Dynamic Projection on Feshbach Molecules: A Probe of Pairing and Phase Fluctuations

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We describe and justify a simple model for the dynamics associated with rapid sweeps across a Feshbach resonance, from the atomic to the molecular side, in an ultracold Fermi system. The model allows us to relate the observed molecule momentum distribution to equilibrium properties of the initial state. In particular, the dependence of the total molecule number on the sweep rate is found to be a sensitive probe of pairing in the initial state, whether condensed or not. This can be used to establish the presence of a phase fluctuation induced ''pseudogap'' phase in these systems.

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Experiments with ultracold fermions near a Feshbach resonance (FR) opened a new window to the study of strongly interacting condensates [1–3]. They can access the strongly coupled regime intermediate between weak pairing BCS superfluidity and Bose Einstein condensation (BEC) of molecules, where deviations from mean field theory [4–6] are expected to be large. In addition, the ability to rapidly vary the interaction parameters provides a unique opportunity to study quantum dynamics far from equilibrium [7]. The focus of recent experiments has been to utilize rapid magnetic field sweeps across the FR, in order to probe *equilibrium* properties of the condensate in the crossover region [2,3]. The idea was to convert Cooper pairs in the initial state, which would otherwise unbind during free expansion, into molecules. The fact that the molecule momentum distribution depended on the start position has been offered as strong indication that indeed properties of the initial equilibrium state were being accessed. However, precise connections to such properties are lacking.

In this Letter we formulate an approach that allows us to relate equilibrium properties of such strongly interacting fermions to measurements in the dynamical experiments. Our approach targets the regime of ''fast'' magnetic field sweeps. Roughly, this is when the conversion efficiency of atoms into molecules changes significantly with ramp rate. Empirically in the ^{40}K system this implies a ramp rate faster than $1/20$ G$/\mu$s [2], while it was too fast to be accessed in ^{6}Li [3]. The physics in this regime turns out to have a remarkable simplicity.

Consider for a moment the extreme limit of an infinitely fast sweep. Then, we can apply the sudden approximation and simply use the initial state to evaluate the final population of molecules. This picture was advocated by Regal *et al.* [2] (see also [8]). Subsequent theoretical studies [9] used the same assumption to estimate the fraction of condensed molecules as a function of the detuning of the initial state from resonance. The molecule momentum distribution in this approach is given by

$$n_{\mathbf{q}} = \langle b^{\dagger}_{\mathbf{q}} b_{\mathbf{q}} \rangle_i, \quad b^{\dagger}_{\mathbf{q}} = \int d\mathbf{k}\, \varphi_f(k) c^{\dagger}_{(\mathbf{q}/2)+\mathbf{k}\uparrow} c^{\dagger}_{(\mathbf{q}/2)-\mathbf{k}\downarrow}, \tag{1}$$

where $\varphi_f(k)$ is the molecular wave function (WF) at the end of the ramp, deep in the molecular side of the resonance. The average $\langle \cdots \rangle_i$ is taken over the initial state, which in Ref. [9] was assumed to be a BCS WF [5]. This gives a bimodal momentum distribution, with a peak at $\mathbf{q} = 0$ due to Cooper pairs projected to molecules, as well as molecules at $\mathbf{q} \neq 0$ due to pairwise projection of atoms belonging to different Cooper pairs. Although this is roughly what is seen in the experiments, it is unsatisfactory in two important respects. (i) Mean field theory is used to calculate the initial state, although in the crossover regime fluctuations are expected to play an important role. (ii) The approach ignores the dynamical aspects of the experiment and is by definition unable to predict the dependence of measured quantities (e.g., conversion efficiency and molecular condensate fraction) on ramp rate.

Both of these issues are addressed in this Letter. (i) We go beyond mean field theory, using RPA [10] to include Gaussian phase fluctuations (or ''noncondensed Cooper pairs''). In the BCS to BEC crossover regime, these sharply reduce the observed condensate fraction relative to the mean field result of Ref. [9], even at zero temperature. For fast sweeps at low temperature this leads us to predict a surprising nonmonotonic behavior of the molecule condensate fraction versus detuning of the initial state from resonance. Point (ii) raised above is addressed by an effective model for the dynamics. For fast sweeps we argue that the time evolution of the system can be approximated by a ''sudden'' part followed by an ''adiabatic'' time evolution part. The point at which the time evolution changes character depends on the ramp rate, the sudden evolution persisting to larger detuning at higher ramp rates. So, we will be using Eq. (1), but with the effective molecular WF, φ that depends on the ramp rate. In this way we are able to obtain the parametric dependence of various measured quantities, such as conversion efficiency into molecules and molecular condensate fraction on the ramp rate, and the parameters of the initial state. At these fast sweep rates, we find that the conversion of Cooper pairs into molecules is vastly more efficient than that of uncorrelated pairs of atoms. This applies both to condensed and noncondensed Cooper pairs, and ultimately results from a short distance singularity present in the Cooper pair WF, which allows them to have a non-negligible overlap even with small sized molecules. Since these dynamical measurements are equally sensitive to noncondensed Cooper pairs, they can potentially probe the phase fluctuation induced pseudogap phase (where thermal and quantum phase fluctuations destroy the condensate but pairing remains). Details such as the momentum distribution of noncondensed pairs may also be accessed.

