Fermion-Mediated BCS-BEC Crossover in Ultracold ^{40}K Gases

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Studies of Feshbach resonance phenomena in fermionic alkali gases have drawn heavily on the intuition afforded by a Fermi-Bose theory which presents the Feshbach molecule as a featureless Bose particle. While this model may provide a suitable platform to explore the ^{6}Li system, we argue that its application to ^{40}K, where the hyperfine structure is inverted, is inappropriate. Introducing a three-state Fermi model, where a spin state is shared by the open and closed channel states, we show that effects of "Pauli blocking" appear in the internal structure of the condensate wave function.

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Fermionic alkali atomic gases present a unique environment in which to control and explore the crossover between BCS and Bose-Einstein condensation (BEC) [1,2]. Already the creation of a molecular BEC phase from a degenerate Fermi gas of atoms has been reported by several experimental groups [3], while studies of fermionic pair condensation in the crossover regime are under way [4]. The facility to control the strength of the atomic pair interaction in the Fermi system relies on a magnetically tuned Feshbach resonance (FR) phenomenon involving the multiple scattering of atoms from open channel states into a molecular bound state formed from neighboring closed channel states. Current theories of the FR treat the molecular bound state as a featureless bosonic particle, and characterize the total system by a Fermi-Bose theory [5] familiar from studies of polariton condensation [6] as well as models of bipolaronic superconductivity [7]. While the Feshbach molecule (FM) involves spin states different from the scattering states, the molecular boson can be regarded as distinct. However, if a spin state is shared, the validity of the Fermi-Bose theory as a microscopic model of the FR is called into question [8].

Nowhere is this scenario illustrated more clearly than ^{40}K. To understand why, let us consider the Hamiltonian of a single fermionic alkali atom of integer nuclear spin I and electron spin $s = \frac{1}{2}$:

$$\hat{H}_{\text{atom}} = A\mathbf{s} \cdot \mathbf{I} + \mathbf{B} \cdot (2\mu_e \mathbf{s} - \mu_n \mathbf{I}). \tag{1}$$

Here A denotes the strength of the hyperfine interaction and $\mathbf{B}$ the magnetic field, while μ_e and μ_n denote the electron and nuclear magnetic moments, respectively. The Hamiltonian preserves only the quantum number $m_F = m_s + m_I$, but the eigenstates can be labeled by their total atomic spin at zero magnetic field $|F, m_F\rangle$ since the energy varies smoothly with field. In the ^{6}Li system ($I = 1$), the hyperfine interaction is positive, and the lowest energy states form a doublet with total spin $F = \frac{1}{2}$. By contrast, in the ^{40}K system ($I = 4$), the hyperfine interaction is negative and the hyperfine structure is inverted such that the lowest eigenstate is the one of highest weight, viz. $F_{\max} = -m_F = \frac{9}{2}$ [9]. Now, if we ignore inelastic collisions or interactions that involve spin flips, the interatomic interaction is specified by a two-body potential that depends only on the electron spin:

$$V(\mathbf{r}_1 - \mathbf{r}_2) = V_c(\mathbf{r}_1 - \mathbf{r}_2) + V_s(\mathbf{r}_1 - \mathbf{r}_2)\mathbf{s}_1 \cdot \mathbf{s}_2. \tag{2}$$

Therefore, it preserves the *total* spin projection of the two-body system $M_F = m_{F,1} + m_{F,2}$, and any scattering process between atomic states that conserves M_F is allowed. If one considers only low-energy, s-wave scattering—the regime relevant to experiment—interactions involving identical fermions are forbidden and the subspace of interacting atomic states is further restricted. Specifically, in the ^{6}Li system, the interaction provides a mechanism to affect a FR through the coupling of the lowest two $F = \frac{1}{2}$ (open channel) states to the higher energy bound state formed from all pairs of hyperfine states, involving the $F = \frac{3}{2}$ (closed channel) states, that satisfy the condition $M_F = \frac{1}{2} - \frac{1}{2} = 0$. Crucially, the constraint on M_F is even more restrictive in ^{40}K allowing the two states $|\frac{9}{2}, -\frac{9}{2}\rangle$ and $|\frac{9}{2}, -\frac{7}{2}\rangle$ that constitute the open channel to couple to only *one* closed channel state $|\frac{7}{2}, -\frac{7}{2}\rangle$ (Fig. 1). Thus, the FM

