High Temperature Expansion Applied to Fermions near Feshbach Resonance

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We show that, apart from a difference in scale, all of the surprising recently observed properties of a *degenerate* Fermi gas near a Feshbach resonance persist in the high temperature Boltzmann regime. In this regime, the Feshbach resonance is unshifted. By sweeping across the resonance, a thermal distribution of bound states (molecules) can be reversibly generated. Throughout this process, the interaction energy is negative and continuous. We also show that this behavior must persist at lower temperatures unless there is a phase transition as the temperature is lowered. We rigorously demonstrate universal behavior near the resonance.

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At present, much experimental activity is concentrated on degenerate quantum gases near a Feshbach resonance [1–5] where the nominally weak effective interactions are strongly enhanced. By applying a magnetic field, which moves the energy of a bound molecular state relative to the scattering continuum, the interactions can be tuned by many orders of magnitude. The scattering length diverges to negative/positive infinity when the molecular energy is infinitesimally above/below threshold. At resonance, the scattering cross section is limited only by *unitarity* ($\sigma = 4\pi/k^2$, where k is the relative momentum of the two atoms) and is *universal* (independent of the microscopic physics). The universal nature of the unitarity limit leads to a challenging many-body problem, since there are no small parameters readily identifiable for the application of perturbation theory.

Recently, a sequence of beautiful experiments on Fermi gases have found unexpected and dramatic behavior near unitarity, including a universal interaction energy [1,2] and the reversible interconversion of atoms and molecules [4]. The former demonstrates the effects of unitary scattering on bulk properties, and the latter suggests the possibility of an equilibrium phase with atoms and molecules in chemical equilibrium. Several of the experimental results are not well understood, and some even appear to be mutually contradictory [2]. In the following, we summarize these experiments and the fundamental questions that they raise. We refer to the range of magnetic fields on either side of the resonance where the scattering length a_{sc} is positive or negative as the "+'ve" and "−'ve" side of the resonance.

(I) Universal interaction energy.—Thomas's group at Duke [1] has studied a gas containing two spin states of fermionic ^{6}Li (which has a Feshbach resonance around 855 G). The experiment is performed on the negative side at 910 G. Upon release from the trap, the Fermi gas undergoes *anisotropic* expansion for temperatures between $0.1T_F$ and $3.5T_F$. This anisotropy can be explained by collisional hydrodynamics with a *universal* interaction energy proportional to the Fermi energy $\mathcal{E}_F$.

(II) Properties near resonance.—More recently, Salomon's group directly measured the interaction energy of the same ^{6}Li system, at temperatures between $0.5T_F$ and T_F. (a) Crossing the resonance from the negative side, they find that the interaction energy ϵ_{int} remains *negative and continuous* across the resonance, despite the expected infinite jump of the scattering length. They find an interaction energy similar to that of the Duke group, convincingly demonstrating that ϵ_{int} remains roughly constant over the temperature range $0.1T_F$ to T_F. (b) Approaching the resonance from the opposite side, ϵ_{int} is positive but drops to a negative value at a field of 700 G, roughly 150 G before the resonance is reached. (c) The three-body recombination rate is maximal at 700 G, rather than at 855 G, a result consistent with the work of Ketterle's group at MIT [3]. (d) The anisotropy of the expansion (which is a measure of the interaction strength) is maximal at 855 G. While (a) through (c) seem to indicate that the resonance is shifted from 855 to 700 G by many-body effects, (d) is consistent with an unshifted resonance.

(III) Conversion between atoms and molecules.—Very recently, Jin's group at JILA has studied a gas consisting of two spin states of fermionic ^{40}K [4]. They show that molecules are produced as one crosses the resonance from the −'ve to the +'ve side. Moreover, this process is reversible. This experiment, performed at $T = 0.1T_F$, finds no significant shift of the original resonance.

