Dressed Feshbach molecules in the BEC-BCS crossover

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We present the RPA theory of the BEC-BCS crossover in an atomic Fermi gas near a Feshbach resonance that includes the relevant two-body atomic physics exactly. This allows us to determine the probability \( Z \) for the dressed molecules in the Bose-Einstein condensate to be in the closed channel of the Feshbach resonance and to compare with the recent experiments of Partridge et al.\textsuperscript{6} with \( ^{6}\text{Li} \). We determine for this extremely broad resonance also the condensate density of the dressed molecules throughout the BEC-BCS crossover.

**Introduction.** — The superfluid phase in an atomic Fermi gas near a Feshbach resonance realizes a fundamentally new state of matter, which shows a macroscopic coherence between atom pairs and molecules that is controlled by the applied magnetic field. As a result, such a gas offers the exciting possibility to study in great detail the crossover between the Bose-Einstein condensation (BEC) of diatomic molecules and the Bose-Einstein condensation of atomic Cooper pairs, i.e., the Bardeen-Cooper-Schrieffer (BCS) transition.\textsuperscript{1-4} In fact, the BEC-BCS crossover region is presently already actively being explored by a number of experimental groups around the world.\textsuperscript{2,5,7,8}

In more detail the physics of the BEC-BCS crossover occurring near a Feshbach resonance can be understood as follows: The superfluid phase of the gas is always associated with a Bose-Einstein condensate of pairs, but the wave function of the pairs or dressed molecules is given by the linear superposition

\[
|\mathbf{r}⟩\chi_{\text{dressed}}(\mathbf{r}) = \sqrt{Z}χ_{m}(\mathbf{r})|\text{closed}⟩ + \sqrt{1-Z}χ_{\text{aa}}(\mathbf{r})|\text{open}⟩.
\]

In the BEC limit the applied magnetic field is taken such that the bare molecular energy level lies far below the threshold of the two-atom continuum and we have \( Z \simeq 1 \). In that case we are dealing with a Bose-Einstein condensate of tightly-bound diatomic molecules and the spatial part of the pair wave function is equal to the bare molecular wave function \( χ_{m}(\mathbf{r}) \). The spin part of the pair wave function is then equal to \(|\text{closed}⟩\), i.e., the spin state of the closed channel that causes the Feshbach resonance.\textsuperscript{11} In the BCS limit the bare molecular energy level lies far above the threshold of the two-atom continuum and can be adiabatically eliminated. We then have that \( Z \simeq 0 \) and the spatial part of the pair wave function equals the usual BCS wave function for atomic Cooper pairs \( χ_{\text{aa}}(\mathbf{r}) \). This Cooper-pair wave function depends also on the magnetic field, because the effective attraction between the atoms after the adiabatic elimination of the bare molecular state depends on the energy of that state. The spin state of the Cooper pairs is, however, always equal to the spin state \(|\text{open}⟩\) of the open channel of the Feshbach problem.

The probability \( Z \) plays therefore a crucial role in the description of the BEC-BCS crossover since it quantifies the amount of coherence between the atom pairs and the bare molecules in the gas. Unfortunately, however, the various theories\textsuperscript{12-16,17,18,19,20} that are presently being used to understand the outcome of the experiments are unable to accurately determine this quantity. This comes about because, either \( Z \) is assumed to be zero from the outset, the many-body theory does not incorporate the two-body Feshbach physics exactly, or the theory is able to determine only the total number of bare molecules in the gas and thus requires an additional assumption about the total number of dressed molecules to extract \( Z \). This situation is particularly unsettling because of the recent \( ^{6}\text{Li} \) experiments of Partridge et al.\textsuperscript{16}, which have used the photodissociation rate to measure the value of \( Z \) throughout the crossover regime. In view of the above situation it is pressing to develop an ab initio many-body theory for the calculation of \( Z \). How that may be achieved is the main topic of this Letter.

**BEC-BCS crossover theory.** — Introducing creation and annihilation operators for the bare molecules and atoms, the effective grand-canonical hamiltonian of the gas with chemical potential \( μ \) becomes\textsuperscript{11,21,22}

\[
H = \int d\mathbf{x} \left( \frac{-\hbar^2 \nabla^2}{2m} + \delta - 2\mu \right) ψ_{m}(\mathbf{x}) (1) + \sum_{σ=↑,↓} \int d\mathbf{x} ψ_{σ}^{†}(\mathbf{x}) \left( -\frac{\hbar^2 \nabla^2}{2m} - μ \right) ψ_{σ}(\mathbf{x}) + g \int d\mathbf{x} \left( ψ_{m}^{†}(\mathbf{x})ψ_{↑}(\mathbf{x})ψ_{↓}(\mathbf{x}) + ψ_{↑}^{†}(\mathbf{x})ψ_{m}^{†}(\mathbf{x})ψ_{m}(\mathbf{x}) \right) + \frac{4πa_{\text{bg}}\hbar^2}{m} \int d\mathbf{x} ψ_{m}^{†}(\mathbf{x})ψ_{↑}^{†}(\mathbf{x})ψ_{↑}(\mathbf{x})ψ_{↓}(\mathbf{x}) ,
\]

