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

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].*

Introducing the Fourier transformed operators,

$$\hat{b}_{\mathbf{k}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{r}} e^{-i\mathbf{k}\cdot\mathbf{r}} \hat{b}_{\mathbf{r}}, \qquad \hat{b}^\dagger_{\mathbf{k}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{r}} e^{i\mathbf{k}\cdot\mathbf{r}} \hat{b}^\dagger_{\mathbf{r}},$$

we obtain

$$\hat{H}(U=0) = \sum_{\mathbf{k}} (\epsilon_{\mathbf{k}} - \mu) \hat{b}^\dagger_{\mathbf{k}} \hat{b}_{\mathbf{k}} \quad \text{with} \quad \epsilon_{\mathbf{k}} = -2t \sum_{i=1}^{d} \cos(k_i).$$

The ground state of $\hat{H}(U=0)$ is a BEC with all particles in the $\mathbf{k} = 0$ one-particle state: $|\psi\rangle \propto (\hat{b}^\dagger_{\mathbf{k}=0})^{N_p} |\text{vac}\rangle$ (N_p is the total number of particles).

The intersite hopping term favors the delocalization of particles whereas the local repulsion tends to suppress high occupancy of a given site. More precisely, by delocalizing the particles, the energy gain is $\mathcal{O}(t)$ whereas putting several particles on the same site implies an energy cost $\mathcal{O}(U)$. If $t \gg U$, the local repulsion should not play an important role, and we expect the bosons to delocalize and the system to be superfluid. On the other hand, if $U \gg t$, we expect sites with a large occupancy number to be essentially forbidden. This leads us to consider two cases. i) If the mean boson density is integer, for instance $n = 1$, we expect that all sites will be occupied by a single boson; moving a boson would indeed imply a site with double occupancy, which is very unlikely since this corresponds to a very high energy cost when $U \gg t$. The same reasoning can be made if there are two bosons per site on average, etc. ii) If the density is not an integer, it is always possible for the bosons to move without changing the occupancy of the sites. For instance, in the case where n is slightly larger than one, most sites will have a one-boson occupancy and a few sites will be doubly occupied; some of the particles can then move without changing the number of doubly-occupied sites. We therefore expect the system to be superfluid in that case, regardless of the strength of the local repulsion.

To summarize, we expect the system to be always superfluid when the density is not integer, and to undergo a superfluid–Mott-insulator transition at a critical value of t/U when the density is integer. This phase transition, which occurs at zero temperature, and is thus driven by quantum (not thermal) fluctuations, is an example of a quantum phase transition.

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

The Bogoliubov theory is a Gaussian-fluctuation theory about the saddle-point solution where all particles are in the condensate. It therefore assumes that the fluctuations are small (otherwise considering only Gaussian fluctuations would not be sufficient), i.e. that the condensate density does not significantly differs

from the full density. It is justified in the limit $t \gg U$ but cannot be used to describe the superfluid–Mott-insulator transition.

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

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

Using

$$\begin{aligned} \hat{b}^\dagger_{\mathbf{r}} \hat{b}_{\mathbf{r}'} &= (\psi^* + \delta\hat{b}^\dagger_{\mathbf{r}})(\psi + \delta\hat{b}_{\mathbf{r}'}) \\ &= |\psi|^2 + \psi\delta\hat{b}^\dagger_{\mathbf{r}} + \psi^*\delta\hat{b}_{\mathbf{r}'} + \mathcal{O}(\delta\hat{b}^\dagger_{\mathbf{r}}\delta\hat{b}_{\mathbf{r}'}) \\ &= -|\psi|^2 + \psi\hat{b}^\dagger_{\mathbf{r}} + \psi^*\hat{b}_{\mathbf{r}'} + \mathcal{O}(\delta\hat{b}^\dagger_{\mathbf{r}}\delta\hat{b}_{\mathbf{r}'}), \end{aligned}$$