Here, we focus on the Fermi gas near a Feshbach resonance. Far from resonance, the interaction energy is $\epsilon_{int} = g n_\uparrow n_\downarrow$, where $g = 4\pi\hbar^2 a_{sc}/M$, and $n_\uparrow$ and $n_\downarrow$ are the number densities of the two spin components. (We consider the case $n_\uparrow = n_\downarrow = n/2$.) A key question is how this nonuniversal form of ϵ_{int} turns into a universal function near resonance [see (I) and (II)]. Moreover, how does this function reflect the existence of molecules, and what signatures do these molecules have if they exist? Equally important is whether the original resonance is shifted in a many-body medium [see (II)]. To use methods where errors can be estimated precisely, we consider the Boltzmann regime. In this case, physical quantities can be

calculated systematically through a high temperature series expansion, and yet the issues of the emergence of universal behaviors at unitarity still remain.

One might wonder whether the phenomena in the Boltzmann regime have any relevance to current ultralow temperature experiments. The connection is simply that *in the absence of any phase transition in the normal state,* the thermodynamic functions in the Boltzmann regime are analytically continuations (in T and n) of those in the degenerate regime. This analytic continuation imposes strong constraints on the phase diagram, allowing one to qualitatively understand the physics at all temperatures. In fact, apart from a difference in scale, the *exact* results in the Boltzmann regime show *all of the features* discovered in experiments (I), (II), and (III). Surprisingly, the high temperature results, which should work well when $n_\uparrow\lambda^3 = n_\downarrow\lambda^3 = n\lambda^3/2 \ll 1$ (where $\lambda = h/\sqrt{2\pi M k_B T}$ is the thermal wavelength and k_B is Boltzmann's constant), agree reasonably well with the ENS (Ecole Normale Supérieure) experiments [2] performed at $n\lambda^3/2 = (4/3\sqrt{\pi})(T_F/T)^{3/2} \sim 1.6$ [see point (E) later]. In the following, we derive the interaction energy density in the Boltzmann regime, then draw a series of conclusions labeled below as (A) to (D).

At high temperatures, or low densities, the grand partition function $\mathcal{Z} = \mathrm{Tr} e^{-(H-\mu N)/k_B T}$ can be expanded in the fugacity $z = e^{\mu/k_B T}$ [6,7]. To second order in z, where interaction effects first appear, the partition function is $\mathcal{Z} = \mathcal{Z}^{(0)} + 2\sqrt{2}(Vz^2/\lambda^3)b_2$, where the superscript "0" denotes quantities for noninteracting systems, and $b_2 = \sum_\nu [e^{-\beta E_\nu^{(2)}} - e^{-\beta[E_\nu^{(2)}]^{(0)}}]$ is the second virial coefficient,

$$b_2 = \sum_b e^{|E_b|/k_B T} + \sum_\ell \gamma_\ell \int_0^\infty \frac{dk}{\pi} \frac{d\delta_\ell(k)}{dk} e^{-\hbar^2 k^2/m k_B T}, \quad (1)$$

where $\gamma_\ell = 2\ell + 1$, the sum is over all integers $\ell = 0, 1, \ldots$, E_b is the energy of the two body bound state, and $\delta_\ell(k)$ is the phase shift of the ℓth partial wave [8].

A standard thermodynamic calculation [9] shows that, to lowest nontrivial order in $n\lambda^3$, the energy density is

$$\epsilon = \frac{3nk_B T}{2}\left(1 + \frac{n\lambda^3}{2^{7/2}}\right) + \epsilon_{\mathrm{int}} \equiv \epsilon_{\mathrm{kin}} + \epsilon_{\mathrm{int}}, \quad (2)$$

where ϵ_{kin} and ϵ_{int} are, respectively, the kinetic and interaction energy densities:

$$\epsilon_{\mathrm{int}} = \frac{3k_B T n}{2}(n\lambda^3)\left[-\frac{b_2}{\sqrt{2}} + \frac{\sqrt{2}}{3} T \frac{\partial b_2}{\partial T}\right]. \quad (3)$$

Since the contributions of partial waves with $\ell \geq 1$ in Eq. (1) are a factor of $n\lambda^3$ smaller than the s-wave contributions, we ignore them in subsequent discussions.