where the two hyperfine states of the atoms are denoted by \(|↑⟩\) and \(|↓⟩\), and the magnetic-moment difference \( Δμ_{\text{mag}} \) between the hyperfine states \(|\text{closed}⟩\) and \(|\text{open}⟩ = (|↑⟩ - |↓⟩)/\sqrt{2} \) gives the so-called detuning from resonance \( δ = Δμ_{\text{mag}}(B - B_{0}) \). Note that the atom-molecule coupling constant \( g \) and the background scattering length \( a_{\text{bg}} \) depend on the magnetic field \( B \) in such a manner that the total scattering length \( a = a_{\text{bg}} - mg^2/4π\hbar^2δ \) agrees with the Feshbach reso-
nance of interest. This is especially important for the broad Feshbach resonance near 834 Gauss that is used in all $^6$Li experiments up to date 22,23.

From now on we consider only the most interesting region close to resonance, where $a_{bg} \ll a$ and the effective interaction between the atoms is dominated by the resonant part $-g^2/\delta$. This suggests that the last term in the right-hand side of Eq. 1 can be neglected altogether. This is, however, not true because we can neglect this term only after we have included its effect on the atom-molecule coupling 25. Physically, the reason for this subtlety is that the above Hamiltonian is an effective Hamiltonian that is only valid for low energies. However, to properly account for the two-body physics near a Feshbach resonance also high-energy states are needed. The main effect of these high-energy states is to renormalize the atom-molecule coupling to $g(k) \equiv g/(1 + ika_{bg})$, where $k$ is the relative momentum of the atoms involved in the coupling 11,24. Only after having performed this substitution are we allowed to neglect the background interaction between the atoms.

Without the background interaction the atomic part of the Hamiltonian is quadratic. Using standard functional methods the fermionic fields can thus be integrated out exactly. This leads to an effective action for the molecules that at sufficiently low temperatures has a minimum at a nonzero value of $|\langle \psi_m(x) \rangle|^2 \equiv \sqrt{Z n_{mc}}$, where we introduced the dressed molecular condensate density $n_{mc}$. Neglecting fluctuations at this point leads to a mean-field theory of the BEC-BCS crossover. As mentioned in the introduction, however, this mean-field theory is unable to calculate the probability $Z$ since it only determines the bare molecular condensate density $|\langle \psi_m(x) \rangle|^2$. We therefore also consider the quadratic fluctuations around the minimum of the effective molecular action, i.e., we consider the Bogoliubov theory of the bare molecules.

As expected with a spontaneously broken $U(1)$ symmetry associated with the presence of a Bose-Einstein condensate, the gaussian fluctuations are determined by normal and anomalous self energies of the bare molecules, which at zero temperature reduce to

\[
\begin{align*}
\hbar \Sigma_{11}(k, i\omega) &= \int \frac{dk'}{(2\pi)^3} |g(k')|^2 \left\{ \frac{|u_a(k'_+)|^2|v_a(k'_-)|^2}{i\omega + \hbar \omega_a(k'_+) - \hbar \omega_a(k'_-)} - \frac{|v_a(k'_+)|^2|v_a(k'_-)|^2}{i\omega + \hbar \omega_a(k'_+) + \hbar \omega_a(k'_-)} + \frac{1}{2\epsilon(k')} \right\}, \\
\hbar \Sigma_{12}(k, i\omega) &= 2 \int \frac{dk'}{(2\pi)^3} |g(k')|^2 \left\{ u_a(k'_+)v_a(k'_-)u_a(k'_-)v_a(k'_+) \frac{\hbar \omega_a(k'_+)}{(\hbar \omega_a(k'_+)) + \hbar \omega_a(k'_-)} + \frac{1}{2\epsilon(k')} \right\}.
\end{align*}
\]

