University of California at San Diego – Department of Physics – Prof. John McGreevy

Physics 212C QM Spring 2023
Assignment 10 ("Final Exam") – Solutions

Due 11:00am Wednesday, June 14, 2023

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1. **Antiferromagnet from fermions.** In lecture, we discussed the idea of getting a magnet from a Mott insulator, where the electrons are stuck in place by mutual repulsion, but can still have a spin degree of freedom. In such a system, what determines the interactions between the spins?

   Consider the hamiltonian

$$\mathbf{H} = -t\sum_{\sigma}\left(\mathbf{c}^\dagger_{1\sigma}\mathbf{c}_{2\sigma} + h.c.\right) + U\left(\mathbf{n}_{1\uparrow}\mathbf{n}_{1\downarrow} + \mathbf{n}_{2\uparrow}\mathbf{n}_{2\downarrow}\right) \equiv \mathbf{H}_t + \mathbf{H}_U$$

   with $t, U > 0$. Here the $\mathbf{c}$s are canonical fermion operators: $\{\mathbf{c}_{i\sigma}, \mathbf{c}^\dagger_{j\sigma'}\} = \delta_{ij}\delta_{\sigma\sigma'}$, $\{\mathbf{c}_{i\sigma}, \mathbf{c}_{j\sigma'}\} = 0$. $\sigma = \uparrow, \downarrow$ labels the electron spin and $\mathbf{n}_{i\sigma} \equiv \mathbf{c}^\dagger_{i\sigma}\mathbf{c}_{i\sigma}$ is the number operator. This is the fermionic Hubbard model on just two sites, $i = 1, 2$.

   In this problem we will think about the sector of states with exactly two electrons *i.e.* we only consider states $|\psi\rangle$ with

$$\left(\sum_{i,\sigma}\mathbf{n}_{i\sigma} - 2\right)|\psi\rangle = 0.$$

   (a) First, enumerate all the states with two electrons (make sure to be careful about defining their signs).

   Let's call them

$$|1\rangle \equiv \mathbf{c}^\dagger_{1\uparrow}\mathbf{c}^\dagger_{2\uparrow}|0\rangle = |\uparrow,\uparrow\rangle \tag{1}$$
$$|2\rangle \equiv \mathbf{c}^\dagger_{1\uparrow}\mathbf{c}^\dagger_{2\downarrow}|0\rangle = |\uparrow,\downarrow\rangle \tag{2}$$
$$|3\rangle \equiv \mathbf{c}^\dagger_{1\downarrow}\mathbf{c}^\dagger_{2\uparrow}|0\rangle = |\downarrow,\uparrow\rangle \tag{3}$$
$$|4\rangle \equiv \mathbf{c}^\dagger_{1\downarrow}\mathbf{c}^\dagger_{2\downarrow}|0\rangle = |\downarrow,\downarrow\rangle \tag{4}$$
$$|5\rangle \equiv \mathbf{c}^\dagger_{1\uparrow}\mathbf{c}^\dagger_{1\downarrow}|0\rangle = |\uparrow\downarrow,\cdot\rangle \tag{5}$$
$$|6\rangle \equiv \mathbf{c}^\dagger_{2\uparrow}\mathbf{c}^\dagger_{2\downarrow}|0\rangle = |\cdot,\uparrow\downarrow\rangle \quad . \tag{6}$$

   Note that the order in which we create the fermions is a sign convention which we are defining here.

(b) Next, consider $U/t = \infty$. How many groundstates does the system have if there are two electrons in total? Write down these ground states.

States $|5\rangle, |6\rangle$ have energy U, and states $|1\rangle, \cdots, |4\rangle$ have energy 0, so they are the degenerate groundstates, *i.e.*$X = \text{span}\{|1\rangle, \cdots |4\rangle\}$.

Now consider $U/t \gg 1$ (but not infinite). We will do degenerate perturbation theory to find an effective Hamiltonian action on the degenerate groundspace, X.

(c) Show that at first order in t/U, the perturbing hamiltonian $\mathbf{H}_t$ always takes us out of the degenerate subspace, X.

If in any of the states $|1\rangle$ through $|4\rangle$ we move a single fermion, it leads to two fermions on top of each other, which costs energy U.