We now motivate the model dynamics via physical arguments and derive the consequences for the system of interest. Later we perform a nontrivial check by showing that this simple scheme indeed reproduces the physics in a nontrivial toy model (the Dicke model) which is solved numerically without approximations. In what follows we concentrate on a *wide* FR, relevant to experiments in ^{40}K [2] and ^{7}Li [3]. That is, $g_s \equiv g\sqrt{n/2} \gg \epsilon_f$, where g is the coupling between the open and closed channels and n is the atom density. The problem reduces to spin-$\frac{1}{2}$ fermions interacting via a contact potential

$$\mathcal{H} = \psi_\sigma^\dagger\left(-\frac{\nabla 2}{2m} - \mu\right)\psi_\sigma - u\psi_\uparrow^\dagger\psi_\downarrow^\dagger\psi_\downarrow\psi_\uparrow, \tag{2}$$

where we set $\hbar = 1$ throughout. Ultraviolet divergences are avoided in the standard fashion by writing all physical results in terms of an s-wave scattering length a instead of u. Near resonance the scattering length diverges as $a \approx -mg^2/4\pi\nu$, where m is the atomic mass and ν is the detuning in energy units, which is related to the magnetic detuning via the magnetic moment difference $\Delta\mu$ between closed and open channels: $\nu = \Delta\mu(B - B_0)$.

Our two stage approximation of the dynamics is depicted graphically in Fig. 1. For slow sweeps, atoms are converted adiabatically to weakly bound Feshbach molecules (FMs) [11]. The binding energy of these molecules is $E_b = -1/(ma^2) \propto \nu^2$ (for $k_f a \ll 1$). Now consider a change in the detuning parameter at a constant rate $\dot{\nu}$. Once the binding energy is large enough, such that $\dot{E}_b \ll E_b^2$, the time evolution is expected to be adiabatic. So, for a given sweep rate $\dot{\nu}$, there is a characteristic detuning ν_*, which marks a dynamic crossover for the system. At ν_*, $\dot{E}_b \approx E_b^2$ [12]. Our simplified two stage model for the dynamics approximates the change up to ν_* as sudden, while the rest is considered as perfectly adiabatic. Thus the WF at the initial state is effectively "projected" on FMs that occur at detuning ν_*. These molecules evolve adiabatically into more tightly bound ones corresponding to the final value of the field, while the rest of the atomic population remains unbound.

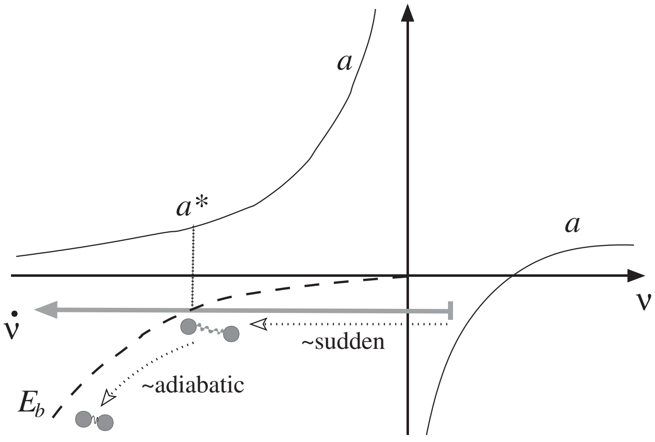

FIG. 1. Model dynamics. Field sweep is effectively sudden up to detuning ν_* depending on the sweep rate $\dot{\nu}$. At this point the scattering length (and molecule size) is a_*. The molecule is assumed to evolve adiabatically from there.

