Two-component Fermi gas with a resonant interaction

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We consider a two-component Fermi gas interacting via a Feshbach molecular state. It is shown that an important energy scale is $E_g = g^2 m^3/(64 \pi^2)$ where $g$ is the Feshbach coupling constant and $m$ the mass of the particles. Only when $E_g \gg \epsilon_F$ where $\epsilon_F$ is the Fermi energy can the gas be expected to enter a universal state in the unitarity limit on the atomic side of the resonance where there are no molecules present. The universal state is distinct from the molecular gas state on the other side of the resonance. We furthermore calculate the energy of the gas for this universal state and our results are related to current experiments on $^6$Li and $^{40}$K.

One of the most interesting recent developments within the field of ultracold atom gases is the use of Feshbach resonances to manipulate the effective atom-atom interaction. By controlling an external magnetic field, the Feshbach molecular state can be tuned to an energy close to the scattering atoms. In this case, the vacuum atom-atom scattering is unitarity limited with a diverging scattering length $a$ and the system is strongly interacting. Thus, it is possible with the atomic gases to address the important question of the nature of a many-body system with an interaction characterized by $|a| \to \infty$. Indeed, remarkable experimental progress concerning this question has been made in recent months with several groups reporting results for two-component atomic Fermi ($^6$Li and $^{40}$K) gases interacting via a closed channel Feshbach molecular state close to resonance [1, 2, 3, 4].

In this paper, we examine the problem of a two-component Fermi gas interacting via a Feshbach molecular state close to zero energy. We show that only for sufficiently broad resonances with $E_g \gg \epsilon_F$ can the gas be expected to exhibit universal behavior close to resonance on the $a < 0$ when there are no molecules. The possibility of such universal behavior when $|a| \to \infty$ has been examined by a number of authors [3, 4, 5, 6]. The basic idea is that $|a|$ is not a relevant length scale in this limit and that the thermodynamic quantities of the gas therefore should only depend on the density $n$ and the temperature $T$. The gas is in this sense universal since its properties are independent of the specific details of the interaction. The energy per particle for a Fermi gas with $T \ll T_F$ where $T_F$ is the Fermi temperature is predicted to scale as $E/N = 3\epsilon_F(1 + \beta)/5$ in the universal limit and various values for the constant $\beta$ has been predicted [2, 4, 6]. For a Bose gas with $|a| \to \infty$, it was argued that $E/N \propto n^{-2/3}$ [7]. Similar results were derived for bosonic three particle states [8]. We will in the present paper calculate $\beta$ for a Fermi gas in the universal limit for $E_g \gg \epsilon_F$ taking into account two-body scattering in a medium. Our results are finally related to the present experiments on the atomic gases.

The explicit model considered here consists of atoms with mass $m$ in two hyperfine states denoted $\uparrow$ and $\downarrow$ being coupled to a closed channel with a Feshbach molecule. The Hamiltonian describing this interacting mixture of atoms and molecules (described as point bosons) is

$$
\hat{H} = \hat{H}_0 + \sum_{k \sigma \q} \frac{g_{\text{bare}}(q)}{\sqrt{\mathcal{V}}} [\hat{b}^\dagger_k \hat{\Phi}_{k/2+\q}^\dagger \hat{\Phi}_{k/2-\q} + \text{h.c}]
$$
$$
+ \sum_{k \sigma \q \q'} \frac{V(q, q')}{\mathcal{V}} \hat{a}^\dagger_k \hat{\Phi}_{k+q}^\dagger \hat{\Phi}_{k-q} \hat{a}^\dagger_{k+q} \hat{\Phi}_{k+q}'
$$

with $\hat{H}_0 = \sum_{k \sigma} \epsilon_k \hat{a}^\dagger_k \hat{a}_k + \sum_{k} E_{k,\text{bare}} \hat{b}^\dagger_k \hat{b}_k$. Here $E_{k,\text{bare}} = 2\epsilon_{\text{bare}} + K^2/4m$, where $2\epsilon_{\text{bare}}$ is the energy of a bare molecule with momentum zero measured with respect to the energy of a pair of atoms at rest in the open channel, $\epsilon_k = k^2/2m$ is the kinetic energy of an atom, $g_{\text{bare}}(q)$ is the bare molecule-atom coupling matrix element, $V$ is the non-resonant interaction between atoms, and $\mathcal{V}$ is the volume of the system.