(d) Recall that at second order, the matrix elements of the effective Hamiltonian take the form

$$\langle a| \mathbf{H}_{\text{eff}} |b\rangle = -\sum_{n \notin X} \langle a| \mathbf{H}_t |n\rangle \frac{1}{\langle n| \mathbf{H}_U |n\rangle} \langle n| \mathbf{H}_t |b\rangle$$

where $|a\rangle, |b\rangle$ belong to the degenerate subspace X, and $|n\rangle$ does not. Show that the effective Hamiltonian is (up to an additive constant)

$$\mathbf{H}_{\text{eff}} = J \vec{\mathbf{S}}_1 \cdot \vec{\mathbf{S}}_2$$

where $\vec{\mathbf{S}}_i \equiv \frac{1}{2} \mathbf{c}_i^\dagger \vec{\sigma} \mathbf{c}_i$. Find the value of J in terms of t and U.

The nonzero matrix elements are

$$\langle 2| \mathbf{H}_t |6\rangle = t, \langle 2| \mathbf{H}_t |5\rangle = -t, \langle 3| \mathbf{H}_t |6\rangle = -t, \langle 3| \mathbf{H}_t |5\rangle = +t.$$

This gives *e.g.*

$$(\mathbf{H}_{\text{eff}})_{2,2} = \frac{\langle 2| \mathbf{H}_t |5\rangle \langle 5| \mathbf{H}_t |2\rangle}{-U} + \frac{\langle 2| \mathbf{H}_t |6\rangle \langle 6| \mathbf{H}_t |2\rangle}{-U} = -2\frac{t^2}{U}$$

while

$$(\mathbf{H}_{\text{eff}})_{2,3} = \frac{\langle 2| \mathbf{H}_t |5\rangle \langle 5| \mathbf{H}_t |3\rangle}{-U} + \frac{\langle 2| \mathbf{H}_t |6\rangle \langle 6| \mathbf{H}_t |3\rangle}{-U} = +2\frac{t^2}{U}$$

Therefore, the effective hamiltonian is

$$h = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & -\frac{2t^2}{U} & +\frac{2t^2}{U} & 0 \\ 0 & \frac{2t^2}{U} & -\frac{2t^2}{U} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

The eigenvalues of h are $0, 0, 0, -\frac{4t^2}{U}$ and the eigenvectors are, respectively, $|\uparrow\uparrow\rangle$, $\frac{|\uparrow\downarrow\rangle+|\downarrow\uparrow\rangle}{\sqrt{2}}$, $|\downarrow\downarrow\rangle$ (with eigenvalue zero) and $\frac{|\uparrow\downarrow\rangle-|\downarrow\uparrow\rangle}{\sqrt{2}}$ with eigenvalue $-4\frac{t^2}{U}$. This should look familiar: the groundstate is the total $\mathsf{SU}(2)$ singlet, and the total $\mathsf{SU}(2)$ triplet is the excited state. The whole thing is $\mathsf{SU}(2)$ symmetric, and this is the same spectrum as

$$\mathbf{H}_{\text{eff}} = +\frac{4t^2}{U}\vec{\mathbf{S}}_1 \cdot \vec{\mathbf{S}}_2$$

(plus a constant).

(e) Now redo the whole problem for hard-core bosons. (By hard-core, I mean we forbid $\left(\mathbf{b}^\dagger_{i\uparrow}\right)^2$ but allow $\mathbf{b}^\dagger_{i\uparrow}\mathbf{b}^\dagger_{i\downarrow}$.) Compare the answer.

The only difference is that we erase the relative signs on the matrix elements

$$\langle 2|\,\mathbf{H}_t\,|6\rangle = t, \langle 2|\,\mathbf{H}_t\,|5\rangle = t, \langle 3|\,\mathbf{H}_t\,|6\rangle = t, \langle 3|\,\mathbf{H}_t\,|5\rangle = +t.$$

This has the consequence that

$$h = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{2t^2}{U} & +\frac{2t^2}{U} & 0 \\ 0 & \frac{2t^2}{U} & \frac{2t^2}{U} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

whose spectrum is $0, 0, 0, \frac{4t^2}{U}$ with the same respective eigenvectors, and now the singlet is the excited state. It is a ferromagnet

$$\mathbf{H}^{\text{bosons}}_{\text{eff}} = -\frac{4t^2}{U}\vec{\mathbf{S}}_1 \cdot \vec{\mathbf{S}}_2.$$

2. **Relative number and relative phase eigenstates.** Consider a collection of N identical bosons, each of which can be in one of two orthonormal single-particle states

$$\mathbf{a}^\dagger\,|0\rangle\,, \mathbf{b}^\dagger\,|0\rangle\,.$$

Assume N is even.

