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Competition between BCS-pairing and "moth-eaten effect" in BEC–BCS crossover

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ABSTRACT

We study the change in condensation energy from a single pair of fermionic atoms to a large number of pairs interacting via the reduced BCS potential. We find that the energy-saving due to correlations decreases when the pair number increases because the number of empty states available for pairing gets smaller ("moth-eaten effect"). However, this decrease dominates the 3D kinetic energy increase of the same amount of noninteracting atoms only when the pair number is a sizable fraction of the number of states available for pairing. As a result, in BEC–BCS crossover of 3D systems, the condensation energy per pair first increases and then decreases with pair number while in 2D, it always is controlled by the "moth-eaten effect" and thus simply decreases.

1. Introduction

It was known for a long time that a 3D system with a weak attractive potential cannot sustain a bound state. Cooper however showed that in the presence of a frozen Fermi core, a pair of electrons with opposite spins can form a bound state with zero total momentum, no matter how weak the attraction is [1]. Note that this "single pair" state already is a many-body state because, even if the frozen core electrons do not interact, they still, because of Pauli blocking, provide a finite density of states which is of importance for pairing. Turning to more than one pair is difficult due to the Pauli exclusion principle between a fixed number of paired electrons. To overcome this difficulty, Bardeen, Cooper and Schrieffer proposed an ansatz for the many-body state in the grand canonical ensemble – with pair number not fixed – which in the presence of a frozen core, leads to an energy lower than the free electron energy, even in the limit of an arbitrarily small potential [2]. Gor'kov and Melik-Barkhudarov then showed that the frozen core is not mandatory, provided that one uses a renormalized attraction measured through the low energy scattering amplitude [3]. Later on, Eagles [4], Leggett [5] and also Nozières and Schmitt-Rink [6] extended the BCS idea to bridge molecular BEC with Cooper pairing. To do it, they vary the potential amplitude while using a BCS-like grand canonical wave function without frozen core, i.e., all **k** states are involved. Their work raises the complementary question: how, when the potential is fixed but too weak to hold a bound state, the solution evolves from a single unbound pair to a very large number of pairs which always have a bound state solution. The grand canonical nature of the BCS ansatz makes it inherently many-body, so a direct connection to the one-pair solution is not really possible.

Five years after the BCS milestone paper, Richardson [7] and Gaudin [8], succeeded to write the exact eigenstate for N pairs interacting via the reduced BCS potential, in terms of N parameters solution of N coupled equations. The condensation energy obtained from the BCS ansatz, has been recovered in the infinite N limit [9–11].

A decade ago, one of us has developed a new framework [12] for many-body effects between composite bosons. Most of its applications dealt with semiconductor excitons. Recently, we have extended this framework to Cooper pairs and rederived Richardson–Gaudin equations [13]. We have also succeeded to obtain an analytical solution of these equations [14,15] whose energy exactly matches the energy obtained through the BCS ansatz. The Richardson–Gaudin approach is all the most suitable to investigate the change in condensation energy from 1 to N pairs when the pairing potential stays constant, because it allows us to handle a fixed number of pairs with Pauli blocking treated exactly.

When one electron pair is added to a system already having N pairs, the Pauli exclusion principle shows up in two different ways. (i) Pairing (binding) has to use a smaller phase space, so that the energy saving per pair due to the attracting potential must be smaller in the case of $(N + 1)$ pairs than for N pairs since they have less freedom to construct the most favorable correlated state. This binding decrease is the so-called "moth-eaten effect" [14]. (ii)

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In the absence of attraction, the additional fermion pair fills the next $\mathbf{k}$-level due to Pauli blocking; so its energy also depends on the N other pairs. Of course, these two effects must be handled self-consistently. However, it is enlightening to separate them in order to build some intuition. The binding energy decrease resulting from the "moth-eaten effect" driven by Pauli blocking, scales as N/N_Ω, where N is the number of pairs at hands and N_Ω the maximum number of pairs in the potential layer which scales as the sample volume. By contrast, the average kinetic energy for free pairs scales as ϵ_F, i.e., $(N/L^3)^{2/3}$, where L^3 is the sample volume in 3D. When N is small, this dominates the "moth-eaten effect", so, the condensation energy per pair, which results from the energy difference without and with potential, must increase. For larger N, however, the "moth-eaten effect" dominates and the condensation energy per pair finally decreases.

This understanding points out an important aspect of the BEC–BCS crossover. It is usually introduced at the two-body level, a bound-state appearing when the attraction passes some threshold. The many-body solution is then seen as the effective potential threshold turning to zero for the system to condense at vanishing potential. The present work proposes a somewhat different understanding which better bridges 2-body to N-body systems in a BEC–BCS crossover: as the pair number increases, a correlated state develops at a lower but still finite potential.

The paper is organized as follows.

In Section 2.1, we describe the model. We recall the single pair case and then turn to a qualitative understanding of the many-pair system through the condensation energy change when the pair number increases. We show that this change is quite different in 2D, with a constant density of state, and 3D with a density of state which cancels at zero energy. To support this understanding, in Section 3, we carefully study two pairs through the resolution of the corresponding Richardson–Gaudin equations with a $\sqrt{\epsilon}$ density of state: we show that a binding indeed develops when turning from one to two pairs for a potential set exactly equal to the threshold value for one pair. We then conclude in Section 4.

