

Simple Mean-Field Theory for a Zero-Temperature Fermionic Gas at a Feshbach Resonance

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We present a simple two-channel mean-field theory for a zero-temperature two-component Fermi gas in the neighborhood of a Feshbach resonance. Our results agree with recent experiments on the bare-molecule fraction as a function of magnetic field [Partridge *et al.*, Phys. Rev. Lett. **95**, 020404 (2005)]. Even in this strongly coupled gas of ⁶Li, the experimental results depend on the structure of the molecules formed in the Feshbach resonance and, therefore, are not universal.

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Introduction.—Magnetoassociation creates a molecule from a pair of colliding atoms when one of the spins flips in the presence of a magnetic field tuned near a Feshbach resonance [1,2]. Nevertheless, the ultracold community as a whole has eschewed molecules in Feshbach-resonant interactions, relying instead on an all-atom single-channel model characterized solely by a tunable *s*-wave scattering length [3]. In this Letter we promote a simple molecule-explicit two-channel mean-field theory to replace all-atom theories. We find good agreement with experiments [4] that should present a severe test for theories of all ilk.

Our approach is built around two species of fermionic atoms that magnetoassociate into bosonic “bare” molecules. In the experiments [4], a laser spectroscopy probe is applied that detects bare molecules only. Below resonance, where thermodynamics favors molecules, the challenge for single-channel theories is to produce two types of molecules out of the same atoms, bare molecules seen by the probe and something else. Instead, our two-channel model simply states that bare molecules come “dressed” with atom pairs. Second, a typical all-atom theory rests on the notion of universality, whereby the interactions between atoms can be lumped into a scattering length and microscopic details of the physics do not matter. Our approach also mimics universal behavior on the atom side of the resonance for strong atom-molecule coupling. However, the experiments [4] cover a wide magnetic-field range on both sides of the resonance and, according to our results, certain molecular physics details are needed to satisfactorily match theory and the experiments. Universality does not hold despite strong interactions. Elementary as our mean-field theory is, it neatly bypasses two limitations of all-atom theories.

Model.—As before [5,6], we study two fermionic species of atoms ($c_{\mathbf{k}\uparrow}$ and $c_{\mathbf{k}\downarrow}$) that magnetoassociate into bosonic molecules ($b_{\mathbf{k}}$) within a version of the Bose-Fermi model [7] used to describe superconductivity beyond the usual weak-coupling limit [8]. The corresponding microscopic Hamiltonian is

$$\frac{H}{\hbar} = \sum_{\mathbf{k}} \left[\left(\frac{1}{2} \epsilon_{\mathbf{k}} + \delta \right) b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}} + \epsilon_{\mathbf{k}} (c_{\mathbf{k}\uparrow}^{\dagger} c_{\mathbf{k}\uparrow} + c_{\mathbf{k}\downarrow}^{\dagger} c_{\mathbf{k}\downarrow}) \right] + \sum_{\mathbf{k}, \mathbf{k}'} \kappa_{\mathbf{k}, \mathbf{k}'} (b_{\mathbf{k}+\mathbf{k}'}^{\dagger} c_{\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} + c_{\mathbf{k}\uparrow}^{\dagger} c_{\mathbf{k}\downarrow}^{\dagger} b_{\mathbf{k}+\mathbf{k}'}). \quad (1)$$

Here $\hbar \epsilon_{\mathbf{k}} = \hbar^2 k^2 / 2m$ is the kinetic energy for an atom with wave vector \mathbf{k} , δ is the detuning controlled by the magnetic field ($\delta > 0$ corresponds to an open dissociation channel for the molecules), and $\kappa_{\mathbf{k}, \mathbf{k}'}$ are the atom-molecule coupling coefficients for two atoms with momenta $\hbar \mathbf{k}$ and $\hbar \mathbf{k}'$.