we obtain the mean-field Hamiltonian

$$\begin{aligned} \hat{H}_{\mathrm{MF}} &= -t \sum_{\langle \mathbf{r},\mathbf{r}' \rangle} [-|\psi|^2 + \psi\hat{b}^\dagger_{\mathbf{r}} + \psi^*\hat{b}_{\mathbf{r}'} + \mathrm{H.c.}] + \sum_{\mathbf{r}} \Big(-\mu \hat{b}^\dagger_{\mathbf{r}}\hat{b}_{\mathbf{r}} + \frac{U}{2} \hat{b}^\dagger_{\mathbf{r}}\hat{b}^\dagger_{\mathbf{r}}\hat{b}_{\mathbf{r}}\hat{b}_{\mathbf{r}} \Big) \\ &= -2t \sum_{\langle \mathbf{r},\mathbf{r}' \rangle} [-|\psi|^2 + \psi\hat{b}^\dagger_{\mathbf{r}} + \psi^*\hat{b}_{\mathbf{r}}] + \sum_{\mathbf{r}} \Big(-\mu \hat{b}^\dagger_{\mathbf{r}}\hat{b}_{\mathbf{r}} + \frac{U}{2} \hat{b}^\dagger_{\mathbf{r}}\hat{b}^\dagger_{\mathbf{r}}\hat{b}_{\mathbf{r}}\hat{b}_{\mathbf{r}} \Big). \end{aligned}$$

The sum over $\mathbf{r}'$ gives a factor $2d$ (the number of nearest-neighbor sites on the hypercubic lattice) divided by 2 (since the pairs $\langle \mathbf{r}, \mathbf{r}' \rangle$ and $\langle \mathbf{r}', \mathbf{r} \rangle$ are identical), hence Eq. (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.*

A non-zero order parameter $\psi = \langle \hat{b}_{\mathbf{r}} \rangle$ spontaneously breaks the U(1) symmetry of the Hamiltonian (1), which is a signature of superfluidity. On the other hand, for $\psi = 0$, the mean-field Hamiltonian $\hat{H}_{\mathrm{MF}}$ describes decoupled sites (the intersite hopping term vanishes) and the ground state is then (trivially) an insulator.

2.3) *We now consider the Hamiltonian $\hat{H}_{\mathrm{eff}}(\hat{b}^\dagger, \hat{b})$ 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 $\hat{H}_{\mathrm{eff}}(\psi = 0)$ 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?

The single-site effective Hamiltonian

$$\hat{H}_{\mathrm{eff}}(\psi = 0) = -\mu\hat{n} + \frac{U}{2}\hat{n}(\hat{n} - 1)$$

is diagonal is the number-occupation basis. The eigenstates are the states $|n\rangle$ (defined by $\hat{n}|n\rangle = n|n\rangle$) with energies $\epsilon_n = -\mu n + (U/2)n(n-1)$. The ground state $|n_0\rangle$ is defined by $\epsilon_{n_0} = \min_n \epsilon_n \equiv a_0$. The value of n_0 can be found graphically by considering ϵ_n/U vs μ/U for all values of n. One easily finds that n_0 is determined by the condition $n_0 - 1 < \mu/U < n_0$. Thus the integer n_0 increases by one each time μ/U is integer (Fig. 1).

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*

[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 $|n\rangle = \frac{(\hat{b}^\dagger)^n}{\sqrt{n!}}|\mathrm{vac}\rangle$ is the normalized eigenstate of the occupation-number operator $\hat{n}$.

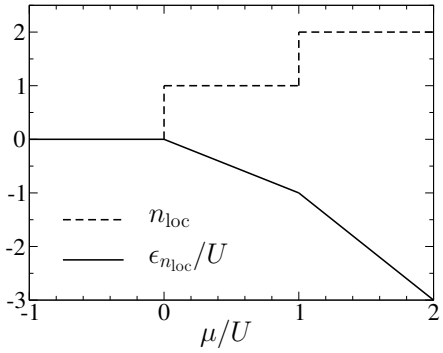


Figure 1: n_0 and ϵ_{n_0}/U *vs* μ/U.