Far from resonance the phase shift is $\delta(k) = -a_{\mathrm{sc}}k$ for small k. Because of the Gaussian cutoff in Eq. (1), no errors are made by using this expression for all k. In the absence of bound states, we then have $b_2 = -a_{\mathrm{sc}}/(\sqrt{2}\lambda)$, and hence $T\partial b_2/\partial T = b_2/2$. Equation (3) then reduces to the usual expression $\epsilon_{\mathrm{int}} = g n_\uparrow n_\downarrow$, with $n_\uparrow = n_\downarrow = n/2$.

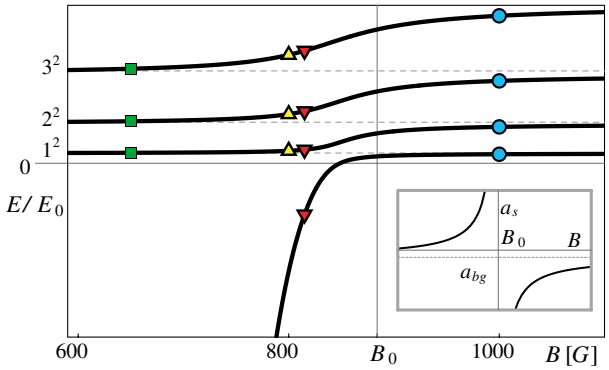

FIG. 1 (color online). Energy levels of a two body system in the center of mass frame calculated from the phase shift and the boundary condition in the text, with $R = 14\ \mu$m, $B_0 = 855$ G, $\Delta B = 325$ G, and $a_{bg} = -120$ nm. The vertical scale is expanded to isolate individual energy levels. The dotted lines are energy levels of a noninteracting system, $E_n^{(0)} = E_0 n^2$, $E_0 = \hbar^2(\pi/R)^2/M$, $n = 1, 2, 3$. Passing from $B > B_0$ to $B < B_0$, the lowest state in the continuum becomes bound. Light (yellow) upright and dark (red) inverted triangles indicate states at the same field with and without the bound state occupied. The interaction energies due to thermal occupation of these states, and those marked by circles and squares, are shown in Fig. 2 by the same symbols. The inset shows the behavior of the scattering length.

To evaluate ϵ_{int} near a Feshbach resonance we use the expression for the phase shift valid for $k \ll b^{-1}$, where b is the range of the potential [10]

$$k\cot\delta(k) = -\frac{1}{a_{\mathrm{sc}}} + \frac{r_0 k^2}{2}, \quad (4)$$

where $r_0(\sim b)$ is the effective range and a_{sc} is the s-wave scattering length. As a function of magnetic field, a_{sc} varies as $a_{\mathrm{sc}} = a_{\mathrm{bg}}(1 - \frac{\Delta B}{B - B_0})$, where B_0 and ΔB are the location and the width of the resonance, and a_{bg} is the background scattering length away from resonance. The region $B > B_0$ and $B < B_0$ where $a_{\mathrm{sc}} < 0$ and $a_{\mathrm{sc}} > 0$ are referred to as the $-$'ve and the $+$'ve sides of the resonance. For a temperature range such that the thermal wavelength is larger than the range of the potential, $\lambda > b$, we can use Eq. (4) in Eq. (1) where the integral is cut off at λ^{-1}. Near resonance, λ/a_{sc}, $r_o/a_{\mathrm{sc}} \to 0$, and Eqs. (1) and (4) imply that up to terms of order r_0/a_{sc}

$$b_2 = \sum_b e^{|E_b|/k_B T} - \frac{\mathrm{sgn}(a_{\mathrm{sc}})}{2}[1 - \mathrm{erf}(x)]e^{x^2}, \quad (5)$$

