

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

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Organization

- Lectures: In-person teaching, start on Oct. 18, 2021.
 - Mondays: 14:15 - 16:00 (Theresienstr. 37, A348)
 - Tuesdays: 12:15 - 14:00 (Theresienstr. 41, C111)
- Tutorial sessions: with Johannes Halbinger (JOHANNES.HALBINGER@PHYSIK.UNI-MUENCHEN.DE), start on Oct. 26, 2021.
 - 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, February 22, 2022, 10:00-12:00, room A348: Closed book exam but one sheet of notes allowed, no electronic devices allowed, 120 minutes.
- Website: Website: https://www2.physik.uni-muenchen.de/lehre/vorlesungen/wise_21_22/TVI_TMP-TA4/index.html

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)

Literature

- [Altland] Alexander Altland and Ben Simons, *Condensed Matter Field Theory*, Cambridge University Press, 2nd Edition
- [Cardy] John Cardy, *Scaling and Renormalization in Statistical Physics*, Cambridge Lecture Notes in Physics
- [Kamenev] Alex Kamenev, *Field Theory of Non-Equilibrium Systems*, Cambridge University Press
- [Kopietz] Peter Kopietz, Lorenz Bartosch, Florian Schütz, *Introduction to the Functional Renormalization Group*, Lecture Notes in Physics
- [Franz] Marcel Franz and Laurens Molenkamp, *Topological Insulators*, in Contemporary Concepts of Condensed Matter Sciences, Vol 6, Elsevier. In particular Chapter 1.
- [Hasan] M. Hasan and C. Kane, *Topological Insulators*, Rev. Mod. Phys. 82, 3045 (2010)

Contents (short)

1. Renormalization Group (Phase transitions, universality, scaling hypothesis, mean-field-theory, Gaussian approximation, Wilsonian RG, functional RG)
2. Non-Equilibrium (Keldysh formalism, kinetic equation)
3. Topology (Berry Phase, Integer Quantum Hall Effect, Topological Insulators)

Part I

Renormalization Group

1 Introduction

- Phase transitions in mostly classical systems, phenomenological point of view: Power laws, critical exponents, universality.
Can be understood from scaling hypothesis.
- Simple microscopic description of phase transitions.
 - Mean-field theory (MFT) neglects fluctuations.
 - Gaussian approximation takes simple fluctuations into account which are exactly tractable.
- Quantum phase transitions: What is different from classical phase transitions when quantum mechanics is involved?
- Wilsonian RG:
 - Rather a set of ideas than one coherent theory. Requires experience for application (many examples and exercises).
Here: Only condensed matter application (skip high-energy physics viewpoint)
 - Justification for scaling hypothesis and microscopic calculation of critical exponents.
 - Deeper understanding of phase diagrams and emergent scales [i.e. magnetic impurity coupled by J to metal of bandwidth D and DOS at Fermi level ν_0 : $T_K \sim D \exp(-1/(2\nu_0 J))$].
 - A given model can behave very differently at varying length- or energy scales. RG will connect physics at different energy scales and provides simplified effective models valid for certain scales.
- functional RG (fRG): Implement RG idea in a formally exact way, on the level of correlation functions, useful also for quantitative calculations beyond critical exponents.

2 Phase transitions, universality and the scaling hypothesis

Goal:

- Phase transitions mostly in classical systems, phenomenological point of view: Power laws, critical exponents, universality.
Can be understood from scaling hypothesis.

2.1 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

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

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

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

We can add more coupling constants like magnetic field h , doping p and so on. In general, with k coupling constants $g_{1,2,3,\dots,k}$, we have to consider $f(g_1, g_2, \dots, g_k)$.

- In the k -dimensional coupling space, $f(g_1, g_2, \dots, g_k)$ is almost everywhere analytic (locally described by convergent power series, $f(g) = a_0 + a_1(g - g_0) + a_2(g - g_0)^2 + \dots$).
- Phases: Domains in coupling space where f is analytic are called “phases” of the system, they can be often described by **order parameters**, that are only non-vanishing in a particular phase.
- There might be points, lines or other manifolds with dimension $< k$ so that f exhibits some kind of non-analyticity. Those describe phase transitions. Note that non-analyticity can only come from infinite summation in $\text{Tr} \dots$, so infinite systems are required.
- Classification of phase transition:
 - First order (discontinuous): There is at least one $i \in 1, \dots, k$ so that at the phase boundary $\partial f / \partial g_i$ is discontinuous.
 - Second order (continuous): For all $i \in 1, \dots, k$, 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, not driven by thermal- but by quantum fluctuations. Same classification as above, for more details see Sec. 4.

2.2 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 ($s_i = \pm 1$)

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

At $h = 0$, we have a \mathbb{Z}_2 symmetry for H under $s_i \rightarrow -s_i$ for all i . The partition function for the Ising model is known exactly for $D=1$ (see Ex. 2.4.1) and for $D=2$ at $h = 0$ [Onsager, 1944].

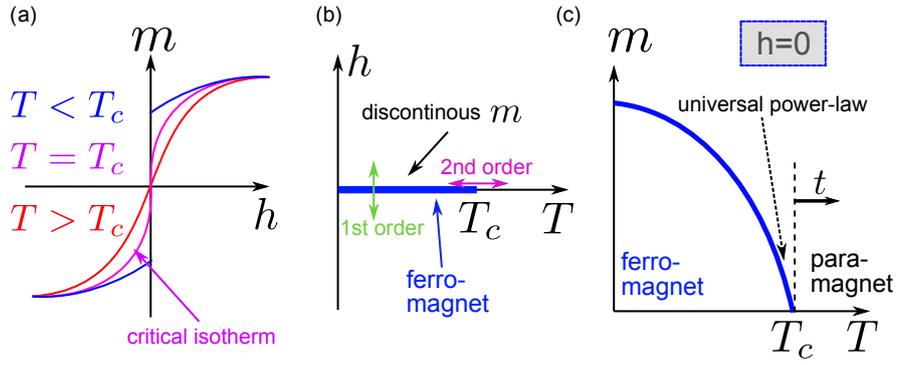


Figure 1: (a,b,c) Various sketches of the magnetization of a classical Ising model for dimension $D \geq 2$. (d) The connected correlation function in real-space close to a phase transition point with regions of power-law and exponential decay.

- Consider magnetization $m(T, h) = -\frac{\partial f(T, h)}{\partial h} = \lim_{V \rightarrow \infty} \frac{1}{V} \langle \sum_i s_i \rangle$ and plot it as a function of h with T as a parameter (Fig. 1a). If we are in $D=2$ with short-range couplings and have a discrete symmetry group (like \mathbb{Z}_2 , “Mermin-Wagner theorem”), 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

$$m \equiv -\lim_{h \rightarrow 0^+} \frac{\partial f(T, h)}{\partial h} = \lim_{h \rightarrow 0} \lim_{V \rightarrow \infty} \frac{1}{V} \left\langle \sum_i s_i \right\rangle \quad (4)$$

(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. Under the \mathbb{Z}_2 -symmetry, we would have $m_0 \rightarrow -m_0$.
- **Critical exponent:** Slightly below the critical temperature $T \lesssim T_c$, we can fit the measured magnetization to $m \propto (T_c - T)^\beta$ (for $T \leq T_c$). The dimensionless number $\beta > 0$ is a critical exponent.
- **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.
 - 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 .
 - * Difference to magnet: $\int d\mathbf{r} n(\mathbf{r}) = \text{const.}$, leads to coexistence of gas and liquid at 1st order line.
 - * Exponent β : $n_{\text{liquid}} - n_{\text{gas}} \propto (T_c - T)^\beta$

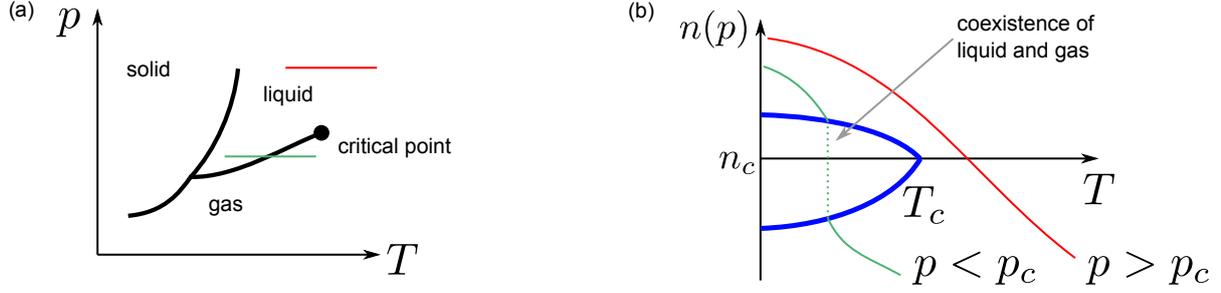


Figure 2: (a) Phase diagram of a simple fluid in the temperature pressure plane. (b) Curves of constant pressure in the temperature-density plane. The blue region for $T < T_c$ is the coexistence region for liquid and gas.

* Where is the \mathbb{Z}_2 symmetry? Lattice gas approximation, correspondence $s_i = +1 \hat{=} \text{occupied site}$ / $-1 \hat{=} \text{empty site}$ \rightarrow Ising model, emergent \mathbb{Z}_2 symmetry close to critical point.

- Other thermodynamic observables with their own critical exponents (historical notation). Definition: $t \equiv (T - T_c)/T_c$.

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

Correlation function, anomalous dimension and correlation length exponent

- Consider spatial correlations of local order parameter $m(\mathbf{r})$. Subtract non-decaying contribution:

$$G(\mathbf{r}) = \langle m(\mathbf{r})m(0) \rangle - \langle m \rangle^2 \quad (5)$$

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

$$G(r \rightarrow \infty) \propto \begin{cases} 1/r^{D-2+\eta} & : t = 0 \\ e^{-r/\xi} / \sqrt{\xi^{D-3} r^{D-1}} & : t \neq 0 \end{cases} \quad (6)$$

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

- At criticality $t = 0$:
 - $G(r)$ decays with a power-law, defines universal **anomalous dimension** $\eta > 0$.
 - There is **no characteristic length scale**.
 - 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

$$\xi \propto |t|^{-\nu} \quad (7)$$

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).

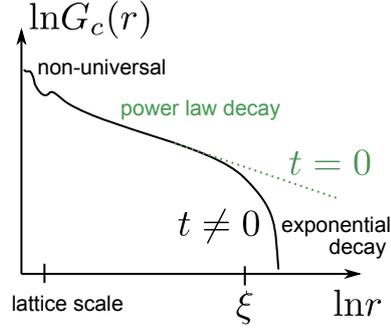


Figure 3: The connected correlation function in real-space close to a phase transition point with regions of power-law and exponential decay.

2.3 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:

$\alpha = 2 - D/y_t$	$\beta = (D - y_h)/y_t$	$\gamma = (2y_h - D)/y_t$	$\delta = y_h/(D - y_h)$	$\nu = 1/y_t$	$\eta = D + 2 - 2y_h$
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- This can be understood from a scaling hypothesis for the free energy and the correlation function (justified later from 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):

$$f_{sing}(t, h) = b^{-D} f_{sing}(b^{y_t} t, b^{y_h} h) \quad (8)$$

with an arbitrary dimensionless scale factor b .

- Since b was arbitrary, let $b^{y_t} = 1/|t|$ and thus $b = |t|^{-1/y_t}$:

$$f_{sing}(t, h) = |t|^{D/y_t} \underbrace{f_{sing}\left(\pm 1, \frac{h}{|t|^{y_h/y_t}}\right)}_{\equiv \Phi_{\pm}\left(\frac{h}{|t|^{y_h/y_t}}\right)} \quad (9)$$

- Assume that around the phase transition, derivatives of f are dominated by its singular part (“ \simeq ” signs):

$$m(t, h) \simeq -\frac{\partial f_{sing}}{\partial h} = |t|^{(D-y_h)/y_t} \Phi'_{\pm}\left(\frac{h}{|t|^{y_h/y_t}}\right) \quad (10)$$

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 .

- δ (critical isotherm): We need to let $t \rightarrow 0$ in Eq. (10). 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 δ .

Scaling hypothesis for correlation function

- Make a scaling hypothesis for the singular part of the correlation function

$$G_{sing}(r; t, h) = b^{-2(D-y_h)} G_{sing}(r/b; b^{y_t} t, b^{y_h} h) \quad (11)$$

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

$$G_{sing}(r; t, h = 0) = |t|^{2(D-y_h)/y_t} \underbrace{G_{sing}(r|t|^{1/y_t}; \pm 1, 0)}_{\equiv \Psi_{\pm}(r|t|^{1/y_t}; \pm 1, 0)} \quad (12)$$

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

$$\Psi_{\pm}(r|t|^{1/y_t}; \pm 1, 0) \propto (r|t|^{1/y_t})^{-2(D-y_h)} \quad (13)$$

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

$$2 - \alpha = 2\beta + \gamma = \beta(\delta + 1) \quad (14)$$

– hyperscaling relations (involving the $G(r)$ -exponents)

$$\begin{aligned} 2 - \alpha &= D\nu \\ \gamma &= (2 - \eta)\nu \end{aligned}$$

Dynamical critical exponent

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

$$\tau_c \propto \xi^z \propto |t|^{-\nu z} \quad (15)$$

- z is the **dynamical critical exponent**.
- **Critical slowing down:** Order parameter fluctuations decay slower and slower as one gets closer and closer to the critical point.
See Ex. 2.4.2 for an application involving z .

2.4 Exercises

2.4.1 Classical Ising model in 1D: Exact solution

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

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

$$\mathbf{T} = \begin{pmatrix} e^{(J+h)/T} & e^{-J/T} \\ e^{-J/T} & e^{(J-h)/T} \end{pmatrix} \quad (16)$$

2. Using the eigenvalues of \mathbf{T} , show that in the thermodynamic limit the free energy per spin reads

$$f(h, T) = -J - T \ln \left[\cosh(h/T) + \sqrt{\sinh^2(h/T) + e^{-4J/T}} \right]. \quad (17)$$

Show that one can approximate

$$f(h, T) = \begin{cases} -J - T e^{-2J/T} & : h = 0, \\ -J - |h| - T e^{-4J/T} e^{-2|h|/T} & : h \neq 0, \end{cases} \quad (18)$$

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 calculations needed).

2.4.2 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

$$t(\tau) \propto -\lambda\tau \quad (19)$$

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

$$\tilde{t} \propto \lambda^{1/(1+\nu z)}. \quad (20)$$

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

$$l \propto \lambda^{-\nu/(1+\nu z)}. \quad (21)$$

The remarkable prediction of Eq. 21 connects *static* critical exponents z, ν to the observable l measured in a *dynamic* experiment. 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.

3 Mean-field theory and Gaussian approximation

Goal:

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

3.1 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!).
- Idea: Split s_i into average value $m \in \mathbb{R}$ and **fluctuation**:

$$s_i = \underbrace{\langle s_i \rangle}_m + \delta s_i \quad (22)$$

- Fluctuation: More than one most likely $\{s_i\}_i$ configuration contributes to the partition function

$$\mathcal{Z} = \sum_{\{s_i = \pm 1\}} e^{-\beta H} \quad (23)$$

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

$$s_i s_j = (m + \delta s_i)(m + \delta s_j) = m^2 + m(\delta s_i + \delta s_j) + \delta s_i \delta s_j \simeq m^2 + m(\delta s_i + \delta s_j) = -m^2 + m(s_i + s_j) \quad (24)$$

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 $\mathcal{Z} = \sum_{\{s_i = \pm 1\}} e^{-\beta H}$ in mean-field approximation:

$$\mathcal{Z}_{MF} = \sum_{\{s_i = \pm 1\}} e^{-\beta \frac{NzJ}{2} m^2 + \sum_i \beta (h + zJm) s_i} \quad (25)$$

$$= e^{-\beta \frac{NzJ}{2} m^2} \prod_i \left[\sum_{s_i = \pm 1} e^{\beta (h + zJm) s_i} \right] \quad (26)$$

$$= e^{-\beta \frac{NzJ}{2} m^2} \{2 \cosh [\beta (h + zJm)]\}^N \quad (27)$$

$$= e^{-\beta N \mathcal{L}_{MF}(T, h; m)} \quad (28)$$

Note that m is yet to be determined.

- **Landau-function:**

$$\mathcal{L}_{MF}(T, h; m) = \frac{zJ}{2} m^2 - T \ln [2 \cosh [\beta (h + zJm)]] \quad (29)$$

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 $\mathcal{L}_{MF}(T, h; m)$.

$$\left. \frac{\partial \mathcal{L}_{MF}(T, h; m)}{\partial m} \right|_{m=m_0} \stackrel{!}{=} 0 \quad (30)$$

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

$$m_0 \stackrel{!}{=} \tanh [\beta ((h + zJm_0))] \quad (31)$$

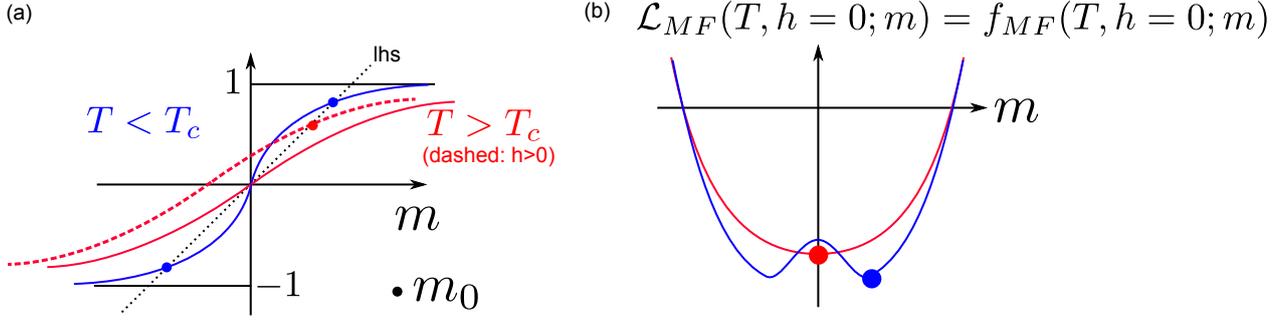


Figure 4: Mean-field approximation for the Ising model. Panel (a) shows the graphical solution of Eq. (31) and panel (b) the Landau function above (red) and below (blue) the critical temperature.

- For $h \neq 0$, there is always at least one non-trivial solution, see Fig. 4a. If there are two solutions, one has to find the global minimum of $\mathcal{L}_{MF}(T, h; m)$.
- Free energy density: Once m_0 is determined as a function of T, h , we find:

$$f_{MF}(T, h) = \mathcal{L}_{MF}(T, h; m_0(T, h)) \quad (32)$$

Mean-field critical temperature

- Set $h = 0$ to find critical temperature: Compare the slopes on the left and the right-hand-side of Eq. (31). Obtain two non-zero m_0 -solutions below a critical temperature

$$T_{c, MF} \equiv zJ. \quad (33)$$

- Example: Hyper-cubic lattice in D -dimensions: $z = 2D \rightarrow T_{c, MF}^D = 2DJ$.
Exact results: $T_c^{D=1} = 0$, $T_c^{D=2} = 2.269J$ ($\sinh(2J/T_c) = 1$). Monte-Carlo simulations for $D \geq 3$.
Comparison to mean-field (relative):

D	1	2	3	4	5	6	7
$T_c^D/T_{c, MF}^D$	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. 4b):

$$\mathcal{L}_{MF}(T, h; m) = f + \frac{r}{2}m^2 + \frac{u}{4!}m^4 - hm + \dots \quad (34)$$

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

$$f = -T \ln 2 \quad (35)$$

$$r = \frac{T_{c, MF}}{T} (T - T_{c, MF}) \simeq T - T_{c, MF} \quad (36)$$

$$u = 2T(T_{c, MF}/T)^4 \simeq 2T_c \quad (37)$$

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

$$rm_0 + \frac{u}{6}m_0^3 = h \quad (38)$$

- 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 $\beta_{D=2}^{Ising} = 0.125$ or $\beta_{D=3}^{Ising} = 0.327$.

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

- Remark: ν, η pertain to $G(r)$ which cannot be described in MFT as spatially homogeneous order parameter is assumed.

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

Heuristic derivation of continuum field theory

- Heuristic steps to continuum field theory (detail in Ex. 3.4.1): Consider again

$$\mathcal{Z} = \sum_{\{s_i = \pm 1\}} \exp[-\beta H] = \sum_{\{s_i = \pm 1\}} \exp \left[\beta J \sum_{\langle ij \rangle} s_i s_j + \beta h \sum_i s_i \right] \quad (39)$$

Smooth discrete spins $s_i = \pm 1$ over a region $V_{\mathbf{r}}$ of volume $[1/\Lambda_0]^D$ and use the field $\varphi(\mathbf{r})$ instead of the spins.

- Result: $\varphi(\mathbf{r})$ and space coordinate \mathbf{r} are **now continuous**.
- **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:

$$\mathcal{Z} = \int \mathcal{D}[\varphi] e^{-S_{\Lambda_0}[\varphi]} \quad (40)$$

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

$$S_{\Lambda_0}[\varphi] = \int d^D \mathbf{r} \left[f_0 - h_0 \varphi(\mathbf{r}) + \frac{r_0}{2} \varphi^2(\mathbf{r}) + \frac{c_0}{2} [\nabla \varphi(\mathbf{r})]^2 + \frac{u_0}{4!} \varphi^4(\mathbf{r}) \right] \quad (41)$$

$$\stackrel{(FT)}{=} V f_0 - h_0 \varphi(\mathbf{k} = 0) + \frac{1}{2} \int_{\mathbf{k}} \left[r_0 + c_0 k^2 \right] \varphi(-\mathbf{k}) \varphi(\mathbf{k}) \quad (42)$$

$$+ \frac{u_0}{4!} \int_{\mathbf{k}_{1,2,3,4}} (2\pi)^D \delta(\mathbf{k}_1 + \dots + \mathbf{k}_4) \varphi(\mathbf{k}_1) \varphi(\mathbf{k}_2) \varphi(\mathbf{k}_3) \varphi(\mathbf{k}_4)$$

with (see Ex. 3.4.1, $a =$ lattice-constant of hyper-cubic lattice)

$$f_0 \equiv -a^{-D} \ln 2 \quad (43)$$

$$h_0 \equiv \beta h a^{-1-D/2} \quad (44)$$

$$r_0 \equiv \frac{T - T_c}{a^2 T_c} \quad (45)$$

$$c_0 \equiv 1/(2D) \quad (46)$$

$$u_0 \equiv 2a^{D-4} \quad (47)$$

- 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 $1/\Lambda_0$.
- Used $\varphi(\mathbf{r}) \equiv \int_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} \varphi(\mathbf{k})$ and $\frac{1}{V} \sum_{\mathbf{k}} \rightarrow (2\pi)^{-D} \int_{-\infty}^{+\infty} d^D \mathbf{k} \equiv \int_{\mathbf{k}}$
- 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 $\Lambda_0 \rightarrow \infty$.

Recovering mean-field theory

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

$$\mathcal{Z} \simeq \int_{-\infty}^{+\infty} \frac{d\bar{\varphi}}{\sqrt{2\pi}} e^{-S_{\Lambda_0}[\bar{\varphi}]} = \int_{-\infty}^{+\infty} \frac{d\bar{\varphi}}{\sqrt{2\pi}} \exp \left[-V \left(f_0 + \frac{r_0}{2} \bar{\varphi}^2 + \frac{u_0}{4!} \bar{\varphi}^4 - h_0 \bar{\varphi} \right) \right] \quad (48)$$

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

$$0 \stackrel{!}{=} \frac{\partial S_{\Lambda_0}[\bar{\varphi}]}{\partial \bar{\varphi}} \Big|_{\bar{\varphi}=\bar{\varphi}_0} = r_0 \bar{\varphi}_0 + \frac{u_0}{6} \bar{\varphi}_0^3 - h_0 = 0 \quad (49)$$

This is the same as the MF equation (34) if we identify

$$\bar{\varphi} \propto m \quad (50)$$

$$r_0, u_0, h_0 \propto r, u, h \quad (51)$$

(proportionality factors will be worked out in the exercise)

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

$$S_{\Lambda_0}[\bar{\varphi} \propto m] = \beta N \mathcal{L}_{MF}(T, h; m) \quad (52)$$

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

3.3 Gaussian approximation

Truncating the action

- Split $\varphi(\mathbf{r})$ in homogeneous part and fluctuation (c.f. idea of MFT, 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, we had to discard the quadratic order fluctuation terms $\delta s_i \delta s_j$.
Now: **Keep** $\delta\varphi(\mathbf{k})\delta\varphi(-\mathbf{k})$ -terms, evaluate 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. (41):

$$\begin{aligned} S_{\Lambda_0}[\bar{\varphi}_0 + \delta\varphi] &= V \left[f_0 + \frac{r_0}{2} \bar{\varphi}_0^2 + \frac{u_0}{4!} \bar{\varphi}_0^4 \right] + \underbrace{\left[r_0 \bar{\varphi}_0 + 4 \frac{u_0}{4!} \bar{\varphi}_0^3 \right]}_{\rightarrow 0} \delta\varphi(\mathbf{k} = 0) \\ &\quad + \frac{1}{2} \int_{\mathbf{k}} \left[r_0 + c_0 k^2 + \frac{4 \cdot 3}{2} \cdot 2 \frac{u_0}{4!} \bar{\varphi}_0^2 \right] \delta\varphi(\mathbf{k}) \delta\varphi(-\mathbf{k}) \end{aligned}$$

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

$$S_{\Lambda_0}[\varphi] = \begin{cases} V f_0 + \frac{1}{2} \int_{\mathbf{k}} [r_0 + c_0 k^2] \delta\varphi(\mathbf{k}) \delta\varphi(-\mathbf{k}) & : T > T_c \\ V \left[f_0 - \frac{3}{2} \frac{r_0^2}{u_0} \right] + \frac{1}{2} \int_{\mathbf{k}} [-2r_0 + c_0 k^2] \delta\varphi(\mathbf{k}) \delta\varphi(-\mathbf{k}) & : T < T_c \end{cases} \quad (53)$$

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:

$$\alpha = \begin{cases} 2 - D/2 & : D < 4 \\ 0 & : D \geq 4 \end{cases} \quad (54)$$

Correlation function in Gaussian approximation: η, ν

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

$$\varphi(\mathbf{r}) = \bar{\varphi}_0 + \delta\varphi(\mathbf{r}) \quad (55)$$

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

$$G(\mathbf{r}) = \langle \delta\varphi(\mathbf{r})\delta\varphi(0) \rangle = \int_{\mathbf{k},\mathbf{k}'} e^{i\mathbf{k}\cdot\mathbf{r}} \underbrace{\langle \delta\varphi(\mathbf{k})\delta\varphi(\mathbf{k}') \rangle}_{(2\pi)^D \delta(\mathbf{k}+\mathbf{k}') G(\mathbf{k})} = \int_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} G(\mathbf{k}) \quad (56)$$

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

$$G_0(\mathbf{k}) = \frac{1}{c_0} \frac{1}{\xi^{-2} + k^2} \quad (57)$$

The subscript 0 stands for ‘‘Gaussian approximation’’ and we defined

$$c_0 \xi^{-2} \equiv \begin{cases} r_0 & : T > T_c, \\ -2r_0 & : T < T_c. \end{cases} \quad (58)$$

- In Ex. 3.4.2 we find the FT in Eq. (56)

$$G_0(\mathbf{r}) = \frac{1}{c_0} \int_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} \frac{1}{\xi^{-2} + k^2} \stackrel{D \gtrsim 2}{\sim} \begin{cases} 1/r^{D-2} & r \ll \xi \\ e^{-r/\xi} / \sqrt{\xi^{D-3} r^{D-1}} & r \gg \xi \end{cases} \quad (59)$$

which confirms our postulate in Eq. (6).

- 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 $\xi = \infty$:

$$\boxed{\nu = 1/2, \eta = 0} \quad (60)$$

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. (42):

$$S_{\Lambda_0}[\varphi] = V f_0 + \frac{1}{2} \int_{\mathbf{k}} [r_0 + c_0 k^2] \varphi(-\mathbf{k})\varphi(\mathbf{k}) + \frac{u_0}{4!} \int_{\mathbf{k}_{1,2,3,4}} (2\pi)^D \delta(\mathbf{k}_1 + \dots + \mathbf{k}_4) \varphi(\mathbf{k}_1)\varphi(\mathbf{k}_2)\varphi(\mathbf{k}_3)\varphi(\mathbf{k}_4) \quad (61)$$

- 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

$$S_{\Lambda_0}[\varphi] = V f_0 + \frac{1}{2} \int_{\tilde{\mathbf{k}}} \underbrace{[1 + \tilde{k}^2]}_{\simeq 1 \text{ for small } k} \tilde{\varphi}(-\tilde{\mathbf{k}})\tilde{\varphi}(\tilde{\mathbf{k}}) + \frac{1}{4!} \left(\frac{u_0 \xi^{4-D}}{c_0^2} \right) \int_{\tilde{\mathbf{k}}_{1,2,3,4}} (2\pi)^D \delta(\tilde{\mathbf{k}}_1 + \dots + \tilde{\mathbf{k}}_4) \tilde{\varphi}(\tilde{\mathbf{k}}_1)\tilde{\varphi}(\tilde{\mathbf{k}}_2)\tilde{\varphi}(\tilde{\mathbf{k}}_3)\tilde{\varphi}(\tilde{\mathbf{k}}_4) \quad (62)$$

- Relative strength of quartic part:

$$\tilde{u}_0 = u_0 \xi^{4-D} / c_0^2. \quad (63)$$

- For $D < 4$: Regardless of how small u_0 , if $\xi \propto |t|^{-\nu}$ diverges as $t \rightarrow 0$, the relative strength of the quartic part diverges. \rightarrow Gaussian approximation to critical exponents (defined in the limit $t \rightarrow 0$) 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: $D_{low} = 1$, $D_{up} = 4$.

3.4 Exercises

3.4.1 Derivation of continuum φ^4 -field theory for Ising model

In this exercise, you formally derive the continuum field theory Eq. (42) starting from the partition function Eq. (39).

1. Use the identity

$$e^{\frac{1}{2}\mathbf{s}^T[\mathbf{A}^{-1}]\mathbf{s}} = \sqrt{\det\mathbf{A}} \int \mathcal{D}[x] e^{-\frac{1}{2}\mathbf{x}^T\mathbf{A}\mathbf{x} + \mathbf{x}^T\mathbf{s}} \quad (64)$$

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 $\int \mathcal{D}[x] \equiv \prod_{i=1}^N \int_{-\infty}^{+\infty} dx_i / \sqrt{2\pi}$ and \mathbf{A} is a real and symmetric $N \times N$ matrix with entries a_{ij} . Show that

$$\mathcal{Z} = \frac{1}{\sqrt{\det\tilde{\mathbf{J}}}} \int \mathcal{D}[x] \exp\left[-\frac{1}{2}\mathbf{x}^T\tilde{\mathbf{J}}^{-1}\mathbf{x} + \sum_{i=1}^N \ln[2 \cosh(x_i + \beta h)]\right] \equiv \frac{1}{\sqrt{\det\tilde{\mathbf{J}}}} \int \mathcal{D}[x] e^{-\tilde{S}[\mathbf{x}]} \quad (65)$$

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 $\varphi \equiv \tilde{\mathbf{J}}^{-1} \mathbf{x}$ which can be interpreted as a spatially fluctuating order parameter as $\langle \varphi_i \rangle_{\tilde{S}} = \langle s_i \rangle = m$. Confirm:

$$\mathcal{Z} = \sqrt{\det\tilde{\mathbf{J}}} \int \mathcal{D}[\varphi] \exp\left[-\frac{1}{2}\varphi^T\tilde{\mathbf{J}}\varphi + \sum_{i=1}^N \ln[2 \cosh([\tilde{\mathbf{J}}\varphi]_i + \beta h)]\right] \equiv \sqrt{\det\tilde{\mathbf{J}}} \int \mathcal{D}[\varphi] e^{-S[\varphi]} \quad (66)$$

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

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

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 $N \equiv V/a^D \rightarrow \infty$. In this case use

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

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. (42) with the given values for h_0 , r_0 , c_0 and u_0 .

3.4.2 Fourier transformation of gapped quadratic 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 $G_0(\mathbf{k}) = [\xi^{-2} + k^2]^{-1}$ for $D > 2$ 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?).

4 Quantum phase transitions

Goal:

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

4.1 Overview

- Quantum phase transitions (QPT) are driven by quantum fluctuations (non-commuting parts of the Hamiltonian that compete to minimize ground-state energy). Thus it is 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”):

$$\hat{H}_{TFIM} = -J \sum_{\langle i,j \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z - \Gamma \sum_i \hat{\sigma}_i^x \quad (67)$$

Control parameter: $r = \Gamma/J$. The two non-commuting terms in \hat{H}_{TFIM} compete between ferromagnetic state $|\uparrow\uparrow \dots \uparrow\rangle$ (or $|\downarrow\downarrow \dots \downarrow\rangle$) and paramagnetic state $|\rightarrow\rightarrow\rangle$. (Mean-field analysis in $\Gamma - T$ -plane: Ex. 4.4.1)

- 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,...).

4.2 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 :

$$H(p, q) = H_{kin}(p) + H_{pot}(q) \quad (68)$$

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

$$\mathcal{Z}_C = \int dpdq \exp[-\beta H(p, q)] = \underbrace{\int dp \exp[-\beta H_{kin}(p)]}_{\rightarrow f_{reg}} \int dq \exp[-\beta H_{pot}(q)] \quad (69)$$

- 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 .
- 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 $[\hat{H}_{kin}, \hat{H}_{pot}] \neq 0$, then

$$e^{\hat{H}_{kin} + \hat{H}_{pot}} \neq e^{\hat{H}_{kin}} e^{\hat{H}_{pot}} \quad (70)$$

- 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)

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

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)

$$\mathcal{Z}_Q \simeq \text{Tr} \left[e^{-\beta \hat{H}/N} \right]^N \simeq \text{Tr} \left[1 + \Delta\tau \tilde{h} \hat{\sigma}^z + \Delta\tau \Gamma \hat{\sigma}^x \right]^N = \text{Tr} \begin{pmatrix} 1 + \Delta\tau \tilde{h} & \Delta\tau \Gamma \\ \Delta\tau \Gamma & 1 - \Delta\tau \tilde{h} \end{pmatrix}^N \quad (71)$$

The matrix can be expressed as the transfer matrix of the 1D *classical* Ising model in a longitudinal magnetic field, c.f. Ex. 2.4.1.

$$\mathbf{T} = \begin{pmatrix} e^{\beta_c(J+h)} & e^{-\beta_c J} \\ e^{-\beta_c J} & e^{\beta_c(J-h)} \end{pmatrix} \quad (72)$$

- Example 2: Interacting fermions

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

- Example 3: TFIM in Eq. (67) maps to anisotropic classical 2D Ising model, see Ex. 4.4.2. Thus expect generalized Landau-Ginzburg-Wilson action Eq. (41) for order parameter φ .

$$S[\varphi(\mathbf{r}, \tau)] = \int d^D \mathbf{r} \int_0^\beta d\tau \left[f_0 + \frac{r_0}{2} \varphi^2 + \frac{c_0}{2} [\nabla_{\mathbf{r}} \varphi]^2 + \frac{u_0}{4!} \varphi^4 - h_0 \varphi + \frac{c_1}{2} [\partial_\tau \varphi]^2 \right] \quad (73)$$

- Zero temperature limit $T \rightarrow 0 \Leftrightarrow \beta \rightarrow \infty$:
 - \mathcal{Z}_Q can be seen as $D+1$ -dimensional classical path integral \mathcal{Z}_C in infinite $D+1$ -dimensional space.
 - QPT in D -space dimensions is equivalent to a classical (thermal) phase transition in $D+1$ space dimension.

- Remarks:
 - Role of temperature T :
 - * Classical: T just multiplies coupling constants, i.e. in Ising model $\beta J \equiv K$.
 - * Quantum: Temperature controls length of τ -dimension in integral expression for partition function.
 - After mapping: Classical $D + 1$ -dimensional system may be unusual and 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 $G(\tau) \rightarrow G(t = i\tau)$
 - * ok for scaling arguments and power-laws
 - * spoils precise mapping of dynamic time-dependent quantities
 - If resulting action $S[q(\tau)]$ becomes negative or complex, it cannot be interpreted as a classical action. [Sign-problem!]

4.3 Scaling around continuous QPT

Scaling at $T = 0$

- Scaling hypothesis for free energy Eq. (8) extended for quantum case:

$$f_{sing}(r - r_c) = b^{-\left(\underbrace{1 + 1 + \dots + 1}_{D} + z\right)} f_{sing}([r - r_c] b^{y_r})$$

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

$$\begin{aligned} \xi &\sim |r - r_c|^{-\nu}, \\ \xi_\tau &\sim \xi^z \sim |r - r_c|^{-z\nu}, \end{aligned}$$

- From scaling hypothesis, repeat derivation of scaling forms of thermodynamic observables and correlation functions, e.g.:

$$O(r - r_c, k, i\omega_n) = \xi^{d_O} O(k\xi, \omega_n\xi_\tau) \quad (74)$$

where k =momentum, ω_n =Matsubara frequency (momentum along τ -axis).

- Remarks:
 - d_O is scaling dimension, see RG. For correlation function $O = G$, we had $d_G = 2 - \eta$.
 - Interpretation: There is no other length scale than ξ , no other time-scale than ξ_τ .
 - Ansatz also holds for real frequencies, $i\omega_n \rightarrow \omega + i0$.

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

- Effect of $T > 0$ (Fig. 5a):
 - τ -direction becomes finite. Leads to “slab”-geometry with $\tau \in [0, \beta]$ and infinite extent in \mathbf{r} .
 - Formal description: “Finite-size scaling”

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

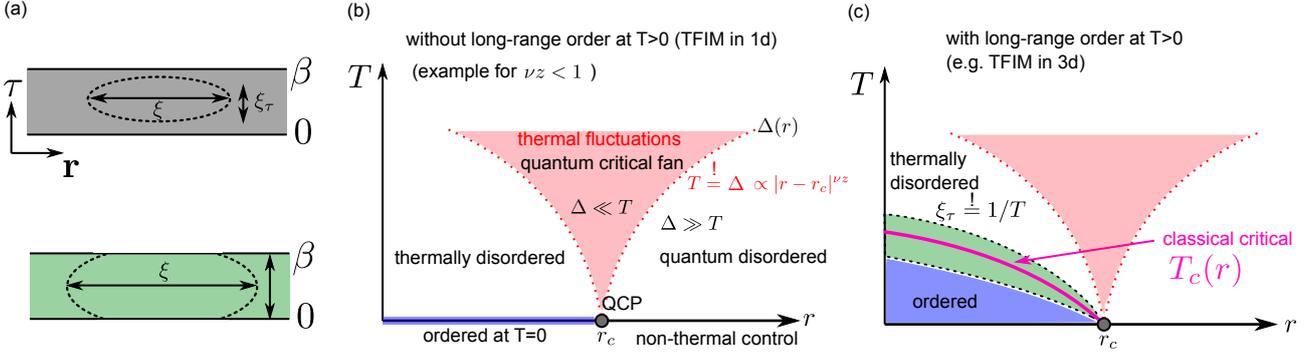


Figure 5: Finite temperature phase diagrams in the presence of a quantum critical point.

- Consequence: Characteristic energy scale $L_\tau = \beta = T^{-1}$, characteristic length scale $L_\tau^{1/z}$:

$$O(r - r_c, k, \omega, T) = L_\tau^{d_O/z} O\left(k L_\tau^{1/z}, \omega L_\tau, L_\tau / \xi_\tau\right) \quad (75)$$

- Two alternative consequences of reduced dimension D in “slab”-geometry:
 1. Absence of phase transition (Fig. 5b), order for $r < r_c$ only at $T = 0$.
 2. Phase transition in D -dimensional *classical universality class* (Fig. 5c). Find critical temperature $T_c(r)$.
Crossover happens when $\xi_\tau \sim |r - r_c|^{-z\nu} \stackrel{!}{=} \beta$ (green region).
- *Quantum critical region/fan* (red region in Fig. 5):
 - At $T = 0$ temporal fluctuation time-scale goes like $\tau_c \sim \xi_\tau \sim \xi^z$ (c.f. Eq. (15)).
 - QM: Relate τ_c to fluctuation energy scale / gap $\Delta = \hbar/\tau_c \propto \xi^{-z} \propto |r - r_c|^{\nu z}$ with power $\nu z > 0$. (Note that possibly $\nu z > 1 \rightarrow$ concave).
 - $T > 0$: Will system notice gap? Depends on $T \lesseqgtr \Delta$.
 - Within quantum critical fan:
Physics dominated by *thermal excitations of the quantum critical ground state*.
Finite-T scaling form Eq. (75): Neglect last argument: $L_\tau / \xi_\tau \sim |r - r_c|^{\nu z} / T \sim \Delta / T \ll 1$. Leads to:

$$O(k, \omega, T) = L_\tau^{d_O/z} O\left(k L_\tau^{1/z}, \omega L_\tau\right) \quad (76)$$

4.4 Exercises

4.4.1 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. (67). 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 $m^z(\Gamma, T)$:

$$\tanh\left(\beta z \sqrt{[m^z]^2 + (\Gamma/z)^2}\right) = \sqrt{[m^z]^2 + (\Gamma/z)^2} \quad (77)$$

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

- 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 $D = 1$.

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

Consider the 1D TFIM in Eq. (67) in one spatial dimension (1D) with $J = 1$ and L_x sites with periodic boundary conditions:

$$\hat{H} = - \sum_i \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z - \Gamma \sum_i \hat{\sigma}_i^x \quad (78)$$

In this exercise, we show the equivalence of the quantum partition function $\mathcal{Z}_{1D,q} = \text{Tr}_{1D} e^{-\beta_q \hat{H}}$ 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 $K_x = J_x \beta_c, K_y = J_y \beta_c$),

$$\mathcal{Z}_{2D,c} = \text{Tr}_{2D} e^{K_x \sum_{i,j} \sigma_{i,j} \sigma_{i+1,j} + K_y \sum_{i,j} \sigma_{i,j} \sigma_{i,j+1}}. \quad (79)$$

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.

- 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 $|\sigma_1, \sigma_2, \dots, \sigma_{L_x}\rangle$, $\{\sigma_i\}_{i=1, \dots, L_x} = \pm 1$. Then use these results to show

$$\mathcal{Z}_{2D,c} = (2 \sinh [2K_y])^{L_y L_x / 2} \text{Tr} \left(\left[e^{K_x \sum_i \tilde{\sigma}_i^z \hat{\sigma}_{i+1}^z} e^{\sum_i \tilde{K}_y \hat{\sigma}_i^x} \right]^{L_y} \right) \quad (80)$$

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

- Use the Trotter-formula $\mathcal{Z}_{1D,q} \simeq \text{Tr}_{1D} \left[e^{-\beta_q \hat{H} / L_y} \right]^{L_y}$ 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 there is only a QPT in the \hat{H} for $L_x \rightarrow \infty$ and $T_q \rightarrow 0$.
- It is known that anisotropy in the 2D classical Ising model does not change the critical exponents. 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. 4.4.1 overestimate the exact Γ_c ?

4.4.3 Transverse field Ising model in 1D (II): Exact eigenenergies

Here we are interested in finding the exact eigenenergy spectrum of the 1D TFIM in Eq. 78. We will find the gap Δ as a function of Γ and confirm the above value of its critical strength.

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

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

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 $i \neq i'$.

- 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

$$\hat{H} = \sum_k \left(2[\Gamma - \cos k] c_k^\dagger c_k - i \sin k [c_{-k}^\dagger c_k^\dagger + c_{-k} c_k] - \Gamma \right) \quad (81)$$

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

$$\hat{H} = \sum_k E_k \gamma_k^\dagger \gamma_k + \text{const.} \quad (82)$$

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 ?)

5 Wilsonian renormalization group

Goal:

- Renormalization group (RG) = Set of ideas, not one coherent theory.
Requires experience for application (\rightarrow examples and exercises).
- study interacting systems 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.
- Examples for length scales: Lattice spacing $a \ll$ correlation length $\xi \ll$ system size L .
- Justification for scaling hypothesis, universality and approximate calculation of critical exponents.
- Deeper understanding of phase diagrams and emergent scales [i.e. Kondo temperature].
- Here: Only condensed matter application (skip high-energy physics viewpoint)

5.1 Basic idea of the RG

- Partition function as path integral over field Φ (bosonic/fermionic/mixed), coupling constants $\mathbf{g} = (g_1, g_2, g_3, \dots)$.
(See, e.g. Ex. 3.4.1 for the derivation of ϕ^4 -theory from Ising model):

$$\mathcal{Z}(\mathbf{g}) = \int \mathcal{D}[\Phi] e^{-S_{\Lambda_0}[\Phi, \mathbf{g}]} \quad (83)$$

- RG-Idea: Iterative integration over Φ in Eq. (83) (Simplifying assumptions needed for generic case.)
Head towards low-energy / long-distance effective theory.
- Two steps:

1. Mode elimination:

For momentum-shell RG in Fig. 6a (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

$$\Lambda = \Lambda_0/b, \quad b > 1. \quad (84)$$

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

$$\Phi(\mathbf{k}) = \underbrace{\Theta(\Lambda - k)\Phi(\mathbf{k})}_{\Phi^<} + \underbrace{\Theta(k - \Lambda)\Phi(\mathbf{k})}_{\Phi^>} \quad (85)$$

and define

$$\mathcal{Z} = \int \mathcal{D}[\Phi^<] \int \mathcal{D}[\Phi^>] e^{-S[\Phi^< + \Phi^>, \mathbf{g}]} = \int \mathcal{D}[\Phi^<] e^{-S_{\Lambda}^<[\Phi^<, \mathbf{g}^<]} \quad (86)$$

Remark:

- Integration in the last step can only be carried out approximately in practice.
- Set of coupling constants \mathbf{g} is usually enlarged and must be truncated.

2. Rescaling:

Re-scale momenta and fields such that $S_{\Lambda}^<[\Phi^<, \mathbf{g}^<]$ has the same form as S_{Λ_0} .

In momentum-shell RG: Stretch momenta from $k \in [0, \Lambda]$ to $k' \in [0, \Lambda_0]$:

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

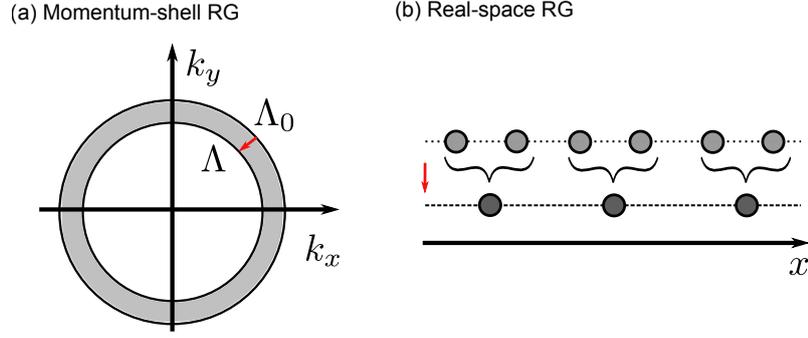


Figure 6: Different incarnations of the RG mode-elimination step.

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

$$\boxed{\mathbf{g}' = \mathcal{R}(b; \mathbf{g})} \quad (87)$$

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

$$i\omega \rightarrow i\omega' = i\omega b^z \quad (88)$$

- Remark: RG-trafo 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

$$\mathbf{g}'' = \mathcal{R}(b'; \underbrace{\mathcal{R}(b; \mathbf{g})}_{\mathbf{g}'}) = \mathcal{R}(b'b; \mathbf{g}) \quad (89)$$

- 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:

$$\mathbf{g}^{(n)} = \mathcal{R}(b; \mathbf{g}^{(n-1)}) = \mathcal{R}(b^n; \mathbf{g}) \quad (90)$$

- In limit $n \rightarrow \infty$, it holds $\Lambda = \Lambda_0/b^n \xrightarrow{n \rightarrow \infty} 0$.

Thus we have integrated out all degrees of freedom, obtain \mathcal{Z} . However, as the RG cannot be carried out exactly, this is usually not what is done.

- Incarnations of mode-elimination step:

1. Momentum-shell RG (Wilson), as outlined above. Requires translational invariant systems. See Sec. 5.4.
2. Real-space RG (Migdal-Kadanoff): For spin systems, decimate certain lattice sites by partial traces over Hilbert space. See Sec. 5.2 for clean 1D system and Sec. 5.7.1 for disordered 1D system. Hard to generalize to $D = 2, 3, \dots$
3. Functional RG (Wegner, Wetterich): Formally exact version of momentum-shell RG (1), go from the level of coupling parameters $g_i^{(n)}$ to vertex functions $\Gamma_\Lambda(K_1, K_2, \dots)$ which depend smoothly on cutoff. See Sec. 6.
4. Numerical RG (Wilson): For impurity models (interacting site + non-interacting bath), numerical implementation, for some “poor-man” version, see Sec. 5.5.

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

- Recall 1D classical Ising model

$$H = -J \sum_{i=1}^N s_i s_{i+1} - h \sum_{i=1}^N s_i - E_0 \quad (91)$$

where E_0 is an energy offset and N assumed even.

- Recall transfer matrix solution (Ex. 2.4.1) for partition function:

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

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

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

RG step

- Mode elimination step: Carry out trace $\sum_{\{s_i\}} = \sum_{\{s_{i \text{ even}}\}} \sum_{\{s_{i \text{ odd}}\}}$ only for *even* sites i :

$$\mathcal{Z}_{N'}(f', g', \tilde{h}') = \text{Tr} [(T')^{N'}] \quad (92)$$

with $N' = N/2$ and

$$T' \equiv T^2 = e^{2\tilde{f}} \begin{pmatrix} e^{2g+2\tilde{h}} + e^{-2g} & e^{\tilde{h}} + e^{-\tilde{h}} \\ e^{\tilde{h}} + e^{-\tilde{h}} & e^{2g-2\tilde{h}} + e^{-2g} \end{pmatrix}. \quad (93)$$

Important: \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 $\{f', g', \tilde{h}'\}$:

$$T' \stackrel{!}{=} e^{\tilde{f}'} \begin{pmatrix} e^{g'+\tilde{h}'} & e^{-g'} \\ e^{-g'} & e^{g'-\tilde{h}'} \end{pmatrix} \quad (94)$$

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

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

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

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

Remarks:

- Exact relations are peculiar to $D=1$. For $D=2,3,\dots$ 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 ($\zeta = 1$).

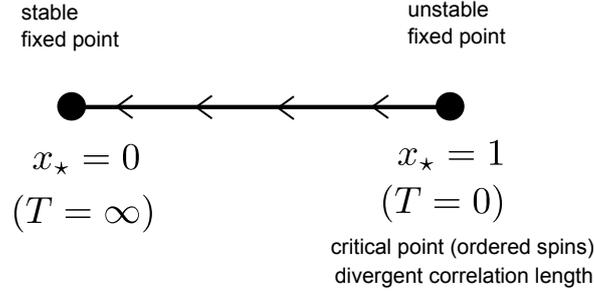


Figure 7: RG flow of the dimensionless coupling $x = \tanh(J/T)$ for the Ising model in 1D.