I got this problem from Leggett's book, *Quantum Liquids*, Appendix 2B.

(a) Construct a basis of this Hilbert space made of eigenstates $|M\rangle$ of the 'relative number' operator

$$\mathbf{M} \equiv \frac{1}{2}\left(\mathbf{a}^\dagger\mathbf{a} - \mathbf{b}^\dagger\mathbf{b}\right).$$

How many such states are there? What are the possible eigenvalues of $\mathbf{M}$?

There are $N+1$ such states, labelled by how many of the N particles we put in the $\mathbf{a}$ orbital:

$$|M\rangle = A_{NM} \left(\mathbf{a}^\dagger\right)^{N/2+M} \left(\mathbf{b}^\dagger\right)^{N/2-M} |0\rangle \,, A_{NM} = \frac{1}{\sqrt{(N/2+M)!(N/2-M)!}}$$

$M = -N/2, -N/2+1 \cdots N/2-1, N/2$ for N even and $M = -N/2 - \frac{1}{2}, -N/2+\frac{1}{2}, \cdots N/2-\frac{1}{2}$ for N odd.

(b) Now consider the 'relative phase' states

$$|\varphi, c, s\rangle \equiv \frac{1}{\sqrt{N!}} \left(ce^{\mathbf{i}\varphi/2}\mathbf{a}^\dagger + se^{-\mathbf{i}\varphi/2}\mathbf{b}^\dagger\right)^N |0\rangle \,,$$

where $c^2+s^2=1$ and $c, s > 0$. Expand this state in the basis above. Where is the peak of $P_M(\varphi, c, s)$, the probability of finding M when measuring $\mathbf{M}$ in this state?

$$\begin{aligned} |\varphi, c, s\rangle &= \frac{1}{N!}\sum_{M=0}^{N} \binom{N}{M} \left(\mathbf{a}^\dagger ce^{\mathbf{i}\varphi/2}\right)^{N/2+M} \left(\mathbf{b}^\dagger se^{-\mathbf{i}\varphi/2}\right)^{N/2-M} & (7)\\ &= |C_M| e^{\mathbf{i}M\varphi} |M\rangle \,, \quad |C_M| = c^{N/2+M} s^{N/2-M} A_{NM}. & (8) \end{aligned}$$

$P_M = |C_M|^2 = c^{N+2M}s^{N-2M}|A_{NM}|^2$. Using Stirling, the maximum occurs at

$$\begin{aligned} 0 &= \partial_M \left(\log |C_M|^2\right) \\ &\simeq \partial_M \big((N+2M)\log c + (N-2M)\log s \\ &\qquad -(N/2-M)\log(N/2-M) - (N/2+M)\log(N/2+M)\big) \\ &= \log \frac{c^2}{s^2}\frac{N/2-M}{N/2+M} & (9) \end{aligned}$$

which is solved by

$$\bar{M} = N\left(c^2 - s^2\right).$$

(c) Show that

$$|M\rangle = A\int_0^{2\pi} d\varphi e^{-\mathbf{i}M\varphi} |\varphi, c, s\rangle$$

and find the constant A.

$$
\begin{aligned}
&A \int_0^{2\pi} đ\varphi e^{-\mathbf{i}M\varphi} \left|\varphi, c, s\right\rangle && (10)\\
&= A \int_0^{2\pi} đ\varphi e^{-\mathbf{i}M\varphi} \sum_{M'} |C_{M'}| e^{\mathbf{i}M'\varphi} \left|M'\right\rangle && (11)\\
&= A |C_M| \left|M\right\rangle && (12)
\end{aligned}
$$

so $A = \frac{1}{|C_M|}$.

(d) [Bonus question] What is the 'relative phase' operator diagonalized by the 'relative phase' states? Consider

$$
\hat{\varphi} \equiv -\mathbf{i}\arg\left(\frac{\mathbf{a}^\dagger \mathbf{b}}{\sqrt{(N/2 - \mathbf{M})(N/2 + \mathbf{M} + 1)}}\right)
$$

and show that it satisfies (approximately, at large N)

$$
[\mathbf{M}, \hat{\varphi}] = -\mathbf{i}.
$$

(e) [Bonus question] What needs to be fixed above if N is odd?