where $x = \lambda/(\sqrt{2\pi}a_{\mathrm{sc}})$ and $\mathrm{erf}(x)$ is the error function. We can then evaluate ϵ_{int} using Eqs. (3) and (5). At the same time, it is useful to look at the effect of phase shifts on the energy levels. In a box of size R, the wave vector k is changed from its noninteracting value $k_0 = \ell\pi/R$ ($\ell = 1, 2, 3, \ldots$) to $k \sim k_0 - \delta(k_0)/R$ through the boundary

condition $\sin[kR + \delta(k)] = 0$ at a large distance R. Scattering states and bound states correspond to the real and the imaginary k solution of this boundary condition. The energies of the lowest few states in the center of mass frame ($E = \hbar^2 k^2/M$) are shown in Fig. 1. As one passes through the resonance from the $-$'ve side, the lowest state in the continuum turns into a bound state, causing $\delta(k = 0)$ to change abruptly from 0 to π. The corresponding interaction energy $\epsilon_{\rm int}$ calculated from Eqs. (3) and (5) are shown in Fig. 2. Despite the simplicity of the calculation, considerable information can be deduced.

(A) Approaching the resonance from the $-$'ve side, $\epsilon_{\rm int}$ follows a "negative branch" $\epsilon_{\rm int}^{(-)}$ which is negative and decreases monotonically (see Fig. 2). $\epsilon_{\rm int}^{(-)}$ evolves from the (temperature independent) nonuniversal form $g n_\uparrow n_\downarrow$ far from resonance to a (temperature dependent) universal form $-\epsilon_0 = -(3nk_BT/2)(n\lambda^3/2^{3/2})$ at resonance, and continues on to the $+$'ve side. This universal form, which follows from the fact that $b_2 = 1/2$ and $\partial b_2/\partial T = 0$ at resonance ($x = 0$) [6], is the high temperature analog of universal interaction found in (I) and (II).

(B) Despite the change in sign of the scattering length, the interaction energy $\epsilon_{\rm int}^{(-)}$ remains negative across the resonance (shown in Fig. 2) because of the thermal population $\langle n_b \rangle$ of bound states that exist when $a_{\rm sc}$ is positive,

$$\langle n_b \rangle = \frac{2\sqrt{2}z^2}{\lambda^3} e^{-E_b/k_BT} = n\left(\frac{n\lambda^3}{\sqrt{2}}\right) e^{|E_b|/k_BT} + \ldots . \quad (6)$$

Although proportional to the small factor $n\lambda^3$, $\langle n_b \rangle$ is macroscopic in the thermodynamic limit. Equation (6) in turn implies that *in a bulk system, the original resonance* (at field B_0) *cannot be shifted to the positive side* (to $B_1 < B_0$) *at a lower temperature unless there is a phase transition for all magnetic fields between* B_1 *and* B_0 *where* $\langle n_b \rangle$ *disappears as temperature is lowered from the Boltzmann regime* (see Fig. 3). So far, such a phase transition has not been observed. Should future experiments rule out such a transition in ^{6}Li, one must then conclude that the resonance in the ENS experiment [2] is not shifted. The absence of a shift of the resonance is also consistent with the findings in Ref. [4] for ^{40}K.

