations $\langle S_j^\alpha S_{j+n}^\alpha\rangle \sim (-1)^n/n$). Snapshot of a correlated region is shown in Fig. 35.
- We (= an experimentalist's neutron which also has $S = 1/2$) can flip one spin at energy cost $\sim J$. This is a $|S| = 1$ excitation ($S = 1/2 \to S = -1/2$).
- Follow idea of magnons: Gain kinetic energy by moving the excitation by the $S_j^+ S_{j+1}^- + h.c.$ terms in H.
- We see that two domain walls ("kinks") emerge which move *independently* and carry away only spin $S = 1/2$. They are called *spinons*.
- Compare to magnon in 1D FM (Ising) setting: Can only move the flipped spin as a whole (↑↑↓↑↑↑ → ↑↑↑↓↑↑↑ → ↑↑↑↑↓↑↑ → ...)
- Spinon: Example of a *fractionalized* excitation. (Other example: Fractional quantum Hall effect where electron charge is fractionalized, e.g. $\nu = 1/3$ plateau state.)
- Separating spinons does not cost further energy (deconfined). → Spinons are well-defined quasi-particles. From Bethe ansatz: $\omega_k = \frac{\pi J}{2}|\sin k|$ (sharp dispersion!)
- The same strategy does *not* work in $D = 2, 3, ...$ due to the region of flipped spins (-----) left behind which would create an energy cost proportional to separation.
- Remark: The discussion above draws intuition from Ising limit but stays qualitatively correct in Heisenberg case. The domain walls are then smoothed out.
- Spinons in neutron scattering experiment: Besides $\Delta S = 1$, neutron deposits momentum q and a tell-tale energy ω_q. How does ω_q look as a function of q?

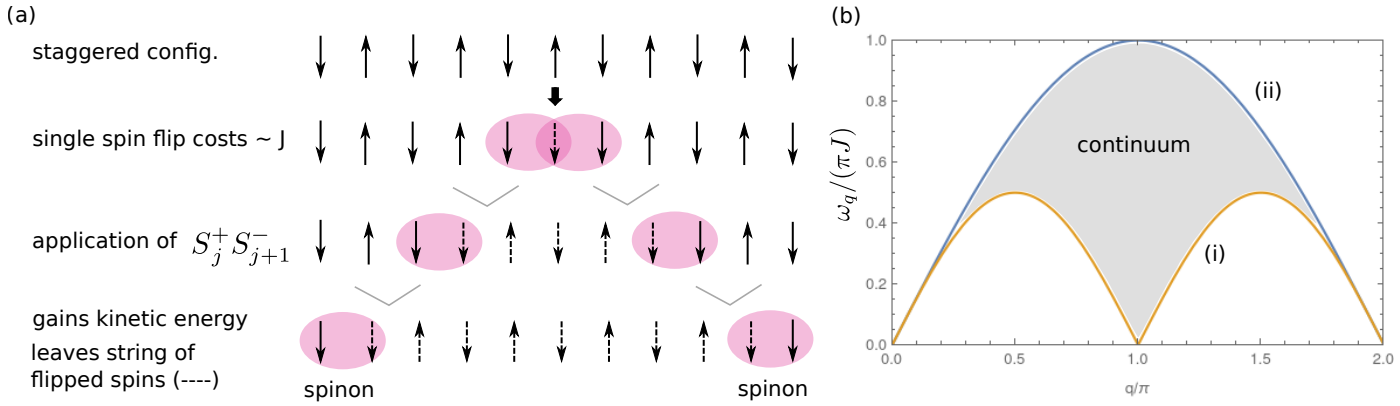


Figure 35: (a) Schematic sketch of spinon excitations (red) that emerge from a local spin-flip. (b) Continuum in ω_q for elastic neutron scattering as indirect experimental evidence for spinons.

