Atom-Molecule Coexistence and Collective Dynamics Near a Feshbach Resonance of Cold Fermions

R. A. Barankov and L. S. Levitov

Department of Physics, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, Massachusetts 02139, USA

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Degenerate Fermi gas interacting with molecules near a Feshbach resonance is unstable with respect to the formation of a mixed state, in which atoms and molecules coexist as a coherent superposition. A theory of this state is developed using a mapping to the Dicke model, treating the molecular field in the single mode approximation. The results are accurate in the strong coupling regime relevant for current experimental efforts. The exact solution of the Dicke model is exploited to study stability, phase diagram, and nonadiabatic dynamics of the molecular field in the mixed state.

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Feshbach resonance scattering [1–4], at which pairs of atoms can bind to form molecules at the same energy, has been used to demonstrate new coherence phenomena in cold atom systems. Those include, notably, the reversible coherent atom-molecule transitions [5,6] which can be accompanied by the Bose-Einstein condensation (BEC) of molecules [7–9]. Recently, in search of fermionic condensation, the focus shifted to Feshbach resonance in cold fermion systems [10–12].

The physics near the resonance is sensitive to the effects of quantum statistics. In particular, at positive detuning from the resonance, molecules can coexist with fermions [13–16], stabilized by Pauli blocking of decay into the states below the Fermi level. The stability and properties of the mixed state depend on the interaction effects. Below we argue that the interactions enhance the stability of the atom-molecule mixture, and lead to molecules and atom pairs hybridizing to form a coherent state. We address the problem of molecules interacting with atoms by mapping it onto the Dicke problem [17] of two-level systems coupled to a Bose field. This problem, being exactly solvable [18], allows to describe the experimentally relevant regime of strong coupling. In the Feshbach resonance case, the two-level systems represent fermion pair states which can be occupied or empty, while the Bose field represents molecules.

The coupling to molecules at positive detuning from Feshbach resonance enhances pairing interaction between fermions, which is expected to stimulate BCS superfluidity [13–16,19–21]. In addition, as noted in Refs. [13,14], the strong coupling BCS condensation, with the critical temperature up to a fraction of E_F, may depend on the presence of molecular field. This conclusion was strengthened by a microscopic analysis [20,21]. Ref. [16] studied fermion-molecule coexistence at positive detuning using an effective theory of strong coupling formulated in terms of low energy parameters. It was noted that strong many-body effects exist even for detuning well above the Fermi energy.

In this Letter, we focus on the effects of molecule-atom hybridization and develop an approach allowing to handle this problem in the strong coupling regime. This is of interest, since the experiment deals with systems where the atom-molecule coupling, measured in the Fermi energy units, is very large. We will see that molecule-atom mixing occurs in this situation in the range of detuning much larger than the Fermi energy, i.e., on the energy scale very different from that of fermionic condensate. The energy scale for the latter, set by the pairing interaction strength, expected to reach $0.2E_F$ at best [21], is much smaller than the atom-molecule interaction. Thus, accurate results can be obtained with the help of a simple analysis which ignores direct pairing interaction between fermions and relies on the exact solution of the atom-molecule dynamics.

Below we analyze stability of fermions with respect to molecule formation, and obtain a phase diagram. There is a fairly wide region around the resonance, spanning both positive and negative detuning, where atoms and molecules coexist, forming a coherent state. At strong coupling, this region has width of the order of g^2n/E_F, a quantity which different estimates [15,16] put between few tens and few hundred E_F for current experiments [10–12]. Also, we exploit the Dicke problem solution to obtain nonlinear oscillations of the molecular field, in which population coherently oscillates between molecular and atomic components. The results of stability analysis are verified by comparing to the exact solution and to the thermodynamic ground state properties.

