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Problem 13.1: The BCS ground state · · · · · · · · · · · · [Oral | 4 pt(s)]

ID: ex_bcs_ground_state:fqt2425

> **Learning objective**
>
> The BCS theory describes conventional superconductors. Here you study the BCS ground state wave-function as an example for a *quasiparticle vacuum*, i.e., the ground state of a non-interacting fermionic theory. This problem also serves as an exercise for calculations in the formalism of second quantization.

We consider the famous BCS state (named after J. Bardeen, L. N. Cooper, J. R. Schrieffer)

$$|\Omega\rangle = \prod_{\boldsymbol{k}} \left(u_{\boldsymbol{k}} + v_{\boldsymbol{k}}\, c_{\boldsymbol{k},\uparrow}^{\dagger} c_{-\boldsymbol{k},\downarrow}^{\dagger} \right) |0\rangle \,, \tag{1}$$

where $u_{\boldsymbol{k}}, v_{\boldsymbol{k}} \in \mathbb{C}$ with $|u_{\boldsymbol{k}}|^2 + |v_{\boldsymbol{k}}|^2 = 1$ and the fermionic operator $c_{\boldsymbol{k},\sigma}^{\dagger}$ creates a fermion with momentum $\boldsymbol{k}$ and spin $\sigma \in \{\uparrow,\downarrow\}$. The product runs over the Brillouin zone of the lattice (which we do not specify here).

a) Show that the BCS state $|\Omega\rangle$ is normalized.   **1**pt(s)

b) Calculate $\langle\Omega|\, c_{\mathbf{q},\uparrow}^{\dagger} c_{-\mathbf{q},\downarrow}^{\dagger} \,|\Omega\rangle$ and $\langle\Omega|\, c_{\mathbf{q},\sigma}^{\dagger} c_{\mathbf{q},\sigma} \,|\Omega\rangle$ for a given wave vector $\boldsymbol{q}$.   **1**pt(s)

c) Introduce the new *quasiparticle* operators $\alpha_{\mathbf{k},\sigma}$ via   **1**pt(s)

$$\alpha_{\mathbf{k},\uparrow} = u_{\mathbf{k}} c_{\mathbf{k},\uparrow} - v_{\mathbf{k}} c_{-\mathbf{k},\downarrow}^{\dagger}, \qquad \alpha_{-\mathbf{k},\downarrow} = v_{\mathbf{k}} c_{\mathbf{k},\uparrow}^{\dagger} + u_{\mathbf{k}} c_{-\mathbf{k},\downarrow}, \tag{2}$$

    Prove that the new operators obey the fermionic anticommutation relations. Show that $\alpha_{\mathbf{k},\sigma}\,|\Omega\rangle = 0$ for all $\mathbf{k}$ and σ and write down a Hamiltonian for which $|\Omega\rangle$ is the ground state (the *quasiparticle vacuum*).

d) What choice of $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ makes $|\Omega\rangle$ the ground state of free fermions (with eigenmodes $c_{\mathbf{k},\sigma}$) ?   **1**pt(s) In this case, what does $\alpha_{\mathbf{k},\sigma}^{\dagger}$ describe for $|\boldsymbol{k}| \lesssim k_F$ where k_F denotes the Fermi wave vector?

Problem 13.2: Gross-Pitaevskii Equation · · · · · · · · [Written | 3 pt(s)]

ID: ex_gross_pitaevskii_equation:fqt2425

> **Learning objective**
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> We consider a system of identical bosons and determine its the ground state. As we will see, the effect of weak interactions between the particles can be studied approximately by means of a variational principle leading to the so-called Gross-Pitaevskii equation.

Consider N non-interacting bosons of mass m in a one-dimensional harmonic trap $U_{\text{trap}}(x) = \frac{1}{2} m \omega^2 x^2$.

a) Write down the ground state wave function for N bosons. What is the generalization to an   1pt(s)
arbitrary potential $U(x)$ with the single-particle ground state wave function $\phi_0(x)$?

b) Now introduce a contact interaction of the form $V(x_i - x_j) = V_0\delta(x_i - x_j)$ between the particles.   1pt(s)
The Hamiltonian of this system is given by

$$H = \sum_{i=1}^{N} \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_i^2} + U(x_i) \right) + V_0 \sum_{i<j} \delta(x_i - x_j) . \tag{3}$$

Write down the expectation value of this Hamiltonian with respect to the ground state wave
function of the non-interacting system for an *arbitrary* external potential $U(x)$ as calculated
in a).

c) We treat the system by a variational principle where we approximate the ground state by a   1pt(s)
product wave function that minimizes the energy expectation value of H (this ansatz is known as
Hartree-Fock approximation; the result of this minimization procedure is an exact eigenstate *only*
for $V_0 = 0$, i.e., non-interacting bosons). Our variational parameter is the rescaled single-particle
wave function $\psi(x)$ defined as

$$\psi(x) = \sqrt{N}\phi_0(x) . \tag{4}$$

The solution of the variational principle $\psi(x)$ will differ from the single-particle ground state
wave function of non-interacting bosons due to the interaction between the particles.

Show that the variational principle that minimizes the energy expectation value calculated in b)
leads to the Gross-Pitaevskii equation

$$\mu\psi(x) = -\frac{\hbar^2}{2m}\partial_x^2\psi(x) + U(x)\psi(x) + V_0|\psi(x)|^2\psi(x) \tag{5}$$

with the chemical potential μ. Note the non-linearity due to the interaction V_0!

Hints:

- Using the expression calculated in b), neglect all terms of order $1/N$ and treat the expectation value
as a functional of the complex-valued function $\psi(x)$. The result should read

$$E[\psi, \psi^*] = \int dx \left(\frac{\hbar^2}{2m}|\partial_x\psi(x)|^2 + U(x)|\psi(x)|^2 + \frac{1}{2}V_0|\psi(x)|^4 \right) . \tag{6}$$

- Minimize this functional with respect to $\psi(x)$ and $\psi^*(x)$ with the constraint

$$N = \int dx\, |\psi(x)|^2 . \tag{7}$$

This constraint can be taken into account by the method of Lagrange multipliers where the chemical
potential μ is the Lagrangian multiplier that fixes the particle number (7).