(f) Now for the real physics content of the problem. Suppose we think our system wants to macroscopically occupy the two orbitals associated with $\mathbf{a}$ and $\mathbf{b}$. We could do this in two different ways: a state of definite relative number:

$$
\left|F\right\rangle \equiv \left(\mathbf{a}^\dagger\right)^{N_A} \left(\mathbf{b}^\dagger\right)^{N_B} \left|0\right\rangle, \quad N_A + N_B = N
$$

or a state of definite relative phase:

$$
\left|G\right\rangle \equiv \left(\alpha \mathbf{a}^\dagger + \beta \mathbf{b}^\dagger\right)^N \left|0\right\rangle.
$$

Notice that the latter is a simple BEC in a particular linear combination of the two orbitals. Based on a variational estimate, which of these states is favored energetically by the interaction

$$
\mathbf{H}_{\text{int}} = U_0 \mathbf{b}^\dagger \mathbf{b} \mathbf{a}^\dagger \mathbf{a}
$$

if $U_0 > 0$?

To do a variational calculation, first we have to normalize the states. Let me redefine

$$
\left|F\right\rangle \equiv \frac{\left(\mathbf{a}^\dagger\right)^{N_A}}{\sqrt{N_A!}} \frac{\left(\mathbf{b}^\dagger\right)^{N_B}}{\sqrt{N_B!}} \left|0\right\rangle, \quad N_A + N_B = N
$$

$$|G\rangle \equiv \frac{1}{\sqrt{N!}}\left(\alpha \mathbf{a}^\dagger + \beta \mathbf{b}^\dagger\right)^N |0\rangle$$

so that they are normalized. The latter requires that $|\alpha|^2 + |\beta|^2 = 1$, which we can parametrize as $\alpha = ce^{\mathbf{i}\varphi/2}, \beta = se^{-\mathbf{i}\varphi/2}$ as above.

$|F\rangle$ is an eigenstate of H_{int}:

$$\langle F|H_{\text{int}}|F| = U_0 N_A N_B. \tag{13}$$

To compute $\left\langle \hat{N}_A \hat{N}_B \right\rangle$ in the state $|G\rangle$, we could just use the calculation above that says $N_A - N_B = 2M = 2N(c^2 - s^2)$. But let's do it exactly:

$$\left\langle G|\hat{N}_A|G\right\rangle = \frac{1}{N!}\sum_{m_1,m_2}\binom{N}{m_1}\binom{N}{m_2}\alpha^{m_1}\bar{\alpha}^{m_2}\beta^{N-m_1}\bar{\beta}^{N-m_1}\underbrace{\langle m_2, N-m_2|\,\hat{N}_A\,|m_1, N-m_1\rangle}_{=\delta_{m_1,m_2}m_1}$$

$$= \sum_m \binom{N}{m}|\alpha|^{2m}|\beta|^{2(N-m)}m \tag{14}$$

$$= |\alpha|^2\partial_{|\alpha|^2}\sum_m \binom{N}{m}|\alpha|^{2m}|\beta|^{2(N-m)} \tag{15}$$

$$= |\alpha|^2\partial_{|\alpha|^2}(|\alpha|^2 + |\beta|^2)^N \tag{16}$$

$$= |\alpha|^2 N. \tag{17}$$

Similarly, $\left\langle G|\hat{N}_B|G\right\rangle = |\beta|^2 N$. So to compare F and G, we should set $|\alpha|^2 = c^2 = N_A/N, |\beta|^2 = s^2 = N_B/N = 1 - |\alpha^2$. The energy expectation can be computed by the same method:

$$\langle G|H_{\text{int}}|G\rangle = U_0\left\langle G|\hat{N}_B\hat{N}_B|G\right\rangle \tag{18}$$

$$= U_0|\alpha|^2\partial_{|\alpha|^2}|\beta|^2\partial_{|\beta|^2}\left(|\alpha|^2 + |\beta|^2\right)^N \tag{19}$$

$$= U_0 N(N-1)|\alpha|^2|\beta|^2 \tag{20}$$

$$= U_0\frac{N-1}{N}N_A N_B \tag{21}$$

which is slightly smaller than (13) at finite N.