The main object to calculate here is the thermodynamic potential of the gas $\Omega = -k_B T \ln \mathcal{Z} + \mathcal{Z} \equiv \text{Tr}\{\exp[-\beta(\hat{H}-\mu \hat{N}_F - 2\mu \hat{N}_B)]\}$. Here, $\hat{N}_F = \sum_{k \sigma} \hat{a}^\dagger_k \hat{a}_k$ and $\hat{N}_B = \sum_{k} \hat{b}^\dagger_k \hat{b}_k$ are the number of bare atoms and molecules respectively and $\mu$ is the chemical potential. We assume an equal density of the two atomic hyperfine states and a total density $n = k_B^2/3\pi^2$. Also, the molecules and atoms are assumed to be in equilibrium. Using the ladder approximation (or the Gaussian approximation for the partition function), the thermodynamic potential can after some algebra be expressed as

$$
\frac{\Omega}{V} = \frac{\Omega_0}{V} + \int \frac{d^3 k}{(2\pi)^3} \int \frac{d\omega}{\pi} e^{i\omega 0 - 1} \times 
\text{Im Tr ln}[1 - (V + g_{\text{bare}} D_0(K, \omega) g_{\text{bare}}) G_0^{(2)}(K, \omega)].
$$

Here $\Omega_0$ is the thermodynamic potential of an ideal gas of non-interacting atoms and molecules described by $\hat{H}_0$. We omit for brevity here and in the rest of the paper a small positive imaginary part to the frequencies in the (retarded) Greens functions which should really be evaluated at $\omega + i \delta$. The free molecule Greens function is $D_0(K, \omega)^{-1} = \omega - F_{k_b}^\dagger + 2\mu$ and the two particle Greens function $G_0^{(2)}(K, \q, \omega) = [\hat{f}(\xi_{k/2+\q}) + \hat{f}(\xi_{k/2-\q}) - 1]/[\xi_{k/2+\q} + \xi_{k/2-\q} - \omega]$ describes the free propagation of a pair of atoms with COM momentum $K$ and relative momentum $\q$ in the presence of the medium. Here $\xi_k = \epsilon_k - \mu$ and $f(x) = (\exp(x/k_B T) + 1)^{-1}$. 


Fermi function. The trace in Eq. (1) refers to integration over the momentum variables appearing in the matrices $V(q,q')$ and $g_{bare}(q)G_0^{(2)}g_{bare}(q')$. Various forms of Eq. (1) have been discussed in the literature in connection with the BCS-BEC crossover problem [11]. For the present purposes, it is convenient to rewrite Eq. (1) as

$$\Omega = \Omega_0 + \Delta \Omega + \Pi(\omega)$$

where $\Delta \Omega$ describes the propagation of a pair of atoms interacting only via the background interaction in the ladder approximation. $D^{-1} - \Pi$ is the molecule Greens function with the self energy $\Pi(\omega) = \text{Tr}[g_{bare}G_0^{(2)}(K,\omega)g_{bare}]$ [12]. Equation (2) is convenient since it separates the corrections to $\Omega$ coming over the momentum variables appearing in the matrix

$$\Delta \Omega = \int \frac{d^3K}{(2\pi)^3} \int \frac{d\omega}{\pi} [\text{ImTr} \ln[G_0^{(2)}(K,\omega)/G_{bg}^{(2)}(K,\omega)] + \text{ImTr} \ln[D_0(K,\omega)/D(K,\omega)]) \frac{(\omega^2/k_BT - T)^{-1}}{\pi}. (2)$$

where $G_{bg}^{(2)} = G_0^{(2)} - V$ describes the propagation of a pair of atoms interacting only via the background interaction in the ladder approximation. $D^{-1} - \Pi$ is the molecule Greens function with the self energy $\Pi(\omega) = \text{Tr}[g_{bare}G_0^{(2)}(K,\omega)g_{bare}]$ [12]. Equation (2) is convenient since it separates the corrections to $\Omega$ coming from the Feshbach molecule from the effects of the background (non-resonant) interaction. Since we focus in the effects of the resonant part of the interaction, we will in the rest of this paper only consider the molecule term in Eq. (2). The $\text{Im}[D_0(K,\omega)]$ term in Eq. (2) is trivial as it simply cancels the bare molecule contribution to $\Omega_0$.

