ICFP M2 Advanced Quantum Mechanics: Homework Problem

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Bardeen–Cooper–Schrieffer theory: Ultracold Fermi gas in the BCS regime

We consider N identical fermions in a three–dimensional box–like potential. Each fermion has two accessible internal states, labelled $|\uparrow\rangle$ and $|\downarrow\rangle$. We assume that N is even, and that the two states are equally populated: $N_\uparrow = N_\downarrow = N/2$ (for odd N, this amounts to neglecting the effect of a mismatch between $N_\uparrow$ and $N_\downarrow$ by a single particle).

The Pauli exclusion principle precludes any short–ranged interaction between two fermions in the same internal state. By contrast, two fermions in different internal states $|\uparrow\rangle$ and $|\downarrow\rangle$ may exhibit short–ranged interactions, which we model using a contact potential characterised by its scattering length a. The value of a may be tuned to take positive values (repulsive interactions) or negative ones (attractive interactions) using a Feshbach resonance.

The goal of this problem is to characterise the ground state and low–energy excitations of this many–body system in the case where $k_F a$ is small and negative, with k_F being the Fermi wavevector. In this case, there is no two–body bound state, but the system is affected by the Cooper instability: the long–ranged pairing of fermions with opposite momenta and spins is energetically favoured. The many–body ground state will be found to consist of multiple long–ranged pairs; the low–energy excitation spectrum is related to the particle–hole spectrum of ideal Fermi gases, and it exhibits a gap. It satisfies Landau's criterion for superfluidity.

The problem deals with fermions. Nevertheless, the commutator $[A, B]_- = AB - BA$ of two operators A and B plays a role in multiple questions. ***The answers to all questions and all required equations are given in the text, so that you may explore the whole problem even without providing a full answer to each question.***

1 The Bardeen–Cooper–Schrieffer (BCS) wavefunction

1.1 Wavefunction with a well–defined number of particles

We assume that N is even, and we introduce the N–fermion wavefunction $|\Psi_N\rangle$ consisting of pairs, defined by:

$$\Psi_N(\boldsymbol{r}_1, \dots, \boldsymbol{r}_N) = \mathcal{A}\left[\phi(\boldsymbol{r}_1, \boldsymbol{r}_2)\,|\chi_{12}\rangle, \dots \phi(\boldsymbol{r}_{N-1}, \boldsymbol{r}_N)\,|\chi_{N-1,N}\rangle\right] \ , \tag{1}$$

where $\mathcal{A}$ is the antisymmetriser acting on the fermionic positions $\boldsymbol{r}_1, \dots, \boldsymbol{r_N}$, $\phi(\boldsymbol{r}_i, \boldsymbol{r}_j)$ is the spatial wavefunction of the pair involving the fermions i and j, and $|\chi_{ij}\rangle$ is the corresponding two–fermion internal state.

1. In a spatially uniform system whose volume is Ω, justify that $\phi(\boldsymbol{r}_i, \boldsymbol{r}_j) = \varphi(\boldsymbol{r}_j - \boldsymbol{r}_i)/\sqrt{\Omega}$.
2. Recall which partial wave plays the most important role in low–temperature quantum collisions, and justify the name 's–wave pairing mechanism'. Identify an additional symmetry satisfied by the wavefunction ϕ, and explain why $|\chi\rangle$ is the singlet state $|\chi\rangle = (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$.
   Hint: The centrifugal barrier plays a role in the discussion.

1.2 Creation and destruction operators, commutation relations

In order to write $|\Psi_N\rangle$ in second–quantised notation, we introduce the operator $b^\dagger$:

$$b^\dagger \quad = \quad \int d^3r_1\, d^3r_2\, \phi(\boldsymbol{r}_1, \boldsymbol{r}_2)\, \hat{\Psi}^\dagger_\uparrow(\boldsymbol{r}_1)\, \hat{\Psi}^\dagger_\downarrow(\boldsymbol{r}_2) \ , \tag{2}$$

where the field operator $\hat{\Psi}^\dagger_\sigma(\boldsymbol{r})$ creates a particle with the spin $\sigma = \uparrow$ or $\downarrow$ at the point $\boldsymbol{r}$.

