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Superfluidity of an Atomic Fermi Gas near the Unitarity Limit

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Abstract—We show that the thermodynamic properties of an atomic Fermi gas near the unitarity limit for Feshbach scattering is not universal as long as the resonance is narrow on the scale of the Fermi energy. In view of ongoing quantum Monte Carlo simulations, we explore this behavior within a mean-field approach extended to a finite temperature by means of a model potential, which allows for a tuning of the scattering phase shift and its energy dependence. Our results may be relevant for constructing a complete theoretical description of the crossover from a Bose–Einstein condensation (BEC) of composite bosons to a Bardeen–Cooper–Schrieffer (BGS) type \cite{11} of superfluid \cite{12} to a Bose–Einstein condensation with respect to the occurrence of superfluidity. An additional question concerning the observability is also connected to the dynamical processes actually involved in the formation of the pairs, which could be sufficiently slow as to require a nontrivial, nonequilibrium theoretical analysis.

Second, crossover theories must be able to give a quantitative description of the BCS and BEC limits. From a general point of view, we may distinguish theories in which the interactions are parametrized by the scattering length \cite{23} from those in which the presence of molecular states of two fermions is explicitly included, together with their coupling to the unpaired states \cite{24}. The two approaches can be formally connected to each other \cite{25} and lead to the common concept that the formation of Cooper pairs and their condensation to the lowest energy state are not simultaneous events. The account of the BCS limit in atomic Fermi gases is relatively easy, as most theories start from a BCS-like ground state \cite{26–29} along the lines of and beyond the seminal works by Leggett \cite{30} and Nozières and Schmitt-Rink \cite{31}. As for the BEC limit, the crossover order parameter must be consistent with the results of the four-fermion scattering problem \cite{32}, according to which the bosonic pairs interact with each other through the effective scattering length $a_B = 0.6a$.

The present work addresses a third question, namely, the behavior across resonance in the unitarity limit $|a| \to \infty$. Here, the thermodynamic properties are expected to be independent of the scattering length, based on the remark that the only available length scale is the interparticle distance \cite{33}. However, this argu-
ment fails in the case of narrow resonances, where the scattering phase shift significantly changes over the energy range of the Fermi energy [34], and a second length scale, namely, the effective range, plays a role. While actual measurements involve broad resonances and are consistent with a universal value of the interaction energy in the unitarity limit, the present study is motivated both by the availability of narrow resonances in, e.g., $^6$Li, and by the theoretical motivation of providing a complete description of the crossover physics.

We thus develop a model that is able to interpolate between the two limits of a broad resonance, where the interaction behavior is completely encapsulated by the scattering length resulting from the low-energy renormalization, and of a narrow resonance in a broad Fermi sea, where large values of scattering energies need to be sampled. We model a minimal interaction potential that is able to reproduce and independently tune the three relevant features of a Feshbach resonance, namely, the detuning and the width of the resonance, and the background scattering length $a_{bg}$. The thermodynamic properties of the atomic gas in the unitarity limit are investigated as functions of the resonance width by resorting to a mean-field solution of the BCS-like equations. The results are discussed as a guide to the ongoing quantum Monte Carlo simulations, which can provide a more refined account of the interactions. While the basic results have been published elsewhere [35], here we extend the analysis of the model to a finite temperature.

**A BARRIER-WELL MODEL OF THE FESHBACH RESONANCE**

We model the presence of a Feshbach resonance by the interaction potential

$$V(r) = \begin{cases} 
-V_0 & r < r_0 \\
V_1 & r_0 < r < r_1 \\
0 & \text{otherwise}
\end{cases} \quad (1)$$

that is displayed in Fig. 1. This is characterized by an attractive well with depth $V_0$ and width $r_0$ and a barrier with height $V_1$ and width $r_1 - r_0 \equiv r_w$. This barrier-well model allows us to incorporate the essential energy-dependence of the scattering physics into a single-channel scattering scheme, since the well can support resonant states with a width dependent on the tunneling through the potential barrier.

We emphasize that, in the many-body perspective, the problem is still characterized by three distinct parameters measured on the scale of the particle density $n$. These are the diluteness $nr_0^3$, the interaction strength $na^3$, and the width $\Delta \nu$ of the resonance on the scale of the Fermi energy $E_F = \hbar^2k_F^2/2m$ with $k_F = (3\pi^2n)^{1/3}$. $\Delta \nu$ can be expressed in terms of the matrix element $g$ for the coupling between the closed and open channels as

$$\Delta \nu = g\sqrt{n},$$

which enters the resonance-superfluidity Hamiltonian, as was pointed out in [36].

