BEC-BCS crossover in an optical lattice

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We present the microscopic theory for the BEC-BCS crossover of an atomic Fermi gas in an optical lattice, showing that the Feshbach resonance underlying the crossover in principle induces strong multiband effects. Nevertheless, the BEC-BCS crossover itself can be described by a single-band model since it occurs at magnetic fields that are relatively far away from the Feshbach resonance. A criterion is proposed for the latter, which is obeyed by most known Feshbach resonances in ultracold atomic gases.

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I. INTRODUCTION

Ever since the compelling work of DeMarco and Jin [1], the study of degenerate Fermi gases has been at the forefront of ultracold atomic physics. Much of the impetus behind current research in this field was provided by the successful experimental investigation in the last two years of the crossover between the Bose-Einstein condensate (BEC) of molecules and the Bardeen-Cooper-Schrieffer (BCS) state of Bose-Einstein condensed Cooper pairs [2–8]. The pairing observed in an unequal spin mixture is presently under intense scrutiny [9,10]. Another exciting direction being explored lately is the physics of ultracold Fermi gases in an optical lattice [11]. The latter gives, for instance, the possibility to experimentally solve the famous positive-U Hubbard model with repulsive on-site interactions, which is believed to embody the physics of high-temperature superconductors [12,13]. The negative-U Hubbard model with an attractive on-site interaction [14] can also be explored. This model is interesting, for example, because, at half filling, particle-hole symmetry leads to an exact SO(4) symmetry. Therefore, the physics at half filling is analogous with that of the SO(5) theory proposed for high-temperature superconductors [15–17]. Moreover, at low filling fractions, a BEC-BCS crossover takes place. This is the subject of the present paper.

In the atomic gases of interest, studying the BEC-BCS crossover demands the exploitation of a Feshbach resonance [18,19]. As a result, the physics is much richer than in the negative-U Hubbard model and requires a multiband description. This is elucidated in Fig. 1. In the absence of an optical lattice, and including solely two-body effects, a dressed molecule formally exists only below the Feshbach resonance with a binding energy that, near resonance, depends quadratically on the magnetic field. Its binding energy is shown as the dashed-dotted line. Above the Feshbach resonance, the dressed molecule is merely a resonance state because it then has a finite lifetime due to the possibility of decaying into the atomic continuum [20], as represented by the dotted line continuation.

Placing the system in a sufficiently deep optical lattice, the bare (closed-channel) molecular state of the Feshbach resonance interacts primarily with a discrete set of atomic states instead of an atomic continuum. Thus, a dressed molecule now exists for all magnetic fields and its energy, plotted as dashed lines, shows a number of avoided crossings before it ultimately becomes a resonance in the continuum above the optical lattice potential.

Using this result, we can restate the interacting problem for deep optical lattices in terms of atoms and dressed molecules emerging from the on-site two-body solution. The binding energy of these dressed molecules obtained from our exact solution of the on-site Feshbach problem is in good agreement with recent experimental data [21,22], showing the validity of this approach. Many-body physics enters if we allow both the atoms and the dressed molecules to hop to

