Problem Set 3:

Handout: Thu, Dec. 3, 2020; Solutions: Fri, Dec. 11, 2020

Problem 1 Spontaneous symmetry breaking in the extended Bose-Hubbard model

In this problem, we will study the 1D extended Bose-Hubbard model in a periodic chain with $j = 1...L$ sites. We consider hard-core bosons $(\hat{a}_j^\dagger)^2 = 0$ described by the following Hamiltonian,

$$\hat{\mathcal{H}} = -t \sum_j \left(\hat{a}_{j+1}^\dagger \hat{a}_j + \text{h.c.} \right) + V \sum_j \hat{n}_{j+1} \hat{n}_j + W \sum_j \hat{n}_{j+2} \hat{n}_j. \tag{1}$$

(1.a) Describe the low-energy spectrum of $\hat{\mathcal{H}}$ for $t = W = 0$ at half-filling, i.e. $N = L/2$ in a chain of even length $L \in 2\mathbb{Z}_{>0}$. Determine *all* low-energy eigenstates for $t = 0$ whose energy is $E \leq V$.

(1.b) Consider the two degenerate ground states $|\Psi_1\rangle$ and $|\Psi_2\rangle$ found in (1.a). Treat $t \ll V$ perturbatively (still for $W = 0$) and discuss lowest-order non-trivial corrections to the ground state energies. Argue why the resulting energy splitting of the perturbed ground states scales as $t \times (t/V)^{L/2}$. I.e. the resulting energy gap is exponentially small in system size. In practice, this will lead to *spontaneous breaking of the discrete translational symmetry*.

(1.c) Discuss how the situation from (1.a) and (1.b) changes if L is odd instead of even and $N = (L-1)/2$. Describe the low-energy eigenstates, and discuss how spontaneous symmetry breaking is affected.

(1.d) Now consider a periodic chain whose length is a multiple of 3, i.e. $L \in 3\mathbb{Z}_{>0}$. For $t = 0$ and $N = 2/3 \times L$ show that *purely repulsive interactions* $V, W > 0$ *lead to pairing* in the ground state.

Problem 2 Full counting statistics

The *full counting statistics* of a quantum mechanical observable $\hat{\mathcal{O}}^\dagger = \hat{\mathcal{O}}$ for a density matrix $\hat{\rho}$ is described by the probability distribution $p_\mathcal{O}$ to measure its eigenvalue $\mathcal{O} \in \mathbb{R}$:

$$p_\mathcal{O} = \sum_n \delta(\mathcal{O} - o_n) \langle o_n | \hat{\rho} | o_n \rangle, \tag{2}$$

where $\hat{\mathcal{O}} = \sum_n o_n |o_n\rangle\langle o_n|$.

(2.a) Show that $p_\mathcal{O}$ can be calculated as the Fourier transform of the generating functional

$$Z(\phi) = (2\pi)^{-1/2} \text{tr} \left(\hat{\rho} \; e^{i\phi\hat{\mathcal{O}}} \right), \qquad \phi \in \mathbb{R}. \tag{3}$$

I.e., numerical calculation of $Z(\phi)$ is sufficient to obtain easy access (via Fourier transform) to the full counting statistics of $\hat{\mathcal{O}}$.

(2.b) Consider a Néel product state $|\mathrm{N}_z\rangle = \prod_j |\sigma = (-1)^j\rangle_j$. Calculate the full counting statistics p_{M_z} of the staggered magnetization

$$\hat{M}_z = \sum_j (-1)^j \hat{S}^z_j. \tag{4}$$

(2.c) Consider an ensemble of Néel product states pointing in a random direction, as described by the density matrix

$$\hat{\rho} = Z^{-1} \int d^2\mathbf{\Omega}\ \hat{R}_{\mathbf{\Omega}} |\mathrm{N}_z\rangle\langle \mathrm{N}_z| \hat{R}^\dagger_{\mathbf{\Omega}} \tag{5}$$

Here $\mathbf{\Omega}$ denotes a solid angle, $\hat{R}_{\mathbf{\Omega}}$ rotates spins pointing along $\pm z$ into spins pointing along $\pm\mathbf{\Omega}$ (see also problem 1.b), and Z ensures normalization. Calculate the full counting statistics p_{M_z} of the staggered magnetization! *Hint:* You don't need to use the result from (2.a)!

(2.d) In (2.c) we considered a classical ensemble of unentangled product states. Discuss how you expect the full counting statistics p_{M_z} to change when quantum fluctuations are included and the product states in the ensemble are replaced by more realistic quantum states with local entanglement. (This problem is about physical intuition rather than mathematical rigor, and no calculation is expected.)

Problem 3 Gutzwiller description of the superfluid-to-Mott transition

To analyze the superfluid-to-Mott transition in the Bose-Hubbar model, consider the following type of *Gutzwiller variational states*:

$$|\Psi_{\mathrm{G}}[f_n]\rangle = \prod_{\boldsymbol{j}} \left(\sum_{n=0}^{m} \frac{f_n}{\sqrt{n!}} (\hat{a}^\dagger_{\boldsymbol{j}})^n \right) |0\rangle, \tag{6}$$

with variational parameters $f_0, ..., f_m$ satisfying (for normalization):

$$\sum_{n=0}^{m} |f_n|^2 = 1. \tag{7}$$

(3.a) Derive expressions for the variational kinetic and interaction energies $\langle \hat{\mathcal{H}}_t \rangle$ and $\langle \hat{\mathcal{H}}_U + \hat{\mathcal{H}}_\mu \rangle$.

(3.b) Discuss for which parameters f_n the $U(1)$ symmetry of the Bose-Hubbard model remains unbroken in the Gutzwiller state. Write down explicit expressions for the $n = 1, 2, 3, ...$ Mott insulating states.

(3.c) Consider the case $t = 0$ without the kinetic (or tunneling) term. Derive the critical values $\mu_c^{(n)}$ of the chemical potential where transitions between different Mott states take place. Of which order is this phase transition?

(3.d) To analyze the stability of the Mott insulating states with n bosons per site, make the following ansatz:

$$f_n = \sqrt{1 - 2|\alpha|^2}, \qquad f_{n-1} = \alpha, \qquad f_{n+1} = \alpha^*, \qquad f_{m \neq n-1,n,n+1} = 0, \tag{8}$$

for a small $\alpha \in \mathbb{C}$ with $|\alpha| \ll 1$. Calculate the variational energy $E_{\mathrm{tot}}(\alpha)$ to second order in α, in the middle of the Mott plateau at $\mu = U(n - 1/2)$.

(3.e) Using the result from (3.d) for $E_{\rm tot}(\alpha)$, show for $n \gg 1$ that the superfluid-to-Mott transition point is estimated to be at

$$U = 4nzt \tag{9}$$

by this Gutzwiller description, and still working at $\mu = U(n - 1/2)$. Derive a better estimate valid also for smaller n.

(3.f) Explain how one can conclude from the Gutzwiller theory that the superfluid breaks the $U(1)$ symmetry. Which order do you expect the phase transition found in (3.e) to have?