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

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

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

$$e^{g'} \pm e^{-g'} = \sqrt{\cosh(2g)} \left(1 \pm \frac{1}{\cosh(2g)} \right) \quad (95)$$

that

$$\tanh g' = \frac{1 + \frac{1}{\cosh(2g)}}{1 - \frac{1}{\cosh(2g)}} \quad (96)$$

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

$$\boxed{\tanh g' = \tanh^2 g} \quad (97)$$

$$\boxed{\tilde{f}' = 2\tilde{f} + \ln [2 \cosh(g)] + \ln \left[\frac{\cosh(g)}{\cosh(g')} \right]} \quad (98)$$

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. 7:

$$\boxed{x_{n+1} = x_n^2} \quad (99)$$

- *Fixed point:* Configuration x_* that does not change under Eq. 99.
 - Unstable fixed point at $x_* = 1$.
 - Stable fixed point at $x_* = 0$.
- One may interpret either T or J as changing under RG: if one chooses T , it increases under the flow to $T = \infty$ at the stable fixed point, or stays at $T = 0$ at the unstable fixed point.

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 ($\tilde{H} = \beta H$):

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

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

$$\xi' \equiv \xi(x') \stackrel{above}{=} \xi(x)/2. \quad (100)$$

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

$$\xi(x^2) = \xi(x)/2 \quad (101)$$

- The equation has the solution

$$\xi(x) = -\frac{a_0}{\ln(x)} \quad (102)$$

where a_0 is arbitrary length scale, it can be taken to physical (initial) lattice constant a .

- Use Eq. 102 to obtain correlation length at low temperature: Use $g = J/T \gg 1$ in:

$$x = \tanh g \simeq 1 - 2e^{-2g} \quad (103)$$

and then obtain from Eq. (102)

$$\xi \simeq \frac{a}{2} e^{2J/T} \quad (104)$$

- 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 $b = 3, 4, \dots$ to get

$$\tanh g' = \tanh^b g \quad (105)$$

$$\tilde{f}' = b\tilde{f} + (b-1) \ln [2 \cosh(g)] + \ln \left[\frac{\cosh(g)}{\cosh(g')} \right] \quad (106)$$

- Analytically continue for arbitrary real b (natural for momentum shell-RG):

$$\boxed{b \equiv e^l = 1 + l + \mathcal{O}(l^2)} \quad (107)$$

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

For $l \rightarrow 0$, write the RG iteration in form of a differential equation:

$$x_l = x_0^b = x_0^{1+l+\mathcal{O}(l^2)} = x_0 \left(1 + l \ln x_0 + \mathcal{O}(l^2)\right)$$

$$\frac{x_l - x_0}{l} = x_0 \ln x_0 + \mathcal{O}(l)$$

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

$$\boxed{\partial_l x \equiv \frac{\partial x}{\partial l} \equiv \beta(x) = x \ln x} \quad (108)$$

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

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

$$\partial_l g = D_g g + \dots \quad (109)$$

- Example: For the 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

$$\partial_l \tilde{f} = D \tilde{f} + \dots \quad (110)$$

5.3 General properties of RG flows

- Goal: Understand
 - relation between RG fixed points and critical points
 - microscopic justification of scaling hypothesis and identification of critical exponents

Fixed points and critical surface

- Recall RG trafo $\mathbf{g}' = \mathcal{R}(b > 1; \mathbf{g})$ from Eq. (87) for general couplings $\mathbf{g} = \{g_1, g_2, \dots\}$. The RG trafo of the correlation length is $\xi(\mathbf{g}') = \xi(\mathbf{g})/b$, see Eq. (100).

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

$$\mathbf{g}^* = \mathcal{R}(b; \mathbf{g}^*)$$

$$\xi(\mathbf{g}^*) = \xi(\mathbf{g}^*)/b$$

- Classification of fixed points according to the two possible solutions for $\xi(\mathbf{g}^*)$:
 - *Trivial* fixed point: $\xi(\mathbf{g}^*) = 0$
 - *Critical* fixed point: $\xi(\mathbf{g}^*) = \infty$
- Example: Square-lattice Ising model (2D) RG flow in Fig. 8 (projected onto $\beta J - \beta J'$ plane):
 - 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
 - Basin of attraction for critical f.p. = critical surface (critical manifold), has also $\xi = \infty$
Reason: $\xi(\mathbf{g}) = b^n \xi(\mathbf{g}^{(n)})$ and for \mathbf{g} on the critical line, we have $\mathbf{g}^{(n)} \xrightarrow{n \rightarrow \infty} \mathbf{g}^*$ for which $\xi(\mathbf{g}^*) = \infty$. 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.
→ Reason to study vicinity of the critical f.p. (next).
 - Careful: Critical fixed point (●) is not the same as critical point (■, on critical surface).

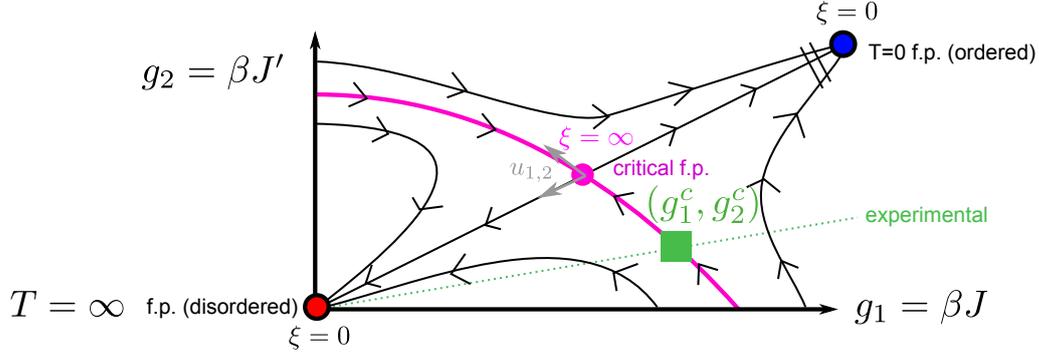


Figure 8: RG-flow of the 2D Ising model, projected to the dimensionless (next-)nearest neighbor couplings J (J').

Local RG flow close to fixed point

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

$$\delta \mathbf{g}' = \mathbf{g}' - \mathbf{g}^* = \mathcal{R}(b; \mathbf{g}) - \mathcal{R}(b; \mathbf{g}^*) \equiv \mathbf{R}(b; \mathbf{g}^*) \cdot \delta \mathbf{g} \quad (111)$$

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

$$R_{ij}(b; \mathbf{g}^*) \equiv \left. \frac{\partial \mathcal{R}_i(b; \mathbf{g})}{\partial g_j} \right|_{\mathbf{g}=\mathbf{g}^*} \quad (112)$$

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

$$\mathbf{v}_\alpha^T \cdot \mathbf{R}(b; \mathbf{g}^*) = \mathbf{v}_\alpha^T \cdot \lambda_\alpha \quad (113)$$

The $\{\mathbf{v}_\alpha^T\}$ 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}_α^T and obtain the *scaling variables*

$$u_\alpha \equiv \mathbf{v}_\alpha^T \cdot \delta \mathbf{g} = \sum_i v_{\alpha,i} \cdot \delta g_i \quad (114)$$

- The RG transformation doesn't mix the α (see grey arrows in Fig. 8):

$$u'_\alpha = \lambda_\alpha u_\alpha \quad (115)$$

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

$$\mathbf{R}(b; \mathbf{g}^*) \cdot \mathbf{R}(b'; \mathbf{g}^*) = \mathbf{R}(bb'; \mathbf{g}^*) = \mathbf{R}(b'; \mathbf{g}^*) \cdot \mathbf{R}(b; \mathbf{g}^*) \quad (116)$$

- Eigenvectors: Commuting matrices have the same eigenvectors $\rightarrow \mathbf{v}_\alpha^T$ are independent of b .
- Eigenvalues: Must satisfy $\lambda_\alpha(b)\lambda_\alpha(b') \stackrel{!}{=} \lambda_\alpha(bb')$, thus

$$\lambda_\alpha(b) = b^{y_\alpha} \quad (117)$$

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

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

$$\boxed{u'_\alpha = b^{y_\alpha} u_\alpha, \quad \partial_l u_\alpha = y_\alpha u_\alpha} \quad (118)$$

Warning: Due to the linearization in Eq. (111), 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 $\partial_l u_\alpha = 0 u_\alpha + \# u_\alpha^2 + \dots$ 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):

$$\partial_l t = y_t t, \quad \partial_l h = y_h h \quad (119)$$

or

$$t' = b^{y_t} t, \quad h' = b^{y_h} h \quad (120)$$

with $y_t > 0$ and $y_h > 0$. (We will compute $y_{t,h}$ approximately in Sec. 5.4 using φ^4 -theory.)

- Recall: RG preserves the partition function

$$\mathcal{Z}_N(t, h) = \mathcal{Z}_{N/b^D}(t' = b^{y_t} t, h' = b^{y_h} h) \quad (121)$$

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

- For the free energy density, we find

$$f \sim -\frac{1}{N} \ln \mathcal{Z}_N = -\frac{1}{b^D} \frac{1}{N/b^D} \ln \mathcal{Z}_{N/b^D} \quad (122)$$

and we read off:

$$\boxed{f_{sing}(t, h) = b^{-D} f_{sing}(t' = b^{y_t} t, h' = b^{y_h} h)} \quad (123)$$

- Restriction to singular part (“*sing*”) is caused by the neglect of
 - higher-order in t, h flow
 - marginal or irrelevant couplings
- We confirmed the scaling hypothesis from Eq. (8).
Critical exponents (i.e. $\nu = 1/y_t$) are related to the linearized RG flow close to the 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 $G(\mathbf{r})$

- Recall definition, assume $k_{1,2} < \Lambda_0/b$ and employ the RG step $\delta\varphi(\mathbf{k}) = \zeta_b \delta\varphi'(\mathbf{k}')$, $\mathbf{k} = \mathbf{k}'/b$:

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

By comparison, we find

$$G(\mathbf{k}; \mathbf{g}) = \zeta_b^2 b^{-D} G(b\mathbf{k}; \mathbf{g}') \quad (124)$$

- Convention: Parametrization

$$\zeta_b \equiv b^{1+D/2} \sqrt{Z_b} \quad (125)$$

so that

$$G(\mathbf{k}; \mathbf{g}) = b^2 Z_b G(b\mathbf{k}; \mathbf{g}') \quad (126)$$

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

$$\partial_l Z_l \equiv -\eta_l Z_l. \quad (127)$$

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

$$G(\mathbf{k}; \mathbf{g}) = b^{2-\eta} G(b\mathbf{k}; \mathbf{g}'). \quad (128)$$

At a fixed point $\mathbf{g} = \mathbf{g}' = \mathbf{g}^*$, this can be solved as

$$G(\mathbf{k}) = |\mathbf{k}|^{-2+\eta} \quad (129)$$

- Conclusion:

Anomalous dimension η introduced in Eq. (6) connected to microscopic RG via field rescaling factor ζ .

- 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

$$h\varphi(\mathbf{k} = 0) = h'\varphi'(\mathbf{k}' = 0) = h'\zeta_b^{-1}\varphi(\mathbf{k} = 0) \quad (130)$$

Read off $h' = \zeta_b h$, compare to $h' = b^{y_h} h$. Find

$$\zeta_b = b^{y_h} \quad (131)$$

Insert in Eq. (124). Consider only relevant couplings $\mathbf{g} = (t, h)$ (singular part only):

$$G_{sing}(\mathbf{k}; t, h) = b^{-D} b^{2y_h} G_{sing}(b\mathbf{k}; b^{y_t} t, b^{y_h} h) \quad (132)$$

which is the Fourier-transformation of the scaling hypothesis in Eq. (11).

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

- Goals:

- Find flow equations for ϕ^4 -theory beyond engineering dimensions.
- Mode elimination step via perturbation theory in u_0 .
- Analysis of flow diagram and critical exponents (for $\epsilon \equiv 4 - D \ll 1$)

RG flow equations

- Recall ϕ^4 -theory (Ginzburg-Landau-Wilson action) from Eq. (42).
Set magnetic field to zero, assume high-temperature regime $r_0 > 0$:

$$S_{\Lambda_0}[\varphi] = V f_0 + \frac{1}{2} \int_{\mathbf{k}}^{\Lambda_0} [r_0 + c_0 k^2] \varphi(-\mathbf{k}) \varphi(\mathbf{k}) + \frac{u_0}{4!} \int_{\mathbf{k}_{1,2,3,4}}^{\Lambda_0} (2\pi)^D \delta(\mathbf{k}_1 + \dots + \mathbf{k}_4) \varphi(\mathbf{k}_1) \varphi(\mathbf{k}_2) \varphi(\mathbf{k}_3) \varphi(\mathbf{k}_4) \quad (133)$$

- 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:

$$S_{\Lambda_0}[\varphi] = S_{\Lambda}[\varphi^<] + S_{\Lambda, \Lambda_0}[\varphi^>] + S_{mix}[\varphi^<, \varphi^>] \quad (134)$$

– “Smaller part” $S_{\Lambda}[\varphi^<]$ is like $S_{\Lambda_0}[\varphi]$ but with $\int_{\mathbf{k}}^{\Lambda_0} \varphi(\mathbf{k}) \dots \rightarrow \int_{\mathbf{k}}^{\Lambda} \varphi^<(\mathbf{k}) \dots$

– “Larger part” $S_{\Lambda, \Lambda_0}[\varphi^>]$ is similar with $\int_{\mathbf{k}}^{\Lambda_0} \varphi(\mathbf{k}) \dots \rightarrow \int_{|\mathbf{k}| > \Lambda}^{\Lambda_0} \varphi^>(\mathbf{k}) \dots$

– “Mixing term”: Of order u_0 . Possibilities of picking 2 $\varphi^<$ -fields of the 4 φ fields $6 = \binom{4}{2}$:

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

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

$$e^{-S_{\Lambda}[\varphi^<, f^<, r^<, c^<, u^<]} = e^{-S_{\Lambda}[\varphi^<, f_0, r_0, c_0, u_0]} \int \mathcal{D}[\varphi^>] e^{-S_{\Lambda, \Lambda_0}[\varphi^>] - S_{mix}[\varphi^<, \varphi^>]} \quad (135)$$

or

$$S_{\Lambda}[\varphi^<, f^<, r^<, c^<, u^<] = S_{\Lambda}[\varphi^<, f_0, r_0, c_0, u_0] - \ln \left[\int \mathcal{D}[\varphi^>] e^{-S_{\Lambda, \Lambda_0}[\varphi^>] - S_{mix}[\varphi^<, \varphi^>]} \right] \quad (136)$$

Expand the ln in powers of u_0 :

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

- Consider leading-in- u_0 corrections to quadratic/quartic parts of $S_{\Lambda}[\varphi^<, f^<, r^<, c^<, u^<]$: Need to keep terms of order $u_0 \varphi^<^2$ and $u_0^2 \varphi^<^4$.

→ 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, $S_{\Lambda, \Lambda_0}^0[\varphi^>] = \frac{1}{2} \int_{|\mathbf{k}| > \Lambda}^{\Lambda_0} [r_0 + c_0 k^2] \varphi^>(-\mathbf{k}) \varphi^>(\mathbf{k})$.

Notation:

$$\langle \dots \rangle_{0, >} \equiv \frac{\int \mathcal{D}[\varphi^>] e^{-S_{\Lambda, \Lambda_0}^0[\varphi^>]} \dots}{\int \mathcal{D}[\varphi^>] e^{-S_{\Lambda, \Lambda_0}^0[\varphi^>]}} \quad (137)$$

We then have

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

- In light of Eq. (136), we compare the parts of order $(\varphi^<)^2$ [terms $\sim \varphi^<$ or $\sim (\varphi^<)^3$ vanish] and read off

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

After comparison of both sides, we find

$$\boxed{c^< = c_0} \tag{138}$$

$$\boxed{r^< = r_0 + \frac{u_0}{2} \int_{\Lambda}^{\Lambda_0} \frac{d^D k}{(2\pi)^D} \frac{1}{r_0 + c_0 k^2} \simeq r_0 + u_0 \frac{K_D \Lambda_0^{D-1} (\Lambda_0 - \Lambda)}{2(r_0 + c_0 \Lambda_0^2)}} \tag{139}$$

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. 3.4.2).

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

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

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 $G_0(\mathbf{k}) = 1/(r_0 + c_0 k^2)$ and carefully consider all the δ -functions:

$$\begin{aligned}
\dots &= \int_{\mathbf{k}_{1,2}}^{\Lambda} \int_{|\mathbf{k}_{3,4}|>\Lambda}^{\Lambda_0} (2\pi)^D \delta(\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3 + \mathbf{k}_4) \int_{\mathbf{q}_{1,2}}^{\Lambda} (2\pi)^D \delta(\mathbf{q}_1 + \mathbf{q}_2 - \mathbf{k}_3 - \mathbf{k}_4) \varphi^<(\mathbf{q}_1) \varphi^<(\mathbf{k}_1) \varphi^<(\mathbf{q}_2) \varphi^<(\mathbf{k}_2) \\
&\times -2 \frac{1}{2} \left(6 \frac{u_0}{4!} \right)^2 \frac{1}{(r_0 + c_0 k_3^2) (r_0 + c_0 k_4^2)} \\
&= \int_{\mathbf{k}_{1,2}}^{\Lambda} \int_{\mathbf{q}_{1,2}}^{\Lambda} (2\pi)^D \delta(\mathbf{q}_1 + \mathbf{q}_2 + \mathbf{k}_1 + \mathbf{k}_2) \varphi^<(\mathbf{q}_1) \varphi^<(\mathbf{k}_1) \varphi^<(\mathbf{q}_2) \varphi^<(\mathbf{k}_2) \\
&\times -2 \frac{1}{2} \left(6 \frac{u_0}{4!} \right)^2 \int_{|\mathbf{k}_{3,4}|>\Lambda}^{\Lambda_0} (2\pi)^D \delta(\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3 + \mathbf{k}_4) \frac{1}{(r_0 + c_0 k_3^2) (r_0 + c_0 k_4^2)}
\end{aligned}$$

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

$$\boxed{u^< = u_0 - \underbrace{4! 2 \frac{1}{2} \left(6 \frac{u_0}{4!} \right)^2}_{\frac{3}{2} u_0^2} \int_{\Lambda}^{\Lambda_0} \frac{d^D k}{(2\pi)^D} \frac{1}{(r_0 + c_0 k^2)^2} \simeq u_0 - \frac{3}{2} u_0^2 \frac{K_D \Lambda_0^{D-1} (\Lambda_0 - \Lambda)}{(r_0 + c_0 \Lambda_0^2)^2}} \tag{140}$$

- 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 $u(\mathbf{k}_{1,2,3}) = u^{(0)} + u^{(1)}k_1 + \dots$ are less relevant than $u^{(0)}$ because $[u^{(1)}] = [u^{(0)}] \times [length]$ under rescaling they have a smaller engineering dimension than $u^{(0)}$.

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

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

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 $\Lambda = \Lambda_0 e^{-l}$:

$$\begin{aligned} r' &= e^{2l} \left[r_0 + u_0 \frac{K_D \Lambda_0^{D-1} (\Lambda_0 - \Lambda_0 e^{-l})}{2(r_0 + c_0 \Lambda_0^2)} \right] \\ &= r_0 + 2lr_0 + u_0 \frac{K_D \Lambda_0^D l}{2(r_0 + c_0 \Lambda_0^2)} + \mathcal{O}(l^2) \\ \partial_l r_l &= 2r_l + \frac{u_l}{2} \frac{K_D \Lambda_0^D}{r_l + c_0 \Lambda_0^2} \end{aligned}$$

and likewise

$$\partial_l u_l = (4 - D)u_l - \frac{3}{2} u_l^2 \frac{K_D \Lambda_0^D}{(r_l + c_0 \Lambda_0^2)^2} \quad (141)$$

- Clean up by defining dimensionless couplings:

$$\bar{r}_l \equiv r_l \frac{1}{c_0 \Lambda_0^2}, \quad \bar{u}_l \equiv u_l \frac{K_D}{c_0^2 \Lambda_0^{4-D}} \quad (142)$$

in terms of which

$$\boxed{\partial_l \bar{r}_l = 2\bar{r}_l + \frac{1}{2} \frac{\bar{u}_l}{\bar{r}_l + 1}} \quad \boxed{\partial_l \bar{u}_l = (4 - D)\bar{u}_l - \frac{3}{2} \frac{\bar{u}_l^2}{(\bar{r}_l + 1)^2}} \quad (143)$$

Wilson-Fisher fixed point for $D > 4$

- Analyze the flow given by Eq. (143) above, see Fig. 9 for flow diagrams at $D = 4.5$, $D = 3.8$ and $D = 3$.
 - For $D > 4$, we only have the Gaussian critical fixed point, $(\bar{u}_*, \bar{r}_*) = (0, 0)$. ($\rightarrow D_{up} = 4$)
 - 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.

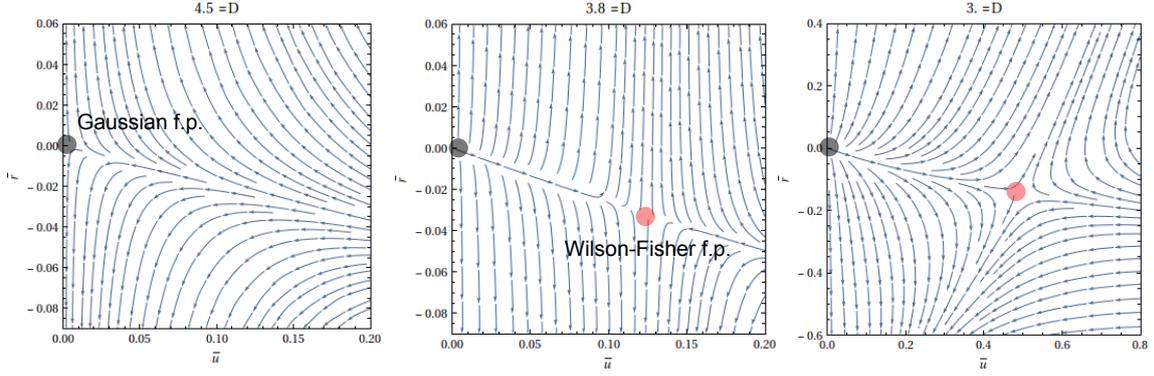


Figure 9: RG flow of the ϕ^4 -theory above and below $D = 4$ according to Eq. (143).

Critical exponents in $D < 4$: ϵ -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 fixed point conditions are

$$\begin{aligned} 0 &= 2\bar{r}_* + \frac{1}{2} \frac{\bar{u}_*}{\bar{r}_* + 1}, \\ 0 &= \epsilon \bar{u}_* - \frac{3}{2} \frac{\bar{u}_*^2}{(\bar{r}_* + 1)^2}. \end{aligned}$$

Without the $\mathcal{O}(\bar{u}_*^3)$ terms, can only reliably solve for \bar{r}_*, \bar{u}_* up to $\mathcal{O}(\epsilon)$: $\bar{u}_* = \frac{2}{3}\epsilon + \mathcal{O}(\epsilon^2)$ and $\bar{r}_* = -\epsilon/6 + \mathcal{O}(\epsilon^2)$.

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

$$\partial_l \begin{pmatrix} \delta\bar{r}_l \\ \delta\bar{u}_l \end{pmatrix} = \begin{pmatrix} 2 - \frac{\epsilon}{3} & \frac{1}{2} + \frac{\epsilon}{12} \\ 0 & -\epsilon \end{pmatrix} \begin{pmatrix} \delta\bar{r}_l \\ \delta\bar{u}_l \end{pmatrix} \quad (144)$$

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

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

- 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. 5.3, we find

$$\boxed{\nu \equiv \frac{1}{y_2} = \frac{1}{2} + \frac{\epsilon}{12} + \mathcal{O}(\epsilon^2)} \quad (145)$$

- Remark: One often lets $\epsilon \rightarrow 1$ at the end of this calculation, which yields $\nu_{1-loop} = 0.58$ and the exact value is $\nu_{ex} \simeq 0.63$. Recall MFT / Gaussian fixed point: $\nu = 0.5$. Systematic improvement $\mathcal{O}(\epsilon)$ is possible in a two-loop calculation (way more complicated!).

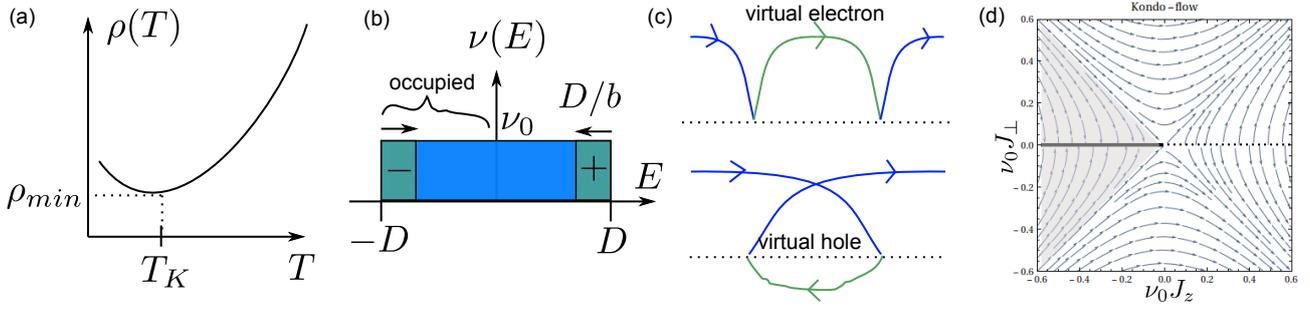


Figure 10: Kondo problem: (a) Typical resistance versus temperature curve for metals with magnetic impurities. (b) Flat density of states assumed for host system with bandwidth $2D$. (c) Diagrams for virtual electron or virtual hole excitations. (d) Poor man's scaling: Flow diagram in the $\nu_0 J_z - \nu_0 J_\perp$ -plane.

5.5 Example: Kondo-Effect and poor-man scaling

- In metals with magnetic impurities (local quantum spin-1/2), the resistance does have a minimum in temperature and then increases again (Fig. 10a).
- Unusual, since well-known mechanisms would lead to further decaying or constant resistance as $T \rightarrow 0$:
 - electron-electron scattering $\rho \sim T^2$
 - electron-phonon scattering $\rho \sim T^5$
 - non-magnetic impurity scattering $\rho \sim \text{const.}$
- Model for single impurity \mathbf{S} at $\mathbf{r} = 0$ with local spin-exchange interaction to non-interacting finite-size V bath of electrons $c_{\mathbf{r}\sigma}$

$$H = \sum_{\mathbf{k}, \sigma} \underbrace{(\varepsilon_{\mathbf{k}} - \mu)}_{\xi_{\mathbf{k}}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + 2J \mathbf{s}_{\mathbf{r}=0} \cdot \mathbf{S} = H_0 + H_{int}$$

We use $c_{\mathbf{r}\sigma} = \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} c_{\mathbf{k}\sigma}$ and find for the spin operator of the itinerant electrons at $\mathbf{r} = 0$:

$$s_{\mathbf{r}=0}^\alpha = \frac{1}{2} c_{\mathbf{r}=0\sigma}^\dagger \tau_{\sigma, \sigma'}^\alpha c_{\mathbf{r}=0\sigma'} = \frac{1}{2} \sum_{\mathbf{k}, \mathbf{k}'} c_{\mathbf{k}\sigma}^\dagger \tau_{\sigma, \sigma'}^\alpha c_{\mathbf{k}'\sigma'} \quad (146)$$

- Expand Pauli matrices, generalize to anisotropic Kondo model with $S^\pm = S^x + iS^y$. Assume flat density of states (per spin, with units [1/energy]), $\nu(E) \equiv \sum_{\mathbf{k}} \delta(E - \xi_{\mathbf{k}}) \equiv \nu_0$ (Fig. 10b):

$$H = \sum_{\mathbf{k}, \sigma} \xi_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + J_z \sum_{\mathbf{k}, \mathbf{k}'} \left(c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}'\uparrow} - c_{\mathbf{k}\downarrow}^\dagger c_{\mathbf{k}'\downarrow} \right) S^z + J_\perp \sum_{\mathbf{k}, \mathbf{k}'} \left(c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}'\downarrow} S^- + c_{\mathbf{k}\downarrow}^\dagger c_{\mathbf{k}'\uparrow} S^+ \right) \quad (147)$$

- Perturbation theory for resistivity ρ in J [Kondo,1964]:

$$\rho = \rho_0 \left(1 - 4J\nu_0 \ln(T/D) + \mathcal{O}(J^3) \right) \quad (148)$$

- explains increase of $\rho(T)$ as $T \rightarrow 0$
- identifies a temperature at which perturbation theory breaks down (second term $\mathcal{O}(1)$): $T_K \sim D \exp\left(-\frac{1}{\# \nu_0 J}\right)$
- Wilson solved the problem using **numerical RG** (NRG): Below the *crossover* temperature T_K , the impurity \mathbf{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

- Goal: Derive T_K using RG based on Hamiltonian and a "run-away-flow".
- Plan for RG:
Ground state of H_0 is filled Fermi sea up to $E = 0$. States $|\psi_{-/+}\rangle$ with at least one hole/electron in the lower/upper band-edge $D/b < |\xi_{\mathbf{k}}| < D$ are highly excited with energy $\geq D/b$.
Integrate out these high-energy states (take them into account as virtual states in perturbation theory), see how $J_{z,\perp}$ flows.
- Formal setup of perturbation theory: Divide Hilbert-space into $|\psi_{-/+}\rangle$ -like states and the rest $|\psi_0\rangle$,

$$H |\psi\rangle = \begin{pmatrix} H_{--} & H_{-0} & \simeq 0 \\ H_{0-} & H_{00} & H_{0+} \\ \simeq 0 & H_{+0} & H_{++} \end{pmatrix} \begin{pmatrix} |\psi_{-}\rangle \\ |\psi_0\rangle \\ |\psi_{+}\rangle \end{pmatrix}, \quad (149)$$

As H_0 does not change between the sectors, the off-diagonal terms are $\sim J$.

- We write Schrödinger equation for $|\psi_0\rangle$ -states:

$$(H_{00} + \underbrace{H_{0+} \frac{1}{E - H_{++}} H_{+0}}_{\text{virtual electron}} + \underbrace{H_{0-} \frac{1}{E - H_{--}} H_{-0}}_{\text{virtual hole}}) |\psi_0\rangle = E |\psi_0\rangle \quad (150)$$

- 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.
- Preparation: From $[E - H_0, c_{\mathbf{q}\sigma}] = \xi_{\mathbf{q}} c_{\mathbf{q}\sigma}$ we find

$$c_{\mathbf{q}\sigma} \frac{1}{E - H_0} = \frac{1}{E - H_0 - \xi_{\mathbf{q}}} c_{\mathbf{q}\sigma}, \quad c_{\mathbf{q}\sigma}^\dagger \frac{1}{E - H_0} = \frac{1}{E - H_0 + \xi_{\mathbf{q}}} c_{\mathbf{q}\sigma}^\dagger \quad (151)$$

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

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

- 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. Find

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

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

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

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

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

- We are interested in energies close to the ground-state energy E_0 of H_0 . \rightarrow Approximate all denominators by $1/(-D)$.
- Result: Virtual $S^z S^z$ -processes give rise to non-magnetic scattering terms that do not depend on the spin of the scattered electrons. 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* $c_{\mathbf{q}+\sigma}^\dagger$

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

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

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

which is the same as in the virtual electron term.

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

$$J_z(b) = J_z + 2\nu_0 J_{\perp}^2 (1 - 1/b) \quad (152)$$

- Remaining processes ($S^z S^+ = S^+/2, \dots$) analogously lead to:

$$J_{\perp}(b) = J_{\perp} + 2\nu_0 J_{\perp} J_z (1 - 1/b) \quad (153)$$

- No need for re-scaling, as the Hamiltonian stays in its initial form. We can interpret $J_{z,\perp}(b)$ as the result of iterative application of perturbation theory, integrating out bath electrons with $|\xi_{\mathbf{k}}| \in [D/b, D]$.
- 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:

$$\boxed{\partial_l (J_z \nu_0) = 2 (J_{\perp} \nu_0)^2, \quad \partial_l (J_{\perp} \nu_0) = 2 (J_{\perp} \nu_0) (J_z \nu_0)} \quad (154)$$

Interpretation of flow and Kondo scale

- The flow diagram is shown in Fig. 10(d). There is a line of fixed points at $J_{\perp} = 0$.
- Observations: $(J_z \nu_0)^2 - (J_{\perp} \nu_0)^2 = \text{const}$. Follows from $\partial_l(\dots) = 0$.
- $J_z \nu_0$ 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 $|J_{\perp}| \leq |J_z|$ (grey).

In particular, 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 energy scale does that happen?

- Specialize to $J_{\perp} = J_z \equiv J$ with $0 < \nu_0 J \ll 1$. Find the Kondo scale $D_l \equiv T_K$ where strong coupling is reached.

Integrate the flow

$$\frac{d(\nu_0 J)}{(\nu_0 J)^2} = 2dl \rightarrow \frac{1}{J_l \nu_0} - \frac{1}{J \nu_0} = 2l = 2 \ln \left(\frac{D}{D_l} \right) \quad (155)$$

The flow has to terminate at $D_l \equiv T_K$ when the dimensionless running coupling constant $J_l \nu_0$ becomes $\mathcal{O}(1)$.

$$\underbrace{\frac{1}{J_l \nu_0}}_{\mathcal{O}(1)} - \underbrace{\frac{1}{J \nu_0}}_{\gg 1} = 2 \ln \left(\frac{D}{T_K} \right) \quad (156)$$

We neglect the left term and are left with $\frac{1}{J \nu_0} \simeq 2 \ln \left(\frac{D}{T_K} \right)$ or

$$\boxed{T_K \simeq D \exp \left(-\frac{1}{2J \nu_0} \right)} \quad (157)$$

- Note: This result does *not* depend on the exact value $\mathcal{O}(1)$ where we stopped the flow.

5.6 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. 11(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 $m^* \gtrsim m_0$.
- Here: RG perspective.

Model

- Modeling:

$$H_0 = \sum_{\mathbf{k}, \sigma} (\varepsilon_{\mathbf{k}} - \mu) c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} \quad (158)$$

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, $\varepsilon_{\mathbf{k}} = -t \sum_{\mu=1}^D \cos k_{\mu} \simeq -Dt + \frac{t}{2} k^2$.

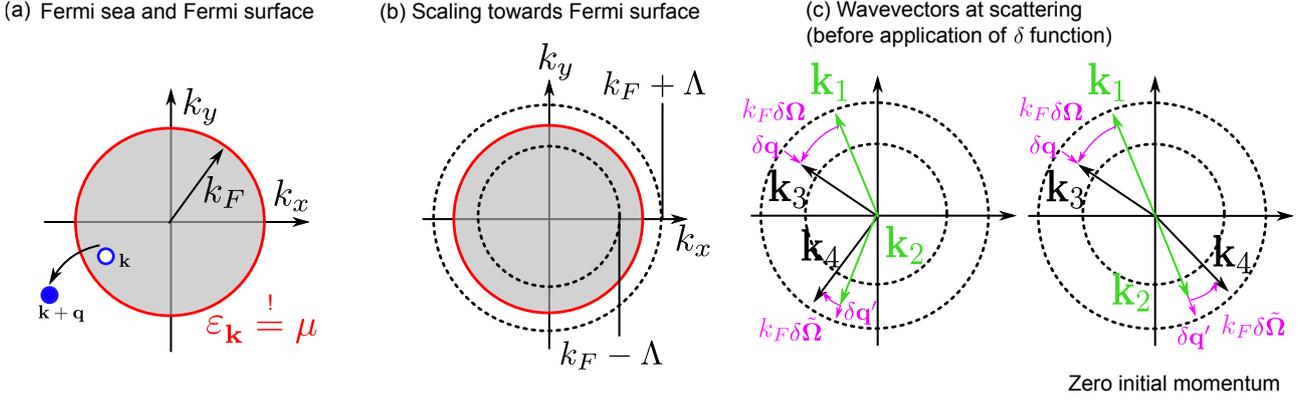


Figure 11: Landau's Fermi liquid theory: (a) Definition of Fermi sea (grey) and Fermi surface (red). (b) Scaling towards Fermi surface.

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

$$\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}} = \frac{(\mathbf{k} + \mathbf{q})^2}{2m} - \frac{k^2}{2m} = \frac{\mathbf{k}}{m} \cdot \mathbf{q} + \mathcal{O}(q^2) \simeq \mathbf{v}_F \cdot \mathbf{q} \quad (159)$$

where $\mathbf{v}_F = \partial_{\mathbf{k}} \varepsilon_{\mathbf{k}}|_{k=l_F}$ 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. 11(b).

Gaussian action

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

$$S_0 = \int d\tau \int d\Omega \int_{-\Lambda}^{+\Lambda} \frac{dq}{2\pi} \bar{\psi}(\tau, q, \Omega) [\partial_\tau + v_F q] \psi(\tau, q, \Omega) \quad (160)$$

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: Integration over $\psi^>$ with $q \in \pm(\Lambda/b, \Lambda)$ decouples from integration over $\psi^<$, 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 :

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

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

$$\int d\tau \int d\Omega \int_{-\Lambda}^{+\Lambda} \frac{dq}{2\pi} m\bar{\psi}\psi \rightarrow \int d\tau' \int d\Omega \int_{-\Lambda}^{+\Lambda} \frac{dq'}{2\pi} \underbrace{mb}_{m'=by_m} \bar{\psi}'\psi' \quad (161)$$

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,

$$\mathbf{k}_i = (k_F + q_i)\mathbf{\Omega}_i \quad (162)$$

with $\mathbf{\Omega}_i = \left(\cos \phi_i \sin \theta_i, \sin \phi_i \sin \theta_i, \cos \theta_i \right)^T$:

$$S_{int} = \int d\tau \prod_{i=1}^4 \int d\Omega_i \int_{-\Lambda}^{+\Lambda} \frac{dq_i}{2\pi} \bar{\psi}_1 \bar{\psi}_2 \psi_3 \psi_4 U(1, 2, 3, 4) \delta^D(\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3 - \mathbf{k}_4) \quad (163)$$

- Rescaling for δ -function: The q_i scale to zero, but the k_F stay fixed. Thus

$$\delta^D(\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3 - \mathbf{k}_4) \simeq \frac{1}{k_F} \delta^D(\mathbf{\Omega}_1 + \mathbf{\Omega}_2 - \mathbf{\Omega}_3 - \mathbf{\Omega}_4) \quad (164)$$

and the δ -function does not change under rescaling.

- Rescaling of interaction U :

$$S_{int} = \int d\tau' \prod_{i=1}^4 \int d\Omega_i \int_{-\Lambda}^{+\Lambda} \frac{dq'_i}{2\pi} \bar{\psi}_1 \bar{\psi}_2 \psi_3 \psi_4 b^{1-4+4 \times (1/2)} U(1, 2, 3, 4) \frac{1}{k_F} \delta(\mathbf{\Omega}_1 + \mathbf{\Omega}_2 - \mathbf{\Omega}_3 - \mathbf{\Omega}_4) \quad (165)$$

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

$$y_U = -1 \quad (166)$$

- Surprising result: Electron-electron interactions are irrelevant.
Strong argument for why Fermi-Liquid theory works.
Electron interaction becomes weaker and weaker as energy is lowered and nearly free electron gas is good description of conductor.

Interactions revisited

- Q: Superconductivity is interaction driven phenomenon.
How can we ever get superconductivity if interactions become weaker and weaker at low energy?
What is wrong with our argument?
- Parameterize scattering process $\mathbf{k}_{1,2} \rightarrow \mathbf{k}_{3,4}$ with

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

so that

$$\delta^D(\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3 - \mathbf{k}_4) = \delta^D(k_F \delta\mathbf{\Omega} + \delta\mathbf{q} + k_F \delta\tilde{\mathbf{\Omega}} + \delta\tilde{\mathbf{q}}) \quad (167)$$

- 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 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:

$$\delta^D(\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3 - \mathbf{k}_4) = \delta^{D-1}\left(k_F\delta\mathbf{\Omega} + k_F\delta\tilde{\mathbf{\Omega}}\right) \delta(\delta\mathbf{q} + \delta\tilde{\mathbf{q}}) \quad (168)$$

- Now, we get an additional factor b upon rescaling

$$\delta(\delta\mathbf{q} + \delta\tilde{\mathbf{q}}) = \delta\left(\frac{\delta\mathbf{q}' + \delta\tilde{\mathbf{q}}'}{b}\right) = b\delta(\delta\mathbf{q}' + \delta\tilde{\mathbf{q}}') \quad (169)$$

which yields $y_U = 0$.

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

$$U(\mathbf{\Omega}_1, -\mathbf{\Omega}_1, \mathbf{\Omega}_3, -\mathbf{\Omega}_3) \equiv V(\mathbf{\Omega}_1, \mathbf{\Omega}_3) \stackrel{rot. invariant}{=} V(\mathbf{\Omega}_1 \cdot \mathbf{\Omega}_3) \quad (170)$$

are marginal under re-scaling!

- Comment:

- Interactions are always irrelevant, but for special kinematics can offset this.
- Many Feynman diagrams are irrelevant, unless certain momentum restrictions apply, see Fig. 12(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. 12(b) to understand fate of interaction. Expand $V(\mathbf{\Omega}_1 \cdot \mathbf{\Omega}_3)$ to angular momentum channels L . Then find the flow [Shankar, Rev. Mod. Phys. 66, 129 (1994)]:

$$\partial_l V_L = -\frac{1}{4\pi} V_L^2 \quad (171)$$

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: Can generate effectively attractive interaction from phonons.

- Attractive interaction leads to superconductivity: Solve flow

$$V_L(l) = \frac{V_L(0)}{1 + lV_L(0)/(4\pi)} \quad (172)$$

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

$$\Lambda_\star = \Lambda e^{-l_\star} = e^{-4\pi/|V_L(0)|} \triangleq T_c^{BCS} \quad (173)$$

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.

- Repulsive interaction: Is 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.

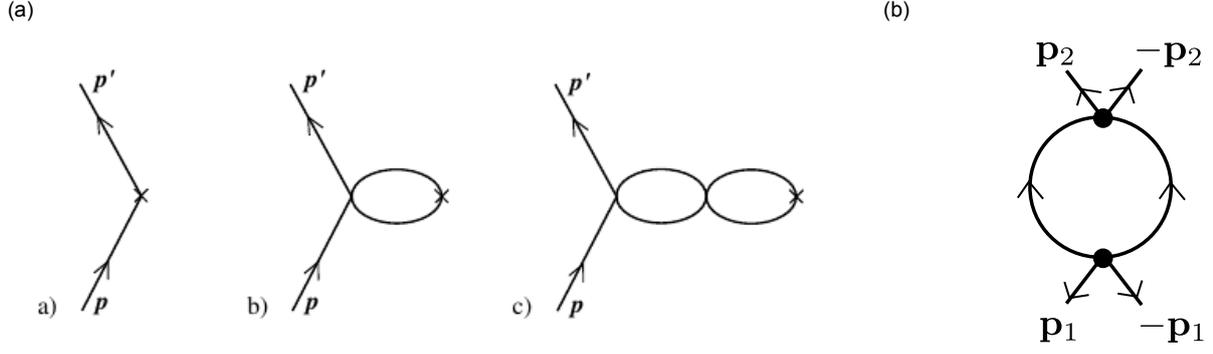


Figure 12: (a) The loop corrections ii),iii) to scattering i) from \mathbf{p} to \mathbf{p}' are generally invariant unless $\mathbf{p} = \mathbf{p}'$ when they become marginal. (b) One-loop renormalization of marginal interaction.

5.7 Exercises

5.7.1 Real-space RG for disordered Heisenberg chain

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

$$H = \sum_i J_i \mathbf{S}_i \cdot \mathbf{S}_{i+1}. \quad (174)$$

1) Decimation scheme: 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 $J_{n\pm 1} \ll \Omega$. 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, $J_{n-1, n+2}^{eff} \mathbf{S}_{n-1} \cdot \mathbf{S}_{n+2}$, with

$$J_{n-1, n+2}^{eff} = \frac{J_{n-1} J_{n+1}}{2\Omega} \quad (175)$$

which is much smaller than $J_{n\pm 1}$. 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. It 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 $P_\Omega(J)$. To facilitate the math, introduce

$$\zeta_i \equiv \ln(\Omega/J_i) \in [0, \infty), \quad (176)$$

neglect the factor 2 in Eq. (175) and define the RG flow parameter to be

$$\Gamma \equiv \ln(\Omega_0/\Omega) \quad (177)$$

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

$$\frac{\partial P_\Gamma(\zeta)}{\partial \Gamma} = \frac{\partial P_\Gamma(\zeta)}{\partial \zeta} + P_\Gamma(0) \int d\zeta_l \int d\zeta_r P_\Gamma(\zeta_l) P_\Gamma(\zeta_r) \delta(\zeta - \zeta_l - \zeta_r) \quad (178)$$

which conserves the total probability.

3) Solve the flow equation (178) by rewriting it for the distribution function $Q(x)$ of the quantity $x \equiv \zeta/\Gamma$. You should find

$$0 = (x+1) \frac{\partial Q(x)}{\partial x} + Q(x) + Q(0) \int dx_l \int dx_r Q(x_l) Q(x_r) \delta(x - x_l - x_r) \quad (179)$$

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

$$P_\Omega(J) = \frac{1}{\Gamma(\Omega)\Omega} \left(\frac{\Omega}{J}\right)^{1-1/\Gamma(\Omega)}. \quad (180)$$

Define the typical J at RG-time Γ as the J that corresponds to the mean of ζ . Show that $J_{typ} = \Omega^2/\Omega_0$ and argue why our initial strong disorder assumption is better and better fulfilled as we iterate the flow. It turns out that our solution (180) 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

$$n = n_0/\Gamma^2 \quad (181)$$

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

- 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 $E \sim L^{-z}$.)
- 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 the susceptibility of a free spin, $\chi \sim 1/T$.

5.7.2 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,

$$\begin{aligned} \partial_l u &= y_u u + A(u, v) \\ \partial_l v &= y_v v + B(u, v) \end{aligned}$$

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:

$$\begin{aligned} A(u, v) &= a_1 u^2 + a_2 uv + a_3 v^2 + \dots \\ B(u, v) &= b_1 u^2 + b_2 uv + b_3 v^2 + \dots \end{aligned}$$

In the $u - v$ plane, plot the flow (u_l, v_l) parameterized by $l \in [0, 2]$ starting from the points $(0.2, 0)$ and $(0.2, 0.3)$. Use $A(u, v) = -uv$ and $B(u, v) = -u^2$ and a computer (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 don't need to consider the irrelevant couplings in a scaling equation like Eq. (8).

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. (42). As a preparation, consider the Gaussian action without interaction term:

$$S_{\Lambda_0}[\varphi] = -h_0 \varphi(\mathbf{k} = 0) + \frac{1}{2} \int_{\mathbf{k}}^{\Lambda_0} [r_0 + c_0 k^2] \varphi(-\mathbf{k}) \varphi(\mathbf{k}) \quad (182)$$

- (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

$$S_{\Lambda_0}^{int}[\varphi] = \frac{u_0}{4!} \int_{\mathbf{k}_{1,2,3,4}}^{\Lambda_0} (2\pi)^D \delta(\mathbf{k}_1 + \dots + \mathbf{k}_4) \varphi(\mathbf{k}_1) \varphi(\mathbf{k}_2) \varphi(\mathbf{k}_3) \varphi(\mathbf{k}_4) \quad (183)$$

disregard the terms generated by momentum shell integration (they will be considered in Sec. 5.4) 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 $f_{sing}(t, h)$ 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 has the scaling form

$$m(t, h, u) = b^{y_h - D} m(b^{y_t} t, b^{y_h} h, b^{y_u} u), \quad (184)$$

set $h = 0$ and derive the scaling relation

$$m(t, 0, u) = |t|^{-(y_h - D)/y_t} m(\pm 1, 0, |t|^{-y_u/y_t} u). \quad (185)$$

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 $\beta = 1/2$.

5.7.3 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

$$\partial_t r = 2r - 24r(g_1 + g_2) \quad (186)$$

$$\partial_t g_1 = (4 - D)g_1 - 8(n + 8)g_1^2 - 48g_1g_2 \quad (187)$$

$$\partial_t g_2 = (4 - D)g_2 - 72g_2^2 - 96g_1g_2 \quad (188)$$

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.

5.7.4 One-loop flow equations for the $O(N)$ -symmetric φ^4 -theory

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

$$S[\boldsymbol{\varphi}] = \frac{1}{2} \int_{\mathbf{k}}^{\Lambda_0} [r_0 + c_0 k^2] \sum_{i=1}^N |\varphi_i(\mathbf{k})|^2 + \frac{u_0}{4!} \int_{\mathbf{r}} \sum_{i,j=1}^N \varphi_i^2(\mathbf{r}) \varphi_j^2(\mathbf{r}). \quad (189)$$

1. Show that the action is invariant under $O(N)$ rotations, $\varphi_i \rightarrow \sum_{j=1}^N M_{ij} \varphi_j$ 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

$$\partial_l \bar{r} = 2\bar{r} + \frac{(N+2)\bar{u}}{6(1+\bar{r})}, \quad \partial_l \bar{u} = \underbrace{(4-D)}_{\epsilon} \bar{u} - \frac{(N+8)\bar{u}^2}{6(1+\bar{r})^2} \quad (190)$$

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 $j > \dots < i$ which carry 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 $D = 3$ and $N = 3$ find an approximation for ν of the three-dimensional Heisenberg universality class governing magnetic phase transitions in classical spin systems. The exact value is $\nu = 0.71$.

5.7.5 Kondo impurity in gapless fermionic system

The Kondo impurity described by the Hamiltonian in Eq. (147) 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,

$$\nu(E) \equiv \sum_{\mathbf{k}} \delta(E - \xi_{\mathbf{k}}) \stackrel{!}{=} \begin{cases} C |E|^r & : |E| \leq D \\ 0 & : |E| > D \end{cases} \quad (191)$$

with $r \geq 0$.

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

For the isotropic case $J_{\perp} = J_z = J$, 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 discussed in the lecture.