The key approximation is to treat the boson operators $b_{\mathbf{k}}$ and $b_{\mathbf{k}}^{\dagger}$ as classical conjugate variables. Then the hierarchy of the equations of motion for fermion correlation functions truncates exactly at the level of pair correlations. As a technical approximation, we only keep the zero-momentum bosons, i.e., a uniform molecular condensate. We write fermion occupation numbers and pair correlations as a function of free-atom energy $\hbar \epsilon \equiv \hbar \epsilon_{\mathbf{k}}$ as $P(\epsilon) = \langle c_{\mathbf{k}\downarrow}^{\dagger} c_{\mathbf{k}\downarrow} \rangle = \langle c_{\mathbf{k}\uparrow}^{\dagger} c_{\mathbf{k}\uparrow} \rangle$, $C(\epsilon) = \langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \rangle$, and, given the invariant atom number N arising from the conserved quantity $\hat{N} = 2b_0^{\dagger} b_0 + \sum_{\mathbf{k}} (c_{\mathbf{k}\uparrow}^{\dagger} c_{\mathbf{k}\uparrow} + c_{\mathbf{k}\downarrow}^{\dagger} c_{\mathbf{k}\downarrow})$, define the molecular amplitude $\beta = \sqrt{2/N} b_0$ such that $|\beta|^2$ is the fraction of atoms converted into molecules. The result is the equations of motion [5]

$$i\dot{C}(\epsilon) = 2\epsilon C(\epsilon) + \frac{1}{\sqrt{2}} \Omega \beta f(\epsilon) [1 - 2P(\epsilon)], \quad (2)$$

$$i\dot{P}(\epsilon) = \frac{1}{\sqrt{2}} \Omega f(\epsilon) [\beta C^*(\epsilon) - \beta^* C(\epsilon)], \quad (3)$$

$$i\dot{\beta} = \delta \beta + \frac{3\Omega}{2\sqrt{2}\epsilon_F^{3/2}} \int d\epsilon \sqrt{\epsilon} f(\epsilon) C(\epsilon). \quad (4)$$

Here $\Omega = \sqrt{N} \kappa_{0,0}$ is the atom-molecule Rabi frequency, and $f(\epsilon)$ [with $f(0) = 1$] conveys the energy dependence of atom-molecule coupling. Since the coupling coefficient $\kappa_{0,0}$ is inversely proportional to the square root of the

quantization volume V , the Rabi frequency is proportional to the square root of the invariant density $\rho = N/V$. Finally, $\hbar\epsilon_F = \hbar^2(3\pi^2\rho)^{2/3}/2m$ is the usual Fermi energy for a two-component gas which, so far, arises simply because the sum over wave vectors is replaced by an integral over the frequencies.

The objective is to find the steady state of Eqs. (2)–(4) at zero temperature. These equations admit solutions of the form $C(\epsilon; t) \equiv C(\epsilon)e^{-2i\mu t}$, $\beta(t) \equiv \beta e^{-2i\mu t}$ and $P(\epsilon; t) \equiv P(\epsilon)$, where $\hbar\mu$ and $2\hbar\mu$ are recognized as the chemical potentials for atoms and molecules. In fact, there are too many solutions. We therefore impose the condition of *maximal pairing*, whereby atoms only come in pairs of $\mathbf{k} \uparrow$ and $-\mathbf{k} \downarrow$. This is technically the usual BCS ansatz, but here it is not so much an ansatz as a natural consequence of how a pair of atoms couples to a molecule. In mathematical terms we have $|C(\epsilon)|^2 = P(\epsilon) - P^2(\epsilon)$. Equations (2) and (4) then give the counterpart of the gap equation in BCS theory,

$$\delta - 2\mu = \frac{3\Omega^2}{8\epsilon_F^{3/2}} \int d\epsilon f^2(\epsilon) \left(\frac{\sqrt{\epsilon}}{\sqrt{(\epsilon - \mu)^2 + \Delta(\epsilon)^2}} - \frac{1}{\sqrt{\epsilon}} \right), \quad (5)$$

where $\Delta(\epsilon) = f(\epsilon)\beta\Omega/\sqrt{2}$ is the analog of the pairing gap. Depending on the form of the coupling function $f(\epsilon)$, the theory may present an ultraviolet divergence that needs to be renormalized [5,6,9–11]. As we [5,6,9] and others have done before, the term $\propto 1/\sqrt{\epsilon}$ has been added into the integrand manually and the corresponding (possibly infinite) constant on the left-hand side has been absorbed into a redefinition of the detuning δ . One more equation is needed, and is found from the conservation of atom number \hat{N} that holds for the mean-field equations (2)–(4) as well. We have

$$\beta^2 + \frac{3}{4\epsilon_F^{3/2}} \int d\epsilon \sqrt{\epsilon} \left(1 - \frac{\epsilon - \mu}{\sqrt{(\epsilon - \mu)^2 + \Delta(\epsilon)^2}} \right) = 1. \quad (6)$$