We consider the problem of a Fermi gas interacting with molecules in a single mode approximation which takes into account only the lowest energy molecular state:

$$\mathcal{H} = \sum_{\alpha=p,\sigma} \epsilon_p^{(0)} a_\alpha^+ a_\alpha + g\sum_p (b^+ c_p + \text{H.c.}) + \omega b^+ b, \quad (1)$$

($\epsilon_p^{(0)} = p^2/2m$) with $a_{p\sigma}$, $a_{p\sigma}^+$ and b, b^+ the atom and molecule operators, σ the fermion spin, and ω the energy of a molecule. The atom pair creation and annihilation

operators $c_p = \frac{1}{\sqrt{2}}(a_{-p\downarrow}a_{p\uparrow} + a_{p\downarrow}a_{-p\uparrow})$, $c_p^+ = \frac{1}{\sqrt{2}} \times (a_{p\uparrow}^+ a_{-p\downarrow}^+ + a_{-p\uparrow}^+ a_{p\downarrow}^+)$ describe pairs of fermions in a spin singlet state that undergo conversion into molecules at Feshbach resonance. The approximation (1) is justified by the analysis below which finds that the energy gained by a formation of a mixed atom-molecule state, with all molecules occupying one state, is large compared to E_F.

The utility of the single mode approximation (1) is that it turns a difficult many-body problem into a well-known exactly solvable problem. The mapping is achieved by identifying the pair operators c_p^+, c_p with pseudospin Pauli operators [22], $\sigma_p^\pm \equiv \frac{1}{2}(\sigma_p^x \pm i\sigma_p^y)$, and noting that their product gives the particle number operator $n_p = a_p^+ a_p$ in the subspace of the many-body Hilbert space in which both states p and $-p$ are simultaneously filled or empty, $2c_p^+ c_p \equiv n_p + n_{-p} = 0, 2$. More formally, defining $\sigma_p^z = [\sigma_p^+, \sigma_p^-]$, one verifies that the standard Pauli spin commutation relations hold:

$$[\sigma_p^+, \sigma_p^z] = -2\sigma_p^+, \qquad [\sigma_p^-, \sigma_p^z] = 2\sigma_{p.}^- \tag{2}$$

This enables one to bring the Hamiltonian (1) to the form containing the spin variables only,

$$\mathcal{H} = \sum_p{}' \left(\epsilon_p^{(0)} \sigma_p^z + gb\sigma_p^+ + gb^+ \sigma_p^- \right) + \omega b^+ b, \tag{3}$$

where the sum is taken over singlet pair states with momenta p and $-p$. We note that the states with $n_p + n_{-p} = 1$, with only one of the p and $-p$ particle states filled and the other one empty, are decoupled and do not participate in the dynamics defined by (3). The reason for this decoupling is that these states have not enough particles to form a molecule, but also one particle too many to contribute to molecule dissociation.

The spin-boson problem (3) is the Dicke model of quantum optics [17,18,23]. Hepp and Lieb [18] found that the Hamiltonian (3) is integrable, and constructed exact many-body states. Besides the total particle number

$$N = 2b^+ b + \sum_p (1 + \sigma_p^z), \tag{4}$$

there are also infinitely many nontrivial conserved quantities underpinning the exact solubility.

Here we employ the Hamiltonian (3) to assess stability of the Fermi gas with respect to molecule formation. The spin dynamics described by (3) is of the Bloch form, $\dot{\sigma} = i[\mathcal{H}, \sigma] = 2\mathbf{h}_p \times \sigma$, with an effective magnetic field $\mathbf{h}_p = (gb', gb'', p^2/2m)$, where $b = b' + ib''$ is a c-number describing the molecular state.