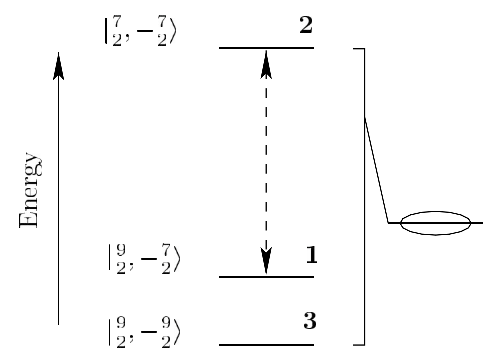

FIG. 1. Atomic states involved in the FR for ^{40}K, where the Fermi gas is initially prepared in the two lowest eigenstates. The coupling between states allowed by the selection rules is represented by a dotted line. The FM is formed from $|\frac{7}{2}, -\frac{7}{2}\rangle$ and the lowest eigenstate $|\frac{9}{2}, -\frac{9}{2}\rangle$.

involves only a hybridization of states $|\frac{9}{2},-\frac{9}{2}\rangle$ and $|\frac{7}{2},-\frac{7}{2}\rangle$, which competes with the pairing of the scattering states $|\frac{9}{2},-\frac{9}{2}\rangle$ and $|\frac{9}{2},-\frac{7}{2}\rangle$. The aim of this Letter is to explore the integrity of FR phenomena in the *three-state* Fermi system and assess the extent to which the nature of the bound state impinges on the mean-field characteristics of the system.

Although, in the three-state basis, the majority of matrix elements of the two-body pair interaction (2) remain nonzero, the low-energy properties of the system may be characterized by just a subset of elements. Labeling the spin states $|\frac{9}{2},-\frac{7}{2}\rangle$, $|\frac{7}{2},-\frac{7}{2}\rangle$, and $|\frac{9}{2},-\frac{9}{2}\rangle$ by indices $i=1$, 2, and 3, respectively, the FM is created by the direct density interaction U between species 2 and 3. At the same time, the exchange contribution g, which allows a transfer of particles between states 1 and 2, induces an effective pair interaction in the open channel. As such, any direct density interaction between species 1 and 3 (repulsive in the physical system) can be subsumed into this contribution. Therefore, at its simplest level, the FR of the three-state Fermi system can be modeled by the Hamiltonian,

$$\begin{aligned}\hat{H}-\sum_{i=1}^{3}\mu_i\hat{N}_i=&\sum_{\mathbf{k}i}(\epsilon_{\mathbf{k}i}-\mu_i)a_{\mathbf{k}i}^\dagger a_{\mathbf{k}i}\\&+\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}}U_{\mathbf{q}}a_{\mathbf{k}2}^\dagger a_{\mathbf{k}'3}^\dagger a_{\mathbf{k}'-\mathbf{q}3}a_{\mathbf{k}+\mathbf{q}2}\\&+\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}}[g_{\mathbf{q}}a_{\mathbf{k}1}^\dagger a_{\mathbf{k}'3}^\dagger a_{\mathbf{k}'-\mathbf{q}3}a_{\mathbf{k}+\mathbf{q}2}+\text{H.c.}],\end{aligned}\tag{3}$$

where the fermion operator $a_{\mathbf{k}i}$ indexes species i, $\hat{N}_i=\Sigma_{\mathbf{k}}a_{\mathbf{k}i}^\dagger a_{\mathbf{k}i}$, and, defining E_i as the corresponding eigenvalue of the atomic interaction (1), $\epsilon_{\mathbf{k}i}=\hbar^2\mathbf{k}^2/2m+E_i$. Since the system is not in chemical equilibrium, and the Hamiltonian separately conserves the particle number N_3 and N_1+N_2, the free energy is characterized by two chemical potentials μ_3 and $\mu_1=\mu_2\equiv\mu_{12}$. Anticipating that the coupled system is prepared with a roughly equal population of open channel states, we use the chemical potentials to impose the condition $N_1+N_2=N_3\equiv N/2$. Without loss of generality, one can absorb E_1 and E_3 into a redefinition of the respective chemical potentials, while the detuning $E_2\equiv\nu>0$ can be used to adjust the relative energy level separation of state 2. Finally, for simplicity, we consider the case where $g_q=\gamma U_q$.

