LMU LUDWIG-MAXIMILIANS-UNIVERSITÄT MÜNCHEN

Fakultät für Physik im SoSe 2022
TMP - TA3: Condensed Matter Many-Body-Physics and Field Theory I
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https://www2.physik.uni-muenchen.de/lehre/vorlesungen/sose_22/TMP-TA3/index.html

Sheet 4:

Hand-out: Friday, May 20, 2022[1]

Problem 1 Symmetries of the Hubbard models

In this problem we prove several symmetries of the 'plain-vanilla' Bose and Fermi-Hubbard models on a square lattice introduced in the lecture.

(1.a) Find explicit expressions for the unitary operators $\hat{U}$, in terms of fermionic operators $\hat{c}^{(\dagger)}_{\boldsymbol{j},\sigma}$ corresponding to the following symmetries $\hat{U}^\dagger \hat{\mathcal{H}}_{\rm FH} \hat{U} = \hat{\mathcal{H}}_{\rm FH}$ of the Fermi-Hubbard model $\hat{\mathcal{H}}_{\rm FH}$: (i) global charge conservation; (ii) global $\hat{S}^z$ conservation.

(1.b) From your results in (1.a), specify the corresponding symmetry groups and derive the resulting conserved quantities.

(1.c) Extend your results from (1.a) and (1.b) to the total particle-number conservation in the case of the Bose-Hubbard model.

(1.d) Find a similar unitary transformation $\hat{U}$ which describes lattice translational symmetry in the Bose / Fermi Hubbard model, and derive the corresponding conserved quantity.

Problem 2 Correlation functions of non-interacting fermions

In this problem we discuss the Fermi-Hubbard model in the non-interacting limit $U = 0$. We work in the Heisenberg picture, where operators are time dependent:

$$\hat{A}(t) = e^{i\hat{\mathcal{H}}t} \hat{A} e^{-i\hat{\mathcal{H}}t}, \qquad \hat{A} \equiv \hat{A}(0); \tag{1}$$

here $\hat{\mathcal{H}}$ is the system Hamiltonian – in this exercise $\hat{\mathcal{H}} = \hat{\mathcal{H}}_{\rm FH}(U = 0)$ – and t denotes time.

(2.a) Calculate $\hat{c}(t)$ and $\hat{c}^\dagger(t)$ in the Heisenberg picture. Start by diagonalizing the free hopping Hamiltonian using Fourier modes.

(2.b) The free-fermion *propagator* in real space is defined as

$$\mathcal{G}_{\sigma\sigma'}(\boldsymbol{r}, t; \boldsymbol{r}', t') = -i \langle {\rm FS} | \mathcal{T} \hat{c}_\sigma(\boldsymbol{r}, t) \hat{c}^\dagger_{\sigma'}(\boldsymbol{r}', t') | {\rm FS} \rangle, \tag{2}$$

where we denote by $|{\rm FS}\rangle$ the non-interacting ground state (Fermi-sea) at a given filling with fermions, and we introduced the time-ordering operator:

$$\mathcal{T} \hat{A}(t) \hat{B}(t') = \hat{A}(t)\hat{B}(t')\theta(t - t') \pm \hat{B}(t')\hat{A}(t)\theta(t' - t) \tag{3}$$

[1] If you would like to present your solution(s), feel free to send them to Felix Palm until Fri, May 27.

with $\theta(\tau)$ the step function and $\pm$ signs referring to bosons $(+)$ and fermions $(-)$ respectively. Show that for a system invariant under spatial and temporal translations this propagator can be written as

$$\mathcal{G}_{\sigma\sigma'}(\boldsymbol{r},t;\boldsymbol{r}',t') = \int \frac{d^dk}{(2\pi)^d} \int \frac{d\omega}{2\pi}\, e^{i[\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}')-\omega(t-t')]}\, \mathcal{G}_{\sigma\sigma'}(\boldsymbol{k},\omega). \tag{4}$$

Furthermore, find the explicit form of the propagtor $\mathcal{G}_{\sigma\sigma'}(\boldsymbol{k},\omega)$ in momentum and frequency space.