In the following, we require that the diluteness condition $nr_0^3 \ll 1$ is always satisfied, while staying within the unitarity limit $na^3 \gg 1$. We thus vary the width of the resonance by tuning the parameter $\Delta \nu/E_F$. The parameters of the model potential can in principle be adjusted to reproduce the scattering properties of an atomic sample [10]. Here, we choose two sets of parameters that are suitable for illustrating the physical behavior of the system. We fix the scattering length to a large and positive value $a = 5000a_0$, with the Bohr radius $a_0$, so as to stay on the BEC side of the resonance under unitarity-limited conditions. This is large compared to the interparticle spacing as determined from the density $n = 1.054 \times 10^{14}$ cm$^{-3}$. The range $r_0$ of the potential is first taken to be $r_0 = 500a_0$, so that $nr_0^3 = 0.002 \ll 1$. The results are compared with those arising from the use of a second set of parameters that correspond to a larger range of the potential $r_0 = 2000a_0$. This value is small enough to ensure that $nr_0^3 = 0.1 < 1$ but large enough to appreciate on a single energy scale both the scattering and many-body effects.

The above requirements fix two out of the four parameters of the model potential. Then, we tune the values of the barrier height $V_0$ and the barrier width $r_1$ (which are not independent parameters) in order to

\begin{align*}
V(r) &= \begin{cases} 
-V_0 & r < r_0 \\
V_1 & r_0 < r < r_1 \\
0 & \text{otherwise}
\end{cases} \\
\Delta \nu &= g\sqrt{n},
\end{align*}
change $\Delta v$. This is accomplished by solving the scattering problem for $V(r)$ in the standard way [37] and thus determining the two-body scattering function $\Psi(r)$ and the $T$ matrix [35].

The $T$ matrix contains all the necessary information. The scattering length $a$ is simply determined from its definition:

$$\frac{4\pi\hbar^2}{m}a = \lim_{k \to 0} T(k).$$

As to the width of the resonance, this is physically related to the tunneling rate through the barrier. The link is made explicit by presenting the usual relation $T(k) = 2\pi\hbar^2/[S(k) - 1]/(mk)$ and noticing that the Feshbach form for the $S$ matrix in the one-resonance parametrization is

$$S(k) = e^{-2ik_a} \left[ 1 - \frac{2k|g|^2}{4\pi\hbar^2 \left( \sqrt{\frac{\hbar^2}{m}} + \frac{ik|g|^2}{m} \right)} \right].$$

Alternatively, one may express the $g$ parameter in terms of the effective range defined as [37] $R_{\text{eff}} \equiv -(4\pi\hbar^2/m)(d^2 T(k)^{-1}/dk^2)|_{k = 0}$. By inspection, we obtain

$$|g|^2 = \frac{8\pi\hbar^4}{m^2 R_{\text{eff}}}.$$  

where we have removed the background $a_{bg} = 0$. This form in Eq. (4) agrees with the expression in [34]. In the unitarity limit, $R_{\text{eff}}$ evidently sets the second relevant length scale, besides the interparticle spacing. The dimensionless width in units of the Fermi energy is then the ratio $g/\hbar n/E_F$, or alternatively $nR_{\text{eff}}$.  

THE NON-LOCAL BCS EQUATIONS

We can now find the equilibrium state of the Fermi gas interacting via the non-local potential interaction modeled by $V(r)$. This is a suitable foundation for the eventual input into the quantum Monte Carlo schemes that are needed to include the many-particle correlations beyond the perturbative approach.

The ground state is determined within the usual variational BCS scheme that utilizes the wavefunction [11]:

$$|\Phi_0 \rangle = \Pi_k (u_k + \nu_k a_k^+ \uparrow d_{-k, \downarrow}^+ )|0\rangle,$$  

where $a_k^\dagger$ is the creation operator for electrons of spin $\sigma$. $\Phi_0$ is normalized, yielding the condition $|u_k|^2 + |\nu_k|^2 = 1$. The expected value of the ground-state energy at $T = 0$ is

$$E_0 = \sum_k 2\varepsilon_k |v_k|^2 + \sum_{kk'} V_{kk'} u_k^\dagger v_k^\dagger u_{k'}^\dagger v_{k'}^\dagger + \sum_{kk'} V_{kk'} u_k^\dagger u_{k'}^\dagger v_k^\dagger v_{k'}^\dagger,$$

where $\varepsilon_k = \hbar^2 k^2/2m$.