Here we have also introduced the BCS dispersion $\hbar \omega_a(k) = \sqrt{(\epsilon(k) - \mu)^2 + |g(k)|^2Z n_{mc}}$, the bare atomic dispersion $\epsilon(k) = \hbar^2k^2/2m$, the usual BCS coherence factors $u_a(k)$ and $v_a(k)$, and the notation $k'_\pm = k/2 \pm k'$. In terms of the above self energies the minimum of the effective action is determined by the exact Hugenholtz-Pines relation $2\mu = \delta + \hbar \Sigma_{11}(0,0) - \hbar \Sigma_{12}(0,0)$, which turns out to be equal to a modified BCS gap equation

\[
\delta - 2\mu = \int \frac{dk}{(2\pi)^3} |g(k)|^2 \left( \frac{1}{2\hbar \omega(k)} - \frac{1}{2\epsilon(k)} \right).
\]

Finally, we also need the equation of state, which we for consistency reasons 11 obtain by differentiating the thermodynamic potential with respect to the chemical potential. Including the effect of the fluctuations we obtain for the total density of atoms

\[
n = -\text{Tr}[G_a] + 2Z n_{mc} - \text{Tr}[G_m] + \frac{1}{2} \text{Tr} \left[ G_m \frac{\partial \Sigma}{\partial \mu} \right],
\]

where $G_a$ and $G_m$ are the Nambu ($2 \times 2$)-matrix Green’s functions of the bare atoms and molecules, respectively. For a given density and magnetic field the last two equations determine only the bare molecular condensate density and the chemical potential. Hence, we need a third equation to determine also $Z$.

**Dressed molecules.** — Before we derive this missing equation, let us first discuss in some more detail the physics behind the maybe somewhat unexpected equation of state in Eq. 4. The first two terms that represent the mean-field theory without fluctuations that is most often used in the recent literature 14,15,16,18. Because of the absence of fluctuations all the molecules are Bose-Einstein condensed and there is no depletion. The third term precisely corresponds to this depletion. Finally, the fourth term physically describes the dressing of the bare atoms and molecules. This can be made more clear by reformulation the equation of state in terms of dressed atoms and molecules, instead of bare atoms and molecules. Since every dressed molecule contains two atoms, we expect the contribution $2n_{mc}$ from the condensate of dressed molecules. Indeed, in the BEC limit it can be shown explicitly that the atomic density $-\text{Tr}[G_a] = 2 \int dk |v_a(k)|^2/(2\pi)^3$ contains exactly the expected contribution $2(1 - Z)n_{mc}$ of paired atoms in the Bose-Einstein condensate of dressed molecules. The
atomic density does, however, not contain the paired atoms associated with the dressed molecules that are not in the Bose-Einstein condensate. This omission is repaired by the fluctuation corrections which contain both the associated changes in the atomic density and twice the total density of dressed molecules that are not Bose-Einstein condensed, i.e., twice the dressed molecular depletion.

We are now in a position to determine $Z$. In principle it is equal to the residue of the pole of $G_{m;11}(0,i\omega)$ at $\omega = 0$. To understand the physics of that result better it is useful to consider the spectral function of the bare molecules with zero momentum, i.e., $\rho_m(0,\omega) = -\text{Im}(G_{m;11}(0,\omega+i0))/\pi$. This spectral function is closely related to the density of states of the molecules at zero momentum and thus gives detailed information on the dressed molecular content of the gas. Most importantly for our purpose, the Bose-Einstein condensate of dressed molecules gives rise to a delta-function in the spectral function exactly at zero frequency. The strength of this delta function is precisely $Z$, because this is the probability to take a bare molecule out of the Bose-Einstein condensate of dressed molecules. Besides this bound-state contribution, the spectral function contains also a contribution from the continuum of atomic scattering states. In the BEC limit of the crossover the continuum contribution only occurs at positive frequency and starts at a frequency of $-2\mu/\hbar \simeq 2\hbar/ma^2$ as shown in Fig. 1a. In the BCS limit the continuum contribution occurs both at positive and negative frequencies, which start at a frequency of about $\pm 2g\sqrt{Z n_{\text{mc}}}/\hbar$, respectively, due to the gap that exists for the creation of an atomic quasiparticle-quasihole pair. This is shown in Fig. 1b. The negative frequency part of the spectral function is especially important, because it determines the depletion of the Bose-Einstein condensate of dressed molecules. Physically it represents the dressed molecules that are stabilized by the Fermi sea $\mathbf{2Q}$. Making use of the above physical picture, we finally obtain the desired result,

$$Z = \frac{1 - \Sigma^{(1)}_{11}}{(1 - \Sigma^{(1)}_{11})^2 + \Sigma_{12} \left(\Sigma^{(2)}_{12} - \Sigma^{(2)}_{11}\right)},$$

where $\Sigma^{(n)}_{ij} \equiv (-i)^n \partial^n \Sigma_{ij}(0,0)/\partial \omega^n$.