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 $x = n_0 + 1/2$].

Treating the Hamiltonian $D(-\psi^* \hat{b} - \psi \hat{b}^\dagger)$ within second-order perturbation theory, one finds

$$\begin{aligned} E^{(2)} &= D|\psi|^2 + \sum_{\substack{n=0 \\ (n\neq n_0)}}^{\infty} \frac{|\langle n| - D(\psi^* \hat{b} + \psi \hat{b}^\dagger)|n_0\rangle|^2}{\epsilon_{n_0} - \epsilon_n} \\ &= D|\psi|^2 + D^2 \sum_{\substack{n=0 \\ (n\neq n_0)}}^{\infty} \frac{|\psi^* \sqrt{n_0}\delta_{n,n_0-1} + \psi\sqrt{n_0+1}\delta_{n,n_0+1}|^2}{\epsilon_{n_0} - \epsilon_n} \\ &= D|\psi|^2 + D^2|\psi|^2 \left(\frac{n_0+1}{\mu - Un_0} - \frac{n_0}{\mu - U(n_0-1)} \right), \end{aligned}$$

where the first contribution in the rhs, $D|\psi|^2$, comes from the $|\psi|^2$ term in (2).

The value of the order parameter is obtained by requiring the energy $E(|\psi|^2)$ to be minimum. a_4 should be positive for the energy to be bounded from below. $|\psi|$ vanishes if $a_2 \geq 0$ and takes a non-zero value if $a_2 < 0$. The Mott insulator is thus stable for $a_2 \geq 0$ and the transition to the superfluid phase occurs for $a_2 = 0$, i.e.

$$\frac{1}{D} = -\frac{n_0+1}{\mu - Un_0} + \frac{n_0}{\mu - U(n_0-1)} = -\frac{\delta\mu + Ux}{\delta\mu^2 - U^2/4}.$$

Solving for $\delta\mu$, we find two solutions,

$$\delta\mu_\pm = -\frac{D}{2} \pm \frac{1}{2}(D^2 - 4DUx + U^2)^{1/2}.$$

For $t = 0$, $\delta\mu_\pm = \pm U/2$. When increasing D, the two solutions merge when $D/U = 2n_0 + 1 - 2\sqrt{n_0^2 + n_0}$ and $\delta\mu_+ = \delta\mu_- = -D/2$, i.e. $\mu_+ = \mu_- = -D/2 + U(n_0 - 1/2)$. For each value of n_0, we thus find a lobe defined by $\mu_-(D) < \mu < \mu_+(D)$ (with $D_{\rm max}/U = 2n_0 + 1 - 2\sqrt{n_0^2 + n_0}$), where the system is insulating (Mott insulator) (Fig. 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 the Mott insulator. Show that there is a special point of the transition line where the superfluid–Mott-insulator transition occurs at constant density.*

The value of the order parameter ψ is obtained by minimizing the energy $E(|\psi|^2)$. In the Mott insulator, $\psi = 0$ and $E = a_0 = \epsilon_{n_0}$. Since the grand canonical Hamiltonian includes the term $-\mu\hat{N}$, the energy E is actually the $T = 0$ grand potential so that the density is given by $n = -\partial E/\partial\mu$, i.e. $n = n_0$ and the compressibility $\kappa = n^{-2}\partial n/\partial\mu = 0$. The system is incompressible, which is usually associated with a gap in the one-particle excitation spectrum (see Sec. 3). In the superfluid phase, $|\psi|^2 = -a_2/2a_4$ and $E = \epsilon_{n_0} - a_2^2/4a_4$, hence

$$n = n_0 + \frac{a_2}{2a_4}\frac{\partial a_2}{\partial\mu} - \frac{a_2^2}{4a_4^2}\frac{\partial a_4}{\partial\mu}.$$

