Chapter 2
The BEC–BCS Crossover: Some History and Some General Observations

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Abstract While the experimental realization in ultracold Fermi alkali gases of the phenomenon we now call the "BEC–BCS crossover" was attained only in the last few years, theoretical considerations of this issue go back a lot further, and refer to other systems as well. In the first part of this chapter we review some of this history, while in the second half we make some general comments on the current theoretical situation with respect to the specific ultracold-gas implementation.

2.1 Introduction

It is by now well accepted that a system of Fermi particles with two different "species" equally populated, and an attractive interspecies interaction, may exhibit a behavior that as the strength of the interaction is decreased varies continuously from a Bose-Einstein condensate of tightly bound di-fermionic molecules to Cooper pairing of weakly attracting independent fermions. While the experimental realization, in dilute ultracold Fermi alkali gases, of this so-called "BEC–BCS crossover" has been attained only in the last few years, related theoretical considerations have a much longer history and have been put forward also in the context of systems other than the dilute ultracold gases (excitons, metallic superconductivity, nuclear matter ...). In the first half of this chapter, we shall give a brief review, which is not claimed to be exhaustive, of the early history of the theory, and in the second half make some general comments on the current theoretical situation with respect to the specific alkali-gas implementation.

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At the outset we would like to emphasize an important aspect in which the ultracold Fermi gases that have been the subject of intense experimental study in the last few years differ from the other physical systems in which a "BEC–BCS crossover" has been studied theoretically: they are "naturally" *dilute*, in the sense that the inter-fermion interaction is short-ranged, with an effective radius r_0, which under typical experimental conditions is orders of magnitude smaller than the average inter-fermion separation. This permits a kind of theoretical simplification that does not in general apply to these other systems, and is part of the subject of the second half of this chapter.

2.2 Some Prehistory

While the many people who worked on the theory of Bose-Einstein condensation (hereafter BEC) in liquid helium in the years between London's proposal of this phenomenon in 1938 and the work of BCS in 1957 were presumably conscious, in the back of their minds, that the ^{4}He atom is actually a composite of six fermions, no particular attention seems to have been paid to this state of affairs; with hindsight this is hardly surprising, since the minimum energy scale relevant to dissociation of the atom into its fermionic components (tens of eV) is several orders of magnitude greater than that involved in BEC of the liquid (a few K), and thus it is usually an excellent approximation, in the context of the latter, to treat the atom as a simple structureless boson. The first person to make the explicit suggestion that pairs of fermions (electrons) with an effectively attractive interaction might form a molecular-like object with bosonic statistics and thus undergo BEC appears to have been Ogg [1], in the context of a very specific superconducting system (an alkali metal-ammonia solution); however, Ogg speculated that this mechanism might more generally be the explanation of superconductivity. This idea was taken up a few years later by Schafroth [2] and amplified in the paper of Schafroth et al. [3]; however, it proved very difficult to use this approach to calculate specific experimental quantities. Following the work of Bardeen et al. [4] (hereafter BCS), further work was done, mainly by Blatt and coworkers, along the lines developed in ref. [3]; see for example ref. [5]. This work emphasized the point of view that Cooper pairing in a weakly interacting Fermi gas could be viewed as a form of BEC (of pairs of electrons); the qualitative considerations developed in it foreshadow some of those that resurfaced subsequently in the context of the crossover problem. However, following the successful explanation by the BCS theory of most of the experimental properties of the then-known superconductors and its consequent rapid acceptance by the community, there seems to have been a tendency in the late 1950s and early 1960s to emphasize the differences rather than the similarities between the phenomena of BEC and of Cooper pairing.

One important development that, at least with hindsight, pulls rather strongly in the opposite direction is the seminal paper of Yang [6] on off-diagonal long-range order (ODLRO). We will discuss the application of this idea (or rather of a closely

related one) to the crossover problem in the second part of this chapter, but here note that Yang in effect showed that the generalized definition of BEC given by Penrose and Onsager [7] for a simple Bose system such as ^{4}He could be generalized to apply to a fermionic system provided one replaces the single-boson density matrix by the two-fermion one. (For details, see below). However, it seems to have been some time before the full significance of this observation was appreciated by the community.

Meanwhile, attempts were being made to apply BCS-like ideas to Fermi systems other than the electrons in metals. In the case of liquid ^{3}He and heavy nuclei, the situation seemed to be fairly close to that envisaged in the original BCS work, in the sense that the pairing interaction was likely to be so weak that the radius of any pairs formed would be much greater than the inter-fermion distance, just as it is in (pre-1970s) superconducting metals; in modern terminology, one is automatically in the "BCS limit." In the present context, a more interesting case is that of excitons in semimetals or semiconductors. That the tightly-bound excitons in a semiconductor are effectively bosons and might therefore undergo (nonequilibrium) BEC had been pointed out in the early 1960s by Moskalenko [8] and by Blatt et al. [9]; however, in 1965 Keldysh and Kopaev [10], and independently des Cloizeaux [11], pointed out that in a semimetal (a crystal in which the groundstate corresponds to partial filling of the conduction band with partial depletion of the valence band), or in a narrow-gap semiconductor where the exciton binding energy exceeds the gap, a process analogous to Cooper pairing can take place, the components of the pair now bring an electron and a hole. The resulting state is not superconducting (since the pair is electrically neutral) but rather forms an "excitonic insulator." It was appreciated that in a real solid one might be in a regime intermediate between the "exciton BEC" and "excitonic insulator" regimes, and in 1968 Keldysh and Kozlov [12] studied the problem of exciton condensation taking explicit account of the fermionic nature of the component electrons and holes. While they mainly concentrated on the corrections to simple BEC behavior arising from the fermionic statistics, their technique, which is diagrammatic in nature, can in principle be applied for arbitrary density of the electron-hole liquid. Since then a great deal of work has been done along similar lines for this system.

