Nonequilibrium dynamics and thermodynamics of a degenerate Fermi gas across a Feshbach resonance

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We consider a two-species degenerate Fermi gas coupled by a diatomic Feshbach resonance. We show that the resulting superfluid can exhibit a form of coherent BEC-to-BCS oscillations in response to a nonadiabatic change in the system’s parameters, such as for example a sudden shift in the position of the Feshbach resonance. In the narrow resonance limit, the resulting soliton-like collisionless dynamics can be calculated analytically. In equilibrium the thermodynamics can be accurately computed across the full range of BCS-BEC crossover, with corrections controlled by the ratio of the resonance width to the Fermi energy.

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Recent experimental advances to control interactions in trapped degenerate gases by tuning (via magnetic field) through a Feshbach resonance (FR), led to observation of long-sought after molecular Bose-Einstein condensation in bosonic \[ ^{85}\text{Rb} \] and fermionic atomic gases \[ ^{2}\text{H} \text{g} \]. Such tunability allows studies of these systems in previously unexplored regimes, as exemplified by recent JILA and MIT experiments \[ ^{2}\text{H} \text{g} \], that appear to observe paired fermionic condensates along the crossover between the BCS regime of weakly-paired, strongly overlapping Cooper pairs, and the BEC regime of tightly bound, weakly-interacting diatomic molecules. An even more exciting possibility, unavailable in other related (e.g., superconductors and superfluids in condensed matter) systems, is the nonadiabatic switching of system’s parameters, thereby allowing access to highly coherent and nonequilibrium quantum states of matter. For bosonic \[ ^{85}\text{Rb} \] atoms, this was recently spectacularly realized in experiments by Donley et al \[ ^{4}\]. Using short magnetic field pulses that briefly bring the system close to a nearby FR, they observed coherent oscillations in the atomic condensate that can be interpreted as Rabi oscillations between atomic and molecular condensates \[ ^{4}\].

Stimulated by these experimental advances, in this paper we study a zero-temperature collisionless dynamics of a two-species degenerate atomic Fermi gas near a FR, that can be tuned through the Fermi sea. The goal is to understand the evolution of the system following a nonadiabatic change in an externally-controlled system’s parameter, such as the detuning of the FR, \( \omega_{0} \), relative to the Fermi energy, \( \epsilon_{F} \).

Our main result is the demonstration that such a system exhibits an integrable soliton-like solutions, corresponding to collective coherent oscillations of the Fermi gas between BCS- and BEC-like paired superfluid states. This dynamics is a paired-fermions analog of the atomic-to-molecular condensate Rabi oscillations observed by Donley et al in trapped bosonic gases. In the narrow Feshbach resonance limit we calculate the frequency and amplitude of these oscillations and find their analytic form. Our work directly builds on the recent discovery by Barankov, Levitov, and Spivak \[ ^{1}\] of integrable dynamics in the BCS model following a sudden change in the negative s-wave scattering length.

Complementing our study of dynamics, we also analyze the thermodynamics along the full range of the BCS-BEC crossover \[ ^{3}\]. We show that for a FR that is narrow compared to the Fermi energy, and a background scattering length \( a_{bg} \) that is short compared to the interatomic spacing, \( n^{-1/3} \), low-temperature thermodynamics can be accurately computed analytically \[ ^{8}\].

Our starting point is the Hamiltonian \[ ^{9}\]

\[
H = \sum_{p,\sigma} \epsilon_{p} \hat{a}_{p,\sigma}^{\dagger} \hat{a}_{p,\sigma} + \sum_{p} \left( \epsilon_{0} + \frac{\epsilon_{p}}{2} \right) \hat{b}_{p}^{\dagger} \hat{b}_{p} + \sum_{p,q} \frac{g}{\sqrt{p}} \left( \hat{b}_{q} \hat{a}_{p+q,\uparrow}^{\dagger} \hat{a}_{p,\downarrow}^{\dagger} + \hat{b}_{q}^{\dagger} \hat{a}_{p,\downarrow} \hat{a}_{p+q,\uparrow} \right) (1)
\]

describing fermionic atoms, created by \( \hat{a}_{p,\sigma}^{\dagger} \), with momentum \( p \), “spin” \( \sigma = \uparrow, \downarrow \), and kinetic energy \( \epsilon_{p} = p^{2}/2m \), that are coupled to diatomic molecular (resonant) states created by \( \hat{b}_{p}^{\dagger} \). The position and the width (molecular lifetime) of the FR are respectively controlled by the bare detuning energy \( \epsilon_{0} \) and coupling \( g \), the former easily experimentally tunable by a magnetic field. We have neglected nonresonant atom-atom and molecule-molecule interactions that we expect near a FR to be subdominant to the resonant scattering.

