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Sheet 4:

Hand-out: Friday, May 12, 2023

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 $\hat{c}_{j,\sigma}^{(\dagger)}$ corresponding to the following symmetries $\hat{U}^\dagger \hat{\mathcal{H}}_{\text{FH}} \hat{U} = \hat{\mathcal{H}}_{\text{FH}}$ of the Fermi-Hubbard model $\hat{\mathcal{H}}_{\text{FH}}$: (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:

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

here $\hat{\mathcal{H}}$ is the system Hamiltonian – in this exercise $\hat{\mathcal{H}} = \hat{\mathcal{H}}_{\text{FH}}(U = 0)$ – 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

$$\mathcal{G}_{\sigma\sigma'}(\mathbf{r}, t; \mathbf{r}', t') = -i \langle \text{FS} | \mathcal{T} \hat{c}_\sigma(\mathbf{r}, t) \hat{c}_{\sigma'}^\dagger(\mathbf{r}', t') | \text{FS} \rangle, \quad (2)$$

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

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

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

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

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

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

$$K(\mathbf{r}, t; \mathbf{r}', t') = \langle \text{FS} | \mathcal{T} \hat{n}(\mathbf{r}, t) \hat{n}(\mathbf{r}', t') | \text{FS} \rangle, \quad (5)$$

with the normal-ordered density operator

$$\hat{n}(\mathbf{r}, t) = \sum_{\sigma} \hat{c}_{\sigma}^{\dagger}(\mathbf{r}, t) \hat{c}_{\sigma}(\mathbf{r}, t) - \rho \quad (6)$$

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 ($\hat{n}_j = \hat{a}_j^{\dagger} \hat{a}_j$)

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

Here μ is a chemical potential which controls the density $\langle \hat{n}_j \rangle$ 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 $\langle \hat{a}_j \rangle = \Psi/z$ with a \mathbb{C} -valued order parameter Ψ , by writing

$$\hat{a}_j = \underbrace{\hat{a}_j - \langle \hat{a}_j \rangle}_{\delta \hat{a}_j} + \langle \hat{a}_j \rangle \equiv \delta \hat{a}_j + \Psi/z, \quad (8)$$

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:

$$\hat{\mathcal{H}}_{\text{BH}} \approx \hat{\mathcal{H}}_{\text{MF}} = \sum_j \left[\frac{U}{2} \hat{n}_j (\hat{n}_j - 1) + \mu \hat{n}_j - t \left(\Psi \hat{a}_j^{\dagger} + \text{h.c.} \right) \right] \quad (9)$$

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

$$\hat{\mathcal{H}}_{\text{MF}} = \sum_j \hat{\mathcal{H}}_j^0, \quad (10)$$

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

$$\langle \psi_0(\Psi) | \hat{\mathcal{H}}_j^0(\Psi) | \psi_0(\Psi) \rangle = \min. \quad (11)$$

Derive a formal equation for Ψ minimizing this energy.