5.7.6 RG approach for the Sine-Gordon model

The Sine-Gordon-Model is a well-known model of mathematical physics with applications from high-energy physics, non-linear physics to condensed matter physics (Josephson junction arrays, disordered quantum wires with electron interactions, ...). We here perform the RG analysis for the Sine-Gordon action:

$$S[\phi] = \int_0^L dx \int_0^{\beta} d\tau \left(\frac{-1}{2\pi K u} \phi \nabla^2 \phi + \frac{2g}{(2\pi\xi)^2} \cos(\sqrt{8}\phi) \right), \quad (192)$$

where $\phi(x, \tau)$ is a real dimensionless bosonic field; $\nabla^2 = u^2 \partial_x^2 + \partial_{\tau}^2$ with u being a velocity; ξ is the UV scale in the real space; $K > 0$ is a dimensionless parameter which reflects compressibility of the underlying quantum liquid and $g \geq 0$ is the interaction. We will study an infinite sample at zero temperature: $L \rightarrow \infty$; $\beta = 1/T \rightarrow \infty$.

1. Re-scale x such that we get an isotropic derivative, $\nabla^2 = \partial_x^2 + \partial_\tau^2$. Rewrite the action Eq. (192) in Fourier-space. Impose a sharp UV-cutoff Λ on the (1+1)-momentum \mathbf{k} .
2. In order to renormalize g , split the field ϕ into a “smaller” part $\phi^<$ with $|\mathbf{k}| \leq \Lambda(l) \equiv \Lambda e^{-l}$ and the remaining “larger” part $\phi^>$. Expand the mixing term to order $\mathcal{O}(g)$, integrate out the fast modes, and do the re-scaling step. You should obtain the flow equation

$$\partial_l g(l) = 2g(l) [1 - K(l)]. \quad (193)$$

Hint: You should use the identity $\cos y = (e^{+iy} + e^{-iy})/2$ and the complex Gaussian integral

$$\int \prod_{i=1}^N d[Re\phi_i] d[Im\phi_i] \exp \left[-\phi_i^* [A]_{ij} \phi_j + b_i^* \phi_i + \phi_i^* c_i \right] = \frac{\pi^N}{\det A} \exp \left[b_i^* [A^{-1}]_{ij} c_j \right]. \quad (194)$$

3. Renormalization of K is given by terms of order $\mathcal{O}(g^2)$ which you don't have to compute. You can use

$$\partial_l [K^{-1}] = g^2 K(l) C, \quad (195)$$

where $C > 0$ is a constant. Sketch and analyze the RG flow diagram in the $K > 0, g \geq 0$ plane. Where are the stable and unstable fixed points (fixed lines)? For $g > 0$, what is the condition for the initial parameters (g, K) to avoid a run-away flow? Hint: Find an invariant of the flow equation.

6 Functional RG

Goals:

- implement RG idea in a formally exact way, on the level of imaginary time correlation functions
- functional RG (fRG) keeps track of momentum- and frequency-dependence
- get quantitative results beyond critical exponents and "∼" sign, but requires (super-)computers

6.1 Functional methods

Partition function and conventions

- Assume partition function \mathcal{Z} can be written as unconstrained functional integral.

$$\mathcal{Z} = \int \mathcal{D}[\Phi] \exp[-\underbrace{(S_0[\Phi] + S_1[\Phi])}_{S[\Phi]}] \quad (196)$$

- Treat classical and quantum systems, fermionic and bosonic particles in *one* formalism: Superfield $\Phi = (\Phi_{\alpha_1}, \Phi_{\alpha_2}, \dots)$ with (anti-)commutation properties encoded by $\Phi_{\alpha_1} \Phi_{\alpha_2} = \zeta \Phi_{\alpha_2} \Phi_{\alpha_1}$.
- Gaussian part in (anti-)symmetrized notation:

$$S_0[\Phi] = -\frac{1}{2} \int_{\alpha} \int_{\alpha'} \Phi_{\alpha} [\mathbf{G}_0^{-1}]_{\alpha\alpha'} \Phi_{\alpha'} \equiv -\frac{1}{2} (\Phi, \mathbf{G}_0^{-1} \Phi) \quad (197)$$

Product is defined as $(\Phi, \Psi) \equiv \int_{\alpha} \Phi_{\alpha} \Psi_{\alpha}$. Statistics is encoded in $\zeta = \pm 1$ for bosons/fermions. We assume properly (anti-)symmetrized \mathbf{G}_0 , i.e. in each sector

$$\zeta \mathbf{G}_0 = \mathbf{G}_0^T \quad (198)$$

- Examples: (recall $\frac{1}{\beta V} \sum_{\omega, \mathbf{k}} \rightarrow \int \frac{d\omega}{2\pi} \int \frac{d\mathbf{k}}{(2\pi)^D} \equiv \int_{\omega} \int_{\mathbf{k}}$)

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

$$S_0[\varphi] = \frac{1}{2} \int_{\mathbf{k}} [r_0 + c_0 k^2] \varphi_{-\mathbf{k}} \varphi_{+\mathbf{k}} \quad (199)$$

leads to

$$[\mathbf{G}_0^{-1}]_{\mathbf{k}\mathbf{k}'} = -(2\pi)^D \delta^D(\mathbf{k} + \mathbf{k}') [r_0 + c_0 k^2] \quad (200)$$

2. Spinless fermions: Need two types of fields, $\{\Phi_{\alpha}\} \rightarrow \{\psi_{i\omega, \mathbf{k}}, \bar{\psi}_{i\omega, \mathbf{k}}\}$, $\zeta = -1$, abbreviate $K \equiv (i\omega, \mathbf{k})$,

$$\int_{\omega} \int_{\mathbf{k}} \equiv \int_K$$

Now $\alpha = (\psi, K)$ or $(\bar{\psi}, K)$.

Recall that Fourier-transform of (independent!) Grassmann fields $\bar{\psi}$ and ψ are oppositely defined:

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

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

Green functions and generating functionals

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

$$G_{\alpha_1 \dots \alpha_n}^{(n)} = \frac{\int \mathcal{D}[\Phi] e^{-S[\Phi]} \Phi_{\alpha_n} \dots \Phi_{\alpha_1}}{\int \mathcal{D}[\Phi] e^{-S[\Phi]}} = \langle \Phi_{\alpha_n} \dots \Phi_{\alpha_1} \rangle \quad (201)$$

- Sourcefield trick: Want to write generating functional

$$G_{\alpha_1 \dots \alpha_n}^{(n)} = \frac{\delta^n \mathcal{G}[J]}{\delta J_{\alpha_n} \dots \delta J_{\alpha_1}} \Big|_{J=0} \quad (202)$$

This is achieved by introducing sourcefields J :

$$\mathcal{G}[J] \equiv \frac{\int \mathcal{D}[\Phi] e^{-S[\Phi] + (J, \Phi)}}{\underbrace{\int \mathcal{D}[\Phi] e^{-S[\Phi]}}_{\mathcal{Z}}} \quad (203)$$

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 .
- $G_{\alpha_1 \dots \alpha_n}^{(n)}$ are fully (anti-)symmetric under index exchange.
- The $G_{\alpha_1 \dots \alpha_n}^{(n)}$ can be seen as the expansion coefficients of $\mathcal{G}[J]$ (now the index-ordering matches!)

$$\mathcal{G}[J] = \sum_{n=0}^{\infty} \frac{1}{n!} \int_{\alpha_1 \dots \alpha_n} G_{\alpha_1 \dots \alpha_n}^{(n)} J_{\alpha_1} \dots J_{\alpha_n} \quad (204)$$

- *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]

$$\begin{aligned} \mathcal{G}_c[J] &= \ln \left(\frac{\mathcal{Z}}{\mathcal{Z}_0} \mathcal{G}[J] \right) = \ln \left(\frac{\int \mathcal{D}[\Phi] e^{-S[\Phi] + (J, \Phi)}}{\int \mathcal{D}[\Phi] e^{-S_0[\Phi]}} \right) = \sum_{n=0}^{\infty} \frac{1}{n!} \int_{\alpha_1 \dots \alpha_n} G_{c, \alpha_1 \dots \alpha_n}^{(n)} J_{\alpha_1} \dots J_{\alpha_n} \quad (205) \\ G_{c, \alpha_1 \dots \alpha_n}^{(n)} &= \frac{\delta^n \mathcal{G}_c[J]}{\delta J_{\alpha_n} \dots \delta J_{\alpha_1}} \Big|_{J=0} \end{aligned}$$

- Example: Relation between connected and disconnected GFs

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

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

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

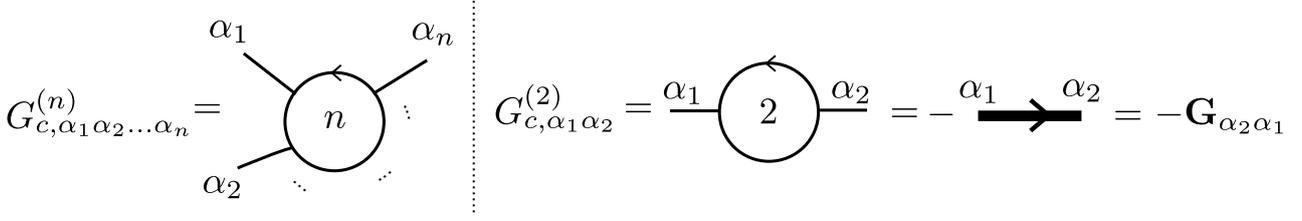


Figure 13: Graphical representation of the connected Green function (left) and its two-point version also called the propagator (right).

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

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

$$e^{\mathcal{G}_{0c}[J]} = \frac{\int \mathcal{D}[\Phi] e^{-\frac{1}{2}(\Phi, \mathbf{G}_0^{-1}\Phi) + (J, \Phi)}}{\int \mathcal{D}[\Phi] e^{-S_0[\Phi]}} \quad (206)$$

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

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

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

$$\mathcal{G}_{0c}[J] = -\frac{1}{2}(J, \mathbf{G}_0^T J) = -\frac{1}{2} \int_{\alpha} \int_{\alpha'} [\mathbf{G}_0]_{\alpha\alpha'} J_{\alpha'} J_{\alpha} \quad (207)$$

so that

$$\boxed{G_{0c, \alpha'\alpha}^{(2)} = \langle \Phi_{\alpha} \Phi_{\alpha'} \rangle_0 = \frac{\delta^2 \mathcal{G}_{0c}[J]}{\delta J_{\alpha} \delta J_{\alpha'}} \Big|_{J=0} \stackrel{(207)}{=} -[\mathbf{G}_0]_{\alpha\alpha'}} \quad (208)$$

- Definition: Differential operator to generate matrix in superfield space

$$\left[\frac{\delta}{\delta J} \otimes \frac{\delta}{\delta J} \right]_{\alpha\alpha'} \equiv \frac{\delta^2}{\delta J_{\alpha} \delta J_{\alpha'}} \quad (209)$$

so that from above

$$\mathbf{G}_0 = - \left(\frac{\delta}{\delta J} \otimes \frac{\delta}{\delta J} \right) \mathcal{G}_{0c}[J] \Big|_{J=0} \quad (210)$$

Propagator and self-energy

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

$$\mathbf{G} \equiv - \left(\frac{\delta}{\delta J} \otimes \frac{\delta}{\delta J} \right) \mathcal{G}_c[J] \Big|_{J=0} \quad (211)$$

and we read off (see right part of Fig. 13)

$$G_{c, \alpha\alpha'}^{(2)} = \langle \Phi_{\alpha'} \Phi_{\alpha} \rangle = -\mathbf{G}_{\alpha'\alpha} \quad (212)$$

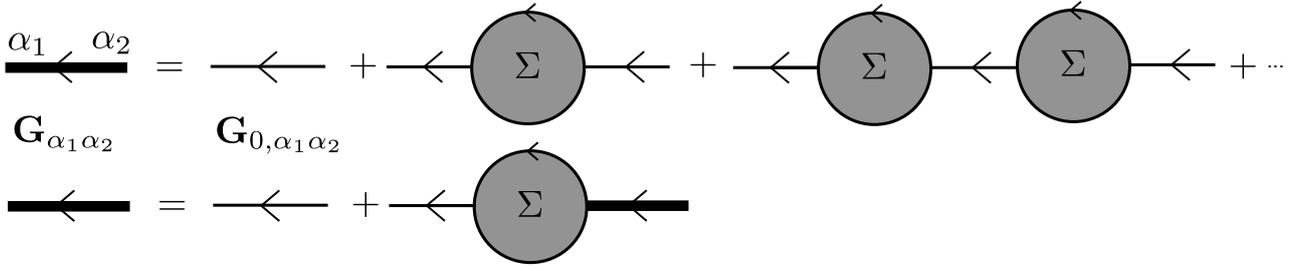


Figure 14: Graphical representation of the Dyson equation.

- The *self-energy* defined as difference between Greens function and Gaussian Greens function,

$$\boxed{\mathbf{G}^{-1} = \mathbf{G}_0^{-1} - \Sigma} \quad (213)$$

and it follows Dyson's equation:

$$\begin{aligned} \mathbf{G} &= \mathbf{G}_0 + \mathbf{G}_0 \Sigma \mathbf{G}_0 + \mathbf{G}_0 \Sigma \mathbf{G}_0 \Sigma \mathbf{G}_0 + \dots \\ &= \mathbf{G}_0 + \mathbf{G}_0 \Sigma \mathbf{G} \end{aligned} \quad (214)$$

With \mathbf{G}_0 represented by a thin line, we have the graphical representation in Fig. 14.

Alternative representation of $\mathcal{G}_c[J]$ (without $\int \mathcal{D}[\Phi] \dots$)

- We use

$$(\Phi_\alpha)^n e^{(J, \Phi)} = \left(\frac{\delta}{\delta J_\alpha} \right)^n e^{(J, \Phi)} \quad (215)$$

to write

$$e^{-S_1[\Phi] + (J, \Phi)} = e^{-S_1[\frac{\delta}{\delta J}] + (J, \Phi)} \quad (216)$$

- Use this in definition of $\mathcal{G}_c[J]$, Eq. (205), and pull out $S_1[\frac{\delta}{\delta J}]$ from the integral

$$e^{\mathcal{G}_c[J]} \equiv \frac{\int \mathcal{D}[\Phi] e^{-S[\Phi] + (J, \Phi)}}{\int \mathcal{D}[\Phi] e^{-S_0[\Phi]}} = e^{-S_1[\frac{\delta}{\delta J}]} \frac{\int \mathcal{D}[\Phi] e^{-S_0[\Phi] + (J, \Phi)}}{\int \mathcal{D}[\Phi] e^{-S_0[\Phi]}} = e^{-S_1[\frac{\delta}{\delta J}]} e^{\mathcal{G}_{0c}[J]} \quad (217)$$

Use Eq. (207) to conclude:

$$\boxed{e^{\mathcal{G}_c[J]} = e^{-S_1[\frac{\delta}{\delta J}] - \frac{1}{2}(J, \mathbf{G}_0^T J)}} \quad (218)$$

Amputated connected Green function

- Motivation: Later, want to start fRG-flow from $\mathbf{G}_0^{\Lambda=\infty} = 0$, but from (218) have then

$$\mathcal{G}_c(\mathbf{G}_0 = 0) = 0 \quad (219)$$

- 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):

$$\mathcal{G}_{ac}[\bar{\Phi}] = \ln \left(\frac{\int \mathcal{D}[\Phi] e^{-S_0[\Phi] - S_1[\Phi + \bar{\Phi}]}}{\mathcal{Z}_0} \right) = \sum_{n=0}^{\infty} \frac{1}{n!} \int_{\alpha_1 \dots \alpha_n} G_{ac, \alpha_1 \dots \alpha_n}^{(n)} \bar{\Phi}_{\alpha_1} \dots \bar{\Phi}_{\alpha_n} \quad (220)$$

$$G_{ac, \alpha_1 \dots \alpha_n}^{(n)} = \frac{\delta^n \mathcal{G}_{ac}[\bar{\Phi}]}{\delta \bar{\Phi}_{\alpha_n} \dots \delta \bar{\Phi}_{\alpha_1}} \Big|_{\bar{\Phi}=0} \quad (221)$$

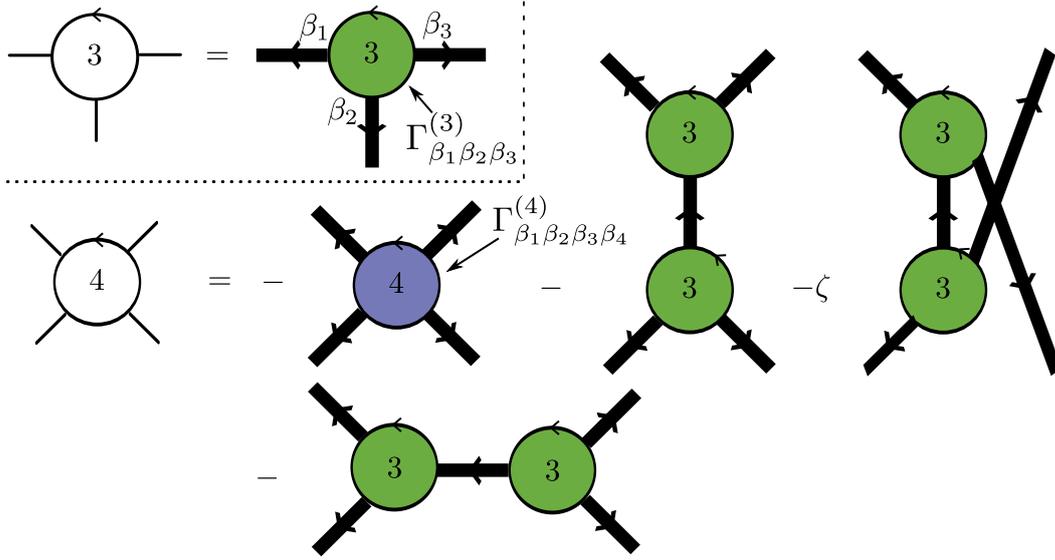


Figure 15: Tree expansion for the three- and four-point connected Green functions.

- Relation between $\mathcal{G}_{ac}[\bar{\Phi}]$ and $\mathcal{G}_c[J]$: Use shift of variable in Eq. (220), $\Phi' = \Phi + \bar{\Phi}$,

$$\mathcal{G}_{ac}[\bar{\Phi}] = \mathcal{G}_c\left[-\left(\mathbf{G}_0^T\right)^{-1}\bar{\Phi}\right] + \frac{1}{2}\left(\bar{\Phi}, \mathbf{G}_0^{-1}\bar{\Phi}\right) \quad (222)$$

Remarks:

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

$$e^{\mathcal{G}_{ac}[\bar{\Phi}]} = e^{-\frac{1}{2}\left(\frac{\delta}{\delta\bar{\Phi}}, \mathbf{G}_0^T \frac{\delta}{\delta\bar{\Phi}}\right)} e^{-\mathcal{S}_1[\bar{\Phi}]} \quad (223)$$

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 (214) for G where essential block Σ was called self-energy.
- Anticipate similar structure for $G_c^{(n)}$ for $n > 2$.
Define irreducible vertex $\Gamma_{\alpha_1\alpha_2\dots\alpha_n}^{(m)}$ (filled circle) as the part of the diagrams for $G_c^{(n)}$ ($n \geq m$) which cannot be separated by cutting a propagator line $G_c^{(2)}$.
The irreducible vertex can be understood as the true interaction between particles.
This leads to the *tree-expansion*. Tree diagrams are diagrams without loops.
- Final goal: Write fRG flow equations on the basis of $\Gamma_{\alpha_1\alpha_2\dots\alpha_n}^{(n)} \rightarrow \Gamma_{\alpha_1\alpha_2\dots\alpha_n}^{(n),\Lambda}$.
- Next goal: Find expression for generating functional $\Gamma[\bar{\Phi}]$ for $\Gamma_{\alpha_1\alpha_2\dots\alpha_n}^{(n)}$ such that

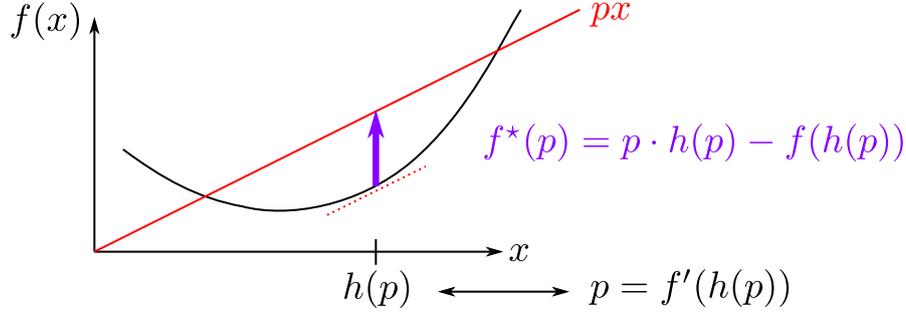
$$\Gamma_{\alpha_1\dots\alpha_n}^{(n)} = \frac{\delta^n \Gamma[\bar{\Phi}]}{\delta\bar{\Phi}_{\alpha_n}\dots\delta\bar{\Phi}_{\alpha_1}} \Big|_{\bar{\Phi}=0} \Leftrightarrow \Gamma[\bar{\Phi}] = \sum_{n=0}^{\infty} \frac{1}{n!} \int_{\alpha_1\dots\alpha_n} \Gamma_{\alpha_1\dots\alpha_n}^{(n)} \bar{\Phi}_{\alpha_1}\dots\bar{\Phi}_{\alpha_n} \quad (224)$$

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

$$f^*(p) \equiv p \cdot h(p) - f(h(p)) \quad (225)$$

$$p = f'(h(p)) \quad (226)$$

and it follows $(f^*)'(p) = h(p) = (f')^{-1}(p)$, i.e. the derivatives of f and f^* are inverse to each other. To find $f^*(p)$ graphically, 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 $f^*(p)$.



- Legendre transform in thermodynamics (different sign-convention):

Relate internal energy U which depends on entropy S , volume V , particle number N (*extensive* variables)

$$U = U(S, V, N) \quad (227)$$

$$dU \equiv TdS - pdV + \mu dN \quad (228)$$

to free energy F which depends on temperature T (*intensive* variable, “slope” of U with respect to S)

$$F \equiv -TS + U \quad (229)$$

$$dF = -TdS - SdT + dU = -SdT - pdV + \mu dN \quad (230)$$

Need to replace all S in F by inverting $T = dU(S, V, N)/dS$.

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

$$\Gamma[\bar{\Phi}] = \underbrace{(J[\bar{\Phi}], \bar{\Phi}) - \mathcal{G}_c[J[\bar{\Phi}])}_{\equiv \mathcal{L}[\bar{\Phi}]} - S_0[\bar{\Phi}] \quad (231)$$

$$\bar{\Phi}_\alpha \equiv \frac{\delta \mathcal{G}_c[J]}{\delta J_\alpha} \quad (232)$$

Remarks:

- Contribution $S_0[\bar{\Phi}] \sim \bar{\Phi}^2$ in Eq. (231) is a convenience convention that “shifts” only $\Gamma_{\alpha_1 \alpha_2}^{(2)}$.
- In Eq. (231), replace all sources J by the inverted relation Eq. (232). Note that $\bar{\Phi}_\alpha = \langle \Phi_\alpha \rangle|_J$ with *non-vanishing* sources.
- From now on, assume there is no spontaneous symmetry breaking, i.e. as $J \rightarrow 0$ one has $\bar{\Phi}_\alpha = \langle \Phi_\alpha \rangle|_{J \rightarrow 0} = 0$. This can be lifted, using $\bar{\Phi} = \delta \bar{\Phi} + \bar{\Phi}^0$, see [Kopietz].

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

- Express J in terms of $\bar{\Phi}$: We have

$$\frac{\delta \mathcal{L}[\bar{\Phi}]}{\delta \bar{\Phi}_\alpha} = \frac{\delta (J, \bar{\Phi}) - \delta \mathcal{G}_c[J]}{\delta \bar{\Phi}_\alpha} = \zeta_\alpha J_\alpha + \left(\frac{\delta J}{\delta \bar{\Phi}_\alpha}, \bar{\Phi} \right) - \int_{\alpha'} \frac{\delta J_{\alpha'}}{\delta \bar{\Phi}_\alpha} \underbrace{\frac{\delta \mathcal{G}_c[J]}{\delta J_{\alpha'}}}_{\bar{\Phi}_{\alpha'}} = \zeta_\alpha J_\alpha \quad (233)$$

or

$$J_\alpha = \zeta_\alpha \frac{\delta \mathcal{L}[\bar{\Phi}]}{\delta \bar{\Phi}_\alpha} \quad (234)$$

2. Chain-rule: Applying the chain-rule and using (1.), we get

$$\frac{\delta}{\delta \bar{\Phi}_\alpha} = \int_{\alpha'} \left[\frac{\delta J_{\alpha'}}{\delta \bar{\Phi}_\alpha} \right] \frac{\delta}{\delta J_{\alpha'}} \stackrel{(1.)}{=} \int_{\alpha'} \left[\frac{\delta^2 \mathcal{L}[\bar{\Phi}]}{\delta \bar{\Phi}_\alpha \delta \bar{\Phi}_{\alpha'}} \zeta_{\alpha'} \right] \frac{\delta}{\delta J_{\alpha'}} \quad (235)$$

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

$$\frac{\delta}{\delta \bar{\Phi}} = \left(\left[\frac{\delta}{\delta \bar{\Phi}} \otimes \frac{\delta}{\delta \bar{\Phi}} \right] \mathcal{L}[\bar{\Phi}] \right) \mathbf{Z} \frac{\delta}{\delta J} \quad (236)$$

3. Use chain rule for $\frac{\delta}{\delta \bar{\Phi}}$ on $\bar{\Phi} \equiv \frac{\delta \mathcal{G}_c[J]}{\delta J}$ (Eq. 232):

$$\mathbf{1} = \frac{\delta}{\delta \bar{\Phi}} \bar{\Phi} \stackrel{(232)}{=} \frac{\delta}{\delta \bar{\Phi}} \frac{\delta \mathcal{G}_c[J]}{\delta J} \stackrel{(2.)}{=} \left(\left[\frac{\delta}{\delta \bar{\Phi}} \otimes \frac{\delta}{\delta \bar{\Phi}} \right] \mathcal{L}[\bar{\Phi}] \right) \mathbf{Z} \left(\left[\frac{\delta}{\delta J} \otimes \frac{\delta}{\delta J} \right] \mathcal{G}_c[J] \right) \quad (237)$$

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

$$\boxed{\left[\frac{\delta}{\delta J} \otimes \frac{\delta}{\delta J} \right] \mathcal{G}_c[J] = \mathbf{Z} \left(\left[\frac{\delta}{\delta \bar{\Phi}} \otimes \frac{\delta}{\delta \bar{\Phi}} \right] \mathcal{L}[\bar{\Phi}] \right)^{-1}} \quad (238)$$

Tree expansion

- In identity (238) above, expand both sides in powers of J_α and compare coefficients. For the r.h.s. we 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 $\Gamma_{\alpha\alpha'}^{(2)}$: Use

$$\left(\frac{\delta}{\delta J_\alpha} \otimes \frac{\delta}{\delta J_{\alpha'}} \right) \mathcal{G}_c[J] |_{J=0} \equiv -\mathbf{G}_{\alpha\alpha'} = G_{c,\alpha'\alpha}^{(2)} \quad (239)$$

and get ($J \rightarrow 0$ yields $\bar{\Phi} \rightarrow 0$)

$$-\mathbf{Z}\mathbf{G}^{-1} = \left[\frac{\delta}{\delta \bar{\Phi}} \otimes \frac{\delta}{\delta \bar{\Phi}} \right] \mathcal{L}[\bar{\Phi}] |_{\bar{\Phi}=0} = \left[\frac{\delta}{\delta \bar{\Phi}} \otimes \frac{\delta}{\delta \bar{\Phi}} \right] \left(\Gamma[\bar{\Phi}] + S_0[\bar{\Phi}] \right) |_{\bar{\Phi}=0} = \left[\frac{\delta}{\delta \bar{\Phi}} \otimes \frac{\delta}{\delta \bar{\Phi}} \right] \Gamma[\bar{\Phi}] |_{\bar{\Phi}=0} - \left[\mathbf{G}_0^\Gamma \right]^{-1} \quad (240)$$

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

$$\left[\frac{\delta}{\delta \bar{\Phi}} \otimes \frac{\delta}{\delta \bar{\Phi}} \right] \Gamma[\bar{\Phi}] |_{\bar{\Phi}=0} = -\left[\mathbf{G}^\Gamma \right]^{-1} + \left[\mathbf{G}_0^\Gamma \right]^{-1} = \Sigma^\Gamma \quad (241)$$

and taking matrix elements

$$\Gamma_{\alpha_1\alpha_2}^{(2)} = [\Sigma]_{\alpha_1\alpha_2} \quad (242)$$

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

$$\mathbf{U}[\bar{\Phi}] \equiv \left(\left[\frac{\delta}{\delta \bar{\Phi}} \otimes \frac{\delta}{\delta \bar{\Phi}} \right] \Gamma[\bar{\Phi}] \right)^\Gamma - \underbrace{\left(\left[\frac{\delta}{\delta \bar{\Phi}} \otimes \frac{\delta}{\delta \bar{\Phi}} \right] \Gamma[\bar{\Phi}] |_{\bar{\Phi}=0} \right)^\Gamma}_{\Sigma} = \sum_{n=1}^{\infty} \frac{1}{n!} \int_{\alpha_1 \dots \alpha_n} \left[\Gamma_{\alpha_1 \dots \alpha_n}^{(n+2)} \right] \bar{\Phi}_{\alpha_1} \dots \bar{\Phi}_{\alpha_n} \quad (243)$$

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

$$\frac{\delta}{\delta \bar{\Phi}} \otimes \frac{\delta}{\delta \bar{\Phi}} \mathcal{L}[\bar{\Phi}] = \frac{\delta}{\delta \bar{\Phi}} \otimes \frac{\delta}{\delta \bar{\Phi}} \Gamma[\bar{\Phi}] - \left[\mathbf{G}_0^\Gamma \right]^{-1} = \mathbf{U}^\Gamma[\bar{\Phi}] + \Sigma^\Gamma - \left[\mathbf{G}_0^\Gamma \right]^{-1} = \mathbf{U}^\Gamma[\bar{\Phi}] - \left[\mathbf{G}^\Gamma \right]^{-1} \quad (244)$$

- In order to connect to Eq. (238), we need to expand the inverse of the above

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

- Expand left (in J 's) and right (in $\bar{\Phi}$'s). Use definitions $[\mathbf{G}_{c,\alpha_1 \dots \alpha_n}^{(n+2)}]_{\alpha\alpha'} \equiv G_{c,\alpha\alpha'\alpha_1 \dots \alpha_n}^{(n+2)}$ (for lhs) and $[\mathbf{\Gamma}_{\alpha_1 \dots \alpha_n}^{(n+2)}]_{\alpha\alpha'} \equiv \Gamma_{\alpha\alpha'\alpha_1 \dots \alpha_n}^{(n+2)}$ (for expansion of $\mathbf{U}[\bar{\Phi}]$ rhs). Take the transpose of the matrix structure.

$$\begin{aligned} \sum_{n=0}^{\infty} \frac{1}{n!} \int_{\alpha_1} \dots \int_{\alpha_n} \mathbf{G}_{c,\alpha_1 \dots \alpha_n}^{(n+2)} J_{\alpha_1} \dots J_{\alpha_n} &= - \sum_{\nu=0}^{\infty} \sum_{n_1=1}^{\infty} \dots \sum_{n_\nu=1}^{\infty} \frac{1}{n_1! \dots n_\nu!} \int_{\beta_1^1} \dots \int_{\beta_{n_1}^1} \dots \int_{\beta_{n_\nu}^\nu} \dots \int_{\beta_{n_\nu}^\nu} \quad (245) \\ &\times \underbrace{\mathbf{G}(\mathbf{\Gamma}_{\beta_1^\nu \dots \beta_{n_\nu}^\nu}^{(n_\nu+2)}) \dots \mathbf{G}(\mathbf{\Gamma}_{\beta_1^1 \dots \beta_{n_1}^1}^{(n_1+2)})}_{\times \nu} \mathbf{G} \mathbf{Z} \bar{\Phi}_{\beta_1^1} \dots \bar{\Phi}_{\beta_{n_1}^1} \dots \bar{\Phi}_{\beta_{n_\nu}^\nu} \dots \bar{\Phi}_{\beta_{n_\nu}^\nu} \end{aligned}$$

- For final comparison of J -coefficients, we still need to trade $\bar{\Phi}$ for J :

$$\bar{\Phi}_\beta = \frac{\delta \mathcal{G}_c[J]}{\delta J_\beta} = \sum_{n=0}^{\infty} \frac{1}{n!} \int_{\alpha_1} \dots \int_{\alpha_n} G_{c,\beta\alpha_1 \dots \alpha_n}^{(n+1)} J_{\alpha_1} \dots J_{\alpha_n} \quad (246)$$

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

- Symmetrization:

- Assume that $G_{c,\alpha_1 \dots \alpha_n}^{(n)}$ (on lhs) and $\Gamma_{\alpha_1 \dots \alpha_n}^{(n)}$ are symmetrized with respect to label exchange. Need to symmetrize rhs.

- Symmetrization operator \mathcal{S} :

Consider function $F_{\alpha_1 \dots \alpha_n}$ of n superlabels $\alpha_1 \dots \alpha_{n_1} | \alpha_{n_1+1} \dots \alpha_{n_1+n_2} | \alpha_{n_1+n_2+1} \dots \alpha_n$, grouped into ν groups, $n_1 + n_2 \dots + n_\nu = n$ such that $F_{\alpha_1 \dots \alpha_n}$ is already properly symmetrized for exchange of labels inside groups.

We get a fully symmetric function from

$$\mathcal{S}_{\alpha_1 \dots \alpha_{n_1}; \dots; \alpha_{n-n_\nu+1} \dots \alpha_n} (F_{\alpha_1 \dots \alpha_n}) = \frac{1}{n_1! \dots n_\nu!} \sum_{P \in S_n} \text{sgn}_\xi(P) F_{\alpha_{P(1)} \dots \alpha_{P(n)}} \rightarrow n! / (n_1! \dots n_\nu!) \text{ distinct terms} \quad (247)$$

with

$$\bar{\Phi}_{\alpha_1} \dots \bar{\Phi}_{\alpha_n} = \text{sgn}_\xi(P) \bar{\Phi}_{\alpha_{P(1)}} \dots \bar{\Phi}_{\alpha_{P(n)}}. \quad (248)$$

Example:

If $F_{\alpha_1 \alpha_2}$ is not yet symmetrized, we have $\nu = 2$ blocks with $n_{1,2} = 1$ and $\mathcal{S}_{\alpha_1; \alpha_2} (F_{\alpha_1 \alpha_2}) = F_{\alpha_1 \alpha_2} + \text{sgn}_\xi F_{\alpha_2 \alpha_1}$.

If $F_{\alpha_1 \alpha_2}$ is already symmetrized, we have $\nu = 1$ block with $n_1 = 2$ and then $\mathcal{S}_{\alpha_1 \alpha_2} (F_{\alpha_1 \alpha_2}) = F_{\alpha_1 \alpha_2}$.

- Full expression for $\mathbf{G}_{c,\alpha_1 \dots \alpha_n}^{(n+2)}$ including \mathcal{S} : Ex. (6.5.2).

Examples

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

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

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

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

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

$$\boxed{G_{c,\alpha_1\alpha_2\alpha_3}^{(3)} = \int_{\beta_1,\beta_2,\beta_3} [\mathbf{G}]_{\alpha_1\beta_1} [\mathbf{G}]_{\alpha_2\beta_2} [\mathbf{G}]_{\alpha_3\beta_3} \Gamma_{\beta_1\beta_2\beta_3}^{(3)}} \quad (249)$$

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

$$\mathbf{G}_{c,\alpha_1\alpha_2}^{(4)} = -\frac{1}{2} \int_{\beta_{1,2}} \mathbf{G} \Gamma_{\beta_1\beta_2}^{(4)} \mathbf{G} \cdot \mathbf{Z} \mathcal{S}_{\alpha_1;\alpha_2} \left[G_{c,\beta_1\alpha_1}^{(2)} G_{c,\beta_2\alpha_2}^{(2)} \right] \quad (250)$$

and we insert the matrix structure

$$G_{c,\alpha_3\alpha_4\alpha_1\alpha_2}^{(4)} = -\frac{1}{2} \int_{\beta_{1,2}} [\mathbf{G}]_{\alpha_3\beta_3} \Gamma_{\beta_3\beta_4\beta_1\beta_2}^{(4)} [\mathbf{G}]_{\alpha_4\beta_4} \left[G_{c,\beta_1\alpha_1}^{(2)} G_{c,\beta_2\alpha_2}^{(2)} + \zeta G_{c,\beta_1\alpha_2}^{(2)} G_{c,\beta_2\alpha_1}^{(2)} \right] \quad (251)$$

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 $G_{c,\beta\alpha}^{(2)} = -\mathbf{G}_{\alpha\beta}$ and some ζ -independent index shuffles

$$\boxed{G_{c,\alpha_1\alpha_2\alpha_3\alpha_4}^{(4)} = -\int_{\beta_{1,2,3,4}} [\mathbf{G}]_{\alpha_1\beta_1} [\mathbf{G}]_{\alpha_2\beta_2} [\mathbf{G}]_{\alpha_3\beta_3} [\mathbf{G}]_{\alpha_4\beta_4} \Gamma_{\beta_1\beta_2\beta_3\beta_4}^{(4)}} \quad (252)$$

This reproduces the term with the blue circle in Fig. 15. The general case for $G_c^{(4)}$ including the three-point vertices $\Gamma^{(3)}$ is treated in Ex. 6.5.2.

6.2 Exact fRG flow equations for generating functionals

Cutoff procedure

- Idea: Modify the Gaussian propagator:

$$\begin{aligned}
\mathbf{G}_0 &\rightarrow \mathbf{G}_{0,\Lambda} \\
S_0[\Phi] &\rightarrow S_{0,\Lambda}[\Phi] = -\frac{1}{2} \left(\Phi, [\mathbf{G}_{0,\Lambda}]^{-1} \Phi \right)
\end{aligned}$$

- Requirements:

For vanishing cutoff ($\Lambda = 0$), we recover the original theory.

For infinite cutoff, particles do not 'move' and all generating functional are simply known.

$$\mathbf{G}_{0,\Lambda} = \begin{cases} \mathbf{G}_0 & (\Lambda \rightarrow 0) \\ 0 & (\Lambda \rightarrow \infty) \end{cases} \quad (253)$$

- Strategy / workflow:

- Derive exact hierarchy of differential equations for generating functionals $\mathcal{G}_\Lambda[J]$ etc. when Λ is varied (fRG flow equations).
- Find initial conditions for generating functionals at $\Lambda = \infty$
- Close or truncate the hierarchy of flow equations and solve them (numerically).
- Extract physical results at $\Lambda = 0$

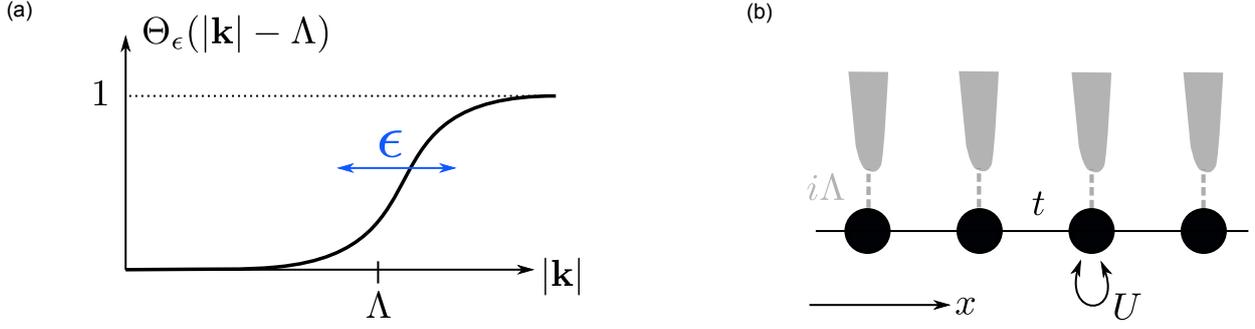


Figure 16: (a) Multiplicative cutoff in momentum space. (b) Sketch of a reservoir cutoff which is diagonal in real space.

Cutoff types and examples

- Multiplicative cutoff: $\mathbf{G}_{0,\Lambda} \equiv \Theta_\Lambda \mathbf{G}_0$ with $\Theta_{\Lambda=0} = \mathbf{1}$ and $\Theta_{\Lambda=\infty} = \mathbf{0}$.
- 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 $\Theta_\Lambda = \theta_\epsilon(|\mathbf{k}| - \Lambda)$ which is a step function broadened on a scale ϵ . As Λ lowers, this switches on smaller and smaller momentum modes iteratively, see Fig. 16(a).
 - For quantum systems, cutoff can switch off small Matsubara frequencies: $\Theta_\Lambda = \theta(|i\omega_n| - \Lambda)$. This works also for \mathbf{G}_0 that are not momentum diagonal.
 - Reservoir cutoff: $\mathbf{R}_\Lambda = i\Lambda$, $\mathbf{G}_{0,\Lambda} = \frac{1}{i\omega - H + i\text{sgn}(\omega_n)\Lambda}$, couples a virtual reservoir to the system which is removed as $\Lambda \rightarrow 0$. See Fig. 16(b).
 - If \mathbf{G}_0 involves several field-types, one can chose different cutoffs for fermions and bosons.
 - Non-RG type cutoffs: $\Theta_\Lambda = e^{-\Lambda}$, effectively switches on interaction strength. One can also design cutoffs that let the chemical potential or the temperature flow. The benefit is that each point along the flow corresponds to a physical system.
- *Morris-Lemma*: If we work with sharp cutoffs, we encounter the ambiguous expression $\delta(x) f(\theta(x))$. This is to be interpreted as:

$$\delta(x) f(\theta(x)) = \delta(x) \int_0^1 dt f(t) \quad (254)$$

Proof: We regularize $\theta(x)$ and $\delta(x)$ by their smooth counterparts $\partial_x \theta_\epsilon(x) = \delta_\epsilon(x)$.

$$\begin{aligned} \delta(x) f(\theta(x)) &\rightarrow \lim_{\epsilon \rightarrow 0} \delta_\epsilon(x) f(\theta_\epsilon(x)) \\ &= \lim_{\epsilon \rightarrow 0} \left[\frac{d\theta_\epsilon(x)}{dx} \right] \frac{d}{d\theta_\epsilon(x)} \int_0^{\theta_\epsilon(x)} dt f(t) \\ &= \lim_{\epsilon \rightarrow 0} \frac{d}{dx} \int_0^{\theta_\epsilon(x)} dt f(t) \\ &= \frac{d}{dx} \lim_{\epsilon \rightarrow 0} \int_0^{\theta_\epsilon(x)} dt f(t) \\ &= \frac{d}{dx} \theta(x) \int_0^1 dt f(t) \\ &= \delta(x) \int_0^1 dt f(t) \end{aligned}$$

Application: $\delta(x) \theta(x) = \delta(x) \frac{1}{2}$ which amounts to setting $\theta(x=0) = 1/2$.

Flow of $\mathcal{G}_\Lambda [J]$ (disconnected Green functions)

- The cutoff dependence of all generating functionals arises only from $\mathbf{G}_{0,\Lambda}$.
- Λ -dependence of generating functional for disconnected Green functions \mathcal{G} :

$$\begin{aligned}\mathcal{G}_\Lambda [J] &= \frac{1}{\mathcal{Z}_\Lambda} \int \mathcal{D}[\Phi] e^{-S_{0,\Lambda}[\Phi] - S_1[\Phi] + (J,\Phi)} \\ \mathcal{Z}_\Lambda &= \int \mathcal{D}[\Phi] e^{-S_{0,\Lambda}[\Phi] - S_1[\Phi]}\end{aligned}$$

We differentiate with respect to Λ :

$$\begin{aligned}\partial_\Lambda \mathcal{G}_\Lambda [J] &= \frac{1}{\mathcal{Z}_\Lambda} \int \mathcal{D}[\Phi] \frac{1}{2} \underbrace{\left(\Phi, \partial_\Lambda [\mathbf{G}_{0,\Lambda}]^{-1} \Phi \right)}_{\rightarrow \left(\frac{\delta}{\delta J}, [\partial_\Lambda \mathbf{G}_{0,\Lambda}^{-1}] \frac{\delta}{\delta J} \right)} e^{-S_{0,\Lambda}[\Phi] - S_1[\Phi] + (J,\Phi)} - \left(\frac{\partial_\Lambda \mathcal{Z}_\Lambda}{\mathcal{Z}_\Lambda} \right) \mathcal{G}_\Lambda [J] \\ &= \frac{1}{2} \left(\frac{\delta}{\delta J}, [\partial_\Lambda \mathbf{G}_{0,\Lambda}^{-1}] \frac{\delta}{\delta J} \right) \mathcal{G}_\Lambda [J] - (\partial_\Lambda \ln \mathcal{Z}_\Lambda) \mathcal{G}_\Lambda [J]\end{aligned}$$

and finally obtain

$$\partial_\Lambda \mathcal{G}_\Lambda [J] = \frac{1}{2} \text{Tr} \left\{ [\partial_\Lambda \mathbf{G}_{0,\Lambda}^{-1}] \left(\frac{\delta}{\delta J} \otimes \frac{\delta}{\delta J} \mathcal{G}_\Lambda \right)^T \right\} - (\partial_\Lambda \ln \mathcal{Z}_\Lambda) \mathcal{G}_\Lambda [J]. \quad (255)$$

Flow of $\mathcal{G}_{c,\Lambda} [J]$ (connected Green functions)

- Use definition

$$\mathcal{G}_\Lambda [J] = \frac{\mathcal{Z}_{0,\Lambda}}{\mathcal{Z}_\Lambda} e^{\mathcal{G}_{c,\Lambda}[J]}, \quad (256)$$

take ∂_Λ on both sides,

$$\partial_\Lambda \mathcal{G}_\Lambda = \frac{\mathcal{Z}_{0,\Lambda}}{\mathcal{Z}_\Lambda} e^{\mathcal{G}_{c,\Lambda}[J]} \left[\partial_\Lambda \mathcal{G}_{c,\Lambda} + \partial_\Lambda \ln \left(\frac{\mathcal{Z}_{0,\Lambda}}{\mathcal{Z}_\Lambda} \right) \right] \quad (257)$$

- Solve for $\partial_\Lambda \mathcal{G}_{c,\Lambda}$:

$$\partial_\Lambda \mathcal{G}_{c,\Lambda} = (\partial_\Lambda \mathcal{G}_\Lambda) \frac{\mathcal{Z}_\Lambda}{\mathcal{Z}_{0,\Lambda}} e^{-\mathcal{G}_{c,\Lambda}[J]} - \partial_\Lambda \ln \left(\frac{\mathcal{Z}_{0,\Lambda}}{\mathcal{Z}_\Lambda} \right) \quad (258)$$

and re-express all $\mathcal{G}_\Lambda [J]$ in Eq. (255) by $\mathcal{G}_{c,\Lambda} [J]$: After a straightforward calculation, we obtain

$$\partial_\Lambda \mathcal{G}_{c,\Lambda} [J] = \frac{1}{2} \left(\frac{\delta \mathcal{G}_{c,\Lambda}}{\delta J}, [\partial_\Lambda \mathbf{G}_{0,\Lambda}^{-1}] \frac{\delta \mathcal{G}_{c,\Lambda}}{\delta J} \right) + \frac{1}{2} \text{Tr} \left\{ [\partial_\Lambda \mathbf{G}_{0,\Lambda}^{-1}]^T \left(\frac{\delta}{\delta J} \otimes \frac{\delta}{\delta J} \mathcal{G}_{c,\Lambda} \right) \right\} - \partial_\Lambda \ln (\mathcal{Z}_{0,\Lambda}) \quad (259)$$

- We saw earlier from Eq. 218 that $\mathcal{G}_{c,\Lambda \rightarrow \infty} [J] = 0$.

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.

Flow of $\mathcal{G}_{ac,\Lambda} [\bar{\Phi}]$ (amputated connected Green functions) - Polchinski Equation

- Initial condition: Recall Eq. (223),

$$e^{\mathcal{G}_{ac}[\bar{\Phi}]} = e^{-\frac{1}{2} \left(\frac{\delta}{\delta \bar{\Phi}}, \mathbf{G}_0^T \frac{\delta}{\delta \bar{\Phi}} \right)} e^{-S_1[\bar{\Phi}]} \quad (260)$$

and find

$$\lim_{\Lambda \rightarrow \infty} \mathcal{G}_{ac,\Lambda} [\bar{\Phi}] = -S_1 [\bar{\Phi}] \quad (261)$$

- Flow equation follows from differentiating Eq. (260):

$$\begin{aligned}
e^{\mathcal{G}_{ac}} \partial_{\Lambda} \mathcal{G}_{ac} &= \partial_{\Lambda} e^{\mathcal{G}_{ac}} \\
&= -\frac{1}{2} \left(\frac{\delta}{\delta \bar{\Phi}}, \left[\partial_{\Lambda} \mathbf{G}_{0,\Lambda}^T \right] \frac{\delta}{\delta \bar{\Phi}} \right) \underbrace{e^{-\frac{1}{2} \left(\frac{\delta}{\delta \bar{\Phi}}, \mathbf{G}_{0,\Lambda}^T \frac{\delta}{\delta \bar{\Phi}} \right)} e^{-S_1[\bar{\Phi}]} }_{e^{\mathcal{G}_{ac,\Lambda}}} \\
&= e^{\mathcal{G}_{ac,\Lambda}} \left[-\frac{1}{2} \left(\frac{\delta \mathcal{G}_{ac,\Lambda}}{\delta \bar{\Phi}}, \left[\partial_{\Lambda} \mathbf{G}_{0,\Lambda}^T \right] \frac{\delta \mathcal{G}_{ac,\Lambda}}{\delta \bar{\Phi}} \right) - \frac{1}{2} \left(\frac{\delta}{\delta \bar{\Phi}}, \left[\partial_{\Lambda} \mathbf{G}_{0,\Lambda}^T \right] \frac{\delta}{\delta \bar{\Phi}} \right) \mathcal{G}_{ac,\Lambda} \right]
\end{aligned}$$

- We find the **Polchinski Equation**, (Polchinski, 1984):

$$\partial_{\Lambda} \mathcal{G}_{ac,\Lambda} = -\frac{1}{2} \left(\frac{\delta \mathcal{G}_{ac,\Lambda}}{\delta \bar{\Phi}}, \left[\partial_{\Lambda} \mathbf{G}_{0,\Lambda}^T \right] \frac{\delta \mathcal{G}_{ac,\Lambda}}{\delta \bar{\Phi}} \right) - \frac{1}{2} \text{Tr} \left(\left[\partial_{\Lambda} \mathbf{G}_{0,\Lambda}^T \right] \left(\frac{\delta}{\delta \bar{\Phi}} \otimes \frac{\delta}{\delta \bar{\Phi}} \mathcal{G}_{ac,\Lambda} \right)^T \right) \quad (262)$$

- Problem: For sharp cutoffs, the first term contains δ -function that is not integrated over (no loops!).