In the context of the ultracold alkali gases, however, it turns out that a rather simple, and as far as present experiments go, at least qualitatively correct picture can be obtained by a very simple generalization of the original BCS technique, which we will refer to as the "naïve ansatz". The motivation for this approach is the following observation, which was certainly appreciated from very early days (see e.g. ref. [13], and references cited therein), that the coordinate-space form of the standard BCS wave function is formally identical to that of a Bose condensate of tightly bound di-fermionic molecules, the only (but crucial!) difference being that the ratio of the pair radius to the mean interparticle spacing is very small in the BEC case and very large in the BCS one. In hindsight this might seem to lead naturally to the conjecture that a reasonable description of the intermediate regime (the "crossover") might be obtained by simply using this form of wave function (or the corresponding BCS particle-nonconserving one) as a variational ansatz over the whole of the range of coupling.

The first person to implement this program explicitly was Eagles in 1969 [14]. He was motivated by experiments that showed that the semiconductor $SrTiO_3$ become superconducting when doped with Zr. Eagles argued that in such a case the electron gas might be very dilute, so that the size of any pairs formed might be much smaller than the mean inter-electron distance; in that case the system would look like a Bose condensate of tightly-bound di-electronic "molecules." Using the BCS form of inter-electron attraction with a cutoff that is tied to the chemical potential μ ("Fermi energy" in the language of ref. [14]) he wrote down the BCS gap equation for an arbitrary strength of interaction, and also the equation expressing the conservation of total (average) particle member; he then solved this pair of equations numerically over the whole crossover regime (in his notation the point where the quantity A of Eq. 2.7 goes through zero is what would nowadays be called the unitarity limit). While the specific choice of the form of interaction, which for $\mu > 0$ depends explicitly on the Fermi energy and hence on density, makes it difficult to compare Eagles' results quantitatively with those obtained subsequently in the context of the dilute ultracold alkali gases, all the qualitative factors that appear in the latter—the change in sign of μ on the "BEC" side of unitarity, the different significance of the "gap" Δ on the two sides of this point, the fact that over much of the crossover regime the superconducting transition temperature T_c is of the order of the free-gas Fermi temperature, and the existence, in the BEC limit, of a wide temperature range where pairing occurs without superconductivity—are to be found in this early paper.

By the late 1970s there had been a couple of experimental developments that tended to focus attention on the crossover problem. First, the long-predicted phenomenon of Cooper pairing in liquid ^{3}He had been experimentally realized, and it was discovered that there were not one but three different paired states, with different structures of their internal wave functions; this tended to re-focus attention on the similarities, rather than the differences, between diatomic molecules and Cooper pairs. Secondly, since dilute spin-polarized atomic hydrogen (a Bose system) was being cooled into a regime close to degeneracy, it was plausible that in the future it would also be possible to cool atomic deuterium, a Fermi system, into the degeneracy regime and possibly even down to the temperature for onset of pairing. (In the event, deuterium turned out to be notoriously refractory in a cryogenic context, and to this day it has not to our knowledge even been cooled into the quantum regime.)

Motivated by these considerations, and unaware at the time of Eagles' work, one of the present authors (A. J. L.) considered [15, 16] in 1980 the crossover problem in the context of a dilute ultracold Fermi gas. The model studied was of a dilute degenerate gas of fermions with the two spin species equally populated, interacting by an interatomic potential that has a strong but finite short-range repulsion but a fairly weak attraction at larger distances, and is tuned so that one is close to the onset of a two-body bound state; thus the low-energy s-wave scattering length a_s is large compared to the range r_0 of the potential and can have either sign. It is intuitively clear that in this limit there is only one physically relevant dimensionless ratio in the problem, namely that of a_s to the mean interparticle spacing, or equivalently $k_F a_s$ where k_F is the Fermi wave vector of the noninteracting atomic gas, so that rather generally one would expect that at $T = 0$ both the chemical potential μ and

the gap (pairing field) Δ could have the form $\varepsilon_F f(k_F a_s)$, where ε_F is the Fermi energy of the noninteracting gas. To obtain approximate forms of $f(k_F a_s)$, ref. [15] wrote down explicitly the "naïve" ansatz for the many-body wave function (see part 2 of this chapter), argued that the Hartree and Fock terms in the energy contribute only uninteresting constants and thus arrived at the standard BCS gap equation, with however the more general form of the pairing matrix element $V_{kk'}$ corresponding to the (semi)realistic form of interatomic potential. Eliminating the high-momentum part of $V_{kk'}$ in favor of the experimentally measurable quantity a_s by a standard renormalization procedure, and solving the resulting gap equation simultaneously with the equation expressing number conservation in a way similar to that done by Eagles earlier, one is able to obtain the general behavior of the dimensionless functions $f_\mu(k_F a_s)$ and $f_\Delta(k_F a_s)$. As we will see in part 2, these results of the naïve ansatz appear to contribute a good starting point for discussion of the realistic alkali gas problem at $T = 0$.