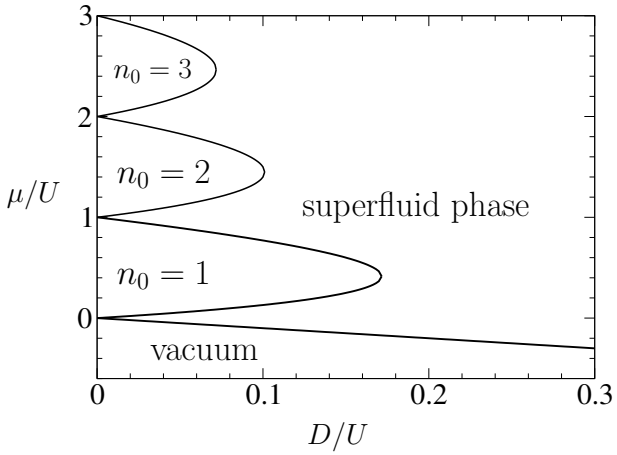


Figure 2: Mean-field phase diagram of the Bose–Hubbard model showing the first three Mott lobes, the vacuum ($n_0 = 0$) and the superfluid phase.

The density is equal to n_0 if (using the fact that $a_2 < 0$ in the superfluid phase)

$$\frac{\partial a_2}{\partial \mu} - \frac{a_2}{2a_4}\frac{\partial a_4}{\partial \mu} = 0.$$

As we move closer and closer to the transition line, i.e. $a_2 \to 0^-$, this condition remains fulfilled only if $\partial a_2/\partial\mu \to 0$. Thus the transition occurs at fixed density if both conditions $a_2 = 0$ and $\partial a_2/\partial\mu = 0$ are satisfied, which corresponds to the tip of the Mott lobe where the tangent to the transition line is vertical.

There are therefore two ways to induce the transition from the Mott insulator to the superfluid phase. One can either increase the ratio t/U at fixed density (tip of the Mott lobe, this is a multi-critical point as two parameters must fine tuned) or change the density (i.e. dope the Mott insulator) at fixed t/U (any point on the transition line except the tip of the lobe, this is the generic transition). We conclude that the Mott-insulator–superfluid transition belongs to two different universality classes.

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,

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

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 $S_{\text{loc}}[b^*, b]$.*

$$S[b^*, b, \psi^*, \psi] = S_{\text{loc}}[b^*, b] + \int_0^\beta d\tau \left[\sum_{\mathbf{r},\mathbf{r}'} \psi^*_{\mathbf{r}} t^{-1}_{\mathbf{r},\mathbf{r}'} \psi_{\mathbf{r}'} - \sum_{\mathbf{r}} (\psi^*_{\mathbf{r}} b_{\mathbf{r}} + \text{c.c.}) \right],$$

where $t^{-1}_{\mathbf{r},\mathbf{r}'}$ should be understood as the inverse of the matrix $t_{\mathbf{r},\mathbf{r}'}$.

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*

$$S[\psi^*,\psi] = \sum_{\mathbf{k},\omega_n} \psi^*(\mathbf{k},i\omega_n)\big[t_{\mathbf{k}}^{-1} + G_{\rm loc}(i\omega_n)\big]\psi(\mathbf{k},i\omega_n), \tag{6}$$

where $t_{\mathbf{k}}$ is the Fourier transform of $t_{\mathbf{r},\mathbf{r}'} = t_{\mathbf{r}-\mathbf{r}'}$ and $G_{\rm loc}(i\omega_n)$ is the local Green function obtained from $S_{\rm loc}$. 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?