Within this model, a faster sweep rate simply moves the break point ν_* to larger negative detuning, leading to effective projection of the initial WF on smaller FMs. We can establish a precise connection between the sweep rate and the size of the effective molecule WF. The typical size of the FM at ν_* is the scattering length $a_*(\nu_*)$. Using $E_b = -1/(ma^2)$ and the relation between the scattering length and the detuning ν quoted earlier, with the break condition $E_b^2(a_*) = dE_b(a_*)/dt$, we obtain

$$k_f a_* = (3\pi g_s^2/4\dot{\nu})^{1/3}. \tag{3}$$

This result is valid if the effective projection takes place in the regime $k_f a_{bg} \ll k_f a_* \ll 1$, where a_{bg} is the background scattering length far from resonance. If the sweep rate is too slow, the effective projection would occur in the strongly interacting regime, while for excessively fast sweep rate, one would have to consider occupation of the closed channel in the final state.

To determine the final molecule distribution within the two stage model, we need to calculate the following correlation function, in the initial state:

$$n_{\mathbf{q}} = \int d^3k d^3k' \varphi_{\mathbf{k}}^* \varphi_{\mathbf{k}'} \langle c_{(\mathbf{q}/2)+\mathbf{k}\uparrow}^\dagger c_{(\mathbf{q}/2)-\mathbf{k}\downarrow}^\dagger c_{(\mathbf{q}/2)-\mathbf{k}'\downarrow} c_{(\mathbf{q}/2)+\mathbf{k}'\uparrow}\rangle. \tag{4}$$

The size of the molecular pair WF $\varphi_{\mathbf{k}}$ is a_*, as prescribed by the model dynamics. First consider the mean field (BCS) approximation of the initial state. In this case, (4) may be factorized (as in Ref. [9]) to obtain

$$n_{\mathbf{q}} = \left|\int d^3k \varphi_{\mathbf{k}} \langle c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger\rangle\right|^2 \delta(\mathbf{q}) + \int d^3k |\varphi_{\mathbf{k}}|^2 \langle n_{(\mathbf{q}/2)+\mathbf{k}\uparrow}\rangle\langle n_{(\mathbf{q}/2)-\mathbf{k}\downarrow}\rangle. \tag{5}$$

The first contribution gives the condensed part of the distribution. In fact, this is just the square of the overlap between the final molecule WF and the "Cooper pair WF." The second term, containing the normal expectation values, gives the noncondensed part of the distribution. To make further progress, we note that if the molecule size a_* is much smaller than the interparticle spacing, we can replace the exact WF with a box WF in momentum space of the same spatial extent. We take $\varphi_{\mathbf{k}} = \sqrt{3/4\pi}a_*^{3/2}$ for $k < 1/a_*$ and $\varphi_{\mathbf{k}} = 0$ outside this sphere. Now $\varphi_{\mathbf{k}}$ serves as a cutoff to the relative momentum integrals. Using this in (5), the number of normal molecules is found to be $N_n = (N/2)(k_f a_*)^3$, where N is the total atom number. This result is easily understood in terms of the overlap of a random pair of atoms in the Fermi sea, with a molecular WF. The conversion efficiency is then proportional to the ratio of the molecule volume to that occupied on average by nearby atoms. In contrast, the number of condensed molecules calculated from (5) is

$$N_0 = \frac{6Va_*^3}{(2\pi)^2}\left|\int_0^{a_*^{-1}} \frac{dkk^2\Delta/2}{\sqrt{\Delta^2+\xi_k^2}}\right|^2 = \frac{9N}{8}\left(\frac{\Delta}{\epsilon_f}\right)^2 k_f a_*. \quad (6)$$

The last step relies on the high momentum divergence of the integral, due to which it depends crucially on the high momentum cutoff. The result (6) will have important consequences on interpretation of experiments, and it is worthwhile to remark on its physical origin. The number of condensed molecules is proportional to the square of the overlap of the molecular WF φ with the Cooper pair WF φ_c. The molecule WF is appreciable only within a region $r < a_*$, where $\varphi(r) \sim a_*^{-3/2}$. Thus, it probes the Cooper pair WF at very short distances, much smaller than the interparticle spacing, where $\varphi_c(r) \propto 1/r$. Therefore $|\langle\varphi|\varphi_c\rangle|^2 \propto a_*$, which is a much larger overlap than might be naively expected. Note that, in solid state systems where a natural short distance cutoff exists, these features are absent and hence have not been emphasized.

Combining the mean field results, we can obtain the condensate fraction N_0/N_n in the molecule distribution: $f_{\mathrm{MF}} = [1 + 4/9(\epsilon_f/\Delta)^2(k_f a_*)^2]^{-1}$. It decreases exponentially for large positive initial detuning because $\Delta/\epsilon_f \sim e^{-1/k_f a}$. Close to resonance, on the other hand, $\Delta \sim \epsilon_f$, so for sufficiently fast sweep rates ($k_f a_* \ll 1$), $f_{\mathrm{MF}} \sim 1$. This is because Cooper pairs are converted into molecules more efficiently, and within the mean field approximation all of them are condensed. However, in the same region, close to the resonance, we expect phase fluctuations to be important (Cooper pairs at finite momenta), which will lead to $f < 1$.