In the following, we present the results of a numerical mean-field analysis of the Hamiltonian (3) across the FR. However, before doing so, it is instructive to anticipate some qualitative aspects of the phenomenology that emerge from the numerics. In contrast to the Fermi-Bose model, the FR Hamiltonian (3) is complicated by the three-fermion character of the system, but the bare interaction of particles in the open channel can still be enhanced by the formation of a two-body resonance out of the three-state basis. In practice, this is achieved by affecting an "optimal" rearrangement of the basis states wherein, by exploiting the exchange interaction, states 1 and 2 hybridize into the orthogonal combination,

$$\begin{aligned}b_{\mathbf{k}1'}^\dagger&=\cos\phi_{\mathbf{k}}a_{\mathbf{k}1}^\dagger+\sin\phi_{\mathbf{k}}a_{\mathbf{k}2}^\dagger,\\b_{\mathbf{k}2'}^\dagger&=-\sin\phi_{\mathbf{k}}a_{\mathbf{k}1}^\dagger+\cos\phi_{\mathbf{k}}a_{\mathbf{k}2}^\dagger,\end{aligned}$$

such that the condensation energy associated with the pairing of states $1'$ and 3 is maximized. In this case, imposing the particle number constraint, one can propose the variational ansatz for the ground state wave function,

$$|\Phi\rangle=\prod_{\mathbf{k}}[\cos\theta_{\mathbf{k}}+\sin\theta_{\mathbf{k}}a_{\mathbf{k}3}^\dagger b_{-\mathbf{k}1'}^\dagger]|0\rangle,\tag{4}$$

the integrity of which is supported by the numerical analysis below. Here, $\theta_{\mathbf{k}}$ encodes the overall strength of the condensate, while $\phi_{\mathbf{k}}$ defines its distribution between the two pairing channels: since the open channel state 3 participates in *both* condensate fractions, $\langle a_3a_1\rangle$ and $\langle a_3a_2\rangle$, there is an inherent frustration due to Pauli exclusion not present in the Fermi-Bose system. Since the exchange interaction contributes indirectly to pair formation, the hybridization (as reflected through $\phi_{\mathbf{k}}$), itself, depends on the strength of the condensate. To maintain contact with the physical system, we hereafter limit our considerations to situations in which the Fermi energy of the unperturbed system, $\epsilon_F=\hbar^2k_F^2/2m$, lies far enough below ν that the auxiliary state $2'$ remains unpopulated in the ground state. In this case, the particle number constraint translates to the condition $\mu_{12}=\mu_3\equiv\mu$.

Considerable insight can be gained from analytical solutions of the variational mean-field equations in the dilute (BEC) and dense (BCS) limits (cf. Ref. [1]). When characterized by a local contact potential $U(\mathbf{r})=-U_0L^3\delta(\mathbf{r})$, such an analysis reveals a phase diagram characterized by three dimensionless parameters, $u_0\equiv U_0N(E_0)$, γ, and ν/E_0, where $E_0=\hbar^2k_0^2/2m$ represents the UV cutoff set by the range of the interaction $1/k_0$, and $N(\epsilon)$ denotes the density of states. At low densities $\epsilon_F\to0$, the system develops a molecular bound state and enters a BEC phase when $\nu<\nu_c$ where, defining $f(z)=1-\sqrt{z}\arctan(1/\sqrt{z})$,

$$f\left(\frac{\nu_c}{2E_0}\right)=\frac{1}{u_0(\gamma^2u_0+1)}\tag{5}$$

(see Fig. 2). In particular, one may note that the exchange contribution γ enhances the bare interaction u_0 expanding the domain of the BEC phase while, in the absence of a direct interaction, $u_0=0$, the exchange can, by itself, induce pairing in the open channel.

