Tutorial class 4: Superfluid–Mott-insulator transition in a Bose gas

We consider the Bose-Hubbard model,

$$\hat{H} = -t \sum_{\langle \mathbf{r},\mathbf{r}' \rangle} \left(\hat{b}^\dagger_{\mathbf{r}} \hat{b}_{\mathbf{r}'} + \text{H.c.} \right) + \sum_{\mathbf{r}} \left(-\mu \hat{b}^\dagger_{\mathbf{r}} \hat{b}_{\mathbf{r}} + \frac{U}{2} \hat{b}^\dagger_{\mathbf{r}} \hat{b}^\dagger_{\mathbf{r}} \hat{b}_{\mathbf{r}} \hat{b}_{\mathbf{r}} \right), \tag{1}$$

describing bosons moving on a lattice and subject to a local (on-site) interaction ($U > 0$). t denotes the hopping amplitude and $\langle \mathbf{r}, \mathbf{r}' \rangle$ pairs of nearest-neighbor sites) (note that $\langle \mathbf{r}, \mathbf{r}' \rangle = \langle \mathbf{r}', \mathbf{r} \rangle$). The chemical potential μ fixes the mean boson density (i.e. the mean number of bosons per site). We assume an hypercubic d-dimensional lattice with N sites and take the lattice spacing a as the unit length, i.e. we set $a = 1$. We consider only the zero-temperature thermodynamic limit: $T \to 0$ and $N \to \infty$.

1) Superfluid–Mott-insulator transition

1.1) Diagonalize the Hamiltonian in the absence of interactions ($U = 0$); what is the ground state? How does the local repulsion affect the boson dynamics? Deduce that, depending on the boson density and the strength of the interactions, the ground state is either a superfluid or an insulator (referred to as a Mott insulator) [consider the limits $t/U \gg 1$ and $t/U \ll 1$ and distinguish between integer and non-integer densities].

1.2) Does the Bogoliubov theory appear appropriate to study the transition between the superfluid state and the Mott insulator?

2) Mean-field theory

We consider the intersite hopping term in the Hamiltonian within mean-field theory: We write $\hat{b}_{\mathbf{r}} = \psi + \delta\hat{b}_{\mathbf{r}}$, where the order parameter $\psi = \langle \hat{b}_{\mathbf{r}} \rangle$ is assumed uniform, and linearize the hopping term with respect to $\delta\hat{b}_{\mathbf{r}}$.[1]

2.1) What is the mean-field Hamiltonian $\hat{H}_{\text{MF}}$? Show that it can be written as the sum of decoupled single-site Hamiltonians, i.e. $\hat{H}_{\text{MF}} = \sum_{\mathbf{r}} \hat{H}_{\text{eff}}(\hat{b}^\dagger_{\mathbf{r}}, \hat{b}_{\mathbf{r}})$, with

$$\hat{H}_{\text{eff}}(\hat{b}^\dagger, \hat{b}) = -\mu \hat{b}^\dagger \hat{b} + \frac{U}{2} \hat{b}^\dagger \hat{b}^\dagger \hat{b} \hat{b} - 2dt(\psi^* \hat{b} + \psi \hat{b}^\dagger - |\psi|^2). \tag{2}$$

2.2) Explain why the state with a non-zero order parameter is superfluid whereas the state characterized by $\psi = 0$ is a Mott insulator.

2.3) We now consider the Hamiltonian $\hat{H}_{\text{eff}}(\hat{b}^\dagger, \hat{b})$ of a single-site. We want to compute the ground-state energy

$$E(|\psi|^2) = a_0 + a_2|\psi|^2 + a_4|\psi|^4 + \mathcal{O}(|\psi|^6) \tag{3}$$

in powers of $|\psi|^2$. Write $\hat{H}_{\text{eff}}(\psi = 0)$ in terms of the occupation-number operator $\hat{n} = \hat{b}^\dagger \hat{b}$. Determine the eigenstates and their energies. What is the ground-state energy a_0 and the number n_0 of bosons (on the site); represent a_0/U and n_0 graphically as a function of μ/U?

2.4) Compute $E^{(2)} = a_2|\psi|^2$ using second-order perturbation theory.[2] What should be the sign of a_4 for the expansion (3) to make sense? What is the condition for the Mott insulator to be stable? Show that, in the plane $(2dt, \mu/U)$, the phase diagram consists of a set of Mott lobes (labeled by the integer n_0) surrounded by the superfluid phase [use the notations $D = 2dt$, $\delta\mu = \mu - U(n_0 - 1/2)$ and $x = n_0 + 1/2$].

2.5) Determine the value of the order parameter and the mean density of bosons in the Mott insulator and in the superfluid phase as a function of n_0, a_2 and a_4. Deduce that the compressibility $\kappa = n^{-2} dn/d\mu$ vanishes in

[1] This is analogous to the usual mean-field theory used in classical spin models such as the Ising model.

[2] Recall that $\hat{b}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$ and $\hat{b}|n\rangle = \sqrt{n}|n-1\rangle$, where $|n\rangle = \frac{(\hat{b}^\dagger)^n}{\sqrt{n!}}|\text{vac}\rangle$ is the normalized eigenstate of the occupation-number operator $\hat{n}$.

the Mott insulator. Show that there is a special point of the transition line where the superfluid–Mott-insulator transition occurs at constant density.