(2.c) Calculate the density-density correlation function

$$K(\boldsymbol{r},t;\boldsymbol{r}',t') = \langle \mathrm{FS}|\mathcal{T}\hat{n}(\boldsymbol{r},t)\hat{n}(\boldsymbol{r}',t')|\mathrm{FS}\rangle, \tag{5}$$

with the normal-ordered density operator

$$\hat{n}(\boldsymbol{r},t) = \sum_\sigma \hat{c}^\dagger_\sigma(\boldsymbol{r},t)\hat{c}_\sigma(\boldsymbol{r},t) - \rho \tag{6}$$

and the average density per site ρ.

Problem 3 Mean-field theory of the Bose-Hubbard model

Here we study a simple mean-field description of the ground state in the Bose-Hubbard model, described by the Hamiltonian ($\hat{n}_{\boldsymbol{j}} = \hat{a}^\dagger_{\boldsymbol{j}}\hat{a}_{\boldsymbol{j}}$)

$$\hat{\mathcal{H}}_{\mathrm{BH}} = -t\sum_{\langle \boldsymbol{i},\boldsymbol{j}\rangle}\left(\hat{a}^\dagger_{\boldsymbol{j}}\hat{a}_{\boldsymbol{i}} + \text{h.c.}\right) + \frac{U}{2}\sum_{\boldsymbol{j}}\hat{n}_{\boldsymbol{j}}(\hat{n}_{\boldsymbol{j}}-1) + \mu\sum_{\boldsymbol{j}}\hat{n}_{\boldsymbol{j}}. \tag{7}$$

Here μ is a chemical potential which controls the density $\langle \hat{n}_{\boldsymbol{j}}\rangle$ in the ground state. Consider a general lattice with a one-site unit-cell and coordination number z (i.e. the number of nearest-neighbor sites is z everywhere).

(3.a) Expand the hopping part of the Bose-Hubbard Hamiltonian around a mean-field $\langle \hat{a}_{\boldsymbol{j}}\rangle = \Psi/z$ with a $\mathbb{C}$-valued order parameter Ψ, by writing

$$\hat{a}_{\boldsymbol{j}} = \underbrace{\hat{a}_{\boldsymbol{j}} - \langle \hat{a}_{\boldsymbol{j}}\rangle}_{\delta\hat{a}_{\boldsymbol{j}}} + \langle \hat{a}_{\boldsymbol{j}}\rangle \equiv \delta\hat{a}_{\boldsymbol{j}} + \Psi/z, \tag{8}$$

and dropping all terms of order $(\delta\hat{a})^2$.

(3.b) Replace the hopping part of the Bose-Hubbard Hamiltonian by its mean-field expression from (3.a) to derive the mean-field Hamiltonian:

$$\hat{\mathcal{H}}_{\mathrm{BH}} \approx \hat{\mathcal{H}}_{\mathrm{MF}} = \sum_{\boldsymbol{j}}\left[\frac{U}{2}\hat{n}_{\boldsymbol{j}}(\hat{n}_{\boldsymbol{j}}-1) + \mu\hat{n}_{\boldsymbol{j}} - t\left(\Psi\hat{a}^\dagger_{\boldsymbol{j}} + \text{h.c.}\right)\right] \tag{9}$$

(3.c) The mean-field Hamiltonian takes the general form

$$\hat{\mathcal{H}}_{\mathrm{MF}} = \sum_{\boldsymbol{j}}\hat{\mathcal{H}}^0_{\boldsymbol{j}}, \tag{10}$$

where each $\hat{\mathcal{H}}_{\boldsymbol{j}}^0$ acts only on the local particle-number Hilbertspace on site $\boldsymbol{j}$. Assuming a fixed given $\Psi \in \mathbb{C}$, one can numerically find the ground state $|\psi_0(\Psi)\rangle$ of $\hat{\mathcal{H}}_{\boldsymbol{j}}^0$. Then the overall ground state of the mean-field Hamiltonian is determined by the condition that (why?)

$$\langle\psi_0(\Psi)|\hat{\mathcal{H}}_{\boldsymbol{j}}^0(\Psi)|\psi_0(\Psi)\rangle = \min. \tag{11}$$

Derive a formal equation for Ψ minimizing this energy.