At around the same time there occurred a development that, although little noticed at the time, foreshadowed a central theme in the study of the BEC–BCS crossover: in his thesis, Modawi [17] suggested the use of a Feshbach resonance to enhance the transition temperature of atomic deuterium by several orders of magnitude (although even after the enhancement it would still be depressingly low). For reasons unconnected with physics, this work was never published (though cf. [18], pp. 626–627).

In 1985 Nozières and Schmitt-Rink [19] returned to the crossover problem and generalized the earlier work to consider both the effects of a crystalline lattice and the behavior of the critical temperature in the intermediate regime. They pointed out that while in the BCS limit the presence of a lattice makes no qualitative difference, in the BEC limit it changes the situation enormously, since the tightly-bound pairs then sit on individual lattice sites and can move only by a "correlated hopping" process involving as an intermediate stage the virtual ionization of a pair; for the "negative-U Hubbard model" that they use the matrix element for motion of the bosons is thus t^2/U, which in this limit is much smaller than that (t) for the original fermions, in contrast to the continuum case where the two quantities are of the same order of magnitude. As to the behavior of the critical temperature, they carried out a calculation that combines a simple "ring" approximation for the thermodynamic potential with the standard Thouless criterion for the instability of the normal state so as to obtain the behavior of T_c as a function of the coupling strength; while they recover the expected results that T_c is given in the weak-coupling (BCS) limit by the standard BCS formula and in the opposite limit by the expression for the condensation temperature of a dilute Bose gas, their most important conclusion is that the transition is, at least in this approximation, a *continuous* function of the coupling strength.

As is well known, a new ingredient was added to the mix with the discovery in 1986 of the cuprate (high-temperature) superconductors, an electronic system in which the (presumed) formation of Cooper pairs seems to take place at intermediate values of coupling strength. This prompted an explosion of work on the crossover problem that we will not attempt to review here; much of this work prior to 1995 is reviewed in [20].

2.3 Some General Remarks on the Crossover Problem

In this section we will discuss the "standard" model of the BEC–BCS crossover problem, by which we mean the following. We consider an ultracold gas of N fermionic atoms with two hyperfine species equally populated, in volume V, and take the standard thermodynamic limit $N, V \to \infty$, $N/V \equiv n = \text{const.}$; as is conventional, we label the two relevant hyperfine species by a spin index $\sigma = \pm 1$. The atoms are taken to interact via an interatomic central potential $V(r)$, which will typically consist of a strongly repulsive hard core, an attractive region of depth 1–5 eV at 2–3 Å, and a more weakly attractive Van der Waals tail of the form $-C/r^6$; the "van der Waals length" $l_{\mathrm{vdW}} \equiv (mC/\hbar^2)^{1/4}$, which determines the "typical" radius of the most weakly bound molecular state, will be taken to be 50–100 Å. We assume that we can apply a variable uniform static magnetic field to the system so as to tune it through a Feshbach resonance, that is, a value H_{res} of the field at which the zero-energy scattering state of our two hyperfine species (which together define the "open" channel) is degenerate with the most weakly bound molecular state of a second pair of hyperfine species (the "closed" channel), which may or may not have one species in common with the open channel; the detuning between these two states will be denoted $\delta(H) = \text{const.}(H - H_{\mathrm{res}})$. For simplicity we shall assume that the resonance is "broad", i.e. that the Fermi energy of the gas calculated in the absence of interaction is much smaller than the characteristic "width" δ_c of the two-body resonance (for details, see e.g. ref. [21], Chap. 4); when this condition is satisfied, there is a wide interval ($\delta_c \ll \delta < 0$) of magnetic field close to the resonance where although molecules are formed, they are almost entirely in the open channel (see e.g. Fig. 4.2 of ref. [21]); we will always assume unless otherwise noted that $|\delta| < \delta_c$. Thus, except when we are explicitly considering the "closed-channel fraction," it will be adequate to eliminate the closed channel from the problem entirely, in favor of an extra magnetic-field-dependent term in the open-channel potential $V(r)$. The resulting zero-energy s-wave scattering length in the open channel, which is of course a function of δ (or H) and tends to $\pm\infty$ at the position of the (normalized [21]) resonance (the "unitary limit"), will be denoted simply a_s.

It is convenient to introduce the dimensionless parameter $\xi \equiv -1/(k_{\mathrm{F}} a_s)$, where $k_{\mathrm{F}} \equiv (3\pi^2 n)^{1/3}$ is the Fermi wave vector of the noninteracting gas; then the "BEC limit" corresponds to $\xi \to -\infty$ and the "BCS limit" to $\xi \to +\infty$, and generally speaking we expect the "crossover" to correspond to the regime $|\xi| \lesssim 1$. In the following we shall always assume the dilute-gas limit, i.e. that $k_{\mathrm{F}} l_{\mathrm{vdW}} \ll 1$ (it would probably actually be adequate for most of our purposes to assume another weaker condition, but we may as well play safe). As we shall see, this condition simplifies some aspects of the problem considerably; since the highest densities so far obtained in the ultracold Fermi gases have been only $\sim 10^{-13}\mathrm{cm}^{-2}$, it has certainly been well satisifed in all experiments to date.