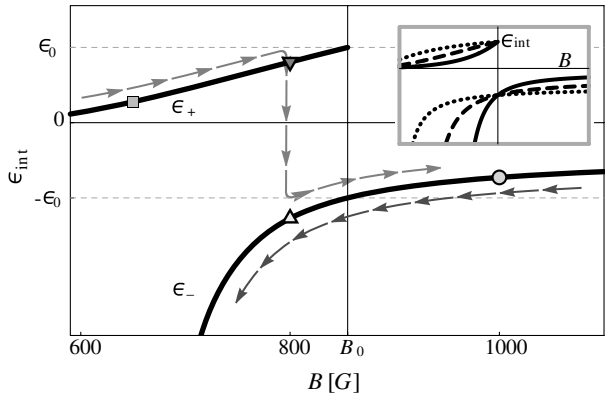

FIG. 2. Interaction energy. The energies $\epsilon_{\rm int}^{(\pm)}$ increase monotonically as the field is increased, reaching the universal value $\pm\epsilon_0$ at resonance, where $\epsilon_0 = (3nk_BT/2)(n\lambda^3/2^{3/2})$. The negative branch, $\epsilon_{\rm int}^{(-)}$, is continuous across the resonance, while $\epsilon_{\rm int}^{(+)}$ will jump to $\epsilon_{\rm int}^{(-)}$ if the bound state is occupied (say, at the field labeled by the triangle). Inset shows the temperature dependence: solid, dashed, and dotted lines correspond to $T = 1$, 10, and 100 μK.

(C) Approaching the resonance from the $+$'ve side, if the bound states are not occupied $\epsilon_{\rm int}$ will follow a "positive branch" $\epsilon_{\rm int}^{(+)} > 0$ that increases monotonically, evolving from $g n_\uparrow n_\downarrow$ to $\epsilon_0 = (3nk_BT/2)(n\lambda^3/2^{3/2})$ at resonance (see Fig. 2). However, a gas containing only scattering states is not in true equilibrium, as the latter requires that all states, including bound states, are thermally populated. As pointed out by Petrov [11], the three-body collisions that convert scattering states into bound states can lead to chemical equilibrium only if the released energy is insufficient to eject the particles from the trap. If one is sufficiently far from the resonance, then the molecular binding energy is larger than the trap depth, and the three-body collisions instead lead to loss. The sudden drop in the interaction energy near 700 G in the ENS experiment [2] is consistent with the production of trapped molecules. Moreover, Jochim *et al.* [5] have directly observed the equilibration of atom/molecule populations near this field. This scenario also predicts that the development of an equilibrium molecular population will coincide with a peak in the three-body loss rate. This peak is observed at ENS [2], MIT [3], and Innsbruck [5].

(D) The extension of $\epsilon_{\rm int}^{(-)}$ to the positive side of the resonance is due to the population of the bound state that becomes available there. If the system is brought across the resonance adiabatically, quasiequilibrium is maintained and the process is reversible. Consequently, molecules generated on the positive side will turn back to atoms when the system is brought back to the negative side. This is consistent with the experiments on ^{40}K [4].

(E) The experiment at ENS was performed at temperature $T = 3.5$ μK and degeneracy factor $T/T_F = 0.6$,

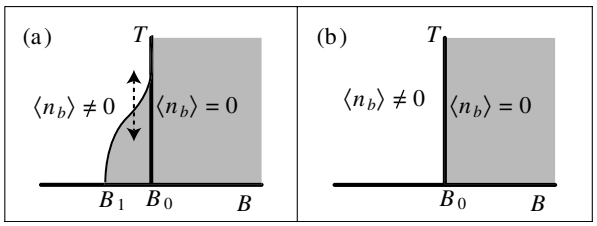

FIG. 3. Schematic phase diagrams. Because the original resonance (B_0) is unshifted at high temperature, a shift in resonance at low temperature ($B_1 < B_0$) will imply a phase boundary as shown in (a), which means that $\langle n_b \rangle$ will disappear (or appear) as temperature is lowered (or raised) along the path indicated by the double-headed arrow. The phase diagram for an unshifted resonance is shown in (b).

