Heavy-Light Fermion Mixtures at Unitarity

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We investigate fermion pairing in the unitary regime for a mass ratio corresponding to a 6Li-40K mixture using Quantum Monte Carlo methods. The ground-state energy and the average light and heavy particle excitation spectrum for the unpolarized superfluid state are nearly independent of the mass ratio. In the majority light system, the polarized superfluid is close to the energy of a phase separated mixture of nearly fully polarized normal and unpolarized superfluid. For a majority of heavy particles, we find an energy minimum for a normal state with a ratio of ~3:1 heavy to light particles. A slight increase in attraction to $k_Fa \approx 2.5$ yields a ground state energy of nearly zero for this ratio. A cold unpolarized system in a harmonic trap at unitarity should phase separate into three regions, with a shell of unpolarized superfluid in the middle.

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Superfluid pairing and the equation of state of cold trapped atoms in the unitary regime have recently been the subject of intense theoretical and experimental investigation [1, 2]. These systems are closely related to strongly interacting fermions in other regimes, such as neutron matter [3, 4] and dense quark matter [5], and hence are useful as prototypes and benchmarks in many areas of physics. At unitarity, all physical quantities are simply given by dimensionless numbers times the relevant free Fermi gas quantity. Theoretical predictions based upon Quantum Monte Carlo (QMC) calculations for these dimensionless numbers – including the ground-state superfluid energy $\xi = E_{sf}/E_{FG} \approx 0.4$ [1, 3, 8], the pairing gap $\eta = \Delta/E_F \approx 0.5$ [1, 3, 8], and the first-order phase transition between an unpolarized superfluid and a normal state at finite polarization or concentration $x_c = n_1/n_1 \approx 0.44$ [10, 11, 12] – are in good agreement with recent experiments [13, 14, 15].

An intriguing variation of this problem is pairing between particles with different masses, which is within experimental reach [16, 17] and has sparked considerable theoretical interest [18, 19, 20, 21, 22, 23, 24]. The most promising candidate is a mixture of 6Li and 40K s-wave Feshbach resonances, for which the mass ratio $r \approx 6.5$. A heavy-light fermion mixture may be more likely to exhibit exotic phases, like Larkin-Ovchinnikov-Fulde-Ferrell phases [22], while for higher mass ratios or more attractive interactions Efimov states are expected to appear.

We consider an interaction of the form:

$$H = \sum_{i=1, N_l} -\frac{\hbar^2}{2m_l} \nabla_i^2 + \sum_{j=1, N_h} -\frac{\hbar^2}{2m_h} \nabla_j^2 + \sum_{i,j} V(r_{ij}),$$

(1)

where $\hbar$ denotes a heavy particle and $l$ denotes a light particle, with a mass ratio $r = m_h/m_l$, and a zero-range interaction between light and heavy particles with strength tuned to infinite scattering length in the unequal-mass pair. Mean-field BCS theory for unequal-mass pairing predicts a simple scaling of the equation of state in terms of the reduced mass $m_r = m_l m_h/(m_l + m_h)$. If we define the average chemical potential by $\bar{\mu} = (\mu_l + \mu_h)/2$ then $\bar{\mu}$ and the pairing gap $\Delta$ remain unchanged in units of the reduced Fermi energy $E_{F(r)}^2 = \frac{\hbar^2}{4m_r}(3\pi^2 n)^{2/3} = \frac{\hbar^2 k_F^2}{4m_r}$, where $n$ is the total particle density.

The heavy and light excitation energies naturally depend upon the masses $m_h$ and $m_l$ individually. The energies of the heavy and light excitations are:

$$E_{h(l)}(k) = \frac{\xi_{h(l)}(k) - \mu_{h(l)}(k)}{2} + \left(\frac{\xi_{h(l)}(k) + \xi_{h(l)}(k)}{2}\right)^2 + \Delta^2(k),$$

(2)

where $\xi_{h(l)}(k) = \frac{\hbar^2 k^2}{2m_{h(l)}} - \mu_{h(l)}$. Even so, the average of $E_{h}(k)$ and $E_{l}(k)$ depends only upon the reduced mass $m_r$, as does the gap $\Delta(k)$.

There is no a priori reason to believe that the BCS results should be accurate. We have performed QMC calculations of the homogeneous superfluid phase, examining the quasi-particle dispersion as a function of the momentum. The methods are those employed previously in the equal-mass case [3, 8], using a modified Pöschl-Teller potential with an effective range of $r_0/12$, where $4/3\pi r_0^3 = 1/n$. The superfluid and normal phase trial wave functions are of the same form as used previously, and provide fixed-node upper bounds to the energy; the superfluid wave function has been variationally re-optimized. Of course, new physics corresponding to quite different nodal structures of more exotic trial functions (for example LOFF phases) is not excluded.

For a mass ratio of 6.5, we obtain a ground-state energy...
The energy of the light (heavy) particle is calculated by subtracting the local energy and the mass of the particles. For a pure BCS state, the quasi-particle excitation energies in each branch is significantly lower than the minimum energy at equal masses. We find this average (calculated by subtracting $\bar{\mu}$) to be $\eta(r = 6.5) = 0.38(4)$, in comparison to the calculated value $\eta(r = 1) = 0.50(5)$ in the equal-mass case. The individual spectra are also important. For example, radio frequency response experiments, which have been used to explore the gap in the equal-mass case [14], could be designed to be sensitive to the individual light and heavy particle dispersion relations.

Away from equal populations, we explore the phase diagram at zero temperature by considering normal and gapless superfluid states using from 60 to 90 particles. For calculations of the normal state, the trial wave functions dictating the nodes are taken from free-particle Slater determinants with filled-shell configurations in periodic boundary conditions. In Fig. 2 we plot the ground-state energy versus the polarization $P = (N_h - N_l)/(N_h + N_l)$, in units of $E_{F,G}^{m}$.

