Atom-molecule coexistence and collective dynamics near a Feshbach resonance of cold fermions

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Degenerate Fermi gas interacting with molecules near Feshbach resonance is unstable with respect to formation of a mixed state in which atoms and molecules coexist as a coherent superposition. Theory of this state is developed using a mapping to the Dicke model, treating 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 molecular field in the mixed state.

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 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 in a macroscopic system 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 molecular 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 greatly enhance 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 [20,13–16,21,22]. In addition, as noted by Timmermans et al. [13] and Holland et al. [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 carried out by Ohashi and Griffin [21], by Milstein et al. [22], who refine the approach of Ref. [14]. Bruun and Pethick [16] studied noncondensed molecules coexisting with the Fermi gas 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. The important role of molecular field at positive detuning has been reemphasized recently by Falco and Stoof [15], who argued that a BCS-BEC crossover takes place in this region.

In this article, 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 0.2 $E_F$ at best [22], 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 $g^2 n / E_F$, 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:

$$H = \sum_{\mathbf{p},\alpha} \frac{p^2}{2m} \alpha_\mathbf{p,\alpha}^+ \alpha_\mathbf{p,\alpha} + g \sum_{\mathbf{p}} \left( b^+ c_\mathbf{p} + \text{h.c.} \right) + \omega b^+ b \quad (1)$$

with $a_\mathbf{p}$, $a_\mathbf{p}^+$ and $b$, $b^+$ the atom and molecule operators, $\alpha$ the fermion spin, and $\omega$ the energy of a molecule.
The atom pair creation and annihilation operators \( c_p = \frac{1}{\sqrt{2}} (a_{-p} a_p + a_p a_{-p}) \), \( c_p^+ = \frac{1}{\sqrt{2}} (a_{-p}^+ a_{-p} + a_p^+ a_p) \) 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 \( E_F \), which allows to limit consideration to a single molecular state.

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 [24]

\[
c_p = \sigma_p^- = \frac{1}{2}(\sigma_p^- - i\sigma_p^y), \quad c_p^+ = \sigma_p^+ = \frac{1}{2}(\sigma_p^+ + i\sigma_p^y) \tag{2}
\]

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, \( 2\sigma_p^+ c_p \equiv n_p + n_{-p} = 0, 2 \). More formally, defining \( \sigma_p^0 = [\sigma_p^+, \sigma_p^-] \), one verifies that the standard Pauli spin commutation relations hold:

\[
[\sigma_p^+, \sigma_p^-] = -2\sigma_p^0, \quad [\sigma_p^0, \sigma_p^-] = 2\sigma_p^-
\tag{3}
\]

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

\[
\mathcal{H} = \sum_p \left( \frac{p^2}{2m} \sigma_p^0 + gb\sigma_p^+ + gb^+\sigma_p^- \right) + \omega b^+ b \tag{4}
\]

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 (4). The reason for this decoupling is that these states do not have enough particles to form a molecule, but also one particle too many to contribute to molecule dissociation.

The spin-boson problem (4) is the Dicke model of quantum optics [17–19]. Hepp and Lieb [18] found that the Hamiltonian (4) is integrable, and constructed exact many-body states. Besides the total particle number

\[
N = 2b^+ b + \sum_p (1 + \sigma_p^0) \tag{5}
\]

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

The problem (4) resembles in many ways the BCS pairing problem. The latter is also integrable, which allows to obtain the full energy spectrum, and to construct nontrivial conserved quantities in a closed form [23]. In fact, the above pseudospin trick has its roots in the BCS problem, where it was invented by Anderson [24] as an interpretation of Bogoliubov mean field theory.

Here we employ the Hamiltonian (4) to assess stability of the Fermi gas with respect to molecule formation. The spin dynamics described by (4) is of the Bloch form, \( \dot{\sigma} = i[H, \sigma] = 2hp \times \sigma \), with an effective magnetic field \( h_p = (gb', gb'', p^2/2m) \), where \( b = b' + ib'' \) is a c-number describing the molecular state in macroscopic limit.

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

\[
i\dot{\sigma}_p^+ = -(p^2/m)\sigma_p^+ + gb\sigma_p^z, \quad i\dot{\sigma}_p^- = (p^2/m)\sigma_p^- - gb^*\sigma_p^z \tag{6}
\]

\[
i\dot{\sigma}_p^z = gb\sigma_p^+ - gb^*\sigma_p^-, \quad \dot{b} = \gamma \sum_p \sigma_p^- + \omega b \tag{7}
\]

From a mathematical standpoint, Eqs.(6),(7) describe collective dynamics of a Bloch spin 1/2 ensemble, with the coupling between the spins provided by the ‘magnetic field’ \( h_p \), 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 \( \sigma_p^z \) describes the number of pairs.