Flow of $\Gamma[\bar{\Phi}]$ (irreducible vertices) - Wetterich Equation

- Augment definition of $\Gamma[\bar{\Phi}]$ with Λ :

$$\begin{aligned}
\Gamma_{\Lambda}[\bar{\Phi}] &= \left(J_{\Lambda}[\bar{\Phi}], \bar{\Phi} \right) - \mathcal{G}_{c,\Lambda} \left[J_{\Lambda}[\bar{\Phi}] \right] + \frac{1}{2} \left(\bar{\Phi}, \left[\mathbf{G}_{0,\Lambda} \right]^{-1} \bar{\Phi} \right) \\
\bar{\Phi} &= \frac{\delta \mathcal{G}_{c,\Lambda}[J]}{\delta J}
\end{aligned} \quad (263)$$

Note that now, the $J_{\Lambda}[\bar{\Phi}]$ are also Λ -dependent.

- Simple initial conditions:

$$\boxed{\lim_{\Lambda \rightarrow \infty} \Gamma_{\Lambda}[\bar{\Phi}] = -\lim_{\Lambda \rightarrow \infty} \mathcal{G}_{ac,\Lambda}[\bar{\Phi}] = S_1[\bar{\Phi}]} \quad (264)$$

Proof: Start from relation between \mathcal{G}_c and \mathcal{G}_{ac} , Eq. (222)

$$\mathcal{G}_{ac,\Lambda}[\bar{\Phi}] = \mathcal{G}_{c,\Lambda} \left[- \underbrace{\left(\mathbf{G}_{0,\Lambda}^T \right)^{-1} \bar{\Phi}}_{\equiv J[\bar{\Phi}]} + \frac{1}{2} \left(\bar{\Phi}, \mathbf{G}_{0,\Lambda}^{-1} \bar{\Phi} \right) \right] \quad (265)$$

To connect the rhs to Γ , we prepare for the use of the Legendre transform with respect to the $J[\bar{\Phi}]$:

$$\begin{aligned}
\bar{\Phi}'_{\alpha} &\equiv \frac{\delta \mathcal{G}_{c,\Lambda}[J]}{\delta J_{\alpha}} \\
&= \int_{\beta} \frac{\delta \bar{\Phi}_{\beta}}{\delta J_{\alpha}} \frac{\delta \mathcal{G}_{c,\Lambda}[J]}{\delta \bar{\Phi}_{\beta}} \\
&= - \int_{\beta} \left[\mathbf{G}_{0,\Lambda}^T \right]_{\beta\alpha} \frac{\delta}{\delta \bar{\Phi}_{\beta}} \left(\mathcal{G}_{ac,\Lambda}[\bar{\Phi}] - \frac{1}{2} \left(\bar{\Phi}, \left(\mathbf{G}_{0,\Lambda} \right)^{-1} \bar{\Phi} \right) \right) \\
\bar{\Phi}' &= -\mathbf{G}_{0,\Lambda} \frac{\delta \mathcal{G}_{ac,\Lambda}[\bar{\Phi}]}{\delta \bar{\Phi}} + \bar{\Phi}
\end{aligned}$$

On the right hand side of Eq. (265), we apply the Legendre transform $\mathcal{G}_{c,\Lambda}[J[\bar{\Phi}']] = \left(J[\bar{\Phi}'], \bar{\Phi}' \right) - \Gamma_{\Lambda}[\bar{\Phi}'] + \frac{1}{2} \left(\bar{\Phi}', \left[\mathbf{G}_{0,\Lambda} \right]^{-1} \bar{\Phi}' \right)$:

$$\mathcal{G}_{ac,\Lambda}[\bar{\Phi}] = \left(J, \bar{\Phi}' \right) - \Gamma_{\Lambda}[\bar{\Phi}'] + \frac{1}{2} \left(\bar{\Phi}', \mathbf{G}_{0,\Lambda}^{-1} \bar{\Phi}' \right) + \frac{1}{2} \left(\bar{\Phi}, \mathbf{G}_{0,\Lambda}^{-1} \bar{\Phi} \right)$$

and insert the prepared $\bar{\Phi}'$ to express the right-hand side in $\bar{\Phi}$. After a short calculation, we obtain

$$\mathcal{G}_{ac,\Lambda}[\bar{\Phi}] = -\Gamma_{\Lambda} \left[\bar{\Phi} - \mathbf{G}_{0,\Lambda} \frac{\delta \mathcal{G}_{ac,\Lambda}}{\delta \bar{\Phi}} \right] + \frac{1}{2} \left(\frac{\delta \mathcal{G}_{ac,\Lambda}}{\delta \bar{\Phi}}, \mathbf{G}_{0,\Lambda}^T \frac{\delta \mathcal{G}_{ac,\Lambda}}{\delta \bar{\Phi}} \right) \quad (266)$$

from which the claim follows as $\lim_{\Lambda \rightarrow \infty} \mathbf{G}_{0,\Lambda} = 0$.

- The flow for $\Gamma_\Lambda [\bar{\Phi}]$ follows by taking ∂_Λ of the defining equation (263):

$$\begin{aligned}\partial_\Lambda \Gamma_\Lambda [\bar{\Phi}] &= \left(\partial_\Lambda J_\Lambda [\bar{\Phi}], \bar{\Phi} \right) - \partial_\Lambda \left(\mathcal{G}_{c,\Lambda} [J_\Lambda [\bar{\Phi}]] \right) + \frac{1}{2} \left(\bar{\Phi}, \partial_\Lambda [\mathbf{G}_{0,\Lambda}]^{-1} \bar{\Phi} \right) \\ &= \left(\partial_\Lambda J_\Lambda [\bar{\Phi}], \bar{\Phi} \right) - \underbrace{\left(\partial_\Lambda J_\Lambda, \frac{\delta \mathcal{G}_{c,\Lambda} [J]}{\delta J} \right)}_{\bar{\Phi}} - \partial_\Lambda \mathcal{G}_{c,\Lambda} [J] |_{J=J_\Lambda[\bar{\Phi}]} + \frac{1}{2} \left(\bar{\Phi}, \partial_\Lambda [\mathbf{G}_{0,\Lambda}]^{-1} \bar{\Phi} \right)\end{aligned}$$

The first two terms cancel. For the third term we use the flow of the connected functional Eq. (259).

$$\begin{aligned}\partial_\Lambda \Gamma_\Lambda [\bar{\Phi}] &= -\frac{1}{2} \left(\frac{\delta \mathcal{G}_{c,\Lambda}}{\delta J}, \left[\partial_\Lambda \mathbf{G}_{0,\Lambda}^{-1}, \frac{\delta \mathcal{G}_{c,\Lambda}}{\delta J} \right] \right) - \frac{1}{2} \text{Tr} \left\{ \left[\partial_\Lambda \mathbf{G}_{0,\Lambda}^{-1} \right]^T \left(\frac{\delta}{\delta J} \otimes \frac{\delta}{\delta J} \mathcal{G}_{c,\Lambda} \right) \right\} \\ &\quad + \partial_\Lambda \ln (\mathcal{Z}_{0,\Lambda}) + \frac{1}{2} \left(\bar{\Phi}, \partial_\Lambda \mathbf{G}_{0,\Lambda}^{-1} \bar{\Phi} \right)\end{aligned}$$

and the brown terms cancel.

- We recall the relation between second functional derivatives of $\mathcal{G}_{c,\Lambda}$, \mathcal{L}_Λ and Γ_Λ :

$$\left(\frac{\delta}{\delta J} \otimes \frac{\delta}{\delta J} \mathcal{G}_{c,\Lambda} \right) = \left(\frac{\delta}{\delta \bar{\Phi}} \otimes \frac{\delta}{\delta \bar{\Phi}} \mathcal{L}_\Lambda [\bar{\Phi}] \right)^{-1} = \left(\frac{\delta}{\delta \bar{\Phi}} \otimes \frac{\delta}{\delta \bar{\Phi}} \Gamma_\Lambda [\bar{\Phi}] - [\mathbf{G}_{0,\Lambda}^T]^{-1} \right)^{-1} \quad (267)$$

and find the **Wetterich Equation** (Wetterich, 1993)

$$\partial_\Lambda \Gamma_\Lambda [\bar{\Phi}] = -\frac{1}{2} \text{Tr} \left\{ \underbrace{\left[\partial_\Lambda \mathbf{G}_{0,\Lambda}^{-1} \right]}_{-\partial_\Lambda \mathbf{R}_\Lambda} \left(\frac{\delta}{\delta \bar{\Phi}} \otimes \frac{\delta}{\delta \bar{\Phi}} \Gamma_\Lambda [\bar{\Phi}] - [\mathbf{G}_{0,\Lambda}^T]^{-1} \right)^{-1} \right\} + \partial_\Lambda \ln (\mathcal{Z}_{0,\Lambda}) \quad (268)$$

- The first term is sometimes more conveniently expressed with the regulator \mathbf{R}_Λ .
- Two strategies for solution of Wetterich equation:
 1. Vertex expansion: Expand both sides in powers of fields $\bar{\Phi}$ and find flow equation for vertices $\Gamma_{\alpha_1 \dots \alpha_n}^{(n)}$ (\rightarrow next Sec. 6.3)
 2. Derivative expansion: Make ansatz $\Gamma_\Lambda [\bar{\Phi}] = \int_{\mathbf{r}} U_\Lambda (\rho) + \mathcal{O}([\nabla \bar{\Phi}]^2)$ with $\rho = \bar{\Phi}^2$ a scalar. The arbitrary functions $U_\Lambda (\rho)$ fulfill flow equations $\partial_\Lambda U_\Lambda (\rho) = f (\Lambda, U_\Lambda^{(j, \dots)} (\rho), \rho, \dots)$. For more details, see [Kopietz, Ch. 9].

6.3 Vertex expansion: Flow of $\Gamma_{\alpha_1 \dots \alpha_n}^{(n)}$

Preparations

- Preparation I: From the section on tree expansion, recall Eq. (243) and augment all quantities with subscript Λ :

$$\frac{\delta}{\delta \bar{\Phi}} \otimes \frac{\delta}{\delta \bar{\Phi}} \Gamma_\Lambda [\bar{\Phi}] - [\mathbf{G}_{0,\Lambda}^T]^{-1} = \mathbf{U}_\Lambda^T [\bar{\Phi}] - [\mathbf{G}_\Lambda^T]^{-1} \quad (269)$$

$$\mathbf{U}_\Lambda [\bar{\Phi}] = \sum_{n=1}^{\infty} \frac{1}{n!} \int_{\alpha_1 \dots \alpha_n} \Gamma_{\Lambda, \alpha_1 \dots \alpha_n}^{(n+2)} \bar{\Phi}_{\alpha_1} \dots \bar{\Phi}_{\alpha_n} \quad (270)$$

Now, the Dyson equation is required to hold for each Λ :

$$[\mathbf{G}_\Lambda]^{-1} = [\mathbf{G}_{0,\Lambda}]^{-1} - \Sigma_\Lambda \quad (271)$$

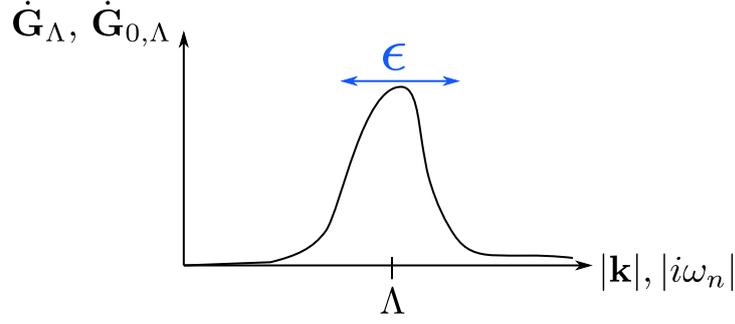


Figure 17: Sketch of the single scale propagator for a multiplicative cutoff in momentum or Matsubara frequency.

- Preparation II:

$$\mathcal{Z}_{0,\Lambda} = \int \mathcal{D}[\Phi] e^{\frac{1}{2}\Phi_\alpha [\mathbf{G}_{0,\Lambda}^{-1}]_{\alpha\beta} \Phi_\beta} \propto e^{-\frac{1}{2}\text{Tr}[\mathbf{Z}\ln(-\mathbf{G}_{0,\Lambda}^{-1})]} \quad (272)$$

so that

$$\partial_\Lambda \ln(\mathcal{Z}_{0,\Lambda}) = -\frac{1}{2}\text{Tr}[\mathbf{Z}\mathbf{G}_{0,\Lambda}(\partial_\Lambda \mathbf{G}_{0,\Lambda}^{-1})] = -\frac{1}{2}\text{Tr}[\mathbf{G}_{0,\Lambda}^T(\partial_\Lambda \mathbf{G}_{0,\Lambda}^{-1})] \quad (273)$$

- Substitute preparations in Eq. (268) and get

$$\partial_\Lambda \Gamma_\Lambda[\bar{\Phi}] = -\frac{1}{2}\text{Tr}\left(\left[\partial_\Lambda \mathbf{G}_{0,\Lambda}^{-1}\right] \left\{ \left(\mathbf{U}_\Lambda^T[\bar{\Phi}] - [\mathbf{G}_\Lambda^T]^{-1}\right)^{-1} + \mathbf{G}_{0,\Lambda}^T \right\}\right) \quad (274)$$

The term $\{\dots\}$ can be written in a series expansion (drop Λ subscript)

$$\begin{aligned} \left(\mathbf{U}^T - [\mathbf{G}^T]^{-1}\right)^{-1} + \mathbf{G}_0^T &= -\left(\mathbf{G}^T + \mathbf{G}^T \mathbf{U}^T \mathbf{G}^T + \mathbf{G}^T \mathbf{U}^T \mathbf{G}^T \mathbf{U}^T \mathbf{G}^T + \dots\right) + \mathbf{G}_0^T \\ &= -\mathbf{G}^T \mathbf{U}^T \left(1 + \mathbf{G}^T \mathbf{U}^T + \mathbf{G}^T \mathbf{U}^T \mathbf{G}^T \mathbf{U}^T + \dots\right) \mathbf{G}^T - \mathbf{G}^T + \mathbf{G}_0^T \\ \left\{ \mathbf{G}^T = \left([\mathbf{G}_0^T]^{-1} - \Sigma^T\right)^{-1} \right\} &= -\mathbf{G}^T \mathbf{U}^T \frac{1}{1 - \mathbf{G}^T \mathbf{U}^T} \mathbf{G}^T - \mathbf{G}_0^T \Sigma^T \frac{1}{1 - \mathbf{G}_0^T \Sigma^T} \mathbf{G}_0^T \end{aligned}$$

which we place back into Eq. (274) to obtain

$$\partial_\Lambda \Gamma_\Lambda[\bar{\Phi}] = -\frac{1}{2}\text{Tr}\left(\dot{\mathbf{G}}_\Lambda \mathbf{U}_\Lambda^T[\bar{\Phi}] \underbrace{\left(1 - \mathbf{G}_\Lambda^T \mathbf{U}_\Lambda^T[\bar{\Phi}]\right)^{-1}}_{\sum_{\nu=0}^{\infty} (\mathbf{G}_\Lambda^T \mathbf{U}_\Lambda^T[\bar{\Phi}])^\nu} + \dot{\mathbf{G}}_{0,\Lambda} \Sigma_\Lambda^T \frac{1}{1 - \mathbf{G}_{0,\Lambda}^T \Sigma_\Lambda^T}\right) \quad (275)$$

with the *single-scale propagator*,

$$\dot{\mathbf{G}}_\Lambda \equiv -\mathbf{G}_\Lambda \left[\partial_\Lambda \mathbf{G}_{0,\Lambda}^{-1}\right] \mathbf{G}_\Lambda \stackrel{Ex.}{=} \frac{1}{1 - \mathbf{G}_{0,\Lambda} \Sigma_\Lambda} \left[\partial_\Lambda \mathbf{G}_{0,\Lambda}\right] \frac{1}{1 - \Sigma_\Lambda \mathbf{G}_{0,\Lambda}} \quad (276)$$

and its non-interacting version,

$$\dot{\mathbf{G}}_{0,\Lambda} \equiv -\mathbf{G}_{0,\Lambda} \left[\partial_\Lambda \mathbf{G}_{0,\Lambda}^{-1}\right] \mathbf{G}_{0,\Lambda} = \partial_\Lambda \mathbf{G}_{0,\Lambda}. \quad (277)$$

For RG-type cutoffs the single-scale propagator has support only close to the (momentum-, frequency-) scale Λ , see Fig. 17.

Expansion of $\partial_\Lambda \Gamma_\Lambda [\bar{\Phi}]$ in fields

- Expansion of Eq. (275) in powers of fields: For lhs use,

$$\partial_\Lambda \Gamma_\Lambda [\bar{\Phi}] = \sum_{n=0}^{\infty} \frac{1}{n!} \int_{\alpha_1 \dots \alpha_n} \partial_\Lambda \Gamma_{\Lambda, \alpha_1 \dots \alpha_n}^{(n)} \bar{\Phi}_{\alpha_1} \dots \bar{\Phi}_{\alpha_n}, \quad (278)$$

for rhs use Eq. (270).

- The field independent second term on the rhs yields

$$\begin{aligned} \partial_\Lambda \Gamma_\Lambda^{(0)} &= -\frac{1}{2} \text{Tr} \left(\dot{\mathbf{G}}_{0,\Lambda} \Sigma_\Lambda^T \frac{1}{1 - \mathbf{G}_{0,\Lambda}^T \Sigma_\Lambda^T} \right) \\ &= -\frac{1}{2} \text{Tr} \left(\dot{\mathbf{G}}_{0,\Lambda} \Sigma_\Lambda^T \left[1 + \mathbf{G}_{0,\Lambda}^T \Sigma_\Lambda^T + \mathbf{G}_{0,\Lambda}^T \Sigma_\Lambda^T \mathbf{G}_{0,\Lambda}^T \Sigma_\Lambda^T + \dots \right] \right) \\ &= -\frac{1}{2} \text{Tr} \left([1 + \Sigma_\Lambda \mathbf{G}_{0,\Lambda} + \Sigma_\Lambda \mathbf{G}_{0,\Lambda} \Sigma_\Lambda \mathbf{G}_{0,\Lambda} + \dots] \Sigma_\Lambda \dot{\mathbf{G}}_{0,\Lambda} \mathbf{Z} \right) \end{aligned}$$

We finally pull the right Σ_Λ in the brackets and move the left out. The $\dot{\mathbf{G}}_{0,\Lambda} \mathbf{Z}$ can be rotated to the front. We are left with:

$$\boxed{\partial_\Lambda \Gamma_\Lambda^{(0)} = -\frac{1}{2} \text{Tr} \left(\mathbf{Z} \dot{\mathbf{G}}_{0,\Lambda} \Sigma_\Lambda \frac{1}{1 - \mathbf{G}_{0,\Lambda} \Sigma_\Lambda} \right)} \quad (279)$$

Interpretation: This yields the flow of the interaction-correction to the free energy $F = -T \log \mathcal{Z}$ (up to factor T):

$$F - F_0 = -T \log (\mathcal{Z}/\mathcal{Z}_0) = -T G_c^{(0)} = -T (-\Gamma^{(0)}) = T \Gamma^{(0)} \rightarrow \text{link to thermodynamics} \quad (280)$$

- Higher-order terms $\partial_\Lambda \Gamma_{\Lambda, \alpha_1 \dots \alpha_n}^{(n \geq 1)}$: The derivation is similar to tree expansion, but a bit simpler as now there are no J -sourcefields involved. We pick n of the $\bar{\Phi}$ -fields on both sides,

$$\begin{aligned} \frac{1}{n!} \partial_\Lambda \Gamma_{\Lambda, \alpha_1 \dots \alpha_n}^{(n)} &= \\ &- \frac{1}{2} \sum_{\nu=1}^{\infty} \sum_{n_1, 2, \dots, \nu=1}^{\infty} \frac{\delta_{n, n_1 + \dots + n_\nu}}{n_\nu! n_{\nu-1}! \dots n_1!} \text{Tr} \left(\dot{\mathbf{G}}_\Lambda \Gamma_{\Lambda, \alpha_{n-n_\nu+1} \dots \alpha_n}^{T(n_\nu+2)} \left[\mathbf{G}_\Lambda^T \Gamma_{\Lambda, \alpha_{n-n_\nu-n_{\nu-1}+1} \dots \alpha_{n-n_\nu}}^{T(n_{\nu-1}+2)} \right] \dots \left[\mathbf{G}_\Lambda^T \Gamma_{\Lambda, \alpha_1 \dots \alpha_{n_1}}^{T(n_1+2)} \right] \right) \end{aligned}$$

To (anti-)symmetrize the rhs, sum over all $n!$ permutations of the labels $\alpha_1 \dots \alpha_n$ with correct sign. We can also take the transpose in the trace (but don't need to reverse the order due to \mathcal{S})

$$\boxed{\begin{aligned} \partial_\Lambda \Gamma_{\Lambda, \alpha_1 \dots \alpha_n}^{(n)} &= -\frac{1}{2} \sum_{\nu=1}^{\infty} \sum_{n_1, 2, \dots, \nu=1}^{\infty} \delta_{n, n_1 + \dots + n_\nu} \mathcal{S}_{\alpha_1 \dots \alpha_{n_1}; \dots; \alpha_{n-n_\nu+1} \dots \alpha_n} \\ &\times \text{Tr} \left(\mathbf{Z} \dot{\mathbf{G}}_\Lambda \Gamma_{\Lambda, \alpha_{n-n_\nu+1} \dots \alpha_n}^{(n_\nu+2)} \mathbf{G}_\Lambda \Gamma_{\Lambda, \alpha_{n-n_\nu-n_{\nu-1}+1} \dots \alpha_{n-n_\nu}}^{(n_{\nu-1}+2)} \dots \mathbf{G}_\Lambda \Gamma_{\Lambda, \alpha_1 \dots \alpha_{n_1}}^{(n_1+2)} \right) \end{aligned}}$$

Example: Flow of vertices with even number of legs

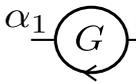
- Assume all vertices with odd number of external legs vanish. For $n = 1$, this is clear as we assumed no vacuum expectation values $\langle \bar{\Phi}_\alpha \rangle = 0$.
- For $n = 2$, have $\nu = 1$ and $n_1 = 2$ ($\nu = 2$ and $n_{1,2} = 1$ would involve $\Gamma^{(3)}$) so that

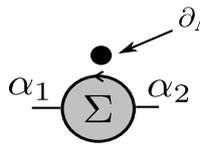
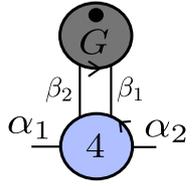
$$\partial_\Lambda \Gamma_{\Lambda, \alpha_1 \alpha_2}^{(2)} = \partial_\Lambda [\Sigma_\Lambda]_{\alpha_1 \alpha_2} = -\frac{1}{2} \text{Tr} \left(\mathbf{Z} \dot{\mathbf{G}}_\Lambda \Gamma_{\Lambda, \alpha_1 \alpha_2}^{(4)} \right) = -\frac{1}{2} \left[\dot{\mathbf{G}}_\Lambda \right]_{\beta_1 \beta_2} \Gamma_{\Lambda, \beta_1 \beta_2 \alpha_1 \alpha_2}^{(4)} \quad (281)$$

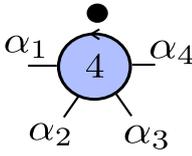
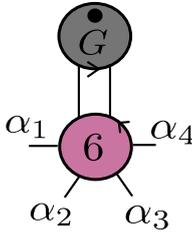
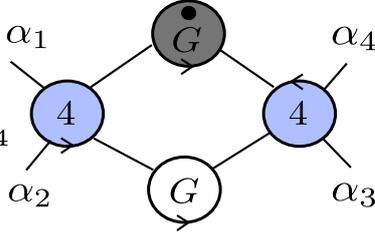
- For $n = 4$ (effective interaction) we have either $\nu = 1$ ($n_1 = 4$) or $\nu = 2$ ($n_1 = 2 = n_2$)

$$\partial_\Lambda \Gamma_{\Lambda, \alpha_1 \dots \alpha_4}^{(4)} = -\frac{1}{2} \text{Tr} \left(\mathbf{Z} \dot{\mathbf{G}}_\Lambda \Gamma_{\Lambda, \alpha_1 \alpha_2 \alpha_3 \alpha_4}^{(6)} + \mathcal{S}_{\alpha_1 \alpha_2; \alpha_3 \alpha_4} \left\{ \mathbf{Z} \dot{\mathbf{G}}_\Lambda \Gamma_{\Lambda, \alpha_3 \alpha_4}^{(4)} \mathbf{G}_\Lambda \Gamma_{\Lambda, \alpha_1 \alpha_2}^{(4)} \right\} \right)$$

and we do not consider the flow of the $n = 6$ vertex.

single-scale propagator:  $= \dot{\mathbf{G}}_{\alpha_1 \alpha_2}$ full propagator:  $= \mathbf{G}_{\alpha_1 \alpha_2} = \overleftarrow{\alpha_1 \alpha_2}$

flow of self energy:  $= -\frac{1}{2}$  All quantities depend on Λ !
(skipped in diagrammatic notation)

flow of effective interaction:  $= -\frac{1}{2}$  $- \frac{1}{2} \mathcal{S}_{\alpha_1 \alpha_2; \alpha_3 \alpha_4}$ 

6.4 Two examples:

fRG for φ^4 -theory, vertex expansion, relation to Wilsonian RG, anomalous dimension η

Goals:

- See vertex expansion at work for non-trivial classical mechanics field theory
- Recover RG flow equations found for coupling *constants* in Wilsonian momentum-shell RG
- Re-scaled vertices, truncation strategy based on relevance.
- Estimate anomalous dimension η from \mathbf{k} -dependence of self-energy.

Preparations

- Only single type of bosonic field with momentum index, $\Phi_\alpha \rightarrow \varphi_{\mathbf{k}}$, $\zeta = +1$.
- Stay in the disordered phase, zero magnetic field $\rightarrow \langle \varphi_{\mathbf{k}=0} \rangle = 0$. For generalization to ordered phase, see [Kopietz], Ch. 8.
- Recall action for φ^4 -theory, assign $S_{0,1}$ in non-standard way:

$$S[\varphi] = \underbrace{\frac{1}{2} \int_{\mathbf{k}} [c_0 k^2] \varphi(-\mathbf{k}) \varphi(\mathbf{k})}_{S_0[\varphi]} + \underbrace{\frac{r_0}{2} \int_{\mathbf{k}} \varphi(-\mathbf{k}) \varphi(\mathbf{k}) + \frac{u_0}{4!} \int_{\mathbf{k}_{1,2,3,4}} (2\pi)^D \delta(\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3 + \mathbf{k}_4) \varphi(\mathbf{k}_1) \varphi(\mathbf{k}_2) \varphi(\mathbf{k}_3) \varphi(\mathbf{k}_4)}_{S_1[\varphi]}$$

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)
- would simplify calculation in the ordered phase (and keeps consistency with [Kopietz] book)
- Use multiplicative sharp cutoff in momentum space:

$$G_{0,\Lambda}(\mathbf{k}) = \frac{\Theta(k - \Lambda)}{c_0 k^2} \quad (282)$$

Note: Due to the cutoff $k \leq \Lambda_0$ implicit in the $S[\varphi]$, we can start the flow at $\Lambda = \Lambda_0$.

- Dictionary for convention used in fRG flow equations:

$$\left[\mathbf{G}_{(0,\Lambda)} \right]_{\mathbf{k}\mathbf{k}'} = -(2\pi)^D \delta(\mathbf{k} + \mathbf{k}') G_{(0,\Lambda)}(\mathbf{k}) = -\langle \varphi_{\mathbf{k}} \varphi_{\mathbf{k}'} \rangle \quad (283)$$

$$\left[\dot{\mathbf{G}}_{\Lambda} \right]_{\mathbf{k}\mathbf{k}'} = -(2\pi)^D \delta(\mathbf{k} + \mathbf{k}') \dot{G}_{\Lambda}(\mathbf{k}) \quad (284)$$

$$\left[\Sigma_{\Lambda} \right]_{\mathbf{k}\mathbf{k}'} = +(2\pi)^D \delta(\mathbf{k} + \mathbf{k}') \Sigma_{\Lambda}(\mathbf{k}) \quad (285)$$

$$G_{\Lambda}^{-1}(\mathbf{k}) = G_{0,\Lambda}^{-1}(\mathbf{k}) + \Sigma_{\Lambda}(\mathbf{k}) \quad (286)$$

or

$$G_{\Lambda}(\mathbf{k}) = \frac{1}{G_{0,\Lambda}^{-1}(\mathbf{k}) + \Sigma_{\Lambda}(\mathbf{k})} = \frac{\Theta(k - \Lambda)}{c_0 k^2 + \Theta(k - \Lambda) \Sigma_{\Lambda}(\mathbf{k})} \quad (287)$$

- Single scale propagator:

$$\begin{aligned} \dot{G}_{\Lambda}(\mathbf{k}) &= -G_{\Lambda}(\mathbf{k}) \left[\partial_{\Lambda} G_{0,\Lambda}^{-1}(\mathbf{k}) \right] G_{\Lambda}(\mathbf{k}) \\ &= \frac{\dot{G}_{0,\Lambda}(\mathbf{k})}{[1 + G_{0,\Lambda}(\mathbf{k}) \Sigma_{\Lambda}(\mathbf{k})]^2} \\ \left\{ \dot{G}_{0,\Lambda} = \partial_{\Lambda} G_{0,\Lambda} \right\} &= \frac{-\delta(k - \Lambda)}{c_0 k^2 \left[1 + \frac{\Theta(k - \Lambda)}{c_0 k^2} \Sigma_{\Lambda}(\mathbf{k}) \right]^2} \end{aligned} \quad (288)$$

fRG flow equations

- For vertices, in accordance with Eq. (283), we take out a momentum-conserving delta-function out of $\Gamma^{(n)}$ and define

$$\Gamma_{\Lambda, \mathbf{k}_1 \dots \mathbf{k}_n}^{(n)} \equiv (2\pi)^D \delta(\mathbf{k}_1 + \dots + \mathbf{k}_n) \Gamma_{\Lambda}^{(n)}(\mathbf{k}_1, \dots, \mathbf{k}_n) \quad (289)$$

where $\Gamma_{\Lambda}^{(n)}(\mathbf{k}_1, \dots, \mathbf{k}_n)$ only really depends on $n - 1$ momenta.

- Recall the general fRG flow equations for vertices, we truncate $\Gamma^{(6)} \stackrel{!}{=} \Gamma_{\Lambda_0}^{(6)} = 0$ and drop all vertices of odd order since we restrict ourselves to the disordered phase.

$$\begin{aligned} \partial_{\Lambda} [\Sigma_{\Lambda}]_{\alpha_1 \alpha_2} &= -\frac{1}{2} \int_{\beta_1 \beta_2} \left[\dot{\mathbf{G}}_{\Lambda} \right]_{\beta_1 \beta_2} \Gamma_{\Lambda, \beta_1 \beta_2 \alpha_1 \alpha_2}^{(4)} \\ \partial_{\Lambda} \Gamma_{\Lambda, \alpha_1 \dots \alpha_4}^{(4)} &= -\frac{1}{2} \text{Tr} \left(\mathcal{S}_{\alpha_1 \alpha_2; \alpha_3 \alpha_4} \left\{ \mathbf{Z} \dot{\mathbf{G}}_{\Lambda} \Gamma_{\Lambda, \alpha_3 \alpha_4}^{(4)} \mathbf{G}_{\Lambda} \Gamma_{\Lambda, \alpha_1 \alpha_2}^{(4)} \right\} \right) \end{aligned}$$

- Insert preparations:

$$\begin{aligned} \partial_{\Lambda} \Sigma_{\Lambda}(\mathbf{k}) &= \frac{1}{2} \int_{\mathbf{k}'} \dot{G}_{\Lambda}(\mathbf{k}') \Gamma_{\Lambda}^{(4)}(\mathbf{k}', -\mathbf{k}', \mathbf{k}, -\mathbf{k}) \\ \partial_{\Lambda} \Gamma_{\Lambda}^{(4)}(\mathbf{k}_{1,2,3,4}) &= - \int_{\mathbf{k}} \dot{G}_{\Lambda}(\mathbf{k}) \\ &\times \left\{ \Gamma_{\Lambda}^{(4)}(\mathbf{k}, -\mathbf{k} + \mathbf{k}_1 + \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4) G_{\Lambda}(-\mathbf{k} + \mathbf{k}_1 + \mathbf{k}_2) \Gamma_{\Lambda}^{(4)}(+\mathbf{k} - \mathbf{k}_1 - \mathbf{k}_2, -\mathbf{k}, \mathbf{k}_1, \mathbf{k}_2) \right. \\ &\quad \left. + (\mathbf{k}_2 \leftrightarrow \mathbf{k}_3) + (\mathbf{k}_2 \leftrightarrow \mathbf{k}_4) \right\} \end{aligned}$$

and the factor of 1/2 has been canceled against the $(\mathbf{k}_1 \leftrightarrow \mathbf{k}_3)$, $(\mathbf{k}_1 \leftrightarrow \mathbf{k}_4)$, $(\mathbf{k}_{1,2} \leftrightarrow \mathbf{k}_{3,4})$ terms.

- Initial conditions (momentum independent): $\Sigma_{\Lambda_0} = r_0$ and $\Gamma_{\Lambda_0}^{(4)} = u_0$.

Recovering Wilsonian momentum shell RG

- Assume coupling *constants*, i.e. momentum independence of $\Sigma_\Lambda(\mathbf{k}) \stackrel{!}{=} r_\Lambda$ and $\Gamma_\Lambda^{(4)}(\mathbf{k}_{1,2,3,4}) \stackrel{!}{=} u_\Lambda$.
- Set momenta to zero at left-hand-side of fRG flow equations.
- From self-energy flow equation:

$$\begin{aligned}\partial_\Lambda r_\Lambda &= \frac{1}{2} \int_{\mathbf{k}} \dot{G}_\Lambda(\mathbf{k}) \Gamma_\Lambda^{(4)}(\mathbf{k}, -\mathbf{k}, 0, 0) \\ &= \frac{u_\Lambda}{2} \int_{\mathbf{k}} \dot{G}_\Lambda(\mathbf{k})\end{aligned}$$

Careful: Integrand

$$\dot{G}_\Lambda(\mathbf{k}) = \frac{-\delta(k - \Lambda)}{c_0 k^2 \left[1 + \frac{\Theta(k - \Lambda)}{c_0 k^2} \Sigma_\Lambda(\mathbf{k})\right]^2} \quad (290)$$

requires Morris' lemma: We use $\int_0^1 dt [1 + tx]^{-2} = -\frac{1}{x[1+tx]} \Big|_{t=0}^{t=1} = \frac{1}{1+x}$ and find

$$\dot{G}_\Lambda(\mathbf{k}) = -\frac{\delta(k - \Lambda)}{c_0 k^2 + \Sigma_\Lambda(k)} \quad (291)$$

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:

$$\begin{aligned}\partial_\Lambda r_\Lambda &= \frac{-u_\Lambda K_D}{2} \int_0^\infty k^{D-1} \cdot dk \frac{\delta(k - \Lambda)}{c_0 k^2 + \Sigma_\Lambda(k)} \\ &= -\frac{u_\Lambda}{2} \frac{K_D \Lambda^{D-1}}{c_0 \Lambda^2 + r_\Lambda}\end{aligned}$$

- From 4-point vertex flow equation:

$$\begin{aligned}\partial_\Lambda u_\Lambda &= -3u_\Lambda^2 \int_{\mathbf{k}} \dot{G}_\Lambda(\mathbf{k}) G_\Lambda(\mathbf{k}) \\ &= 3u_\Lambda^2 K_D \int dk k^{D-1} \frac{\delta(k - \Lambda) \Theta(k - \Lambda) c_0 k^2}{[c_0 k^2 + \Theta(k - \Lambda) r_\Lambda]^3} \\ \{Morris\} &= 3u_\Lambda^2 K_D \int dk k^{D-1} \delta(k - \Lambda) \int_0^1 dt \frac{t c_0 k^2}{[c_0 k^2 + t r_\Lambda]^3} \\ &= \frac{3}{2} u_\Lambda^2 K_D \int dk k^{D-1} \delta(k - \Lambda) \frac{1}{[c_0 k^2 + r_\Lambda]^2} \\ &= \frac{3K_D}{2} \frac{u_\Lambda^2 \Lambda^{D-1}}{[c_0 \Lambda^2 + r_\Lambda]^2}\end{aligned}$$

- We move to dimensionless quantities as before,

$$\bar{r}_\Lambda = \frac{r_\Lambda}{c_0 \Lambda^2}, \quad \bar{u}_\Lambda = K_D \frac{u_\Lambda}{c_0^2 \Lambda^{4-D}}, \quad (292)$$

and introduce l as $\Lambda = \Lambda_0 e^{-l}$ 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. 5.4

$$\partial_l \bar{r}_l = 2\bar{r}_l + \frac{1}{2} \frac{\bar{u}_l}{1 + \bar{r}_l} \quad (293)$$

$$\partial_l \bar{u}_l = (4 - D)\bar{u}_l - \frac{3}{2} \frac{\bar{u}_l^2}{[1 + \bar{r}_l]^2} \quad (294)$$

- Back to fRG: Options to solve flow equations.

1. Treat full momentum dependence numerically: Expensive, vertex $\tilde{\Gamma}_l^{(4)}$ depends on three D -dimensional momenta. Symmetries, form-factors and other tricks can be applied \rightarrow Master- & PhD-thesis.
2. Analytical approximations and further simplifications. \rightarrow This lecture. Goal: Find η .
Work with re-scaled flow equations to make strategy transparent.

Re-scaled flow equations (preparation for η)

- Idea: Make the vertices dimensionless functions of dimensionless momenta $\mathbf{k} = \Lambda\mathbf{q}$. Use $l = \ln(\Lambda_0/\Lambda)$ as flow parameter.
- Useful for analytic considerations, because canonical (engineering) dimensions at given fixed point can be read off directly.
- Motivation: Substitute $\mathbf{k} = \Lambda\mathbf{q}$ and vertices in action,

$$\begin{aligned}
S[\varphi] &= \frac{1}{2} \int_{\mathbf{k}} [c_0 k^2] \varphi(-\mathbf{k}) \varphi(\mathbf{k}) + \frac{1}{2} \int_{\mathbf{k}} \Sigma_{\Lambda_0}(\mathbf{k}) \varphi(-\mathbf{k}) \varphi(\mathbf{k}) \\
&\quad + \sum_{n=4,6,\dots} \frac{1}{n!} \int_{\mathbf{k}_1, \dots, \mathbf{k}_n} (2\pi)^D \delta(\mathbf{k}_1 + \dots + \mathbf{k}_n) \Gamma_{\Lambda_0}^{(n)}(\mathbf{k}_1, \dots, \mathbf{k}_n) \varphi(\mathbf{k}_1) \dots \varphi(\mathbf{k}_n) \\
&= \frac{1}{2} \int_{\mathbf{q}} \Lambda^{D+2} [c_0 q^2] \varphi(-\mathbf{q}\Lambda) \varphi(\mathbf{q}\Lambda) + \frac{1}{2} \int_{\mathbf{q}} \Lambda^D \Sigma_{\Lambda_0}(\mathbf{q}\Lambda) \varphi(-\mathbf{q}\Lambda) \varphi(\mathbf{q}\Lambda) \\
&\quad + \sum_{n=4,6,\dots} \frac{1}{n!} \int_{\mathbf{q}_1, \dots, \mathbf{q}_n} (2\pi)^D \delta(\mathbf{q}_1 + \dots + \mathbf{q}_n) \Lambda^{(n-1)D} \Gamma_{\Lambda_0}^{(n)}(\mathbf{q}_1, \dots, \mathbf{q}_n \Lambda) \varphi(\mathbf{q}_1 \Lambda) \dots \varphi(\mathbf{q}_n \Lambda)
\end{aligned}$$

and introduce new fields $\varphi'(\mathbf{q})$ such that the first term is $1/2 \int_{\mathbf{q}} q^2 \varphi'(-\mathbf{q}) \varphi'(\mathbf{q})$. This is of course pointless if there is a contribution $\Sigma_{\Lambda_0}(\mathbf{q}\Lambda) \sim q^2 + \dots$, so need to take this possibility into account via

$$\Lambda^{D+2} c_0 \underbrace{\left(1 + \frac{\partial \Sigma_{\Lambda_0}(\mathbf{k})}{\partial (c_0 k^2)} \Big|_0\right)}_{\equiv 1/Z} \varphi(-\mathbf{q}\Lambda) \varphi(\mathbf{q}\Lambda) \stackrel{!}{=} \varphi'(-\mathbf{q}) \varphi'(\mathbf{q}) \quad (295)$$

Apply the replacements $\varphi(\mathbf{q}\Lambda) \Lambda^{D/2+1} c_0^{1/2} Z^{-1/2} = \varphi'(\mathbf{q})$ in the n-field term:

$$\Lambda^{(n-1)D} \Gamma_{\Lambda_0}^{(n)}(\mathbf{q}_1 \Lambda) \dots \varphi(\mathbf{q}_n \Lambda) = \Lambda^{(n-1)D} Z^{n/2} c_0^{-n/2} \Lambda^{-n(D+2)/2} \Gamma_{\Lambda_0}^{(n)} \varphi'(\mathbf{q}_1) \dots \varphi'(\mathbf{q}_n) \quad (296)$$

Introducing Λ (or l), the blue terms combine to the dimensionless flowing vertex (tilde notation):

$$\boxed{\tilde{\Gamma}_l^{(n)}(\mathbf{q}_1, \dots, \mathbf{q}_n) \equiv \Lambda^{D(n/2-1)-n} \left(\frac{Z}{c_0}\right)^{n/2} \Gamma_{\Lambda}^{(n)}(\mathbf{q}_1 \Lambda, \dots, \mathbf{q}_n \Lambda)} \quad (297)$$

and then the definition of Z_l can be rewritten:

$$\boxed{Z_l = 1 - \frac{\partial \tilde{\Gamma}_l^{(2)}(\mathbf{q}, -\mathbf{q})}{\partial q^2} \Big|_{\mathbf{q}=0}} \quad (298)$$

- Remark: The definition of Z depends on the field theory in question, the chosen $G_{0,\Lambda}$ and the renormalization scheme. For fermionic systems, Z is often related to $i\omega$ -derivative of self-energy.
- Recall definition of anomalous dimension (c.f. scaling for correlation function, see Sec. 5.3)

$$\begin{aligned}
\eta_l &= -\partial_l \ln Z_l = -\frac{1}{Z_l} \partial_l Z_l = -\Lambda Z_l \frac{\partial [\partial_{\Lambda} \Sigma_{\Lambda}(\mathbf{k})]}{\partial (c_0 k^2)} \Big|_{\mathbf{k}=0} \\
\eta &= \lim_{l \rightarrow \infty} \eta_l
\end{aligned} \quad (299)$$

- Introduce re-scaled propagators (scale as inverse $\Gamma^{(2)}$):

$$\begin{aligned}
\tilde{G}_l(\mathbf{q}) &= \frac{c_0 \Lambda^2}{Z_l} G_{\Lambda}(\mathbf{k} = \Lambda\mathbf{q}), \\
\dot{\tilde{G}}_l(\mathbf{q}) &= -\frac{c_0 \Lambda^3}{Z_l} \dot{G}_{\Lambda}(\mathbf{k} = \Lambda\mathbf{q})
\end{aligned}$$

where the sign makes up for the sign in $\partial_l f_l = -\Lambda \partial_{\Lambda} f_{\Lambda}$.

- Flow for re-scaled two-point vertex: (product/chain rule, short calculation):

$$\partial_l \tilde{\Gamma}_l^{(2)}(\mathbf{q}) = (2 - \eta_l - \mathbf{q} \partial_{\mathbf{q}}) \tilde{\Gamma}_l^{(2)}(\mathbf{q}) + \dot{\Gamma}_l^{(2)}(\mathbf{q}) \quad (300)$$

$$\dot{\Gamma}_l^{(2)}(\mathbf{q}) = \frac{1}{2} \int_{\mathbf{q}'} \dot{G}_l(\mathbf{q}') \tilde{\Gamma}_l^{(4)}(\mathbf{q}', -\mathbf{q}', \mathbf{q}, -\mathbf{q}) = -\frac{Z_l}{c_0 \Lambda} \partial_{\Lambda} \Sigma_{\Lambda}(\mathbf{k}) \quad (301)$$

Note: Combining Eq. (301) and (299), we get

$$\eta_l = \lim_{q \rightarrow 0} \frac{\partial \dot{\Gamma}_l^{(2)}(q)}{\partial q^2} \quad (302)$$

- Flow for re-scaled four-point vertex:

$$\partial_l \tilde{\Gamma}_l^{(4)}(\mathbf{q}_{1,2,3,4}) = \left(4 - D - 2\eta_l - \sum_{i=1}^4 \mathbf{q}_i \partial_{\mathbf{q}_i} \right) \tilde{\Gamma}_l^{(4)}(\mathbf{q}_{1,2,3,4}) + \dot{\Gamma}_l^{(4)}(\mathbf{q}_{1,2,3,4}) \quad (303)$$

$$\begin{aligned} \dot{\Gamma}_l^{(4)}(\mathbf{q}_{1,2,3,4}) = & - \int_q \dot{G}_l(\mathbf{q}) \tilde{G}_l(\mathbf{q} + \mathbf{q}_1 + \mathbf{q}_2) \\ & \times \left\{ \tilde{\Gamma}_l^{(4)}(\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}, -\mathbf{q} - \mathbf{q}_1 - \mathbf{q}_2) \tilde{\Gamma}_l^{(4)}(\mathbf{q} + \mathbf{q}_1 + \mathbf{q}_2, -\mathbf{q}, \mathbf{q}_3, \mathbf{q}_4) + (\mathbf{q}_2 \leftrightarrow \mathbf{q}_3) + (\mathbf{q}_2 \leftrightarrow \mathbf{q}_4) \right\} \end{aligned} \quad (304)$$

- Integral form of flow equations (check by differentiation):

$$\tilde{\Gamma}_l^{(2)}(\mathbf{q}) = \exp \left[2l - \int_0^l d\tau \eta_{\tau} \right] \tilde{\Gamma}_{l=0}^{(2)}(e^{-l} \mathbf{q}) + \int_0^l dt \exp \left[2t - \int_{l-t}^l d\tau \eta_{\tau} \right] \dot{\Gamma}_{l-t}^{(2)}(e^{-t} \mathbf{q}) \quad (305)$$

$$\begin{aligned} \tilde{\Gamma}_l^{(4)}(\mathbf{q}_{1,2,3,4}) = & \exp \left[(4 - D)l - 2 \int_0^l d\tau \eta_{\tau} \right] \tilde{\Gamma}_{l=0}^{(4)}(e^{-l} \mathbf{q}_{1,2,3,4}) \\ & + \int_0^l dt \exp \left[(4 - D)t - 2 \int_{l-t}^l d\tau \eta_{\tau} \right] \dot{\Gamma}_{l-t}^{(4)}(e^{-t} \mathbf{q}_{1,2,3,4}) \end{aligned} \quad (306)$$

Truncation scheme based on relevance

- Idea: In flow equations for re-scaled vertices (300) and (303), consider parantheses

$$\begin{aligned} \partial_l \tilde{\Gamma}_l^{(2)} &= (2 - \eta_l - \mathbf{q} \partial_{\mathbf{q}}) \tilde{\Gamma}_l^{(2)} + \dot{\Gamma}_l^{(2)} \\ \partial_l \tilde{\Gamma}_l^{(4)} &= \left(4 - D - 2\eta_l - \sum_{i=1}^4 \mathbf{q}_i \partial_{\mathbf{q}_i} \right) \tilde{\Gamma}_l^{(4)} + \dot{\Gamma}_l^{(4)} \end{aligned}$$

Up to the term η_l , they contain the canonical (engineering) dimension of vertex at the Gaussian fixed point. The remaining terms give loop-corrections.

- $\tilde{\Gamma}_l^{(2)}$ -term: $\tilde{\Gamma}_l^{(2)}(0) = \tilde{r}_l$ relevant with dimension 2, contribution $\sim q^2$ is marginal because $q \partial_q q^n = n q^n$. We have to keep it (c.f. Eq. 298):

$$\tilde{\Gamma}_l^{(2)}(\mathbf{q}) = \tilde{r}_l + (1 - Z_l) q^2 \quad (307)$$

- $\tilde{\Gamma}_l^{(4)}$ -term: $\tilde{\Gamma}_l^{(4)}(0) = \tilde{u}_l / K_D = \tilde{u}_l$ has canonical dimension $4 - D$, relevant in $D < 4$. Keep this term. Finite- \mathbf{q} parts are irrelevant for $D > 3$.
- $\tilde{\Gamma}_l^{(6)}$ -term: $\tilde{\Gamma}_l^{(6)}(0)$ has canonical dimension $(n - D[n/2 - 1])|_{n=6} = 6 - 2D$, irrelevant in $D > 3$, discard.
- Careful in $D = 3$: $\tilde{\Gamma}_l^{(6)}$ and contributions $\tilde{\Gamma}_l^{(4)} \sim q$ are marginal! Will become marginally irrelevant if $\eta_l \sim \tilde{u}_l^2$ is considered.

- Flow equations so far are like in momentum-shell RG but with η :

$$\partial_l \bar{r}_l = (2 - \eta) \bar{r}_l + \frac{1}{2} \frac{\bar{u}_l}{1 + \bar{r}_l} \quad (308)$$

$$\partial_l \bar{u}_l = (4 - D - 2\eta) \bar{u}_l - \frac{3}{2} \frac{\bar{u}_l^2}{(1 + \bar{r}_l)^2} \quad (309)$$

Flow of η_l from $\eta_l = \lim_{q \rightarrow 0} \frac{\partial \dot{\Gamma}_l^{(2)}(q)}{\partial q^2}$

- Goal: Close set of flow equations, find flow for Z_l .
- Momentum dependence of $\tilde{\Gamma}_l^{(2)}$ generated by momentum dependence of $\tilde{\Gamma}_l^{(4)}$, see Eq. (300). This comes from the Green function momentum dependence of the $\partial_l \tilde{\Gamma}_l^{(4)}(\mathbf{q}_{1,2,3,4})$ flow equation (we keep $\tilde{\Gamma}_l^{(4)}$ momentum independent on the rhs). We get

$$\dot{\Gamma}_l^{(4)}(\mathbf{q}_{1,2,3,4}) = -\tilde{u}_l^2 \underbrace{\left\{ \int_{\mathbf{q}} \dot{G}_l(\mathbf{q}) \tilde{G}_l(\mathbf{q} + \mathbf{q}_1 + \mathbf{q}_2) + (2 \leftrightarrow 3) + (2 \leftrightarrow 4) \right\}}_{\equiv \dot{\chi}_l(\mathbf{q}_1 + \mathbf{q}_2)}$$

The “bubble” $\dot{\chi}_l(\mathbf{q}) = f(\bar{r}, q)$ can be found analytically in $D = 3$.

