Problem set 9

April 22, 2013

to submit before the 10$^{\text{th}}$ of May

1 $T = 0$: BCS ground state

Let us consider a balanced (same density) mixture of N fermionic atoms (we can equivalently think of electrons in a metal), $N/2$ with spin $\sigma =\uparrow$ and $N/2$ with spin $\sigma =\downarrow$, described by the creation (annihilation) single particle operators in momentum (or wavevector $\mathbf{k} = \mathbf{p}/\hbar$) space $\hat{c}^\dagger_{\mathbf{k}\sigma}$ ($\hat{c}_{\mathbf{k}\sigma}$):

$$\{\hat{c}^\dagger_{\mathbf{k}\sigma}, \hat{c}_{\mathbf{k}'\sigma'}\} = \delta_{\sigma,\sigma'}\delta_{\mathbf{k},\mathbf{k}'} \qquad \{\hat{c}^\dagger_{\mathbf{k}\sigma}, \hat{c}^\dagger_{\mathbf{k}'\sigma'}\} = 0 = \{\hat{c}_{\mathbf{k}\sigma}, \hat{c}_{\mathbf{k}'\sigma'}\} \ . \tag{1}$$

Let us consider the pair operator

$$\hat{b}^\dagger_{\mathbf{k}} = \hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}^\dagger_{-\mathbf{k}\downarrow} \qquad \hat{b}_{\mathbf{k}} = \hat{c}_{-\mathbf{k}\downarrow}\hat{c}_{\mathbf{k}\uparrow} \ . \tag{2}$$

1. Evaluate the commutators $[\hat{b}_{\mathbf{k}}, \hat{b}_{\mathbf{k}'}]$, $[\hat{b}^\dagger_{\mathbf{k}}, \hat{b}^\dagger_{\mathbf{k}'}]$, and $[\hat{b}_{\mathbf{k}}, \hat{b}^\dagger_{\mathbf{k}'}]$ and comment if the operator $\hat{b}_{\mathbf{k}}$ has bosonic statistics or not. Establish if a limit does exist in which you can describe it as a bosonic operator — N.B. pairs $\hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}^\dagger_{-\mathbf{k}\downarrow}$ form a tightly bound molecule when average occupation numbers $n_{\mathbf{k}\sigma}$ are overall small and spread in momentum.

Let us now consider the following two ground states describing a superposition of $N/2$ pairs. The first is a Fock state, a state with a definite number of particles, N:

$$|\Psi_N\rangle = \sum_{\mathbf{k}_1} \cdots \sum_{\mathbf{k}_{N/2}} \prod_{i=1}^{N/2} \varphi_{\mathbf{k}_i} \hat{b}^\dagger_{\mathbf{k}_i} |0\rangle \ , \tag{3}$$

2. Describe which form the wavefunction $\varphi_{\mathbf{k}_i}$ needs to have in order that the Fock state $|\Psi_N\rangle$ describes a (non-interacting) Fermi sea at $T = 0$ filled up to the Fermi energy $\varepsilon_F = \hbar^2 k_F^2/2m$.

The second state, is the BCS ground state, i.e., a coherent superposition of pairs all with the same phase:

$$|\Psi_\phi\rangle = \prod_{\mathbf{k}} \left(u_{\mathbf{k}} + e^{i\phi} v_{\mathbf{k}} \hat{b}^\dagger_{\mathbf{k}}\right) |0\rangle = \prod_{\mathbf{k}} \left(\cos\theta_{\mathbf{k}} + e^{i\phi} \sin\theta_{\mathbf{k}} \hat{b}^\dagger_{\mathbf{k}}\right) |0\rangle \ . \tag{4}$$