3. Show that $|\Psi_N\rangle = \dfrac{1}{\sqrt{(N/2)!}}\, b^{\dagger N/2}\,|\text{vac}\rangle$.

We wish to express $b^\dagger$ in terms of the creation operators $c^\dagger_{\boldsymbol{k},\sigma}$, creating a particle with the spin σ in the plane–wave state $|\boldsymbol{k}\rangle$ defined by $\langle \boldsymbol{r}|\boldsymbol{k}\rangle = e^{i\boldsymbol{k}\cdot\boldsymbol{r}}/\sqrt{\Omega}$, where Ω is the volume of the system. These states satisfy $\langle \boldsymbol{k}_1|\boldsymbol{k}_2\rangle = \delta_{\boldsymbol{k}_1,\boldsymbol{k}_2}$.

4. Show that $\langle \boldsymbol{r}_1, \boldsymbol{r}_2|\phi\rangle$ expands onto the plane waves as follows:

$$\langle \boldsymbol{r}_1, \boldsymbol{r}_2|\phi\rangle = \sum_{\boldsymbol{k}} \phi_{|\boldsymbol{k}|}\, e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_1-\boldsymbol{r}_2)}/\Omega \quad = \sum_{\boldsymbol{k}} \phi_k\, \langle \boldsymbol{r}_1|\boldsymbol{k}\rangle\, \langle \boldsymbol{r}_2|(-\boldsymbol{k})\rangle \ . \tag{3}$$

Hints: *(a)* First, accounting for the spatial symmetry of $\varphi(\boldsymbol{r}) = \varphi(r)$, show that its Fourier coefficients φ_k depend only on $k = |\boldsymbol{k}|$.
(b) Equation (3) enforces the condition $\sum_{\boldsymbol{k}} |\phi_k|^2 = 1$.

5. Express $\hat{\Psi}^\dagger_\sigma(\boldsymbol{r})$ in terms of the creation operators $c^\dagger_{\boldsymbol{k},\sigma}$, and conclude:

$$b^\dagger = \sum_{\boldsymbol{k}} \phi_k\, c^\dagger_{\boldsymbol{k}\uparrow} c^\dagger_{-\boldsymbol{k}\downarrow} \ . \tag{4}$$

6. Show that the bosonic commutators for b satisfy:

$$[b,b]_- = [b^\dagger, b^\dagger]_- = 0 \quad \text{and} \quad [b, b^\dagger]_- = \sum_{\boldsymbol{k}} |\phi_k|^2 (1 - n_{\boldsymbol{k}\uparrow} - n_{\boldsymbol{k}\downarrow}) \ . \tag{5}$$

May $b^\dagger$ be considered a true bosonic creation operator?

1.3 The BCS wavefunction and its normalisation

We relax the assumption of a fixed number of particles, and consider instead instead the state $|\Psi_{\text{BCS}}\rangle$, whose total particle number is not fixed:

$$|\Psi_{\text{BCS}}\rangle = \frac{1}{\mathcal{N}} \exp\left(\sqrt{N_p}\, b^\dagger\right) |\text{vac}\rangle \quad \text{with } N_p = N/2. \tag{6}$$

In Eq. (6), $\mathcal{N}$ is a normalisation factor.

7. What is the average pair number? What is the standard deviation of the pair number?
Explain why, for large N, the state $|\Psi_{\text{BCS}}\rangle$ closely mimics the N–particle state $|\Psi_N\rangle$.
Hint: The results of the supplementary exercise on coherent states may be useful.

8. Show that the wavefunction $|\Psi_{\text{BCS}}\rangle$ may be written as:

$$\mathcal{N}\,|\Psi_{\text{BCS}}\rangle = \prod_{\boldsymbol{k}} \exp(\sqrt{N_p}\, \phi_k\, c^\dagger_{\boldsymbol{k}\uparrow} c^\dagger_{-\boldsymbol{k}\downarrow})\, |\text{vac}\rangle \quad = \prod_{\boldsymbol{k}} \left(1 + \sqrt{N_p}\, \phi_k\, c^\dagger_{\boldsymbol{k}\uparrow} c^\dagger_{-\boldsymbol{k}\downarrow}\right) |\text{vac}\rangle \ . \tag{7}$$