The effective action of the ψ field is given by

$$S[\psi^*,\psi] = \int_0^\beta d\tau \left[\sum_{\mathbf{r},\mathbf{r}'} \psi^*_{\mathbf{r}} t^{-1}_{\mathbf{r},\mathbf{r}'}\psi_{\mathbf{r}'} + \langle S'\rangle_{\rm loc} - \frac{1}{2}(\langle S'^2\rangle_{\rm loc} - \langle S'\rangle^2_{\rm loc})\right],$$

where

$$S' = -\sum_{\mathbf{r}} \int_0^\beta d\tau (\psi^*_{\mathbf{r}} b_{\mathbf{r}} + \text{c.c.}).$$

One finds

$$\langle S'\rangle = 0$$

since $\langle b_{\mathbf{r}}\rangle_{\rm loc} = \langle b^*_{\mathbf{r}}\rangle_{\rm loc} = 0$, and

$$\begin{aligned}\langle S'^2\rangle_{\rm loc} &= \int_0^\beta d\tau d\tau' \sum_{\mathbf{r},\mathbf{r}'} \langle[\psi^*_{\mathbf{r}}(\tau)b_{\mathbf{r}}(\tau) + \text{c.c.}][\psi^*_{\mathbf{r}'}(\tau')b_{\mathbf{r}'}(\tau') + \text{c.c.}]\rangle_{\rm loc} \\ &= -2\sum_{\mathbf{r}} \int_0^\beta d\tau d\tau'\, \psi^*_{\mathbf{r}}(\tau) G_{\rm loc}(\tau-\tau')\psi_{\mathbf{r}}(\tau')\end{aligned}$$

since $\langle b_{\mathbf{r}}(\tau)b_{\mathbf{r}'}(\tau')\rangle_{\rm loc} = \langle b^*_{\mathbf{r}}(\tau)b^*_{\mathbf{r}'}(\tau')\rangle_{\rm loc} = 0$ and $\langle b_{\mathbf{r}}(\tau)b^*_{\mathbf{r}'}(\tau')\rangle_{\rm loc} = -\delta_{\mathbf{r},\mathbf{r}'}G_{\rm loc}(\tau-\tau')$. Hence Eq. (6), with

$$t_{\mathbf{k}} = \frac{1}{N}\sum_{\mathbf{r},\mathbf{r}'} e^{-i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} t_{\mathbf{r},\mathbf{r}'} = 2t\sum_{\nu=1}^{d}\cos k_\nu.$$

The propagator $\mathcal{G}$ is given by

$$\mathcal{G}(\mathbf{k},i\omega_n) = \frac{-1}{t_{\mathbf{k}}^{-1} + G_{\rm loc}(i\omega_n)}.$$

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

$$G_{\rm loc}(i\omega_n) = \frac{n_0+1}{i\omega_n + \mu - Un_0} - \frac{n_0}{i\omega_n + \mu - U(n_0-1)} \tag{7}$$

in the zero-temperature limit.

For $\tau > 0$, using the basis $\{|n\rangle\}$,

$$\begin{aligned}G_{\rm loc}(\tau) &= -\frac{1}{Z_{\rm loc}}\text{Tr}\big[e^{-(\beta-\tau)\hat{H}_{\rm loc}}\hat{b}e^{-\tau\hat{H}_{\rm loc}}\hat{b}^\dagger\big] \\ &= -\frac{1}{Z_{\rm loc}}\sum_{n,m=0}^{\infty} e^{-(\beta-\tau)\epsilon_n}\langle n|\hat{b}|m\rangle e^{-\tau\epsilon_m}\langle m|\hat{b}^\dagger|n\rangle \\ &= -\frac{1}{Z_{\rm loc}}\sum_{n=0}^{\infty} e^{-(\beta-\tau)\epsilon_n - \tau\epsilon_{n+1}}|\langle n+1|\hat{b}^\dagger|n\rangle|^2 \\ &= -\frac{1}{Z_{\rm loc}}\sum_{n=0}^{\infty} e^{-(\beta-\tau)\epsilon_n - \tau\epsilon_{n+1}}(n+1)\end{aligned}$$

with $Z_{\rm loc} = \sum_n e^{-\beta\epsilon_n}$. We deduce

$$G_{\rm loc}(i\omega_n) = \int_0^\beta d\tau\, e^{i\omega_n\tau} G_{\rm loc}(\tau) = -\frac{1}{Z_{\rm loc}} \sum_{m=0}^{\infty} (m+1) \frac{e^{-\beta\epsilon_{m+1}} - e^{-\beta\epsilon_m}}{i\omega_n + \epsilon_m - \epsilon_{m+1}}.$$

Since $\min \epsilon_n = \epsilon_{n_0}$, we finally find (7) for $T \to 0$.