So far our approach deals with bare atoms and molecules that would emerge if the Feshbach-resonance interaction were suddenly turned off. In more practical terms, the sample breaks up into atoms and bare molecules if the magnetic field is switched quickly enough far enough away from the Feshbach resonance. However, the rate of change of the detuning that separates quick from slow is $|\dot{\delta}| \simeq \Omega^2$ [5,9], and fast switching may be a tall order for the 834 G Feshbach resonance in ${}^6\text{Li}$. Fortunately alternative methods to measure the bare-molecule fraction exist, e.g., a measurement [12] of the magnetic moment per atom [13], or a laser spectroscopic probe that couples only to the bare molecules [4]. Here we, of course, focus on the latter.

An alternative angle helps with the interpretation of the results. Let us initially take a single zero-momentum dressed molecule. The available state space is spanned by the states with either one molecule at zero momentum and

no atoms, $b_0^\dagger|0\rangle$, or no molecule and pairs of atoms $\mathbf{k} \uparrow$ and $-\mathbf{k} \downarrow$, $c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger|0\rangle$, where $|0\rangle$ is the particle vacuum. We are at liberty to write the state vector as

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}}\beta(t)b_0^\dagger|0\rangle + \frac{1}{\sqrt{N}}\sum_{\mathbf{k}} C_{\mathbf{k}}(t)c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger|0\rangle. \quad (7)$$

Assuming self-consistently that the C coefficients only depend on energy, $C_{\mathbf{k}}(t) \equiv C(\epsilon; t)$, the Hamiltonian (1) gives the time dependent Schrödinger equations for the coefficients β and $C(\epsilon)$ that coincide with Eqs. (2) and (4), except that in the counterpart of Eq. (2) we have unity in lieu of the factor $[1 - 2P(\epsilon)]$. Were it not for this factor that obviously reflects the Pauli exclusion principle, our mean-field theory would represent a collection of independent dressed molecules.

A stationary state of the form (7) is a molecule dressed with atom pairs [5,6,9,13,14]. With the same renormalization that was applied in Eq. (5), the dressed molecule is dissociated for $\delta > 0$ and has one bound state for $\delta < 0$. The latter is the bound state that molecular spectroscopy [15,16] detects in a dilute gas. The effect of our renormalization scheme is to put the position of the Feshbach resonance at the detuning $\delta = 0$ both for an individual molecule and, by implication, for a dilute gas.

The properties of a dressed molecule depend on the coupling function $f(\epsilon)$, which may be obtained in principle from molecular structure calculations. Setting $f(\epsilon) \equiv 1$ corresponds to a contact interaction for the conversion between atoms and molecules. In reality, though, the interaction has a finite range. Corresponding to a nonzero spatial range, there is a range in energy; at high enough atom energies the coupling between two bare atoms and a bare molecule must vanish. As before [5,6,9], we use here the model in which we simply cut off the coupling at an energy $\hbar M$ and write $f(\epsilon) = \theta(M - \epsilon)$, where θ is the Heaviside unit step function. The binding energy $2\hbar|\mu|$ of an isolated dressed molecule for a negative detuning $-|\delta|$ may be solved from the transcendental equation

$$|\delta| - 2|\mu| - \frac{3}{4}\sqrt{|\mu|}\sqrt{\bar{\omega}} \arctan \sqrt{\frac{M}{|\mu|}} = 0, \quad (8)$$

with $\bar{\omega} = \Omega^4/\epsilon_F^3$. While Ω and ϵ_F depend on the density, in the single-molecule parameter $\bar{\omega}$ the density dependence duly cancels. Given the binding energy, the bare-molecule fraction β^2 in the dressed-molecule state vector (7) is easily found. A substantial molecular component, say, $\beta^2 > 1/2$, emerges in the contact-interaction case $M = \infty$ for detunings $\delta < -(7\pi^2/512)\bar{\omega} \sim -0.1\bar{\omega}$ and in the case $M \ll \bar{\omega}$ for detunings $\delta < -(3/4)\sqrt{M\bar{\omega}}$. Until further notice all results are for the contact interaction, $M = \infty$.