9. Show that the BCS wavefunction, normalised such that $\langle \Psi_{\text{BCS}}|\Psi_{\text{BCS}}\rangle = 1$, reads:

$$|\Psi_{\text{BCS}}\rangle = \prod_{\boldsymbol{k}} \left(u_k + v_k c^\dagger_{\boldsymbol{k}\uparrow} c^\dagger_{-\boldsymbol{k}\downarrow}\right) |\text{vac}\rangle \quad \text{with} \quad u_k = \frac{1}{\sqrt{1 + N_p|\phi_k|^2}} \text{ and } v_k = \frac{\sqrt{N_p}\,\phi_k}{\sqrt{1 + N_p|\phi_k|^2}} \ . \tag{8}$$

What are the values of u_k and v_k in the absence of any interaction between the particles?

2 The BCS Hamiltonian

2.1 Full BCS Hamiltonian

We start from the Hamiltonian for N fermions, written using second–quantisation operators:

$$H \quad = \quad \sum_{\boldsymbol{k},\sigma} \epsilon_k\, c^\dagger_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma} \quad + \quad \frac{g}{\Omega} \sum_{\boldsymbol{k},\boldsymbol{k}',\boldsymbol{q}} c^\dagger_{\boldsymbol{k}+\frac{\boldsymbol{q}}{2},\uparrow}\, c^\dagger_{-\boldsymbol{k}+\frac{\boldsymbol{q}}{2},\downarrow}\, c_{\boldsymbol{k}'+\frac{\boldsymbol{q}}{2},\downarrow}\, c_{-\boldsymbol{k}'+\frac{\boldsymbol{q}}{2},\uparrow} \ . \tag{9}$$

In Eq. (9), the spin index $\sigma =\uparrow$ or $\downarrow$, the operator $c^\dagger_{\boldsymbol{k},\sigma}$ creates a fermion in the single–particle state $|\boldsymbol{k}\rangle$ whose energy is $\epsilon_{\boldsymbol{k}} = \hbar^2 k^2/(2m)$, and the operator $c_{\boldsymbol{k},\sigma}$ is the corresponding annihilation operator. The coupling constant $g = 4\pi\hbar^2 a/m$ is related to the scattering length a and encodes the nature (repulsive for $a > 0$, attractive for $a < 0$) and the strength of the two–body interaction between opposite–spin fermions. Finally, Ω is the total volume of the system.

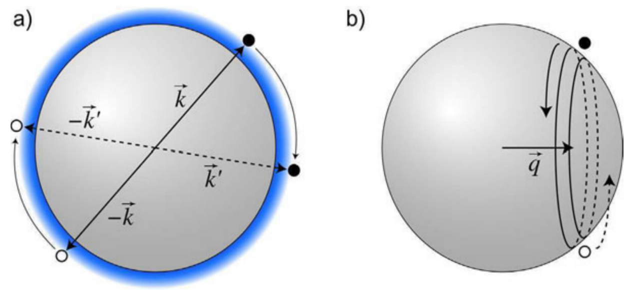

Figure 1 Two particles scattering on top of the Fermi sea. *(a)* Particles with equal and opposite momenta may scatter into final states in a narrow shell (shaded in blue) on top of the Fermi sea. *(b)* For non–zero total momentum $2\boldsymbol{q}$, the only accessible final states are in a narrow band of the Fermi surface around a circle of radius $(k_F^2 - q^2)^{1/2}$, with k_F being the Fermi wavevector. Reproduced from Ref. [1].

10. What is the conservation relation satisfied by the momenta involved in the interaction term? Which property of the two–body interaction potential does it reflect?

11. Explain why pairs with the total linear momentum $\boldsymbol{q} = \boldsymbol{0}$ play the most important role in the pairing mechanism. HINT: Consider two fermions colliding at the Fermi surface, with the total linear momentum $2\boldsymbol{q}$. You may refer to Figure 1.