In order to be able to express our result in terms of observables only, we use the low energy effective theory developed in ref. [12]. We therefore write $\hat{z}D^{-1}(K,\omega) = \omega - E_K + g^2 m^{3/2} (4\pi)^{-1} \sqrt{\omega - \hat{\Pi}(K,\omega)}$ where $E_K = K^2/2m + 2\nu - 2\mu$ and $\hat{\omega} = \omega + 2\mu - K^2/2m$. Here $2\nu$ is the energy of the molecule taking into account the high energy dressing by the atoms but excluding the threshold effects which are explicitly treated by the $\sqrt{\omega - \hat{\Pi}}$ term. The wave function renormalization of the molecule given by $\hat{z}$ is due to the coupling to high energy atoms. The constant $\mu$ yields the coupling between this dressed molecule and the atoms and $\hat{\Pi}$ gives the medium corrections to the molecule self energy $\Pi$. Explicit expressions for these quantities are given in ref. [12] and will not be repeated here. The point is that $\hat{z}$ and $2\nu$ can be extracted from experiments without any arbitrary assumptions of the behavior of the bare quantities.

It is easy to show that Eq. (2) reproduces the two-body term in the virial expansion of $\Omega$ in the Boltzmann regime [13]. This expansion has been used to prove that a gas of atoms interacting via a closed channel resonant (zero energy) Feshbach molecule exhibits universal behavior in the non-degenerate limit [6]. We will presently examine under which conditions such universal behavior persists in the low temperature degenerate regime.

We split $\Delta \Omega$ into a contributions coming from undamped and damped two particle states. This is done by writing Eq. (2) (neglecting the background parts) as

$$\Delta \Omega = \int \frac{d^3K}{2\pi^3} \int \frac{d\omega}{\pi} \frac{f(\xi_{K+q/2} - q)}{\Pi(\omega,K,\xi_{K+q/2} + \xi_{K/2} - q)/g^2} \times \arctan \left[ \frac{\Pi(\omega,K,\xi_{K+q/2} + \xi_{K/2} - q)/g^2}{\sqrt{q^2/m - 2\nu - \text{Re} \Pi(\omega,K,\xi_{K+q/2} + \xi_{K/2} - q)}} \right]. (3)$$

where $\Delta \Omega_M = k_BT \sum_k \log[1 - \exp(\omega_K/k_BT)][1 - \partial_k \Pi(K,\omega_K)]$ is the contribution from the undamped molecular states with energy $\omega_K$. The energies $\omega_K = \omega_K + K^2/2m - 2\mu$ are determined by $\omega_K = 2\nu + g^2 m^{3/2} (4\pi)^{-1} \sqrt{\omega_K + \text{Re} \Pi(K,\omega_K)}$ with $\omega_K \leq K^2/2m - 2\mu$ since $\text{Im} \Pi(K,\omega) \neq 0$ for $\omega > K^2/2m - 2\mu$. It is easy to show that $\Pi(K,\omega) \geq 0$ for $\omega \leq K^2/2m - 2\mu$, i.e. the medium only increases the molecule energies. There will therefore be no undamped molecules below the Fermi sea for $\nu > 0$. To arrive at the second term in Eq. (3) from Eq. (2), we have divided and multiplied by $\text{Im} \Pi$ and performed the $\omega$ integration. Using Eq. (3), we can analyze under which conditions the interacting gas will exhibit universal thermodynamics.

As explained above, the universal thermodynamics hypothesis states that the thermodynamic quantities should depend only on $T$ and $n$ in the unitarity limit when $|a| \to \infty$. For the specific system considered here, the scattering length is $4\pi a_{\text{res}}/m = -g^2 / 2\nu$. The thermodynamic potential depends therefore in general on $\nu, T$, and $g$ and we write $\Omega(T,\mu,\nu,g)$. If such a gas is to exhibit universal thermodynamic behavior, we must have $\Omega(T,\mu,\nu,g) \sim \Omega(T,\mu)$ close to resonance, i.e. the thermodynamics become independent of the specific details of the resonance.