Defining the anomalous (normal) density, $\kappa_{\mathbf{k},ji}=\langle\Phi|a_{-\mathbf{k}i}a_{\mathbf{k}j}|\Phi\rangle(\rho_{\mathbf{k},ji}=\langle\Phi|a_{\mathbf{k}i}^\dagger a_{\mathbf{k}j}|\Phi\rangle)$, when deep within the BEC phase $\nu\ll\nu_c$, a linearization of the variational equations shows that the total condensate wave function involves the coherent superposition of components

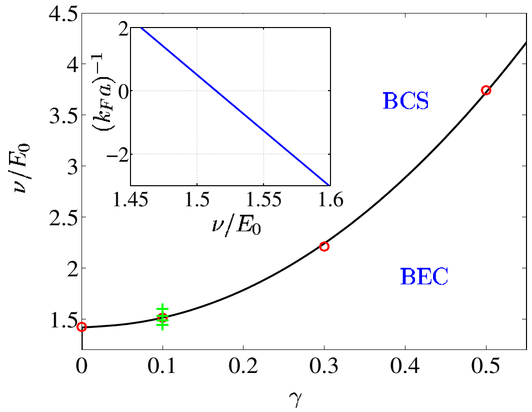

FIG. 2 (color online). Phase diagram of the FR Hamiltonian (3). The solid line shows the boundary separating the BEC and BCS-like phases in the dilute system as inferred from the variational analysis (5) with $u_0 \equiv U_0 N(E_0) = 3.76$. The points marked on the curve are obtained from the numerical mean-field analysis in the limit of low density, and, in order of increasing γ, they correspond to the ratios $N_1/N_3 \simeq 0\%$, 30%, 73%, and 90%, respectively. The intersection of the curve with the ν-axis translates into the binding energy of the molecular state associated with the bare potential $U_{\mathbf{q}}$. The density distributions displayed in Fig. 3 are drawn from the range shown by crosses at $\gamma = 0.1$. Inset: The dependence of the scattering length a on the detuning ν, as inferred from the numerics, can be well approximated by the relation $(k_F a)E_0/(\nu_c - \nu) \simeq 35$.

$$\kappa_{\mathbf{k},13} = \frac{1}{2}\sin 2\theta_{\mathbf{k}} \cos\phi_{\mathbf{k}} \simeq \frac{\alpha\Delta_{13}}{2(\epsilon_{\mathbf{k}1} - \mu)},$$
$$\kappa_{\mathbf{k},23} = \frac{1}{2}\sin 2\theta_{\mathbf{k}} \sin\phi_{\mathbf{k}} \simeq \frac{(\alpha^{-1} + \gamma^{-1})\alpha\Delta_{13}}{2(\epsilon_{\mathbf{k}1} - \mu) + \nu}, \tag{6}$$

where, to leading order, the condensate order parameter $\Delta_{13} = \gamma U_0 \Sigma_{\mathbf{k}}^{k_0} \kappa_{\mathbf{k},13}$ (and the partner $\Delta_{23} = U_0 \Sigma_{\mathbf{k}}^{k_0} \kappa_{\mathbf{k},23}$) remain unspecified. Here, for $|\mu| \ll \nu$, the chemical potential, $\mu = -|\mu|$ (which asymptotes to half the molecular bound state energy), is determined by the self-consistency condition $\alpha^{-1} = \gamma u_0 f(|\mu|/E_0)$ with the coefficient $\alpha \equiv \Delta_{23}/\Delta_{13}$ determined by the relation,

$$\frac{1}{u_0} \simeq \left(1 + \frac{\gamma}{\alpha}\right) f\left(\frac{\nu}{2E_0}\right). \tag{7}$$