- Two spinons are created that carry $q = k_1 + k_2$ and $\omega_q = \omega_{k_1} + \omega_{k_2} \sim |\sin k_1| + |\sin k_2|$. Thus there are many possibilities, expect continuum signal and no sharp features (only individual spinon has sharp ω_k).
- Limiting cases (i): $k_1 = q, k_2 = 0$ or $k_1 = 0, k_2 = q$ leads to $\omega_q = \frac{\pi J}{2}|\sin q|$. (ii): $k_1 = k_2 = q/2$ leads to $\omega_q = 2 \times \frac{\pi J}{2}|\sin(q/2)|$.
- With all intermediate cases, obtain the continuum with boundaries from the limiting cases in Fig. 35(b). This has been measured in $KCuF_3$ where the magnetic Cu atoms are arranged in well isolated chains [Tennant et al., (1993)].

- - - - 06.02.2023

18 Non-magnetic states: Variational wavefunctions and parent Hamiltonians

- Use variational principle and educated guesses for variational wavefunctions to better understand non-magnetic ground states.
- Similar philosophy as in fractional quantum Hall effect (e.g. Laughlin's wavefunction)
- Focus on $S = 1/2$ (can be generalized to any S)
- Parent Hamiltonian: A (contrived) Hamiltonian for which variational wavefunction is exact. Might still offer insights for more realistic models close in parameter space.

Valence-bond states

- For a given lattice, let Λ_α be a configuration of bonds (ij) such that each lattice site belongs to one bond. See Fig. 36(a) for an example on the square lattice.
- For each Λ_α, define a product state of singlets

$$|\alpha\rangle = \prod_{(i,j)\in\Lambda_\alpha} \left(|\uparrow_i\downarrow_j\rangle - |\downarrow_i\uparrow_j\rangle\right)/\sqrt{2} \tag{52}$$

with $\mathbf{S}_{tot}\,|\alpha\rangle = 0$ (c.f. Marshall's theorem).

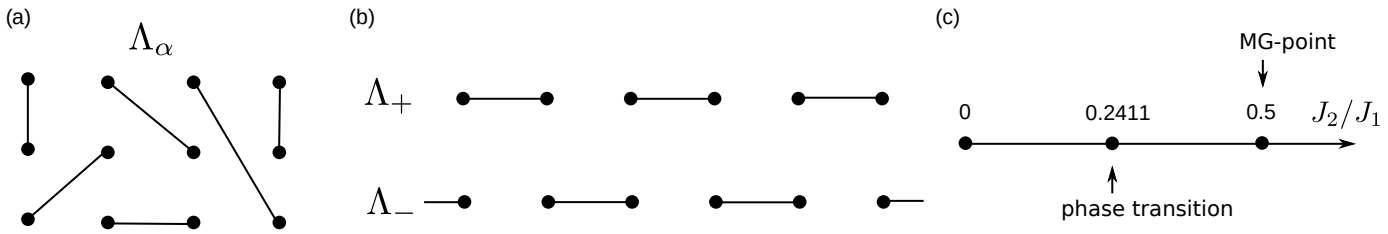


Figure 36: (a) Schematic sketch of possible configuration Λ_α for square lattice. (b) Spin chain: Two n.n. choices for Λ_α. (c) Numerical phase diagram of the AFM $J_1 - J_2$-Heisenberg chain (58).

- The state $|\alpha\rangle$ breaks translational symmetry, and Λ_α determines spin-correlations:

$$\langle\alpha|\mathbf{S}_k \cdot \mathbf{S}_l|\alpha\rangle = \begin{cases} 3/4 & : k = l \\ -3/4 & : (kl) \in \Lambda_\alpha \\ 0 & : otherwise \end{cases} \tag{53}$$

  The correlations are short-range if Λ_α contains bonds of finite size.

- General valence-bond state (still spin singlet): Pick $c_\alpha \in \mathbb{C}$,

$$|\{c_\alpha\}\rangle = \sum_\alpha c_\alpha |\alpha\rangle \tag{54}$$

  Note: Such a general valence-bond state can restore translational symmetry.

- Resonating valence bond state (RVB): $|\{c\}_\alpha\rangle$ with macroscopically many $|\alpha\rangle$ contributing. (This was first proposed by Phil Anderson for the frustrated n.n. triangular lattice AFM.)