12. Conclude that the Hamiltonian may be approximated by:

$$H_{\mathrm{BCS}} \;=\; \sum_{\boldsymbol{k},\sigma} \epsilon_k \, c^\dagger_{\boldsymbol{k}\sigma}\, c_{\boldsymbol{k}\sigma} \;+\; \frac{g}{\Omega} \sum_{\boldsymbol{k},\boldsymbol{k}'} c^\dagger_{\boldsymbol{k}\uparrow}\, c^\dagger_{-\boldsymbol{k}\downarrow}\, c_{\boldsymbol{k}'\downarrow}\, c_{-\boldsymbol{k}'\uparrow} \;. \tag{10}$$

2.2 Effective quadratic Hamiltonian and its diagonalisation

We assume that the double–annihilation operator $c_{\boldsymbol{k}\uparrow}\, c_{-\boldsymbol{k}\downarrow}$ fluctuates only weakly about its non–zero expectation value $C_k = \langle c_{\boldsymbol{k}\uparrow} c_{-\boldsymbol{k}\downarrow}\rangle$, which we assume to be real. Therefore, we write:

$$c_{\boldsymbol{k}\uparrow}\, c_{-\boldsymbol{k}\downarrow} \;=\; C_k \,+\, (c_{\boldsymbol{k}\uparrow}\, c_{-\boldsymbol{k}\downarrow} \,-\, C_k) \;, \tag{11}$$

where the operator within the parentheses yields fluctuations that are small compared to C_k. The isotropy of the system implies that C_k only depends on $k = |\boldsymbol{k}|$. We introduce the 'gap parameter' Δ defined in terms of the C_k as:

$$\Delta \;=\; \frac{g}{\Omega} \sum_{\boldsymbol{k}} C_k \;. \tag{12}$$

13. Show that $\langle c^\dagger_{\boldsymbol{k}\uparrow} c^\dagger_{-\boldsymbol{k}\downarrow}\rangle = -C_k$ and $\langle c_{\boldsymbol{k}'\downarrow} c_{-\boldsymbol{k}'\uparrow}\rangle = -C_{k'}$. Conclude that, up to first order in the operators $(c_{\boldsymbol{k}\uparrow} c_{-\boldsymbol{k}\downarrow} - C_k)$, Eq. (10) reduces to a quadratic Hamiltonian:

$$H_{\mathrm{BCS}} \approx H_{\mathrm{eff}} = -\frac{\Delta^2}{g/\Omega} + \sum_{\boldsymbol{k}} \left[\epsilon_k \left(c^\dagger_{\boldsymbol{k}\uparrow} c_{\boldsymbol{k}\uparrow} + c^\dagger_{-\boldsymbol{k}\downarrow} c_{-\boldsymbol{k}\downarrow} \right) - \Delta \left(c^\dagger_{\boldsymbol{k}\uparrow} c^\dagger_{-\boldsymbol{k}\downarrow} + c_{-\boldsymbol{k}\downarrow} c_{\boldsymbol{k}\uparrow} \right) \right] \;. \tag{13}$$

In order to diagonalise the quadratic Hamiltonian of Eq. (13), we perform a Bogoliubov transformation, i.e. we introduce the new 'quasi–particle' operators $\gamma_{\boldsymbol{k}\uparrow}$ and $\gamma^\dagger_{-\boldsymbol{k}\downarrow}$ defined by:

$$\begin{pmatrix} c_{\boldsymbol{k}\uparrow} \\ c^\dagger_{-\boldsymbol{k}\downarrow} \end{pmatrix} = \begin{pmatrix} u_k & v_k \\ -v_k & u_k \end{pmatrix} \begin{pmatrix} \gamma_{\boldsymbol{k}\uparrow} \\ \gamma^\dagger_{-\boldsymbol{k}\downarrow} \end{pmatrix} \;, \tag{14}$$

where the real numbers u_k and v_k depend on $k = |\boldsymbol{k}|$. We shall now choose them such that:

$$H_{\mathrm{eff}} - \mu \hat{N} = E_G^{\mathrm{GC}} + \sum_{\boldsymbol{k}} E_k \left(\gamma^\dagger_{\boldsymbol{k}\uparrow} \gamma_{\boldsymbol{k}\uparrow} + \gamma^\dagger_{-\boldsymbol{k}\downarrow} \gamma_{-\boldsymbol{k}\downarrow} \right) \;. \tag{15}$$

In Eq. (15), $\hat{N}$ is the total particle number operator. The chemical potential μ sets the average value $N = \langle \hat{N} \rangle$. The grand–canonical ground–state energy E_G^{GC} is related to the true ground–state energy E_G through $E_G^{\mathrm{GC}} = E_G - \mu N$.