3. **Mean field theory for the Bose-Hubbard model.**

Consider again the Bose-Hubbard model

$$H_{BH} = \sum_i\left(-\mu n_i + \frac{U}{2}n_i(n_i - 1)\right) + \sum_{ij} b_i^\dagger w_{ij} b_j$$

on a lattice with uniform coordination number z. The hopping matrix is $w_{ij} \equiv w$ if ij share a link, and zero otherwise.

We'll consider a variational approach to mean field theory. We'll find the best product-state wavefunction $|\Psi_{\text{var}}\rangle = \otimes_i |\psi_i\rangle$, and minimize the BH energy $\langle\Psi_{\text{var}}| H_{BH} |\Psi_{\text{var}}\rangle$ over all ψ_i. We can parametrize the single-site states as the groundstates of the mean-field hamiltonian:

$$H_{\text{MF}} = \sum_i h_i = \sum_i \left(-\mu n_i + \frac{U}{2} n_i(n_i - 1) - \psi^\star b_i - \psi b_i^\dagger \right).$$

Here ψ is an effective field that incorporates the effects of the neighboring sites. Notice that nonzero ψ breaks the $\mathsf{U}(1)$ boson number conservation: particles can hop out of the site we are considering. This also means that nonzero ψ will signal SSB.

What does this simple approximation give up? For one, it assumes the groundstate preserves the lattice translation symmetry, which doesn't always happen. More painfully, it also gives up on any entanglement at all in the groundstate. Phases for which entanglement plays an important role will not be found this way.

We want to minimize over ψ the quantity

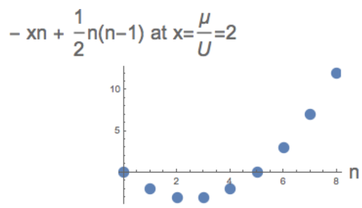
$$\begin{aligned}
\mathcal{E}_0 \equiv \frac{1}{M} \langle\Psi_{\text{var}}| H_{BH} |\Psi_{\text{var}}\rangle &= \frac{1}{M} \left(\langle\Psi_{\text{var}}| \left(\underbrace{H_{BH} - H_{MF}}_{= \sum w b^\dagger b + \psi^\star b + h.c.} + H_{MF} \right) |\Psi_{\text{var}}\rangle \right) \\
&= \frac{1}{M} E_{MF}(\psi) + zw \left\langle b^\dagger \right\rangle \langle b \rangle + \langle b \rangle \psi^\star + \left\langle b^\dagger \right\rangle \psi. \qquad (22)
\end{aligned}$$

Here z is the coordination number of the lattice (the number of neighbors of a site, which we assume is the same for every site), M is the number of sites, and $\langle .. \rangle \equiv \langle\Psi_{\text{var}}| .. |\Psi_{\text{var}}\rangle$.

(a) Make sure the previous discussion makes sense to you.

(b) First consider $w = 0$, no hopping. What is the optimal value of ψ? What is the optimal single-site state as a function of μ/U?

Then $\psi = 0$ (neighbors don't matter), and the single-site state is a number eigenstate $|\psi_i\rangle = |n_0(\mu/U)\rangle$, where $n_0(x) = 0$ for $x < 0$, and $n_0(x) = \lceil x \rceil$, (the ceiling of x, *i.e.* , the next integer larger than x), for $x > 0$. Precisely when μ/U is an integer, there is a twofold degeneracy per site.



That is, the groundstate has n_0 bosons when $(n_0-1)U < \mu < nU$.

(c) We can find the boundaries of the region where $\psi = 0$ (the Mott insulator phase) by Taylor expanding $\mathcal{E}_0$ in powers of ψ, following Landau: $\mathcal{E}_0 = \mathcal{E}_0^0 + r|\psi|^2 + \mathcal{O}(|\psi|^4)$.
Using second order perturbation theory (in the $\psi b^\dagger + \psi^\star b$ terms of the mean field hamiltonian) or otherwise, derive the form of r as a function of μ/U. The answer is

$$r = \chi_0(n_0)\left(1 - zw\chi_0(n_0)\right)$$

where

$$\chi_0(n_0) \equiv \frac{n_0+1}{Un_0-\mu} + \frac{n_0}{\mu - U(n_0-1)}, \tag{23}$$

and n_0 is the integer which minimizes $Un(n-1) - \mu n$.