Conversely, deep within the BCS-like phase, for $|\mathbf{k}| \lesssim k_F$, $\phi_{\mathbf{k}} \simeq \nu^{-1}(\alpha^{-1} + \gamma^{-1})\alpha\Delta_{13} \cot\theta_{\mathbf{k}} \ll 1$, and the condensate wave function acquires the familiar form

$$\kappa_{\mathbf{k},13} \simeq \frac{1}{2}\sin 2\theta_{\mathbf{k}} \simeq \frac{1}{2}\frac{\alpha\Delta_{13}}{[(\epsilon_{\mathbf{k}} - \mu)^2 + |\alpha\Delta_{13}|^2]^{1/2}},$$

with $\mu \simeq \epsilon_F$, while $\kappa_{\mathbf{k},23} \simeq (\phi_{\mathbf{k}}/2)\sin 2\theta_{\mathbf{k}}$. For $|\mathbf{k}| \gg k_F$, the solution converges to the low-density asymptotic (6). Once again, with $\epsilon_F \ll \nu$, α is determined by (7) while

$$\Delta_{13} = \frac{8\epsilon_F}{e^2}\exp\left[-\sqrt{\frac{E_0}{\epsilon_F}}\left(\frac{1}{\alpha\gamma u_0} - 1\right)\right].$$

From the variational analysis, two striking features emerge: first, in both BEC and BCS-like phases, the condensate wave function is characterized by two length scales. Deep within the BEC regime, the FM has a size $k_0\xi_{23} = [E_0/(\nu/2 + |\mu|)]^{1/2}$, while that of the molecule formed from open channel states, $k_0\xi_{13} = (E_0/|\mu|)^{1/2}$, diverges at the crossover. In the BCS-like phase, the FM is increased in size $k_0\xi_{23} = [E_0/(\nu/2 - \epsilon_F)]^{1/2}$, while the range of the Cooper pair of open channel states is set by the coherence length $\xi_{13} = v_F/|\alpha\Delta_{13}|$. Second, in the BCS-like phase, Pauli exclusion has the effect of substantially depleting the normal density $\rho_{\mathbf{k},22} = \sin^2\theta_{\mathbf{k}}\sin^2\phi_{\mathbf{k}}$ and, with it, the condensate fraction $\kappa_{\mathbf{k},23}$ in the range $|\mathbf{k}| < k_F$. Both features are clearly visible in the numerically inferred density distributions below (Fig. 3).

With this background, let us turn to the results of the numerical mean-field analysis. Specifically, the ground

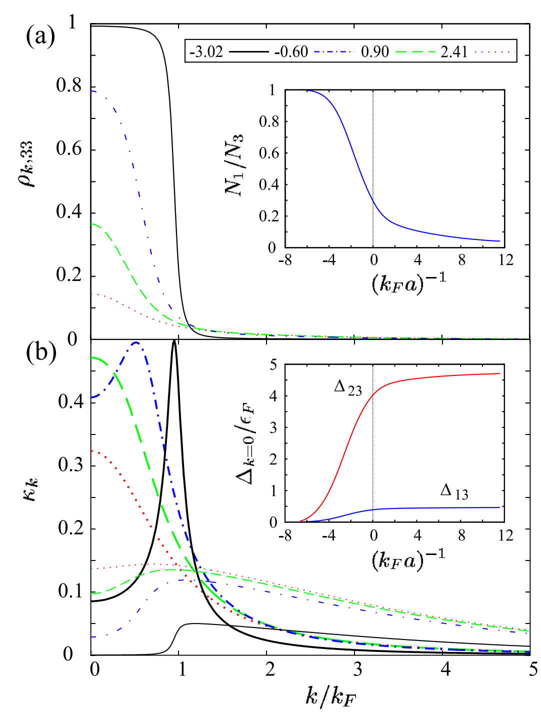

FIG. 3 (color online). Density distribution of (a) $\rho_{k,33}$ and (b) $\kappa_{k,13}$ and $\kappa_{k,23}$ for the range of scattering lengths $(k_F a)^{-1}$ shown by the crosses in Fig. 2. At $k = 0$, we have $\kappa_{13} > \kappa_{23}$. The inset in (a) shows the ratio of particles N_1/N_3 in the ground state as a function of the scattering length $(k_F a)^{-1}$. Note that the relative weight of the 1 state on the "BCS side" of the resonance increases dramatically from 30% at the crossover to almost 100% as $(k_F a)^{-1} \to -\infty$. The inset in (b) shows the condensate fractions Δ_{13} and Δ_{23} as a function of the scattering length $(k_F a)^{-1}$.