Main features.—In the limit of weak coupling, $\Omega \ll \epsilon_F$, the relevant demarcation points for the detuning δ are 0 (Feshbach resonance) and $2\epsilon_F$; 2 because it takes two atoms to make a molecule. For $\delta < 0$ the system is a condensate of bare molecules, for $\delta > 2\epsilon_F$ a weak-

coupling BCS superfluid. For $0 < \delta < 2\epsilon_F$ we have an atom-molecule mixture in which all atoms from the Fermi sea above the energy $\hbar\delta/2$ have been converted into bare molecules with the energy $\hbar\delta$, so that $\beta^2 = 1 - [\delta/(2\epsilon_F)]^{3/2}$. As has been noted before [5,6,14,17,18], the Fermi sea of atoms blocks the decay of the molecules even if the molecules are above the dissociation threshold.

In the intermediate case with $\Omega \simeq \epsilon_F$ numerical results show a continuous transformation from bare molecules to dressed molecules, to a nondescript mixture of atoms and molecules, and finally to a weak-coupling BCS as the detuning is varied from well below the Feshbach resonance to well above it. Typical ^{40}K experiments [19] with $\Omega \simeq 4\epsilon_F$ [5,6] belong to this category. In the present approach the calculated fraction of bare molecules at the Feshbach resonance is 6%, and ca. 8% for non-zero temperature [6,14], enough to cast ambiguity on the observation [19] of fermionic condensation.

For the 834 G Feshbach resonance in ^6Li , $\Omega \gg \epsilon_F$. The coupling is now so strong that dissociation of above-threshold molecules is no longer Pauli blocked [6], which may bring universal single-channel models into play. Since the term universality comes in many shades, we frame the issues somewhat along the lines of Refs. [20–22], in the order of increasing degree of universality. First, there are single-channel theories where atoms and their interactions are the building blocks, and explicit molecules are absent. The question is, do single-channel and two-channel descriptions give the same results? Second, can the relevant atom-atom or atom-molecule interactions be rolled into a single parameter, such as a scattering length, so that the results of either theory or experiments are independent of the microscopic physics of the interactions? Third, given the interaction parameter, will the system reach a unitarity limit that does not even depend on this parameter anymore as the interaction strength increases?

Zero-temperature strong-coupling BCS theory is a single-channel model characterized entirely by the scattering length, and gives results that are independent of the scattering length when the scattering length tends to infinity. In this strong form of universality the BCS theory agrees with experiments carried out close to the Feshbach resonance [23–25], although it may or may not be quantitatively accurate [26,27]. Moreover, as may be deduced easily from the arguments of Ref. [20], in the case $\Omega \gg \epsilon_F$ and uniformly for all detunings $\delta > 0$, our two-channel mean-field theory and the standard BCS theory give the same results. The product of Fermi wave number and scattering length, $k_F a$, is the dimensionless scaling parameter of the BCS theory. The translation into our model reads $k_F a \equiv -3\pi\Omega^2/8\epsilon_F\delta$.

On the other hand, on the side of large negative detunings and in the limit of strong interaction, the two-channel theory scales with the dressed-molecule parameter $\delta/\bar{\omega}$. This parameter cannot be expressed in terms of $k_F a$ and experimental constants such as atom mass, so that BCS and

two-channel theories are not equivalent. As the normalization equation in the BCS theory is Eq. (6) sans the explicit β^2 , an increasing fraction of bare molecules signals an increasing discrepancy between single- and two-channel mean-field theories.

Nonuniversal experiments.—Our two-channel theory covers all parameter regions, and has different scaling properties on different sides of the resonance. It is therefore of particular interest that the Rice group has recently measured [4] the bare-molecule fraction of a Fermi gas over a wide range of magnetic fields across the resonance. Comparisons between theory and experiment are complicated by the fact that the experimental density varies substantially between data points taken at different magnetic fields. Density information can be recovered from a representation of the data in terms of the parameter $k_F a$ [4], but $k_F a$ is not a scaling variable in our theory and we cannot use it unambiguously as the abscissa when plotting the calculated results. For these reasons we use the average of the Fermi energies deduced from the quoted values of $k_F a$ as our parametrization of the density. Since the interaction-strength parameter scales weakly with density, $\Omega/\epsilon_F \propto \rho^{-1/6}$, we still expect a qualitatively valid comparison with experiments.