A convenient general description of the crossover behavior, which does not assume any particular ansatz for the many-body wave function or density matrix, may be given in terms of the formalism developed by Yang [6]. Suppose that the energy

eigenstates of the N-body system are $\Psi_N^{(n)}(\mathbf{r}_1\sigma_1\mathbf{r}_2\sigma_2\ldots\mathbf{r}_N\sigma_N)$ with energies E_n and the system is in thermal equilibrium at some inverse temperature $\beta \equiv (k_B T)^{-1}$. (We could generalize the formalism also to discuss nonequilibrium states, but this is not necessary for our present purposes). Then define the reduced two-body density matrix

$$\begin{aligned}\rho_2(\mathbf{r}_1\sigma_1\mathbf{r}_2\sigma_2 : \mathbf{r}_1'\sigma_1'\mathbf{r}_2'\sigma_2') &\equiv Z^{-1}(\beta)\sum_n \exp(-\beta E_n)\left\{\sum_{\sigma_3\ldots\sigma_N}\iint\ldots d\mathbf{r}_3\ldots d\mathbf{r}_N\right.\\ &\left.\times\Psi_N^{(n)}(\mathbf{r}_1\sigma_1\mathbf{r}_2\sigma_2\ldots\mathbf{r}_N\sigma_N)\Psi_N^{*(n)}(\mathbf{r}_1'\sigma_1'\mathbf{r}_2'\sigma_2'\ldots\mathbf{r}_N'\sigma_N')\right\}\\ &\equiv\left\langle\psi_{\sigma_1}^\dagger(\mathbf{r}_1)\psi_{\sigma_2}^\dagger(\mathbf{r}_2)\psi_{\sigma_2'}(\mathbf{r}_2')\psi_{\sigma_1'}(\mathbf{r}_1')\right\rangle, \qquad (2.1)\end{aligned}$$

where $Z(\beta)$ is the partition function. The quantity ρ_2, regarded as a matrix function of its indices, is Hermitian and thus can be diagonalized with real eigenvalues:

$$\rho_2(\mathbf{r}_1\sigma_1\mathbf{r}_2\sigma_2 : \mathbf{r}_1'\sigma_1\mathbf{r}_2'\sigma_2) = \sum_i n_i\chi_i(\mathbf{r}_1\sigma_1\mathbf{r}_2\sigma_2)\chi_i^*(\mathbf{r}_1'\sigma_1'\mathbf{r}_2'\sigma_2'), \qquad (2.2)$$

where the eigenfunctions $\chi(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2)$ must be antisymmetric under the exchange $\mathbf{r}_1\sigma_1 \leftrightarrows \mathbf{r}_2, \sigma_2$.

As shown by Yang, the n_i must satisfy the condition

$$\sum_i n_i = N(N-1). \qquad (2.3)$$

Intuitively, the eigenvalue n_i can be interpreted as "the number of atomic pairs which occupy the two-particle state $\chi_i(\mathbf{r}_1\sigma_1\mathbf{r}_2\sigma_2)$." Assuming that the translational symmetry of the Hamiltonian is not spontaneously broken, the quantity ρ_2 must be invariant under the total translation operation $\mathbf{r}_i \to \mathbf{r}_i + \eta, \mathbf{r}_j' \to \mathbf{r}_j' + \eta (i, j = 1, 2)$, and hence the eigenfunctions χ_i can be chosen to be eigenstates of the center-of-mass momentum:

$$\chi_i(\mathbf{r}_1\sigma_1\mathbf{r}_2\sigma_2) = \exp i\mathbf{K}\cdot(\mathbf{r}_1+\mathbf{r}_2)/2\,\widetilde{\chi}_i(\mathbf{r}_1-\mathbf{r}_2, \sigma_1\sigma_2). \qquad (2.4)$$

By a similar argument they can be chosen to be eigenfunctions of the total spin and its z-component:

$$\widetilde{\chi}_i(\mathbf{r}_1-\mathbf{r}_2, \sigma_1\sigma_2) = \overset{\approx}{\chi}_i(\mathbf{r}_1-\mathbf{r}_2)\zeta_i(S, m), \qquad (2.5)$$

where $\zeta_i(S, m)$ is one of the four simultaneous eigenstates of total spin $S(= 0, 1)$ and total z-projection of spin $m(= 0, 1)$ of a pair of spin-1/2 particles. (It would also be possible to use the rotational invariance of ρ_2 to choose the functions $\overset{\approx}{\chi}_i(\mathbf{r}_1-\mathbf{r}_2)$ to be eigenstates of the relative orbital angular momentum, but it is convenient not to do so, at least for the moment.) Evidently, one would expect not only the eigenvalues

n_i but also the eigenfunctions χ_i (or at least the $\approx$-components thereof) to depend both on the temperature and on the detuning δ (which controls the scattering length $a_s(\delta)$).

We can divide the possible forms of the eigenfunctions $\chi(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2)$ (Eq. 2.4) into three classes according to the center of mass momentum $\mathbf{K}$ and whether the relative wave function $\widetilde{\chi}(\mathbf{r}_1 - \mathbf{r}_2)$ is or is not bound as a function of $|\mathbf{r}_1 - \mathbf{r}_2| \equiv r$ (i.e. whether or not it tends to zero faster than r^{-2} as $r \to \infty$). (A) $\widetilde{\chi}$ unbound, $\mathbf{K}$ any (B) $\widetilde{\chi}$ bound, $\mathbf{K} = 0$ (C) $\widetilde{\chi}$ bound, $\mathbf{K} \neq 0$. It should be noted that the number of eigenfunctions with eigenvalue ~ 1 in class A is always of order N^2, even in the extreme BEC limit; this is simply because even in this limit, if we pick two fermions at random it is highly likely that they will belong to different molecules and will be uncorrelated. Classes (B) and (C) together intuitively describe any bound pairs that form in the system, and the number of relevant eigenfunctions in these two classes can be at most of order N; crudely speaking, the onset of pairing, e.g. with decreasing temperature, corresponds to the point at which the sum of eigenvalues N_{BC} in these two classes becomes of order N. The onset of condensation corresponds to the point, if any, at which the quantity N_B becomes of order N; the usual assumption is that there is then only a single relevant form of $\widetilde{\chi}$, i.e. one gets "simple" BEC or a generalization of it. In this case the onset of condensation is equivalent, in our infinite geometry, to the onset of off-diagonal long-range order as defined by Yang [6]. With these definitions it is clear that there is no fundamental conceptual distinction between BEC and Cooper pairing; the only differences (which are of course crucial in a practical sense) lie in the ratio of the pair radius to the mean interparticle spacing and in the nature of the low-lying excitation spectrum.