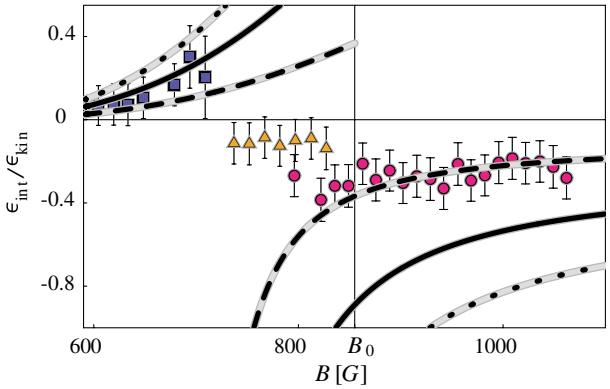

FIG. 4 (color online). The ratio $\epsilon_{\rm int}/\epsilon_{\rm kin}$ for $T = 3.5\ \mu$K. Squares (circles) show data from Ref. [2], which agrees with ϵ^+ (ϵ^-). Triangles do not fall on either curve and probably reflect a nonequilibrium situation. The dashed, solid, and dotted lines are for $T/T_F = 1.2$, 0.6, and 0.4, respectively.

corresponding to $n\lambda^3/2 = 1.6$. Using the same temperature, we have plotted the ratio $\epsilon_{\rm int}/\epsilon_{\rm kin}$ in Fig. 4 for $T/T_F = 1.2$, 0.6, and 0.4, corresponding to $n\lambda^3/2 =$ 0.6, 1.6, and 3.0. Although our result on interaction energy should be accurate only when $n\lambda^3/2 < 1$, we also plot it at higher phase space densities (i.e., extending it to regions $n\lambda^3/2 > 1$) to indicate its temperature dependence. Moreover, these extensions are the leading terms of the interaction energy in powers of $n\lambda^3/2$. On the positive side all three of our curves are consistent with the experimental data, while on the negative side the $T/T_F = 1.2$ curve is closest. The fact that the $B > B_0$ data match this higher temperature curve may be due to higher order terms in the high temperature expansion or systematic differences in the density/temperature of the sample on the two sides of the resonance. In any case, it is clear that a Fermi gas in the Boltzmann regime exhibits all the phenomena seen in current experiments. Equally important is the fact that the exact high temperature results near unitarity force one to conclude the existence of a phase where atoms and molecules are in chemical equilibrium.

Having shown that the behavior of the quantum gas in the Boltzmann regime has all the characteristics seen in experiments at lower temperatures, we reiterate that the two regimes are connected by the analyticity of the thermodynamic functions. Despite the divergent scattering length, at small fugacity z (or equivalently small density $n\lambda^3$) the probablility of particle collisions is small, leading to our systematic perturbative scheme.

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[8] Equation (1) is obtained by noting that the wave vector k is changed by the phase shift from the noninteracting value k_0, which leads to the change of density state given by $d\delta(k)/dk$. The details are given in [7].

[9] Using the relation $PV = k_B T \ln\mathcal{Z}$, the pressure is $P(T, \mu) = P^{(0)}(T, \mu) + 2\sqrt{2}(k_B T z^2/\lambda^3) b_2$, where $P^{(0)}(T, \mu)$ is the pressure for a two component noninteracting Fermi gas. The fugacity expansion for $P^{(0)}(T, \mu)$ (see Chap. 5 in [10]) gives $P(T, \mu) = 2\lambda^{-3} k_B T(z - 2^{-5/2} z^2 + \sqrt{2} b_2 z^2)$. Using the Gibbs-Duham relation $dP = n d\mu + s dT$, where n is the number density and s is the entropy density, the density is $n(T, \mu) = 2\lambda^{-3}(z - 2^{-3/2} z^2 + 2\sqrt{2} b_2 z^2 + \ldots)$, which is inverted to produce $z = (n\lambda^3/2) + (2^{-3/2} - 2\sqrt{2} b_2) \times (n\lambda^3/2)^2 + \ldots$. Similarly, it is straightforward to show that $s = 5P/(2T) - \mu n/T + 2\sqrt{2} k_B T z^2 \lambda^{-3} \partial b_2/\partial T$. The energy density, $\epsilon = Ts + \mu n - P$, then becomes $\epsilon = (3 k_B T z/\lambda^3) \times \{1 + z[-2^{-5/2} + \sqrt{2} b_2 + (2\sqrt{2}/3) T(\partial b_2/\partial T)]\}$, which can be written in the form of Eq. (2).

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