3. Show that $|\Psi_\phi\rangle$ is a normalized (i.e., $\langle\Psi_\phi|\Psi_\phi\rangle = 1$) coherent state of pairs condensed in the zero center of mass momentum. Evaluate the average

number of particles in the BCS ground state $\bar{N} = \langle\Psi_\phi|\hat{N}|\Psi_\phi\rangle$ and the variance $\sigma = \sqrt{\langle\Psi_\phi|\hat{N}^2|\Psi_\phi\rangle - \langle\Psi_\phi|\hat{N}|\Psi_\phi\rangle^2}$, and show that $\sigma/\bar{N} \to 0$ in the thermodynamic. Finally, show that the Fock state can be written as the following linear superposition of the BCS coherent state:

$$|\Psi_N\rangle = (\text{norm}) \int_0^{2\pi} \frac{d\phi}{2\pi} |e^{-i\phi N/2}\Psi_\phi\rangle \; . \tag{5}$$

2 Variational calculation

Consider the following Hamiltonian describing the interacting Fermi gas (in this simplified description, interactions are included only between fermions with opposite spins):

$$\hat{H} - \mu\hat{N} = \sum_{\mathbf{k}\sigma} \xi_{\mathbf{k}} \hat{c}^\dagger_{\mathbf{k}\sigma}\hat{c}_{\mathbf{k}\sigma} + \frac{1}{V}\sum_{\mathbf{k}_1\mathbf{k}_2\mathbf{q}} U_{\mathbf{k}_1-\mathbf{k}_2} \hat{c}^\dagger_{\mathbf{k}_1+\frac{\mathbf{q}}{2}\uparrow}\hat{c}^\dagger_{-\mathbf{k}_1+\frac{\mathbf{q}}{2}\downarrow}\hat{c}_{-\mathbf{k}_2+\frac{\mathbf{q}}{2}\downarrow}\hat{c}_{\mathbf{k}_2+\frac{\mathbf{q}}{2}\uparrow} \; , \tag{6}$$

where $\xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu$.

4. Evaluate the Hamiltonian expectation value $\langle\Psi_\phi|\hat{H}-\mu\hat{N}|\Psi_\phi\rangle$ (without loss of generality you can assume the phase to be zero, $\phi = 0$) and show that the functions $u_{\mathbf{k}} = \cos\theta_{\mathbf{k}}$ and $v_{\mathbf{k}} = \sin\theta_{\mathbf{k}}$ that minimise this expectation value have to satisfy the following equation:

$$0 = 2\xi_{\mathbf{k}}\tan 2\theta_{\mathbf{k}} - 2\Delta_{\mathbf{k}} \tag{7}$$

$$\Delta_{\mathbf{k}} = -\frac{1}{2V}\sum_{\mathbf{k}'} U_{\mathbf{k}-\mathbf{k}'}\sin 2\theta_{\mathbf{k}'} = -\frac{1}{V}\sum_{\mathbf{k}'} U_{\mathbf{k}-\mathbf{k}'}\langle\Psi_\phi|\hat{c}_{-\mathbf{k}'\downarrow}\hat{c}_{\mathbf{k}'\uparrow}|\Psi_\phi\rangle \; . \tag{8}$$

   Show that for a model interaction

$$U_{\mathbf{k}-\mathbf{k}'} = \begin{cases} -|U_0| & |\xi_{\mathbf{k}}|, |\xi_{\mathbf{k}'}| < \hbar\omega_D \\ 0 & \text{otherwise} \end{cases} \tag{9}$$

   the gap equation can be solved, giving $\Delta = \hbar\omega_D/\sinh(1/N(\varepsilon_F)|U_0|)$. What do the coefficients $u^2_{\mathbf{k}}$, $v^2_{\mathbf{k}}$, and $u_{\mathbf{k}}v_{\mathbf{k}}$ represent physically? Plot them as a function of the wavevector $\mathbf{k}$ in the weak-coupling limit $\Delta \ll \hbar\omega_D \ll \varepsilon_F$.