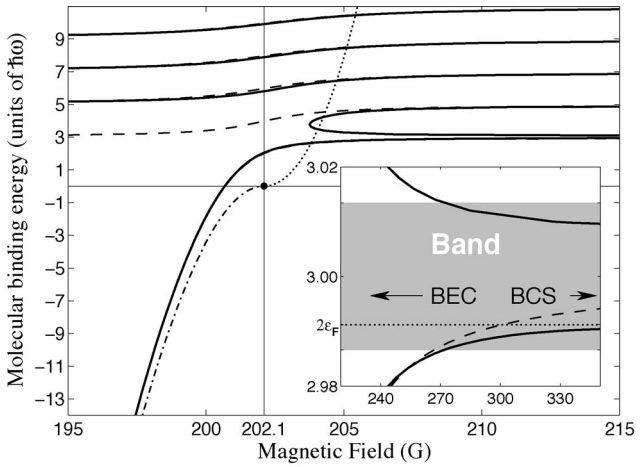

FIG. 1. Comparison of the dressed molecular binding energy at various magnetic fields for the homogenous, the on-site two-body, and the many-body cases corresponding to the dashed-dotted, dashed, and solid lines, respectively. We use ^{40}K atoms near the Feshbach resonance at $B_0=202.1$ G and with a filling fraction of 0.1. The on-site harmonic oscillator frequency ω is $2\pi\times 58275$ Hz, which corresponds to a lattice with wavelength $\lambda=806$ nm and a Rabi frequency of $\Omega_R=2\pi\times 1.43$ GHz. In the homogeneous case, the molecules become short-lived resonances above B_0 and this is indicated by a dotted curve. The inset shows the two-particle continuum associated with the lowest Bloch band. The two-body binding energy crosses through twice the Fermi energy at $B\simeq 300$ G, demonstrating that the BEC-BCS crossover occurs far from B_0. The upper curve in the inset corresponds to the hole-particle symmetric solution of the BCS gap equation.

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adjacent lattice sites [23]. In particular, for the low filling fractions considered, the two-body binding energy of the dressed molecules passes through the Fermi sea in the lowest Bloch band, as shown in the inset of Fig. 1. It is due to this phenomenon that the BEC-BCS crossover occurs in this resonantly interacting case [24]. The interaction of the molecules with the Fermi sea further clads the dressed molecules with many-body effects, resulting in a change of the binding energy such that it only asymptotically reaches twice the Fermi energy at high magnetic fields, as shown by the solid line. Mathematically, this arises because the two-body pole at $3\hbar\omega$ in the self-energy of the molecules is replaced by the famous logarithmic BCS singularity at twice the Fermi level. By placing the system in an optical lattice, we thus find that the BEC-BCS crossover takes place rather far from the resonance. Consequently, as we shall show below, we may always use the single-band approximation to describe the BEC-BCS crossover for all experimentally relevant Feshbach resonances.

II. BEC-BCS CROSSOVER THEORY IN THE LATTICE

We now begin with an outlay of our general BEC-BCS crossover theory in the lattice before discussing the specific case of ^{40}K. The second-quantized grand-canonical Hamiltonian in the presence of an optical lattice potential $V(\mathbf{x})$ is

$$H = \int d\mathbf{x}\psi_{\mathrm{m}}^{\dagger}(\mathbf{x})\left[-\frac{\hbar^2\nabla^2}{4m} + \delta - 2\mu + 2V(\mathbf{x})\right]\psi_{\mathrm{m}}(\mathbf{x}) + \sum_{\sigma=\uparrow,\downarrow}\int d\mathbf{x}\psi_{\sigma}^{\dagger}(\mathbf{x})\left[-\frac{\hbar^2\nabla^2}{2m} - \mu + V(\mathbf{x})\right]\psi_{\sigma}(\mathbf{x}) + g\int d\mathbf{x}\left[\psi_{\mathrm{m}}^{\dagger}(\mathbf{x})\psi_{\uparrow}(\mathbf{x})\psi_{\downarrow}(\mathbf{x}) + \psi_{\downarrow}^{\dagger}(\mathbf{x})\psi_{\uparrow}^{\dagger}(\mathbf{x})\psi_{\mathrm{m}}(\mathbf{x})\right], \tag{1}$$

where $\psi_{\sigma}(\mathbf{x})$ are the atomic and $\psi_{\mathrm{m}}(\mathbf{x})$ the molecular annihilation operators, and μ is the chemical potential. The atom-molecule coupling is given by $g=\hbar\sqrt{4\pi a_{\mathrm{bg}}\Delta B\Delta\mu_{\mathrm{mag}}/m}$, where a_{bg} is the background scattering length, ΔB is the width of the Feshbach resonance, $\Delta\mu_{\mathrm{mag}}$ is the difference in magnetic moments between the closed and open channels of the Feshbach resonance, and m is the atomic mass [20,24]. The detuning from resonance is $\delta=\Delta\mu_{\mathrm{mag}}(B-B_0)$, where B_0 is the value of the magnetic field B at the resonance. It gives the location of the bare molecular level with respect to the atomic continuum in the absence of the lattice.