Let us first briefly consider the molecular side of the resonance with $\nu \leq 0$. Since $\mu \leq \nu$, the system in this case consists of a pure molecular gas with essentially no atoms present for $T \ll T_F$ and we need only to consider $\Delta \Omega_M$ in Eq. (3). We therefore also have $\Pi = 0$ and the molecule energies are given by $\omega = -(\sqrt{E_g} - 2\nu - \sqrt{E_g})$. We have introduced the energy $E_g = g^4 m^3/(64\pi^2)$ which determines the range of energies for which threshold effects are important. So universality for $\nu \leq 0$ is straightforward to understand within the present model: For $-E_g < 2\nu < 0$, we simply obtain an ideal gas of molecules with energy $\omega = -h^2/(ma_{\text{res}}^2)$. However, this result ignores the molecule-molecule interactions, which are not included in the present formalism. Such effects could be important for $\nu \leq 0$ where there is a macroscopic number of molecules [14].

The main purpose of the present paper is to examine the $a_{\text{res}} < 0 (\nu > 0)$ side of the resonance where there are no undamped molecules and $\Delta \Omega_M$ in Eq. (3) can be ignored. The only place where $\nu$ and $g$ enter in the expression for $\Omega$ is then in the argument of the arctan(...) where $\nu$ appear explicitly and $g^2$ enters since $\Pi \propto g^2$. The molecule self energy $\Pi$ scales as $\sim O(g^2 m^{3/2}/4\pi)$ [12]. From this it follows that in order to make the argument of the arctan(...) independent of $g^2$ and $\nu$, we must have $g^2 m^{3/2}/4\pi \gg \epsilon_T$. Only in this case will the $\Pi$ terms in the arctan(...) dominate and thus cancel the $g^2$ and $\nu$ dependence even when $\nu \gg \epsilon_T$. The reason for the requirement $\nu \ll \epsilon_T$ is that $\mu \ll \nu$ from particle conservation. When $\nu \ll \epsilon_T$ we have $\mu \sim \nu$ due to the presence of damped molecules; i.e., $\mu$ and the thermodynamics of the gas will depend critically on $\nu$ when $0 \leq \nu \ll \epsilon_T$. It
should be noted that for $\nu/\epsilon_F \to 0$, we of course approach the pure molecular gas state for $\nu \leq 0$ described above; the state of the gas changes continuously across the resonance. What we have shown here however is that the gas approaches a different universal state independent of $(g, \nu)$ for $\nu \gg \epsilon_F$ only if the resonance is sufficiently broad with $g^2 \gg 4\pi k_F m^{-2}$. This state is characterized by strongly correlated atom pairs with no real molecules present. The condition for universality on the $a_{\text{res}} < 0$ side can also be written

$$E_g \gg \epsilon_F.$$  \hspace{1cm} (4)

In terms of the scattering length $4\pi a_{\text{res}}/m = g^2/2\nu$, Eq. 4 can be written as $k_F|a_{\text{res}}| \gg 1$ even when $\nu \gg \epsilon_F$. Thus, the condition for universality on the atomic side of the resonance simply states that the coupling must be so strong that one can reach the unitarity regime $k_F|a_{\text{res}}| \gg 1$ before there is a significant population of molecules. The $g^2$ in the denominator of the arctan(...) may be regarded as arising from an effective range term. We can then identify the effective range for the effective interaction mediated by the Feshbach molecule as $r_{\text{eff}} = -8\pi m^{-2}g^{-2}$. Using this, we can finally write Eq. 4 in the illuminating way $k_F|a_{\text{eff}}| \ll 1$, i.e. universality can only be reached if the effective range of the interaction is small.