Example: Heisenberg AFM chain

- Consider again Hamiltonian (44), we still want to understand ground-state better.
- Due to n.n. nature of H, use n.n. valence bond states $\Lambda_\pm$ of Fig. 36(b). Use both to avoid translational symmetry breaking. Since $\langle+|H|+\rangle = \langle-|H|-\rangle$, the $c_\pm$ are not suitable for variational calculation.
- Check how state $|\pm\rangle$ performs against Néel state $|N\rangle$:

$$\begin{aligned} \langle N|H|N\rangle &= -\frac{1}{4}JN = -\frac{2}{8}JN \\ \langle\pm|H|\pm\rangle &= -\frac{3}{4}\frac{J}{2}N = -\frac{3}{8}JN \end{aligned}$$

  The valence-bond state gives a tighter bound on the g.s. energy.
  Fact: The true g.s. is in fact similar to valence-bond state, but with macroscopically many and long-ranged contributions $|\alpha\rangle$.

Majumdar-Ghosh Hamiltonian

- Q: Is there a H so that $|\pm\rangle$ of Fig. 36(b) is exact g.s.? Yes, but need to add next-n.n. coupling.
- Majumdar-Ghosh Hamiltonian with $K > 0$ (non-bipartite!):

$$H_{MG} = K \sum_i \left(\mathbf{S}_i \cdot \mathbf{S}_{i+1} + \frac{1}{2}\mathbf{S}_i \cdot \mathbf{S}_{i+2} \right) \tag{55}$$

Proof that $|\pm\rangle$ are g.s. of H_{MG}:

- Define $\mathbf{J}_i = \mathbf{S}_{i-1} + \mathbf{S}_i + \mathbf{S}_{i+1}$ so that $\mathbf{J}_i \cdot \mathbf{J}_i$ has eigenvalues $J_i(J_i+1)$ with $J_i = 1/2$ or $3/2$ (addition of angular momenta).
- Projector to $J_i = 3/2$ case: $P_i = (\mathbf{J}_i \cdot \mathbf{J}_i - 3/4)/3$. (Check: $P_i^2 = P_i$, however $[P_i, P_j] \neq 0$!)
- Rewrite

$$\begin{aligned} P_i &= \frac{1}{3}\left[(\mathbf{S}_{i-1} + \mathbf{S}_i + \mathbf{S}_{i+1})(\mathbf{S}_{i-1} + \mathbf{S}_i + \mathbf{S}_{i+1}) - \frac{3}{4}\right] \\ &= \frac{1}{2} + \frac{2}{3}(\mathbf{S}_{i-1} \cdot \mathbf{S}_i + \mathbf{S}_{i-1} \cdot \mathbf{S}_{i+1} + \mathbf{S}_i \cdot \mathbf{S}_{i+1}) \end{aligned}$$

  so that we have twice a n.n.-bond and one next-n.n.-bond as in H_{MG}.
- Express H_{MG} with P_i:

$$H_{MG} = \frac{3}{4}K\sum_i P_i - \frac{3NK}{8} \tag{56}$$

- In $|\pm\rangle$, the $J_i = 3/2$ cannot appear. Indeed $\mathbf{J}_i = \mathbf{S}_{i-1} + (\mathbf{S}_i + \mathbf{S}_{i+1}) = (\mathbf{S}_{i-1} + \mathbf{S}_i) + \mathbf{S}_{i+1}$ and either the first or second parentheses refer to total spin zero, so only $J_i = 1/2$ is possible. Thus

$$H_{MG}|\pm\rangle = -\frac{3NK}{8}|\pm\rangle \tag{57}$$

- Lower bound for g.s. energy E_0: The lowest eigenvalue of H_{MG} cannot be smaller than the sum of the lowest eigenvalues of its individual terms. The lowest eigenvalue of P_i is 0, thus $E_0 \geq -\frac{3NK}{8}$ which is saturated by the eigenvalue of $|\pm\rangle$.