The Bloch equations of motion for the spin components $\sigma_p^\pm$, σ_p^z, and b take the form

$$i\dot{\sigma}_p^+ = -2\epsilon_p^{(0)}\sigma_p^+ + gb\sigma_p^z, \quad i\dot{\sigma}_p^- = 2\epsilon_p^{(0)}\sigma_p^- - gb\sigma_p^z, \tag{5}$$

$$i\dot{\sigma}_p^z = 2gb\sigma_p^+ - 2gb^*\sigma_p^-, \qquad i\dot{b} = g\sum_p{}'\sigma_p^- + \omega b. \tag{6}$$

From a mathematical standpoint, Eqs. (5) and (6) describe collective dynamics of a Bloch spin 1/2 ensemble, with the coupling between the spins provided by the "magnetic field" $\mathbf{h}_p$ transverse components which depend on the spin variables via an equation for b. Physically, the transverse spin components $\sigma_p^\pm$ characterize coherence between the filled and unfilled pair state, while σ_p^z describes the number of pairs.

Since the field b is a c-number, the operator Eqs. (5) and (6) are linear, and thus the spin expectation values are subject to evolution equations of the form identical to (5) and (6). In the absence of molecules, we have $b = 0$, and all the spins are aligned in the $\pm z$ direction, with probabilities determined by occupation of pair states: $\langle \sigma_p^z \rangle = p_\uparrow - p_\downarrow = n_p^2 - (1 - n_p)^2 = 2n_p - 1$, where $n_p = (e^{\beta(\epsilon_p^{(0)} - \mu)} + 1)^{-1}$ in thermal equilibrium. This state, containing only fermions but no molecules, $\langle b \rangle = \langle \sigma_p^\pm \rangle = 0$, is stationary for the problem (5) and (6).

To assess stability with respect to molecule formation, we linearize Eqs. (5) and (6), introducing $\delta\sigma_p^-, \delta b \propto e^{-i\lambda t}$, $\delta\sigma_p^+, \delta b^* \propto e^{i\lambda^* t}$. From the coupled linear equations for $\delta\sigma_p^-$ and δb, we obtain the eigenvalue equation

$$\lambda = \omega + g^2 \sum_p \frac{\langle \sigma_p^z \rangle}{2\epsilon_p^{(0)} - \lambda}. \tag{7}$$

To make the formally divergent sum over p well-behaved, we renormalize ω by subtracting the term $\delta\omega = g^2 \sum_p (2\epsilon_p^{(0)})^{-1}$. The shift $\omega \to \omega - \delta\omega$ brings the position of the Feshbach resonance to $\omega = 0$ for zero particle density, while Eq. (7) transforms to

$$\lambda = \omega + g^2 \sum_p \left(\frac{2n_p - 1}{2\epsilon_p^{(0)} - \lambda} + \frac{1}{2\epsilon_p^{(0)}} \right) \tag{8}$$

with the sum now converging at large p.

The solution of Eq. (8) can be real or complex, depending on the value of ω. Complex-valued $\lambda = \lambda' + i\lambda''$ indicates an instability, with λ'' describing the instability growth rate. Numerical analysis of Eq. (8) and simple analytic arguments reveal that the instability occurs in an interval $\omega_0 < \omega < \omega_1$ with $\omega_{0,1}$ being a function of temperature. The values $\omega_{0,1}$ can be inferred by noting that the complex λ becomes real at $\omega = \omega_{0,1}$, which gives the condition $\lambda'' = 0$. When does Eq. (8) admit real solutions? This is possible for $\lambda = 2\mu \equiv p_F^2/m$, since $2n_p - 1$ changes sign at the Fermi energy, and for $\lambda \leq 0$. (For all positive λ except $\lambda = 2\mu$, the residue $\langle \sigma_p^z \rangle = 2n_p - 1$ generates a finite imaginary part of λ.) With $\lambda = 2\mu$, one obtains

$$\omega_1 = 2\mu + \frac{g^2}{2} \sum_p \left(\frac{1 - 2n_p}{\epsilon_p^{(0)} - \mu} - \frac{1}{\epsilon_p^{(0)}} \right), \tag{9}$$

while ω_0 is determined by a root $\lambda < 0$ of Eq. (8) which

can be found numerically. This indicates that atoms are stable at $\omega > \omega_1$, metastable at $\omega < \omega_0$, and at $\omega_0 < \omega < \omega_1$ can exist only in a state coherently mixed with the molecules (Fig. 1). We note that, since $\omega_0 < 0$ and $\omega_1 > 2\mu$, coexistence is favored by interaction. Moreover, at strong interaction, the detuning range where coexistence takes place becomes very large: $\Delta\omega \simeq g^2 n/E_F \gg E_F$.