- Split the four-point vertex as

$$\tilde{\Gamma}_l^{(4)}(\mathbf{q}_{1,2,3,4}) = \tilde{u}_l + \gamma_l(\mathbf{q}_{1,2,3,4}) \quad (310)$$

and use the integral form 306 with $\gamma_{l=0} = 0$. This yields

$$\begin{aligned} \tilde{\Gamma}_l^{(4)}(\mathbf{q}_{1,2,3,4}) &= \exp \left[(4 - D)l - 2 \int_0^l d\tau \eta_\tau \right] \tilde{u}_{l=0} \\ &\quad - \int_0^l dt \exp \left[(4 - D)t - 2 \int_{l-t}^l d\tau \eta_\tau \right] \tilde{u}_{l-t}^2 \left\{ \dot{\chi}_{l-t}([\mathbf{q}_1 + \mathbf{q}_2]e^{-t}) + (2 \leftrightarrow 3) + (2 \leftrightarrow 4) \right\} \end{aligned}$$

and we can read off the flow equations $\partial_l \bar{u}_l = \dots$ as above coming from the first term in $\dot{\chi}_l(\mathbf{q}) = \dot{\chi}_l(0) + \delta \dot{\chi}_l(\mathbf{q})$. The second term gives rise to

$$\gamma_l(\mathbf{q}_{1,2,3,4}) = - \int_0^l dt \exp \left[(4 - D)t - 2 \int_{l-t}^l d\tau \eta_\tau \right] \tilde{u}_{l-t}^2 \left\{ \delta \dot{\chi}_{l-t}([\mathbf{q}_1 + \mathbf{q}_2]e^{-t}) + (2 \leftrightarrow 3) + (2 \leftrightarrow 4) \right\} \quad (311)$$

- We feed the result for \tilde{u}_l and γ_l into $\dot{\Gamma}_l^{(2)}(q)$:

$$\begin{aligned} \dot{\Gamma}_l^{(2)}(\mathbf{q}) &= \frac{1}{2} \int_{\mathbf{q}'} \dot{G}_l(\mathbf{q}') \tilde{\Gamma}_l^{(4)}(\mathbf{q}', -\mathbf{q}', \mathbf{q}, -\mathbf{q}) \\ &= \tilde{u}_l \frac{1}{2} \int_{\mathbf{q}'} \dot{G}_l(\mathbf{q}') + \frac{1}{2} \int_{\mathbf{q}'} \dot{G}_l(\mathbf{q}') \gamma_l(\mathbf{q}', -\mathbf{q}', \mathbf{q}, -\mathbf{q}) \\ &= \frac{\bar{u}_l}{2(1 + \bar{r}_l)} - \int_{\mathbf{q}'} \frac{\delta(q' - 1)}{1 + \bar{r}_l} \int_0^l dt \exp \left[(4 - D)t - 2 \int_{l-t}^l d\tau \eta_\tau \right] \tilde{u}_{l-t}^2 \delta \dot{\chi}_{l-t}([\mathbf{q}' + \mathbf{q}]e^{-t}) \end{aligned}$$

- Use this in Eq. (302). After a short calculation:

$$\eta_l = \lim_{q \rightarrow 0} \frac{\partial \dot{\Gamma}_l^{(2)}(\mathbf{q})}{\partial q^2} = \int_0^l dt K(l, t) \bar{u}_{l-t}^2 e^{-2 \int_{l-t}^l d\tau \eta_\tau} \quad (312)$$

$$K(l, t) = -\frac{1}{2DK_D [1 + \bar{r}_l]} \left[(D - 1) e^{-(D-3)t} \dot{\chi}'_{l-t}(e^{-t}) + e^{-(D-2)t} \dot{\chi}''_{l-t}(e^{-t}) \right]$$

- Equations (308), (309), (312) are a closed system of equations that can be solved numerically.
- Since η_l is small, the flow of \bar{r}, \bar{u} will look not much different from Fig. 9.
- Tune to critical manifold flowing into Wilson-Fisher fixed point: Get a finite $\eta = \lim_{l \rightarrow \infty} \eta_l, \bar{u}_*, \bar{r}_*$. Then Eq. (312) turns into self-consistency equation for $l \rightarrow \infty$:

$$\eta = \bar{u}_*^2 \int_0^\infty dt K(\infty, t) e^{-2t\eta} \quad (313)$$

Evaluate and compare to precise value for the $D = 3$ Ising universality class $\eta = 0.036$:

- In $\epsilon = 4 - D$ in leading order: $\eta = \epsilon^2/54 \xrightarrow{\epsilon=1} 0.018$.
- Numerically in $D = 3$: $\eta = 0.101$.

fRG for spinful fermions

Goal: Derive flow equations for fermions, use them in Ex. 6.5.5 for single-impurity Anderson model (SIAM).

Preparations

- Need two types of fields for creation and annihilation operator, $\{\Phi_\alpha\} \rightarrow \{\psi_{K\sigma}, \bar{\psi}_{K\sigma}\}$, $\zeta = -1$, abbreviate $K \equiv (i\omega, \mathbf{k})$ (the quantities that are usually conserved at a vertex) and $\sigma = \uparrow, \downarrow$ is the spin index. Now $\alpha = (\psi, K, \sigma)$ or $(\bar{\psi}, K', \sigma')$. Generalize spinless case from the beginning of Sec. 6.1,

$$S_0[\bar{\psi}, \psi] = - \sum_{\sigma, \sigma'} \int_{K', K} \bar{\psi}_{K'\sigma'} \underbrace{G_0^{-1}(K)}_{i\omega \delta_{K, K'} \delta_{\sigma'\sigma} - H_{K'\sigma'; K\sigma}} \psi_{K\sigma}$$

$$\left[\mathbf{G}_0^{-1} \right]_{(\bar{\psi}, K', \sigma'), (\psi, K, \sigma)} = \delta_{K, K'} \delta_{\sigma\sigma'} (i\omega \delta_{K, K'} \delta_{\sigma'\sigma} - H_{K'\sigma'; K\sigma}) = \left[G_0^{-1} \right]_{K'\sigma'; K\sigma} \quad (314)$$

- Full Green function, propagate from $1' = (K', \sigma')$ (creation) to $1 = (K, \sigma)$ (annihilation). Minus sign and definition of $G_{11'}$ with $\psi, \bar{\psi}$ not explicitly specified is fermionic **convention**.

$$\boxed{\mathbf{G}_{\psi_1 \bar{\psi}_{1'}} = - \langle \psi_1 \bar{\psi}_{1'} \rangle \equiv G_{11'}} \quad (315)$$

- The above two points require the following assignments (also hold with cutoff Λ):

$$\mathbf{G} = \begin{pmatrix} 0 & \mathbf{G}_{\psi\bar{\psi}} \\ \mathbf{G}_{\bar{\psi}\psi} & 0 \end{pmatrix} = \begin{pmatrix} 0 & G \\ \zeta G^T & 0 \end{pmatrix}$$

$$\mathbf{G}^{-1} = \begin{pmatrix} 0 & [\mathbf{G}^{-1}]_{\psi\bar{\psi}} \\ [\mathbf{G}^{-1}]_{\bar{\psi}\psi} & 0 \end{pmatrix} = \begin{pmatrix} 0 & \zeta (G^{-1})^T \\ G^{-1} & 0 \end{pmatrix} = \mathbf{G}_0^{-1} - \Sigma$$

$$\Sigma = \begin{pmatrix} 0 & [\Sigma]_{\psi\bar{\psi}} \\ [\Sigma]_{\bar{\psi}\psi} & 0 \end{pmatrix} = \begin{pmatrix} 0 & \zeta \Sigma^T \\ \Sigma & 0 \end{pmatrix}$$

and we read off

$$G^{-1} = G_0^{-1} - \Sigma. \quad (316)$$

The above conventions are summarized in Fig. 18.

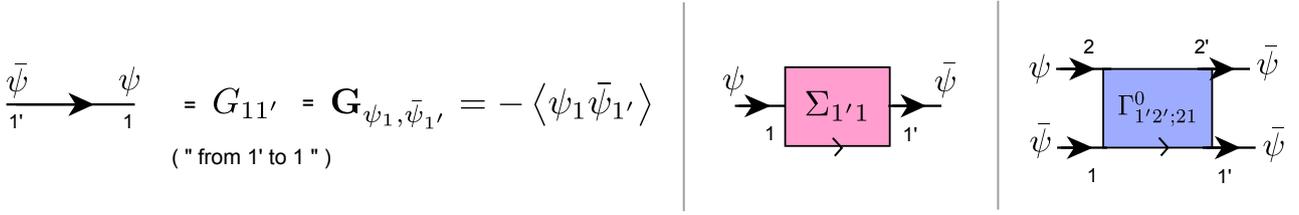


Figure 18: Diagrammatic conventions for fermionic field theories.

Interaction and vertex

- Assume total spin is conserved in bare scattering ($\{\sigma_1, \sigma_2\} \rightarrow \{\sigma_1, \sigma_2\}$).

$$S_1[\bar{\psi}, \psi] = \frac{1}{2} \sum_{\sigma_1, 2} \int_{K'_1 K'_2 K_1 K_2} \delta_{K'_1 + K'_2, K_2 + K_1} U_{\sigma_1 \sigma_2} (K'_1, K'_2; K_2, K_1) \bar{\psi}_{K'_1 \sigma_1} \bar{\psi}_{K'_2 \sigma_2} \psi_{K_2 \sigma_2} \psi_{K_1 \sigma_1} \quad (317)$$

The function U is symmetric under simultaneous exchange within first *and* last index pair.

$$U_{\sigma_1 \sigma_2} (K'_1, K'_2; K_2, K_1) = U_{\sigma_2 \sigma_1} (K'_2, K'_1; K_1, K_2) \quad (318)$$

The function U is not to be confused with the (bare) one-line irreducible vertex which is (anti-)symmetric under exchange of *all* of its arguments.

- *Partially* symmetrized vertex (can exchange within first *or* last index pair):

$$S_1[\bar{\psi}, \psi] = \frac{1}{(2!)} \int_{K'_1 \sigma'_1 K'_2 \sigma'_2 K_1 \sigma_1 K_2 \sigma_2} \delta_{K'_1 + K'_2, K_2 + K_1} \times \Gamma_0^{(4)} (K'_1 \sigma'_1, K'_2 \sigma'_2; K_2 \sigma_2, K_1 \sigma_1) \times \bar{\psi}_{K'_1 \sigma'_1} \bar{\psi}_{K'_2 \sigma'_2} \psi_{K_2 \sigma_2} \psi_{K_1 \sigma_1} \quad (319)$$

$$\Gamma_0^{(4)} (K'_1 \sigma'_1, K'_2 \sigma'_2; K_2 \sigma_2, K_1 \sigma_1) = \delta_{\sigma'_1 \sigma_1} \delta_{\sigma'_2 \sigma_2} U_{\sigma_1 \sigma_2}^{(4)} (K'_1, K'_2; K_2, K_1) - \delta_{\sigma'_1 \sigma_2} \delta_{\sigma'_2 \sigma_1} U_{\sigma_1 \sigma_2}^{(4)} (K'_1, K'_2; K_1, K_2) \quad (320)$$

- Superfield vertex with full (anti-)symmetry:

$$S_1[\Phi] = \frac{1}{4!} \int_{\alpha_1, 2, 3, 4} \Gamma_{\alpha_1 \alpha_2 \alpha_3 \alpha_4}^{(4), 0} \Phi_{\alpha_1} \Phi_{\alpha_2} \Phi_{\alpha_3} \Phi_{\alpha_4} \quad (321)$$

which leads to

$$\Gamma_{\alpha_1 = (\bar{\psi} K'_1 \sigma'_1), \alpha_2 = (\bar{\psi} K'_2 \sigma'_2), \alpha_3 = (\psi K_2 \sigma_2), \alpha_4 = (\psi K_1 \sigma_1)}^{(4), 0} = \delta_{K'_1 + K'_2, K_2 + K_1} \Gamma_0^{(4)} (K'_1 \sigma'_1, K'_2 \sigma'_2; K_2 \sigma_2, K_1 \sigma_1) \quad (322)$$

and $\Gamma_{\alpha_1 \alpha_2 \alpha_3 \alpha_4}^{(4)}$ 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 chose 2 = 6 possibilities to pick two $\bar{\psi}$ and two ψ fields in α -sums.

The fully (anti-)symmetric vertex is distinguished from the partially (anti-)symmetric vertex by the semicolon (;).

- In graphical representation of 4-point vertex and self-energy, $\bar{\psi}$ is outgoing arrow, ψ is in-going arrow. (Opposite to Green functions!)

Flow equations in $\Gamma^{(4)}$ truncation scheme

- From the general case above, we take the flow equations in terms of fully symmetric Γ :

$$\partial_\Lambda \Gamma_{\Lambda, \alpha_1 \alpha_2}^{(2)} = -\frac{1}{2} [\dot{\mathbf{G}}_\Lambda]_{\beta_1 \beta_2} \Gamma_{\Lambda, \beta_1 \beta_2 \alpha_1 \alpha_2}^{(4)} \quad (323)$$

and

$$\begin{aligned} \partial_\Lambda \Gamma_{\Lambda, \alpha_1 \dots \alpha_4}^{(4)} &= -\zeta \frac{1}{2} [\dot{\mathbf{G}}_\Lambda]_{\beta_1 \beta_2} [\mathbf{G}_\Lambda]_{\beta_3 \beta_4} \\ &\quad \{ \Gamma_{\Lambda, \beta_2 \beta_3 \alpha_3 \alpha_4}^{(4)} \Gamma_{\Lambda, \beta_4 \beta_1 \alpha_1 \alpha_2}^{(4)} + \Gamma_{\Lambda, \beta_2 \beta_3 \alpha_4 \alpha_1}^{(4)} \Gamma_{\Lambda, \beta_4 \beta_1 \alpha_3 \alpha_2}^{(4)} + \zeta \Gamma_{\Lambda, \beta_2 \beta_3 \alpha_2 \alpha_4}^{(4)} \Gamma_{\Lambda, \beta_4 \beta_1 \alpha_1 \alpha_3}^{(4)} \\ &\quad + \zeta \Gamma_{\Lambda, \beta_2 \beta_3 \alpha_3 \alpha_1}^{(4)} \Gamma_{\Lambda, \beta_4 \beta_1 \alpha_4 \alpha_2}^{(4)} + \Gamma_{\Lambda, \beta_2 \beta_3 \alpha_3 \alpha_2}^{(4)} \Gamma_{\Lambda, \beta_4 \beta_1 \alpha_4 \alpha_1}^{(4)} + \Gamma_{\Lambda, \beta_2 \beta_3 \alpha_1 \alpha_2}^{(4)} \Gamma_{\Lambda, \beta_4 \beta_1 \alpha_3 \alpha_4}^{(4)} \} \end{aligned} \quad (324)$$

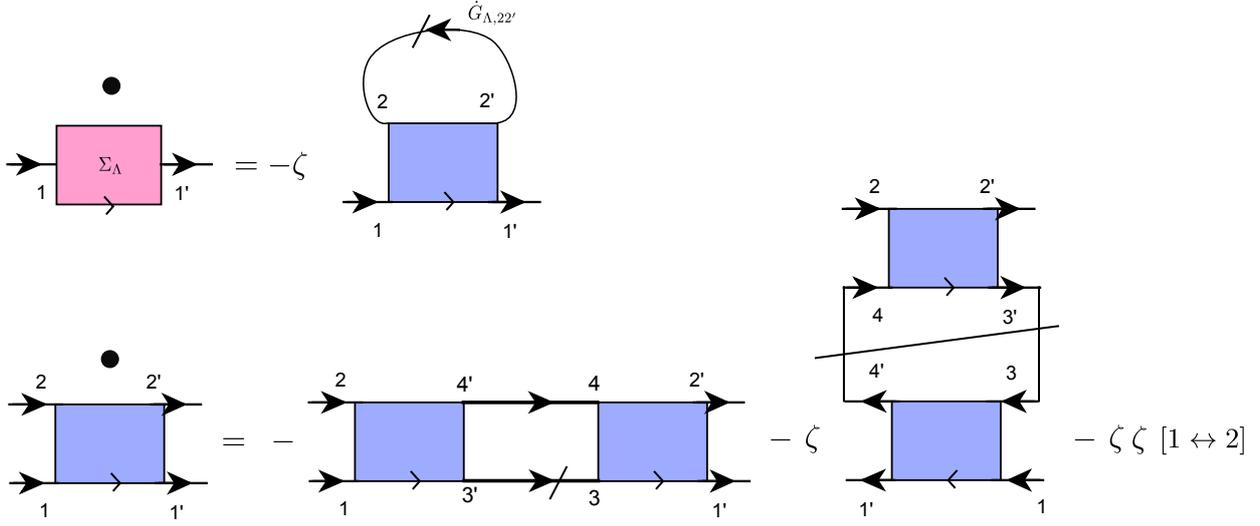


Figure 19: Fermionic fRG flow equations in diagrammatic convention. The last term amounts to exchanging the labels 1 and 2 in the previous diagram and multiplying the statistical factor ζ . The dash over a pair of propagators denotes a sum of the type $G\dot{G} + \dot{G}G$, see Eq. (326).

- Setting $j = (\underbrace{\psi K_j \sigma_j}_j)$ and $j' = (\underbrace{\bar{\psi} K_{j'} \sigma_{j'}}_{j'})$ [so the primes indicate $\bar{\psi}$] and picking $\alpha_1, \alpha_2 = 1'1$ for $\Gamma^{(2)}$, and similar $\alpha_1 \alpha_2 \alpha_3 \alpha_4 = 1'2'21$ for $\Gamma^{(4)}$, we obtain (see Fig. 19):

– For self energy:

$$\begin{aligned}
\partial_\Lambda \Sigma_{\Lambda, 1'1} &= \partial_\Lambda \Gamma_{\Lambda, \alpha_1 = \bar{\psi}_{1'}, \alpha_2 = \psi_1}^{(2)} \\
&= - \int_{22'} \frac{1}{2} \left([\dot{\mathbf{G}}_\Lambda]_{22'} \Gamma_{\Lambda, 22'1'1}^{(4)} + [\dot{\mathbf{G}}_\Lambda]_{2'2} \Gamma_{\Lambda, 2'2'1'1}^{(4)} \right) \\
&= -\zeta \int_{22'} [\dot{\mathbf{G}}_\Lambda]_{22'} \Gamma_{\Lambda, 1'2'21}^{(4)}
\end{aligned}$$

and we insert the conventions from above

$$\partial_\Lambda \Sigma_{\Lambda, 1'1} = -\zeta \int_{22'} \dot{G}_{\Lambda, 22'} \Gamma_\Lambda^{(4)}(1'2'; 21) \quad (325)$$

– Interaction vertex (see Ex. 6.5.4 for details):

$$\begin{aligned}
&\delta_{K'_1+K'_2, K_1+K_2} \partial_\Lambda \Gamma_\Lambda^{(4)}(1'2'; 21) = \quad (326) \\
&-\delta_{K'_3+K'_4, K_1+K_2} \delta_{K'_1+K'_2, K_3+K_4} \Gamma_\Lambda^{(4)}(1'2'; 43) \left[\dot{G}_{\Lambda, 33'} G_{\Lambda, 44'} \right] \Gamma_\Lambda^{(4)}(3'4'; 21) \\
&-\delta_{K'_3+K'_2, K_2+K_4} \delta_{K'_1+K'_4, K_3+K_1} \zeta \left(\dot{G}_{\Lambda, 33'} G_{\Lambda, 44'} + \dot{G}_{\Lambda, 44'} G_{\Lambda, 33'} \right) \Gamma_\Lambda^{(4)}(1'4'; 31) \Gamma_\Lambda^{(4)}(3'2'; 24) \\
&-\delta_{K'_4+K'_1, K_3+K_2} \delta_{K'_2+K'_3, K_4+K_1} \zeta^2 \left(\dot{G}_{\Lambda, 33'} G_{\Lambda, 44'} + \dot{G}_{\Lambda, 44'} G_{\Lambda, 33'} \right) \Gamma_\Lambda^{(4)}(1'4'; 32) \Gamma_\Lambda^{(4)}(3'2'; 14)
\end{aligned}$$

6.5 Exercises

6.5.1 Generating Functions for toy model

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

$$\begin{aligned}
s_0(\varphi) &= -\frac{\varphi^2}{2G_0}, \\
s_1(\varphi) &= \frac{u}{4!} \varphi^4,
\end{aligned}$$

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 $I_0 = Z$. This exercise should familiarize you with the concept of generating function(al)s in a simple setting.

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!*)

$$g_c(j), g_{ac}(\bar{\varphi}), \gamma(\bar{\varphi}) \quad (327)$$

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.

$$g_c(j) = \sum_{n=0}^{\infty} \frac{1}{n!} g_c^{(n)} j^n. \quad (328)$$

The Legendre transform should be denoted by

$$l(\varphi) = j(\varphi)\varphi - g_c(j(\varphi)), \\ \varphi = \partial_j g_c.$$

Show explicitly the two relations:

$$g_{ac}(\bar{\varphi}) = g_c(-G_0^{-1}\bar{\varphi}) + \bar{\varphi}^2/(2G_0), \\ 1 = \left(\frac{\partial^2 l}{\partial \varphi^2} \right) \left(\frac{\partial^2 g_c}{\partial j^2} \right).$$

2. Derive the following relations:

$g_c^{(0)} = \ln [Z/Z_0]$	$g_c^{(2)} = g^{(2)}$	$g_c^{(4)} = g^{(4)} - 3 [g^{(2)}]^2$
$g_{ac}^{(0)} = g_c^{(0)}$	$g_{ac}^{(2)} = G_0^{-2} [g_c^{(2)} + G_0]$	$g_{ac}^{(4)} = G_0^{-4} g_c^{(4)}$
$l^{(0)} = -g_c^{(0)}$	$l^{(2)} = [g_c^{(2)}]^{-1}$	$l^{(4)} = - [g_c^{(2)}]^{-4} g_c^{(4)}$
$\gamma^{(0)} = l^{(0)}$	$\gamma^{(2)} = l^{(2)} + G_0^{-1}$	$\gamma^{(4)} = l^{(4)}$

3. Use the results of part 1.) and 2.) to calculate the irreducible vertices 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. 6.5.3 to compare perturbation theory to the fRG for this toy model. You should obtain:

$$\gamma^{(0)} = \frac{u}{8} G_0^2 - \frac{u^2}{12} G_0^4, \quad \gamma^{(2)} = -\frac{u}{2} G_0 + \frac{5u^2}{12} G_0^3, \quad \gamma^{(4)} = u - \frac{3u^2}{2} G_0^2. \quad (329)$$

6.5.2 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. (245), (246) and (247) to find

$$\mathbf{G}_{c, \alpha_1 \dots \alpha_n}^{(n+2)} = - \sum_{\nu=0}^{\infty} \sum_{n_1=1}^{\infty} \dots \sum_{n_\nu=1}^{\infty} \frac{1}{n_1! \dots n_\nu!} \int_{\beta_1^1} \dots \int_{\beta_{n_1}^1} \dots \int_{\beta_1^\nu} \dots \int_{\beta_{n_\nu}^\nu} \\ \left(\sum_{m_1^1=1}^{\infty} \dots \sum_{m_{n_1}^1=1}^{\infty} \right) \dots \left(\sum_{m_1^\nu=1}^{\infty} \dots \sum_{m_{n_\nu}^\nu=1}^{\infty} \right) \delta_{n, \sum_{i=1}^{\nu} \sum_{j=1}^{n_i} m_j^i} \\ \times \mathbf{G} \left\{ \Gamma_{\beta_1^\nu \dots \beta_{n_\nu}^\nu}^{(n_\nu+2)} \mathbf{G} \right\} \dots \left\{ \Gamma_{\beta_1^1 \dots \beta_{n_1}^1}^{(n_1+2)} \mathbf{G} \right\} \mathbf{Z} \\ \times \mathcal{S}_{\alpha_1 \dots \alpha_{m_1^1}; \dots; \alpha_{n-m_{n_\nu}^\nu+1} \dots \alpha_n} \left\{ G_{c, \beta_1^1 \alpha_1 \dots \alpha_{m_1^1}}^{(m_1^1+1)} \dots G_{c, \beta_{n_\nu}^\nu \alpha_{n-m_{n_\nu}^\nu+1} \dots \alpha_n}^{(m_{n_\nu}^\nu+1)} \right\}$$

- Use the above result to derive the complete form of the tree expansion for $G_{c,\alpha_1\alpha_2\alpha_3\alpha_4}^{(4)}$, including the three-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.

6.5.3 fRG for toy-model

Consider the toy-model field theory of Ex. 6.5.1. The goal of this exercise is to derive and solve fRG flow equations for this simple model and compare the results with the exact and perturbative approach.

- Using the general results from the lecture, derive the flow equations for the generating functions $g_c(j)$, $g_{ac}(\bar{\varphi})$, $\gamma(\bar{\varphi})$.
- Use the following cutoff procedure $G_0 \rightarrow G_{0,\Lambda} = -\Lambda$ 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 $n = 0, 2, 4, 6$ and show explicitly

$$\begin{aligned}\partial_\Lambda \gamma_\Lambda^{(0)} &= \frac{1}{2} \frac{\gamma_\Lambda^{(2)}}{1 + \Lambda \gamma_\Lambda^{(2)}}, \\ \partial_\Lambda \gamma_\Lambda^{(2)} &= \frac{1}{2} \frac{\gamma_\Lambda^{(4)}}{(1 + \gamma_\Lambda^{(2)} \Lambda)^2}, \\ \partial_\Lambda \gamma_\Lambda^{(4)} &= \frac{1}{2} \frac{\gamma_\Lambda^{(6)}}{[1 + \Lambda \gamma_\Lambda^{(2)}]^2} - 3 \frac{\Lambda [\gamma_\Lambda^{(4)}]^2}{[1 + \Lambda \gamma_\Lambda^{(2)}]^3}, \\ \partial_\Lambda \gamma_\Lambda^{(6)} &= 45 \frac{\Lambda^2 [\gamma_\Lambda^{(4)}]^3}{[1 + \Lambda \gamma_\Lambda^{(2)}]^4} - 15 \frac{\Lambda \gamma_\Lambda^{(4)} \gamma_\Lambda^{(6)}}{[1 + \Lambda \gamma_\Lambda^{(2)}]^3} + \frac{1}{2} \frac{\gamma_\Lambda^{(8)}}{[1 + \Lambda \gamma_\Lambda^{(2)}]^2}.\end{aligned}$$

- Find the initial conditions for the quantities from 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 $\Lambda = 1$. In three plots over $u \in [0, 0.7]$, compare the following three quantities to the perturbative result of Ex. 6.5.1 and to the exact solution (from direct numerical evaluation of the integrals I_n in Ex. 6.5.1).

$$\begin{aligned}\gamma^{(0)} &= -\ln [Z/Z_0], \\ \gamma^{(2)} &= \Sigma, \\ \gamma^{(4)} &.\end{aligned}$$

6.5.4 Flow of fermionic vertex

Derive the flow equation for the fermionic 4-point vertex shown in Eq. (326) starting from the general equation (324).

6.5.5 Fermionic fRG for single-impurity Anderson model

The single impurity Anderson model ($H + H_l$, SIAM) can be used to model a quantum dot (Hamiltonian H) with single electronic energy level that is connected to one or more metallic leads (electrical contacts, Hamiltonian H_l). Only electrons of opposite spin meeting at the quantum dot are assumed to interact.

$$\begin{aligned}H &= \sum_{\sigma=\uparrow,\downarrow} \varepsilon_\sigma n_\sigma + U (n_\uparrow - 1/2) (n_\downarrow - 1/2) - \sum_l \sum_{\sigma=\uparrow,\downarrow} t_l \left(d_\sigma^\dagger c_{1,l,\sigma} + h.c. \right) \\ H_l &= -t \sum_\sigma \sum_{m=1}^{\infty} \left(c_{m,l,\sigma}^\dagger c_{m+1,l,\sigma} + h.c. \right)\end{aligned}$$

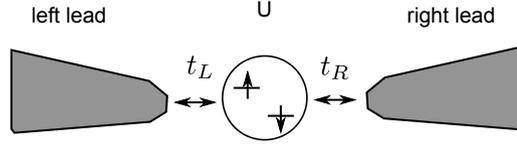


Figure 20: Sketch of the single impurity Anderson model.

Here, $n_\sigma = d_\sigma^\dagger d_\sigma$ describes the occupation of dot electrons with spin $\sigma = \uparrow, \downarrow$ and in $\uparrow \hat{=} +1$, $\downarrow \hat{=} -1$ is understood. The repulsive interaction is $U > 0$. The single-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.

1. The leads are non-interacting and can be integrated out exactly. Show that when seen from the quantum dot, they induce a self-energy for the d -electrons, $\Sigma_{l,\sigma}(i\omega) = |t_l|^2 \mathcal{G}_{l,1,1}(i\omega)$. Here $\mathcal{G}_{l,1,1}(i\omega)$ is the real-space Green function for the isolated lead l for the first site $m = 1$ which you should calculate exactly using the known eigenstates of the semi-infinite lead. Show that in the so called wide-band limit $|\omega| \ll t$,

$$\Sigma_{l,\sigma}(i\omega) = -i \text{sgn}(\omega) |t_l|^2 / t \equiv -i \text{sgn}(\omega) \Gamma_l. \quad (330)$$

As a consequence, the SIAM with left and right lead attached reduces to a single interacting site with a non-interacting Green function

$$G_{0,\sigma}(i\omega) = \frac{1}{i\omega - (V_g + \sigma h/2) + i \text{sgn}(\omega) \Gamma} \quad (331)$$

with $\Gamma = \Gamma_L + \Gamma_R$.

2. Introduce a Matsubara frequency cutoff $G_{0,\Lambda}(i\omega) = \theta(|\omega| - \Lambda) G_0(i\omega)$. In a first step, neglect the flow of the four-point vertex, i.e. set $\Gamma_\Lambda^{(4)}(\omega_1, \sigma, \omega_2, \bar{\sigma}; \omega_2, \bar{\sigma}, \omega_1, \sigma) \equiv U^\Lambda \stackrel{!}{=} U$. Here $\bar{\sigma} = -\sigma$. From the self-energy fRG flow equation, derive the flow of the effective level position $V_\sigma^\Lambda = V_g + \sigma h/2 + \Sigma_\sigma^\Lambda$ (excluding Γ):

$$\partial_\Lambda V_\sigma^\Lambda = \frac{U^\Lambda V_\sigma^\Lambda / \pi}{(\Lambda + \Gamma)^2 + (V_\sigma^\Lambda)^2}. \quad (332)$$

Confirm that the initial condition at large but finite Λ_i reads $V_\sigma^{\Lambda=\Lambda_i} = V_g + \sigma h/2$. Hint: This is not as trivial as it might seem, show that the contribution of the terms $U n_\sigma / 2$ 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 interaction term has to be considered.

3. Set $\Lambda_i = 100$, $h = 0$, $U/\Gamma = 1, 10$ or 25 and solve the flow equation numerically (e.g. with Mathematica) to obtain $V_\sigma \equiv V_\sigma^{\Lambda=0}$ as a function of V_g/U . Plot both the dot occupation $\langle n_\uparrow + n_\downarrow \rangle$ and the conductance $G(V_g)$ across the dot over $V_g/U \in [-4, 4]$. The conductance $g(V_g) = g_\uparrow(V_g) + g_\downarrow(V_g)$ can be calculated from $g_\sigma(V_g) = \frac{e^2}{h} \pi \Gamma \rho_\sigma(0)$ where $\rho_\sigma(\omega) = -\frac{1}{\pi} \text{Im} G_\sigma(\omega + i0^+)$ is the dot spectral function analytically continued to real frequencies. Fact: The simple expression for the conductance stems from the Kubo formula, it only applies for $T = 0$, zero frequency, zero voltage and a single interacting site.
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

$$\partial_\Lambda U^\Lambda = \frac{2 (U^\Lambda)^2 V_\uparrow^\Lambda V_\downarrow^\Lambda / \pi}{\left[(\Lambda + \Gamma)^2 + (V_\uparrow^\Lambda)^2 \right] \left[(\Lambda + \Gamma)^2 + (V_\downarrow^\Lambda)^2 \right]}. \quad (333)$$

Part II

Non-equilibrium and Keldysh formalism

7 Quantum dynamics and real-time Green functions

7.1 Expectation values

- Quantum average of observable O : $\langle O \rangle = \frac{1}{\text{tr}\rho} \text{tr}[O\rho]$ where ρ is the density matrix that describes the state of the system and $\text{tr}\dots = \sum_n \langle n|\dots|n \rangle$ is the sum over expectation values of a basis.
- So far: Thermal equilibrium (in contact with bath of temperature T):
 - Canonical ensemble $\rho = e^{-\beta H}$
 - With particle exchange: Grand canonical ensemble $e^{-(H-\mu N)\beta}$, the trace is also over all particle numbers.
- Non-equilibrium: Not necessarily a bath present, possibly time-dependent Hamiltonian. Assume state is known at $t = t_0 \rightarrow -\infty$, e.g. $\rho(t_0) = e^{-\beta H}$.

7.2 Dynamics in Schrödinger and Heisenberg picture

- Schrödinger picture: State evolves in time, operators have only explicit time dependence,

$$|\psi(t)\rangle = U(t, t_0) |\psi(t_0)\rangle \quad (1)$$

or for density matrix (von-Neumann equation)

$$\rho(t) = U(t, t_0)\rho_0 U(t_0, t) \quad (2)$$

- Preparation: Time ordering operator for general operators A, B , puts *later times to the left*:

$$T_t [A(t)B(t')] = \begin{cases} A(t)B(t') & : t > t' \\ \zeta B(t')A(t) & : t' > t \end{cases} \quad (3)$$

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* :

$$U(t, t_0) = T_t \exp \left[-i \int_{t_0}^t d\tau H(\tau) \right] \quad (4)$$

is solution of Schrödinger equation (since $H(t)$ always appears on the left, interpret exponent as power series):

$$i\partial_t U(t, t_0) = H(t)U(t, t_0). \quad (5)$$

- 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 H : $U(t, t_0) = e^{-iH(t-t_0)}$.

- Time evolution of expectation value of operator O :

$$\langle O \rangle(t) = \frac{1}{\text{tr}\rho_0} \text{tr} [OU(t, t_0)\rho_0 U(t_0, t)] \stackrel{\text{cycl.}}{=} \frac{1}{\text{tr}\rho_0} \text{tr} \left[\underbrace{U(t_0, t)OU(t, t_0)}_{\equiv O(t) \text{ Heisenberg pic.}} \rho_0 \right] = \langle O(t) \rangle \quad (6)$$

7.3 Zoo of real-time Green functions

Goal: Above: Expectation values with single time argument, now: *two* time arguments.

- Operators A, B :
 - $A(t), B(t)$ in Heisenberg picture.
 - do not need to be hermitian.
 - with $\zeta = \pm 1$ for bosonic or fermionic operators

- Greater and lesser GF [correlation functions]:

$$\begin{aligned} G_{AB}^>(t, t') &= -i \langle A(t)B(t') \rangle \\ G_{AB}^<(t, t') &= -i\zeta \langle B(t')A(t) \rangle \end{aligned}$$

- Retarded and advanced GF [response functions \rightarrow Kubo]:
(with $\theta(0) \equiv 1/2$ and $[A, B]_\zeta = AB - \zeta BA$ is commutator or anti-commutator)

$$\begin{aligned} G_{AB}^R(t, t') &\equiv -i\theta(t-t') \langle [A(t), B(t')]_\zeta \rangle \\ &= +\theta(t-t') (G_{AB}^>(t, t') - G_{AB}^<(t, t')) \end{aligned}$$

$$\begin{aligned} G_{AB}^A(t, t') &\equiv +i\theta(t'-t) \langle [A(t), B(t')]_\zeta \rangle \\ &= +\theta(t'-t) (G_{AB}^<(t, t') - G_{AB}^>(t, t')) \end{aligned}$$

The retarded $G_{AB}^R(t, t')$ is only non-vanishing for $t - t' \geq 0$, the advanced $G_{AB}^A(t, t')$ for $t - t' \leq 0$.

- Relations at time t, t' :

$$\begin{aligned} G_{AB}^{\lessgtr}(t, t') &= -G_{B^\dagger A^\dagger}^{\lessgtr}(t', t)^* \\ G_{AB}^>(t, t') &= \zeta G_{BA}^<(t', t) \\ G_{B^\dagger A^\dagger}^A(t', t) &= G_{AB}^R(t, t')^* \\ G_{BA}^A(t', t) &= \zeta G_{AB}^R(t, t') \end{aligned}$$

Equal time relations [recall $\theta(0) = 1/2$]:

$$\begin{aligned} G^R(t, t) + G^A(t, t) &= 0 \\ G^R(t, t) - G^A(t, t) &= -i [A, B]_\zeta \end{aligned}$$

- Time ordered GF (for computation):

$$\begin{aligned} G_{A,B}^T(t, t') &= -i \langle T_t A(t)B(t') \rangle \\ &= \theta(t-t') G_{AB}^>(t, t') + \theta(t'-t) G_{AB}^<(t, t') \end{aligned}$$

and anti-time ordered GF

$$\begin{aligned} G_{A,B}^{\tilde{T}}(t, t') &= -i \langle \tilde{T}_t A(t)B(t') \rangle \\ &= \theta(t'-t) G_{AB}^>(t, t') + \theta(t-t') G_{AB}^<(t, t') \end{aligned}$$

- Redundancy relation:

$$G_{A,B}^T(t, t') + G_{A,B}^{\tilde{T}}(t, t') - G_{AB}^>(t, t') - G_{AB}^<(t, t') = 0 \quad (7)$$

- For later: Keldysh GF:

$$G_{A,B}^K(t, t') \equiv G_{A,B}^{<}(t, t') + G_{A,B}^{>}(t, t') \quad (8)$$

and the above relations imply the “anti-hermitian” property::

$$G_{A,B}^K(t, t') = -G_{B^\dagger, A^\dagger}^K(t, t')^* \quad (9)$$

Parametrization with hermitian matrix F :

$$\begin{aligned} G^K(t, t') &= \int dt'' \left[G^R(t, t'') F(t'', t') - F(t, t'') G^A(t'', t') \right] \\ &\rightarrow G^K = G^R \cdot F - F \cdot G^A \end{aligned}$$

- Temporal FT for stationary state where $G(t, t') \stackrel{!}{=} G(t - t')$:

$$\begin{aligned} G(\omega) &= \int_{-\infty}^{\infty} dt e^{i\omega t} G(t) \\ G(t) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega t} G(\omega) \end{aligned}$$

7.4 Green functions in thermal equilibrium and Fluctuation-dissipation theorem

- In equilibrium, we can work in frequency representation.
All GFs can be calculated from the *spectral density*:

$$\boxed{A_{A,B}(\omega) \equiv iG_{A,B}^R(\omega) - iG_{B^\dagger, A^\dagger}^R(\omega)^*} \quad (10)$$

- Definition: “Real” and “imaginary” parts of Green function (not the same as for complex numbers).
Applies for retarded, advanced and time-ordered GF:

$$G^{(T,R,A)} = \Re G^{(T,R,A)} + i\Im G^{(T,R,A)} \quad (11)$$

$$\begin{aligned} \Re G_{A,B}^{(T,R,A)}(\omega) &\equiv \frac{1}{2} \left(G_{A,B}^{(T,R,A)}(\omega) + G_{B^\dagger, A^\dagger}^{(T,R,A)}(\omega)^* \right) \\ \Im G_{A,B}^{(T,R,A)}(\omega) &\equiv \frac{1}{2i} \left(G_{A,B}^{(T,R,A)}(\omega) - G_{B^\dagger, A^\dagger}^{(T,R,A)}(\omega)^* \right) \end{aligned}$$

Relations:

$$\boxed{\Re G^R = \Re G^A = \Re G^T} \quad (12)$$

$$\Im G^R = -\Im G^A = -\frac{1}{2} A \quad (13)$$

- Integral relation (only for eq.!): Shift t-integration from real axis to the line $t - i\beta$:

$$\int dt e^{i\omega t} \langle A(t)B(0) \rangle = e^{\omega\beta} \int dt e^{i\omega t} \langle B(0)A(t) \rangle \quad (14)$$

- Use the above to get for retarded and advanced GF:

$$\begin{aligned} \Im G_{A,B}^R(\omega) &= -\Im G_{A,B}^A(\omega) \\ &= -\frac{1}{2} \int_{-\infty}^{\infty} dt e^{i\omega t} \langle A(t)B(0) - \zeta B(0)A(t) \rangle \\ &= -\frac{i}{2} \left(1 - \zeta e^{-\omega\beta} \right) G_{A,B}^{>}(\omega) \end{aligned} \quad (15)$$

and similar for time-ordered GF

$$\Im G_{A,B}^T(\omega) = -\frac{i}{2} \left(1 + \zeta e^{-\omega\beta}\right) G_{A,B}^>(\omega)$$

Combining the last two equations, we find

$$\boxed{\Im G^R = -\Im G^A = \frac{1 - \zeta e^{-\beta\omega}}{1 + \zeta e^{-\beta\omega}} \Im G^T(\omega)} \quad (16)$$

- $\Im G_{A,B}^R(\omega)$ determines full $G_{A,B}^R(\omega)$: Find full retarded GF with $\theta(t) = \frac{1}{2\pi i} \int_{-\infty}^{+\infty} d\omega' \frac{e^{i\omega't}}{\omega - i\eta}$ and convolution:

$$\begin{aligned} G_{A,B}^R(\omega) &= -\frac{1}{2\pi} \int_{-\infty}^{+\infty} d\omega' \frac{1}{\omega' - \omega - i\eta} \int_{-\infty}^{\infty} dt e^{i\omega't} \langle A(t)B(0) - \zeta B(0)A(t) \rangle \\ [(15)] &= \frac{1}{\pi} \int_{-\infty}^{+\infty} d\omega' \frac{\Im G_{A,B}^R(\omega')}{\omega' - \omega - i\eta} \\ &= \frac{1}{\pi} \int_{-\infty}^{+\infty} d\omega' \frac{-\frac{1}{2} A_{A,B}(\omega')}{\omega' - \omega - i\eta} \end{aligned}$$

- Similar:

$$\begin{aligned} G_{A,B}^>(\omega) &= -\frac{i A_{A,B}(\omega)}{1 - \zeta e^{-\omega\beta}} \\ G_{A,B}^<(\omega) &= +\frac{i A_{A,B}(\omega)}{1 - \zeta e^{+\omega\beta}} \end{aligned}$$

- Keldysh GF:

$$\boxed{G_{A,B}^K(\omega) \equiv G_{A,B}^<(\omega) + G_{A,B}^>(\omega) = -i A_{AB}(\omega) \frac{e^{\beta\omega} + \zeta}{e^{\beta\omega} - \zeta} = [G^R(\omega) - G^A(\omega)] \frac{e^{\beta\omega} + \zeta}{e^{\beta\omega} - \zeta}} \quad (17)$$

This is also called the fluctuation - dissipation theorem. It only holds in equilibrium.

Fluctuation is related to the equilibrium correlation function G^{\lessgtr} , dissipation to the imaginary part of the response functions $\Im G^R$.

7.5 Contour ordered Green function

- Assume the state of a system at $t \rightarrow -\infty$, $\rho(-\infty)$ is known. Recall Eq. (6) for expectation value of operator O :

$$\langle O \rangle(t) = \frac{1}{\text{tr}\rho(t)} \text{tr} [U(-\infty, t) O U(t, -\infty) \rho(-\infty)]$$

This is shown schematically in Fig. 21(a) in solid lines.

- Extend the time evolution from $-\infty$ to $+\infty$ (top) and back (bottom), see dashed contour also called *Keldysh-contour*. Formally, insert $1 = U(t, +\infty) U(+\infty, t)$ in front of O :

$$\begin{aligned} \langle O \rangle(t) &= \frac{1}{\text{tr}\rho(t)} \text{tr} [U(-\infty, t) U(t, +\infty) U(+\infty, t) O U(t, -\infty) \rho(-\infty)] \\ &= \frac{1}{\text{tr}\rho(t)} \text{tr} [U(-\infty, +\infty) U(+\infty, t) O U(t, -\infty) \rho(-\infty)] \end{aligned}$$

Note: Operator O could equally well be inserted on backward branch of contour, standard choice: $O/2$ on both branches.

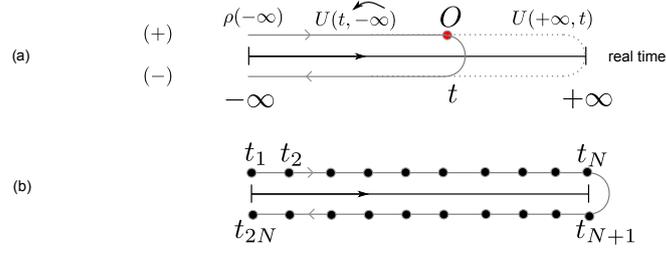


Figure 21: (a) Expectation value $\langle O(t) \rangle$ evaluated on the Keldysh contour. (b) Time-slice convention for the construction of functional integral representation of partition function.

- Two operators A, B on contour (either on top $[+]$ or bottom branch $[-]$):
Define contour ordering operator T_c in analogy to time-ordering operator (move lower branch to left).
Contour-ordered Green function:

$$G_{A,B}(t, t') \equiv -i \langle T_c A_{\pm}(t) B_{\pm}(t') \rangle = \begin{pmatrix} G_{A,B}^T(t, t') & G_{A,B}^<(t, t') \\ G_{A,B}^>(t, t') & G_{A,B}^T(t, t') \end{pmatrix} = \begin{pmatrix} \text{time ordered} & \text{lesser} \\ \text{greater} & \text{anti-time ordered} \end{pmatrix} \quad (18)$$

7.6 Exercises

7.6.1 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

$$H = \frac{1}{2m} p^2 + \frac{1}{2} m \omega_0^2 x^2 \quad (19)$$

where momentum and position operators satisfy $[p, p] = 0 = [x, x]$ and $[p, x] = -i$.

1. Introduce the bosonic creation operator $a = x\sqrt{m\omega_0/2} + ip/\sqrt{2m\omega_0}$ to rewrite 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 $a^\dagger(t)$. Assume thermal equilibrium at temperature T , find the greater and lesser Green functions $G_{aa^\dagger}^{\gtrless}$, the retarded and advanced Green function $G_{aa^\dagger}^{R,A}$ and the time ordered Green function $G_{aa^\dagger}^T$, 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

$$G_{xx}^R(t) = -\theta(t) \frac{1}{m\omega_0} \sin(\omega_0 t). \quad (20)$$

Find the same result from the equation-of-motion technique, which does not require a diagonalization of the Hamiltonian: Take the definition of $G_{xx}^R(t)$, apply two t -derivatives and solve the resulting differential equation.

8 Keldysh functional integral

8.1 Generating function $Z[V]$

- Define time-evolution operator on closed time contour c :

$$U_c \equiv U(-\infty, +\infty) U(+\infty, -\infty) = 1 \quad (21)$$

- Add source-terms: $H(t) \rightarrow H^\pm(t) = H(t) \pm OV(t)$ where $V(t)$ is a function and H^+ is applied on forward branch of c , H^- on backward branch. Thus

$$U_c \rightarrow U_c[V] \quad (22)$$

- “Partition function” (generating function)

$$\boxed{Z[V] \equiv \frac{1}{\text{tr}\rho(-\infty)} \text{tr} \{U_c[V] \rho(-\infty)\}} \quad (23)$$

We can compute $\langle O \rangle(t)$ from generating functional as

$$\langle O \rangle(t) = \frac{i}{2} \frac{\delta Z[V]}{\delta V(t)} \Big|_{V=0} \quad (24)$$

Proof:

$$\begin{aligned} \frac{i}{2} \frac{\delta Z[V]}{\delta V(t)} \Big|_{V=0} &= \frac{i}{2} \frac{1}{\text{tr}\rho(-\infty)} \text{tr} \left\{ \frac{\delta}{\delta V(t)} U_c[V] \rho(-\infty) \right\} \Big|_{V=0} \\ &= \frac{i}{2} \frac{1}{\text{tr}\rho(-\infty)} \\ &\quad \text{tr} \left\{ \frac{\delta U_{-V}(-\infty, +\infty)}{\delta V(t)} U_{+V}(+\infty, -\infty) \rho(-\infty) + U_{-V}(-\infty, +\infty) \frac{\delta U_{+V}(+\infty, -\infty)}{\delta V(t)} \rho(-\infty) \right\} \Big|_{V=0} \end{aligned}$$

and use

$$\begin{aligned} \frac{\delta U_{+V}(+\infty, -\infty)}{\delta V(t)} \Big|_{V=0} &= \frac{\delta}{\delta V(t)} T_t \exp \left[-i \int_{-\infty}^{+\infty} d\tau H(\tau) + OV(\tau) \right] \Big|_{V=0} \\ &= U(+\infty, t) (-iO) U(t, -\infty) \end{aligned}$$

- Remarks:

- Without source field, partition function is normalized: $Z[V=0] = 1$.
- If source-field is different on the two branches, have $U_c[V] \neq 1$ and $Z[V] \neq 1$.