Generalization: $J_1 - J_2$ AFM Heisenberg chain

- Interpolation from n.n. AFM Heisenberg chain to MG-model: AFM $J_1 - J_2$-Heisenberg chain

$$H = \sum_i (J_1 \mathbf{S}_i \cdot \mathbf{S}_{i+1} + J_2 \mathbf{S}_i \cdot \mathbf{S}_{i+2}) \tag{58}$$

- Phase diagram is known numerically, see Fig. 36(c).

	$J_2/J_1 \in [0, 0.2411)$	$J_2/J_1 \in (0.2411, \infty)$
excitations	gapless	gapped
valence-bonds	macroscopically many long-range $\|\alpha\rangle$	dominated by $\|\pm\rangle$
$\|\langle \mathbf{S}_i \cdot \mathbf{S}_{i+n}\rangle\|$	$\sim 1/n^a$ (algebraic decay)	$\sim \exp(-n/\xi)$

19 Kitaev's honeycomb model

Aims:

- Q: Does spin fractionalization and quantum spin liquid exist beyond D=1?
- No realistic parent Hamiltonian is known for D=2 resonating valence-bond state.
- [A. Kitaev, (2006)]: Exactly solvable spin $S = 1/2$ model in D=2. Fractionalization of spin-1/2 in Majorana fermions.
- Proposals for material realization in spin-orbital $J_{eff} = 1/2$ Mott insulators. Most famous material to date: $\alpha - \mathrm{RuCl_3}$.

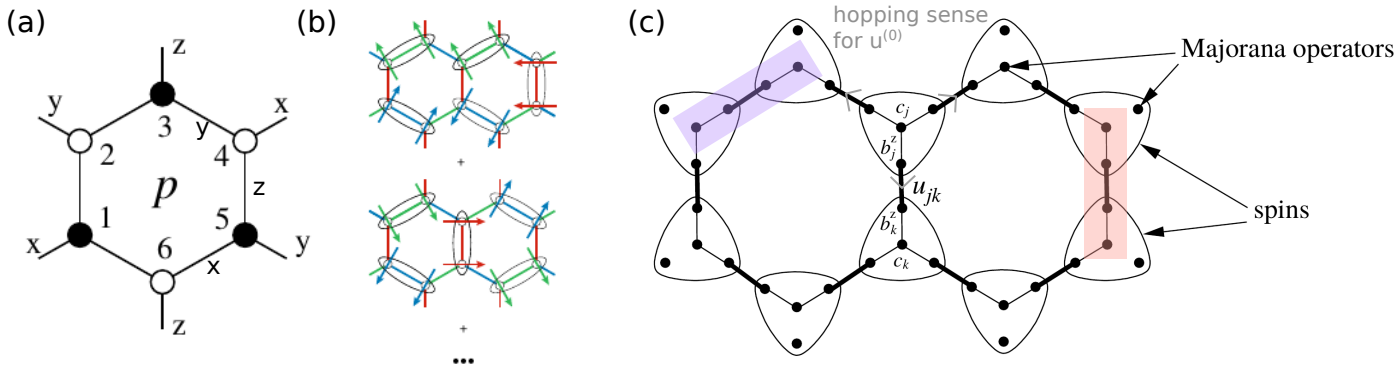


Figure 37: (a) An elementary hexagonal plaquette of the honeycomb lattice with bond directions labeled as x, y, z. (b) For the classical model, the g.s. is highly degenerate and once can expect quantum fluctuations to cause a superposition of these states. (c) The $S = 1/2$ at each lattice site are represented by four Majorana fermions. The resulting Hamiltonian $\tilde{H}$ features interactions between four adjacent Majoranas in the colored regions. (Figures adapted from [Kitaev, (2006)] and [Tagaki et al, Nature 2019])

Spin-Hamiltonian

- Spins $S = 1/2$ on sites of a honeycomb lattice, see Fig. 37(a).
- Ising interactions along links, special feature: Axis of Ising interaction depends on orientation of link ($\rightarrow$ frustration)

$$H = -J_x \sum_{\langle ij \rangle_x} \sigma_i^x \sigma_j^x - J_y \sum_{\langle ij \rangle_y} \sigma_i^y \sigma_j^y - J_z \sum_{\langle ij \rangle_z} \sigma_i^z \sigma_j^z \tag{59}$$