In what follows we focus on molecules with zero center of mass momentum, \( \hat{b}_{0} \), neglecting molecules \( \hat{b}_{p\neq0} \) excited above the molecular condensate. For equilibrium phenomena, this approximation is justified at low temperatures and weak interactions (small \( g \)), for which condensate depletion is small. However, for nonequilibrium dynamics of interest to us, the validity of this approximation is a more delicate issue, as one might generically expect such bosonic finite momentum excitations to be induced by a nonadiabatic shift in the FR. Nevertheless, physically we expect that for an initially homogeneous condensate \[ ^{3}\] and weak interactions the dynamics will
be dominated by \( b_0(t) \). However, on sufficiently long time scales the \( b_{q \neq 0} \) excitations and particle collisions should decohere and damp out the collective BEC-BCS oscillations studied here, allowing a slow relaxation to a new equilibrium state for the shifted FR. Determining this relaxational dynamics is beyond the scope of the present work. We thus replace \( b_q \) by \( b_q \delta_{q,0} \equiv b \delta_{q,0} \).

Expected macroscopic occupation \( \langle \hat{b}^\dagger \hat{b} \rangle \gg 1 \) of the molecular level \( \epsilon_0 \) allows us to neglect quantum molecular fluctuations and replace operators \( \hat{b}(t), \hat{b}^\dagger(t) \) by the corresponding c-numbers \( b(t), b^\dagger(t) \).

We now look for time dependent fermionic operators in terms of reference, time-independent fermions \( \hat{\alpha}_{p\uparrow}, \hat{\alpha}_{p\downarrow} \), related to \( a_{p\sigma}(t) \) through the Bogoliubov amplitudes \( u_p(t), v_p(t) \) by \( \hat{\alpha}_{p\uparrow} = u_p^* \hat{\alpha}_{p\uparrow} + v_p \hat{\alpha}_{p\downarrow} \), \( \hat{\alpha}_{p\downarrow} = u_p^* \hat{\alpha}_{p\downarrow} - v_p \hat{\alpha}_{p\uparrow} \) with a constraint \( u_p^* u_p + v_p^* v_p = 1 \), that ensures fermionic anticommutation relations. The Heisenberg dynamics is then encoded in the equations of motion for \( u_p(t), v_p(t) \), and \( b(t) \)

\[
i \partial_t u_p = -\epsilon_p u_p + \frac{g b^\dagger}{\sqrt{V}} v_p, \quad i \partial_t v_p = \epsilon_p v_p + \frac{g b}{\sqrt{V}} u_p,
\]

\[
i \partial_t b = \epsilon_0 b + \frac{g}{\sqrt{V}} \sum_p u_p^* v_p.
\]

The dynamical evolution equations (2) and (3) preserve pair correlations of fermions. Accordingly, we choose the initial state to be of the BCS type, \( |\Omega(0)\rangle = \prod_p (u_p(0) + v_p(0) a_{p\uparrow}^\dagger a_{p\downarrow}^\dagger) |0\rangle \). As a result of the time evolution the fermion wave function preserves the same form with time dependent factors \( u_p(t) \) and \( v_p(t) \).