14. We require that the operators $\gamma_{\boldsymbol{k}\sigma}$ and $\gamma^\dagger_{\boldsymbol{k}\sigma}$ satisfy fermionic commutation rules. Show that this amounts to the normalisation condition $u_k^2 + v_k^2 = 1$.

15. Write Eq. (15) in terms of commutators:

$$[\gamma_{\boldsymbol{k}\uparrow},\, H_{\mathrm{eff}} - \mu\, \hat{N}]_- \;=\; E_k\, \gamma_{\boldsymbol{k}\uparrow} \quad \text{and} \quad [\gamma^\dagger_{-\boldsymbol{k}\downarrow},\, H_{\mathrm{eff}} - \mu\, \hat{N}]_- \;=\; -E_k\, \gamma^\dagger_{-\boldsymbol{k}\downarrow} \;. \tag{16}$$

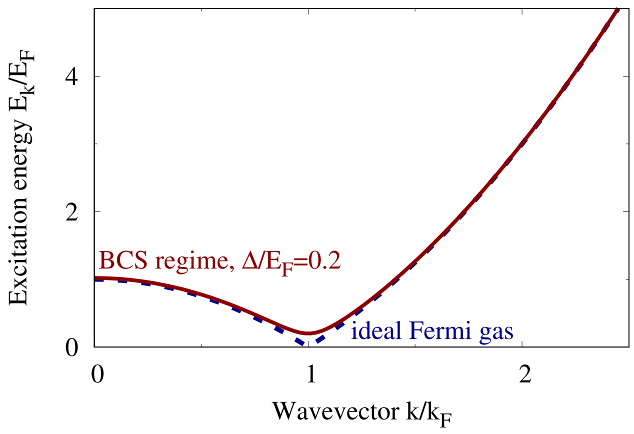

Figure 2 Energy spectrum for the particle and hole excitations in an ideal Fermi gas (dashed blue curve) and in a balanced Fermi gas in the BCS regime (solid red curve). In the latter case, the value of the gap parameter, $\Delta/E_F = 0.2$, is greatly exaggerated to make its smoothing effect near $k = k_F$ apparent.

16. Calculate the commutator $[c_{\boldsymbol{k}\uparrow},\, H_{\rm eff} - \mu N]_-$.
Combine the result with Eq. (16) to establish the *Bogoliubov–de Gennes* equations, which determine u_k and v_k:

$$\begin{pmatrix} (\epsilon_k-\mu) & \Delta \\ \Delta & -(\epsilon_k-\mu) \end{pmatrix} \begin{pmatrix} u_k \\ v_k \end{pmatrix} \quad = \quad E_k \begin{pmatrix} u_k \\ v_k \end{pmatrix} \; . \tag{17}$$

17. Interpret the terms appearing in Eq. (15) and justify that E_k should be chosen to be positive. Conclude:

$$E_k = \sqrt{(\epsilon_k-\mu)^2+\Delta^2}, \qquad u_k^2 = 1 - v_k^2 = \frac{1}{2}\left(1+\frac{\epsilon_k-\mu}{E_k}\right), \qquad \text{and} \qquad u_k\, v_k = \frac{\Delta}{2E_k} \; . \tag{18}$$

18. Check that the grand–canonical ground–state energy is given by:

$$E_G^{\rm GC} = -\frac{\Delta^2}{g/\Omega} - \sum_{\boldsymbol{k}} \left[E_k - (\epsilon_k-\mu)\right] \; . \tag{19}$$

Check that the wavefunction $|\Psi_{\rm BCS}\rangle$ of Eq. (8) is the ground state of $H_{\rm eff}$, that is to say: $\gamma_{\boldsymbol{k}\sigma}\, |\Psi_{\rm BCS}\rangle = 0$.

19. Using Eqs. (15) and (18), determine the low–energy excitation spectrum.
Compare it to the excitation spectrum for an ideal Fermi gas (see Fig. 2).