Since the field \( b \) is a c-number, the operator equations (6),(7) are linear, and thus the spin operators expectation values are subject to evolution equations of the form identical to (6),(7). 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: \( \langle \sigma_p^z \rangle = n_p - n_{-p}^2 = 2n_p - 1 \), where \( n_p = (e^{p^2/(2m - \nu)} + 1)^{-1} \), in thermal equilibrium. This state, containing only fermions but no molecules, \( \langle \sigma_p^z \rangle = 0 \), is stationary for the problem (6),(7).

To assess stability with respect to molecule formation, we linearize Eqs.(6),(7), introducing \( \delta\sigma_p^\pm, \delta b \propto e^{-i\lambda t}, \delta\sigma_p^z, \delta b^\prime \propto e^{i\lambda^\prime t} \). From the coupled linear equations for \( \delta\sigma_p^\pm \) and \( \delta b \) we obtain the eigenvalue equation

\[
\lambda = \omega + g^2 \sum_p \frac{\langle \sigma_p^z \rangle}{p^2/m - \lambda} \tag{8}
\]

To make the formally divergent sum over \( p \) well-behaved, following Ohashi and Griffin [25], we renormalize \( \omega \) by subtracting the term \( \delta\omega = g^2 \sum_p (p^2/m)^{-1} \). The shift \( \omega \rightarrow \omega - \delta\omega \) brings the position of the Feshbach resonance to \( \omega = 0 \) for zero particle density, while Eq.(8) transforms to

\[
\lambda = \omega + g^2 \sum_p \left( \frac{2n_p - 1}{p^2/m - \lambda} + \frac{1}{p^2/m} \right) \tag{9}
\]

with the sum now converging at large \( p \).

The solution of Eq.(9) can be real or complex, depending on the value of \( \omega \). Complex-valued \( \lambda = \lambda' + i\lambda'' \) indicates an instability, with \( \lambda'' \) describing the instability growth rate. Numerical analysis of the solutions of Eq.(9) and simple analytic arguments reveal that (i) the real part \( \lambda' \) is a monotonic function of \( \omega \); (ii) the instability occurs in an interval \( \omega_0 < \omega < \omega_1 \) with the threshold values \( \omega_{0,1} \) being a function of temperature.
The values $\omega_{0,1}$ can be inferred by noting that the complex $\lambda$ becomes real at $\omega = \omega_{0,1}$, which gives the condition $\lambda' = 0$. When does Eq. (9) admit real solutions? This is possible for $\lambda \leq 0$, as well as for $\lambda = 2\mu$, since $\omega_{0,1} = 1$ changes sign at $\mu = p_F$. (For all positive $\lambda$ except $\lambda = 2\mu$ the residue $(\sigma^+_{p}) = 2n_p - 1$ generates a finite imaginary part of $\lambda$.) With $\lambda = 0$, $2\mu$ one obtains

$$\omega_0 = -g^2 \sum_p \frac{2n_p}{p^2/m}, \quad \omega_1 = 2\mu + g^2 \sum_p \left( \frac{1 - 2n_p}{p^2/m - 2\mu} - \frac{1}{p^2/m} \right)$$

(10)

This indicates that atoms are stable at $\omega > \omega_0$, 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: $\Delta\omega \simeq g^2 n/E_F \gg E_F$.

FIG. 1. Phase diagram of coupled atom-molecule system obtained from Eq. (10) 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 developed by Falco and Stoof [15], applied to the conditions of the JILA experiment [10].) Inset: Effective potential schematic illustrating the behavior in the three regions.

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 $n = 2\sum_p n_p \mu = 0.0972(m/\beta)^{3/2}$ which gives $T_c = 0.9885 E_F$. Interestingly, at low temperature $T \ll T_c$, the instability is pushed to higher detuning, $\omega_1 = 2\mu + g^2 n \ln(\mu/T)$, 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 $\Delta\omega = g^2 n/E_F \approx 60\mu$K $\approx 8$ 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 $\sim h/(2m\Delta\omega)^{1/2}$ 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 $r_{p}^{\pm} = (\frac{1}{2}(\sigma_{p}^{z} \pm i\sigma_{p}^{y}))$, and rescaling $gb \rightarrow b$, we write

$$\dot{r}_p^+ = (p^2/m)r_p^- - br_p^+,$$

$$\dot{r}_p^- = 2br_p^- - 2^*r_p^-$$

(11)

(12)