At nonzero momenta the spectral function is similar but now contains two delta functions at the frequencies $\pm \omega_m(k)$, which have the strength $Z|\nu_m(k)|^2$ and $-Z|\nu_m(k)|^2$, respectively, with $|\nu_m(k)|^2 - |\nu_m(k)|^2 = 1$.

This shows explicitly how at long wavelengths our theory leads to a Bogoliubov-like theory for dressed molecules with a wave function renormalization factor $Z$. Moreover, in agreement with the Goldstone theorem, the quasiparticle dispersion $\omega_m(k)$ always turns out to be linear at long wavelengths. In the following we therefore determine also the associated speed of (second) sound throughout the BEC-BCS crossover region.

**FIG. 1:** Spectral functions of the bare $^6$Li$_2$ molecules with zero momentum a) in the BEC limit at 571 Gauss and b) in the BCS limit at 892 Gauss of the crossover occurring near the broad Feshbach resonance of $^6$Li at 834 Gauss. The Fermi energy of the gas is 380 nK.

**FIG. 2:** The solid curve shows the probability $Z$ and the dashed curve the fraction $2Z n_{\text{mc}}/n$ as a function of magnetic field. The Fermi energy $\hbar^2 k_F/2m$ of the gas is 380 nK. The data points are from the experiment of Partridge et al. [10]. In the inset the solid line shows the Bose-Einstein condensate fraction of dressed molecules $2n_{\text{mc}}/n$ and the dashed line the contribution of the fluctuations to the total atomic density. The vertical lines indicate the magnetic fields where $k_F|\alpha| = 1$.

**Results and discussion.** — In Fig. 2 we show our results for $Z$ and compare with the experimental data of Partridge et al. [10]. In general the agreement is satisfactory. This is particularly true at relatively low magnetic fields where $Z$ is determined by two-body physics, which is exactly incorporated into our theory. At higher magnetic fields the theoretical values of $Z$ are somewhat higher than the experimental ones. We believe that the reasons for this are twofold. First, the experiment is performed in an optical trap. As a result the experimental data involves an appropriate average over the den-
sity profile of the gas, which lowers the observed value of $Z$. Second, the photodissociation laser used in the experiment has a width which is much larger than the Fermi energy of the gas. The laser, therefore, has not sufficient resolution to probe only the Bose-Einstein condensate of dressed molecules, and probes also the dressed molecules which are not Bose-Einstein condensed. This second effect should be especially important at high magnetic fields. To disentangle these different effects, however, goes beyond the scope of the present Letter and is left for further investigation.

We also show in Fig. 2 the Bose-Einstein condensate fraction of dressed molecules $2\eta_{\text{mc}}/n$ throughout the BEC-BCS crossover. In qualitative agreement with the poor man’s approach of Ref. [12], the latter fraction is never substantially below the Feshbach resonance and becomes negligible only sufficiently far above the Feshbach resonance when $k_F|\alpha| < 1$. This is an important observation, because in our theoretical description of the experiment of Partridge et al. the molecular probe couples directly to the dressed molecules, which act as distinct entities in the gas since the atom-molecule coupling is much larger than the coupling of the probe laser to the bare molecules. In this manner it is most easy to understand the experimental observation that there is initially an exponential (one-body) decay of a large part of the total atomic density with a rate that is much smaller than the bare molecular photodissociation rate.

For completeness we give in Fig. 2 also the Bose-Einstein condensate fraction of bare molecules $2Z\eta_{\text{mc}}/n$ and the fluctuation corrections to the total atomic density. As expected the fluctuation corrections are very important in the crossover region and become small far away from the Feshbach resonance, where mean-field theory applies. From the fluctuations we also extract the speed of sound of the gas, which is shown in Fig. 3. Note that in the BCS limit the Anderson-Bogoliubov mode is recovered. In combination with the presence of the sharp peaks in the spectral function in Fig. 1b, this shows that also the decoupling of the amplitude and phase fluctuations of the Bose-Einstein condensate of dressed molecules that occurs in the BCS limit is correctly incorporated. We therefore conclude that the RPA-like atom-molecule theory developed here gives an excellent account of the subtle interplay between two-body and many-body physics taking place at the crossover near a Feshbach resonance.

We are very grateful for many helpful remarks and stimulating discussions with Randy Hulet. This work is supported by the Stichting voor Fundamenteel Onderzoek der Materie (FOM) and the Nederlandse Organisatie voor Wetenschappelijk Onderzoek (NWO).

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FIG. 3: The speed of sound as a function of magnetic field. The Fermi energy of the gas is 380 nK. The dashed curves show the Bogoliubov result $\hbar k_F/\sqrt{3m} \equiv v_F/\sqrt{\pi}$ of the Anderson-Bogoliubov mode.
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