The upper temperature at which $\omega_0 = \omega_1$ is determined by the condition $\mu(T) = 0$. For a two-species Fermi gas of total particle density n, one has $n = 2\sum_p n_p(\mu = 0) = 0.0972(m/\beta)^{3/2}$ which gives $T_* = 0.9885E_F$. Interestingly, at low temperature $T \ll T_*$, the instability is pushed to higher detuning, $\omega_1 = 2\mu + g^2\nu\ln(\mu/T)$, due to a BCS-like log divergence at the Fermi level $p = p_F$.

It is instructive to look at the JILA experiment parameters (Fig. 1). The estimate of coupling $\Delta\omega = g^2 n/E_F \simeq 60\ \mu\text{K} \approx 2\pi \times 1.3$ MHz gives a typical energy gained by the system via molecules and atom pairs hybridization, which is much larger than E_F. This leads to pair size in the mixed state $\sim\hbar/(2m\Delta\omega)^{1/2}$ much smaller than fermion wavelength p_F^{-1}. This indicates that the kinetic energy of atoms *and molecules* does not play a significant role, justifying the single mode approximation.

Nonlinear dynamics at instability can be found with the help of the mapping to Bloch spins. Defining $r_p^{\pm} = \langle\sigma_p^{\pm}\rangle$, $r_p^z = \langle\sigma_p^z\rangle$, and rescaling $gb \to b$, we write

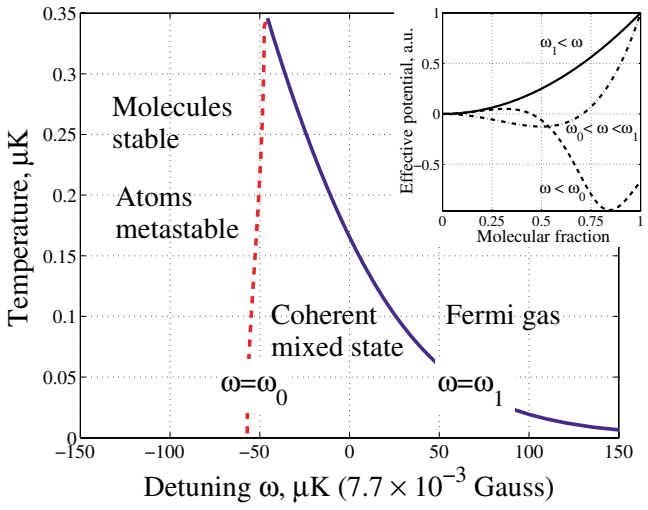

FIG. 1 (color online). Phase diagram of coupled atom-molecule system obtained from Eq. (8) for ^{40}K system [10] at particle density $n \approx 1.8 \times 10^{13}$ cm^{-3}, Fermi energy $E_F = 0.35\ \mu$K, and coupling strength $g^2 n/E_F \approx 60\ \mu$K. (The coupling was estimated using the microscopic theory of Feshbach resonance [15], applied to the conditions of the JILA experiment [10]). Inset: Effective potential schematic illustrating the behavior in the three regions.

$$i\dot{r}_p^- = 2\epsilon_p^{(0)} r_p^- - b r_p^z, \qquad i\dot{r}_p^z = 2b r_p^+ - 2b^* r_p^-, \tag{10}$$

and $i\dot{b} = \omega b + g^2\sum_p r_p^-$. Since the norm is preserved by Bloch time evolution, $|\mathbf{r}_p|^2 = 4r_p^- r_p^+ + (r_p^z)^2$ is conserved for each spin. We apply rotation,

$$r_p^- \to e^{-i\eta t} r_p^-, \qquad r_p^+ \to e^{i\eta t} r_p^+, \qquad b \to e^{-i\eta t} b \tag{11}$$

with the value η to be determined later. This is equivalent to shifting $2\epsilon_p^{(0)} \to \omega_p = p^2/m - \eta$ and $\omega \to \omega - \eta$.