All of the summations entering into Eq. (6) can be easily handled in our isotropic system after performing the angular integration. For the generic function $F(k)$, this procedure amounts to evaluating a one-dimensional integral

$$
\sum_k V_{kk'} F(k) \rightarrow \frac{1}{(2\pi)^3} \int dq q^2 V(k, q) F(q),
$$

with $V(k, q)$ determined from the three-dimensional Fourier transform of the spatial potential

$$V(k, q) = \frac{2\pi}{kq} (V_0 + V_1) \left[ \frac{\sin r_k |k + q|}{|k + q|} - \frac{\sin r_k |k - q|}{|k - q|} \right] - V_1 \left[ \frac{\sin r_k |k + q|}{|k + q|} - \frac{\sin r_k |k - q|}{|k - q|} \right].$$

The BCS solution results from the minimization of the free energy $f = \langle \Phi_0 | H | \Phi_0 \rangle - \mu \langle \Phi_0 | \hat{N} | \Phi_0 \rangle$ with respect to the variational parameters $u_k$, $\nu_k$ and with the chemical potential $\mu$ fixed by the constraint of particle-density conservation. The two resulting self-consistent equations for the isotropic superfluid gap and the particle density are

$$\Delta(k) = \frac{1}{(2\pi)^3} \int dq q^2 V(k, q) \frac{\Delta(q)}{2E(q)},$$

$$n = \frac{1}{(2\pi)^3} \int dk n_k,$$

where

$$n_k = 1 - \frac{\xi(k)}{E(k)}.$$  

In Eqs. (9)–(11), the excitation energy $E(k) = \sqrt{\Delta(k)^2 + \xi(k)^2}$ is expressed in terms of the gap function and of the single-particle energy $\xi(k)$

$$\xi(k) = \epsilon_k - \mu + \frac{1}{2} V_{k=0} = -\sum_k V_{k, k} n_k$$

and contains the Hartree–Fock corrections to the single-particle self-energy (the second and third terms).

Equations (9) and (10) are to be self-consistently solved to find $\Delta(k)$ at each $k$ vector, as well as $\mu$. We find
that the use of three different grids of $k$ points is needed for a sufficiently accurate account of the integrations, due to the presence of two different length scales, $r_0$ and $k_F^{-1}$. The Bogoliubov $u_k$ and $v_k$ functions resulting from the energy minimization are finally evaluated via the expressions

$$u_k = \text{sgn}(\Delta(k)) \frac{1}{\sqrt{2}} \left( 1 + \frac{\xi(k)}{E(k)} \right),$$  \hspace{1cm} (13)$$

$$v_k = \frac{1}{\sqrt{2}} \left( 1 - \frac{\xi(k)}{E(k)} \right).$$  \hspace{1cm} (14)

At a finite temperature, the equations are modified as follows to include the Fermi function $f(k) = \left(\exp\left(\xi(k)/(k_BT)\right) + 1\right)^{-1}$:

$$\Delta(k) = \frac{1}{(2\pi)^3} \int dq \int dq' \frac{\Delta(q)}{2E(q)} (1 - 2f(q)), \hspace{1cm} (15)$$

$$n = \frac{1}{(2\pi)^3} \int dqn_k, \hspace{1cm} (16)$$

$$n_k = 2v_k^2 (1 - f(k)) + 2u_k^2 f(k).$$

The single-particle excitation energy $\xi(k)$ is correspondingly modified by substituting the new $n_k$ from Eq. (16).

**SELF-CONSISTENT RESULTS**

We begin by analyzing the results obtained at the temperature $T = 0$ in the case of a narrow well with $nr_0^3 = 2 \times 10^{-3}$. The gap function $\Delta(k)$ is displayed in Fig. 2 for different values of $g\sqrt{n}/E_F$. The damped oscillatory behavior on the scale of $1/r_0$ is a manifestation of the pairing potential. While the wavelength and damping coefficient of the oscillations are almost independent of the resonance width, the value of $\Delta_0 \equiv \Delta(k = 0)$ is extremely sensitive to it.

This is summarized in Fig. 3, where a BCS-like solution is seen to emerge while the resonance shrinks on the scale of $E_F$. This is signaled by the increasing values of $\Delta_0$ (represented by the squares) and by the chemical potential $\mu$ (circles) becoming large and negative. We also find from the behavior of the ground-state energy (Eq. (6)) that the narrowing of the resonance has the effect of increasing the level of the interactions.