  The signs of $J_{x,y,z}$ do not matter for what follows, they can be flipped by unitary rotations (e.g. flip J_z by applying π-spin rotation around x-axis along every other horizontal zig-zag line).
- Classical picture (spins $\mathbf{S}$ replaced by vector, assume FM interactions): Huge g.s.-degeneracy, can make 1/3 of the bonds happy, see Fig. 37(b). Hope: With quantum effects, have superposition of classical g.s., similar to RVB state.
- Plaquette operator for plaquette p [see Fig. 37(a)] $W_p = \sigma_1^x \sigma_2^y \sigma_3^z \sigma_4^x \sigma_5^y \sigma_6^z$ commutes with H and $W_{p'}$ for p' any other plaquette. We also have $W_p^2 = 1$ so that W_p has eigenvalues $w_p = \pm 1$ (="flux") which can be chosen for each plaquette.
- Unfortunately, this is not quite enough for exact solution: Of each spin, only 1/3 belongs to a plaquette. Thus we have 2 spins per plaquette, but only one constraint.

Majorana Hamiltonian

- Majorana fermion operators: For usual fermions f_a ($a = 1, 2, ...n$), we have $\{f_a, f_b^\dagger\} = \delta_{ab}$. For each a, define the two Majorana operators $\eta_{2a-1} = f_a + f_a^\dagger$ and $\eta_{2a} = (f_a - f_a^\dagger)/i$. It is easy to check that $\eta_j^2 = 1$ and $\{\eta_j, \eta_k\} = 0$ for $j \neq k$.
- Kitaev Majorana spin-representation (c.f. Ex. 14.1): Four Majoranas b_i^x, b_i^y, b_i^z, c_i per site $\tilde{\sigma}_i^x = i b_i^x c_i$, $\tilde{\sigma}_i^y = i b_i^y c_i$, $\tilde{\sigma}_i^z = i b_i^z c_i$. Faithful for $S = 1/2$ only in subspace $D_i = b_i^x b_i^y b_i^z c_i \stackrel{!}{=} 1$ ($D_i^2 = 1$ and $[D_i, H] = 0$ for any spin Hamiltonian, thus $D_i = \pm 1$).
- Projector on physical subspace: $P = \Pi_i P_i$ with $P_i = (1 + D_i)/2$.

- In the Kitaev-Majorana representation, the Hamiltonian reads

$$\tilde{H} = iJ_x \sum_{\langle ij\rangle_x} \left(ib_i^x b_j^x\right) c_i c_j + iJ_y \sum_{\langle ij\rangle_y} \left(ib_i^y b_j^y\right) c_i c_j + iJ_z \sum_{\langle ij\rangle_z} \left(ib_i^z b_j^z\right) c_i c_j \tag{60}$$

  see Fig. 37(b).

- Key fact for exact solution: Extensive set of conserved quantities. Define

$$U_{ij} \equiv \begin{cases} \left(ib_i^x b_j^x\right) & : \langle ij\rangle = x - \text{bond} \\ \left(ib_i^y b_j^y\right) & : \langle ij\rangle = y - \text{bond} \\ \left(ib_i^z b_j^z\right) & : \langle ij\rangle = z - \text{bond} \end{cases} \tag{61}$$

  with $U_{ij} = -U_{ji}$ and see that (i) $\left[\tilde{H}, U_{ij}\right] = 0$, (ii) $[U_{ij}, U_{kl}] = 0$. Since $U_{ij}^2 = 1$, we have eigenvalues $u_{ij} = \pm 1$. These eigenvalues can be chosen individually for each bond.