Since the norm is preserved by Bloch time evolution, $|r_p|^2 = 4r_p^- r_p^+ + (r_p^*)^2$ is conserved for each spin. We apply rotation,

$$r_p^- = A_p b + iB_p b^*, \quad r_p^+ = D_p - C_p b^2$$

(13)

Substituting this into Eqs.(11),(12), from the real part of the equation or $r_p^-$ and from the equation or $r_p^-$ one finds the relations between the ansatz parameters $A_p = \epsilon_p B_p$, $C_p = 2B_p$, while the imaginary part of the equation or $r_p^-$ generates a set of equations

$$B_p \dot{b} + \epsilon_p b - b(D_p - C_p b^2) = 0$$

(14)

The constant of motion $|r_p|^2 = 4r_p^- r_p^+ + (r_p^*)^2$ provides a first integral of Eq.(15):

$$4 \left(\epsilon_p^2 b^2 + \dot{b}^2 \right) + (2b^2 - D_p/B_p)^2 - B_p^{-2}|r_p|^2$$

(16)

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.(16), giving a single equation for $b$ of the form

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

(17)

which is possible with the following choice of constants:

$$D_p/B_p - \epsilon_p^2 = b_-^2 + b_+^2, \quad D_p - |r_p|^2 = 4b_-^2 b_+^2$$

(18)

These equations determine the modulus of $B_p$ and $D_p$ only. The sign has to be determined from initial conditions: $\text{sgn} B_p = \text{sgn} D_p = \text{sgn} r_p^-$.

The solution of Eq. (17) is an elliptic function $b(t) = d n(t, k^2)$ with $k^2 = 1 - b_-^2/b_+^2$ [27], oscillating periodically between $b_-$ and $b_+$. At $b_- < b_+$, the solution
is approximately given by a train of weakly overlapping solitons

\[ b(t) = \sum_n \frac{\gamma}{\cosh \gamma(t - t_n)}, \quad t_n = \tau n \]  

(19)

(Fig. 2), where each soliton in Eq. (19) is a solution of Eq. (17) with \( b_- = 0, b_+ = \gamma \).

![Diagram of soliton train form (19), shown in the inset. The Bloch sphere with different energies obtained for the molecular field of a soliton train.]  

The quantities \( b_\pm \) and the frequency \( \eta \) must be determined from the equation for \( b \). One verifies that Eq. (12) is consistent with the ansatz (14) and obtains

\[ 1 = g^2 \sum_p \frac{r_p^2}{\sqrt{(\epsilon_p + b_-^2 + b_+^2)^2 - 4b_-^2 b_+^2}}, \]  

(20)

\[ \omega = \eta - g^2 \sum_p \left( \frac{\epsilon_p r_p^2}{\sqrt{(\epsilon_p + b_-^2 + b_+^2)^2 - 4b_-^2 b_+^2}} + \frac{1}{p^2/m} \right), \]

Here \( r_p^2 = 2n_p - 1 \) corresponds to the energy distribution \( n_p \) of fermions which depends on the initial state. For the parameters used in Fig. 1, by order of magnitude we estimate \( \gamma, \tau^{-1} \approx g^2 n / E_F \approx 8 \text{ MHz} \). This is much faster than typical energy relaxation rates, which justifies ignoring relaxation effects in the dynamics.

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 \( h_p = (b_0, 0, p^2 / 2m - \mu) \)

which gives \( n_p = 1 / \left( 1 + e^{\beta |h_p|} \right) \). The molecular field \( b_0 \) in the ground state is determined by

\[ \omega = \eta + g^2 \sum_p \left( \frac{\text{sgn} \epsilon_p (1 - 2n_p)}{\sqrt{\epsilon_p^2 + 4b_0^2}} - \frac{1}{p^2/m} \right) \]  

(21)

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

Here we use Eq. (21) 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. (9) for the instability exponent \( \lambda \). The difference, however, is that \( \eta \) defined by Eq. (21) is real, while \( \lambda \) is complex. Atoms’ stability is thus indeed equivalent to the existence of a real-valued solution of Eq. (9). One possibility to have such a solution is to set \( \eta = 2\mu \), which eliminates the log divergence in (21) at \( \epsilon_p = 0 \). The other possibility is to have \( \mu, \eta \leq 0 \). Put together with the properties of equilibrium state at finite \( b_0 \), this confirms the above estimate of the coexistence region (10) 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 \( p_F^{-1} \).

After having completed this work we became aware of the article by Andreev, Gurarie and Radzihovsky [28] which exploits the mapping to the Dicke model, while focusing on the weak coupling limit.

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