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

Physics 212C QM Spring 2020
Assignment 10 ("Final Exam")

Due 12:30pm Friday, June 12, 2020

Please refer to the first homework for submission format and procedures (and replace hw01 by hw10 in the relevant places, of course).

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1. **Brain-warmer: the size of a Cooper pair.** In the Cooper problem, estimate the mean square size of a Cooper pair in terms of the Fermi velocity $v_F \equiv |\vec{\nabla}_k \epsilon_k||_{k_F}$ and the binding energy Δ.

   Hints: (1) Don't forget to normalize the wavefunction. (2) Show that $\int d^d r r^2 |\psi(r)|^2 = \int đ^d k |\vec{\nabla}\psi(k)|^2$. (3) Assume the Fermi surface is round, that v_F and the density of states vary slowly near the Fermi energy, and that $\epsilon_a \gg \epsilon_F$.

2. **Non-BCS superconductivity.** In this problem we describe a series of uncontrolled approximations which display d-wave superconductivity in a model with repulsive interactions; it is something like a model of a cuprate superconductor.

   Recall that starting from the Hubbard model on the square lattice at half-filling with strong repulsive interactions $U \gg t$, we derived an effective antiferromagnetic spin-spin interaction, by the superexchange mechanism. Now consider introducing into this system a small finite density of *holes*. That is, we decrease the filling fraction from half-filling. This will require some of the sites to be unoccupied. It does not, however, require any of the sites to be doubly occupied. An effective description incorporating this information is called the tJ-model:

$$\mathbf{H}_{tJ} = -t \sum_{\langle ij \rangle} \left(\mathbf{c}^\dagger_{i\sigma} \mathbf{c}_{j\sigma} + \mathbf{c}^\dagger_{j\sigma} \mathbf{c}_{i\sigma} \right) + J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$$

   where $\vec{S}_i = \frac{1}{2} \mathbf{c}^\dagger_{i\sigma} \vec{\sigma} \mathbf{c}_{i\sigma}$ and $J = 4t^2/U$. The first term describes the hopping of the holes, and the second term describes an interaction between the spins.

   (a) Using the identity $\sum_a \sigma^a_{\alpha\beta}\sigma^a_{\gamma\delta} = -2\epsilon_{\alpha\gamma}\epsilon_{\beta\delta} + \delta_{\alpha\beta}\delta_{\gamma\delta}$, show that the interaction can be rewritten as

$$\vec{S}_1 \cdot \vec{S}_2 = a \left(\epsilon_{\alpha\gamma} \mathbf{c}^\dagger_{1\alpha} \mathbf{c}^\dagger_{2\gamma} \right) \left(\epsilon_{\beta\delta} \mathbf{c}_{1\beta} \mathbf{c}_{2\delta} \right) + b \mathbf{c}^\dagger_{1\alpha} \mathbf{c}_{1\alpha} \mathbf{c}^\dagger_{2\beta} \mathbf{c}_{2\beta}. \quad (1)$$

   Find a, b.

The first term in (1) is written in a way that suggests a BCS factorization. The second term we will simply ignore without justification[1]. So we will consider the model

$$\mathbf{H}_{tJ-BCS} \equiv -t\sum_{\langle ij\rangle}\left(\mathbf{c}^\dagger_{i\sigma}\mathbf{c}_{j\sigma} + \mathbf{c}^\dagger_{j\sigma}\mathbf{c}_{i\sigma}\right) + aJ\sum_{\langle ij\rangle}\left(\epsilon_{\alpha\gamma}\mathbf{c}^\dagger_{1\alpha}\mathbf{c}^\dagger_{2\gamma}\right)\left(\epsilon_{\beta\delta}\mathbf{c}_{1\beta}\mathbf{c}_{2\delta}\right).$$

