LMU LUDWIG-MAXIMILIANS-UNIVERSITÄT MÜNCHEN

Fakultät für Physik im SoSe 2024
T M1/TV: Advanced Statistical Physics
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https://www2.physik.uni-muenchen.de/lehre/vorlesungen/sose_24/t_m1_advanced-statistical-physics/index.html

Sheet 5:

Hand-out: Friday, May. 17, 2024; Hand-in: Tuesday, May. 28, 2024, 11:59 pm

Problem 1 A quantum phase transition described by mean-field theory – **(sol: Central Exercise)**

In this problem, we consider a quantum mechanical lattice gas of interacting bosons, as described by the so-called *Bose-Hubbard* Hamiltonian $\hat{\mathcal{H}}_{\rm BH}$. On each lattice site $\boldsymbol{j}$ in a d-dimensional hypercubic lattice it is characterized by the bosonic occupation number $\hat{n}_{\boldsymbol{j}}$. It is most convenient to think of each lattice site as a separate harmonic oscillator, with ladder operators $\hat{a}_{\boldsymbol{j}}$ and $\hat{a}^\dagger_{\boldsymbol{j}}$ annihilating and creating an extra particle/excitation respectively (with the commutation relations $[\hat{a}_{\boldsymbol{i}}, \hat{a}^\dagger_{\boldsymbol{j}}] = \delta_{\boldsymbol{i},\boldsymbol{j}}$), such that $\hat{n}_{\boldsymbol{j}} = \hat{a}^\dagger_{\boldsymbol{j}}\hat{a}_{\boldsymbol{j}}$ denotes the number of bosons on site $\boldsymbol{j}$.

The Hamiltonian $\hat{\mathcal{H}}_{\rm BH} = \hat{\mathcal{H}}_U + \hat{\mathcal{H}}_t + \hat{\mathcal{H}}_\mu$ consist of three terms: the local interactions between bosons on the same site,

$$\hat{\mathcal{H}}_U = \frac{U}{2}\sum_{\boldsymbol{j}} \hat{n}_{\boldsymbol{j}}(\hat{n}_{\boldsymbol{j}} - 1), \tag{1}$$

parameterized by an on-site interaction strength U, the hopping term which allows bosons to move (i.e. "hop") between nearest-neighbor lattice sites $\langle \boldsymbol{i}, \boldsymbol{j}\rangle$,

$$\hat{\mathcal{H}}_t = -t\sum_{\langle \boldsymbol{i},\boldsymbol{j}\rangle} \left(\hat{a}^\dagger_{\boldsymbol{i}}\hat{a}_{\boldsymbol{j}} + \text{H.c.}\right), \tag{2}$$

parameterized by the hopping amplitude t; And to control the total particle number N we add the chemical potential term

$$\hat{\mathcal{H}}_\mu = -\mu\sum_{\boldsymbol{j}} \hat{n}_{\boldsymbol{j}} \equiv -\mu\hat{N}, \tag{3}$$

parametrized by μ, which appears as usual when working in the grand-canonical ensemble.

In this exercise we will see that the Bose-Hubbard model has two types of (quantum) phase transitions at zero temperature $T = 0$ when μ/t and U/t are tuned. To analyze them, we consider the following type of *Gutzwiller variational states*:

$$|\Psi_{\rm G}[f_n]\rangle = \prod_{\boldsymbol{j}} \left(\sum_{n=0}^{m} \frac{f_n}{\sqrt{n!}}(\hat{a}^\dagger_{\boldsymbol{j}})^n\right)|0\rangle\,, \tag{4}$$

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

$$\sum_{n=0}^{m} |f_n|^2 = 1. \tag{5}$$

(1.a) (**4 Points**) Explain (in a few words), how Eq. (4) constitutes a mean-field description of the system. Then, derive expressions for the kinetic and interaction energies $E_t = \langle \Psi_{\rm G}| \hat{\mathcal{H}}_t |\Psi_{\rm G}\rangle$ and $E_U = \langle \Psi_{\rm G}| \hat{\mathcal{H}}_U |\Psi_{\rm G}\rangle$, as well as for $E_\mu = \langle \Psi_{\rm G}| \hat{\mathcal{H}}_\mu |\Psi_{\rm G}\rangle$.
Hints: sums do not have to be evaluated at this point; make use of the properties of the harmonic oscillator ladder operators!