Before we enter the general discussion using Yang's formulation, it is instructive to revisit briefly the standard model of the BEC–BCS crossover at $T = 0$. There we write the ground state wave function as

$$\Psi_N^{(0)}(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2, \ldots, \mathbf{r}_N\sigma_N) = \mathscr{A}\left[\phi(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2)\phi(\mathbf{r}_3\sigma_3, \mathbf{r}_4\sigma_4)\ldots\phi(\mathbf{r}_{N-1}\sigma_{N-1}, \mathbf{r}_N\sigma_N)\right], \tag{2.6}$$

where $\mathscr{A}$ is the antisymmetrization operator. The two-body wave function $\phi(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2)$ is regarded as a variational parameter. At this stage, no constraint has yet been put on the form of $\phi(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2)$ except that we require it to be antisymmetric with respect to simultaneous exchange of $(\mathbf{r}_1\sigma_1)$ and $(\mathbf{r}_2\sigma_2)$. In the following, we take the spin structure of $\phi(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2)$ to be a singlet and write the relative spatial wave function as

$$\phi(\mathbf{r}_1 - \mathbf{r}_2) = \sum_{\mathbf{k}} c_{\mathbf{k}} \exp i\mathbf{k}\cdot(\mathbf{r}_1 - \mathbf{r}_2) \tag{2.7}$$

where $c_{-\mathbf{k}} = c_{\mathbf{k}}$ and $a^\dagger_{\mathbf{k}\uparrow}$ is the fermion creation operator for momentum state $\mathbf{k}$ with spin up. Now, if we follow the BCS trick and relax the constraint on the number of particles, we can write the equation which results from minimizing the energy as a

function of the coefficients $c_{\mathbf{k}}$, i.e. the gap equation, in the form (possibly unfamiliar, but completely equivalent to the standard form)

$$2E_{\mathbf{k}}F_{\mathbf{k}} + \sum_{\mathbf{k}'} V(\mathbf{k}-\mathbf{k}')F_{\mathbf{k}'} = 0, \tag{2.8}$$

where $E_{\mathbf{k}} = \sqrt{(\varepsilon_{\mathbf{k}}-\mu)^2 + |\Delta_{\mathbf{k}}|^2}$ is the quasiparticle excitation energy and $\varepsilon_{\mathbf{k}} = \frac{\hbar^2 k^2}{2m}$ is the free particle kinetic energy. $F_{\mathbf{k}} \equiv \frac{c_{\mathbf{k}}}{1+|c_{\mathbf{k}}|^2}$ is the pair wave function. If we compare this with the two-body Schrödinger equation with energy E:

$$(2\varepsilon_{\mathbf{k}} - E)\psi_{\mathbf{k}} + \sum_{\mathbf{k}'} V(\mathbf{k}-\mathbf{k}')\psi_{\mathbf{k}'} = 0, \tag{2.9}$$

we find that for large $|\mathbf{k}|$, $F_{\mathbf{k}}$ has the same structure as $\psi_{\mathbf{k}}$, which suggests that the short-range form of the pair function $F(\mathbf{r}) = \sum_{\mathbf{k}} F_{\mathbf{k}} \exp(i\mathbf{k}\cdot\mathbf{r})$ is the same as that of the two-body wave function. (We shall give a more general argument concerning the short-range form of many-body wave function in the following.) The gap equation (2.9) can be conveniently written in terms of scattering length a_s by a standard renormalization procedure,

$$\frac{1}{V}\sum_{\mathbf{k}}\left[\frac{1}{\varepsilon_{\mathbf{k}}} - \frac{1}{E_{\mathbf{k}}}\right] = \frac{m}{2\pi\hbar^2 a_s}. \tag{2.10}$$

This provides one equation for the gap $\Delta_{\mathbf{k}}$ (which we will take to be independent of $\mathbf{k}$) and the chemical potential μ. Another equation can be obtained by requiring that the average number of particles be N, namely

$$\frac{1}{V}\sum_{\mathbf{k}}\left[1 - \frac{\varepsilon_{\mathbf{k}}-\mu}{E_{\mathbf{k}}}\right] = n. \tag{2.11}$$