8.2 Functional integral representation for $Z[V]$ (Bosons)

General construction

- 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 $l = 1, 2, \dots, M$:

$$H(a^\dagger, a) = \sum_{l,m} t_{lm} a_l^\dagger a_m + \sum_{l,m,n,o} U_{lmno} a_l^\dagger a_m^\dagger a_n a_o \quad (25)$$

- Take standard steps to coherent state functional integral, pay attention to (+) or (-) contour.
- Slice closed time contour c into $2N - 2$ intervals so that $t_1 = -\infty = t_{2N}$ and $t_N = +\infty = t_{N+1}$, see Fig. 21(b).
- Insert resolution of identity operator using 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	$\langle\phi \psi\rangle = e^{\sum_l \phi_l^* \psi_l}$
action of a_l	$a_l \phi\rangle = \phi_l \phi\rangle$	identity	$1 = \int \prod_l \frac{d\phi_l^* d\phi_l}{\pi} e^{-\sum_l \phi_l^* \phi_l} \phi\rangle \langle\phi $ $d(\phi^*, \phi)$
action of a_l^\dagger	$\langle\phi a_l^\dagger = \langle\phi \phi_l^*$	trace	$\text{tr} O = \int d(\phi^*, \phi) e^{-\sum_l \phi_l^* \phi_l} \langle\phi O \phi\rangle$
useful identity	$\langle\phi e^{a^\dagger a} \psi\rangle = e^{\phi^* \psi c}$		

- The last identity is non-standard for equilibrium applications, it can be proven as follows: $f(c) = \langle\phi| e^{a^\dagger a} |\psi\rangle$, $\partial_c f(c) = \langle\phi| a^\dagger a c^{a^\dagger a - 1} |\psi\rangle$. We note that for an arbitrary function g , we have $g(a^\dagger a) a = a g(a^\dagger a - 1)$. This is clear by acting on basis vector $|n\rangle$ which yields $g(a^\dagger a) a |n\rangle = g(n-1) \sqrt{n} |n-1\rangle$ on the left and on the right $a g(a^\dagger a - 1) |n\rangle = \sqrt{n} g(n-1) |n\rangle$. Then we find $\partial_c f(c) = \langle\phi| a^\dagger a c^{a^\dagger a - 1} |\psi\rangle = \langle\phi| a^\dagger e^{a^\dagger a} a |\psi\rangle = \phi^* \psi f(c)$. This can be uniquely solved as $f(c) = e^{c \phi^* \psi}$ since indeed $f(c=1) = \langle\phi|\psi\rangle = e^{\phi^* \psi}$.
- We label time-steps by $j = 1, 2, \dots, 2N$: We use the formula for the trace and $U_c = U_{-\delta t} \dots U_{-\delta t} \cdot 1 \cdot U_{\delta t} \dots U_{\delta t}$ for the second step:

$$\begin{aligned}
Z &= \frac{1}{\text{tr} \rho} \text{tr} \{U_c \rho\} \\
&= \frac{1}{\text{tr} \rho} \int d(\phi_{2N}^*, \phi_{2N}) e^{-\sum_l |\phi_{2N,l}|^2} \langle\phi_{2N}| U_c \rho |\phi_{2N}\rangle \\
&= \frac{1}{\text{tr} \rho} \int \prod_{j=1}^{2N} d(\phi_j^*, \phi_j) \langle\phi_{2N}| U_{-\delta t} |\phi_{2N-1}\rangle \cdots \langle\phi_{N+2}| U_{-\delta t} |\phi_{N+1}\rangle \langle\phi_{N+1}| 1 |\phi_N\rangle \\
&\quad \times \langle\phi_N| U_{\delta t} |\phi_{N-1}\rangle \cdots \langle\phi_2| U_{\delta t} |\phi_1\rangle \langle\phi_1| \rho |\phi_{2N}\rangle \exp \left[-\sum_{j=1}^{2N} \sum_{l=1}^M |\phi_{n,l}|^2 \right]
\end{aligned}$$

Evaluate matrix elements for $\delta t \rightarrow 0$ (keep $[2N-2]dt$ fixed) where we use that H is normal ordered and approximately time-independent on a time-scale δt :

$$\begin{aligned}
\langle\phi_j| U_{\pm\delta t} |\phi_{j-1}\rangle &= \langle\phi_j| e^{\mp i\delta t H(a_l^\dagger, a_l)} |\phi_{j-1}\rangle \\
&= \langle\phi_j| 1 \mp i\delta t H(a_l^\dagger, a_l) + \mathcal{O}(\delta t^2) |\phi_{j-1}\rangle \\
&= \langle\phi_j| \phi_{j-1}\rangle \left[1 \mp i\delta t H(\phi_{j,l}^*, \phi_{j-1,l}) + \mathcal{O}(\delta t^2) \right] \\
&= e^{\phi_j^* \phi_{j-1}} \left[e^{\mp i\delta t H(\phi_{j,l}^*, \phi_{j-1,l})} + \mathcal{O}(\delta t^2) \right]
\end{aligned}$$

Insert in expression for Z (suppress l and recall $\phi_{N+1} = \phi_N$):

$$Z = \frac{1}{\text{tr} \rho} \int \prod_{j=1}^{2N} d(\phi_j^*, \phi_j) \exp \left[\sum_{j=2}^{2N} \phi_j^* \phi_{j-1} - i\delta t \sum_{j=2}^N H(\phi_j^*, \phi_{j-1}) + i\delta t \sum_{j=N+2}^{2N} H(\phi_j^*, \phi_{j-1}) - \sum_{j=1}^{2N} |\phi_j|^2 \right] \langle\phi_1| \rho |\phi_{2N}\rangle \quad (26)$$

Example: Single bosonic mode

- Consider single bosonic mode $H = \omega_0 a^\dagger a$ starting out in equilibrium:

$$\rho(-\infty) \equiv \rho = e^{-\beta H} = e^{-\beta \omega_0 a^\dagger a} \quad (27)$$

- Preparations:

– Normalization: $\text{tr} \rho = \sum_{n=0}^{\infty} e^{-\beta \omega_0 n} = 1/(1 - e^{-\beta \omega_0})$.

– with identity from table: $\langle \phi_1 | e^{-\beta\omega_0 a^\dagger a} | \phi_{2N} \rangle = \exp(e^{-\beta\omega_0} \phi_1^* \phi_{2N})$

- Find matrix iG^{-1} in:

$$Z = \frac{1}{\text{tr}\rho} \int \prod_{j=1}^{2N} d(\phi_j^*, \phi_j) \exp \left[i \sum_{j,j'=1}^{2N} \phi_j^* G_{jj'}^{-1} \phi_{j'} \right] \quad (28)$$

with the $2N \times 2N$ -matrix (here $N = 3$)

$$i [G^{-1}]_{jj'} = \begin{pmatrix} -1 & 0 & 0 & 0 & 0 & e^{-\beta\omega_0} \\ h_- & -1 & 0 & 0 & 0 & 0 \\ 0 & h_- & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 0 & h_+ & -1 & 0 \\ 0 & 0 & 0 & 0 & h_+ & -1 \end{pmatrix} \quad (29)$$

where $h_- = 1 - i\delta t\omega_0$ and $h_+ = 1 + i\delta t\omega_0$.

- Check normalization $Z = 1$: The functional integral yields $1/\det(-iG^{-1})$. Expand the determinant with respect to the top row, use for upper or lower triangular matrix: $\det T = t_{11}t_{22}\dots$,

$$\begin{aligned} \det(-iG^{-1}) &= \det([iG]^{-1}) \\ &= (-1)(-1)^{2N-1} - e^{-\beta\omega_0} (1 - i\delta t\omega_0)^{N-1} 1 (1 + i\delta t\omega_0)^{N-1} \\ &= 1 - e^{-\beta\omega_0} (1 + \delta t^2 \omega_0^2)^{N-1} \\ &= 1 - e^{-\beta\omega_0} \left(1 + (N-1) \frac{\delta t^2 \omega_0^2}{N-1} \right)^{N-1} \\ &\simeq 1 - e^{-\beta\omega_0} \exp[(N-1)\delta t^2 \omega_0^2] \\ \{\delta t N = \text{const.}\} &\simeq 1 - e^{-\beta\omega_0} \end{aligned}$$

As a result, normalization is confirmed:

$$Z = \frac{1 - e^{-\beta\omega_0}}{1 - e^{-\beta\omega_0}} = 1. \quad (30)$$

Continuum limit

- Take continuum limit as $N \rightarrow \infty$, $\delta t \rightarrow 0$ with $N\delta t = \text{const.}$
- For forward branch $\phi_{j=1,2,\dots,N} \rightarrow \phi_+(t)$, $\sum_{j=1}^N \delta t \rightarrow \int_{-\infty}^{+\infty} dt$, and $\phi_j^* \phi_{j-1} - \phi_j^* \phi_j = -\delta t \phi_j^* \frac{\phi_j - \phi_{j-1}}{\delta t} \rightarrow -\phi_+^*(t) \partial_t \phi_+(t)$.
Likewise on backward branch.

- Find:

$$Z = \int_{\phi_+(\infty)=\phi_-(\infty)} D[\phi_+^*, \phi_+, \phi_-^*, \phi_-] e^{iS[\phi_+, \phi_-]} \langle \phi_+(-\infty) | \rho | \phi_-(-\infty) \rangle \quad (31)$$

with

$$\begin{aligned} S[\phi_+, \phi_-] &= + \int_{-\infty}^{+\infty} dt \left[\sum_l \phi_{+,l}^*(t) i \partial_t \phi_{+,l}(t) - H[\phi_+^*(t), \phi_+(t)] \right] \\ &\quad - \int_{-\infty}^{+\infty} dt \left[\sum_l \phi_{-,l}^*(t) i \partial_t \phi_{-,l}(t) - H[\phi_-^*(t), \phi_-(t)] \right] \end{aligned}$$

and

$$D[\phi_+^*, \phi_+, \phi_-^*, \phi_-] \equiv \frac{1}{\text{tr}\rho} \cdot \lim_{N \rightarrow \infty} \int \prod_{j=1}^{2N} d(\phi_j^*, \phi_j) \quad (32)$$

- Remarks:

- Keep in mind: Continuum notation is just an abbreviation for discrete form.
- Compare to equilibrium formalism, $Z = \int D[\phi^*, \phi] e^{-S[\phi]}$ with $S = \int_0^\beta d\tau \phi^*(\tau) \partial_\tau \phi(\tau) + H[\phi^*(\tau), \phi(\tau)]$. 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 $\langle \phi_+(-\infty) | \rho | \phi_-(-\infty) \rangle$. These are the entries of the off-diagonal blocks of $i[G^{-1}]$ in Eq. (29).

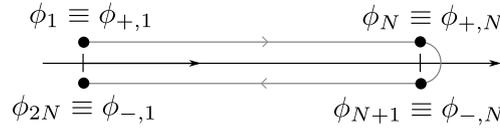
Green functions (for single bosonic mode)

- Find two-point function (no factor of $1/Z!$), use Gaussian integral identity:

$$\langle T_c a_j a_{j'}^\dagger \rangle = \langle \phi_j \phi_{j'}^* \rangle \equiv \frac{1}{\text{tr} \rho} \int \prod_{k=1}^{2N} d(\phi_k^*, \phi_k) \phi_j \phi_{j'}^* \exp \left[i \sum_{k,k'=1}^{2N} \phi_k^* G_{kk'}^{-1} \phi_{k'} \right] = i G_{jj'} \quad (33)$$

- 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)

$$iG = \frac{1}{\det(-iG^{-1})} \begin{bmatrix} 1 & \rho h_+^2 h_- & \rho h_+^2 & \rho h_+^2 & \rho h_+ & \rho \\ h_- & 1 & \rho h_+^2 h_- & \rho h_+^2 h_- & \rho h_+ h_- & \rho h_- \\ h_-^2 & h_- & 1 & \rho h_+^2 h_-^2 & \rho h_+ h_-^2 & \rho h_-^2 \\ h_-^2 & h_- & 1 & 1 & \rho h_-^2 h_+ & \rho h_-^2 \\ h_-^2 h_+ & h_- h_+ & h_+ & h_+ & 1 & \rho h_-^2 h_+ \\ h_-^2 h_+^2 & h_- h_+^2 & h_+^2 & h_+^2 & h_+ & 1 \end{bmatrix} \begin{pmatrix} \phi_1 = \phi_{+,1} \\ \vdots \\ \phi_N = \phi_{+,N} \\ \phi_{N+1} = \phi_{-,N} \\ \vdots \\ \phi_{2N} = \phi_{-,1} \end{pmatrix} \quad (34)$$



- Read off four different propagators $G^{\lessgtr, T, \bar{T}}$ defined above, depending on choice of ϕ_\pm :

$$\begin{aligned} iG_{jl}^< &\equiv \langle \phi_{+,j} \phi_{-,l}^* \rangle = \frac{e^{-\beta \omega_0} h_+^{l-1} h_-^{j-1}}{\det(-iG^{-1})} \\ iG_{jl}^> &\equiv \langle \phi_{-,j} \phi_{+,l}^* \rangle = \frac{h_+^{N-j} h_-^{N-l}}{\det(-iG^{-1})} \\ iG_{jl}^T &\equiv \langle \phi_{+,j} \phi_{+,l}^* \rangle = \frac{h_-^{j-l}}{\det(-iG^{-1})} \begin{cases} 1 & : j \geq l \\ e^{-\beta \omega_0} (h_+ h_-)^{N-1} & : j < l \end{cases} \\ iG_{jl}^{\bar{T}} &\equiv \langle \phi_{-,j} \phi_{-,l}^* \rangle = \frac{h_+^{l-j}}{\det(-iG^{-1})} \begin{cases} e^{-\beta \omega_0} (h_+ h_-)^{N-1} & : j > l \\ 1 & : j \leq l \end{cases} \end{aligned}$$

- Continuum limit, $(h_+ h_-)^N \rightarrow 1$ as before. Use $h_\pm^j = \left(1 \pm i \frac{\delta t j}{j} \omega_0\right)^j \rightarrow e^{\pm i \omega_0 \delta t j} = e^{\pm i \omega_0 t}$, and $\det(-iG^{-1}) = 1 - e^{-\beta \omega_0}$ and the boson number $n_B = \frac{e^{-\beta \omega_0}}{1 - e^{-\beta \omega_0}} = \frac{1}{e^{\beta \omega_0} - 1}$

$$\begin{aligned} iG^<(t, t') &= n_B e^{-i \omega_0 (t-t')} \\ iG^>(t, t') &= (n_B + 1) e^{-i \omega_0 (t-t')} \end{aligned}$$

$$G^T(t, t') = \begin{cases} G^>(t, t') & : t \geq t' \\ G^<(t, t') & : t < t' \end{cases} \quad (35)$$

$$G^{\tilde{T}}(t, t') = \begin{cases} G^>(t, t') & : t' \geq t \\ G^<(t, t') & : t' < t \end{cases} \quad (36)$$

Up to the case $t = t'$ (see below), this is in agreement with the result from the operator formalism in Sec. 7.3 and Ex. 7.6.1.

- Equal times: The last two lines differ from the convention $\theta(0) = 1/2$ put forward in Sec. 7.3! This should not bother us because:
 - In any of the two conventions: $G^R(t, t) + G^A(t, t) = G^T(t, t) - G^{\tilde{T}}(t, t) = 0$ and $G^R(t, t) - G^A(t, t) = G^>(t, t) - G^<(t, t) = -i$ (the commutator). This is what matters for practical calculations.
 - The redundancy relation (7) is modified at equal times:

$$G^T(t, t') + G^{\tilde{T}}(t, t') - G^>(t, t') - G^<(t, t') = \begin{cases} 0 & : t \neq t' \\ 1 & : t = t' \end{cases} \quad (37)$$

The right hand side is defines a manifold of measure zero and does not bother us further in the next section.

Keldysh rotation (for generic bosons)

- Idea: Take into account the redundancy relation (7) in a simple form. Find retarded, advanced and Keldysh Green functions.
- Define new fields in terms of rotation applied to ϕ_{\pm} (analogous for ϕ_{\pm}^*):

$$\begin{aligned} \phi_c(t) &\equiv \frac{1}{\sqrt{2}} (\phi_+(t) + \phi_-(t)) \\ \phi_q(t) &\equiv \frac{1}{\sqrt{2}} (\phi_+(t) - \phi_-(t)) \end{aligned}$$

They are called “classical” and “quantum” components.

- The rotation yields for

$$iG_{\alpha\beta}(t, t') \equiv \langle \phi_{\alpha}(t) \phi_{\beta}^*(t') \rangle \quad (38)$$

with $\alpha, \beta \in \{c, q\}$:

$$G = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} G^T & G^< \\ G^> & G^{\tilde{T}} \end{pmatrix} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \begin{pmatrix} G^K(t, t') & G^R(t, t') \\ G^A(t, t') & 0 \end{pmatrix} \quad (39)$$

and we identify the retarded (R), advanced (A) and Keldysh (K) component introduced above in Sec. 7.3. The zero in the bottom right ($\langle \phi_q(t) \phi_q^*(t') \rangle = 0$) is the consequence of Eq. (37).

- Example for single bosonic mode $H_0 = \omega_0 a^\dagger a$ (see Ex. 7.6.1):

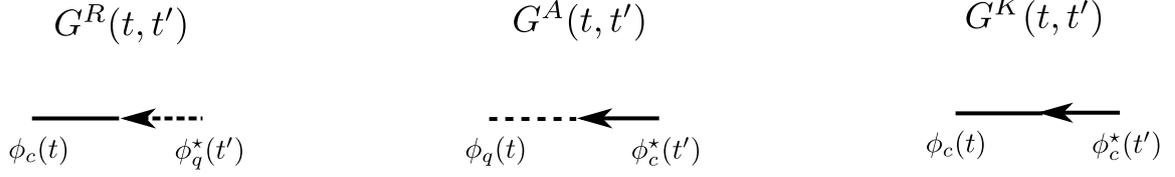
$$G_{aa^\dagger}(t, t') = -ie^{-i\omega_0(t-t')} \begin{pmatrix} 2n_B + 1 & \theta(t-t') \\ -\theta(t'-t) & 0 \end{pmatrix} \quad (40)$$

and the Fourier-trafo is

$$G_{aa^\dagger}(\omega) = \begin{pmatrix} -i2\pi\delta(\omega_0 - \omega) [2n_B + 1] & \frac{1}{\omega - \omega_0 + i\eta} \\ \frac{1}{\omega - \omega_0 - i\eta} & 0 \end{pmatrix} \quad (41)$$

- Graphical representation for $-i \langle \phi_{\alpha}(t) \phi_{\beta}^*(t') \rangle$. Conventions:
 - classical field ϕ_c - solid line

- quantum field ϕ_q - dashed line
- arrow from $\phi_\beta^*(t')$ to $\phi_\alpha(t)$



Keldysh action

- Non-interacting case: Want action $S[\phi_c, \phi_q]$ such that

$$\langle \phi_\alpha(t) \phi_\beta^*(t') \rangle = \int D[\phi_c, \phi_q] \phi_\alpha(t) \phi_\beta^*(t') e^{iS[\phi_c, \phi_q]} \quad (42)$$

reproduces Eq. (39). Need

$$S[\phi_c, \phi_q] = \int_{-\infty}^{+\infty} dt dt' \begin{pmatrix} \phi_c^*(t), \phi_q^*(t) \end{pmatrix} \underbrace{\begin{pmatrix} 0 & [G^{-1}]^A(t, t') \\ [G^{-1}]^R(t, t') & [G^{-1}]^K(t, t') \end{pmatrix}}_{\equiv G^{-1}} \begin{pmatrix} \phi_c(t') \\ \phi_q(t') \end{pmatrix} \quad (43)$$

with the condition:

$$G^{-1} \cdot G = \begin{pmatrix} 0 & [G^{-1}]^A \\ [G^{-1}]^R & [G^{-1}]^K \end{pmatrix} \cdot \begin{pmatrix} G^K & G^R \\ G^A & 0 \end{pmatrix} = \mathbf{1} \equiv \begin{pmatrix} \delta(t-t') & 0 \\ 0 & \delta(t-t') \end{pmatrix} \quad (44)$$

- Written in components, we have the following non-trivial conditions:

$$\begin{aligned} \int dt'' [G^{-1}]^A(t, t'') G^A(t'', t') &= \delta(t-t') \\ \int dt'' [G^{-1}]^R(t, t'') G^R(t'', t') &= \delta(t-t') \\ [G^{-1}]^R G^K + [G^{-1}]^K G^A &= 0 \end{aligned}$$

or

$$\begin{aligned} [G^{-1}]^A &= [G^A]^{-1} \\ [G^{-1}]^R &= [G^R]^{-1} \\ [G^{-1}]^K &= -[G^{-1}]^R \cdot G^K \cdot [G^{-1}]^A = -F \cdot [G^A]^{-1} + [G^R]^{-1} \cdot F \end{aligned}$$

where in the last step, we used $G^K = G^R \cdot F - F \cdot G^A$. Note: $[G^{-1}]^K \neq [G^K]^{-1}$!

- Main features (“Causality structure”, remains intact even with interactions):
 - $S[\phi_c, \phi_q = 0] \leftrightarrow c - c$ block of quadratic action = 0 : 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 $[G^{-1}]^A$ and $[G^{-1}]^R$ of G^{-1} are mutually hermitian conjugated lower and upper triangular matrices in the time-domain. Indeed, in Sec. 7.3 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 keeps information about distribution function.
For the single bosonic mode model, we have $[G^{-1}]^K \propto \eta$, it becomes finite if interactions are added.

External sources

- For the computation of observables, want to include source-fields $Z \rightarrow Z[V]$, see Eq. (23). Recall sources should be different on forward and backward branch, assume the following coupling $V_+(t)\phi_+^*(t)\phi_+(t)$ and $V_-(t)\phi_-^*(t)\phi_-(t)$.
- Keldysh-rotation for source fields:

$$\begin{aligned} V_c(t) &= \frac{1}{2} (V_+(t) + V_-(t)) \\ V_q(t) &= \frac{1}{2} (V_+(t) - V_-(t)) \end{aligned}$$

Note:

- For $V_q = 0$, we have $V_+ = V_-$ and thus $Z[V_c, V_q = 0] = 1$.
- Source-field has only one time argument, $V_{c,q}(t, t') \propto \delta(t - t')$.
- Keldysh action in continuum:

$$S = \int_{-\infty}^{+\infty} dt dt' \left(\phi_c^*(t), \phi_q^*(t) \right) G^{-1}(t, t') \begin{pmatrix} \phi_c(t') \\ \phi_q(t') \end{pmatrix} - \int_{-\infty}^{+\infty} dt \begin{pmatrix} \phi_c^*(t), \phi_q^*(t) \end{pmatrix} \begin{pmatrix} V_q(t) & V_c(t) \\ V_c(t) & V_q(t) \end{pmatrix} \begin{pmatrix} \phi_c(t) \\ \phi_q(t) \end{pmatrix} \quad (45)$$

- Partition function from Gaussian integral

$$Z[V_c, V_q] = \frac{1}{\text{tr}(\rho)} \frac{1}{\det(-iG^{-1} + iV)} = \frac{1}{\det(1 - G \cdot V)} = \exp(-\text{tr} \ln(1 - G \cdot V)) \quad (46)$$

where the trace runs over Keldysh-matrix index and time.

Example (single bosonic mode):

- Compute observable

$$i \frac{\delta Z[V_c, V_q]}{\delta V_q(t)} \Big|_{V_{c,q}=0} = \left\langle \phi_c^*(t)\phi_c(t) + \phi_q^*(t)\phi_q(t) \right\rangle = \left\langle \phi_+^*(t)\phi_+(t) + \phi_-^*(t)\phi_-(t) \right\rangle \quad (47)$$

We compute both sides of Eq. (47) separately:

1. Right-hand side:

- Recall that $\phi_+^*(t)$ is infinitesimally temporally earlier than $\phi_+(t)$. The opposite is true on the backward (-) branch.
- Recall that in the functional integral formalism

$$\left\langle Ta^\dagger(t_1)a(t_2) \right\rangle \hat{=} \left\langle \phi_\pm^*(t_1)\phi_\pm(t_2) \right\rangle \quad (48)$$

- We find:

$$\begin{aligned} \left\langle \phi_+^*(t)\phi_+(t) + \phi_-^*(t)\phi_-(t) \right\rangle &= \left\langle \phi_+^*(t+\eta)\phi_+(t) + \phi_-^*(t-\eta)\phi_-(t) \right\rangle \\ &= \left\langle Ta^\dagger(t+\eta)a(t) + Ta^\dagger(t-\eta)a(t) \right\rangle \\ &= \left\langle a^\dagger(t)a(t) + a(t)a^\dagger(t) \right\rangle \\ &= 2 \left\langle a^\dagger(t)a(t) \right\rangle + 1 \\ &= 2n_B + 1 \end{aligned}$$

2. Left-hand side:

$$\begin{aligned}
i \frac{\delta Z[V_c, V_q]}{\delta V_q(t)} \Big|_{V_{c,q}=0} &= i \frac{\delta \exp(-\text{tr} \ln(1 - G \cdot V))}{\delta V_q(t)} \Big|_{V_{c,q}=0} \\
&= -i \text{tr} \left[(1 - G \cdot V)^{-1} (-G) \frac{\delta V}{\delta V_q(t)} \right] \Big|_{V_{c,q}=0} \\
&= i \int dt' \text{tr}_2 \left[G(t', t) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \delta(t, t') \right] \\
&= i G^K(t, t)
\end{aligned}$$

and we use from Eq. (40) that $iG^K(t, t') = e^{-i\omega_0(t-t')}(2n_B + 1)$ and we obtain the result $2n_B + 1$ already found from the right hand side.

8.3 Exercises

8.3.1 Driven Harmonic oscillator

A quantum harmonic oscillator $H_0 = \omega_0 a^\dagger a$ is coupled to a time-dependent driving field $U(t)$,

$$H(t) = H_0 + U(t) (a + a^\dagger) / \sqrt{2}, \quad (49)$$

where $a^{(\dagger)}$ are bosonic operators and the driving field vanishes for $t \rightarrow \pm\infty$. 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 $t \rightarrow -\infty$.

1. Upgrade $U(t)$ to a source field $U_\pm(t)$. Note that U_\pm couples differently to the fields ϕ, ϕ^* compared to the source V_\pm used in the lecture. 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

$$G(t, t') = \begin{pmatrix} G^K & G^R \\ G^A & 0 \end{pmatrix} (t, t') \quad (50)$$

which you can take from Eq. (40). 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 $n = \langle a^\dagger a \rangle = |\alpha|^2$. We want to find α . Compute the functional derivative $i\delta Z[U_c, U_q] / \delta U_q(t) |_{U_q=0}$ 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 $t \rightarrow \infty$, the coefficient α is given by the Fourier transform of $U_c(t) \equiv U(t)$ (up to an unimportant factor $\sqrt{2}e^{i\varphi}$).
3. Take 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 ?

9 Interactions, self-energy and kinetic equation

9.1 Interactions

- Consider interacting part of bosonic Hamiltonian (now in D-dim real space, contact interaction):

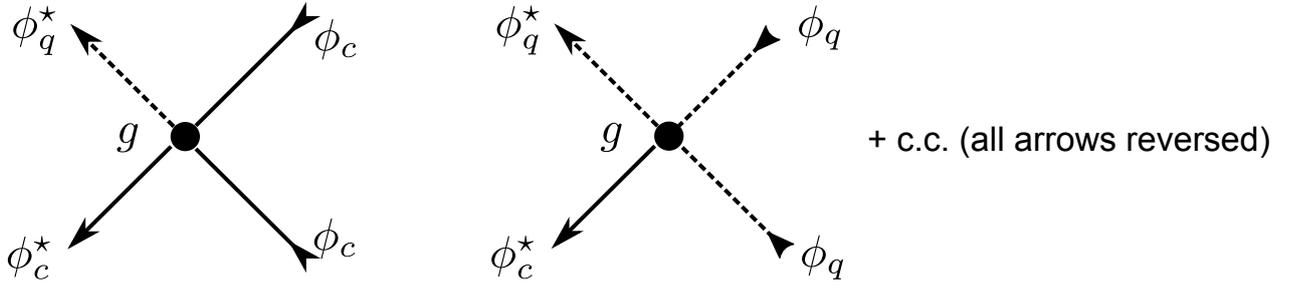
$$H_{int} = g \int d\mathbf{x} a^\dagger(\mathbf{x}) a^\dagger(\mathbf{x}) a(\mathbf{x}) a(\mathbf{x}) \quad (51)$$

which yields in terms of the action:

$$\begin{aligned}
 S_{int} &= -g \int d\mathbf{x} \int_c dt \phi^*(\mathbf{x}, t) \phi^*(\mathbf{x}, t) \phi(\mathbf{x}, t) \phi(\mathbf{x}, t) \\
 &= -g \int d\mathbf{x} \int_{-\infty}^{+\infty} dt [(\phi_+^* \phi_+)^2 - (\phi_-^* \phi_-)^2] \\
 (rot.) &= -g \int d\mathbf{x} \int_{-\infty}^{+\infty} dt [\phi_c^* \phi_q^* \phi_c \phi_c + \phi_c^* \phi_q^* \phi_q \phi_q + c.c.]
 \end{aligned} \tag{52}$$

Remarks:

- S_{int} vanishes for $\phi_q = 0$, just like the quadratic action.
- Diagrammatic notation with the rules defined below Eq. (39).



- Interactions maintain normalization ($Z = 1$): Check via perturbation theory to order g and g^2 , see Ex. 9.4.1.

9.2 Dyson equation

- Although $Z = 1$ is maintained with interactions, the propagators are modified (“dressed”). They are defined as:

$$G = -i \langle \phi_\alpha \phi_\beta^* \rangle = -i \int D[\phi_c, \phi_q] \phi_\alpha \phi_\beta^* e^{iS_0 + iS_{int}} \tag{53}$$

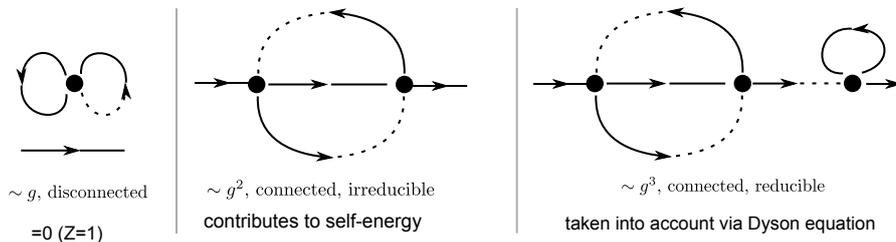
Perturbative expansion in g and Wick-theorem generates various diagrams (internal vertices: sum over Keldysh-indices, integrate over space-time coordinates)

- Disconnected diagrams vanish due to $Z = 1$, they contain $\langle S_{int}^{n>0} \rangle_0 = 0$.
- Irreducible diagrams contribute to the self-energy Σ (without external legs).
- One-line reducible diagrams are taken into account via the Dyson equation (“.” includes t -integrals!).

$$\begin{aligned}
 G &= G_0 + G_0 \cdot \Sigma \cdot G_0 + G_0 \cdot \Sigma \cdot G_0 \cdot \Sigma \cdot G_0 + \dots \\
 &= G_0 + G_0 \cdot \Sigma \cdot G
 \end{aligned}$$

or

$$G = [G_0^{-1} - \Sigma]^{-1} \Leftrightarrow (G_0^{-1} - \Sigma) \cdot G = 1 \tag{54}$$



- The Keldysh self-energy has the same causality structure as G_0^{-1} (similar perturbation theory arguments as for $Z = 1$):

$$\Sigma = \begin{pmatrix} 0 & \Sigma^A \\ \Sigma^R & \Sigma^K \end{pmatrix} \quad (55)$$

The Dyson equation then reads:

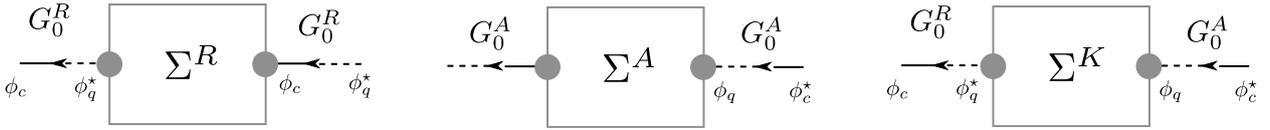
$$\begin{pmatrix} 0 & (G_0^A)^{-1} - \Sigma^A \\ (G_0^R)^{-1} - \Sigma^R & (G_0^{-1})^K - \Sigma^K \end{pmatrix} \cdot \begin{pmatrix} G^K & G^R \\ G^A & 0 \end{pmatrix} = \mathbf{1} \quad (56)$$

Remark: $(G_0^{-1})^K = 2i\eta F$ can be omitted if $\Sigma^K \neq 0$.

- What are the terminal fields for the self-energy diagrams? For the irreducible diagrams appearing in the perturbative expansion of G , we find in components and using Eq. (55),

$$\begin{pmatrix} G^K & G^R \\ G^A & 0 \end{pmatrix} \Big|_{irr} = \begin{pmatrix} G_0^R \cdot \Sigma^K \cdot G_0^A + G_0^K \cdot \Sigma^A \cdot G_0^A + G_0^R \cdot \Sigma^R \cdot G_0^K & G_0^R \cdot \Sigma^R \cdot G_0^R \\ G_0^A \cdot \Sigma^A \cdot G_0^A & 0 \end{pmatrix} \quad (57)$$

This tells us which diagrams should be accounted for as $\Sigma^{R,A,K}$, see the figure below. In other words, Eq. (55) is to be understood in $\phi^* - \phi$ space (while G is a matrix in $\phi - \phi^*$ 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 .



9.3 Kinetic equation

- Assume particles with parabolic dispersion: From the path integral formulation, we recall:

$$(G_0^{R,A})^{-1}(t\mathbf{x}, t'\mathbf{x}') = \delta(t - t') \delta(\mathbf{x} - \mathbf{x}') \left[i\partial_t + \frac{1}{2m} \nabla_{\mathbf{x}}^2 \pm i\eta - V_c(\mathbf{x}, t) \right] \quad (58)$$

- Write the Dyson equation in components. For the diagonal elements,

$$\int dt'' dx'' \left(i\partial_t + \frac{1}{2m} \nabla_{\mathbf{x}}^2 - V_c(\mathbf{x}, t) - \Sigma^{R(A)}(t - t'', \mathbf{x} - \mathbf{x}'') \right) G^{R(A)}(t''\mathbf{x}'', t\mathbf{x}') = \delta(t - t') \delta(\mathbf{x} - \mathbf{x}') \quad (59)$$

which, for $V_c = 0$ (space-time translational invariance) can be solved via Fourier transform of $G^{R(A)}(x, x') = G^{R(A)}(x - x')$:

$$G^{R(A)}(\mathbf{k}, \omega) = \frac{1}{\omega - k^2/(2m) - \Sigma^{R(A)}(\mathbf{k}, \omega)} \quad (60)$$

We see that

- $\text{Re}\Sigma^R(\mathbf{k}, \omega) = \text{Re}\Sigma^A(\mathbf{k}, \omega)$ modifies (“renormalizes”) the dispersion $E = k^2/(2m) \rightarrow k^2/(2m) + \text{Re}\Sigma^{R(A)}(\mathbf{k}, \omega)$ of the particle.
- $\text{Im}\Sigma^R(\mathbf{k}, \omega) = -\text{Im}\Sigma^A(\mathbf{k}, \omega)$ has the meaning of an inverse life-time for a particle in eigenstate \mathbf{k} .

- From the remaining component of the Dyson equation:

$$\underbrace{\left[(G_0^R)^{-1} - \Sigma^R \right]}_{(G^R)^{-1}} \cdot \underbrace{G^K}_{G^R \cdot F - F \cdot G^A} = \Sigma^K \cdot G^A \quad (61)$$

Multiply from the right by $(G_0^A)^{-1} - \Sigma^A = [G^A]^{-1}$:

$$F \cdot \left((G_0^A)^{-1} - \Sigma^A \right) - \left((G_0^R)^{-1} - \Sigma^R \right) \cdot F = \Sigma^K \quad (62)$$

and we obtain the quantum kinetic equation for the matrix F (“distribution matrix”):

$$\boxed{F \cdot (G_0^A)^{-1} - (G_0^R)^{-1} \cdot F = \Sigma^K - (\Sigma^R \cdot F - F \cdot \Sigma^A)} \quad (63)$$

- Usage: Usually, obtain $\Sigma^{R,A,K}$ from perturbation theory. Then use Eq. (63) to find F .

Wigner transform

- Kinetic equation for $F(x_1, x_2)$ [$x = (\mathbf{x}, t)$] is usually too difficult to solve.
- Assume there is separation of intrinsic and extrinsic $[V_c(\mathbf{x}, t)]$ time and length scales (e.g. external potential smooth compared to wavelength of particle).
- Wigner transform for $A(x_1, x_2)$: 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 $\partial_x \partial_p = \nabla_{\mathbf{x}} \nabla_{\mathbf{p}} - \partial_t \partial_\omega$)

$$\boxed{A(x, p) = \int dx' e^{-ipx'} A(x + x'/2, x - x'/2)} \quad (64)$$

and the inverse transform is

$$A(x_1, x_2) = \sum_p e^{ip(x_1 - x_2)} A\left(\frac{x_1 + x_2}{2}, p\right). \quad (65)$$

- Consider Wigner trafo 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. 9.4.2, one shows the following:

If for $A(x, p)$ and $B(x, p)$ the dependence on the central coordinate x is slow, one has (no “.”!)

$$C(x, p) \simeq A(x, p) B(x, p) + \frac{i}{2} (\partial_x A(x, p) \partial_p B(x, p) - \partial_p A(x, p) \partial_x B(x, p)) \quad (66)$$

and corrections would include higher order derivatives $\partial_x^{2,3,4,\dots}$ which are supposed to be weak.

- From this, it follows

$$[A; B] \equiv A \cdot B - B \cdot A \simeq i (\partial_x A(x, p) \partial_p B(x, p) - \partial_p A(x, p) \partial_x B(x, p)) \quad (67)$$

where the notation $[.;.]$ should remind us that we are dealing with “.”.

Wigner transform of kinetic equation

- Idea: Apply the Wigner transform on both sides of the kinetic equation (63).
- Left-hand side: We have with the free particle assumption (58) (can drop $\pm i\eta$ terms in this context):

$$lhs = \left[F; i\partial_t + \frac{1}{2m} \nabla_{\mathbf{x}}^2 - V_c(\mathbf{x}, t) \right] \quad (68)$$

The function $V_c(\mathbf{x}, t) = V_c(x)$ is considered to have slow coordinate dependence only, i.e. $V_c(x, p) = V_c(x)$. Then

$$[F; -V_c(x)] = -i \left(\partial_x F \underbrace{\partial_p V_c(x, p)}_0 - \partial_p F \partial_x V_c(x, p) \right) = i \partial_x V_c(x) \partial_p F \quad (69)$$

Other terms: The Wigner transform of the translational invariant operator $i\partial_t$ is ω , of $\nabla_{\mathbf{x}}^2$ it is $-\mathbf{p}^2$. Also use $\partial_x\partial_p = \nabla_{\mathbf{x}}\nabla_{\mathbf{p}} - \partial_t\partial_\omega$:

$$\begin{aligned} [F; i\partial_t] &= i(\partial_x F \partial_p \omega - \partial_p F \partial_x \omega) = -i\partial_t F \\ \left[F; \frac{1}{2m}\nabla_{\mathbf{x}}^2 \right] &= \frac{-i}{2m} \left(\partial_x F \partial_p \mathbf{p}^2 - \partial_p F \partial_x \mathbf{p}^2 \right) = \frac{-i}{m} \mathbf{p} \nabla_{\mathbf{x}} F \end{aligned}$$

- Right-hand side: Use $\Sigma^A(x, p) = [\Sigma^R(x, p)]^*$:

$$\begin{aligned} rhs &= \Sigma^K - \left(\Sigma^R \cdot F - F \cdot \Sigma^A \right) \\ &= \Sigma^K - F \left(\Sigma^R - \Sigma^A \right) - \frac{i}{2} \left(\partial_x \Sigma^R \partial_p F - \partial_p \Sigma^R \partial_x F \right) + \frac{i}{2} \left(\partial_x F \partial_p \Sigma^A - \partial_p F \partial_x \Sigma^A \right) \\ &= \Sigma^K - 2iF \text{Im} \Sigma^R - i\partial_x [\text{Re} \Sigma^R] \partial_p F + i\partial_p [\text{Re} \Sigma^R] \partial_x F \end{aligned}$$

- Final result: Multiply by i , move all derivatives of F on the lhs and expand $x = (\mathbf{x}, t)$ and $p = (\mathbf{p}, \omega)$.

$$\boxed{\left\{ \left(1 - \partial_\omega [\text{Re} \Sigma^R] \right) \partial_t + \partial_t \tilde{V}(x, p) \partial_\omega + \underbrace{\left(\frac{1}{m} \mathbf{p} + \nabla_{\mathbf{p}} [\text{Re} \Sigma^R] \right)}_{\tilde{\mathbf{v}}_{\mathbf{p}}} \nabla_{\mathbf{x}} - \nabla_{\mathbf{x}} \tilde{V}(x, p) \nabla_{\mathbf{p}} \right\} F = \underbrace{i\Sigma^K + 2F \text{Im} \Sigma^R}_{\text{collision integral}}}$$

(70)

with the effective potential

$$\tilde{V}(x, p) \equiv V_c(x) + \text{Re} \Sigma^R(x, p). \quad (71)$$

- Remark:

- The left-hand side contains the self-energy enhanced single particle dynamics of F .
- The right-hand side of Eq. (70) is called the “collision integral” $I^{\text{coll}}[F]$, it will be caused by interactions or disorder.
- Can use generalized dispersion $\frac{1}{2m}\mathbf{p}^2 \rightarrow \omega_{\mathbf{p}}$. This leads to $\mathbf{v}_{\mathbf{p}} = \frac{1}{m}\mathbf{p} \rightarrow \nabla_{\mathbf{p}}\omega_{\mathbf{p}}$.
- Consider static situation, such that all $\partial_t \rightarrow 0$. The left-hand side is zero for any $F(x, p) = F(\omega)$. The only such function which nullifies the right-hand side is the equilibrium solution

$$F^{\text{eq}}(\omega) = \coth(\omega - \mu) / (2T) \quad (72)$$

Mass-shell approximation

- Shift the energy argument ω of the distribution function F

$$F(\mathbf{x}, t, \mathbf{p}, \omega) = \tilde{F}(\mathbf{x}, t, \mathbf{p}, \underbrace{\omega - \omega_{\mathbf{p}} - \tilde{V}(x, p)}_{\tilde{\omega}}) \quad (73)$$

where $\tilde{\omega}$ is the renormalized energy.

- Express the kinetic equation (70) 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 to

$$\begin{aligned} \partial_t F &= \partial_t \tilde{F} - \left(\partial_t \tilde{V} \right) \partial_\omega \tilde{F} \\ \partial_\omega F &= \partial_\omega \tilde{F} - \left(\partial_\omega \tilde{V} \right) \partial_\omega \tilde{F} \\ \nabla_{\mathbf{x}} F &= \nabla_{\mathbf{x}} \tilde{F} - \left(\nabla_{\mathbf{x}} \tilde{V} \right) \partial_\omega \tilde{F} \\ \nabla_{\mathbf{p}} F &= \nabla_{\mathbf{p}} \tilde{F} - \left(\nabla_{\mathbf{p}} \omega_{\mathbf{p}} + \nabla_{\mathbf{p}} \tilde{V} \right) \partial_\omega \tilde{F} \end{aligned}$$

Use that the external potential is a “slow” function $\nabla_{\mathbf{p}}V_c(x) = 0 = \partial_\omega V_c(x)$, obtain after some straightforward algebra:

$$\left\{ \left(1 - \partial_\omega [\text{Re}\Sigma^R]\right) \partial_t + \tilde{\mathbf{v}}_{\mathbf{p}} \nabla_{\mathbf{x}} - \left(\nabla_{\mathbf{x}} \tilde{V}\right) \nabla_{\mathbf{p}} \right\} \tilde{F} = I^{coll}[\tilde{F}] \quad (74)$$

Observation: The derivative $\partial_{\tilde{\omega}}$ is now absent.

- If $I^{coll}[\tilde{F}]$ 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.
- Quasiparticle approximation: In $I^{coll}[\tilde{F}]$, \tilde{F} always multiplies Wigner trafo of $G^R - G^A \sim$ spectral density. Close to the non-interacting limit $G^R - G^A \sim \delta(\omega - \omega_{\mathbf{p}} - \tilde{V}(x, p))$, i.e. the spectral function peaks as a function of ω peaks at $\tilde{\omega} = 0$. The peak is assumed to be much sharper than the $\tilde{\omega}$ -dependence of \tilde{F} . This means that for given \mathbf{p} , we may focus on

$$\tilde{F}(\mathbf{x}, t, \mathbf{p}, 0) \equiv \tilde{F}(\mathbf{x}, t, \mathbf{p}) \quad (75)$$

which is the *mass-shell restricted distribution function*.

- Kinetic equation for $\tilde{F}(\mathbf{x}, t, \mathbf{p})$:

$$\underbrace{\left\{ \left(1 - \partial_\omega [\text{Re}\Sigma^R]\right) \right\}}_{\tilde{Z}^{-1}} \partial_t + \tilde{\mathbf{v}}_{\mathbf{p}} \nabla_{\mathbf{x}} - \left(\nabla_{\mathbf{x}} \tilde{V}\right) \nabla_{\mathbf{p}} \tilde{F} = I^{coll}[\tilde{F}] \quad (76)$$

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} , \tilde{V} , Eq. (76) is equivalent to the classical Boltzmann equation.
- Classical Boltzmann equation: $f(\mathbf{x}, t, \mathbf{p}) d\mathbf{x} d\mathbf{p}$ = numbers particles in phase-space volume $d\mathbf{x} d\mathbf{p}$. From Liouville theorem, phase space volume preserved under Hamiltonian equation of motion $\dot{\mathbf{x}} = \mathbf{v}(\mathbf{p})$, $\dot{\mathbf{p}} = \mathbf{F}(\mathbf{x}, \mathbf{p})$, propagating to time $t + dt$. Treat collisions that are beyond these equations of motion separately in collision term:

$$\partial_t f + \mathbf{v}_{\mathbf{p}} \cdot \nabla_{\mathbf{x}} f + \mathbf{F} \cdot \nabla_{\mathbf{p}} f = \partial_t f|^{coll} \quad (77)$$

Example for collision integral: Disorder scattering

- Consider non-interacting bosonic Hamiltonian with a static potential:

$$H = \sum_{\mathbf{p}} \omega_{\mathbf{p}} a_{\mathbf{p}}^\dagger a_{\mathbf{p}} + \int d\mathbf{x} V(\mathbf{x}) a^\dagger(\mathbf{x}) a(\mathbf{x}) \quad (78)$$

- Assume $V(\mathbf{x})$ comes from randomly placed impurities, $V(\mathbf{x}) = \sum_{j=1}^N v(\mathbf{x} - \mathbf{r}_j)$ where $\mathbf{r}_{1,2,\dots,N}$ are the N impurity positions.
Assume $\int d\mathbf{x} v(\mathbf{x}) = 0$, i.e. the offset is already taken into account in a shift of $\omega_{\mathbf{p}}$.

- Disorder average for quantity O (integrate over all impurity positions):

$$\overline{O} = \prod_{j=1}^N \left[\frac{1}{V} \int d\mathbf{r}_j O \right] \quad (79)$$

Two examples:

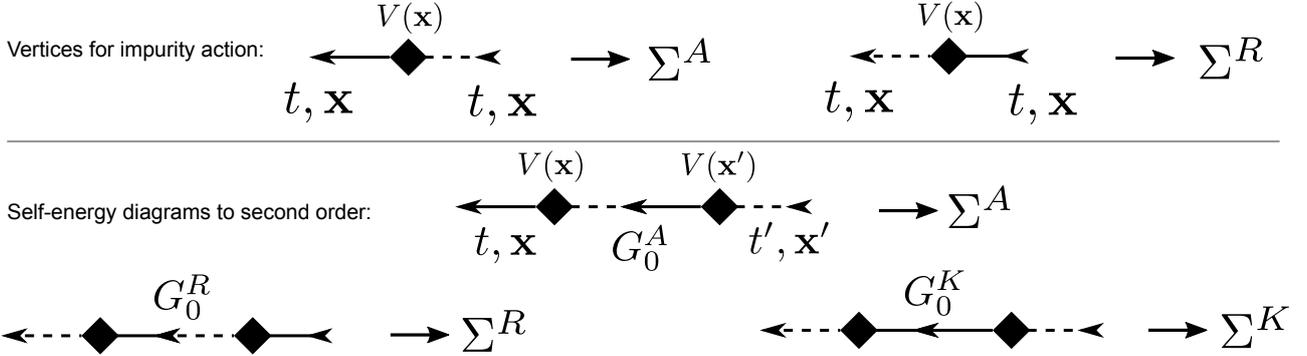
$$\overline{V(\mathbf{x})} = \prod_{j=1}^N \frac{1}{V} \int d\mathbf{r}_j \sum_{j=1}^N v(\mathbf{x} - \mathbf{r}_j) = 0 \quad (80)$$

$$\begin{aligned}
\overline{V(\mathbf{x}_1)V(\mathbf{x}_2)} &= \sum_{j=1}^N \sum_{j'=1}^N \overline{v(\mathbf{x}_1 - \mathbf{r}_j) v(\mathbf{x}_2 - \mathbf{r}_{j'})} \\
&= \sum_{j=1}^N \overline{v(\mathbf{x}_1 - \mathbf{r}_j) v(\mathbf{x}_2 - \mathbf{r}_j)} + \underbrace{\sum_{j \neq j'} \overline{v(\mathbf{x}_1 - \mathbf{r}_j) v(\mathbf{x}_2 - \mathbf{r}_{j'})}}_{\overline{VV}=0} \\
(\text{diag.}) &= \underbrace{N/V}_{n_i} \int d\mathbf{r} v(\mathbf{x}_1 - \mathbf{r}) v(\mathbf{x}_2 - \mathbf{r}) \\
&= n_i \int d\mathbf{r} v(\mathbf{x}_1 - \mathbf{x}_2 - \mathbf{r}) v(-\mathbf{r}) \\
&\equiv K(\mathbf{x}_1 - \mathbf{x}_2)
\end{aligned}$$

- The impurity action for a specific realization is

$$S_V = - \int_{-\infty}^{+\infty} dt \int d\mathbf{x} V(\mathbf{x}) \left[\phi_c^*(\mathbf{x}, t) \phi_q(\mathbf{x}, t) + \phi_q^*(\mathbf{x}, t) \phi_c(\mathbf{x}, t) \right]$$

and the corresponding diagrams are given in the Figure.