We now consider the $a_{\text{res}} < 0$ and $T = 0$ limit of the universal behavior for in more detail. For $T = 0$, we can write $\Delta \Omega/\nu = \mu_I(\mu)$$I$ where $I(\nu/\mu, g^2 m^{3/2}/\sqrt{\mu})$ is the $T = 0$ integral in Eq. 3 expressed in dimensionless variables ($k = k/\sqrt{2m\mu}$ etc.) and $n_I(\mu) = (2\mu)^{3/2}(3\pi^2)^{-1}$. The integral $I$ can be evaluated numerically. In the universal limit $E_g \gg \epsilon_F$, we get $I_{\text{uni}} \simeq -0.3$ for $T = 0$. This immediately gives $\Omega(T = 0, \mu) = -2\mu_I(\mu)(1 - 5I_{\text{uni}}/2)/5$ and $\mu = (2m)^{-3/2}(3\pi^2)^{1/2}(1 - 5I_{\text{uni}}/2)^{-2/3}$. We finally obtain $E/N = 3\epsilon_F(1 + \beta)/5$ with

$$\beta = (1 - 5I_{\text{uni}}/2)^{-2/3} - 1 \simeq -0.3.$$  \hspace{1cm} (5)

Equation 5 gives the $T = 0$ energy correction in the universal limit when all two-particle correlations are evaluated using the ladder approximation. It should be noted that the medium effects giving energy shifts and Pauli blocking through $\Pi$ are significant; if the vacuum values $\text{Im} \Pi_{\text{vac}} = g^2 m^2/4\pi$ and $\Pi = 0$ are used in Eq. 3, we obtain $I_{\text{uni vac}} = 5/8$ which gives $\beta \simeq -0.519$.

To illustrate the conclusions described above, we present results based on a numerical evaluation of Eq. 3. In Fig. 2 we plot the energy per particle $E/N$ as a function of $-k_F a_{\text{res}}$ for two different coupling strengths: $E_{\text{large}} \gg \epsilon_F$ and $E_{\text{small}} \ll \epsilon_F$. For $E_{\text{large}}$, we also plot the energy for two different temperatures $T = 0$ and $T = T_F/4$. The number of particles is fixed while $a_{\text{res}} = -g^2 m/(8\pi\nu)$ is varied through varying $\nu$. We see that for $E_{\text{large}}$, the energy per particle approaches a constant for $-k_F a_{\text{res}} \gg 1$. In agreement with the Eq. 5, we find $E/N \simeq 0.42\epsilon_F$ for $-k_F a_{\text{res}} \gg 1$ and $T = 0$. For the narrow resonance $E_{\text{small}}$, on the other hand, the energy per particle steadily decreases with increasing $-k_F a_{\text{res}}$ and the gas does not reach the universal limit for $a_{\text{res}} < 0$. This is simply because when $-k_F a_{\text{res}} \gtrsim 1$, we already have $\nu \ll \epsilon_F$ for such a small value of $g$, and the depletion of the Fermi sea into the molecular level is significant. Of course, the depletion of the Fermi sea for $\nu \ll \epsilon_F$ also happens for $E_{\text{large}}$. However, since this corresponds to $-k_F a_{\text{res}} \gtrsim g_{\text{large}}^2 m^2/4\pi k_F$, there is a large region of parameter space $1 \ll -k_F a_{\text{res}} \ll g_{\text{large}}^2 m^2/4\pi k_F$ where the thermodynamics of the gas is universal with no molecules present. This is illustrated by the inset, which plots $E/N$ for $E_{\text{large}}$ over a larger range of $-k_F a_{\text{res}}$. In a second inset, we plot $E/N$ for $-k_F a_{\text{res}} \ll 1$. The solid line is the numerical results whereas the dashed line is the Galitskii result $E/N = \epsilon_F[3/5 + 2k_F a_{\text{res}}/(3\pi) + 4(11 - 2\log 2)/(35\pi^2)(k_F a)^2 + ...]$. We see that our theory reproduces the Galitskii result for $-k_F a_{\text{res}} \ll 1$ as it should.

The depletion effect for $\nu \ll \epsilon_F$ is illustrated more clearly in Fig. 2 where we plot the chemical potential $\mu$ and $E/N$ for the same coupling strengths but now as function of $\nu$ for $T = T_F/4$. We also plot the density of (damped) molecules $n_{\text{mol}} = Tr D$ and atoms $n_{\text{atom}} = n - n_{\text{mol}}$ for $E_{\text{large}}$. We see that there is only a significant number of molecules when $\nu \ll \epsilon_F$ as expected. They will eventually become the undamped molecule gas for $\nu < 0$. Of course, for both coupling strengths the gas converges toward a pure molecular state for $\nu < 0$.