So we need to approximate the groundstate of $\mathbf{H}_{MF}$. We can do this in perturbation theory in ψ, that is, $\mathbf{\Delta H} \equiv -\psi\mathbf{b}^\dagger - \psi^\star\mathbf{b}$:

$$|gs\rangle \simeq |n_0\rangle + \sum_n |n\rangle \frac{\langle n|\,\mathbf{\Delta H}\,|n_0\rangle}{E_0(n) - E_0(n_0)} \tag{24}$$

$$= |n_0\rangle + \frac{1}{E_+}|n_0+1\rangle\langle n_0+1|\left(-\psi\mathbf{b}^\dagger\right)|n_0\rangle + \frac{1}{E_-}|n_0-1\rangle\langle n_0-1|\left(-\psi^\star\mathbf{b}\right)|n_0\rangle \tag{25}$$

$$= |n_0\rangle - \psi\frac{\sqrt{n_0+1}}{E_+}|n_0+1\rangle - \psi^\star\frac{\sqrt{n_0}}{E_-}|n_0-1\rangle \tag{26}$$

where

$$E_\pm = E_0(n_0) - E_0(n_0 \pm 1), \quad E_0(n_0) \equiv -\mu n_0 + \frac{U}{2}n_0(n_0-1)$$

This gives

$$E_+ = \mu - Un_0, \quad E_- = -\mu + U(n_0-1).$$

We used $\langle n_0|\,\mathbf{b}\,|n_0+1\rangle = \sqrt{n_0+1}$.
To first order in ψ, then, this gives

$$\langle\mathbf{b}\rangle = \psi\chi_0, \quad \left\langle\mathbf{b}^\dagger\right\rangle = \psi^\star\chi_0$$

where χ_0 is defined in (24). Also using perturbation theory in ψ, the groundstate energy of $\mathbf{H}_{MF}$ is then approximately

$$E_{MF}^0 \simeq E_0(n_0) + \sum_n \frac{|\langle n| \Delta\mathbf{H} |n_0\rangle|^2}{E_0(n) - E_0(n_0)} = E_0(n_0) - \psi\psi^\star \chi_0.$$

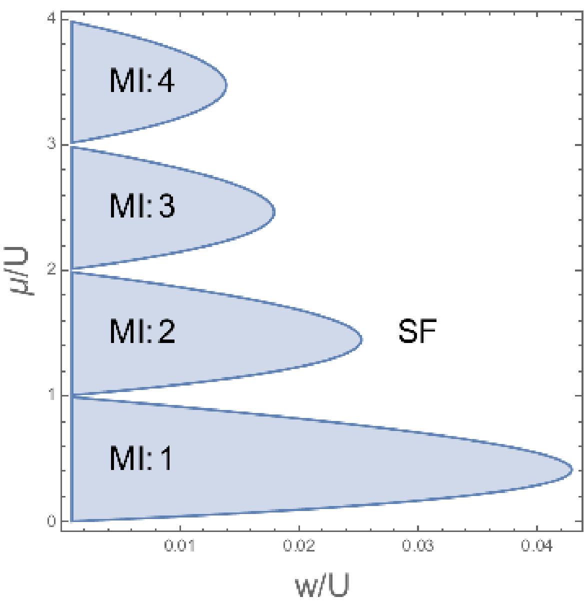
The expectation value of the hamiltonian is then

$$\begin{aligned} \mathcal{E}_0 &= E_0(n_0) + \psi\psi^\star\chi_0 + zw\psi\psi^\star\chi_0^2 - \psi\chi_0\psi^\star - \psi^\star\chi_0\psi & (27) \\ &= E_0(n_0) + \psi\psi^\star\left(-\chi_0 + zw\chi_0^2 + \chi_0 + \chi_0\right) & (28) \end{aligned}$$

and hence

$$r = \chi_0(1 - zw\chi_0).$$

(d) Draw the Mott lobes using this formula.



This figure is for $z = 4$, as for the square lattice.

Note that everywhere in each MI lobe, the expectation $\langle \mathbf{b}^\dagger\mathbf{b}\rangle$ takes exactly the same value, and the same value, n_0 as it does at $w = 0$. This is because the Hamiltonian commutes with the total number operator $\mathbf{N} = \sum_i \mathbf{b}_i^\dagger\mathbf{b}_i$, and the state is uniform so $\langle\mathbf{N}\rangle = M\langle\mathbf{b}^\dagger\mathbf{b}\rangle$. The groundstate at $w = 0$ is an eigenstate of $\mathbf{N}$. Since there is an energy gap in the MI state, the (quantized) eigenvalue of $\mathbf{N}$ cannot change. This means in particular that $\partial_\mu\langle\mathbf{N}\rangle = 0$, the MI state is *incompressible*.