- Find $\Sigma = \begin{pmatrix} 0 & \Sigma^A \\ \Sigma^R & \Sigma^K \end{pmatrix}$ using perturbation theory to the lowest non-trivial order, but keep F general as it will be determined from kinetic equation. From the figure, we have

$$\begin{aligned}
\Sigma^{R,A}(x_1, x_2) &= \delta(t_1 - t_2) \delta(\mathbf{x}_1 - \mathbf{x}_2) V(\mathbf{x}_1) + V(\mathbf{x}_1) G_0^{R,A}(x_1, x_2) V(\mathbf{x}_2) \\
\Sigma^K(x_1, x_2) &= V(\mathbf{x}_1) G_0^K(x_1, x_2) V(\mathbf{x}_2)
\end{aligned}$$

- Take disorder average (omit the \dots on Σ, G): $\overline{V(\mathbf{x}_1)} = 0$ and note that $\overline{V(\mathbf{x}_1)V(\mathbf{x}_2)} = K(\mathbf{x}_1 - \mathbf{x}_2)$ is a function of $\mathbf{x}_1 - \mathbf{x}_2$ only.
- Wigner transform of the right-hand side is simple: Use product \rightarrow convolution rule and $K(\mathbf{p}) = n_i v_{\mathbf{p}} v_{-\mathbf{p}} \stackrel{v(\mathbf{x}) \in \mathbb{R}}{=} n_i |v_{\mathbf{p}}|^2$:

$$\Sigma^{R,A,K}(x, p) = n_i \sum_{\mathbf{p}'} G_0^{R,A,K}(\mathbf{x}, t, \mathbf{p}', \omega) |v_{\mathbf{p}-\mathbf{p}'}|^2 \quad (81)$$

- Find collision integral $I^{coll}[\tilde{F}] = i\Sigma^K + 2\tilde{F}\text{Im}\Sigma^R$ from self-energies in Eq. (81):

$$- 2\tilde{F}\text{Im}\Sigma^R: \text{ use } G_0^{R,A}(\mathbf{x}, t, \mathbf{p}, \omega) = G_0^{R,A}(\mathbf{p}, \omega) = \frac{1}{\omega - \omega_{\mathbf{p}} \pm i\eta},$$

$$2\text{Im}\Sigma^R(x, p) = -i\Sigma^R + i\Sigma^A = -n_i \sum_{\mathbf{p}'} i \underbrace{[G_0^R - G_0^A]}_{A_0 = 2\pi\delta(\omega - \omega_{\mathbf{p}'})}(\mathbf{p}', \omega) |v_{\mathbf{p}-\mathbf{p}'}|^2 \quad (82)$$

– $i\Sigma^K$: Use

$$i\Sigma^K(x, p) = in_i \sum_{\mathbf{p}'} G_0^K(\mathbf{x}, t, \mathbf{p}', \omega) |v_{\mathbf{p}-\mathbf{p}'}|^2 \quad (83)$$

and plug in

$$\begin{aligned} G_0^K(\mathbf{x}, t, \mathbf{p}', \omega) &= (G_0^R \cdot F - F \cdot G_0^A)(\mathbf{x}, t, \mathbf{p}', \omega) \\ \text{[lowest order approx.]} &\simeq -ii [G_0^R - G_0^A](\mathbf{p}', \omega) F(\mathbf{x}, t, \mathbf{p}', \omega) \\ &= -i2\pi\delta(\omega - \omega_{\mathbf{p}'}) F(\mathbf{x}, t, \mathbf{p}', \omega) \end{aligned}$$

so that

$$i\Sigma^K = 2\pi n_i \sum_{\mathbf{p}'} \delta(\omega - \omega_{\mathbf{p}'}) |v_{\mathbf{p}-\mathbf{p}'}|^2 F(\mathbf{x}, t, \mathbf{p}', \omega) \quad (84)$$

- Collect terms and work with \tilde{F} at $\tilde{\omega} = 0$ ($\omega \rightarrow \omega_{\mathbf{p}}$):

$$\boxed{\Gamma^{coll} [\tilde{F}(\mathbf{x}, t, \mathbf{p})] = -2\pi n_i \sum_{\mathbf{p}'} \delta(\omega_{\mathbf{p}} - \omega_{\mathbf{p}'}) |v_{\mathbf{p}-\mathbf{p}'}|^2 [\tilde{F}(\mathbf{x}, t, \mathbf{p}) - \tilde{F}(\mathbf{x}, t, \mathbf{p}')] } \quad (85)$$

- 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}' .
- Rates determined by Fermi's golden rule: $W(\mathbf{p}, \mathbf{p}') \equiv 2\pi n_i \delta(\omega_{\mathbf{p}} - \omega_{\mathbf{p}'}) |\langle \mathbf{p} | v | \mathbf{p}' \rangle|^2$.

9.4 Exercises

9.4.1 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. (52). Hint: Show explicitly that the two rightmost terms in

$$Z = \int D[\phi_c, \phi_q] e^{iS_0 + iS_{int}} = \langle e^{iS_{int}} \rangle_0 = 1 + i \langle S_{int} \rangle_0 - \frac{1}{2} \langle S_{int}^2 \rangle_0 + \dots \quad (86)$$

vanish.

9.4.2 Wigner transform of $C = A \cdot B$

Find the Wigner transform from Eq. (64) 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

$$C(x, p) = \sum_{n, m=0}^{\infty} \frac{(+i)^m (-i)^n}{2^m m! 2^n n!} \partial_x^{(m)} \partial_p^{(n)} A(x, p) \partial_p^{(m)} \partial_x^{(n)} B(x, p) \quad (87)$$

$$\equiv A(x, p) e^{\frac{i}{2} (\overleftarrow{\partial}_x \overrightarrow{\partial}_p - \overleftarrow{\partial}_p \overrightarrow{\partial}_x)} B(x, p) \quad (88)$$

where the arrows show the direction of the differentiation. Hints: With appropriate substitutions, first confirm

$$C(x, p) = \int dx_a \int dx_b \sum_{p_{a,b}} e^{ip_b x_a - ip_a x_b} A\left(x + \frac{x_a}{2}, p + p_a\right) B\left(x + \frac{x_b}{2}, p + p_b\right). \quad (89)$$

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.

10 Keldysh formalism for fermions

Grassmann numbers, fermion coherent states

- Consider fermionic Hamiltonian $H(\{c_j^\dagger, c_j\})$ with $\{c_i, c_j^\dagger\} = \delta_{ij}$ canonical anti-commutation relation for fermionic operators.
- Grassmann numbers ψ :
 - mutually anti-commute $\psi\psi' = -\psi'\psi$, $\rightarrow \psi^2 = 0$.
 - function of Grassmann number via series expansion: $f(\psi) = f_0 + f_1\psi$.
 - Definition of integrals: $\int d\psi 1 = 0$, $\int d\psi \psi = 1$.
 - ψ anti-commutes with fermionic operators, $\{c, \psi\} = \{c^\dagger, \psi\} = 0$.
 - “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:	$\langle\psi \psi'\rangle = e^{\bar{\psi}\psi'} = 1 + \bar{\psi}\psi'$
action of c :	$c \psi\rangle = \psi \psi\rangle$	identity:	$1 = \int d\bar{\psi} d\psi e^{-\bar{\psi}\psi} \psi\rangle \langle\psi $
action of c^\dagger :	$\langle\psi c^\dagger = \langle\psi \bar{\psi}$	trace:	$\text{tr}O = \int d\bar{\psi} d\psi e^{-\bar{\psi}\psi} \langle\psi O -\psi\rangle$
		Gaussian integral:	$\int \Pi_l d\bar{\psi}_l d\psi_l e^{-\bar{\psi}^T \cdot A \cdot \psi} = \det(A)$

- In $\text{tr}O$, 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, $\langle n|\psi\rangle \langle\psi|O|n\rangle = \langle\psi|O|n\rangle \langle n|-\psi\rangle$.

Partition function

- Consider single fermionic level, $H = \varepsilon_0 c^\dagger c$. In thermal equilibrium at $t = -\infty$, we have $\text{tr}\rho = \text{tr}e^{-\beta H_0} = 1 + e^{-\beta\varepsilon_0}$ (no geometric series) and $\langle c^\dagger c \rangle \equiv n_F = 1/(1 + e^{\beta\varepsilon_0})$.
- In definition of Z , add time slices on both branches (ψ_\pm), find in analogy to bosonic case

$$Z = \frac{1}{\text{tr}\rho} \int \Pi_{j=1}^{2N} d\bar{\psi}_j d\psi_j \exp \left[i \sum_{j,j'=1}^{2N} \bar{\psi}_j (G^{-1})_{jj'} \psi_{j'} \right] \quad (90)$$

with (N=3)

$$i (G^{-1})_{jj'} = \begin{pmatrix} -1 & 0 & 0 & 0 & 0 & -e^{-\beta\varepsilon_0} \\ h_- & -1 & 0 & 0 & 0 & 0 \\ 0 & h_- & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 0 & h_+ & -1 & 0 \\ 0 & 0 & 0 & 0 & h_+ & -1 \end{pmatrix} \quad (91)$$

where $h^\pm = 1 \pm i\varepsilon_0 \delta t$ and indeed normalization holds, $Z = \frac{\det(iG^{-1})}{\text{tr}\rho} \stackrel{N \rightarrow \infty}{=} 1$.

- Green functions: $G_{c,c^\dagger} \equiv G$,

$$\begin{aligned} G^<(t, t') &= i n_F e^{-i\varepsilon_0(t-t')} \\ G^>(t, t') &= -i(1 - n_F) e^{-i\varepsilon_0(t-t')} \\ G^T(t, t') &= \theta(t-t') G^>(t, t') + \theta(t'-t) G^<(t, t') \\ G^{\tilde{T}}(t, t') &= \theta(t'-t) G^>(t, t') + \theta(t-t') G^<(t, t') \end{aligned}$$

Keldysh rotation

- Keldysh rotation: Redundancy relation (7) holds also for fermions, take it into account via rotation. Careful: Different convention in comparison to bosonic case [Larkin-Ovchinnikov], rotated fields.

$$\begin{aligned}\psi_{1,2} &\equiv \frac{1}{\sqrt{2}} (\psi_+ \pm \psi_-) \\ \bar{\psi}_{1,2} &\equiv \frac{1}{\sqrt{2}} (\bar{\psi}_+ \mp \bar{\psi}_-)\end{aligned}$$

Note that the “classical-quantum” nomenclature is not used: Grassmann variables never have classical meaning.

- Propagators: For $\alpha, \beta \in \{1, 2\}$

$$-i \langle \psi_\alpha(t) \bar{\psi}_\beta(t') \rangle \equiv G_{\alpha\beta}(t, t') = \begin{pmatrix} G^R & G^K \\ 0 & G^A \end{pmatrix} (t, t') \quad (92)$$

and inverse propagator (with convention above, have *same* structure as G)

$$G^{-1} = \begin{pmatrix} (G^R)^{-1} & (G^{-1})^K \\ 0 & (G^A)^{-1} \end{pmatrix} \quad (93)$$

With the parametrization $G^K = G^R \cdot F - F \cdot G^A$, find

$$(G^{-1})^K = (G^R)^{-1} \cdot F - F \cdot (G^A)^{-1} \quad (94)$$

- Single fermionic level in thermal equilibrium

$$\begin{aligned}G^R(t, t') &= -i\theta(t-t') e^{-i\varepsilon_0(t-t')} \xrightarrow{FT} \frac{1}{\omega - \varepsilon_0 + i\eta} \\ G^A(t, t') &= +i\theta(t'-t) e^{-i\varepsilon_0(t-t')} \xrightarrow{FT} \frac{1}{\omega - \varepsilon_0 - i\eta} \\ G^K(t, t') &= -i(1 - 2n_F) e^{-i\varepsilon_0(t-t')} \xrightarrow{FT} -2\pi i(1 - 2n_F) \delta(\omega - \varepsilon_0) = \tanh\left(\frac{\omega}{2T}\right) (G^R(\omega) - G^A(\omega))\end{aligned}$$

The last identity is the fermionic fluctuation-dissipation theorem.

10.1 Exercises

10.1.1 Drude formula for metallic conductivity

In this exercise, we calculate the Drude conductivity of a non-interacting but disordered metal in three spatial dimensions. The clean metal Hamiltonian of the electrons (spin-less, say) is

$$H_0 = \sum_{\mathbf{p}} (\varepsilon_{\mathbf{p}} - \varepsilon_F) c_{\mathbf{p}}^\dagger c_{\mathbf{p}} \quad (95)$$

with Fermi energy ε_F and the electric and impurity potentials are $U(\mathbf{x}) = -e\mathbf{x} \cdot \mathbf{E}$ and $\sum_{j=1}^N v(\mathbf{x} - \mathbf{x}_j)$, respectively. We assume an isotropic impurity potential $v(\mathbf{x}) = v(x)$ and a parabolic dispersion $\varepsilon_{\mathbf{p}} = |\mathbf{p}|^2/(2m)$. The conductivity σ is defined via the relation between current density and (small) electric field, $\mathbf{j} = \sigma \mathbf{E}$. It is straightforward to show the Boltzmann equation can be derived from the fermionic Keldysh-Dyson equation as in the bosonic case. As in the lecture, we consider the disorder average. We employ the mass-shell approximation, assume weak impurity scattering and neglect self-energy effects on the left hand side of the equation. For the fermionic phase-space distribution function $n_F(\mathbf{x}, t, \mathbf{p}) = [1 - \tilde{F}(\mathbf{x}, t, \mathbf{p})]/2$ (quasiparticle picture valid!), it reads

$$\{\partial_t + \mathbf{v}_{\mathbf{p}} \nabla_{\mathbf{x}} - (\nabla_{\mathbf{x}} U) \nabla_{\mathbf{p}}\} n_F(\mathbf{x}, t, \mathbf{p}) = -2\pi n_i \sum_{\mathbf{p}'} \delta(\varepsilon_{\mathbf{p}} - \varepsilon_{\mathbf{p}'}) |v_{\mathbf{p}-\mathbf{p}'}|^2 [n_F(\mathbf{x}, t, \mathbf{p}) - n_F(\mathbf{x}, t, \mathbf{p}')] \quad (96)$$

1. We assume that the collision integral on the right-hand side of Eq. (96) can be written as $I^{coll} = -\frac{n_F - n_F^{(0)}}{\tau_{tr}(p)}$ where τ_{tr} is known as the “transport mean free time”. We will show the consistency of this “relaxation-time approximation” below, once we have found n_F . Assume a stationary situation with a homogeneous electric field. Expand $n_F = n_F^{(0)} + n_F^{(1)}$ with $n_F^{(0)}$ the equilibrium distribution function and $n_F^{(1)}$ of linear order in the field \mathbf{E} , find $n_F^{(1)}(\mathbf{p})$. Argue that the current density is given by

$$\mathbf{j}(\mathbf{x}, t) = \frac{e}{V} \sum_{\mathbf{p}} \mathbf{v}_{\mathbf{p}} n_F(\mathbf{x}, t, \mathbf{p}) \quad (97)$$

and show that the conductivity at low temperature is determined by the Drude formula

$$\sigma = e^2 \tau_{tr}(p_F) n / m \quad (98)$$

where $n = N/V$ is the (spin-less) electron density and the Fermi wave vector p_F^2 is determined by $p_F^2/(2m) = \varepsilon_F$.

2. Show that for a distribution function of the form found in (1), i.e. $n_F(\mathbf{p}) = n_F^{(0)}(\mathbf{p}) + \mathbf{a}(k) \cdot \mathbf{p}$, the collision integral indeed assumes the relaxation-time form and confirm

$$\tau_{tr}^{-1}(p) = 2\pi n_i \sum_{\mathbf{p}'} \delta(\varepsilon_{\mathbf{p}} - \varepsilon_{\mathbf{p}'}) |v_{\mathbf{p}-\mathbf{p}'}|^2 (1 - \cos \theta') \quad (99)$$

where θ' is the angle between \mathbf{p} and \mathbf{p}' . Discuss the significance of the term $\cos \theta'$ that distinguishes the transport mean free time from the quasiparticle decay time in Eq. (82).

Part III

Topology in condensed matter physics

11 Introduction

- Central goal of condensed matter physics: Characterization of phases of matter. Two ways:
 1. Spontaneously broken symmetries and *local* order parameter.
Example: Magnet, time-reversal is broken, magnetic phase $\langle m \rangle \neq 0$
 2. Topological properties and entanglement in quantum ground state.
Example: Integer quantum Hall effect. Does not break any symmetries, but has quantized transversal conductivity $\sigma_{xy} = ne^2/h$.
Hallmark of “topological phases”: σ_{xy} insensitive to smooth changes in material parameters, does only change at a quantum phase transition where σ_{xx} becomes finite in bulk.

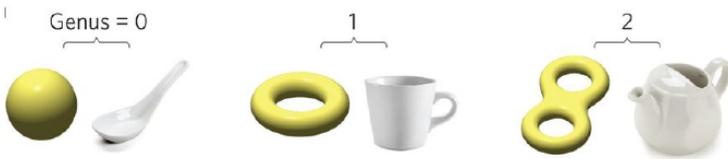
12 Topological band theory (non-interacting)

12.1 Introduction

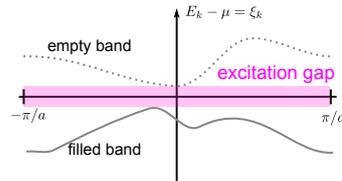
- Topology = branch of mathematics concerned with properties insensitive to smooth deformations.
- Example: Closed 2D surfaces in 3D. If they can be smoothly deformed into each other, they are *topologically equivalent*. They are distinguished by their genus \sim number of holes:
 - sphere \leftrightarrow spoon ($g=0$ holes) \leftrightarrow doughnut \leftrightarrow mug ($g=1$) \leftrightarrow double-doughnut \leftrightarrow teapot ($g=2$), see Fig. 22(a).
 - Topological invariant “Euler characteristic”, via Gauss-Bonnet theorem:
Integral over (local) Gaussian curvature K (e.g. $K = 1/R^2$ for a sphere)

$$\chi = 2 - 2g = \frac{1}{2\pi} \int_S K dA \quad (1)$$

(a) Topology of closed 2D orientable surfaces in 3D



(b) Insulator band structure in 1D



(c) Boundary state

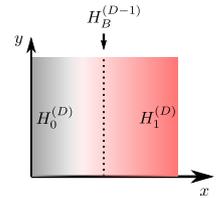


Figure 22: Basics of topology for surfaces in 2D and for insulators.

- Translate concept of topological invariant to electronic insulators [Fig. 22(b)]:
 - Insulator: Material with energy gap E_G for electronic excitations.
 - Gap E_G allows for *principle of adiabatic continuity*:
Two insulators are topologically equivalent, if their Hamiltonians can be smoothly changed into each other while staying in ground state.
 - Consequence: Connecting topologically *inequivalent* insulators will cause closing of gap (topological phase transition).

- Topological classification for general gapped many-body Hamiltonians → problem of current research, not solved yet.
- Simpler: Classification for insulators described by band-theory.
Rests on 2 key assumptions:

1. Electrons are non-interacting (or at least adiabatically connected to non-interacting case).
Important: Pauli principle for occupation of *fermionic* states.

2. Crystalline (translational invariant) material.

Bloch theorem: Crystal momentum \mathbf{k} is a good quantum number, eigenstate at energy $E_n(\mathbf{k})$ is Bloch wave

$$|\psi_n(\mathbf{k})\rangle = e^{i\mathbf{k}\mathbf{r}} |u_{n,\mathbf{k}}\rangle, \quad (2)$$

with $|u_{n,\mathbf{k}}\rangle$ cell-periodic eigenstate of Bloch Hamiltonian $H(\mathbf{k}) = e^{i\mathbf{k}\mathbf{r}} H e^{-i\mathbf{k}\mathbf{r}}$.

Lattice translation: $H(\mathbf{k}) = H(\mathbf{k} + \mathbf{G})$ for reciprocal lattice vector \mathbf{G} . Thus $\mathbf{k} \equiv \mathbf{k} + \mathbf{G}$ defines Brillouin zone (BZ), topology of torus T^D . See Fig. 22(b) for example in D=1.

- Conclusion:

Insulating band structure = Mapping from T^D to space of Bloch Hamiltonians $H(\mathbf{k})$ with energy gap.

- Gapless boundary [Fig. 22(c)]:

Effectively coarse-grained description of inhomogeneous D-dimensional material $H_x^{(D)}$, $x \in [0, 1]$. Let $H_0^{(D)}$ and $H_1^{(D)}$ be topologically in-equivalent. Moving along x , have to cross gapless boundary described by $H_B^{(D-1)}$.

- Two objectives:

- a) Classify topologically distinct insulators $H^D(\mathbf{k})$.

- b) Study gapless boundary theory $H_B^{(D-1)}(\mathbf{k}_\parallel)$ and relate to difference in bulk invariants. (Bulk-boundary correspondence.)

12.2 Berry phase and Chern number

- Goal: For (a), find what takes the role of local curvature “K”.

Loops in k-space: Berry phase

- Observe quantum mechanical phase ambiguity for (Bloch-)states (U(1) transformation)

$$|u_{\mathbf{k}}\rangle \rightarrow e^{i\phi(\mathbf{k})} |u_{\mathbf{k}}\rangle \quad (3)$$

Reminiscent of local gauge trafo in EM if k-space is identified with r-space.

- **Berry-connection:** Defined in analogy to EM vector potential,

$$\begin{aligned} \mathbf{A}(\mathbf{k}) &\equiv i \langle u_{\mathbf{k}} | \nabla_{\mathbf{k}} | u_{\mathbf{k}} \rangle, \\ \mathbf{A}(\mathbf{k}) &\rightarrow \mathbf{A}(\mathbf{k}) - \nabla_{\mathbf{k}} \phi(\mathbf{k}). \end{aligned} \quad (4)$$

Note: $\mathbf{A}(\mathbf{k})$ is a real vector, find this from acting with $\nabla_{\mathbf{k}}$ on $\langle u_{\mathbf{k}} | u_{\mathbf{k}} \rangle = 1$.

- **Berry phase:** Berry-connection is not gauge invariant, but we can integrate it over closed loop c ($\hat{=}$ magnetic flux B through c) and obtain gauge-invariant quantity:

$$\boxed{\gamma_c = \oint_c \mathbf{A} \cdot d\mathbf{k} \text{ mod } 2\pi} \quad (5)$$

Notes:

- γ_c = phase acquired under adiabatic *cyclic* evolution along (closed) loop c in k-space.
- Reason for $\text{mod}2\pi$: Non-smooth “large” gauge trafo $|u_{\mathbf{k}}\rangle \rightarrow e^{i\phi(\mathbf{k})} |u_{\mathbf{k}}\rangle$ with phase-winding around the loop c yields $\delta\gamma_c = \oint_c \nabla_{\mathbf{k}}\phi(\mathbf{k}) \cdot d\mathbf{k} = \mp 2\pi$.
- k-space can be replaced with any other cyclic parameter dependence.

2D surfaces: Berry curvature \mathcal{F}

- Assume the loop c in 2D parameter space is the boundary of the 2D region S_c [Fig. (23)(a)]. If the parameter space is k-space $\mathbf{k} \in T^2$ embedded in \mathbb{R}^3 think about curved surfaces in \mathbb{R}^3 .
- Apply Stokes theorem on right-hand side of Eq. (5) for Berry phase,

$$\boxed{\gamma_c = \int_{S_c} \mathcal{F}(\mathbf{k}) \cdot d^2\mathbf{k}} \quad (6)$$

with $d^2\mathbf{k}$ the surface element in k-space and Berry curvature:

$$\mathcal{F}(\mathbf{k}) \equiv \nabla_{\mathbf{k}} \times \mathbf{A}. \quad (7)$$

- Berry curvature is manifestly gauge invariant for smooth gauge transformations [since then $\nabla_{\mathbf{k}} \times \nabla_{\mathbf{k}}\phi(\mathbf{k}) = 0$].

Example: 2-band model in 2D

- Consider 2x2 hermitian matrix, expand in Pauli matrix basis, ignore $\mathbf{1}$ since it does not affect eigenstates.

$$H(\mathbf{k}) = \mathbf{d}(\mathbf{k}) \cdot \boldsymbol{\sigma} = d_x(\mathbf{k})\sigma_x + d_y(\mathbf{k})\sigma_y + d_z(\mathbf{k})\sigma_z \quad (8)$$

- Eigenvalues $\pm d$, eigenstates using $\hat{\mathbf{d}} = (\cos\phi(\mathbf{k})\sin\theta(\mathbf{k}), \sin\phi(\mathbf{k})\sin\theta(\mathbf{k}), \cos\theta(\mathbf{k}))^T$ are

$$|u_{-}\rangle = \begin{pmatrix} \sin\frac{\theta}{2}e^{-i\phi} \\ -\cos\frac{\theta}{2} \end{pmatrix}, \quad |u_{+}\rangle = \begin{pmatrix} \cos\frac{\theta}{2}e^{-i\phi} \\ \sin\frac{\theta}{2} \end{pmatrix}. \quad (9)$$

- Eigenstates only depend on $\hat{\mathbf{d}} \in S^2$, a point on the unit sphere. Ex. 12.1 shows that for $\hat{\mathbf{d}} = \hat{\mathbf{d}}(\mathbf{k})$,

$$\mathcal{F}_z = \frac{1}{2} \hat{\mathbf{d}} \cdot (\partial_{k_x} \hat{\mathbf{d}} \times \partial_{k_y} \hat{\mathbf{d}}) \quad (10)$$

which is half the two-sphere surface area element.

- For a loop c we find:

$$\gamma_c = \frac{1}{2} \left(\text{Solid angle swept out by } \hat{\mathbf{d}}(\mathbf{k}) \text{ during loop } c \right) \quad (11)$$

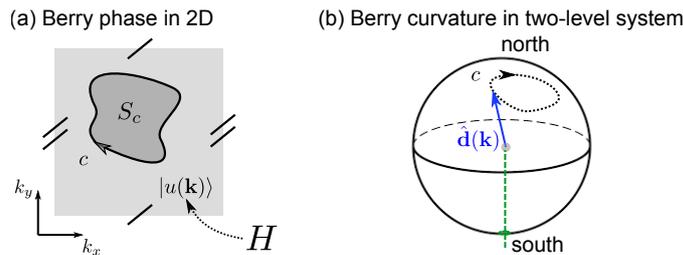


Figure 23: Berry phase and -curvature.

Closed 2D surfaces: Chern number C

- Consequence of Eq. (10) for two-band model:

Berry curvature \mathcal{F} integrated over *closed 2D surface* S (here $S = T^2$) is multiple n of $\frac{1}{2}(4\pi) = 2\pi$, n is the number of times the map $T^2 \rightarrow S^2$ wraps around S^2 .

$$C \equiv \frac{1}{2\pi} \int_{T^2} \mathcal{F} \cdot d^2\mathbf{k} = n \quad (12)$$

This the ‘‘Chern number’’. Remarks:

- C is a topological invariant, compare to Gauss-Bonnet in Eq. (1) where the curvature is now the Berry curvature \mathcal{F} .
- can be generalized to any 2D *closed* surface, $T^2 \rightarrow S$ (without boundary)
- Quantization of C for general $H(\mathbf{k})$ beyond two-band model:
Take loop c on *closed* surface S , then ‘‘inside’’ and ‘‘outside’’ are arbitrary. So

$$\gamma_c = \oint_c \mathbf{A} \cdot d\mathbf{k} = \int_{S_{c,in}} \mathcal{F} d^2\mathbf{k} = - \int_{S_{c,out}} \mathcal{F} d^2\mathbf{k} + 2\pi m \quad (13)$$

where $2\pi m$ with $m \in \mathbb{Z}$ follows since γ_c only defined mod 2π .

Put together S from $S_{c,in}$ and $S_{c,out}$, find for C :

$$C = \frac{1}{2\pi} \int_S \mathcal{F} d^2\mathbf{k} = \frac{1}{2\pi} \int_{S_{c,in}} \mathcal{F} d^2\mathbf{k} + \frac{1}{2\pi} \int_{S_{c,out}} \mathcal{F} d^2\mathbf{k} = \frac{1}{2\pi} [\gamma_c - (\gamma_c - 2\pi m)] = m \quad (14)$$

- Interpretation: C integrates the Berry flux over a closed surface, it counts the number of (EM: magnetic) *monopoles* inside S by detecting their 2π -flux lines.
(see Ex. 12.2, where we work in 3D and including the *inside* of S).

12.3 Topology in 1D

Su-Schrieffer-Heeger (SSH) Model and polarization

- Model conducting polymer acetylene as 1D tight binding model chain.
At half filling, it lowers its energy by a Peierls distortion (dimerization) [see band structure in Fig. 24(a)].
- SSH model with two-site unit-cell for spin-less electrons with dimerization δt :

$$H = \sum_i \underbrace{(t + \delta t)}_{\delta t > 0: \text{''-''}} c_{Ai}^\dagger c_{Bi} + \underbrace{(t - \delta t)}_{\delta t > 0: \text{''-''}} c_{Ai+1}^\dagger c_{Bi} + h.c. \quad (15)$$

- Fourier transform to k -space, two sites per unit cell, get two bands:

$$\begin{aligned} H(k) &= \mathbf{d}(k) \cdot \boldsymbol{\sigma} \\ d_x(k) &= (t + \delta t) + (t - \delta t) \cos ka \\ d_y(k) &= (t - \delta t) \sin ka \\ d_z(k) &= 0 \end{aligned}$$

- Claim: Electrostatic polarization $P \sim \langle r \rangle \sim \langle i\partial_k \rangle$ (with r position operator) is related to Berry phase γ_c via $A(k) = i \langle u_k | \partial_k | u_k \rangle$ [King-Smith, Vanderbilt PRB 47.1651 (1993)]

$$P = \frac{e}{2\pi} \oint_{BZ} A(k) \cdot dk = \frac{e}{2\pi} \gamma_c \quad (16)$$

Notes:

- For finite chain, polarization yields end-charges $P = Q_{end,L} = -Q_{end,R}$. End-charges must cancel for charge neutrality.
- Check: Both sides of Eq. (16) are defined mod e (can add integer charge to end of chain).
- Calculate P from Eq. (11) valid for two-band model (extend 1D k-space $k_x \rightarrow (k_x, k_y = 0)$ and do not vary k_y):

$$P = \frac{e}{2\pi} \frac{1}{2} \left(\text{Solid angle swept out by } \hat{\mathbf{d}}(k_x) \in S^2 \text{ for } k_x \text{ around } S^1 \right)$$

Find solid angle swept out by map $k \rightarrow \hat{\mathbf{d}}(k)$ from $S^1 \rightarrow S^2$ [Fig. 24(b)]:

- $\delta t > 0$: No finite solid angle swept out, $P = 0$.
- $\delta t < 0$: $\hat{\mathbf{d}}(k)$ winds around equator of unit-sphere, $P = \frac{e}{2\pi} \frac{1}{2} (2\pi) = e/2$. For end charges: $Q_{end,L} = -Q_{end,R} = \pm e/2$.
- Interpretation: The extreme case $\delta t = -t$ is easily understood, where only intra-unitcell coupling exists and end-sites provide localized zero-energy states, see Fig. 24(c).
- For $\delta t \in [-t, 0)$: Since γ_c does not change, end-charges are maintained. They are smeared out into the bulk, though. They mutually cancel when $\delta t = 0$ and the bulk gap closes.

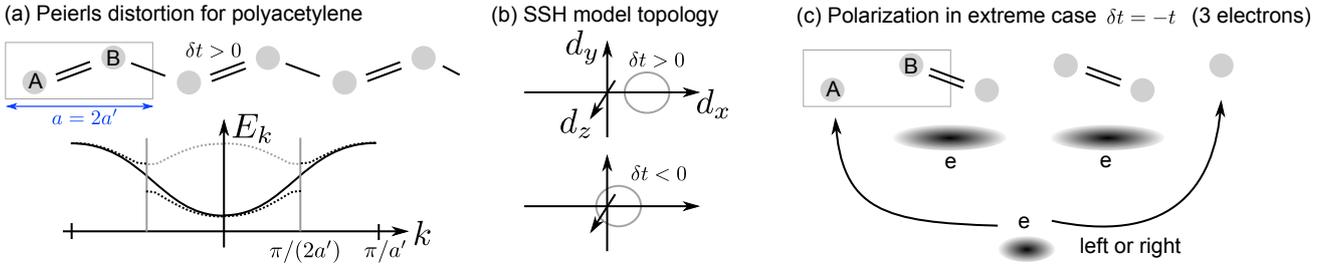


Figure 24: Topology in 1D

Role of chiral symmetry

- For the SSH model (15), $P = \frac{e}{2\pi} \gamma_c$ cannot vary from $\{0, e/2\}$ mod e unless gap closes at some k in BZ. Reason: $d_z(k) = 0$. This is easily violated by onsite energy $\sim c_{Ai}^\dagger c_{Ai}$ or next-nearest neighbor hopping $\sim c_{Ai}^\dagger c_{Ai+1}$.
- Symmetry that enforces $d_z(k) = 0$: Chiral symmetry:

$$\{H(k), \sigma_z\} = 0 \quad (17)$$

Remark: Chiral symmetry...

- can be generalized to arbitrary spatial and matrix dimension, $\{H(k), \Pi\} = 0$.
- causes symmetry of spectrum, $H|\psi\rangle = E|\psi\rangle \xrightarrow{\Pi} \Pi H|\psi\rangle = E\Pi|\psi\rangle \rightarrow H|\psi'\rangle = -E|\psi'\rangle$ with $|\psi'\rangle = \Pi|\psi\rangle$.
- is defined via *Anti*-commutator (note that, usually, symmetries enforce commutator $[S, H] = 0$ and degeneracies)
- Empiric reason for edge-state stability away from $\delta t = -t$ as long as bulk gap is present: No *local* (symmetry preserving) perturbation can move $E = 0$ eigenstate at left end away from $E = 0$. Reason: Need to move chiral partner state at right hand as well. This only works via the bulk, which is gapped. When the gap vanishes, end states can be moved simultaneously in energy to $\pm E \neq 0$ and merge with bands.

- Conclusion:
 - Unless with special symmetry (like chiral symmetry), there is no topology in 1D.
 - All 1D insulating bandstructures are topologically equivalent.

Domain wall states and Jackiw-Rebbi model

- Goal: Find wavefunction of SSH-model boundary state and understand its stability.
- Idea [Fig. 25(a)]: Replace vacuum at the end of topological non-trivial ($\delta t < 0$) section by section with $\delta t > 0$.
The latter is adiabatically connected to vacuum.
- Consider limit $\delta t \ll t$, focus on edge of BZ, $k \simeq \pi/a$. Expand $H(k)$ in lowest order $q = k - \pi/a$, get back to real space with $q \rightarrow -i\partial_x$:

$$H = iv\sigma_x\partial_x + m\sigma_y \quad (18)$$

where $v = ta$ and $m = 2\delta t$. Smoothen domain wall $\delta t = \delta t(x)$, so that $m \rightarrow m(x)$ [Fig. 25(b)].

- H is 1+1D massive Dirac Hamiltonian with spatially changing sign of mass, $m(x \rightarrow -\infty) < 0$ and $m(x \rightarrow +\infty) > 0$.
- Solve Schrödinger Eqn. for localized zero-energy domain wall state $|\psi_0\rangle$:

$$\begin{aligned} 0|\psi_0\rangle &= H|\psi_0\rangle \\ 0 &= i\sigma_x H\psi_0(x) \\ 0 &= -v\partial_x\psi_0(x) - m(x)\sigma_z\psi_0(x) \end{aligned}$$

or

$$\partial_x\psi_0(x) = -\frac{m(x)}{v}\sigma_z\psi_0(x) \quad (19)$$

This can be solved as

$$\psi_0(x) = \mathcal{N} \exp\left(-\int_{-\infty}^{+x} dx' m(x')/v\right) |\uparrow\rangle \quad (20)$$

where $\sigma_z |\uparrow\rangle = |\uparrow\rangle$.

- Remarks:
 - State $\psi_0(x)$ is normalizable for the specific domain wall configuration $m(x \rightarrow -\infty) < 0$ and $m(x \rightarrow +\infty) > 0$. For an opposite domain wall, use $|\downarrow\rangle$.
 - Precise form of the domain wall $m(x)$ does not matter for construction of $\psi_0(x)$.
 - Chiral symmetry $\Pi = \sigma_z$ maps $\psi_0(x)$ to itself, $\sigma_z\psi_0(x) = \psi_0(x)$!
Thus $|\psi_0\rangle$ is its own partner state under chiral symmetry and forced to sit at $E = 0$.
This is artifact of continuum approximation, would not work in finite-dimensional tight-binding matrix model where the number of states has to be even and two domain wall states are required.

Thouless charge pump

- Consider a quantum pump in 1D, i.e. a time-dependent Hamiltonian $H(k, t)$ that varies adiabatically (always gapped) and periodically in time such that

$$H(k, t) = H(k, t + T) \quad (21)$$

- At time $t = 0$, say, polarization $P(t = 0)$ is defined up to e but generically *not* quantized.

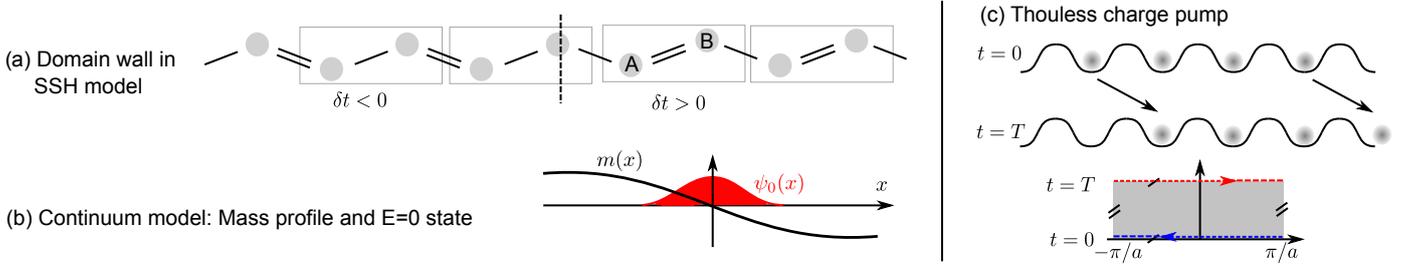


Figure 25: (a) Domain-wall in SSH model. (b) Domain-wall in continuum model and localized zero-energy mode. (c) Thouless charge pump in 1D.

- At time $t = T$, Hamiltonian has not changed, but P might have been changed by ne (recall that P was only defined mode).
- The change in polarization is [Fig. (25)(c)]

$$\Delta P = P(T) - P(0) = \frac{e}{2\pi} \left[\int_{-\pi/a}^{\pi/a} A(k, T) dk - \int_{-\pi/a}^{\pi/a} A(k, 0) dk \right] \stackrel{\text{Stokes}}{=} \frac{e}{2\pi} \int_{-\pi/a}^{\pi/a} \int_0^T \mathcal{F} dk dt \stackrel{\text{closed}}{=} eC \quad (22)$$

In the last step, we used that the grey region that is bounded by the red and blue contour is actually a torus and thus closed, so the Chern number is well defined.

- Conclusion:
Cyclic *families* of 1D-Hamiltonians as in Eq. (21) are classified by the Chern number C . Its value, $C = n$, gives the quantized charge (in units of e) that is pumped per cycle.
- Example for Thouless charge pump: Rice-Mele model (see Ex. 12.3), which is the SSH-model with added on-site terms

$$H_m = m \sum_i \left(c_{Ai}^\dagger c_{Ai} - c_{Bi}^\dagger c_{Bi} \right) \quad (23)$$

and adiabatic periodic modulation $(\delta(t), m(t)) = \left(\cos \frac{2\pi t}{T}, \sin \frac{2\pi t}{T} \right)$.

Idea: Variation in δ -term switches between connection of dimers, synchronized variation in m nudges occupation of dimers to one side.

- Proposal of pump: [Thouless Phys. Rev. B 27, 6083 (1983)],
Experimental realization: Ultra-cold bosons [Lohse et al, Nat. Phys., 12 350 (2016)] @ MPQ and fermions [Nakajima et al, Nat. Phys., 12 296 (2016)].

12.4 Integer quantum Hall effect (QHE)

Phenomenology and classical Hall effect

- QHE is beautiful manifestation of quantum effect on the macroscopic scale (other example: superconductivity).
[Klitzing, Dorda, Pepper, Phys. Rev. Lett., 1980]
- Hall effect: $j_x = \sigma_{xy} E_y$. Requirement for finite j_x is breaking of time reversal symmetry (TRS, more on that symmetry later) $j_x \rightarrow -j_x$.
Conclusion: To get Hall effect, must break TRS. Most simple way for now: External magnetic field.
- Classical Hall effect in 2D metal with perpendicular magnetic field: [Fig. 26(a)]

– Lorentz force $\mathbf{F} = e(\mathbf{E} + \mathbf{v} \times \mathbf{B})$, deflection of current in x -direction canceled by electric field E_y from charge accumulation at the edge.

$$F_y = 0 \leftrightarrow E_y - v_x B_z = 0 \quad (24)$$

- With the current density in x -direction, $j_x = env_x$ with n electron density, find for classical Hall effect:

$$\sigma_{xy}^{(cl.)} = \frac{E_y}{j_x} = \frac{en_e}{B_z} \quad (25)$$

- Experimental data (sufficiently clean, quasi-2D electron gas, e.g. GaAs):
Main finding: Plateaus of Hall conductivity $\sigma_{xy} = ne^2/h$, $\sigma_{xx} = 0$ (bulk gap!) with n an integer up to accuracy 10^{-10} .
Amazing: Independent of material, (modest) imperfections of sample, shape of sample...
- Next: Be agnostic about microscopic models and give two general arguments that explain why σ_{xy} is quantized.
Later: Look at two microscopic models.

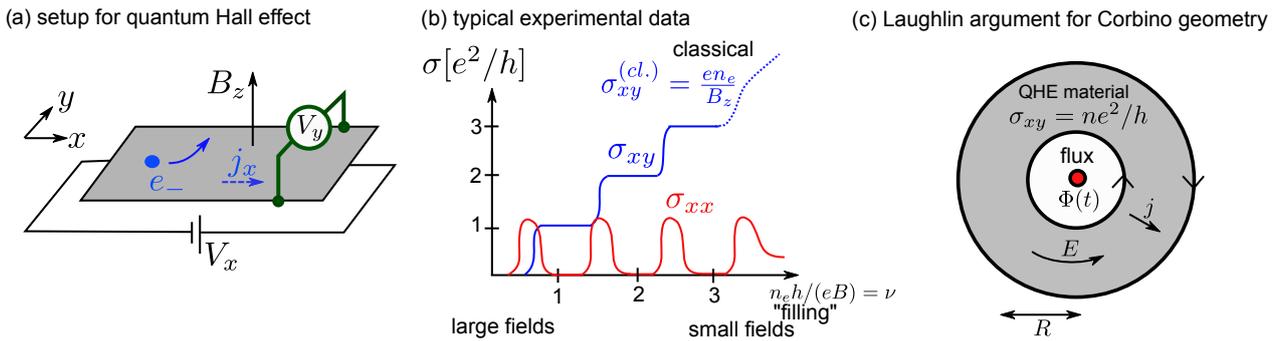


Figure 26: Quantum Hall effect.

Argument 1: Robustness of σ_{xy} via Laughlin argument (relation to 1D charge pump)

- Consider Corbino geometry, which is an annulus of 2D QHE material [Fig. 26(c)].
If the material has $\sigma_{xy} = ne^2/h$, would expect *radial* current j as a response to electric field E applied along azimuthal direction.
- How to apply E ? Insert time-dependent (but adiabatic) magnetic flux $\Phi(t)$ in inner hole, use Faraday effect:

$$\oint d\mathbf{r} \cdot \mathbf{E} = \partial_t \Phi(t) \rightarrow E(R, t) = \frac{1}{2\pi R} \partial_t \Phi(t) \quad (26)$$

- How to measure j ? Find charge ΔQ transferred between inner and outer edge in time ΔT :

$$j = \frac{I}{2\pi R} = \frac{\Delta Q / \Delta T}{2\pi R} \quad (27)$$

- Measure σ_{xy} from E, j :

$$\sigma_{xy} = \frac{j}{E} = \frac{I}{\partial_t \Phi} \quad (28)$$

- Argument for presence of gapless edge states:
 - For finite σ_{xy} and for a gap in the bulk ($\sigma_{xx} = 0$), the transferred charge ΔQ cannot relax across the bulk and must pile up at the edges.
 - As process was adiabatic, edge states must be gapless to absorb the charge.
 - Edge theory is “anomalous”: Charge is not-conserved individually at each edge (unlike stand-alone chain).

- Question: Why is $\sigma_{xy} = ne^2/h$ to such a high precision?
Answer: Laughlin argument [Laughlin, Phys. Rev. B 23, 5632 (1981)].
- Chose special $\Delta\Phi = \Phi_0 = h/e$ (flux quantum) inserted in time ΔT (c.f. Thouless pump): Find transferred charge:

$$\Delta Q = I\Delta T = \sigma_{xy} \underbrace{\Delta T \partial_t \Phi}_{\Phi_0} = \sigma_{xy} \frac{h}{e} \quad (29)$$

- Fact from QM: Vector potential generated by Φ_0 can be removed by (large) gauge-transformation, $H(\Phi = \Phi_0) = H(\Phi = 0)$.
- Hamiltonian of system (and eigenstates) unchanged after time ΔT . Due to adiabatic evolution, system is still in eigenstate.
- Non-interacting system: Only the occupation of (gapless!) single-particle edge states could have changed, thus $\Delta Q/e = n$ is an integer!

It follows:

$$\sigma_{xy} = \frac{\Delta Q}{h/e} = ne^2/h \quad (30)$$

- Note: The Laughlin argument works also with disorder and interactions, it only relies on gauge invariance.

Argument 2: Connection between σ_{xy} and Chern number via Kubo formula

[Thouless, Kohmoto, Nightingale, den Nijs (TKNN), Phys. Rev. Lett 49, 405 (1982)]

- Calculate σ_{xy} for 2D electron system described by Bloch Hamiltonian $H(\mathbf{k})$.
- Kubo formula connects conductivity with retarded current-current correlator: $\sigma_{xy}(\omega) = \frac{1}{\hbar\omega} \int_0^\infty dt e^{i\omega t} \langle [j_x(0), j_y(t)] \rangle$ (use Lehmann representation, $\omega \rightarrow 0$, work at $T = 0$, lazy notation - should have $|u_{\alpha\mathbf{k}}\rangle$ and $|u_{\beta\mathbf{k}'}\rangle$, but along the way we would get $\delta_{\mathbf{k},\mathbf{k}'}$):

$$\sigma_{xy} = i\hbar \sum_{E_\alpha < E_F < E_\beta} \int_{\mathbf{k}} \frac{\langle u_{\alpha\mathbf{k}} | j_y | u_{\beta\mathbf{k}} \rangle \langle u_{\beta\mathbf{k}} | j_x | u_{\alpha\mathbf{k}} \rangle - \langle u_{\alpha\mathbf{k}} | j_x | u_{\beta\mathbf{k}} \rangle \langle u_{\beta\mathbf{k}} | j_y | u_{\alpha\mathbf{k}} \rangle}{[E_\beta(\mathbf{k}) - E_\alpha(\mathbf{k})]^2} \quad (31)$$

- Current density \mathbf{j} : Charge times group velocity $\mathbf{j} = \frac{e}{\hbar} \partial_{\mathbf{k}} H(\mathbf{k})$.
- Side calculation: Use $\partial_{k_i} (E(\mathbf{k}) |u_{\mathbf{k}}\rangle) = \partial_{k_i} (H(\mathbf{k}) |u_{\mathbf{k}}\rangle) = [\partial_{k_i} H(\mathbf{k})] |u_{\mathbf{k}}\rangle + H(\mathbf{k}) (\partial_{k_i} |u_{\mathbf{k}}\rangle)$ in

$$\begin{aligned} \langle u_{\alpha\mathbf{k}} | [\partial_{k_i} H(\mathbf{k})] | u_{\beta\mathbf{k}} \rangle &= \langle u_{\alpha\mathbf{k}} | \partial_{k_i} (E_\beta(\mathbf{k}) | u_{\beta\mathbf{k}} \rangle) - \langle u_{\alpha\mathbf{k}} | H(\mathbf{k}) | \partial_{k_i} u_{\beta\mathbf{k}} \rangle \\ &= [E_\beta(\mathbf{k}) - E_\alpha(\mathbf{k})] \langle u_{\alpha\mathbf{k}} | \partial_{k_i} | u_{\beta\mathbf{k}} \rangle + \underbrace{\langle u_{\alpha\mathbf{k}} | u_{\beta\mathbf{k}} \rangle}_{0} \partial_{k_i} E_\beta(\mathbf{k}) \end{aligned}$$

- Insert in Kubo formula, the energy-denominator cancels:

$$\sigma_{xy} = -\frac{ie^2}{\hbar} \sum_{E_\alpha < E_F < E_\beta} \int_{\mathbf{k}} \left\{ \frac{\langle u_{\alpha\mathbf{k}} | \partial_{k_y} | u_{\beta\mathbf{k}} \rangle \langle u_{\beta\mathbf{k}} | \partial_{k_x} | u_{\alpha\mathbf{k}} \rangle - \langle u_{\alpha\mathbf{k}} | \partial_{k_x} | u_{\beta\mathbf{k}} \rangle \langle u_{\beta\mathbf{k}} | \partial_{k_y} | u_{\alpha\mathbf{k}} \rangle}{-\langle \partial_{k_y} u_{\alpha\mathbf{k}} | u_{\beta\mathbf{k}} \rangle - \langle \partial_{k_x} u_{\alpha\mathbf{k}} | u_{\beta\mathbf{k}} \rangle} \right\}$$

- For the sum over the unfilled bands $\sum_{E_F < E_\beta} |u_{\beta\mathbf{k}}\rangle \langle u_{\beta\mathbf{k}}| = 1 - \sum_{E_{\alpha'} < E_F} |u_{\alpha'\mathbf{k}}\rangle \langle u_{\alpha'\mathbf{k}}|$. The second term (α' -sum) vanishes by symmetry. We find:

$$\begin{aligned} \sigma_{xy} &= \frac{ie^2}{\hbar} \sum_{E_\alpha < E_F} \int_{\mathbf{k}} \left\{ \langle \partial_{k_y} u_{\alpha\mathbf{k}} | \partial_{k_x} u_{\alpha\mathbf{k}} \rangle - \langle \partial_{k_x} u_{\alpha\mathbf{k}} | \partial_{k_y} u_{\alpha\mathbf{k}} \rangle \right\} \\ &= \frac{e^2}{\hbar} \sum_{E_\alpha < E_F} \int_{\mathbf{k}} \left\{ \partial_{k_y} A_x(\alpha, \mathbf{k}) - \partial_{k_x} A_y(\alpha, \mathbf{k}) \right\} \\ &= -\frac{e^2}{\hbar} \sum_{E_\alpha < E_F} \frac{1}{2\pi} \int_{-\pi/a}^{\pi/a} dk_x \int_{-\pi/a}^{\pi/a} dk_y \mathcal{F}_\alpha(\mathbf{k}) \end{aligned}$$

and we find the TKNN-formula:

$$\sigma_{xy} = -\frac{e^2}{h} \sum_{E_\alpha < E_F} C_\alpha \quad (32)$$

- Conclusion: Hall conductivity σ_{xy} is (the negative of) the sum of Chern numbers for each occupied band.

QHE - Model 1: Landau levels (with external B-field)

- Continuum model for free 2D electrons in out-of-plane magnetic field (Landau gauge):

$$H = \frac{1}{2m} (\mathbf{p} - e\mathbf{A})^2$$

$$\mathbf{A} = \mathbf{e}_x B y$$

- H does not depend on x , thus $p_x \rightarrow \hbar k_x$:

$$H = \frac{1}{2m} [p_y^2 + (\hbar k_x - eBy)^2] \quad (33)$$

- For each k_x , this is a 1D harmonic oscillator in y -direction centered at $y_0(k_x) = \hbar k_x / (eB)$. Find Landau levels (LL):

$$H = \hbar\omega_c \left(a^\dagger a + \frac{1}{2} \right),$$

$$\omega_c = \frac{eB}{m} \text{ [cyclotron frequency]}$$

$$E_n = \hbar\omega_c \left(n + \frac{1}{2} \right)$$

See Fig. 27(b) for density of states.