The Fermi energy here is obtained from $\epsilon_F = 7.46 \times 2\pi$ kHz. The detuning in terms of magnetic field B is $\delta = \Delta\mu(B - B_0)/\hbar$, where $\Delta\mu = 2\mu_B$ is the difference in magnetic moments between a molecule and an atom pair, and B_0 is the position of the Feshbach resonance. The standard relation between atom-atom scattering length and magnetic field is $a = a_b[1 + \Delta/(B - B_0)]$, where a_b is the background scattering length and Δ is the magnetic-field width of the Feshbach resonance. For a comparison, we need to modify the conversion of parameters between BCS and our approach to exclude the background scattering length, so that $k_F(a - a_b) = -3\pi\Omega^2/8\delta\epsilon_F$. The relation between Fermi energy and wave number, of course, is $\hbar\epsilon_F = \hbar^2 k_F^2/(2m)$. These observations, together with the known resonance parameters [16], give the molecular parameter $\bar{\omega} = 3.34 \times 2\pi$ THz, enormously large compared with any other frequency scale in the problem. Finally, the Rabi frequency is determined from $\Omega/\epsilon_F = (\bar{\omega}/\epsilon_F)^{1/4} = 146$, which indicates the strong-coupling regime.

We plot in Fig. 1 the bare-molecule fraction β^2 as a function of the magnetic field B from the Rice data (circles) and from our calculations assuming a contact interaction with $M = \infty$ (dashed line). In the experiments the conversion into bare molecules extends a few hundred Gauss below the resonance, while the contact-interaction theory predicts a scale $\sim 0.1\hbar\bar{\omega}/|\Delta\mu| \sim 10$ T and completely misses a qualitative trend in the experimental data. The remedy is to invoke a finite range for atom-molecule conversion. We vary the parameter M until what is essentially the relative root-mean square error between the experiments and the theory is minimized at $M = 254 \times 2\pi$ kHz. The corresponding theory curve is

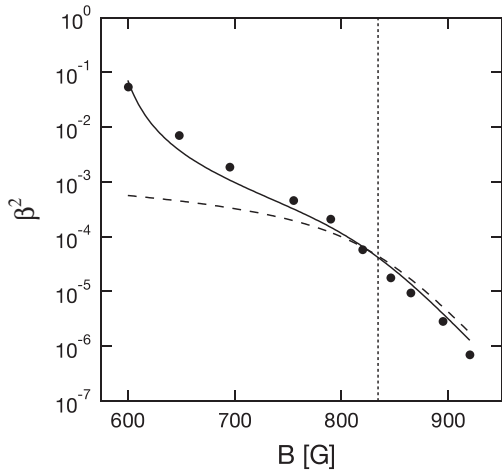


FIG. 1. Bare-molecule fraction in a ${}^6\text{Li}$ gas as a function of magnetic field from experiments [4] (circles), from our theory with a contact interaction for atom-molecule conversion, $M = \infty$, (dashed line), and from our theory with energy cutoff $M = 254 \times 2\pi$ kHz corresponding to a range of the interaction of about $1500a_0$ (solid line). The dotted vertical line marks the position of the Feshbach resonance.

plotted as the solid line. In view of the qualitative assumptions about the Fermi energy in the experiments and the simplistic model for the energy dependence of atom-molecule coupling, the agreement between theory and experiment is now good.

The magnetic-moment data [12] on the bare-molecule fraction covers a much smaller dynamical range than optical spectroscopy, and only on the molecule side of the resonance. The corresponding theory in Ref. [13] is a dressed-molecule argument for $\delta < 0$ that explicitly builds in the background scattering length $a_b = -1405a_0$. Interestingly, when converted into a length via $M = \hbar/(m\ell^2)$, our fitted cutoff M gives $\ell = 1500a_0$.

Conclusions.—A finite cutoff (M) indicates that a contact interaction independent of the details of molecular physics is not sufficient to reach even a qualitative agreement with the experiments (see also [28]). The Rice data manifestly contradicts universality. Besides, experimental detection of a bare-molecule fraction $0 < \beta^2 < 1$ within a presumably molecular gas poses a severe challenge to any single-channel theory. A single-channel model can be retrofitted to include molecules as bound states of atom pairs, which would be the counterpart of our dressed molecules. But what, then, are the separate bare molecules?

We have studied a simple two-channel mean-field theory for a zero-temperature Fermi gas at a Feshbach resonance. The model applies seamlessly across the resonance; no mixing or matching to join the BCS and BEC regimes is needed, or allowed. Our results agree with recent measurements of the fraction of bare molecules at various magnetic fields [4] over a dynamical range of 5 orders of magnitude. Even though the ${}^6\text{Li}$ Fermi gas is strongly coupled, the experimental results are not universal but reflect a finite range of atom-molecule coupling.

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