Following Ref. [3] we utilize Anderson’s spin analogy for the BCS problem [10], and look for a vector-representation of these equations in terms of the variables

\[
S_p = S_p^\uparrow + i S_p^\downarrow = 2 u_p u_p^* - \epsilon_p, \quad S_p^\dagger = v_p \sqrt{V} u_p^* - u_p v_p^*,
\]

that satisfy \( \langle S_p \rangle^2 = S_p^\dagger S_p + S_p S_p^\dagger = 1 \). Equations (2) become

\[
\partial_t S_p = 2i \epsilon_p S_p - \frac{2ig}{\sqrt{V}} b^\dagger S_p^\dagger, \quad \partial_t S_p^\dagger = -2i \epsilon_p S_p^\dagger + \frac{2ig}{\sqrt{V}} b S_p,
\]

\[
\partial_t S_p^\dagger = \frac{ig}{\sqrt{V}} (b^\dagger S_p^\dagger - b S_p),
\]

and have a form of Bloch equations for a spin precessing in an effective (p-dependent) field \(- \frac{2g}{\sqrt{V}} \text{Re} b, \frac{2g}{\sqrt{V}} \text{Im} b, -2 \epsilon_p \), whose azimuthal dynamics is in turn self-consistently determined by molecular \( (b(t)) \) evolution, Eq. (3). It is now straightforward to check that these equations can be solved by an ansatz (for the BCS limit, in the absence of molecules suggested in Ref. [3])

\[
S_p(t) = e^{i \omega t} \left( - (2\epsilon_p - \omega) C_p \Omega(t) + i C_p \hat{\Omega}(t) \right),
\]

\[
S_p^\dagger(t) = C_p \Omega^2(t) - D_p, \quad b(t) = \sqrt{V} \Omega(t) e^{-i \omega t},
\]

provided that the real function \( \Omega(t) \) satisfies

\[
\dot{\Omega}^2 + (\Omega^2 - \Delta_+^2) (\Omega^2 - \Delta_-^2) = 0,
\]

and that \( C_p \) and \( D_p \) satisfy

\[
\frac{D_p^2 - 1}{C_p^2} = \Delta_-^2 \Delta_+^2, \quad 2 D_p C_p = (2\epsilon_p - \omega)^2 + \Delta_-^2 + \Delta_+^2.
\]

Here \( \Delta_+, \Delta_- \), and \( \omega \) are parameters characterizing the periodic instanton-like solution \( \Omega(t) \) expressible in terms an elliptic integral. It follows from Eq. (4) that \( b(t)/\sqrt{V} \) oscillates between the values \( \Delta_-/g \) and \( \Delta_+/g \) (we choose \( \Delta_- < \Delta_+ \)) with a period of oscillations given by

\[
T = \frac{2}{\Delta_+} K \left( 1 - \frac{\Delta_-^2}{\Delta_+^2} \right),
\]

where \( K(m) \) is the complete elliptic integral of the first kind.

A direct substitution of this ansatz into Eq. (3), shows that the solution, Eq. (3) is compatible with the evolution of \( b(t) \) provided that the following two conditions are satisfied:

\[
2\epsilon_p - \omega = \frac{g^2}{2} \int \frac{d^3p}{(2\pi)^3} (2\epsilon_p - \omega) C_p, \quad 1 = -\frac{g^2}{2} \int \frac{d^3p}{(2\pi)^3} C_p.
\]

Eqs. (10), (11) determine \( \omega \) and \( \Delta_+ \) in terms of the experimentally controlled (initial conditions) parameters \( \epsilon_0 \) and \( \Delta_- \). As we will see below, the first of these equations is a nonequilibrium generalization of the BCS gap equation. The second one simply reflects the conservation of the total particle number, \( \frac{dN}{dt} = 0 \), with

\[
N = 2b b^\dagger + V \int \frac{d^3p}{(2\pi)^3} (S_p^\dagger + 1).
\]