- If we could place E_F between LLs, then we could explain experimental observations $\sigma_{xx} = 0$ and $\sigma_{xy} = \nu e^2/h$ if each of the ν filled LL had $|C| = 1$.
This only works if LLs are broadened by disorder. In this case Anderson localization is essential to maintain $\sigma_{xx} = 0$ even though there are states at the Fermi level.
- Degeneracy g of Landau level for finite $L_x \times L_y$ system [Fig. 27(a)]:
 - Finite $L_x \rightarrow$ quantized $k_x = \frac{2\pi}{L_x} n_x$ (“particle in box”).
 - Distance in center-coordinates along y : $\delta y_0 = \hbar \frac{2\pi}{L_x} / (eB)$.
 - Can place $g = L_y / \delta y_0$ wavefunctions in system: $g = L_x L_y \frac{eB}{h}$

- Number of filled Landau levels:

$$\nu = \frac{N}{g} = n_e \frac{h}{eB} \quad (34)$$

- Argument for $\sigma_{xy} = e^2/h$ per LL: Flux pumping [Fig. 27(c)]:
 - Smoothly deform Corbino geometry to torus where we can use LL wavefunction from above.
 - Adiabatically inserting flux quantum Φ_0 changes $k_x \rightarrow k_x + \frac{2\pi}{L_x}$.
 - This moves all y -coordinates by $\delta y = \delta y_0 = \frac{h}{L_x eB}$. All wavefunctions take their top neighbor’s place.
 - We have transferred one of the g states per LL to edge: $\Delta Q = \nu e$. $\sigma_{xy}(LL) = e^2/h$.

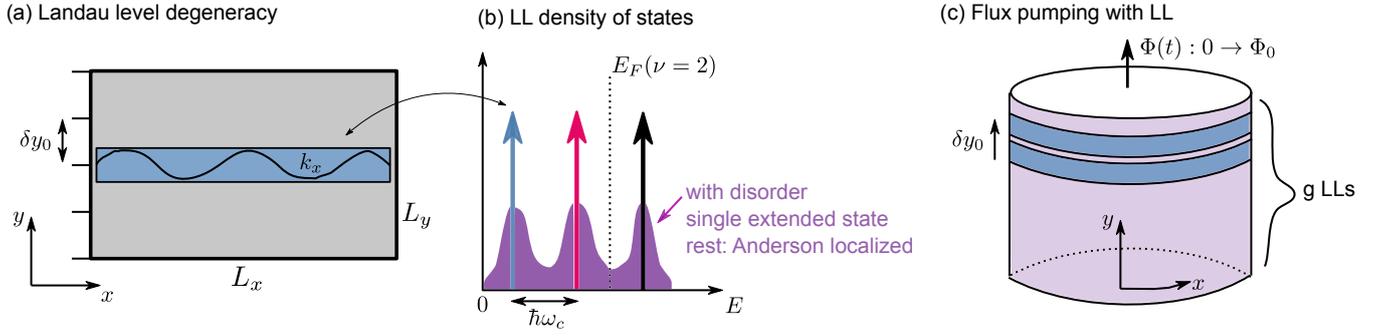


Figure 27: Quantum Hall effect from free electrons in 2D which form Landau levels (LL).

QHE - Model 2: Chern insulators on lattice (without external B-field)

- Chern insulator = bandstructure with $\sigma_{xy} = ne^2/h$ ($n \neq 0$) but without external magnetic field. Need to break time-reversal symmetry internally (complex hoppings, experimentally: Magnetization.)
- Simple 2D model on square lattice: Two get two bands, use two-”color” spinless electrons $\psi_{x,y} = (c_{(x,y),A}, c_{(x,y),B})^T$. Colors are denoted by τ Pauli matrices:

$$H = - \sum_{x,y} \left\{ \psi_{x,y}^\dagger \frac{\tau_z - i\tau_x}{2} \psi_{x+1,y} + \psi_{x,y}^\dagger \frac{\tau_z - i\tau_y}{2} \psi_{x,y+1} + h.c. \right\} + M \sum_{x,y} \psi_{x,y}^\dagger \tau_z \psi_{x,y} \quad (35)$$

- Imposing periodic boundary condition, $H = \sum_{\mathbf{k}} \psi_{\mathbf{k}}^\dagger H(\mathbf{k}) \psi_{\mathbf{k}}$ with $H(\mathbf{k}) = \mathbf{d}(\mathbf{k}) \cdot \boldsymbol{\tau}$ and

$$\mathbf{d}(\mathbf{k}) = (\sin k_x, \sin k_y, M - \cos k_x - \cos k_y) \quad (36)$$

- Band structure $E_{\mathbf{k}} = \pm d(\mathbf{k})$ will be gapless if $M = \{-2, 0, 2\}$. What is the Chern number in gapped phases?

Graphical approach looking at high-symmetry points in 2D-BZ [Fig. 28(a)]:

- $M < -2$: $\hat{\mathbf{d}}$ always points down ($-\mathbf{e}_z$) for \mathbf{k} everywhere, no wrapping of unit-sphere: $C = 0$
- $-2 < M < 0$: At point (π, π) , $\hat{\mathbf{d}}$ points up ($+\mathbf{e}_z$). Thus we have a non-trivial winding and we find $C = +1$ (sign from exact calculation using $\mathcal{F}(\mathbf{k})$ or Eq. (37)).
- $0 < M < 2$: Inverse to previous situation, three points up, one down: $C = -1$.
- $M > 2$: All points up, $C = 0$.
- Alternative formula for Chern number for models $H(\mathbf{k}) = \mathbf{d}(\mathbf{k}) \cdot \boldsymbol{\tau}$ [Kronecker]: Fix vector $\mathbf{d}_0 \neq 0$, find the points \mathbf{k}_i in the BZ where $\mathbf{d}(\mathbf{k}_i)$ points in the \mathbf{d}_0 -direction. Then:

$$C = \sum_{\mathbf{k}_i} \text{sign det} \left(\mathbf{d}_0, \frac{\partial \mathbf{d}}{\partial k_x}, \frac{\partial \mathbf{d}}{\partial k_y} \right) \Big|_{\mathbf{k}=\mathbf{k}_i} \quad (37)$$

Chiral boundary mode = quantum Hall edge state

- Use the lattice model (35) to study topological edge mode for region of, say, $C = 1$.
- Expand Bloch Hamiltonian around point (π, π) , up to terms quadratic in $\mathbf{q} = \mathbf{k} - (\pi, \pi)$:

$$H_{2D-Dirac}(\mathbf{q}) = q_x \sigma_x + q_y \sigma_y + M \sigma_z \quad (38)$$

This is a 2D-Dirac Hamiltonian.

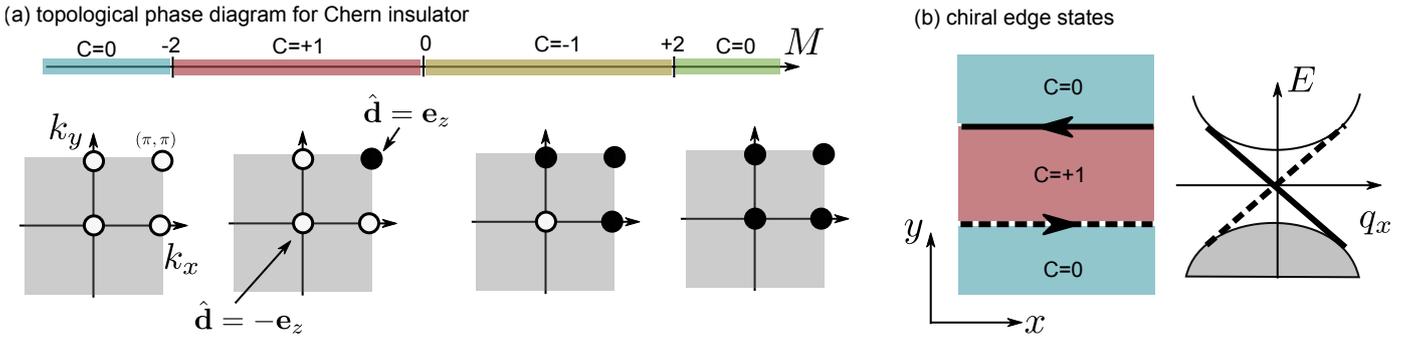


Figure 28: Lattice model for Chern insulator Eq. (35).

- Make parameter M space-dependent $M = M(y)$ so that at $y = 0$ so that as we increase $y < 0$ to $y > 0$, we model transition from $C = 0$ to $C = 1$ or vice versa (in space!).
- Back to Dirac approximation:

$$H_{2D-Dirac}(\mathbf{q}) = q_x \sigma_x - i \partial_y \sigma_y + M(y) \sigma_z \quad (39)$$

- For the last two terms, the Jackiw-Rebbi zero mode construction (20) for domain wall mode in 1D-Dirac Hamiltonian (18) goes through, but with σ_x eigenstates. The first term including $q_x \sigma_x$ leads to a linear dispersion from motion along the boundary:

$$\psi_{\pm}(x, y) = \mathcal{N} e^{-iq_x x} e^{\pm \int_0^y d\tilde{y} M(\tilde{y})} \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix},$$

$$E_{\pm}(q_x) = \pm q_x.$$

- Have one normalizable solution per interface, ψ_- if we go from $m < 0$ at $y < 0$ to $m > 0$ at $y > 0$, and ψ_+ in the opposite case. [Fig. 28(b)]
- The group velocity of ψ_{\pm} is $v_{\pm} = \partial_{q_x} E_{\pm} = \pm 1$. This is a one-way street for wave-packets (“chiral”) with perfect conductance (no backscattering).
- See Fig. 28(b) for chiral edge mode dispersion: Perturbations can change $E_{\pm}(q_x)$, but connectivity with bands and crossing of the gap is protected (like a rubber band)! Generalize for boundary between Chern number $C_{1,2}$: Have $|C_1 - C_2|$ edge states with velocity $\text{sgn}(C_1 - C_2)$.
- Robustness of QHE: Chiral edge modes can never back-scatter, unless bulk becomes gapless and hybridization with partner mode at the other side occurs.

12.5 Symmetries and ten-fold way classification

- General 2nd quantized fermionic Hamiltonian

$$\hat{H} = \sum_{ij} \hat{\psi}_i^{\dagger} h_{ij} \hat{\psi}_j \quad (40)$$

with $h = h^{\dagger}$ a complex hermitian matrix.

Fock-space operators $\hat{\psi}_i^{(\dagger)}$ (with hat!) fulfill fermionic anti-commutation relations (ACR) $\{\hat{\psi}_i, \hat{\psi}_j^{\dagger}\} = \delta_{ij}$, $\{\hat{\psi}_i, \hat{\psi}_j\} = 0 = \{\hat{\psi}_i^{\dagger}, \hat{\psi}_j^{\dagger}\}$.

- The index i can denote (sub-)lattice site, spin, flavor... or a combination thereof.
- Strategy: Specify symmetries by their action on $\hat{\psi}_i^{(\dagger)}$, read off consequences for h .

Unitary symmetry

- Let matrix U that transforms the $\hat{\psi}_i^{(\dagger)}$ as follows:

$$\begin{aligned}\hat{\psi}_j &\rightarrow \sum_k U_{jk} \hat{\psi}_k \equiv \hat{U} \hat{\psi}_j \hat{U}^{-1}, \\ \hat{\psi}_j^\dagger &\rightarrow \sum_k U_{jk}^* \hat{\psi}_k^\dagger \equiv \hat{U} \hat{\psi}_j^\dagger \hat{U}^{-1}.\end{aligned}$$

Here, \hat{U} is a second-quantized operator that acts on Fock space.

- U is a unitary matrix: Since ACR should be preserved, $\delta_{ij} = \{\hat{\psi}_i, \hat{\psi}_j^\dagger\} \rightarrow \hat{U} \{\hat{\psi}_i, \hat{\psi}_j^\dagger\} \hat{U}^{-1} \stackrel{!}{=} \delta_{ij}$ it follows that $UU^\dagger = 1$.
- \hat{U} is a symmetry of the Hamiltonian \hat{H} if

$$\hat{U} \hat{H} \hat{U}^{-1} \stackrel{!}{=} \hat{H} \quad (41)$$

- Special case of non-interacting systems (characterized by h as in Eq. (40)), it follows

$$\hat{H} \rightarrow \hat{U} \hat{H} \hat{U}^{-1} = \sum_{ij} \hat{U} \hat{\psi}_i^\dagger \hat{U}^{-1} h_{ij} \hat{U} \hat{\psi}_j \hat{U}^{-1} = \sum_{ij} \sum_{kl} U_{ik}^* \hat{\psi}_k^\dagger h_{ij} U_{jl} \hat{\psi}_l \stackrel{!}{=} \sum_{kl} \hat{\psi}_k^\dagger h_{kl} \hat{\psi}_l \quad (42)$$

and we read off $U^\dagger h U \stackrel{!}{=} h$ or

$$\boxed{[U, h] = 0} \quad (43)$$

- Can find a basis where both U and h are block diagonal, each block has a common symmetry eigenvalue (colors in Fig. 29)
- Examples:
 - lattice translation: $U = T_{\mathbf{a}}$, eigenstates are Bloch states with eigenvalue $\mathbf{k} = (k_x, k_y, k_z)$.
 - total spin in z-direction: $U = S_{tot}^z = \sum_i S_i^z$, eigenvalue of, i.e. for even number N of spin-half $S_{tot}^z = 0, \pm 1, \dots \pm N/2$.

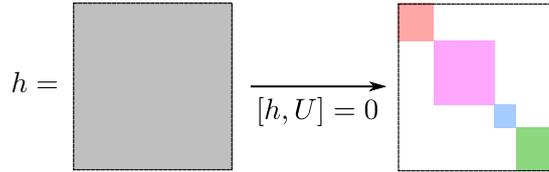


Figure 29: A unitary symmetry diagonalizes the Hamiltonian matrix h in blocks.

Anti-unitary symmetries

- Assume we have exhausted all unitary symmetries and wrote h in block-form. How can we further classify these blocks of h ?
- Important symmetries in nature are realized as anti-unitary operators:

$$\begin{aligned}|\alpha\rangle &\rightarrow \hat{O} |\alpha\rangle \\ \langle\beta|\alpha\rangle &= \langle\hat{O}\alpha|\hat{O}\beta\rangle\end{aligned}$$

- Wigner Theorem: Anti-unitary symmetries must be *anti-linear*, this means $\hat{O} = \hat{U}\mathcal{K}$ with \mathcal{K} the complex conjugation operator and \hat{U} a unitary symmetry.

Time reversal \hat{T}

- Time reversal (motion reversal) \hat{T} is anti-unitary operator:

$$\boxed{\hat{T} = \hat{U}_T \mathcal{K}} \quad (44)$$

Reason: Assert $\hat{x} \rightarrow \hat{x}$ but $\hat{p} \rightarrow -\hat{p}$, consider $[\hat{x}, \hat{p}] = i$, so it is consistent to request $i \rightarrow -i$, thus \hat{T} anti-linear)

- Action on $\hat{\psi}^{(\dagger)}$:

$$\begin{aligned} \hat{\psi}_j &\rightarrow \hat{T} \hat{\psi}_j \hat{T}^{-1} = \sum_k U_{T,jk} \hat{\psi}_k \\ \hat{\psi}_j^\dagger &\rightarrow \hat{T} \hat{\psi}_j^\dagger \hat{T}^{-1} = \sum_k U_{T,jk}^* \hat{\psi}_k^\dagger \end{aligned}$$

- Time reversal invariance for many-body Hamiltonian \hat{H} is defined as:

$$\hat{H} \stackrel{!}{=} \hat{T} \hat{H} \hat{T}^{-1} \quad (45)$$

- For non-interacting systems as in Eq. (40), we find the following condition on h (\mathcal{K} acts on numbers in h , not on $\hat{\psi}$):

$$\boxed{U_T^\dagger h^* U_T = h} \quad (46)$$

Up to unitary rotations, this is a reality condition on h^* .

Note: For Bloch Hamiltonians $h \rightarrow h(\mathbf{k})$ the complex conjugation generalizes to $h^* \rightarrow h^*(-\mathbf{k})$.

- Two types of \hat{T} : Acting with \hat{T} twice, we have $\hat{T} \hat{T} \hat{\psi}_j \hat{T}^{-1} \hat{T}^{-1} = \sum_k (U_T^* U_T)_{jk} \hat{\psi}_k$ which leads to

$$(U_T^* U_T)^\dagger h (U_T^* U_T) = h \quad (47)$$

Since we required that h is an irreducible block, Schur's lemma can be applied, $U_T^* U_T \sim 1$. Since $(U_T^* U_T)$ is unitary, we are left with a phase:

$$U_T U_T^* \stackrel{!}{=} e^{i\phi} \quad (48)$$

but $\det(U_T U_T^*) = \det U_T (\det U_T)^* \in \mathbb{R}$, so $\phi = \{0, \pi\}$ and thus

$$\boxed{\hat{T}^2 = \pm 1 \text{ for } U_T^* U_T = \pm 1} \quad (49)$$

- Example for $\hat{T}^2 = -1$: Spin-1/2 fermions, $\psi = \begin{pmatrix} c_\uparrow \\ c_\downarrow \end{pmatrix}$, combine to yield spin-operator $\hat{\mathbf{S}} = \frac{1}{2} \psi^\dagger \boldsymbol{\sigma} \psi$.

Chose $U_T = i\sigma_y = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$ so that $c_\uparrow \rightarrow c_\downarrow$, $c_\downarrow \rightarrow -c_\uparrow$ we have indeed $U_T U_T^* = -1$ and we flip the spin as expected:

$$\hat{T} \hat{\mathbf{S}} \hat{T}^{-1} = \frac{1}{2} \psi^\dagger [(-i\sigma_y) \boldsymbol{\sigma}^* (i\sigma_y)] \psi = \frac{1}{2} \psi^\dagger [\sigma_y \boldsymbol{\sigma}^* \sigma_y] \psi = -\hat{\mathbf{S}}. \quad (50)$$

- Important consequence for time-reversal symmetric systems with $\hat{T}^2 = -1$: Kramer's degeneracy (two-fold degeneracy of all eigenstates)

Let $\hat{H} |\psi\rangle = E |\psi\rangle$ and assume $\hat{H} = \hat{T} \hat{H} \hat{T}^{-1}$. We have

$$\hat{T} \hat{H} |\psi\rangle = \hat{H} \hat{T} |\psi\rangle = E \hat{T} |\psi\rangle \quad (51)$$

so $|\psi'\rangle \equiv \hat{T} |\psi\rangle$ is also an eigenstate at energy E . To prove degeneracy, show that there is no $c \in \mathbb{C}$ with $c |\psi\rangle \stackrel{!}{=} |\psi'\rangle = \hat{T} |\psi\rangle$. Apply $\hat{T}^2 = -1$, but \hat{T} contains \mathcal{K} , so $c^* c |\psi\rangle = -|\psi\rangle$ but there is no $c \in \mathbb{C}$ with $|c|^2 = -1$.

Particle-hole symmetry \hat{P} (also called charge conjugation)

- Particle hole symmetry $\hat{P} = \hat{U}_P$ is a *unitary* symmetry that exchanges $\psi \leftrightarrow \psi^\dagger$:

$$\begin{aligned}\hat{\psi}_j &\rightarrow \hat{P}\hat{\psi}_j\hat{P}^{-1} = \sum_k (U_{P,jk})^* \hat{\psi}_k^\dagger \\ \hat{\psi}_j^\dagger &\rightarrow \hat{P}\hat{\psi}_j^\dagger\hat{P}^{-1} = \sum_k U_{P,jk} \hat{\psi}_k\end{aligned}$$

From the invariance of the ACR, U_P is a unitary matrix.

- A many-body Hamiltonian \hat{H} is particle-hole symmetric if

$$\hat{H} \stackrel{!}{=} \hat{P}\hat{H}\hat{P}^{-1} \quad (52)$$

- As for time-reversal, we have two kinds of particle-hole symmetry, $\hat{P}^2 = \pm 1$ for $U_P^* U_P = \pm 1$.
- For non-interacting systems Eq. (40), from particle-hole symmetry, it follows: $\text{tr}h = 0$ and

$$\boxed{U_P^\dagger h^* U_P = -h} \quad (53)$$

- For single-particle eigenvector $h \cdot u = \varepsilon u$, we thus have a particle-hole reversed partner state:

$$h(U_P^\dagger u^*) = -\varepsilon(U_P^\dagger u^*) \quad (54)$$

- Example: Superconducting systems in mean-field approximation $V\hat{c}_\uparrow^\dagger\hat{c}_\downarrow^\dagger\hat{c}_\uparrow\hat{c}_\downarrow \rightarrow V\hat{c}_\uparrow^\dagger\hat{c}_\downarrow^\dagger \underbrace{\langle\hat{c}_\uparrow\hat{c}_\downarrow\rangle}_{\Delta} + V\langle\hat{c}_\uparrow^\dagger\hat{c}_\downarrow^\dagger\rangle\hat{c}_\uparrow\hat{c}_\downarrow$

Using Nambu spinors $\hat{\psi}^\dagger = (\hat{c}_\uparrow^\dagger, \hat{c}_\downarrow^\dagger)$, these Hamiltonians can be described by non-interacting Bogoliubov-deGennes (BdG) Hamiltonians.

BdG Hamiltonians have built-in particle-hole symmetry (or “constraint”, see Ex. 12.4).

Chiral symmetry \hat{S}

- Chiral symmetry is combination of time-reversal and particle-hole symmetry and thus an anti-unitary operator on the Fock space:

$$\hat{S} = \hat{T}\hat{P} \quad (55)$$

- If \hat{T} and \hat{P} are broken, their combination can still be a symmetry of \hat{H} :

$$\hat{H} \stackrel{!}{=} \hat{S}\hat{H}\hat{S}^{-1} \quad (56)$$

- Action on $\hat{\psi}$:

$$\hat{\psi}_j \rightarrow \hat{S}\hat{\psi}_j\hat{S}^{-1} = \hat{T}\hat{P}\hat{\psi}_j\hat{P}^{-1}\hat{T}^{-1} = \sum_k \hat{T}(U_{P,jk}^*) \hat{\psi}_k^\dagger \hat{T}^{-1} = \sum_k (U_{P,jk}) \hat{T}\hat{\psi}_k^\dagger \hat{T}^{-1} = \sum_k \underbrace{(U_P U_T^*)}_{\equiv U_S^*}{}_{jk} \hat{\psi}_k^\dagger \quad (57)$$

- Consequence for non-interacting Hamiltonian in Eq. (40):

- Find $\text{tr}h = 0$ and $U_S^\dagger h U_S = -h$ with $U_S = U_P^* U_T$.
- Applying chiral symmetry twice: $(U_S^2)^\dagger h (U_S^2) = h$, use Schur’s lemma: $U_S^2 = e^{i\phi}$. Redefine $U_S \rightarrow e^{i\phi/2} U_S$ [this did not work above for time-reversal!], then $U_S^2 = 1$ and $U_S = U_S^\dagger$.
- Final:

$$\boxed{U_S h U_S = -h \leftrightarrow \{U_S, h\} = 0 \text{ with } U_S^2 = 1} \quad (58)$$

- Consequence for single-particle eigenvalues (see above):

$$hu = \varepsilon u \rightarrow h(U_S u) = -\varepsilon(U_S u) \quad (59)$$

Tenfold way symmetry classification for non-interacting Hamiltonians

- Summary of symmetries for non-interacting Hamiltonian in terms of matrix $h = h^\dagger$ (void of unitary symmetries)

symmetry	non-interacting Hamiltonian h	Bloch Hamiltonian $h(\mathbf{k})$	types
time-reversal	$U_T^\dagger h^* U_T = +h$	$U_T^\dagger h^*(-\mathbf{k}) U_T = +h(\mathbf{k})$	$U_T^* U_T = \pm 1$
particle-hole	$U_P^\dagger h^* U_P = -h$	$U_P^\dagger h^*(-\mathbf{k}) U_P = -h(\mathbf{k})$	$U_P^* U_P = \pm 1$
chiral	$U_S h U_S = -h$	$U_S h(\mathbf{k}) U_S = -h(\mathbf{k})$	$U_S^2 = 1$

- We can assume that there is only one time-reversal (or particle-hole) symmetry:
If there were two time-reversal symmetries, we would combine them to one unitary symmetry $\hat{T}_1 \hat{T}_2$ with $U = U_{T_1} U_{T_2}^*$ and $[U, h] = 0$.
Thus h should be block-diagonalized first.
On each block, $U_{T_1} U_{T_2}^*$ would be a constant, so on each block, there is only a single time-reversal symmetry.
- This argument does not work for the combination $\hat{T}\hat{P}$, as they do not combine to a unitary symmetry (but to chiral!).
- Tenfold-way classification [Altland and Zirnbauer (1997)]:
 - Is h time-reversal symmetric? If yes, how? ($U_T^* U_T = \pm 1$) [3 possibilities “0,+,-”]
 - Is h particle-hole symmetric? If yes, how? ($U_P^* U_P = \pm 1$) [3 possibilities “0,+,-”]
 - If h is neither time-reversal nor particle-hole symmetric (1 out of the 3x3=9 possibilities above):
Does h have chiral symmetry? [split in 2 possibilities]
(In the other 8 cases, the presence of chiral symmetry is uniquely determined.)
- In summary: 10 different cases.
Tabular representation of tenfold-way classification:

class	T	P	S	D=1	D=2	D=3
A	0	0	0	0	\mathbb{Z} (e.g. QHE)	0
AIII	0	0	1	\mathbb{Z} (e.g. SSH)	0	\mathbb{Z}
AI	+	0	0	0	0	0
BDI	+	+	1	\mathbb{Z}	0	0
D	0	+	0	\mathbb{Z}_2 (e.g. Maj. wire)	\mathbb{Z}	0
DIII	-	+	1	\mathbb{Z}_2	\mathbb{Z}_2	\mathbb{Z}
AII	-	0	0	0	\mathbb{Z}_2 (e.g. QSH)	\mathbb{Z}_2 (e.g. TI)
CII	-	-	1	$2\mathbb{Z}$	0	\mathbb{Z}_2
C	0	-	0	0	$2\mathbb{Z}$	0
CI	+	-	1	0	0	$2\mathbb{Z}$

- The right hand side of the 10-fold way table shows the topological classification.
We have already seen the SSH model (1D class AIII) and the Chern insulator or QHE (2D class A) as examples.

12.6 Time reversal invariant topological insulators (in 2D, class AII) (07.01.2022)

- With time-reversal symmetry: Anti-symmetric Berry curvature $\mathcal{F}(\mathbf{k}) = -\mathcal{F}(-\mathbf{k})$ (does not necessarily vanish!), but leads to $C = -C \rightarrow C = 0$.
Consequence: No (quantum) Hall effects with time-reversal symmetry.

- Proof: From time-reversal symmetry, have for eigenvector u of Bloch-Hamiltonian $h(\mathbf{k})$: $u(\mathbf{k}) = U_T^* \cdot u^*(-\mathbf{k})$ and $u^*(\mathbf{k}) = U_T \cdot u(-\mathbf{k})$. Insert in:

$$\begin{aligned}\mathcal{F}_z(\mathbf{k}) &= i [\partial_{k_x} u^*(\mathbf{k})] \cdot [\partial_{k_y} u(\mathbf{k})] - i [\partial_{k_y} u^*(\mathbf{k})] \cdot [\partial_{k_x} u(\mathbf{k})] \\ &= i [\partial_{k_x} u(-\mathbf{k}) U_T^T] \cdot [U_T^* \partial_{k_y} u^*(-\mathbf{k})] - i [\partial_{k_y} u(-\mathbf{k}) U_T^T] \cdot [U_T^* \partial_{k_x} u^*(-\mathbf{k})] \\ \{U_T^T U_T^* = 1\} &= -\mathcal{F}_z(-\mathbf{k})\end{aligned}$$

Quantum spin Hall effect

- Idea: Add spin-ful time-reversal symmetry

$$U_T = i\sigma_y = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \quad (60)$$

to the 2D Chern-insulator Hamiltonian (35) (here called H_0). Recall H_0 was made from two “colors” of spin-less electrons $c_{A,B}$ (suppressed τ -grading).

$$H = \begin{pmatrix} c_{\uparrow}^\dagger & c_{\downarrow}^\dagger \end{pmatrix} \underbrace{\begin{pmatrix} H_0 & 0 \\ 0 & H_0^* \end{pmatrix}}_H \begin{pmatrix} c_{\uparrow} \\ c_{\downarrow} \end{pmatrix} \quad (61)$$

Hamiltonian H is time-reversal symmetric:

$$U_T^\dagger H^* U_T = \sigma_y H^* \sigma_y = H \quad (62)$$

- Edge-state picture: H has two counter-propagating chiral modes at each edge, with opposite spin [Fig. 30(a)].
Note: Time-reversal is local, but maps left-moving to right-moving states ($k_x \leftrightarrow -k_x$) and flips the spin. At time-reversal invariant momentum (TRIM, $k_x = 0$): The two states are Kramers partners.
- Hall conductivities:
 - for charge: $\sigma_{xy} = \frac{e^2}{h} (C_\uparrow + C_\downarrow) = 0$ where $C_{\uparrow,\downarrow}$ are spin-resolved Chern numbers with $C_\uparrow = -C_\downarrow$. (Consistent with $\sigma_{xy} = 0$ for time-reversal symmetric system).
 - for spin: Weigh charge-current by spin, good as long as S_z conserved: $\sigma_{xy}^s = \frac{e^2}{2h} (C_\uparrow - C_\downarrow) = e^2/h$ (if H_0 such that $C_\uparrow = -C_\downarrow = 1$). This is the spin-Hall conductivity.

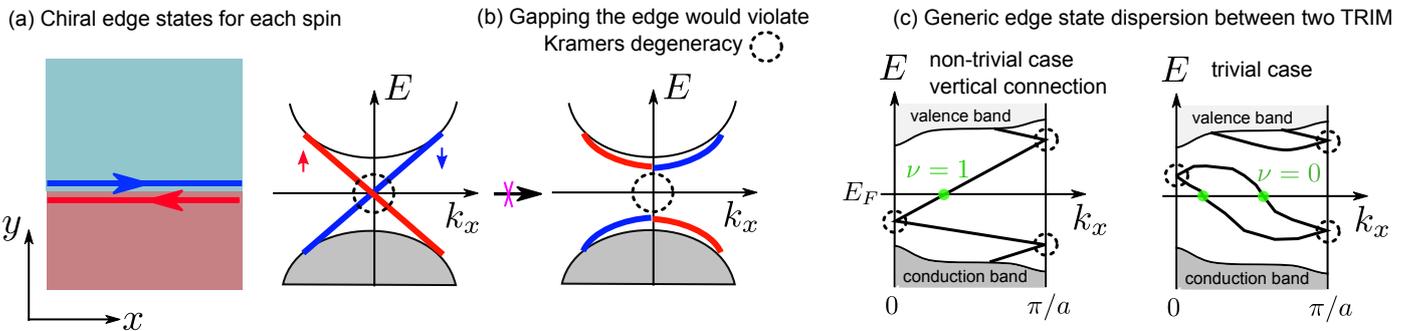


Figure 30: Time-reversal symmetric topological insulator.

Spin-orbit coupling

- Problem I: H is block-diagonal, which is related to the imposed spin-rotation symmetry, $[H, \sigma_z] = 0$. Can we break the latter by terms on the off-diagonal but still preserve time-reversal?
- Answer: Spin-orbit coupling.
Want $H \rightarrow H + H_{SO}$ with $H_{SO} = f_x(\mathbf{k})\sigma_x + f_y(\mathbf{k})\sigma_y$, $f_{x,y} \in \mathbb{R}$. According to Eq. (62), we need $f_{x,y}(\mathbf{k}) \stackrel{!}{=} -f_{x,y}(-\mathbf{k})$, i.e. $f_x(k_x) = \sin k_x$. The resulting terms like $c_{\uparrow}^{\dagger}(\mathbf{k}) \sin(k_x) c_{\downarrow}(\mathbf{k})$ are known as spin-orbit coupling (orbit \sim momentum).
- Reminder: Spin-orbit coupling
 - was introduced in atomic physics a contribution $\lambda_{SO} \hat{\mathbf{S}} \cdot \hat{\mathbf{L}}$, with $\hat{\mathbf{S}}$ spin-1/2 operator and $\hat{\mathbf{L}} = \hat{\mathbf{r}} \times \hat{\mathbf{p}}$, both odd under time-reversal.
 - is a relativistic effect $\lambda_{SO} \sim [\#\text{protons}]^4 \rightarrow$ Spin-orbit coupling more pronounced in materials with heavy elements.

Robustness of edge-states

- Once S_z is no longer conserved, $[H, \sigma_z] \neq 0$, it makes no sense to define spin-Hall conductivity.
- Problem II: Are the edge states robust if time-reversal symmetry is maintained? Or can they be gapped out?
- First answer: Perturbation theory.
 - Let $|\psi\rangle$ and $|\psi'\rangle = \hat{T}|\psi\rangle$ be the degenerate Kramers partner states (at $k_x = 0$).
 - Check for their overlap $\langle \psi | \hat{H}_{SO} | \psi' \rangle$ under the most general time-reversal symmetric perturbation:

$$\begin{aligned}
\langle \psi | \hat{H}_{SO} \hat{T} | \psi \rangle &\stackrel{\text{anti-unitary}}{=} \langle \hat{T} \psi | \hat{T} \hat{H}_{SO} \hat{T} | \psi \rangle^* \\
&\stackrel{[\hat{T}, \hat{H}_{SO}] = 0}{=} \langle \hat{T} \psi | \hat{H}_{SO} \hat{T}^2 | \psi \rangle^* \\
&= -\langle \hat{T} \psi | \hat{H}_{SO} | \psi \rangle^* \\
&= -\langle \psi | \hat{H}_{SO} \hat{T} | \psi \rangle
\end{aligned}$$

- Find: $\langle \psi | \hat{H}_{SO} | \psi' \rangle = 0$. No gap opening in perturbation theory.
- Second answer:
Kramers theorem ties the “knot”, i.e. dashed circle in Fig. 30(a), together. It can only be moved in energy, but not gapped.

Edge states for generic situation and \mathbb{Z}_2 invariant [Fig. 30(c)]:

- Energy of Kramers pairs is not tied to E_F . We might or might not have edge states, their presence can also be accidental (i.e. non-topological).
- Kramers degeneracy is guaranteed for each state at $k_x = 0$ and $\pi/a = -\pi/a$ (part $k < 0$ part of BZ not shown due to time-reversal redundancy).
- Connectivity between states at $k_x = 0$ and π/a fixes value $\nu \in \{0, 1\}$ of \mathbb{Z}_2 topological invariant:
 - $\nu = 1$: Connection of alternating Kramers pairs, odd parity of E_F crossings. Cannot remove crossing, perfect edge conduction $g = e^2/h$.
 - $\nu = 0$: Pairing of Kramers energies, even number of E_F crossings. Can push pair of edge states below E_F , obtain trivial edge.
- \mathbb{Z}_2 nature: Combining two “ $\nu = 1$ ” edges leads to a trivial edge “ $\nu = 0$ ”, since band-crossings away from TRIM are not protected (not avoided).

Scattering theory view-point for disordered edge [Fig. 31]

- Consider left and right clean regions (L,R) with N edge states that have a velocity $v = \partial_k E(k)$ pointing towards the disordered scattering region (incoming). Label states $|n, L\rangle$ and $|n, R\rangle$, $n = 1, 2, \dots, N$.
- Recall that $\nu = N \bmod 2$, so a topologically non-trivial case corresponds to odd N .
- The N time-reversed partners $\hat{T}|n\rangle$ move in the opposite direction away from the scattering region (outgoing)
- Ansatz for scattering states in left and right region:

$$|\Psi, L\rangle = \sum_{n=1}^N \alpha_{n,L} \underbrace{|n, L\rangle}_{in} + \beta_{n,L} \underbrace{\hat{T}|n, L\rangle}_{out}$$

$$|\Psi, R\rangle = \sum_{n=1}^N \alpha_{n,R} \underbrace{|n, R\rangle}_{in} + \beta_{n,L} \underbrace{\hat{T}|n, L\rangle}_{out}$$

The α and β are not independent but related by continuity conditions to eigenstate wavefunctions in the disordered region.

- The unitary $2N \times 2N$ scattering matrix S relates incoming to outgoing amplitudes:

$$\begin{pmatrix} \beta_L \\ \beta_R \end{pmatrix} = S \begin{pmatrix} \alpha_L \\ \alpha_R \end{pmatrix} \quad (63)$$

It is customary to write S in $N \times N$ transmission and reflection blocks:

$$S = \begin{pmatrix} r & t \\ t' & r' \end{pmatrix} \quad (64)$$

The transmission probability is $\text{tr}(t^\dagger t)$ and the Landauer conductance $g = \text{tr}(t^\dagger t) e^2/h$.

- What can be said about $\text{tr}(t^\dagger t)$?

Check how time-reversal acts on S , use $\hat{T}^2 = -1$:

$$\hat{T}|\Psi, L\rangle = \sum_{n=1}^N \alpha_{n,L}^* \underbrace{\hat{T}|n, L\rangle}_{out} - \beta_{n,L}^* \underbrace{|n, L\rangle}_{in}$$

$$\hat{T}|\Psi, R\rangle = \sum_{n=1}^N \alpha_{n,R}^* \underbrace{\hat{T}|n, R\rangle}_{out} - \beta_{n,L}^* \underbrace{|n, L\rangle}_{in}$$

These states still fulfill the Schrödinger equation, thus can read off S :

$$\begin{pmatrix} \alpha_L^* \\ \alpha_R^* \end{pmatrix} = -S \begin{pmatrix} \beta_L^* \\ \beta_R^* \end{pmatrix} \quad (65)$$

Complex conjugate and multiply with $(S^*)^{-1} = S^T$, compare to Eq. (63). We find:

$$S = -S^T \quad (66)$$

or

$$\begin{pmatrix} r & t \\ t' & r' \end{pmatrix} = - \begin{pmatrix} r^T & t'^T \\ t^T & r'^T \end{pmatrix} \quad (67)$$

- Consequence of Eq. (66):

- Try to gap out the edges $\leftrightarrow t = 0 = t'$. Then all states must be reflected back, we require $r^\dagger r = 1 = r'^\dagger r'$.
- Is it possible to have $r^\dagger r = 1$ and $r = -r^T$? Not possible for $N = 1$, for $N = 2$ can take $r = \sigma_y, \dots$
- For odd N : From $r = -r^T$ spectral theory requires to have a single zero eigenvalue (in conflict with $e^{i\phi}$ eigenvalues of unitary matrices).
From $\text{tr} r^\dagger r + \text{tr} t^\dagger t = N$ and the presence of the zero-eigenvalue of $r^\dagger r$, we find that $\text{tr} t^\dagger t \geq 1$.
- Conclusion: The edge cannot localize for odd N ($\nu = 1$) and has a minimum conductance $g = e^2/h$.

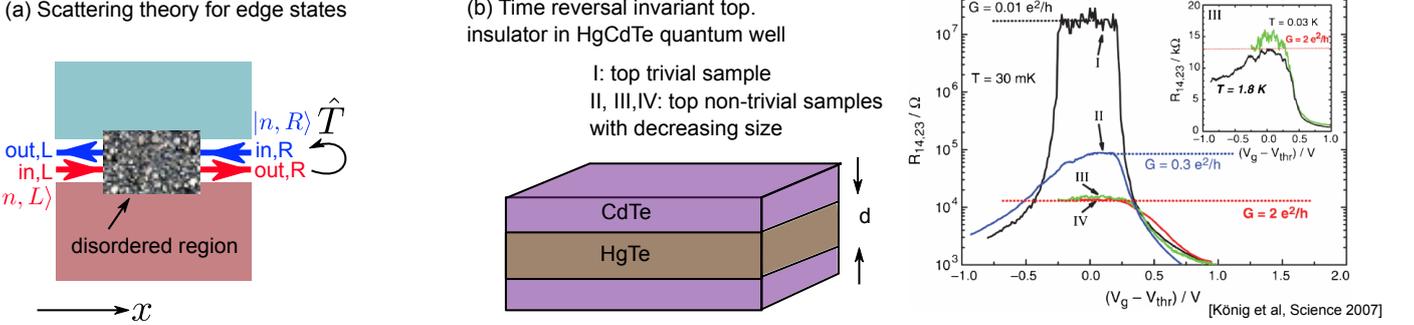


Figure 31: Scattering theory for edge of 2D time-reversal invariant topological insulator in class AII.

Topological bulk invariant

- For Bloch Hamiltonian $H(\mathbf{k})$, define matrix

$$w_{mn}(\mathbf{k}) \equiv u_m^*(\mathbf{k}) \cdot U_T \mathcal{K} \cdot u_n(-\mathbf{k})$$

where n, m run over all occupied bands.

- The matrix $w_{mn}(\mathbf{k})$ is unitary and fulfills $w_{mn}(\mathbf{k}) = -w_{nm}(-\mathbf{k})$. At the four TRIM \mathbf{k}_a (defined by $\mathbf{k}_a = -\mathbf{k}_a + \mathbf{G}$), we then have an antisymmetric matrix

$$w_{mn}(\mathbf{k}_a) = -w_{nm}(\mathbf{k}_a) \equiv (w_a)_{mn} \quad (68)$$

- For an antisymmetric matrix $A = -A^T$, the Pfaffian $\text{Pf}(A)$ is defined, which squares to the determinant, $\text{Pf}(A)^2 = \det A$. Hence

$$\delta_a \equiv \frac{\text{Pf} w_a}{\sqrt{\det w_a}} = \pm 1. \quad (69)$$

- To define the bulk invariant $\nu \in \{0, 1\}$, chose a continuous $u_n(\mathbf{k})$ in the Brillouin zone. As the Chern number vanishes ($C = 0$), this is always possible. Then the branch of $\sqrt{\det w(\mathbf{k})}$ can be specified globally (as $\det w(\mathbf{k})$ does NOT wind around the origin) and we can obtain:

$$(-1)^\nu = \prod_{a=1}^4 \delta_a \quad (70)$$

Experimental realization [Fig. 31(b)] Würzburg experiment: [König et al, Science 318, 766 (2007)]

- Heavy-element semiconductor $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$, where the energy of p- and s-bands inverts when going from CdTe (non-topological) to HgTe (topological).
- Build sandwich structure, tune Fermi energy in band gap via gate, find quantized conductance $G = 2e^2/h$ from two edge states with $\nu > 0$. This only works if sample is small enough, it is still debated what causes backscattering (magnetic impurities or interactions?).

12.7 Topological superconductors

Case study: Kitaev's Majorana wire and possible realization.

Exercises

12.1 Two-band model Show that the states in Eq. (9) are indeed eigenstates for the two-band Hamiltonian in (8). Show that the Berry curvature is given by Eq. (10).

12.2 Weyl points: Topology for gapless points in 3D

1. Consider a generic two-band model in 3D,

$$H(\mathbf{k}) = f_0(\mathbf{k})\mathbf{1} + f_x(\mathbf{k})\sigma_x + f_y(\mathbf{k})\sigma_y + f_z(\mathbf{k})\sigma_z, \quad (71)$$

with $f_{0,x,y,z} \in \mathbb{R}$ and $\mathbf{k} = (k_x, k_y, k_z) \in T^3$. Find the two eigenenergies $E_{\pm}(\mathbf{k})$. Argue that a given band-crossing point at $\mathbf{k} = \mathbf{k}_0$, defined by $E_+(\mathbf{k}_0) = E_-(\mathbf{k}_0) \equiv E_0$, is generically stable, i.e. it cannot disappear under small variations of the functions $f_{0,x,y,z}$. In 2D, why would a band-crossing point generically be unstable?

2. One can expand $H(\mathbf{k})$ around the gapless momentum \mathbf{k}_0 in lowest order in $\mathbf{q} = \mathbf{k} - \mathbf{k}_0$. For a particular choice of $f_{0,x,y,z}$, one would then find the Weyl-Hamiltonian,

$$H_0^W(\mathbf{q}) = v(\sigma_x q_x + \sigma_y q_y + \sigma_z q_z), \quad (72)$$

with the velocity $v > 0$ and up to an energy shift of E_0 . Switch to spherical coordinates and compute the Berry curvature $\mathcal{F}(\mathbf{q})$. Show that the Weyl points \mathbf{k}_0 are quantized sources of Berry flux ("monopoles" in the magnetic analogy), i.e. show by an explicit calculation using that for a two-dimensional closed surface S surrounding \mathbf{k}_0 (i.e. ball), one has Chern number

$$C = \frac{1}{2\pi} \int_S \mathcal{F}(\mathbf{q}) \cdot d\mathbf{S} = 1. \quad (73)$$

Fact: For $v \rightarrow \chi v$ with $\chi = \pm 1$ called the "chirality", this result would generalize to $C = \chi$, i.e. a Weyl point with negative velocity would act as a sink of Berry flux.

3. Argue that in a realistic bandstructure $\mathbf{k} \in T^3$, Weyl points only occur in pairs with $\chi = \pm 1$. That is, there is no single Weyl point! Hint: Think how the monopole flux lines are compatible with the periodic nature of the Brillouin zone.

Remark: Weyl points are indeed ubiquitous even in the band-structure of mundane materials like iron. However, they become only relevant in materials where the Weyl points energy is located close to the Fermi energy. These materials exist, they are called Weyl semimetals and have been recently investigated due to their interesting topological properties.

12.3 Rice-Mele model as Thouless charge pump Consider the Rice-Mele model which is the SSH-Model of Eq. (15) with the additional on-site terms contributed by Eq. (23),

$$H = \sum_i (1 + \delta) c_{Ai}^\dagger c_{Bi} + (1 - \delta) c_{A_{i+1}}^\dagger c_{Bi} + h.c. + m \sum_i (c_{Ai}^\dagger c_{Ai} - c_{Bi}^\dagger c_{Bi}). \quad (74)$$

We have put $t = 1$ to avoid confusion with the time variable. Show that the Hamiltonian can be written as

$$\begin{aligned} H(k) &= \mathbf{d}(k) \cdot \boldsymbol{\sigma}, \\ \mathbf{d}(k) &= ([1 + \delta] + [1 - \delta] \cos ka, [1 - \delta] \sin ka, m). \end{aligned}$$

We define the adiabatic pumping cycle via the following time dependence of the two parameters δ and m :

$$(\delta(t), m(t)) = \left(\cos \frac{2\pi t}{T}, \sin \frac{2\pi t}{T} \right). \quad (75)$$

Show that the pumped charge in the time interval between $t = 0$ and $t = T$ is given by $|\Delta P| = e$. Hint: Argue by considering the direction of $\hat{\mathbf{d}}(k, t)$ at the high-symmetry points $(k, t) = (0, 0), (0, T/2), (\pi/a, 0), (\pi/a, T/2)$. Next, let us see the pump at work in a numerical simulation (use your favorite tool like Mathematica or Python). Consider the Rice-Mele model (74) for a finite length ($i = 1, 2, \dots, L$) and with open boundary conditions (i.e. the chain just terminates at both ends). Work with a chain of $L \simeq 10$ unit-cells and find the instantaneous eigenstates for finely spaced times, e.g. $t/T = 0, 0.01, 0.02, \dots, 1$. Plot the eigenenergies $E_n(t)$ over t/T . Investigate which of the eigenstates are end-states, i.e. localized at the end of the chain. You can add this information in your above energy plot by coloring the data points. Confirm that during a pump cycle (i) the bulk gap stays open, (ii) there emerges an in-gap state localized at the right end from the lower band which gets pushed above the Fermi energy and merges with the upper band. Similar with a left end-state which traverses the gap from high to low energies.

Explain in words and using a sketch how this leads to charge pumping of one electronic charge per cycle if the pump is placed between two leads (electron reservoirs) with their (equal) Fermi energies at or around $E = 0$.

12.4 Symmetry classification of superconductors In this problem, we explore the rich interplay of unitary and anti-unitary symmetries for Bogoliubov-de Gennes (BdG) Hamiltonians describing superconducting systems in mean-field approximation. These second-quantized Hamiltonians

$$\hat{H} = \frac{1}{2} \hat{\psi}^\dagger h_{BdG} \hat{\psi} \quad (76)$$

are defined in terms of Nambu-spinors, $\hat{\psi}^\dagger = (\hat{c}_\uparrow^\dagger, \hat{c}_\downarrow^\dagger, \hat{c}_\uparrow, \hat{c}_\downarrow)$ and $\hat{\psi} = (\hat{c}_\uparrow, \hat{c}_\downarrow, \hat{c}_\uparrow^\dagger, \hat{c}_\downarrow^\dagger)^T$, where \hat{c}_σ with $\sigma = \uparrow, \downarrow$ should be thought of as an N -vector containing possible further (spatial, ...) indices. Note that the Nambu spinors fulfill canonical anti-commutation relations $\{\hat{\psi}_a, \hat{\psi}_b^\dagger\} = \delta_{ab}$ with $a, b = 1, 2, \dots, 4N$. Assume that the zero of energy is shifted such that $\text{tr} h_{BdG} = 0$.

1. Show that due to the redundancy of $\hat{\psi}^\dagger$ and $\hat{\psi}$, it follows that h_{BdG} fulfills

$$\tau_x h_{BdG}^T \tau_x = -h_{BdG} \quad (77)$$

with $\tau_x = \begin{pmatrix} 0 & 1_{2N} \\ 1_{2N} & 0 \end{pmatrix}$ and the matrix Hamiltonian h_{BdG} thus belongs in class D. Show that this leads to the most general form

$$h_{BdG} = \begin{pmatrix} \Xi & \Delta \\ -\Delta^\star & -\Xi^T \end{pmatrix} \quad (78)$$

where $\Xi = \Xi^\dagger$ and $\Delta = -\Delta^T$ are $2N \times 2N$ matrices.

If (spinful) time-reversal symmetry is present for our superconductor, this would lead to the additional symmetry

$$\sigma_y h_{BdG}^\star \sigma_y = h_{BdG}. \quad (79)$$

where σ_y contains two diagonal blocks of $i \begin{pmatrix} 0 & -1_N \\ 1_N & 0 \end{pmatrix}$. What is the symmetry class of such a time-reversal symmetric BdG Hamiltonian?

2. Now assume that the system has an additional *unitary* U(1) spin rotation symmetry around the S^z -axis in spin space. Show that \hat{H} can then be written as

$$\hat{H} = \hat{\Psi}^\dagger \tilde{h}_{BdG} \hat{\Psi} + \text{const.} \quad (80)$$

where $\hat{\Psi}^\dagger = (\hat{c}_\uparrow^\dagger, \hat{c}_\downarrow^\dagger)$. (Hint: Think about which terms $\hat{c}_{\sigma_1}^\dagger \hat{c}_{\sigma_2}^\dagger$ in Eq. (76) are now forbidden.) What is the symmetry classification of \tilde{h}_{BdG} in this case? How does the answer change if in addition, time-reversal symmetry of Eq. 79 is imposed?

3. Bonus: Finally, assume that the system has full $SU(2)$ spin rotation symmetry. What further restriction on \tilde{h}_{BdG} is imposed and what is its symmetry classification? Again, what changes if time-reversal symmetry of Eq. 79 is imposed in addition? (You should find class C and CI, respectively.)