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

Physics 212C QM Spring 2020
Assignment 8

Due 12:30pm Wednesday, May 27, 2020

Please refer to the first homework for submission format and procedures (and replace hw01 by hw08 in the relevant places, of course).

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1. **Brain-warmer.** Consider two single-particle orbitals with wavefunctions $\psi_\alpha(r), \psi_\beta(r)$. Find the position-space wavefunctions

$$\Psi(r_1\sigma, r_2\sigma') \equiv \langle r_1\sigma, r_2\sigma'|\Psi\rangle = \langle 0| \mathbf{a}_{r_2\sigma'}\mathbf{a}_{r_1\sigma}|\Psi\rangle$$

for the four states of two spinful fermions:

$$|S\rangle = \frac{1}{\sqrt{2}}\mathbf{a}^\dagger_{\alpha\sigma}\mathbf{a}^\dagger_{\beta\sigma'}\varepsilon_{\sigma\sigma'}|0\rangle = \frac{1}{\sqrt{2}}\left(\mathbf{a}^\dagger_{\alpha\uparrow}\mathbf{a}^\dagger_{\beta\downarrow} - \mathbf{a}^\dagger_{\alpha\downarrow}\mathbf{a}^\dagger_{\beta\uparrow}\right)|0\rangle$$

$$|A,1\rangle = \mathbf{a}^\dagger_{\alpha\uparrow}\mathbf{a}^\dagger_{\beta\uparrow}|0\rangle\,, \quad |A,0\rangle = \frac{1}{\sqrt{2}}\left(\mathbf{a}^\dagger_{\alpha\uparrow}\mathbf{a}^\dagger_{\beta\downarrow} + \mathbf{a}^\dagger_{\alpha\downarrow}\mathbf{a}^\dagger_{\beta\uparrow}\right)|0\rangle\,, \quad |A,-1\rangle = \mathbf{a}^\dagger_{\alpha\downarrow}\mathbf{a}^\dagger_{\beta\downarrow}|0\rangle\,.$$

Check that the singlet (triplet) indeed has a symmetric (antisymmetric) orbital wavefunction. Check that the labels on the A states correctly label the eigenvalues of the total spin along z, $S^z \equiv \sum_r \frac{1}{2}\mathbf{a}^\dagger_r\sigma^z\mathbf{a}_r$.

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.

   (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 $\mathbf{M}$?

   (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?

(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.

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

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

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 **a** and **b**. We could do this in two different ways: a state of definite relative number:

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

or a state of definite relative phase:

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

Notice that the latter is a simple BEC in a particular linear combination of the two orbitals. 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 $U_0 > 0$?

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

Consider again the Bose-Hubbard model[1]

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

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

[1] My apologies for belatedly redefining $U \to \frac{U}{2}$. The answers look nicer (and (8) is actually correct) with this convention.

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 which 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 ground-state 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

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

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?

(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

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

where

$$\chi_0(n_0) \equiv \frac{n_0 + 1}{Un_0 - \mu} + \frac{n_0}{\mu - U(n_0 - 1)}, \tag{2}$$

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

(d) Draw the Mott lobes using this formula.

4. **Antiferromagnet from fermions.** 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.) 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).

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

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.

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

(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.