We note that Eqs. (3) only determine \( C_p \) and \( D_p \) up to a \( p \)-dependent sign, that one would expect to be fixed by the initial fermion momentum distribution, encoded in \( |\Omega(0)\rangle \). With the exception of a filled Fermi sea initial condition, \( |\Omega(0)\rangle = \Delta_- = 0 \), the solution encoded in \( C_p \) and \( D_p \), Eq. (3), does not correspond to initial conditions \( (u_p(0), v_p(0)) \) characteristic of a ground state of the Hamiltonian (1) for any value of bare detuning \( \epsilon_0 \). Nevertheless, we fix the sign of \( C_p \) so as to most closely match \( n_p = \frac{1}{2} (S_p^\dagger + 1) \) to the initial fermion momentum distribution. For a large positive detuning this corresponds to a Fermi-Dirac step function with discontinuity at the chemical potential \( \mu \), that separates the hole-like and particle-like states. Combining this criterion with Eqs. (3), we find

\[
C_p = \frac{2 \text{sign}(\epsilon_p - \mu)}{\sqrt{[(2\epsilon_p - \omega)^2 + \Delta_-^2 + \Delta_+^2]^2 - 4\Delta_-^2 \Delta_+^2}}.
\]
where, as in equilibrium problem, $\mu$ is implicitly determined by the conserved total particle number $N$, Eq. (12), that reduces to $N = V \int d^3 p (1 - D_p)$.

Equation (10) involves a linearly-divergent integral (11), arising from an unphysical aspect of the model Eq. (8), that the atomic modes with an arbitrarily large energy interact with the molecular ones with equal strength $g$. In a more realistic model, the momentum dependence of the coupling $g$ would cutoff this divergence. As usual, our ignorance of this high energy physics can be buried in a (uv cutoff-dependent) relation between the parameter $\epsilon_0$ appearing in the Hamiltonian and the position of the physical Feshbach resonance, $\omega_0$.

To see this, we calculate the two-atom scattering amplitude within the model Hamiltonian Eq. (1). It is completely determined by the self-energy of the molecules, given by

$$\Sigma(E) = \int \frac{d\omega}{2\pi} \frac{d^3 p}{(2\pi)^3} \frac{ig^2}{\omega^2} \frac{i}{\omega - \epsilon_p + i\nu}(\omega - \epsilon_p + i\nu)$$

$$= i \frac{g^2}{4\pi m^2} \sqrt{E - g^2} \int \frac{d^3 p}{(2\pi)^3} \frac{m}{p^2}, \tag{14}$$

diverges in exactly the same way as the integral in Eq. (11). Since $\Sigma(E)$ enters the retarded molecular propagator $G_R(E) = (E - \epsilon_0 - \Sigma(E))^{-1}$ in combination with $\epsilon_0$, we can trade in $\epsilon_0$ for the physical (“renormalized”) FR detuning $\omega_0$ according to $\omega_0 = \epsilon_0 - g^2 \int \frac{d^3 p}{(2\pi)^3} \frac{m}{p^2}$. This leads to the two-atom scattering amplitude $f = \frac{1}{\sqrt{m \omega_0 + \mathrm{i} g^2/2}}$, that is consistent with the generic form based on unitarity (12) and is identical to that of the Fano-Anderson model (equivalent to our model at the two-body scattering level) (12). We see that the scattering phase changes by $\pi$ as the energy changes from below to above the physical (“renormalized”) FR, $\omega_0$, with finite width for positive detuning, $\omega_0 > 0$, controlled by $\gamma = g^2 m^{3/2}/4\pi$. In contrast for negative detuning, $\omega_0 < 0$, the scattering amplitude has a real pole at negative energy (a bound state in the open channel), that corresponds to a real molecular state (14).

With above renormalization of detuning, the nonequilibrium gap equation (10) becomes

$$\omega_0 - \omega = \frac{g^2}{2} \int \frac{d^3 p}{(2\pi)^3} \left[ \frac{1}{\sqrt{m (\omega - \epsilon_p - \Delta_0/2)}} - \frac{1}{\epsilon_p} \right], \tag{15}$$

where all the integrals are now convergent. This together with the atom conservation condition, (11), the total atom number Eq. (12) (that determines $\mu$), the detuning $\omega_0$, and the initial molecular density $\Delta_0$, allows us to determine the condensate frequency $\omega$, and the molecular density maximum $\Delta_\pm$, that controls the period of oscillations, in accordance with Eq. (13). Although the complete solution requires a numerical evaluation of the integrals, here we will focus on two analytically tractable regimes: (i) $\Delta_+ - \Delta_- \ll \Delta_+$ that corresponds to small amplitude oscillations of the condensate about the BCS-BEC ground state, and (ii) $\Delta_+ \ll \Delta_-$, that corresponds to the evolution of the filled Fermi sea, following a large downward shift in detuning.