The resulting problem possesses real-valued solutions which can be obtained from the standard ansatz [25]

$$r_p^- = A_p b + iB_p\dot{b}, \qquad r_p^z = D_p - C_p b^2. \tag{12}$$

This ansatz automatically satisfies the imaginary part of Eq. (10) for r_p^- as well as the equation for r_p^z, provided that $A_p = \omega_p B_p$, $C_p = 2B_p$, while the real part of Eq. (10) for r_p^- generates a set of equations

$$B_p\ddot{b} + \omega_p A_p b - b(D_p - C_p b^2) = 0. \tag{13}$$

The constant of motion $|\mathbf{r}_p|^2 = 4r_p^- r_p^+ + (r_p^z)^2$ provides a first integral of Eq. (13):

$$4(\omega_p^2 b^2 + \dot{b}^2) + (2b^2 - D_p/B_p)^2 = B_p^{-2}|\mathbf{r}_p|^2, \tag{14}$$

where we expressed A_p and C_p through B_p.

Evidently, since the function $b(t)$ is the same for all spins, the dependence on p has to drop out of Eq. (14), giving a single equation for b of the form

$$\dot{b}^2 = (b^2 - b_-^2)(b_+^2 - b^2), \qquad b_- < b_+, \tag{15}$$

which is possible with the following choice of constants: $D_p/B_p - \omega_p^2 = b_-^2 + b_+^2$, $D_p^2 - |\mathbf{r}_p|^2 = 4b_-^2 b_+^2 B_p^2$. These equations define the modulus of B_p and D_p only. The sign has to be determined from initial conditions: $\text{sgn}B_p = \text{sgn}D_p = \text{sgn}r_p^z$.

The solution of Eq. (15) is an elliptic function $b(t) = b_+\text{dn}(b_+ t, \kappa^2)$ with $\kappa^2 = 1 - b_-^2/b_+^2$ [26], oscillating periodically between b_- and b_+. At $b_- \ll b_+$, the solution is approximately given by a train of weakly overlapping solitons with period $\tau = (2/b_+)\ln(4b_+/b_-)$,

$$b(t) = \sum_n \frac{\gamma}{\cosh\gamma(t - t_n)}, \qquad t_n = \tau n \tag{16}$$

(Fig. 2), where each soliton in Eq. (16) is a solution of Eq. (15) with $b_- = 0$, $b_+ = \gamma$.

The values $b_\pm$ and η are fixed by the equation for b. The latter is consistent with the ansatz (12), giving

$$1 = g^2\sum_p \frac{r_p^z}{\sqrt{(\omega_p^2 + b_-^2 + b_+^2)^2 - 4b_-^2 b_+^2}}, \tag{17}$$

$$\omega = \eta - g^2\sum_p \left(\frac{\omega_p r_p^z}{\sqrt{(\omega_p^2 + b_-^2 + b_+^2)^2 - 4b_-^2 b_+^2}} + \frac{1}{2\epsilon_p^{(0)}}\right),$$