(b) To develop a mean field theory for this model, we will study

$$\mathbf{H}_{\rm MF} = -t\sum_{\langle ij\rangle}\left(\mathbf{c}^\dagger_{i\sigma}\mathbf{c}_{j\sigma} + \mathbf{c}^\dagger_{j\sigma}\mathbf{c}_{i\sigma}\right) + aJ\sum_{\langle ij\rangle}\left(\Delta^\star_{ij}\epsilon_{\alpha\beta}\mathbf{c}_{i\alpha}\mathbf{c}_{j\beta} + \Delta_{ij}\epsilon_{\alpha\beta}\mathbf{c}^\dagger_{i\beta}\mathbf{c}^\dagger_{j\alpha} - |\Delta_{ij}|^2\right)$$

where $\Delta_{ij} = -\left\langle \epsilon_{\alpha\beta}\mathbf{c}_{i\alpha}\mathbf{c}_{j\beta}\right\rangle$. Convince yourself that the groundstate $|\text{MF}\rangle$ of this hamiltonian provides a useful trial wavefunction for $\mathbf{H}_{tJ-BCS}$.

(c) Check that $\Delta_{ij} = \Delta_{ji}$.

(d) Assume a translation-invariant solution: $\Delta_{ij} = \Delta_{i-j} = \Delta_{j-i}$. This reduces the number of parameters to two: Δ_x, Δ_y associated with x-links and y-links. Write $\mathbf{H}_{\rm MF}$ in terms of Fourier modes and $\Delta_k = \Delta_x \cos k_x + \Delta_y \cos k_y$.

(e) Construct the groundstate $|\text{MF}\rangle$ of $\mathbf{H}_{\rm MF}$ by a Bogoliubov transformation.

(f) Compute $\langle \mathbf{c}_{-k\downarrow}\mathbf{c}_{-k\uparrow}\rangle \equiv \langle \text{MF}|\,\mathbf{c}_{-k\downarrow}\mathbf{c}_{-k\uparrow}\,|\text{MF}\rangle$.

(g) Show that the self-consistency condition

$$\Delta_\delta = \sum_k \langle \mathbf{c}_{-k\downarrow}\mathbf{c}_{-k\uparrow}\rangle \cos k_\delta \qquad (2)$$

($\delta = x, y$) is the same as the condition obtained by minimizing the groundstate energy with respect to $\Delta_{x,y}$.

(h) [Bonus problem] The self-consistency condition (2) involves some unfriendly integrals. By doing these integrals numerically, find a solution with $\Delta_x = -\Delta_y$ at small hole-doping. This is a d-wave superconductor.

3. **No anti-damping in equilibrium.** Consider a system governed by a hamiltonian $\mathbf{H}_0$ in its groundstate. Poke the system by a small perturbation of definite frequency and wavenumber via a (time-independent) operator $\mathcal{O}_B$,

$$\mathbf{H} = \mathbf{H}_0 + V, \quad V = \int d^dx\varphi(x,t)\mathcal{O}_B(x) = \int d^dx e^{\mathbf{i}q\cdot x - \mathbf{i}\omega t}\varphi(q,\omega)\mathcal{O}_B(q).$$

[1] A further warning which is irrelevant for actually doing this problem: if we actually project out the doubly-occupied states, the $\mathbf{c}$s are no longer canonical fermion operators. We will nevertheless treat them as such below.

(a) Show that the rate of work done on the system is

$$\frac{dW}{dt} = \frac{d}{dt}\mathrm{tr}\rho(t)\mathbf{H} = \mathrm{tr}\rho(t)\partial_t V.$$

(b) Show that this is

$$\frac{dW}{dt} = \int d^d x \partial_t \varphi(x,t) \langle \mathcal{O}_B \rangle .$$

Using our result for linear response, relate this to the retarded Green's function $G^R_{\mathcal{O}_B\mathcal{O}_B}$.

(c) Now consider the time-averaged work done per unit volume

$$\overline{\frac{dw}{dt}} \equiv \frac{1}{V}\overline{\frac{dW}{dt}}$$

where $\overline{X} \equiv \frac{\omega}{2\pi}\int_0^{2\pi/\omega} dt X(t)$. Using the fact that $G^R(q,\omega)^\star = G^R(-q,-\omega)$, show that

$$\overline{\frac{dw}{dt}} = 2\omega|\varphi(q,\omega)|^2 \mathrm{Im}\, G^R_{\mathcal{O}_B\mathcal{O}_B}(q,\omega).$$

(d) Using the relation to the spectrum of the theory, conclude that the average work done on the system is positive.