state wave function $|\Phi\rangle$ of the three-state Fermi system is determined by minimizing the free energy $\langle\Phi|\hat{H} - \mu\hat{N}|\Phi\rangle$ using a generalized Bogoliubov-Valatin transformation $a_{\mathbf{k}i} = \Sigma_{j=1}^{3}(u_{\mathbf{k},ij}\beta_{\mathbf{k}j} + v^{*}_{\mathbf{k},ij}\beta^{\dagger}_{-\mathbf{k}j})$. Here, we take the most general ansatz for the ground state wave function compatible with the formation of a condensate; i.e., all elements of the matrix coefficients $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ are allowed to acquire nonzero expectation values. For convenience, we choose a model potential $U_{\mathbf{q}}$ that possesses only one bound state (although, in the quasiequilibrium system, the presence of multiple bound states will not change the conclusions qualitatively). We set $U(\mathbf{r}) = -U_0 \exp[-(k_0\mathbf{r})^2/2]$, where the range of the pair interaction is chosen to be much smaller than the average particle separation, viz. $N/(k_0L)^3 \ll 1$.

The numerical procedure involves the minimization of the free energy with respect to the normal and anomalous densities, $\rho_{k,ji} = \Sigma_m v^{*}_{k,jm}v_{k,im}$ and $\kappa_{k,ji} = \Sigma_m v^{*}_{k,jm}u_{k,im}$ where, in the s-wave approximation, the Bogoliubov matrix coefficients u_k and v_k, as well as the densities, depend only on $k \equiv |\mathbf{k}|$. We obtain nonzero values of the off-diagonal component of the density matrix $\rho_{k,12}$, which is consistent with the hybrid character of the ground state, while the observed relations $\langle\Phi|b^{\dagger}_{\mathbf{k}1'}b_{\mathbf{k}1'}|\Phi\rangle = \rho_{k,33}$ and $\langle\Phi|b^{\dagger}_{\mathbf{k}2'}b_{\mathbf{k}2'}|\Phi\rangle = 0$ confirm the validity of the particular variational ansatz (4). For completeness, we note that, once ϵ_F becomes comparable with the detuning, the subsequent population of level $2'$ requires an adjustment of the chemical potentials $\mu_{12} \neq \mu_3$ to comply with the particle number constraint. Within this range, the ground state is eventually no longer encompassed by the reduced variational ansatz (4).

The nature of the ground state can be characterized by monitoring the normal density $\rho_{k,33}$ and the components of the condensate wave function $\kappa_{k,23}$ and $\kappa_{k,13}$. As in single-channel theories involving only two species of fermions, the momentum distribution interpolates smoothly from a BCS-like distribution at $(k_Fa)^{-1} \ll -1$ to a molecular condensate wave function in the BEC regime when $(k_Fa)^{-1} \gg 1$, where $(k_Fa)^{-1}$ denotes the (inverse) scattering length [Fig. 3(a)]. As expected from the variational analysis, a key feature of the condensate wave function is the presence of a robust tail at high momenta which persists into the BCS-like phase [Fig. 3(b)]. (Note that, to infer the total occupation density, the distribution must be weighted by the density of states $\sim k^2$ leading to a significant amplification of the tail.) The existence of two correlation lengths and the effects of exclusion are also emphasized in the variation of the condensate wave function. This is amenable to rough estimation by determining the molecular condensate fraction after a ramp [4]. More subtly, the multicomponent condensate is expected to have a complex collective mode structure [10] that will then influence the dynamical response through the crossover [11]. The most direct signatures are, of course, in spectroscopy [12], because different gap features will correspond to different Raman transitions.

In summary, we have shown that the FR in the ^{40}K system involves a three-state Fermi Hamiltonian. Of course, while the FM remains only sparsely populated, the character of the mean-field ground state shows few qualitative differences from a single-channel theory, as would a Fermi-Bose model in that limit. However, when the FM population is significant, the development of weight in both $(1, 3)$ and $(2, 3)$ fractions is revealed in the appearance of two length scales in the internal condensate wave function. The existence of "Pauli blocking" discriminates this behavior from that of a Fermi-Bose model. We expect signatures of the internal structure of the composite wave function will appear in both the collective mode response of the condensate and in the dynamics of condensate formation [4].

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