The solution of these two equations can be obtained easily in the BEC or BCS limits and in the intermediate regime by numerical means. In the BEC limit, we find that $\mu \to -\frac{\hbar^2}{2ma_s^2}$ and $\Delta \to \frac{4\varepsilon_{\mathrm{F}}}{\sqrt{3\pi k_{\mathrm{F}} a_s}} \sim \sqrt{n}$. In the BCS limit, $\mu \to \varepsilon_{\mathrm{F}}$ and $\Delta \to 8\varepsilon_{\mathrm{F}} e^{-2} \exp\left[-\frac{\pi}{2k_{\mathrm{F}}|a_s|}\right]$, the standard BCS results. At unitarity, we find that the chemical potential $\mu = 0.59\varepsilon_{\mathrm{F}}$ and $\Delta = 0.68\varepsilon_{\mathrm{F}}$. The chemical potential μ goes through zero in the BEC side of the resonance at a value $\xi \sim 1$. The qualitative behavior of the BEC–BCS crossover sketched above is quite satisfactorily tested in experiments. However, there are important effects which are not accounted for in the naïve ansatz even in the BEC and BCS limits. For example, in the BEC limit, the scattering length between molecules turns out to be $0.6a_s$ rather than $2a_s$ as one would get from the naïve ansatz [22]. In the BCS limit, as Gor'kov and Melik-Barkhudarov have shown, there are important polarization contributions to the zero temperature gap parameter [23].

To go beyond the naïve ansatz and discuss the general crossover problem, we first have to examine the sort of approximations that one is allowed to make

in the context of ultracold Fermi gases. In the BEC–BCS crossover model, the scattering length a_s can assume an arbitrarily large value and thus the conventional perturbative calculation using the small gaseousness parameter $\eta \equiv k_F a_s$ is clearly inapplicable. On the other hand, as was pointed out earlier, the actual range of the interaction potential l_{VdW} is small such that $k_F l_{VdW} \ll 1$ is always guaranteed. This suggests that an expansion in binary collisions should be possible. In fact, as we shall see momentarily, such a formulation is exact to the extent that one can describe the system entirely in terms of the s-wave scattering length a_s.

Let us consider then the energy eigenstates $\Psi_N^{(n)}(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2, \ldots, \mathbf{r}_N\sigma_N)$ of the system and ask the following question. Suppose we take two atoms of opposite spin, say at positions $\mathbf{r}_1$ and $\mathbf{r}_2$ with $\sigma_1 \neq \sigma_2$, close together such that $|\mathbf{r}_1 - \mathbf{r}_2| \lesssim l_{VdW}$ while far away (compared with l_{VdW}) to all the other atoms, what will the many-body wave function $\Psi_N^{(n)}(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2, \ldots, \mathbf{r}_N\sigma_N)$ look like? Obviously, in this case, since atoms 1 and 2 cease to interact with the other atoms, the wave function factorizes and we can write it as

$$\Psi_N^{(n)}(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2, \ldots, \mathbf{r}_N\sigma_N) = \mathscr{A}\phi(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2)\Psi_{N-2}^{\prime(n)}(\mathbf{r}_3\sigma_3, \mathbf{r}_4\sigma_4, \ldots, \mathbf{r}_N\sigma_N) \tag{2.12}$$

where $\mathscr{A}$ is the antisymmetrization operator. $\phi(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2)$ is determined by solving the two-body Schrödinger equation in the region $|\mathbf{r}_1 - \mathbf{r}_2| \lesssim l_{VdW}$. Any corrections arise only if a third atom is within a distance $\sim l_{VdW}$ from atoms 1 and 2. Such an event is unlikely for two reasons. Firstly, the phase space associated with this event is a factor $(k_F l_{VdW})^3$ less than that for the two-body encounters. Secondly, in the spin-$\frac{1}{2}$ system we are considering here, two of the three atoms close together must have the same spin orientation, the probability of which is suppressed by the Pauli principle. In fact, by the very formulation of the problem, we have already neglected the higher partial wave scattering, which makes a contribution of order $(k_F l_{VdW})^2$ or higher. Thus, to be consistent, we need not consider three-body processes and the binary expansion becomes exact.[1]

Next, we have to discuss the form of the two-body wave function $\phi(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2)$. We first note that in the crossover model, the spin part of $\phi(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2)$ is necessarily a singlet and will be of no further interest to us. The spatial part of $\phi(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2)$, which we denote as $\widetilde{\phi}(\mathbf{r}_1, \mathbf{r}_2)$, will have a complicated nodal structure in its relative coordinates $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$. However, its short-range form ($|\mathbf{r}| \lesssim l_{VdW}$) should be insensitive to the energy scales of the problem, namely the Fermi energy ε_F and the characteristic width δ_c of the Feshbach resonance. The reason for this is simple: The form of $\widetilde{\phi}(\mathbf{r}_1, \mathbf{r}_2)$ in the region $|\mathbf{r}_1 - \mathbf{r}_2| \lesssim l_{VdW}$ is determined by the competition between the kinetic energy and the deep potential energy, each of which is much larger than ε_F and δ_c. In the region $l_{VdW} \ll r \lesssim a_s, k_F^{-1}$, the form of $\widetilde{\phi}(\mathbf{r}_1, \mathbf{r}_2)$ is fixed by the scattering length. Up to a normalization constant, it is given by

$$\widetilde{\phi}(\mathbf{r}_1 - \mathbf{r}_2) = \text{const.} \times \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}\left(1 - \frac{|\mathbf{r}_1 - \mathbf{r}_2|}{a_s}\right), \tag{2.13}$$

[1] However, in discussing the stability of the system with respect to decay into deeply bound molecular states, such processes are of primary importance.

where we have suppressed the centre of mass dependence which is of no relevance in the discussion below. The whole of the many-body problem can then be viewed as an effort to enforce this particular boundary condition in the many-body wave function. Two routes can be taken in principle. One is to reformulate this boundary condition as a pseudopotential between atoms with opposite spins in the zero-range limit. Another way is to deal with this boundary condition explicitly. We shall follow the second route in the following.