With a lattice potential present, we turn to a description in terms of Bloch bands since plane wave states no longer diagonalize the Hamiltonian. Summing the effects of nearest-neighbor tunneling leads to a dispersion in the lowest band of the optical lattice equal to $\varepsilon(\mathbf{k})=-2t^{\mathrm{a}}[\cos(k_x\lambda/2)+\cos(k_y\lambda/2)+\cos(k_z\lambda/2)]+3\hbar\omega/2$, with λ the wavelength of the lattice laser and $3\hbar\omega/2$ the on-site, ground-state energy of a single atom. The atomic and molecular tunneling amplitudes are given by $t_{\mathrm{a,m}}=4(V_0^3E_{\mathrm{a,m}}^{\mathrm{R}}/\pi^2)^{1/4}\exp(-2\sqrt{V_0/E_{\mathrm{a,m}}^{\mathrm{R}}})$, where V_0 is the peak-to-trough depth of the optical lattice potential and the atomic and molecular recoil energies are $E_{\mathrm{a}}^{\mathrm{R}}=2(\pi\hbar)^2/m\lambda^2$ and $E_{\mathrm{m}}^{\mathrm{R}}=E_{\mathrm{a}}^{\mathrm{R}}/2$. Moreover, the effective on-site atom-molecule coupling $g_b^2=g^2\int d\mathbf{x}|\chi_b(\mathbf{x})|^4$ becomes band dependent, where $\chi_b(\mathbf{x})$ is the Wannier function in band $b=0,1,2,\ldots$ of the optical lattice. In the lowest band, we write this effective coupling as $g'\equiv g_0=g/(2\pi l^2)^{3/4}$ where $l=\sqrt{\hbar/m\omega}$ is the on-site harmonic oscillator length [23].

Obtaining pertinent thermodynamic quantities for this system involves the calculation of the molecular self-energy. We obtain this self-energy by first integrating the fermions out of the partition function exactly. We then perform an random phase approximation (RPA) or Bogoliubov approximation around the mean field $\Delta=g'\langle\psi_{\mathrm{m}}\rangle\equiv g'\sqrt{n_{\mathrm{mc}}^{\mathrm{B}}}$ of the bare molecular condensate. This approach is known to work well in the zero-temperature limit considered here [25]. In the on-site two-body limit, we have $t_{\mathrm{a}}=0$ and $\Delta=0$, leaving dispersionless harmonic oscillator bands with energies $\varepsilon_b=(b+3/2)\hbar\omega$. The two-body molecular self-energy then becomes $\hbar\Sigma(E)=g'^2\sqrt{\pi}G(E-3\hbar\omega)/\hbar\omega$, where the analytic sum over dispersionless bands is encapsulated in the function [26] $G(E)\equiv\Gamma(-E/2\hbar\omega)/\Gamma(-E/2\hbar\omega-1/2)$. The binding energy of the dressed molecules is then found from $E=\delta+3\hbar\omega/2+\hbar\Sigma(E)$.