To obtain such corrections to the mean field result (5), we calculate the correlation function (4) within RPA. The details of the calculation are left to [12]; here we briefly outline the main steps and the results. Following Ref. [10], we consider a path integral representation of the partition function $\mathcal{Z}$ determined by the Hamiltonian (2). The interaction term may be decoupled with a Hubbard-Stratanovitch pair field $\Delta(\mathbf{q}, \omega)$. In order to extract the desired correlation functions, we introduce a source term $J(q)\int d^4k\varphi_k c^\dagger_{(q/2)+k\uparrow}c^\dagger_{(q/2)-k\downarrow} + \text{H.c.}$, where $q \equiv (\mathbf{q}, \omega)$. At $T > 0$ the integral over imaginary frequencies is converted into the usual Matsubara sum. Then, the desired molecular distribution function is $n_{\mathbf{q}} = \mathcal{Z}^{-1}\sum_{\omega\omega'}\delta^2\mathcal{Z}/\delta J(\mathbf{q}, \omega)\delta J^*(\mathbf{q}, \omega')$. While the saddle-point approximation gives us the BCS result, here we go beyond and expand $\Delta(\mathbf{q}, \omega) = \Delta_0\delta(\mathbf{q}) + \eta(\mathbf{q}, \omega)$, where Δ_0 is the saddle-point value of the gap. The RPA approximation involves integrating out the fermions and expanding the resulting effective action to quadratic order in the η and J fields. The poles in the η propagator give the collective mode spectrum. Finally, integrating out the η fields gives us an effective action solely in terms of J, from which the molecular distribution function $n(\mathbf{q})_{\mathrm{MF}} + \delta n_{\mathbf{q}}$ ($\delta n_{\mathbf{q}}$ is the contribution due to fluctuations) may be evaluated.

Assuming that the fluctuation contribution is dominantly from superfluid phonons, we can make a small momentum, small frequency expansion. The J propagator takes the form $F(k_f a_*, k_f a)[(cq)^2 - (i\omega)^2]^{-1}$, where c is the sound velocity. The implied linear dispersion is only an approximation due to the low q and ω expansion: At momenta $q \gtrsim 4mc$, the dispersion becomes quadratic; at $\omega > \Delta$, phase fluctuations can decay into quasiparticle excitations, leading to damping in the BCS limit at $q \gtrsim \Delta/c \approx 1/\xi$.

Carrying out the Matsubara summation, we obtain the RPA correction to the molecule momentum distribution $\delta n(\mathbf{q}) = \coth(cq/2T)F(k_f a_*, k_f a)/(2cq)$. The number of noncondensed molecules due to these fluctuations is found by integrating over $\mathbf{q}$ up to a natural cutoff. As discussed above, such a cutoff is provided in the BCS limit by $q_1 = 1/\xi$, and in the BEC limit by $q_2 = 4mc$. We interpolate between the two limits using $q_0^{-1} = q_1^{-1} + q_2^{-1}$. The function $F(k_f a_*, k_f a)$ can be computed along the crossover

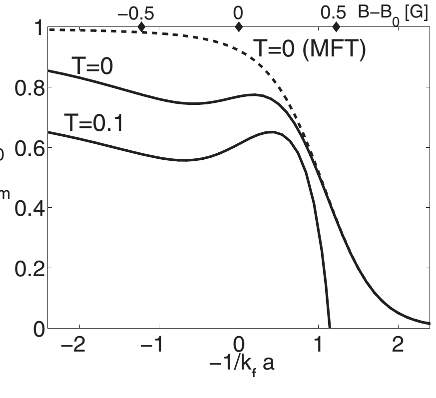

FIG. 2. Calculated molecule condensate fraction versus $-1/k_f a$ in the initial state (bottom axis), and versus magnetic field detuning for parameters of ^{40}K [2] (top axis). The sweep rate corresponds to $k_f a_* = 0.3$. Solid lines include the effect of quantum and thermal phase fluctuations. Dashed line shows the $T = 0$ mean field theory (MFT) result for comparison.

from BCS to BEC [12]. Figure 2 depicts the calculated condensed molecule fraction for sweep rate corresponding to projection at $k_f a_* = 0.3$. The nonmonotonic dependence on detuning toward the BCS limit is due to competition between two effects. On the one hand, decreasing phase fluctuations act to increase the condensed molecule fraction. On the other hand, the ratio ϵ_f/Δ appearing in the normal atom contribution diverges exponentially at large detuning and eventually leads to the vanishing of the molecular condensate fraction.