4. **Particle conservation and the f-sum rule.** [Bonus problem] Consider a collection of N particles (bosons or fermions) governed by a Hamiltonian of the

form

$$\mathbf{H} = \sum_i \frac{\mathbf{p}_i^2}{2m} + \sum_{i<j} V(r_{ij}).$$

Recall that the operator

$$\rho_q = \sum_i e^{-\mathbf{i}q\cdot\mathbf{r_i}}$$

is the Fourier transform of the particle density $\rho(r) = \sum_i \delta^d(r - \mathbf{r_i})$, where $\mathbf{r_i}$ is the position of the ith particle.

(a) Find

$$\partial_t \rho_q = -\mathbf{i}[\rho_q, \mathbf{H}]$$

and show that it can be written in the form

$$[\rho_q, \mathbf{H}] = \vec{q} \cdot \vec{\mathbf{J}}_q$$

where

$$\vec{\mathbf{J}}_q = \frac{1}{2} \sum_i \left(\frac{\vec{\mathbf{p}}_i}{m} e^{-\mathbf{i}q\cdot\mathbf{r_i}} + e^{-\mathbf{i}q\cdot\mathbf{r_i}} \frac{\vec{\mathbf{p}}_i}{m} \right). \tag{29}$$

Interpret this as a continuity equation.

The only ingredient we need is $[\mathbf{q}_i, \mathbf{p}_j] = \mathbf{i}\hbar\delta_{ij}$.

$$\partial_t \rho_q = -\mathbf{i}[\rho_q, \mathbf{H}] = -\mathbf{i} \sum_i \sum_j [e^{-\mathbf{i}q\cdot\mathbf{r_i}}, \frac{\mathbf{p}_j^2}{2m}] \tag{30}$$

$$= -\frac{\mathbf{i}}{2m} (-\mathbf{i}) (\mathbf{i}) \sum_i \vec{q} \cdot \left(\vec{\mathbf{p}}_i e^{-\mathbf{i}q\cdot\mathbf{r_i}} + e^{-\mathbf{i}q\cdot\mathbf{r_i}} \vec{\mathbf{p}}_i \right) \tag{31}$$

where we used $[A, B^2] = B[A, B] + [A, B]B$. This is (30) (times $-\mathbf{i}$). We have

$$\partial_t \rho_q + \mathbf{i}\vec{q} \cdot \vec{\mathbf{J}}_q$$

which, since $\rho_q = \int d^d r e^{\mathbf{i}q\cdot r} \rho(r)$ is the fourier transform of the density operator $\rho(r) = \sum_i \delta^d(r - \mathbf{r_i})$, is the fourier transform in space of the continuity equation

$$\partial_t \rho(r) + \vec{\nabla} \cdot \vec{\mathbf{J}}(r) = 0$$

where

$$\vec{J}(r) = \int đ^d q e^{-\mathbf{i}q\cdot r} \vec{\mathbf{J}}_q = \frac{1}{2} \sum_i \left(\frac{\vec{\mathbf{p}}_i}{m} \delta^d(r - \mathbf{r_i}) + \delta^{\mathbf{d}}(\mathbf{r} - \mathbf{r_i}) \frac{\tilde{\mathbf{p}}_\mathbf{i}}{\mathbf{m}} \right).$$

(b) For later use, compute $[\vec{\mathbf{J}}_q, \rho_q^\dagger]$.

$$[\vec{\mathbf{J}}_q, \rho_q^\dagger] = \frac{1}{2}\sum_{i,j}^{N}[\left(\frac{\vec{\mathbf{p}}_i}{m}e^{-\mathbf{i}q\cdot\mathbf{r_i}} + e^{-\mathbf{i}q\cdot\mathbf{r_i}}\frac{\vec{\mathbf{p}}_i}{m}\right), e^{+\mathbf{i}q\cdot\mathbf{r_j}}] \tag{32}$$

$$= \frac{1}{2}\left(-\mathbf{i}\vec{q}\right)\sum_{ij}\left(\frac{1}{m}e^{+\mathbf{i}q\cdot\mathbf{r_j}}e^{-\mathbf{i}q\cdot\mathbf{r_i}} + e^{-\mathbf{i}q\cdot\mathbf{r_i}}\frac{1}{m}e^{+\mathbf{i}q\cdot\mathbf{r_j}}\right) \tag{33}$$

$$= (-\mathbf{i})(+\mathbf{i})\frac{\vec{q}}{m}\sum_i = \frac{\vec{q}}{m}N. \tag{34}$$