In the many-body case, where t_{a}, t_{m}, and Δ are all nonzero, in general, we work in a regime where the temperature is sufficiently below the Fermi temperature that we may use a zero-temperature approximation. Because of the large band gap in a deep optical lattice, the structure of all bands but the lowest has a negligible effect and they can be taken to be dispersionless, as in the two-body case. However, they cannot be excluded altogether from calculations since, as we have just witnessed, they renormalize the two-body energy levels. The BCS dispersion relation of the fermions is now $\hbar\omega(\mathbf{k})=\sqrt{[\varepsilon(\mathbf{k})-\mu]^2+|\Delta|^2}$, and we can write the normal and anomalous molecular self-energies in terms of the usual coherence factors of BCS theory $|u(\mathbf{k})|^2=\{\hbar\omega(\mathbf{k})+\varepsilon(\mathbf{k})-\mu\}/2\hbar\omega(\mathbf{k})$ and $|v(\mathbf{k})|^2=\{\hbar\omega(\mathbf{k})-[\varepsilon(\mathbf{k})-\mu]\}/2\hbar\omega(\mathbf{k})$ to obtain

$$\hbar\Sigma_{11}(\mathbf{k},i\omega_n) = \frac{g'^2\sqrt{\pi}G(E)}{\hbar\omega} - \frac{g'^2}{i\hbar\omega_n - 3\hbar\omega + 2\mu} + \frac{g'^2}{N_{\mathrm{S}}}\sum_{\mathbf{k}'}\left\{\frac{|u(\mathbf{k}_+)|^2|u(\mathbf{k}_-)|^2}{i\hbar\omega_n - \hbar\omega(\mathbf{k}_+) - \hbar\omega(\mathbf{k}_-)} - \frac{|v(\mathbf{k}_+)|^2|v(\mathbf{k}_-)|^2}{i\hbar\omega_n + \hbar\omega(\mathbf{k}_+) + \hbar\omega(\mathbf{k}_-)}\right\}, \tag{2}$$

$$\hbar\Sigma_{12}(\mathbf{k},i\omega_n) = \frac{2g'^2}{N_{\mathrm{S}}}\sum_{\mathbf{k}'}u(\mathbf{k}_+)v(\mathbf{k}_+)u(\mathbf{k}_-)v(\mathbf{k}_-) \times\frac{\hbar\omega(\mathbf{k}_+) + \hbar\omega(\mathbf{k}_-)}{[\hbar\omega(\mathbf{k}_-) + \hbar\omega(\mathbf{k}_+)]^2 + \hbar^2\omega_n^2}, \tag{3}$$

where $\mathbf{k}_{\pm}=\mathbf{k}'\pm\mathbf{k}/2$, $E=i\hbar\omega_n+2\mu-3\hbar\omega$, N_{S} is the total number of lattice sites and the sums are over the first Brillouin zone only: $k_x',k_y',k_z'\in(-2\pi/\lambda,2\pi/\lambda)$. An equation for

the BCS gap Δ is then found in the form of a Hugenholtz-Pines relation

$$2\mu = \delta + \frac{3\hbar\omega}{2} - 6t^{\mathrm{m}} + \hbar\Sigma_{11}(\mathbf{0},0) - \hbar\Sigma_{12}(\mathbf{0},0). \quad (4)$$

Having these quantities in hand enables us to determine the partition function of the system from the Gaussian effective action of our RPA theory and, via the resulting thermodynamic potential Ω, we can calculate the total number of particles using the identity $N=-\partial\Omega/\partial\mu$. This leads to the equation of state for the total atomic filling fraction $n=N/N_{\mathrm{S}}$ given by

$$n = \mathrm{Tr}[\tau_3 \mathbf{G}_{\mathrm{BCS}}] + 2\frac{|\Delta|^2}{g'^2} - \mathrm{Tr}[\mathbf{G}_{\mathrm{m}}] + \frac{1}{2}\mathrm{Tr}\left[\mathbf{G}_{\mathrm{m}}\frac{\partial\hbar\Sigma}{\partial\mu}\right], \quad (5)$$

where τ_3 is the third Pauli matrix and the 2×2 Nambu space matrices $\mathbf{G}_{\mathrm{BCS}}$, $\mathbf{G}_{\mathrm{m}}$ and Σ are the BCS atomic Green's function, the molecular Green's function, and self-energy matrix composed of Eqs. (2) and (3), respectively.