20. Justify that the minimum value of E_k/k is strictly positive, and conclude that the system exhibits superfluidity.

2.3 Gap and number equations

21. Calculate the gap parameter Δ in the ground state $|\Psi_{\rm BCS}\rangle$ using Eq. (12), and show that:

$$-\frac{1}{g} \quad = \quad \int \frac{d^3k}{(2\pi)^3}\, \frac{1}{2E_k} \tag{20}$$

22. Calculate the average number of particles $N = \langle \hat{N} \rangle$ in the ground state $|\Psi_{\rm BCS}\rangle$, and show that:

$$n = \frac{\langle N \rangle}{\Omega} \quad = \quad \int \frac{d^3k}{(2\pi)^3} \left(1 - \frac{\epsilon_k-\mu}{E_k}\right) \; . \tag{21}$$

3 Calculation of the gap Δ, in the BCS limit, at the temperature $T = 0$

The final step is to obtain μ and Δ as a function of a and N. We focus on the BCS regime, i.e. in the weakly–attractive limit, where $k_F a$ is small and negative. We work at the temperature $T = 0$, so that the system is in its ground state $|\Psi_{\rm BCS}\rangle$. Therefore, the gap equation (Eq. (20)) and the number equation (Eq. (21)) are applicable.

We assume $\mu > 0$ with $|\Delta| \ll \mu$, an assumption to be checked at the end of the calculation.

23. Taking the limit $\Delta \to 0$ in Eq. (21), show that $\mu \approx E_F$.

24. Approximate evaluation of the integral in Eq. (20):
   a) Justify that the integral is dominated by the contribution of wavevectors $\boldsymbol{k}$ such that $k \sim k_F$.
   b) In this region of momentum space, justify that the quantity $\eta = \epsilon_k - \mu$ satisfies $\eta \approx \hbar^2 k_F (k - k_F)/m$.
   c) Under this approximation, show that Eq. (20) reduces to:

$$-\frac{1}{g} \quad \approx \quad \frac{m k_F}{4\pi^2 \hbar^2} \int_{-\bar{\epsilon}}^{\bar{\epsilon}} \frac{d\eta}{(\eta^2 + \Delta^2)^{1/2}} \quad , \tag{22}$$

   where $\bar{\epsilon}$ is an energy cut–off chosen of the order of μ.
   d) Conclude as to the expression for the gap in the BCS regime:

$$\Delta \quad \approx \quad 2\,\bar{\epsilon}\,\exp\left(-\frac{\pi}{2k_F|a|}\right) \;, \tag{23}$$

   and confirm the validity of the assumption $\Delta \ll \mu$.
   HINT: $d[\text{arcsinh}(u)]/du = 1/(1+u^2)^{1/2}$.

25. Explain why reaching the superfluid regime in the BCS limit with ultracold Fermi gases is a particularly challenging goal for experimentalists.

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The approximate approach suggested in question 24 provides the correct exponent in Eq. (23), but not the correct prefactor (the prefactor in Eq. (23) depends on the value of the energy cut–off). The more elaborate approach required to obtain the correct prefactor is briefly sketched e.g. in Ref. [2, Sec. 26.5.2].

Further reading

INTRODUCTORY

- Sà de Melo's popularisation article [3] gives a brief overview of the BEC–BCS crossover in ultracold Fermi gases, and mentions the current related hot topics.
- The (long but accessible) review article by Zwierlein and Ketterle [1] provides an excellent overview of the theory and experiments on ultracold Fermi gases. The BEC–BCS crossover is reviewed in §4.4–4.12, including a discussion of finite–temperature effects.

MORE ADVANCED

- Reference [4, chap. 4] gives an extremely clear and detailed presentation of the BCS theory in the context of condensed–matter systems, including a brief description of the fermionic Josephson effect.
- The link between BCS theory and superconductor phenomenology (Meissner effect, SQUIDs, ...) is presented in Ref. [5, chap. 10].

This problem is directly inspired from Ref. [1, Secs. 4.3–4.5] and Ref. [4, chaps. 4 & 5].

References

[1] W. Ketterle, M. Zwierlein, in *Proc. International School of Physics Enrico Fermi, course CLXIV (Varenna, June 2006)* (2008).

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