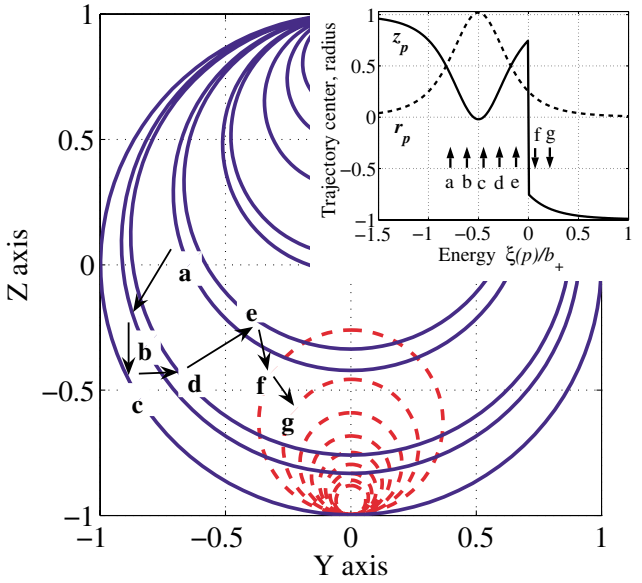

FIG. 2 (color online). Pseudospin precession (12) for fermion pair states corresponding to the soliton train (16) is shown on the Bloch sphere $r_p^{x,y,x} = \langle \sigma_p^{x,y,x} \rangle$. Parameters used: $b_-/b_+ = 0.1$, $\eta - 2E_F = -b_+$, constant density of states. The energies above and below the Fermi level (solid and dashed curves) are chosen as indicated by arrows in the inset. Note that each state completes a full 2π Rabi cycle per soliton. Inset: Radius $r_p = (b_+^2 - b_-^2)/(\omega_p^2 + b_+^2 + b_-^2)$ and center $z_p = (1 - 2n_p)\omega_p^2/(\omega_p^2 + b_+^2 + b_-^2)$ of trajectories *vs* energy $\xi(p) = \epsilon_p^{(0)} - E_F$. Note the absence of particle-hole symmetry.

with $r_p^z = 2n_p - 1$ determined by the initial energy distribution n_p. Equation (17) implies that $\omega_p = 2\epsilon_p^{(0)} - \eta$ changes sign below the Fermi level, $\eta < 2E_F$. Thus there is no particle-hole symmetry in the dynamics even in the case of constant density of states, as illustrated in Fig. 2.

The properties at equilibrium can be understood by considering the limit $b_- \to b_+ = b_0$ when oscillations are absent. The energy distribution n_p can be easily obtained in the pseudospin picture, taking into account that each spin is presented with a tilted field $\mathbf{h}_p = (b_0, 0, \epsilon_p^{(0)} - \mu)$ which gives $n_p = 1/(1 + e^{\beta|\mathbf{h}_p|})$. The molecular field b_0 in the ground state is determined by

$$\omega = \eta + g^2 \sum_p \left(\frac{\mathrm{sgn}\omega_p (1 - 2n_p)}{\sqrt{\omega_p^2 + 4b_0^2}} - \frac{1}{2\epsilon_p^{(0)}} \right) \qquad (18)$$

along with the constraint $N = 2b_0^2/g^2 + 2\sum_p n_p$.

Here we use Eq. (18) to verify the above stability analysis. To determine when the atoms can be stable with respect to hybridizing with molecules, we set $b_0 = 0$ and immediately recover Eq. (8) for the instability exponent λ. The difference, however, is that η defined by Eq. (18) is real, while λ is complex. Atoms' stability is thus indeed equivalent to the existence of a real-valued solution of Eq. (8). One possibility to have such a solution is to set $\eta = 2\mu$, which eliminates the log divergence in (18) at $\omega_p = 0$. The other possibility is to have μ, $\eta \leq 0$. Put together with the properties of equilibrium state at finite b_0, this confirms the above estimate of the coexistence region (8) and the conclusion that pure atom state is metastable at the detuning $\omega < \omega_0$.

In summary, this work provides a phase diagram and an exact solution for the atom-molecule dynamics in the regime of strong coupling. The characteristic energy scales are estimated to be much larger than E_F, which makes the Dicke model approximation ignoring molecular dispersion, as well as the BCS fermion pairing effects, accurate enough. A wide atom-molecule coexistence region is predicted in which atom pairs and molecules hybridize into objects of size much less than Fermi wavelength p_F^{-1}.

Note added.— After having completed this work we became aware of the article by Andreev, Gurarie and Radzihovsky [27], which exploits the mapping to the Dicke model, while focusing on the weak coupling limit.

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