(1.b) (**3 Points**) The so-called *Mott insulating* (MI) states with $n_0 = 1, 2, 3, 4, ...$ correspond to the choice $f_n|_{\rm MI} = e^{i\varphi}\delta_{n,n_0}$, with an arbitrary phase $\varphi \in [0, 2\pi)$. They correspond to having exactly n_0 bosons occupying every lattice site. Show that the energy $E(\varphi) = \langle \Psi_{\rm G}[f_n|_{\rm MI}]| \hat{\mathcal{H}}_{\rm BH} |\Psi_{\rm G}[f_n|_{\rm MI}]\rangle$ is independent of the phase choice φ – this is a manifestation of a continuous $U(1)$ symmetry of the model.

(1.c) (**3 Points**) Consider the case $t = 0$ without the kinetic term. Derive the critical values $\mu_c^{(n_0)}$ of the chemical potential where transitions between different Mott states n_0 and $n_0 + 1$ take place. Which type of phase transition is this (first order or continuous)?

(1.d) (**4 Points**) Now we analyze an additional phase transition obtained when tuning t while U and μ are fixed. From now on, consider the choice $\mu = U(n_0 - 1/2)$. For given integer n_0, make the ansatz

$$f_{n_0}|_\alpha = \sqrt{1 - 2|\alpha|^2}, \qquad f_{n_0-1}|_\alpha = \alpha, \qquad f_{n_0+1} = \alpha^*, \qquad f_{m\neq n_0-1,n_0,n_0+1}|_\alpha = 0, \quad (6)$$

for a small $\alpha \in \mathbb{C}$ with $|\alpha| \ll 1$. Calculate the variational energy $E(\alpha)$ to second order in α and show that it is given by (in d dimensions)

$$\begin{aligned} E(\alpha) &= \langle \Psi_{\rm G}[f_{n_0}|_\alpha]| \hat{\mathcal{H}}_{\rm BH} |\Psi_{\rm G}[f_{n_0}|_\alpha]\rangle \\ &= V\left[-\frac{U}{2}n_0^2 + |\alpha|^2\left(U - 2td(2n_0 + 2\sqrt{n_0(n_0+1)} + 1)\right) + \mathcal{O}(|\alpha^4|)\right]. \end{aligned} \quad (7)$$

(1.e) (**3 Points**) For small U/t, the energy $E(\alpha)$ in Eq. (7) indicates an instability, signaling the transition from a $U(1)$ symmetric Mott insulating state at large U/t to a state with a broken $U(1)$ symmetry (i.e. superfluid state). For $n_0 \gg 1$, show that the superfluid-to-Mott transition point can be estimated to be at

$$(U/t)_c = 8n_0 d. \quad (8)$$

(1.f) (**3 Points**) Sketch $E(\alpha)$ for $\alpha \in \mathbb{C}$ in the complex plane for large $U/t > (U/t)_c$ and small $U/t < (U/t)_c$ respectively. How do you expect $\mathcal{O}(|\alpha|^4)$ corrections to change the result? Discuss the signatures you find in these sketches for a spontaneous breaking of a continuous $U(1)$ symmetry when $U/t < (U/t)_c$!

Problem 2 Solid–solid solutions – (solution: Tutorials)

In this problem we consider a crystalline solid composed of two different types of constituent atoms, denoted type A and B respectively. The energies associated with nearest-neighbor pairs of different types are e_{AA}, e_{BB} and e_{AB} respectively. Assume they satisfy the relation

$$\varepsilon = \frac{1}{2}\left(e_{AA} + a_{BB}\right) - e_{AB} < 0, \tag{9}$$

and consider a lattice with coordination number z (i.e. every lattice site has z nearest neighbors).

(2.a) (**3 Points**) Calculate the Helmholtz free energy in the Bragg-Williams approximation for a homogeneous system in which the concentration of type A atoms is c_A, and the concentration of type B atoms is $c_B = 1 - c_A$.

(2.b) (**3 Points**) For $c_A = c_B = 1/2$, show that the system will phase separate below the critical temperature

$$k_B T_c = \frac{z}{2}|\varepsilon|. \tag{10}$$

(2.c) (**3 Points**) For $c_A \neq c_B$, show that phase separation will occur at a lower temperature than the T_c found in (2.b).

(2.d) (**3 Points**) Calculate the coexistence curve numerically (e.g. using appropriate software such as Mathematica, Matlab etc.) and plot the result in the $k_B T/z|\varepsilon| - c_A$ plane.