2. Physical understanding

2.1. The model

We consider N pairs of fermionic atoms with creation operators $a^\dagger_{\mathbf{k}}$ and $b^\dagger_{\mathbf{k}}$, ruled by the Hamiltonian $H = H_0 + V_{\mathrm{BCS}}$. For same mass atoms, the kinetic part H_0 reads

$$H_0 = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} (a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + b^\dagger_{\mathbf{k}} b_{\mathbf{k}}). \tag{2.1}$$

We take as potential the reduced BCS potential of standard superconductivity, but without its frozen core, namely

$$V_{\mathrm{BCS}} = -v \sum_{\mathbf{k}\mathbf{k}'} w_{\mathbf{k}'} w_{\mathbf{k}} \beta^\dagger_{\mathbf{k}'} \beta_{\mathbf{k}} \tag{2.2}$$

where $\beta^\dagger_{\mathbf{k}} = a^\dagger_{\mathbf{k}} b^\dagger_{-\mathbf{k}}$ while $w_{\mathbf{k}} = 1$ for $0 < \epsilon_{\mathbf{k}} < \Omega$ and zero otherwise, so attraction between zero-moment pairs acts from zero to a sharp cutoff Ω. While this cut-off bears no connection with phonon energies, we can still relate it to a physical quantity, the scattering length, as shown below.

2.2. One pair

The energy E_1 of a single pair in this potential follows from Cooper's equation

$$\frac{1}{v} = \sum_{\mathbf{k}} \frac{\omega_{\mathbf{k}}}{2\epsilon_{\mathbf{k}} - E_1} \equiv S(E_1). \tag{2.3}$$

(i) In 2D, the density of state is constant. By transforming the sum over $\mathbf{k}$ into an integral, we get for negative E,

$$S^{(2D)}(E < 0) = \rho \int_0^\Omega \frac{d\epsilon}{2\epsilon - E} = \frac{\rho}{2} \ln\left(\frac{2\Omega - E}{-E}\right). \tag{2.4}$$

This function tends to infinity when $E \to 0_-$ and to zero as $\rho\Omega/(-E)$ when $E \to -\infty$. A bound state, solution of Eq. (2.3), thus exists no matter how weak v is. It reads $E_1^{(2D)} = -2\Omega\sigma/(1-\sigma)$ with $\sigma = e^{-2/\rho v}$. Note that while ρ increases linearly with sample volume, ρv stays constant.

(ii) In 3D, the density of states can be written as $\rho(\epsilon) = \rho\sqrt{\epsilon/\Omega}$ where ρ now is the density of state at the potential upper boundary. So

$$S^{(3D)}(E < 0) = \rho \int_0^\Omega d\epsilon \frac{\sqrt{\epsilon/\Omega}}{2\epsilon - E} = \rho\left[1 - \sqrt{\frac{-E}{2\Omega}} \mathrm{Arctg} \sqrt{\frac{2\Omega}{-E}}\right] \tag{2.5}$$

tends to ρ when $E \to 0_-$ and to zero as $\frac{2}{3}\rho\Omega/(-E)$ when $E \to -\infty$. A bound state thus exists for v larger than a threshold $v_{\mathrm{th}} = 1/\rho$. For a potential just above threshold, the single pair energy tends to zero as $E_1^{(3D)} \approx -8(\rho v - 1)^2 \Omega/\pi^2$ while far above threshold $E_1^{(3D)} \approx -\frac{2}{3}\rho v \Omega$.

(iii) Using this result, we can relate the s-wave scattering length a_s, commonly used for cold gases, to the potential cut-off Ω via the density of state at this cut-off, $\rho = mL^3\sqrt{2m\Omega}/2\pi^2$. Indeed, for fermion pairs interacting via V_{BCS}, the T-matrix for S-wave reduces to

$$T_k^0 = \frac{-v\omega_k}{1 - vS(2\epsilon_k + i0_+)} \tag{2.6}$$

with, from Eq. (2.5), $S^{(3D)}(2\epsilon_k + i0_+) \simeq \rho(1 + i\pi\sqrt{\epsilon_k/4\Omega})$ for $\epsilon_k \ll \Omega$. The scattering length then follows from the scattering amplitude $f_k^0 = -a_s/(1 + ika_s)$ which depends on the T-matrix as $f_k^0 = -mL^3 T_k^0/4\pi$. So, $a_s \simeq mL^3 v/4\pi(\rho v - 1)$. For v slightly above the single pair threshold $1/\rho$, we find a_s positive with a pair binding energy $E_b \approx -1/ma_s^2$, while below threshold, a_s is negative and no bound state exists.

2.3. N pairs

Richardson [7] and Gaudin [8] showed that the energy of N fermion pairs interacting via V_{BCS} reads as $E_N = R_1 + \cdots + R_N$ where the R_i's follow from N coupled equations

$$\frac{1}{v} = \sum_{\mathbf{k}} \frac{w_{\mathbf{k}}}{2\epsilon_{\mathbf{k}} - R_i} + \sum_{j \neq i} \frac{2}{R_i - R_j}. \tag{2.7}$$

(i) *2D systems*: Very recently [14,16], we have derived a compact solution of these equations when the density of state is constant above a 3D frozen core, as for the N Cooper pairs in standard BCS superconductivity. Using this result for 2D systems which have a constant density of states whatever the electron energy is, we get

$$E_N^{(2D)} = N E_1^{(2D)} + \frac{N(N-1)}{\rho} \frac{1+\sigma}{1-\sigma} \tag{2.8}$$

within under-extensive terms in $(N/\rho)^n$. The energy difference without and with potential leads to a condensation energy per pair $\epsilon_N = [E_N(v = 0) - E_N]/N$ equal to

$$\epsilon_N^{(2D)} = \left[1 - \frac{N-1}{N_\Omega}\right] \frac{2\sigma}{1-\sigma} \Omega \tag{2.9}$$