(c) Consider the object

$$\langle\Phi_0|\,[[\rho_q, \mathbf{H}], \rho_q^\dagger]\,|\Phi_0\rangle$$

where Φ_0 is the groundstate. Compute this by inserting a resolution of the identity $\mathbb{1} = \sum_n |\Phi_n\rangle\langle\Phi_n|$ in terms of energy eigenstates $\mathbf{H}\,|\Phi_n\rangle = (E_0 + \omega_n)\,|\Phi_n\rangle$ and show that it is equal to

$$\langle\Phi_0|\,[[\rho_q, \mathbf{H}], \rho_q^\dagger]\,|\Phi_0\rangle = 2\int d\omega S(q,\omega)$$

where

$$S(q,\omega) = \sum_n \delta(\omega - \omega_n)|\,\langle\Phi_n|\,\rho_q\,|\Phi_0\rangle\,|^2 \tag{35}$$

is the dynamical structure factor.

For free we can replace $\mathbf{H}$ with $\mathbf{H} - E_0$, where E_0 is the groundstate energy, since $[\rho_q, E_0 = 0$. Then there are only two nonzero terms:

$$\langle\Phi_0|\,[[\rho_q, \mathbf{H}], \rho_q^\dagger]\,|\Phi_0\rangle = \langle\Phi_0|\,[[\rho_q, \mathbf{H} - E_0], \rho_q^\dagger]\,|\Phi_0\rangle \tag{36}$$

$$= \langle\Phi_0|\left(\rho_q(\mathbf{H} - E_0)\rho_q^\dagger + \rho_q^\dagger(\mathbf{H} - E_0)\rho_q\right)|\Phi_0\rangle \tag{37}$$

$$= \sum_n \langle\Phi_0|\,\rho_q\,|n\rangle\,\langle n|\,\rho_q^\dagger\,|\Phi_0\rangle\,\omega_n + \langle\Phi_0|\,\rho_q^\dagger\,|n\rangle\,\langle n|\,\rho_q\,|\Phi_0\rangle\,\omega_n$$

$$= \sum_n \omega_n\left(|\,\langle n|\,\rho_q^\dagger\,|\Phi_0\rangle\,|^2 + |\,\langle n|\,\rho_q\,|\Phi_0\rangle\,|^2\right) \tag{38}$$

Now a slightly tricky step: because of time-reversal invariance, there is a degeneracy between states with momentum $\vec{q}$ and $-\vec{q}$. Therefore for each $\vec{q}$ we can find a state $|n'\rangle$ with the same $\omega_n = E_n - E_0$ so that $|\,\langle n|\,\rho_q^\dagger\,|\Phi_0\rangle\,|^2 = |\,\langle n'|\,\rho_q\,|\Phi_0\rangle\,|^2$. Therefore this is

$$\langle\Phi_0|\,[[\rho_q, \mathbf{H}], \rho_q^\dagger]\,|\Phi_0\rangle = 2\sum_n \omega_n|\,\langle n|\,\rho_q\,|\Phi_0\rangle\,|^2$$

which is manifestly what we get if we integrate (36) over ω.

(d) Conclude (by combining the previous parts) that the f-sum rule

$$\int d\omega S(q,\omega) = \frac{N\hbar^2 q^2}{2m}.$$

is true.

On the one hand, we have from the first two parts of the problem

$$[[\rho_q, \mathbf{H}], \rho_q^\dagger] = \vec{q} \cdot [\vec{\mathbf{J}}_q, \mathbf{H}] = \frac{q^2}{m} N.$$

On the other hand, if we take its matrix element in the groundstate, we get by the previous part

$$\langle \Phi_0 | \, [[\rho_q, \mathbf{H}], \rho_q^\dagger] \, | \Phi_0 \rangle = 2 \int d\omega S(q,\omega).$$

Therefore

$$\int d\omega S(q,\omega) = \frac{N q^2}{2m}.$$

Restoring factors of $\hbar$ by dimensional analysis gives the state f-sum rule.