Let us first consider the regime of small oscillations, $\Delta_+ - \Delta_- \ll \Delta_+$ about a BCS-BEC ground state. Limiting our analysis to $\omega > 0$, we find that Eq. (11) constrains $\omega$ to be close to $2\mu$. This together with the condition Eq. (15) gives (at $\Delta_+ = \Delta_+ = \Delta_0$, and $\mu = \omega/2$)

$$\omega_0 - 2\mu = \frac{g^2}{2} \int \frac{d^3 p}{(2\pi)^3} \left[ \frac{1}{\sqrt{\mu - \epsilon_p} + \Delta_0/2} - \frac{1}{\epsilon_p} \right]. \tag{16}$$

This coincides with the BCS-BEC gap equation, that can be derived in the equilibrium treatment of this problem (15). It relates the condensate density $\Delta/g$ to the Feshbach resonance $\omega_0$, with the chemical potential $\mu$ determined by the total atom number equation, Eq. (12). Simple analysis of these equations shows that for large positive detuning, $\omega_0 > \varepsilon_F$, molecules are strongly suppressed, leading the chemical potential to “stick” to $\varepsilon_F$, and to a conventional atomic BCS ground state, with $\Delta(\omega_0) \approx 8e^{-2\varepsilon_F}e^{-\mu(\omega_0)}/g^2v(\varepsilon_F)$ ($\mu(\epsilon) = m^2 \varepsilon^{1/2}/\sqrt{2\pi^2}$ is the atomic density of states). In this far off-resonance BCS regime the accuracy of the mean-field treatment of the equilibrium problem is controlled by the ratio of the width of the FR to Fermi energy, namely by the dimensionless parameter $\gamma^2/\varepsilon_F$ (8).

As the detuning $\omega_0$ is lowered toward and below $\varepsilon_F$, the chemical potential begins to track the detuning, $\mu(\omega_0) \approx \omega_0/2 - O(g^2 \nu(\omega_0)/2)$, with atoms from states between $\varepsilon_F$ and $\mu(\omega_0)$ converting into Bose-condensed molecules. The density of these tightly bound molecules, that coexist with BCS’s Fermi sea determine the gap, which displays a rounded mean-field behavior $\Delta_{\text{equil}}(\omega_0) \approx \sqrt{\frac{\nu^2}{3\pi}} \gamma^{3/2} - \mu(\omega_0)^{3/2}$. In the $g \rightarrow 0$ limit, $\omega_0$ crossing of $\varepsilon_F$ is a genuine quantum transition, with an upper-critical dimension of $d_{\text{uc}} = 2$, and is therefore mean-field in 3d (10). A finite atom-molecule coupling $g$ rounds the transition into a smooth crossover near $\varepsilon_F$, that for small $g$ (i.e., narrow FR, $\gamma^2 \ll \varepsilon_F$) is therefore also accurately described by the mean-field theory summarized by Eqs. (14). Clearly, no additional anomalies appear when the 2-body FR ($\omega_0 = 0$) is crossed, since by that point nearly all atoms are bound up into well-ordered Bose-condensed molecules. One interesting observation is that in this $\mu < 0$ BEC regime the remaining dilute fermionic atoms are paired but are nondegenerate, and therefore realize a “strongly-coupled” BCS state (17).

This picture of the ground state (that can be easily extended to a finite temperature (15)) is qualitatively consistent with recent observations by Regal, et al (2), which find that molecules appear at about 0.5 Gauss above the experimentally determined 2-body FR (in our interpretation corresponding to $\omega_0 \approx 2\varepsilon_F$).
The nonequilibrium solution, Eq. [3] then describes small oscillations about this equilibrium BCS-BEC state, with the period $T = \pi/\Delta$ given by Eq. [4]. Because $\omega \approx 2\mu$ it is easy to see that for a sufficiently small oscillation amplitude, the atomic momentum distribution function $n_p(t) = \frac{1}{2} (S_p(t) + 1)$ only changes near the Fermi surface, $\epsilon_p = \mu$.