The above discussions, when formulated in terms of density matrices, tell us the following. First, in calculating any physical quantities of interest, knowledge of the two-body density matrix is sufficient. Secondly, the short range form of the eigenfunction $\approx\!\!\!\!\!\!\sim\ \chi_i(r)$ associated with the two-body density matrix defined before is determined by the two-body physics only, while in the region $l_{\mathrm{vdW}} \ll r \lesssim a_s, k_{\mathrm{F}}^{-1}$, it is given by $r \approx\!\!\!\!\!\!\sim\ \chi_i(r) \equiv C_i(\xi, T)\overline{\chi}(r)$, where

$$\overline{\chi}(r) = 1 - \frac{r}{a_s}, \quad l_{\mathrm{vdW}} \ll r \lesssim a_s, k_{\mathrm{F}}^{-1} \tag{2.14}$$

and $C_i(\xi, T)$ is the normalization constant, which in principle depends on ξ as well as temperature T. Note that according to the classification used before, for classes (B) and (C), $C_i(\xi, T)$ is of the form $l^{-1/2}$, where l is some microscopic length scale (to be identified later), while for class (A), $C_i(\xi, T)$ is normalized as $L^{-1/2}$, where L is the linear size of the system. We emphasize that $\overline{\chi}(r)$ is of this particular form and common to all $\approx\!\!\!\!\!\!\sim\ \chi_i(r)$ only for the region indicated; its short-range form is the same as that of $\approx\!\!\!\!\!\!\sim\ \chi_i(r)$, except for the normalization $C_i(\xi, T)$. From a many-body point of view, the complicated short-range physics is not interesting and furthermore, as the discussion above has made clear, can be computed without reference to the many-body state (except the normalizations $C_i(\xi, T)$ which we shall take care of explicitly). It is thus desirable to separate the short-range dependence in any physical quantity that we might be interested in computing. The hope is that, once this is done, the part that remains would be insensitive to the short-range complications and hence be universal.

To do this, let us introduce an arbitrary short-range ($\sim l_{\mathrm{vdW}}$) function $s(\mathbf{r})$ that operates only between the opposite spin states and consider the following integral:

$$A \equiv \int d\mathbf{r}_1 d\mathbf{r}_2 s(\mathbf{r}_1 - \mathbf{r}_2) \left\langle \psi_1^\dagger(\mathbf{r}_1)\psi_2^\dagger(\mathbf{r}_2)\psi_2(\mathbf{r}_2)\psi_1(\mathbf{r}_1) \right\rangle. \tag{2.15}$$

Using Eqs. 2.2 and 2.5, we can write the above expression as

$$\sum_i n_i \int d\mathbf{r} s(\mathbf{r}) \left| \approx\!\!\!\!\!\!\sim\ \chi_i(r) \right|^2 \tag{2.16}$$

with the eigenfunction $\approx\!\!\!\!\!\!\sim\ \chi_i(r)$ appearing in the sum corresponding to the singlet spin wave function $\zeta(S = 0, m = 0)$. Now using Eq. 2.14 above, we find

$$A \equiv \sum_i n_i |C_i(\xi, T)|^2 \int dr s(r) |\overline{\chi}(r)|^2$$
$$\equiv h(\xi, T) k_F N \int dr s(r) |\overline{\chi}(r)|^2. \quad (2.17)$$

Here, we have defined a positive definite universal function

$$h(\xi, T) \equiv \sum_i \frac{n_i}{N k_F} |C_i(\xi, T)|^2 > 0 \quad (2.18)$$

and inserted a factor k_F^{-1} to make $h(\xi, T)$ dimensionless. N is the total number of atoms. The structure of $h(\xi, T)$ is clear. Apart from the constant $(N k_F)^{-1}$, it is a weighted sum of the eigenvalues of the two-body density matrix. We emphasize again that all the n_i's appearing in the sum correspond to singlet eigenfunctions. According to the discussion before, if we have a simple BEC, where only one n_i, say n_0, is of order of N, then this term will make the largest contribution $\sim O(1)$, while all the other terms contribute $\sim O(1/N)$. Note that the sum of the latter might still be larger than the contribution from n_0. Typically, as in the theory of superconductivity, n_0 is associated with the eigenfunction χ_0 that is bound in space, namely $C_0(\xi, T) \sim l^{-1/2}$, where l in the case of superconductivity turns out to be given by the zero temperature Ginzburg-Landau coherence length ξ_{GL}. This conclusion is also valid in the BCS limit of the crossover, while in the BEC limit $C_0(\xi, T) \sim a_s^{-1/2}$ and around unitarity, $C_0(\xi, T) \sim k_F^{1/2}$ (see below).

We further note that the integral in Eq. 2.17 is a purely two-body quantity and as such does not depend on the many-body parameters of the system, namely, temperature T and Fermi energy ε_F. Depending on the form of $s(r)$, it might depend on the scattering length a_s in some complicated way, but as its normalization has made clear, it displays no singularity as one approaches unitarity, $a_s = \pm\infty$. Thus, to all intents and purposes, it can be regarded as a known parameter. The function $h(\xi, T)$, on the other hand, incorporates only the many-body physics and thus one expects it to be universal and independent of the particular alkali element under consideration. The physical significance of $h(\xi, T)$ lies in the fact that as far as the short-range physics is concerned, the many-body system looks just like a two-body problem except that one has to normalize the corresponding two-body wave function in the region $l_{VdW} \ll r \lesssim a_s, k_F^{-1}$ by a value determined by $h(\xi, T)$ [see Eq. 2.17]. Once this is recognized, it is easy to see that $h(\xi, T)$ determines the momentum distribution of the many-body system in the region $k_F, a_s^{-1} \ll k \ll l_{VdW}^{-1}$, $n_k = 4\pi k_F n h(\xi, T)/k^4$, where $n = N/V$ is the average density. In the literature, the combination $C = 4\pi k_F n h(\xi, T)$ is referred to as the "Contact" [24].