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

The Mott phase is stable if $-\mathcal{G}(\mathbf{k} = 0, i\omega_n = 0) \geq 0$, which is the usual stability condition for a bosonic theory with quadratic action [if this condition is not satisfied, the Gaussian integral over the field $\psi^{(*)}(\mathbf{k} = 0, i\omega_n = 0)$ is not defined]. Thus the transition line is defined by

$$0 = \frac{1}{t_{\mathbf{k}=0}} + G_{\rm loc}(i\omega_n = 0) = \frac{1}{D} + \frac{n_0 + 1}{\mu - U n_0} - \frac{n_0}{\mu - U(n_0 - 1)},$$

which reproduces the result of the mean-field theory.

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?*

The spectrum is obtained from the pole of the retarded propagator $\mathcal{G}(k, i\omega_n \to \omega + i0^+)$, i.e.

$$\begin{aligned} 0 &= t_{\mathbf{k}}^{-1} + G_{\rm loc}(\omega + i0^+) \\ &= t_{\mathbf{k}}^{-1} + \frac{n_0 + 1}{\omega + \delta\mu - U/2} - \frac{n_0}{\omega + \delta\mu + U/2}. \end{aligned}$$

Solving for ω, we obtain two branches (referred to as the upper and lower Hubbard bands),

$$E_\pm(\mathbf{k}) = -\frac{t_{\mathbf{k}}}{2} \pm \frac{1}{2}\left(t_{\mathbf{k}}^2 - 4xUt_{\mathbf{k}} + U^2\right)^{1/2} - \delta\mu.$$

For $t = 0$,

$$\begin{aligned} E_+(\mathbf{k}) &= -\mu + U n_0 = \epsilon_{n_0+1} - \epsilon_{n_0}, \\ E_-(\mathbf{k}) &= -\mu + U(n_0 - 1) = \epsilon_{n_0} - \epsilon_{n_0-1}. \end{aligned}$$

Thus the upper branch ($E_+(\mathbf{k})$) corresponds to the addition of a particle whereas the lower one ($E_-(\mathbf{k})$) corresponds to the removal of a particle.

One finds

$$E_\pm(\mathbf{k} = 0) = \delta\mu_\pm - \delta\mu.$$

Assuming that the minimum (maximum) of $E_+(\mathbf{k})$ occurs for $\mathbf{k} = 0$ (which can be easily checked by plotting $E_\pm(\mathbf{k})$ vs $\mathbf{k}$ with, e.g., Mathematica), one concludes that at the transition, where $\delta\mu = \delta\mu_+$ or $\delta\mu = \delta\mu_-$, one of the two branches becomes gapless (the upper branch $E_+(\mathbf{k})$ becomes gapless on the upper part of the transition line for a given Mott lobe, and *vice versa* for the lower branch). The tip of the Mott lobe is special, being defined by $\delta\mu_+ = \delta\mu_- = 0$; both branches become gapless simultaneously and $E_+(\mathbf{k} = 0) - E_-(\mathbf{k} = 0)$ vanishes.

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) may take two different values.*

Defining $\epsilon_{\mathbf{k}} = -t_{\mathbf{k}} + D \simeq t\mathbf{k}^2$ for $\mathbf{k} \to 0$, one has

$$E_\pm(\mathbf{k}) = -\delta\mu - \frac{D}{2} + \frac{\epsilon_{\mathbf{k}}}{2} \pm \frac{1}{2}\left(\epsilon_{\mathbf{k}}^2 + 4xU\epsilon_{\mathbf{k}} - 2D\epsilon_{\mathbf{k}} + A^2\right)^{1/2} \quad \text{where} \quad A^2 = D^2 - 4xUD + U^2.$$