4. **One-dimensional atoms.**

(a) **Brain-warmer.** Consider an electron in a one-dimensional 'atom' where the Coulomb potential has been replaced by a delta function:

$$\mathbf{H} = \frac{p^2}{2} - Z\delta(x) \equiv T + V.$$

Find the groundstate energy E_0 and verify the virial theorem:

$$E_0 = -\langle T \rangle = +\frac{1}{2}\langle V \rangle \tag{3}$$

(b) Prove the virial theorem (3) for this example as follows: Argue that in any energy eigenstate $\langle [\mathbf{H}, xp] \rangle = 0$. Then evaluate $[\mathbf{H}, xp]$ in terms of T and V.

For the rest of the problem, we consider the analog of the helium atom, with

$$\mathbf{H} = +\frac{1}{2}\mathbf{p}_1^2 + \frac{1}{2}\mathbf{p}_2^2 - Z\delta(x_1) - Z\delta(x_2) + \delta(x_1 - x_2).$$

The idea is that the two terms proportional to Z are like the potential from the nucleus, while the last term is the inter-electron interaction.

(c) First, ignore the last term and find the groundstate for spinful electrons. Next, treat the last term as a perturbation and find the ground-state energy to first order.

(d) Now use the variational method to improve the estimate of the previous part. Use a trial wavefunction which allows for 'screening,' *i.e.* that the full value of Z may not be seen by the electrons. Find the minimal value of $\langle \mathbf{H} \rangle$.

(e) Here is the fun part of this problem. Consider the Hartree self-consistent field ansatz

$$\Psi(x_1, x_2) = \phi(x_1)\phi(x_2)$$

(times an appropriate spin wavefunction). Explain what is the spin wavefunction and why we do not need Hartree-Fock here. Show that

$$-\frac{1}{2}\partial_x^2 \phi - Z\delta(x)\phi(x) + \phi^3 = \epsilon\phi \tag{4}$$

with $\langle \mathbf{H} \rangle = 2\epsilon - \langle \delta(x_1 - x_2) \rangle$. Find the normalized *analytic* solution to (4) and show that

$$\langle \mathbf{H} \rangle_{\text{Hartree}} = -\left(Z - \frac{1}{4}\right)^2 - \frac{1}{48}.$$

Compare to the results from the previous parts.

5. **Self-consistent field for Helium.** Implement the Hartree-Fock method for the groundstate of Helium.

(a) Convince yourself that Hartree and Hartree-Fock are the same in this case. Explain.

(b) Show that the Hartree equations can be written as

$$-\frac{1}{2}\vec{\nabla}^2\phi + \left(-\frac{Z}{r} + U(r)\right)\phi(r) = \epsilon\phi(r) \tag{5}$$

with

$$U(r) = \int d^3r' \frac{|\phi(r')|^2}{|r - r'|}. \tag{6}$$

Note that the self-consistent potential (6) is automatically spherically symmetric, so the Central-Force Approximation is exact here.

(c) Show that the groundstate energy in this approximation can be written as

$$E_0 = 2\epsilon + 4\pi \int_0^\infty r^2 |\phi(r)|^2 U(r),$$

where $U(r)$ is the self-consistent potential in (6), and ϵ is the eigenvalue in (5).

(d) Find the form of $U(r)$ in (6) for the variational ansatz using hydrogen orbitals. This is a good starting point for an iterative solution of these equations.

Hint: to do the integrals, use

$$\frac{1}{|r_{12}|} = \frac{1}{r_>} \sum_{\ell=0}^{\infty} P_\ell(\cos\theta) \left(\frac{r_<}{r_>}\right)^\ell$$

(where θ is the angle between $\vec{r}_1$ and $\vec{r}_2$, and $r_> = \max(|r_1|, |r_2|)$) and the orthonormality of the Legendre polynomials.

(e) **The fun part.** [Bonus problem] Actually implement the solution of the self-consistent equations (5), (6) numerically. The expected value of the groundstate energy is $E_0 = -2.86168$. What do you find?