In total, the numerical results confirm our conclusion, that the thermodynamics of the gas only exhibit universal behavior when $-a_{\text{res}} k_F \gg 1$ for a sufficiently broad resonance with $E_{\text{large}} \gg \epsilon_F$.

Let us now compare our result for the $T = 0$ universal limit with a number of recent calculations. In ref. 3, the value $\beta \simeq -0.67$ was estimated from an expansion of the on-shell scattering amplitude in powers of $k_F a$ and an approximate momentum average. In ref. 7, the values $\beta \simeq -0.43$ and $\beta \simeq -0.67$ were suggested from two different Padé approximants of the ladder series for the

FIG. 1: The energy per particle $E/N$ in units of $\epsilon_F$ as a function of $-k_F a_{\text{res}}$ for a narrow and a broad resonance.
energy. The $T = 0$ result $\beta \simeq -0.3$ presented in this paper however, is the exact within the ladder approximation excluding superfluid correlations. A fixed node Greens function Monte Carlo calculation with $\sim 40$ particles yields $\beta \simeq -0.46$ and $\beta \simeq -0.56$ when superfluid correlations are excluded and included respectively. It could be interesting to examine in more detail the reasons for the difference between the present diagrammatic result and the Monte Carlo results in ref. $\circ$. One possible reason could be $> 2$ body correlations which cannot be expected to be small in the unitarity limit.

We conclude this paper by relating our results to some of the experiments on atomic gases. First, we examine whether a couple of the experimentally relevant resonances can be expected to exhibit universal thermodynamics. For one such Feshbach resonance at the magnetic field $B_0 \simeq 200$ G for $^{40}$K in the two open channel hyperfine states $|9/2, -9/2\rangle$ and $|9/2, -7/2\rangle$, an analysis yields $k_F|\varepsilon_{\text{res}}| \simeq 15n_{12}^{-1/3}E_F/\nu$ where $n_{12}$ is the density in units of $10^{12}$ cm$^{-3}$ $\Box$. Another case of interest is the $^6$Li Feshbach resonance between the two lowest hyperfine states at $B_0 \simeq 860$ G $\Box$. An estimate of this resonance yields $k_F|\varepsilon_{\text{res}}| = 1.1 \times 10^8n_{12}^{-1/3}\varepsilon_F/\nu_{\text{bare}}$ $\Box$. This shows that these two particular resonances are sufficiently broad (large $g^2$) such that one would expect universal behavior on the $a_{\text{res}} < 0$ side of the resonance. There has recently been a number of measurements of the energy of a $^6$Li gas close to the Feshbach resonance considered above $\Box,\Box,\Box$. In agreement with the conclusions of this paper, they suggest that the properties of the gas indeed become universal in the limit $|a| \to \infty$. The Duke group obtain $\beta = -0.26 \pm 0.07$ on the $a_{\text{res}} < 0$ side of the $^6$Li resonance $\Box$. This value agrees well with Eq. $\Box$. However, the Innsbruck group measures $\beta = -0.88^{+0.15}_{-0.1}$ for the same resonance $\Box$. Finally, the group at ENS obtains $(E_{\text{tot}} - E_{\text{kin}})/E_{\text{kin}} \simeq -0.3$ for $a_{\text{res}} \to -\infty$ $\Box$. But since both the total energy $E_{\text{tot}}$ and the kinetic energy $E_{\text{kin}}$ of the gas are measured for the interacting system this ratio is not identical to the parameter $\beta$ as defined in the present paper. In general, further investigation is needed in order to remove some of the apparent inconsistencies of the results for $|a| \to \infty$ reported so far.

In conclusion, we have shown that a two-component Fermi gas interacting via a Feshbach state can be expected to exhibit universal behavior on the $a_{\text{res}} < 0$ side only when the resonance is sufficiently broad with $E_g \gg \varepsilon_F$. We furthermore calculated the universal parameter $\beta$ taking into account two-body processes in the ladder approximation. Our results were compared to the experimental results when appropriate.

We acknowledge very useful discussions with C. J. Pethick, H. Heiselberg, and S. J. J. M. F. Kokkelmans.

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