At the generic transition (i.e. away from the Mott lobe), $\delta\mu \neq -D/2$ and $A^2 > 0$:

$$E_\pm(\mathbf{k}) = -\delta\mu + \delta\mu_\pm \pm \frac{\mathbf{k}^2}{2m_\pm} + \mathcal{O}(|\mathbf{k}|^4).$$

At the critical point, where $\delta\mu_+ \to 0$, $E^+(\mathbf{k}) \sim \mathbf{k}^2$ and $z = 2$. At the multi-critical point (tip of the Mott lobe), where $\delta\mu = -D/2$ and $A = 0$, one finds

$$E_\pm(\mathbf{k}) \simeq \pm[(4xU - 2D)\epsilon_\mathbf{k}]^{1/2} + \mathcal{O}(\mathbf{k}^2) = \pm c|\mathbf{k}| + \mathcal{O}(\mathbf{k}^2),$$

so that $z = 1$.

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

One has

$$\begin{aligned} t_\mathbf{k}^{-1} + G_{\rm loc}(i\omega_n) &= t_{\mathbf{k}=0}^{-1} + G_{\rm loc}(i\omega_n = 0) + K_3 \mathbf{k}^2 + i\omega_n \left.\frac{\partial G_{\rm loc}(i\omega_n)}{\partial i\omega_n}\right|_{i\omega_n=0} + \frac{(i\omega_n)^2}{2} \left.\frac{\partial^2 G_{\rm loc}(i\omega_n)}{\partial (i\omega_n)^2}\right|_{i\omega_n=0} \\ &= r + K_3 \mathbf{k}^2 + i\omega_n \left.\frac{\partial G_{\rm loc}(i\omega_n)}{\partial i\omega_n}\right|_{i\omega_n=0} + \frac{(i\omega_n)^2}{2} \left.\frac{\partial^2 G_{\rm loc}(i\omega_n)}{\partial (i\omega_n)^2}\right|_{i\omega_n=0} \end{aligned}$$

to $\mathcal{O}(\mathbf{k}^2, \omega_n^2)$ (note that $i\omega_n \equiv i\omega$ is a continuous variable at $T = 0$), where $r = t_{\mathbf{k}=0}^{-1} + G_{\rm loc}(i\omega_n = 0) = -\mathcal{G}^{-1}(\mathbf{k} = 0, i\omega_n = 0)$. Since $G_{\rm loc}(i\omega_n) \equiv G_{\rm loc}(i\omega_n + \mu)$,

$$\frac{\partial G_{\rm loc}(i\omega_n)}{\partial i\omega_n} = \frac{\partial G_{\rm loc}(i\omega_n)}{\partial \mu}, \qquad \left.\frac{\partial G_{\rm loc}(i\omega_n)}{\partial i\omega_n}\right|_{i\omega_n=0} = \frac{\partial G_{\rm loc}(0)}{\partial \mu} = \frac{\partial r}{\partial \mu},$$

hence Eqs. (8,9).

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?*

The transition at constant density occurs at the tip of the Mott lobe where the tangent to the transition line is vertical. Since the transition line is defined by $r(\mu, t, U) = 0$, this implies that $K_1 = 0$. There is then no first-order term in ∂_τ in the effective action (8), which corresponds to a "relativistic" O(2) model in d dimensions or, equivalently, a classical O(2) model in $d + 1$ dimensions (the complex field $\psi = \psi_1 + i\psi_2$ can be seen as a two-component real field). The universality class of the transition is therefore that of the $(d + 1)$-dimensional O(2) model or $(d + 1)$-dimensional XY model, and is characterized by a dynamical critical exponent $z = 1$. The other universality class, corresponding to the generic transition, is known as the dilute-Bose-gas universality class, being in the same universality class as the $T = 0$ transition between the vacuum state (no particles) and the superfluid state that occurs in a Bose gas when varying the chemical potential from negative to positive values.