The other interesting limit, $\Delta_- \to 0$, $\Delta_+ = \Delta$ describes oscillations between a Fermi sea (a normal “metal”, with $\mu = \epsilon_F$) of atoms and bosonic molecules, following a nonadiabatic shift of detuning from $\infty$ down to $\omega_0$. In this regime, Eq. [11, 15] reduce to

$$\omega_0 - \omega = \frac{g^2}{2} \int \frac{d^3p}{(2\pi)^3} \left[ (\epsilon_p - \frac{\omega}{2}) \text{sign}(\epsilon_p - \epsilon_F) - \frac{1}{\epsilon_p} \right],$$

$$1 = -\frac{g^2}{4} \int \frac{d^3p}{(2\pi)^3} \text{sign}(\epsilon_p - \epsilon_F) \frac{(\epsilon_p - \omega/2)^2 + \Delta^2}{4 \epsilon_p}. \quad (17)$$

Simple integration of the atom-number conservation (second) equation above gives

$$\Delta \approx g^2 \nu(\omega/2) \tan^{-1}[2(\epsilon_F - \omega)/\Delta]. \quad (18)$$

The behavior then depends qualitatively on whether the detuning $\omega_0$ is shifted to the BCS ($\omega_0/2 > > \epsilon_F$) or to the BCS-BEC ($0 < \omega_0/2 < \epsilon_F$) regime, i.e., above or below the Fermi surface. In the former case Eq. [18] reduces to $2\epsilon_F - \omega \approx \Delta^2/g^2 \nu(\omega/2) \ll \Delta$, with an exponentially suppressed BCS-like gap $\Delta \propto e^{-\omega/2 \epsilon_F}$ given by the gap (first) equation in Eq. [17]. Hence in this regime, for narrow FR, $\omega \approx 2\epsilon_F$ and oscillations are confined to the vicinity of the Fermi surface.

In contrast, for the detuning shift below the Fermi surface, $0 < \omega_0/2 < \epsilon_F$, it is now Eq. [13] that determines the molecular density. It gives $\Delta \approx g^2 \nu(\omega/2) = \gamma \sqrt{\omega} \times \mathcal{O}(1)$, while the gap equation gives $\omega_0 - \omega = g^2 \nu(\epsilon_F) \times \mathcal{O}(1) \ll \omega_0$, enforcing the molecular energy $\omega_0$ to stick to the detuning $\omega_0$. We note, that, although $\Delta \approx \gamma \sqrt{\omega_0}$ is much larger (scales as $g^2$ rather than exponentially suppressed in $1/g^2$) than for the detuning into the BCS regime, it is much smaller than the equilibrium $\Delta_{\text{equil}}(\omega_0)$, found as the solution to the equilibrium gap equation Eq. [10] in this regime. This suppression of the condensate oscillations is due to energy conservation between the atoms in the Fermi sea and the molecules. For a narrow FR resonance, $\gamma \sqrt{\omega_0} \ll \omega_0 < \epsilon_F$ it is only a small fraction of atoms in the Fermi sea that are in the immediate vicinity (set by the resonance width $\gamma \sqrt{\omega_0}$) of $\omega_0$, that can resonantly bind into molecules. The resulting resonant atom-molecule interconversion leads to a narrow oscillatory depletion of the Fermi sea, illustrated in Fig.11 with a period of oscillations that diverges as $T \propto \frac{1}{\epsilon_F} \ln \left( \frac{\Delta + \epsilon_F}{\Delta - \epsilon_F} \right)$, in the limit of the “normal” Fermi sea ($\Delta_- \to 0$) as the initial condition.

Analysis of the gap and atom-conservation equations shows that the amplitude of the atom-molecule oscillations vanishes as the molecular energy $\omega \approx \omega_0$ approaches zero. This is again enforced by the energy conservation that in the absence of other degrees of freedom (e.g., molecules above a condensate, $b_{\eta \neq 0}$) forbids conversion of molecules at negative energy $\omega_0$ into atoms at positive energy $\epsilon_p$. We leave analysis of the dynamics that incorporates these additional degrees of freedom to future research.

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