III. RESULTS AND DISCUSSION

Although our approach is quite general, the numerical calculations in this paper are for the $B_0=202.1$ G Feshbach resonance of ^{40}K atoms, which has a width of $\Delta B=7.8$ G [2], and for a total filling fraction of 0.1 as an illustrative and experimentally relevant case. For every δ, solving the BCS gap equation, Eq. (4), and the equation of state simultaneously yields self-consistent values for μ and the filling fraction of the bare molecular condensate $n_{\mathrm{mc}}^{\mathrm{B}}=\Delta^2/g'^2$. Since fluctuation effects are expected to be less important away from resonance, in the first instance we neglect the fluctuation contribution reflected by the last two terms on the right-hand side of Eq. (5). In order to examine $n_{\mathrm{mc}}^{\mathrm{B}}$, it proved requisite to include the structure of the higher bands to which intermediate states strongly couple in the neighborhood of the Feshbach resonance. Having done so, the many-body result monotonically approaches the two-body limit in the resonant region as more bands are included in the self-energy calculation. This is clear from Fig. 2. When including higher bands, we used a multiband generalization of Eqs. (2) and (3) that did not factor in any interband coupling other than the already present interaction of the mean field $\Delta_b=g_b\langle\psi_{\mathrm{m}}\rangle$ with the molecular condensate. Although this leads to only qualitative results in the higher bands, the correct two-body physics is obtained and the importance of multiband effects near resonance is well demonstrated.

We also determine the filling fraction of Bose-Einstein condensed dressed molecules as this will provide us with another good indication of where the crossover from a Bose-Einstein condensate of dressed molecules to the BCS state composed of Bose-Einstein condensed Cooper pairs takes place. This fraction is given by $n_{\mathrm{mc}}=n_{\mathrm{mc}}^{\mathrm{B}}/Z$, where Z is the so-called wave-function renormalization factor, which determines the probability amplitude for the dressed molecular wave function, to be in the bare molecular state [20]. This is plotted in the inset of Fig. 3. For this purpose, we did not calculate the true many-body Z, which would involve the full fluctuation calculation [25], but used instead the two-body wave-function renormalization factor given by $Z^{2\mathrm{B}}=1/[1-\partial\hbar\Sigma(E)/\partial E]$, where $\hbar\Sigma(E)$ is the two-body self-energy discussed earlier.

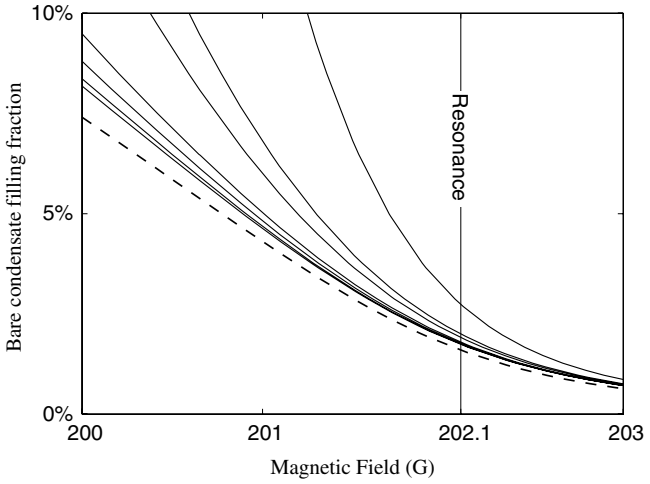

FIG. 2. The filling fraction of the bare molecular condensate, $2n_{\mathrm{mc}}^{\mathrm{B}}/n$, drawn as solid lines, decreases monotonically to the two-body limit as progressively more bands are included, from 1 to 300 in this case. The dashed line is $Z^{2\mathrm{B}}$, which is equivalent to the filling fraction of the molecular condensate in the BEC region shown here.