The total conversion into molecules as a function of sweep rate is due to condensed Cooper pairs, unpaired atoms, and fluctuations (uncondensed pairs). The fluctuation contribution is encoded into the dependence of $F(k_f a_*, k_f a)$ on $k_f a_*$. This is found to be proportional to $k_f a_* \propto (g_s^2/\dot{\nu})^{1/3}$, the same as condensed Cooper pairs. By contrast, conversion of unpaired atoms into molecules is much less efficient and scales as $(k_f a_*)^3 \propto g_s^2/\dot{\nu}$.

These results rely on the two stage model of the dynamics and on the relation (3) that followed from it. We now turn to a nontrivial check of this approximation. We start from the microscopic two channel Hamiltonian [6],

$$H = \sum_{\mathbf{k}\sigma} (\epsilon_{\mathbf{k}} - \mu) c^\dagger_{\sigma\mathbf{k}} c_{\sigma\mathbf{k}} + \sum_{\mathbf{k}} (\epsilon_{\mathbf{k}}/2 + \nu - 2\mu) m^\dagger_{\mathbf{k}} m_{\mathbf{k}} - g \sum_{\mathbf{kq}} (m_{\mathbf{q}} c^\dagger_{\uparrow\mathbf{k}} c^\dagger_{\downarrow\mathbf{q}-\mathbf{k}} + \text{H.c.}) + \mu N, \tag{7}$$

which is regularized by absorbing the high momentum cutoff into renormalized detuning parameter [6]. Note that $m_{\mathbf{q}}$ describes a (bare) closed channel molecule.

We compute the dynamics of (7) within the Dicke model (i.e., keeping only $m_{\mathbf{q}=0}$). The initial state is taken to be the equilibrium solution at detuning $\nu \geq 0$. Then ν is changed at a constant rate to far negative detuning where the equilibrium population of m_0 would be ~96%. The resulting dynamics (see, e.g., [7]) is calculated numerically. Following the experiments, we count the number of molecules in the *final* state, which to a good approximation is $|\langle m_0 \rangle|^2$. According to the two stage model, this is directly related to the number of FMs produced after the sudden stage. The results are summarized in Fig. 3. For initial state at resonance, the dependence on sweep rate fits $1/\dot{\nu}^{1/3}$, as expected from our two stage model. For weak pairing, deep in the BCS regime, the dominant contribution is $1/\dot{\nu}$, although it is strongly suppressed here because the Dicke model neglects molecules with $q \neq 0$.

In summary, we presented a simple model of the dynamics of rapid magnetic field sweeps across the FR. This allowed us to relate the measurements of such dynamical experiments to properties of the initial equilibrium state of the fermions. For rapid sweeps at low temperatures, we predict a nonmonotonic behavior of the final condensed molecule fraction versus detuning, which is a direct signature of the quantum phase fluctuations in the initial state.

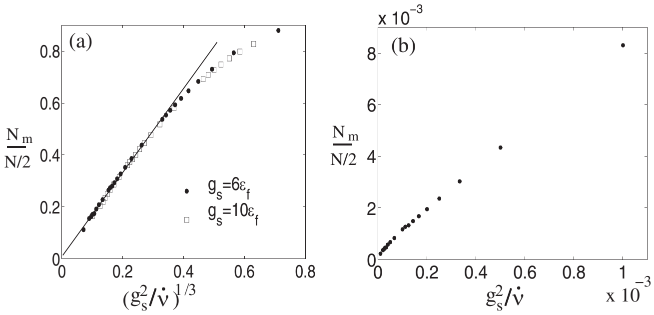

FIG. 3. Simulated Dicke model dynamics: final molecule number as a function of the sweep rate. (a) Initial state at resonance. The curves for different coupling constants g_s fall on a universal curve $\propto 1/\dot{\nu}^{1/3}$ at fast rates, in agreement with (3) and (6). (b) Initial state far detuned ($\nu = 400\epsilon_f$, $g_s = 6\epsilon_f$). $1/\dot{\nu}$ behavior due to unpaired atoms dominates.

In addition, the conversion efficiency to molecules at fast sweep rates is argued to be a sensitive probe of pairing, whether in a condensed state or not. This can be used to establish the presence of a fluctuation induced pseudogap phase. In this regime, we expect enhanced conversion efficiency due to the presence of noncondensed fermion pairs, despite a vanishing condensate fraction.

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