Energy minimization in the BCS state and excitation spectrum (I)

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25th October 2012

Consider a gas of indistinguishable fermionic particles. Each particle of mass m has two possible orthogonal spin states, $|\uparrow\rangle$ and $|\downarrow\rangle$, and the number of "spin-up" particles equals the number of "spin-down" particles. The particles of opposite spins interact through an attractive potential while there is no interaction between particles of the same spin state.

1 Model Hamiltonian

Consider a one-dimensional ($1d$) case where the fermionic mixture is confined in a box of size L with periodic boundary conditions.

a) The zero range potential between particle 1 and particle 2 does not change the spin state and we can model it as follows:

$$V(|x_1 - x_2|) = g\delta(x_1 - x_2), \tag{1}$$

where g is the so-called coupling constant, δ is the Dirac's distribution, and the position of particle 1 and particle 2 is respectively given by x_1 and x_2. Write explicitly the Hamiltonian in second quantization as a function of the field operators $\hat{\psi}_\sigma(x)$, $\hat{\psi}^\dagger_\sigma(x)$ with $\sigma = \uparrow, \downarrow$.

b) Show that the kinetic energy operator of the gas in the k-space may be written as follows:

$$\hat{T} = \sum_k \sum_{\sigma=\uparrow,\downarrow} \epsilon_k \hat{a}^\dagger_{k,\sigma} \hat{a}_{k,\sigma}, \tag{2}$$

where $\hat{a}^\dagger_{k,\sigma}$ is the creation operator of a fermion with spin component σ in a plane wave with wavevector k, and

$$\epsilon_k = \frac{\hbar^2 k^2}{2m}, \tag{3}$$

with m being the mass of a particle.

c) In the grand canonical ensemble show that one can replace ϵ_k with

$$\xi_k = \epsilon_k - \mu, \tag{4}$$

in $\hat{T}$, where μ is the chemical potential.

2 Minimization of the energy

To this end, we have to calculate the expectation value of the Hamiltonian in the coherent state of pairs:

$$|\psi_{BCS}\rangle = \mathcal{N}\,\Pi_k(1+\Gamma_k a^\dagger_{k\uparrow}a^\dagger_{-k\downarrow})|0\rangle\,. \tag{5}$$

a) Calculate the expectation value of the kinetic energy operator, including the chemical potential contribution, as a function of the parameters ξ_k and Γ_k.

b) What is the physical meaning of the quantity

$$\rho_\uparrow \equiv \langle\hat{\psi}^\dagger_\uparrow(x)\hat{\psi}_\uparrow(x)\rangle\ ? \tag{6}$$

Using a result of the previous lecture, calculate the value of $\rho_\uparrow$ as a function of the coefficients Γ_k.

c) Calculate the following quantity

$$\Delta \equiv g\langle\hat{\psi}_\uparrow(x)\hat{\psi}_\downarrow(x)\rangle, \tag{7}$$

as a function of the parameters Γ_k. Does this quantity depend on the position x ?

d) Calculate $\langle\hat{\psi}^\dagger_\uparrow(x)\hat{\psi}_\downarrow(x)\rangle$.

e) Show that the expectation value of the interaction Hamiltonian is:

$$\langle\hat{V}\rangle = \frac{g}{L}\left[\left(\sum_k \frac{\Gamma_k}{1+\Gamma_k^2}\right)^2 + \left(\sum_k \frac{\Gamma_k^2}{1+\Gamma_k^2}\right)^2\right]. \tag{8}$$

f) We shall consider for a moment the non-interacting case, $g=0$. What is the choice of the parameters Γ_k minimizing the expectation value of the complete Hamiltonian ? What is then the state $|\psi_{BCS}\rangle$? Does it coincide with the exact ground state of the gas ?

g) We now turn back to the interacting case and we shall consider an attractive interaction, such that $g<0$. Express the fact that the first derivative of the expectation value of $\hat{H}$ with respect to each Γ_k is zero. We should find the following second degree equation, which we will not try to solve:

$$\Gamma_k^2 + 2\frac{\tilde{\xi}_k}{\Delta}\Gamma_k - 1 = 0, \tag{9}$$

where we have set

$$\tilde{\xi}_k = \epsilon_k - \tilde{\mu} \quad \text{et} \quad \tilde{\mu} = \mu - g\rho_\uparrow. \tag{10}$$

Give a physical interpretation of the shift in the chemical potential μ.