3) Excitation spectrum in the Mott insulator

In this section we go beyond mean-field theory in order to compute the one-particle excitation spectrum in the Mott insulator. Starting from the Euclidean action $S[b^*, b]$ associated with Hamiltonian (1), we rewrite the partition function as a functional integral over two (complex) bosonic fields, b and ψ, using the Hubbard-Stratonovich transformation

$$e^{\int_0^\beta d\tau \sum_{\mathbf{r},\mathbf{r}'} b^*_{\mathbf{r}} t_{\mathbf{r},\mathbf{r}'} b_{\mathbf{r}'}} = \int \mathcal{D}[\psi^*, \psi]\, e^{-\int_0^\beta d\tau \sum_{\mathbf{r},\mathbf{r}'} \psi^*_{\mathbf{r}} t^{-1}_{\mathbf{r},\mathbf{r}'} \psi_{\mathbf{r}'} + \int_0^\beta d\tau \sum_{\mathbf{r}} (\psi^*_{\mathbf{r}} b_{\mathbf{r}} + \text{c.c.})}, \tag{4}$$

where $t_{\mathbf{r},\mathbf{r}'}$ equals t if the sites $\mathbf{r}$ and $\mathbf{r}'$ are nearest neighbors and vanishes otherwise. One can then integrate out the field b in a cumulant expansion,

$$\int \mathcal{D}[b^*, b]\, e^{-S_{\text{loc}}[b^*,b] - S'[b^*,b]} = Z_{\text{loc}}\, e^{-\langle S' \rangle + \frac{1}{2}\left(\langle S'^2 \rangle - \langle S' \rangle^2\right) + \cdots} \tag{5}$$

where the action S' may depend on $\psi^{(*)}$ and the mean value $\langle \cdots \rangle$ is to be taken with the local action S_{loc} corresponding to the limit $t = 0$.

3.1) What is the action $S[b^*, b, \psi^*, \psi]$ obtained from the Hubbard-Stratonovich transformation. Give its expression in terms of $S_{\text{loc}}[b^*, b]$.

3.2) Show that the effective action of the ψ field, obtained from the cumulant expansion (5) retaining only the first- and second-order cumulants, is given by

$$S[\psi^*, \psi] = \sum_{\mathbf{k},\omega_n} \psi^*(\mathbf{k}, i\omega_n) \left[t^{-1}_{\mathbf{k}} + G_{\text{loc}}(i\omega_n)\right] \psi(\mathbf{k}, i\omega_n), \tag{6}$$

where $t_{\mathbf{k}}$ is the Fourier transform of $t_{\mathbf{r},\mathbf{r}'} = t_{\mathbf{r}-\mathbf{r}'}$ and $G_{\text{loc}}(i\omega_n)$ is the local Green function obtained from S_{loc}. What is the expression of the propagator $\mathcal{G}(\mathbf{k}, i\omega_n) = -\langle \psi(\mathbf{k}, i\omega_n) \psi^*(\mathbf{k}, i\omega_n) \rangle$ of the ψ field?

3.3) Compute the finite-temperature Green function $G_{\text{loc}}(\tau) = -\langle T_\tau \hat{b}(\tau) \hat{b}^\dagger(0) \rangle$ for $\tau > 0$ using the occupation-number-state basis $\{|n\rangle\}$.[2] Deduce that

$$G(i\omega_n) = \frac{n_0 + 1}{i\omega_n + \mu - U n_0} - \frac{n_0}{i\omega_n + \mu - U(n_0 - 1)} \tag{7}$$

in the zero-temperature limit.

3.4) What is the condition for the Mott phase to be stable? Does it agree with the result of question 2.4?

3.5) Show that the one-particle spectrum exhibits two branches, $E_+(\mathbf{k})$ and $E_-(\mathbf{k})$. Show that for $t = 0$, one of the excitation energy corresponds to the addition of a particle while the other one corresponds to the removal of a particle. Compute $E_\pm(\mathbf{k} = 0)$. How does the transition to the superfluid phase manifest itself? Why is the transition occurring at constant density special?

3.6) What is the behavior of $E_\pm(\mathbf{k})$ in the limit $\mathbf{k} \to 0$? Show that at the Mott transition $E_\pm(\mathbf{k}) \sim |\mathbf{k}|^z$ where the exponent z (known as the dynamical critical exponent) takes two different values.

4) Low-energy effective action

It is possible to write an effective action for the auxiliary field ψ by expanding $\mathcal{G}^{-1}(\mathbf{k}, i\omega_n)$ in powers of $\mathbf{k}$ and ω_n.

4.1) Show that one obtains

$$S[\psi^*, \psi] = \int_0^\beta d\tau \int d^d r\, \psi^*(\mathbf{r}, \tau) \left(r + K_1 \partial_\tau - K_2 \partial_\tau^2 - K_3 \boldsymbol{\nabla}^2 + \cdots\right) \psi(\mathbf{r}, \tau) + \cdots \tag{8}$$

where

$$r = -\mathcal{G}^{-1}(\mathbf{k} = 0, i\omega_n = 0), \qquad K_1 = -\frac{\partial r}{\partial \mu}. \tag{9}$$

Notice that $G_{\text{loc}}(i\omega_n) \equiv G_{\text{loc}}(i\omega_n + \mu)$, and $\omega_n \equiv \omega$ becomes a continuous variable at $T = 0$.

4.2) How does K_1 behave when the transition occurs at constant density? What can we deduce about the universality class of the superfluid–Mott-insulator transition?