5. Evaluate the ground state energy of the superconducting state with respect to the energy of the normal state.

6. Show that the very same results obtained above can also be obtained by diagonalising the mean-field Bogoliubov Hamiltonian,

$$\hat{H} = \sum_{\mathbf{k}} \begin{pmatrix} \hat{c}^\dagger_{\mathbf{k}\uparrow} & \hat{c}_{-\mathbf{k}\downarrow} \end{pmatrix} \begin{pmatrix} \xi_{\mathbf{k}} & -\Delta_{\mathbf{k}} \\ -\Delta^*_{\mathbf{k}} & -\xi_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} \hat{c}_{\mathbf{k}\uparrow} \\ \hat{c}^\dagger_{-\mathbf{k}\downarrow} \end{pmatrix} + \sum_{\mathbf{k}} \left(\xi_{\mathbf{k}} + \Delta^*_{\mathbf{k}}\langle\hat{b}_{\mathbf{k}}\rangle\right) \; , \tag{10}$$

   by means of the following canonical transformation

$$\begin{pmatrix} \hat{\gamma}_{\mathbf{k}1} \\ \hat{\gamma}^\dagger_{-\mathbf{k}2} \end{pmatrix} = \begin{pmatrix} \cos\theta_{\mathbf{k}} & \sin\theta_{\mathbf{k}} \\ \sin\theta_{\mathbf{k}} & -\cos\theta_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} \hat{c}_{\mathbf{k}\uparrow} \\ \hat{c}^\dagger_{-\mathbf{k}\downarrow} \end{pmatrix} \; . \tag{11}$$

Evaluate the gap equation at finite temperature and evaluate numerically the finite temperature gap $\Delta(T)/\Delta(0)$ as a function of the temperature T/T_c (where $\Delta(T_c) \to 0$). **Optional**: Show that the following asymptotic limits are verified:

$$\Delta(T) \simeq \begin{cases} \Delta(0) - (2\pi\Delta(0)k_B T)^{1/2} e^{-\beta\Delta(0)} & T \ll T_c \\ 1.74\Delta(0)\left(1 - \dfrac{T}{T_c}\right)^{1/2} & T \to T_c^- \, . \end{cases} \tag{12}$$

3 Gap and number equations in the BEC-BCS crossover

We will see in the last two classes that, for a gas of fermionic atoms with a simplified contact interaction potential

$$U_{\mathbf{k}} = U_0 \qquad\qquad \frac{m}{4\pi\hbar^2 a} = \frac{1}{U_0} + \frac{1}{V}\sum_{\mathbf{k}} \frac{1}{2\epsilon_{\mathbf{k}}} \, , \tag{13}$$

gap and number equations can be respectively written in the following form (in terms of dimensionless parameters):

$$\frac{1}{k_F a} = \frac{2}{\pi}\sqrt{\frac{|\mu|}{\varepsilon_F}} \int_0^\infty dy\sqrt{y}\left[\frac{1}{2y} - \frac{1}{2\sqrt{(y\mp 1)^2 + (\frac{\Delta}{\mu})^2}}\right] \tag{14}$$

$$\frac{4}{3} = \left(\frac{|\mu|}{\varepsilon_F}\right)^{3/2} \int_0^\infty dy\sqrt{y}\left[1 - \frac{y \mp 1}{\sqrt{(y\mp 1)^2 + (\frac{\Delta}{\mu})^2}}\right] \, , \tag{15}$$

where $\varepsilon_F = (\hbar k_F)^2/2m$ is the Fermi energy, a the scattering length and the sign $\mp$ refers to respectively the case of positive $\mu > 0$ (BCS side) and negative $\mu < 0$ (BEC side) chemical potential.

7. Solve gap (14) and number (15) equations in the BEC limit ($\frac{1}{k_F a} \gg 1$), using the following approximations $\varepsilon_F \ll \Delta \ll |\mu|$. Find $\frac{\mu}{\varepsilon_F}$ and $\frac{\Delta}{\varepsilon_F}$ as functions of $\frac{1}{k_F a}$ and check *a posteriori* that the $\varepsilon_F \ll \Delta \ll |\mu|$ is satisfied when $\frac{1}{k_F a} \gg 1$.

8. Solve the number equation (15) in the BCS limit ($a < 0$ and $\frac{1}{k_F |a|} \gg 1$) and find an approximate expression of the chemical potential μ.

9. **Optional**: Solve numerically the two coupled equations (14) and (15) across the BEC-BCS crossover and plot both μ/ε_F and Δ/ε_F as a function of $1/k_F a$.