- Hopping Hamiltonian for c_i: The Hilbert space of $\tilde{H}$ splits into eigenspaces that are indexed by the configuration of $u_{\langle ij\rangle}$ denoted by u, $\mathcal{L} = \bigoplus_u \mathcal{L}_u$. Relation between physical w_p and u (in physical subspace):

$$w_p = \prod_{\langle ij\rangle \in \partial p} u_{ij} \tag{62}$$

- Note: Seen from the c-Majoranas, the $u_{ij} = \pm 1$ are similar to Peierls phase factors as from hopping in the presence of a vector potential = gauge field. Thus u_{ij} is called a $\mathbb{Z}_2$ gauge field. A local $\mathbb{Z}_2$ gauge transformation changes $c_i \to -c_i$ and $b_i^\alpha \to -b_i^\alpha$ for all $\alpha = x, y, z$. This does not change $\tilde{\sigma}_i^\alpha = ib_i^\alpha c_i$.

- If restricted to $\mathcal{L}_u$, $\tilde{H}$ is a non-interacting hopping Hamiltonian for the c_i-Majoranas,

$$\tilde{H}_u = iJ_x \sum_{\langle ij\rangle_x} u_{ij} c_i c_j + iJ_y \sum_{\langle ij\rangle_y} u_{ij} c_i c_j + iJ_z \sum_{\langle ij\rangle_z} u_{ij} c_i c_j \tag{63}$$

- Huge simplification: For N lattice sites, we only have to diagonalize $N \times N$ Hamiltonian for c-hopping problem instead of $2^N \times 2^N$ Hamiltonian for the original spin model.

- Procedure for finding the g.s. of H:

  1. Fix some $w_p = \pm 1$ for all p
  2. Find any u satisfying Eq. (62)
  3. Solve the non-interacting Hamiltonian (63) and find its g.s.-energy $E_0(\{w_p\})$ and g.s. $|\psi(\{w_p\})\rangle$
  4. Repeat for all $\{w_p\}$, pick the $\{w_p\}$ than minimizes the energy
  5. Compute physical observables from the state projected to the physical subspace, $P|\psi\rangle$

- Shortcut - *Lieb's theorem*: For lattices with mirror symmetry that does not cut through lattice sites, plaquettes of length 2 mod 4 carry zero flux in the g.s. (plaquettes of length 0 mod 4 carry π-flux).

- Conclude: Set $w_p = +1$ to find the g.s.! Suitable choice of u_{ij} configuration $u^{(0)}$ which is translational invariant: $u_{ij} = +1$ if $i \in$ even sub-lattice, $u_{ij} = -1$ otherwise. See gray arrows in Fig. 37(c).

Spectrum of the Fermions in the Kitaev-Honeycomb model

- Translational invariance of $\tilde{H}_{u^{(0)}}$ suggests spatial Fourier transform. Follow Fig. 38(a) and use the basis $\mathbf{n}_{1,2} = \left(\pm\frac{1}{2}, \frac{\sqrt{3}}{2}\right)$ and reciprocal basis $q_{1,2} = 2\pi\left(\pm 1, \frac{1}{\sqrt{3}}\right)$.

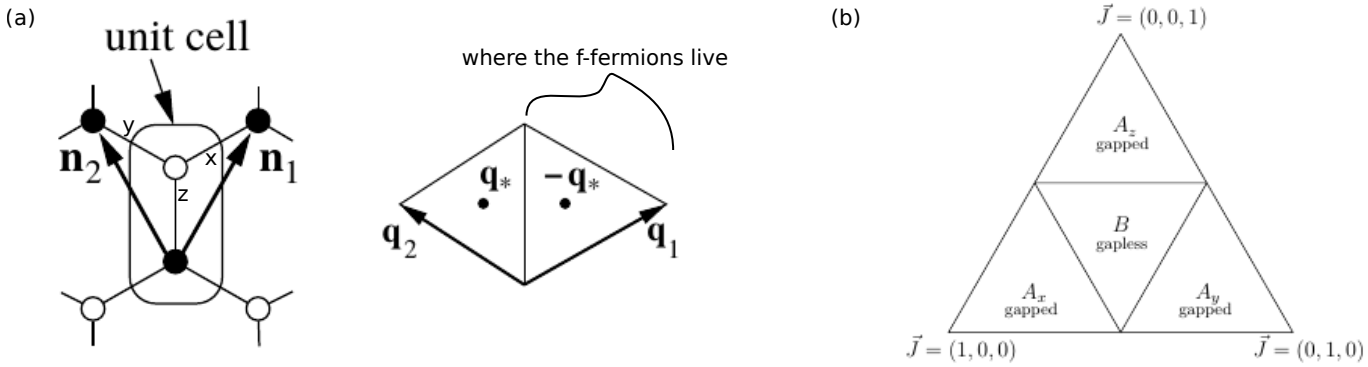


Figure 38: Kitaev honeycomb model: (a) Choice of (reciprocal-) lattice vectors. (b) Ground-state phase diagram. Adapted from [Kitaev, (2006)] and [Kitaev and Laumann, (2009)].