In the following, we consider two representative physical quantities in which the universal function $h(\xi, T)$ plays a central role. Common to those physical quantities is that they can be cast in the form of a short-range function, convoluted with the two-body density matrix. Physically, this means that these physical quantities are sensitive to short-range physics and the many-body physics only enters in the determination of the overall amplitude. For more details, see ref. [25].

As we have discussed before, once we eliminate the closed channel from the problem, the open channel potential $V(r)$ acquires an additional magnetic field dependence, which by appropriate rescaling, can be written in terms of a dimensionless parameter λ and hence $V(r;\lambda)$. Now, if we consider a process in which λ changes adiabatically, then according to general arguments of thermodynamics

$$\left.\frac{\partial E}{\partial \lambda}\right|_S = \left\langle \frac{\partial H}{\partial \lambda} \right\rangle = \left\langle \frac{\partial V(r;\lambda)}{\partial \lambda} \right\rangle, \tag{2.19}$$

where E and S are the total energy and entropy of the system, respectively. The average includes both quantum mechanical and statistical ones. In the last step, we have used the fact that only the interaction term in the Hamiltonian depends on λ. Note that $\frac{\partial V(r;\lambda)}{\partial \lambda}$ is a short-range function and we can use the decomposition established before. Furthermore, by using a relation between the variation of the scattering length a_s and that of the interaction potential (see ref. [21], p. 158),

$$\delta a_s^{-1} = -\frac{m}{\hbar^2}\left[\int_0^\infty dr \frac{\partial V(r;\lambda)}{\lambda} |\overline{\chi}(r)|^2\right]\delta\lambda, \tag{2.20}$$

we find, for fixed density,

$$\left.\frac{\partial E}{\partial \xi}\right|_S = 2\varepsilon_F N h(\xi, T). \tag{2.21}$$

The above relation can be conveniently written, using the theorem of small increments (see ref. [26], p. 50), in terms of the free energy F of the system

$$\left.\frac{\partial F}{\partial \xi}\right|_T = 2\varepsilon_F N h(\xi, T). \tag{2.22}$$

Several conclusions can be drawn immediately. Firstly, since $h(\xi, T)$ is positive definite, the free energy F is a strictly increasing function of ξ. Secondly, if we expand F around $\xi = 0$, taking note that $h(\xi = 0, T)$ is a well-defined quantity, we find that in the vicinity of $\xi = 0$, F increases linearly with ξ. By using other thermodynamic relations, one can write the specific heat, entropy and pressure of the system in terms of the universal function $h(\xi, T)$. For more details, see ref. [25].

A second quantity we consider is the interaction energy of the system. For this we simply replace $s(r)$ by the interaction potential $V(r)$ and we find that interaction energy per particle is given by

$$\frac{\langle V \rangle}{N} = C_V(a_s) k_F h(\xi, T), \tag{2.23}$$

where $C_V(a_s) = \int dr\, V(r)|\overline{\chi}(r)|^2$ is the extracted two-body factor. Note that at unitarity, the interaction energy scales with k_F, rather than ε_F (as a naïve dimension

analysis would suggest). The reason for this lies in the fact that interaction energy is sensitive to short-range physics and is not universal. A rough understanding of the k_F scaling might go as follows. Let us look at the many-body wave function $\Psi_N^{(n)}(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2, \ldots, \mathbf{r}_N\sigma_N)$ and ask what can possibly set the scale for the normalization in the region $l_{\mathrm{VdW}} \ll |\mathbf{r}_i - \mathbf{r}_j| \lesssim a_s, k_F^{-1}, \sigma_i \neq \sigma_j$. At unitarity, the only scale that is relevant in the region indicated is k_F^{-1} and since the radial wave function has dimension $[L]^{-1/2}$, we conclude

$$\lim_{l_{\mathrm{VdW}} \ll |\mathbf{r}_i - \mathbf{r}_j| \lesssim k_F^{-1}} |\mathbf{r}_i - \mathbf{r}_j| \, \Psi_N^{(n)}(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2, \ldots, \mathbf{r}_N\sigma_N) \propto k_F^{1/2}. \tag{2.24}$$

The interaction energy, which depends on the modulus square amplitude of the wave function, turns out to depend linearly on k_F, as obtained above. We note that the same reasoning leads to the conclusion that the average radio-frequency shift and the population of closed channel molecules also scale with k_F at unitarity. For more details concerning the later two quantities, see Refs. [25, 27].

The realization of the existence of the universal function in the many-body physics was first made by Tan based on an analysis of the many-body wave function and some of his results were later re-derived by Braaten and Platter using the operator product expansion, which is the ideal tool to explore the short-range physics in a field theory context [28, 24]. Recently, Combescot et al. [29] have extended the same consideration to two dimensions.

An important consequence of the considerations given above is that it should be possible to check the mutual consistency of experimental results obtained on different physical quantities. This should be particularly useful at unitarity, where the dependence of such quantities on the details of the trap used should disappear.

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