This results in an upper bound for n_{mc}, owing to the fact that $Z^{2\mathrm{B}}$ is always smaller than its many-body counterpart Z. The magnetic field region where this dressed filling fraction decreases from one to zero indicates the position of the BEC-BCS crossover, which is clearly in the same neighborhood as where the two-body molecular energy enters the Fermi sea. From the inset in Fig. 3, we see that the BEC-BCS crossover

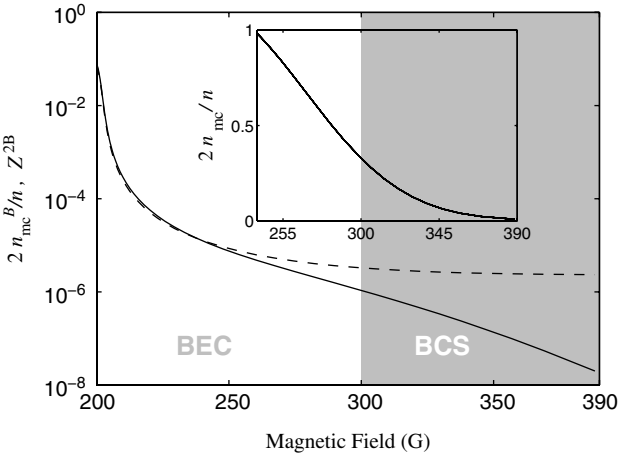

FIG. 3. Two-body wave-function renormalization factor $Z^{2\mathrm{B}}$ (dashed line) plotted together with the filling fraction of the bare molecular condensate $2n_{\mathrm{mc}}^{\mathrm{B}}/n$, including a varying number of bands (solid lines), which shows that a single-band calculation is adequate in the BEC-BCS crossover region of interest. The inset shows the approximate filling fraction of dressed molecules, $2n_{\mathrm{mc}}/n$, in the crossover region. The multiple solid lines of the main graph all lie on top of each other in this high magnetic field region.

is dominated by contributions from the lowest band only; including higher bands in the self-energy calculation does not bring about any apparent change.

In Fig. 3 we compare Z^{2B} to $2n_{mc}^{B}/n$. Indeed, $2n_{mc}^{B}/n$ and Z^{2B} are similar in the BEC limit, since the gas then consists solely of a Bose-Einstein condensate of dressed molecules. This is a result of the fact that in this regime the energies of the atomic states lie far above the dressed molecular state, as seen in Fig. 1, which suppresses many-body effects. The BCS region, however, sees a pronounced difference between the two-body renormalization factors and the bare molecular condensate fraction.

Our solutions of the BCS gap equation confirm the presence of the logarithmic BCS singularity arising at high detuning where the gap then scales as $\Delta \simeq 2t^{\sigma}\exp(-29t^{\sigma}/|U_{\mathrm{eff}}|)$ [14]. Here, $U_{\mathrm{eff}} \simeq -g'^{2}/(\delta+3\hbar\omega-2\mu)$, is the on-site Hubbard attraction of the atoms. In the crossover region, the molecular energy crosses the lowest-band boundary when $\delta \simeq g'^{2}/12t_{a}$. Furthermore, U_{eff} indicates this crossing occurs close to a Feshbach resonance when $\delta \simeq 3\hbar\omega/2$. This leads to the criterion $\Delta B \gg 18t_{a}\sqrt{4\pi\hbar/m\omega}/a_{bg}\Delta\mu_{mag}$, which ensures that the Feshbach resonance and the BEC-BCS crossover are well separated, as required for the applicability of a single-band model to the BEC-BCS crossover in an optical lattice. Most known Feshbach resonances adhere to this criterion.

In conclusion, we have presented the full microscopic many-body theory that describes the BEC-BCS crossover in an optical lattice due to the presence of a Feshbach resonance. Both two-channel physics and the possible effects of higher bands were taken into account. We have shown that in general the BEC-BCS crossover takes place far from the Feshbach resonance, such that a single-band model suffices to accurately describe the BEC-BCS crossover. The many-body Z can only be obtained from the full fluctuation calculation, and this is an important topic of further study.

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