- Sub-lattice index $\lambda = \{\circ, \bullet\}$ goes into a 2x2 grading, $c_{\mathbf{r}_i,\lambda} = \frac{1}{\sqrt{2N}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r}_i} c_{\mathbf{k},\lambda}$ which leads to $(c_{\mathbf{k},\lambda})^\dagger = c_{-\mathbf{k},\lambda}$ and $\mathbf{k}$ is from the BZ of the triangular lattice. We find:

$$\tilde{H}_{u^{(0)}} = \frac{i}{2} \sum_{\mathbf{k}} c_{\mathbf{k},\bullet} \left(J_x e^{-i\mathbf{k}\cdot\mathbf{n}_1} + J_y e^{-i\mathbf{k}\cdot\mathbf{n}_2} + J_z \right) c_{-\mathbf{k},\circ}$$

- We move over to complex (ordinary) f-fermions, treating the Majoranas with $k_x < 0$ as the other species. Thus we need to restrict the $\mathbf{k}$ for $f_{\mathbf{k}\lambda}$ to $k_x > 0$ (primed sum):

$$f_{\mathbf{k},\lambda} \equiv c_{\mathbf{k},\lambda}, \; f^\dagger_{\mathbf{k},\lambda} = c_{-\mathbf{k},\lambda}$$

  Note that $(f_{\mathbf{k},\lambda})^\dagger = f^\dagger_{\mathbf{k},\lambda}$. We get

$$\tilde{H}_{u^{(0)}} = \sum\nolimits'_{\mathbf{k}} \begin{pmatrix} f^\dagger_{\mathbf{k},\bullet} \\ f^\dagger_{\mathbf{k},\circ} \end{pmatrix}^T \begin{pmatrix} 0 & \frac{i}{2}\left(J_x e^{i\mathbf{k}\cdot\mathbf{n}_1} + J_y e^{i\mathbf{k}\cdot\mathbf{n}_2} + J_z \right) \\ c.c. & 0 \end{pmatrix} \begin{pmatrix} f_{\mathbf{k},\bullet} \\ f_{\mathbf{k},\circ} \end{pmatrix} + \text{const.}$$

- The spectrum has gapless Dirac points at $\mathbf{k}^\star$ iff $(...)_{\mathbf{k}=\mathbf{k}^\star} = 0$. This will happen if the $J_{x,y,z}$ fulfill the triangle inequality, $|J_i| \leq |J_j| + |J_k|$, (i,j,k) are permutations of (x,y,z). Otherwise, the spectrum is gapped. This leads to the g.s. phase diagram of Fig. 38(b).

- For the symmetric case $J_x = J_y = J_z$, the gapless condition reads $e^{i\mathbf{k}^\star\cdot\mathbf{n}_1} + e^{i\mathbf{k}^\star\cdot\mathbf{n}_2} = -1$ which is fulfilled for $\mathbf{k}^\star = 2\pi \left(\frac{1}{3}, \sqrt{3} \right)$.

- Further facts:
  - The A-phases are adiabatically connected to Toric code model (a spin model with 4-spin interactions, exotic anyon excitations and topological order).
  - Gapless B-phase can be gapped by breaking time-reversal symmetry, e.g. by physical magnetic field. The Majorana bands carry non-trivial Chern number C, which leads to edge states and a quantized thermal heat conductivity. This was claimed to be measured in $\alpha - \mathrm{RuCl_3}$in [Kasahara et al, Nature 559, 227 (2018)], but the result is highly controversial.