These are nontrivial results, since they are obtained on the BEC side of the resonance. They also suggest that a high-quality resonance leads to a nonuniversal regime in the unitarity limit.

A similar conclusion emerged from the analysis of our previous results obtained for a wider well with $nr_0^3 = 0.125$ [35]. A quantitative comparison between the two cases then shows that narrower wells correspond to larger values of $\Delta_0$. This is seen in Fig. 4, where the temperature behavior of $\Delta_0$ for the well with $nr_0^3 = 0.125$, as evaluated from Eqs. (15) and (16), is

\[ \Delta(k)/E_F, \mu/E_F \]

\[ \Delta_0 = \Delta(k = 0) \text{ (squares)} \text{ and } \mu \text{ (circles) as functions of } g\sqrt{n}/E_F, \text{ with } a = +5000a_0 \text{ and } nr_0^3 = 2 \times 10^{-3}. \]
shown for different values of $g\sqrt{n}/E_F$. The curve at $g\sqrt{n}/E_F = 0.9$ yields $\Delta_0/E_F = 2$, whereas the corresponding value for the narrower well is $\Delta_0/E_F = 9$ (Fig. 3).

Figure 4 once again evidences how narrow resonances favor the emergence of the superfluid state, with regard to both the gap strength and the value of the transition temperature. The smooth temperature behavior of $\Delta_0$ near the transition is a manifestation of the short-ranged, bosonic character of the resulting state.

An analysis of the momentum distribution $n(k)$ further clarifies the overall physical picture. As is seen in the top of Fig. 5, larger values of $g\sqrt{n}/E_F$ lead to a more pronounced normal Fermi-gas character, with larger values of the jump at $k_F$. The momentum distribution typical of a BCS superfluid develops with decreasing values of $g\sqrt{n}/E_F$. It is useful to remark that the $n(k)$ in the top of Fig. 5 with $nr_0^3 = 2 \times 10^{-3}$ varies over a larger range of $k$ vectors than that previously obtained for the case with $nr_0^3 = 0.125$ and displayed in the bottom of Fig. 5 at different temperatures. This demonstrates that the BCS-like solution for narrower wells is accompanied by a more pronounced bosonic character.

A crucial effect of the resonance width is to change the nodal surfaces of the many-body wavefunction. This is evident in Fig. 6, where the BCS pair functions $\Psi(r) = \int d\mathbf{r} \left(\psi_k/\mu_k\right)\exp(i\mathbf{k} \cdot \mathbf{r})$ in the unitarity limit are reported for different values of $g\sqrt{n}/E_F$ and compared with the solution of the two-body scattering problem (dashed line). For broad resonances, the node of the wavefunction is shifted towards larger values of $r$ with respect to the value $r = a$ of the two-body wavefunction. However, the position of the nodes is seen to shift to smaller values of $r$ as the resonance shrinks, until the nodes disappear. These remarks are to be taken into account when resorting to quantum Monte Carlo simu-
Further information that can be extracted from Fig. 6 concerns the average size of the Cooper pair that is related to the spatial extension of the pair wavefunction. Consistently with the above results, the size of the Cooper pair is seen to become smaller while the resonance shrinks. This corresponds to the emergence of an increasingly higher peak in the pair distribution function at $T = 0$ [35], which washes away as the temperature approaches $T_F$ (see Fig. 7).

CONCLUSIONS

We have considered an atomic Fermi gas in the unitarity limit near a Feshbach resonance. To have a flavor of the underlying physics, we have used a mean-field BCS-like approach with a model potential that is able to reproduce the main characteristics of Feshbach resonances. We have found that the thermodynamic properties of the superfluid with a large and positive scattering length on the BEC side of the resonance are sensitively affected by the energy dependence of the phase shift. This supports the conclusion that universality under unitarity conditions holds only for sufficiently broad resonances on the scale of the Fermi energy. Furthermore, narrow resonances favor the occurrence of strong-coupling superfluidity.

A refined account of the interactions is needed, especially around resonance, and, to this aim, we are resorting to quantum Monte Carlo simulations. As the mean-field results have shown, the resonance width is seen to significantly affect the nodal structure of the wavefunction. This remark is accounted for in our combined technique of variational and reptation quantum Monte Carlo. We anticipate that the preliminary data are consistent with the above discussions and will be the subject of a future publication.

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