The circles are QMC calculations of the normal state and the curve is a simple polynomial fit to the normal state results as a function of polarization. The polynomial fit is explicitly tied to the free-particle results at $P = \pm 1$, and to the binding energy $B_{h(l)}$ of a single heavy (light) particle in a sea of light (heavy) particles. With the majority particle number $N_{l(h)}$ and the simulation volume $L^3$ constant, we find $B_h = 0.36 E_F^l = 0.99(5) E_F^{m}$ and $B_l = 2.3 E_F^l = 0.97(5) E_F^{m}$ at $r = 6.5$. With this definition the equal mass binding $B = 0.6 E_F$. At constant total densities, these results correspond to $B_h = 0.76 E_F$, and $B_l = 2.7 E_F$, in rough agreement with results in Ref. 22. By fitting the dispersion of single impurities, we find $m^*_l/m_l = 1.3$ and $m^*_h/m_h = 1.0$.

We find an energy minimum near a polarization of 0.5, corresponding to a ratio of 3:1 heavy to light particles. The small value of the energy indicates a possible collapse of the normal state at a mass ratio smaller than that found in 3-body calculations, where Efimov states and a collapse begin at a mass ratio of 13.6 [19, 24]. At unitarity with this finite range potential we observe collapse (large negative energies and several particles within the interaction range) before $r = 12$. At a mass ratio $r = 6.5$, we find that the energy decreases quickly with interaction strength, reaching zero at $k_F a \approx 2.5$. These few-particle correlations may increase loss rates and limit the effectiveness of standard cooling techniques which sweep from the Bose-Einstein condensation regime to the unitary regime. As the mass ratio increases, the minimum in energy will shift toward higher polarizations. It would be very interesting to examine this evolution and the associ-
lated Fermi or Bose condensates of odd and even clusters of fermions.

We also consider the possibility of polarized superfluids; a simple case is the gapless superfluid where unpaired particles are placed at the minimum of the dispersion curves in Fig. 1. The energies for the gapless superfluid are shown as squares in Fig. 2. Over a range of polarizations $P < 0$, we find the polarized superfluid has a significantly lower energy than the homogeneous normal state at the same density and polarization.

The results displayed in Fig. 2 can be used to determine the stability of these phases. We use a polynomial fit to the normal state to calculate the critical concentrations of heavy and light particles and possible first-order phase transitions that occur between the superfluid and the normal states at finite polarization. This is illustrated in Fig. 3, where we plot the energy normalized to the free-particle energy of the majority species at the relevant density to the 3/5 power as a function of the concentration $x'_c = n_h/n_l$ for the majority light particle case and $x = n_l/n_h$ for the majority heavy particle case. The transition points can be found by equating the pressures and chemical potentials of the normal and superfluid states. For the case of majority light species, the equilibrium concentration of heavy particles is extremely small, $x'_c = 0.02(2)$, indicating equilibrium between a superfluid and a nearly fully polarized sea of light particles. For the majority heavy case the critical concentration is $x_c = 0.49(5)$, near the concentration found for the equal mass case: $x_c = 0.44$ [10]. The transitions indicated in the figure are calculated from the polynomial fits and indicated by dashed lines following the tangent construction used in Ref. [11].

The polarized superfluid results are also shown in Fig. 3. Over a range of polarizations $P < 0$ these states are very close to stability with respect to the phase separated normal state and unpolarized superfluid. It is possible that further generalizations of the trial states, for example by considering inhomogeneous polarized superfluids like LOFF states, would lower the energy and provide a stable polarized superfluid at zero temperature.

The pressures and chemical potentials calculated for the superfluid and normal states can also be used to examine what happens in a harmonic trap. Keeping the chemical potentials $\mu^0_h(l)$ fixed and choosing the state of highest pressure with local chemical potentials $\mu_h(l)(r) = \mu^0_h(l) - V_h(l)(r)$ one can calculate, within the local-density approximation, the density for each species in the trap. In general, the trapping potentials of the two species are unequal; for this analysis we assume harmonic potentials with a strength $m_h \omega^2_h/2$ for the heavy particles equal to twice that of the light potential strength $m_l \omega^2_l/2$, similar to that of a recent experiment on $^6$Li - $^{40}$K mixtures [17].

In Fig. 4 we plot the local polarization as a function of scaled radius for various total polarizations $P_{tot} = (N_h - N_l)/(N_h + N_l)$ where $N_h$ and $N_l$ are the total number of heavy and light particles in the trap. Curves are shown for $P_{tot} = -0.4, 0, 0.4$, and 0.8. The radii are scaled in each case so that within the local density approximation the density falls to zero at $r_{sc} = 1$. In this plot we assume that the polarized superfluid is unstable at $T = 0$. For large total negative polarizations, the equilibrium configuration is an unpolarized ($P = 0$)
superfluid in the center and a nearly fully polarized sea of light particles in the exterior. At a finite temperature the polarized superfluid state at $P < 0$ would appear, similar to what happens in the equal mass case. Because of the small energy differences, we expect finite temperature effects to be even more important here.

Near zero total polarization, in contrast, three distinct regions exist. In the center a normal state is favored with a polarization near $P = 0.5$: this is the lowest-energy normal state of the system described earlier. At larger radius, there is a shell of unpolarized superfluid, and then again in the exterior a region of nearly all light particles, or potentially a polarized superfluid. At this large mass ratio, this unusual configuration is actually lower in energy than a homogeneous superfluid everywhere. Finally, for very large total polarizations the system is normal everywhere, with the polarization smoothly increasing from the center of the trap as the radius increases. This is again analogous to what happens in the equal-mass case for a large total polarization. It would be interesting to confirm this new structure experimentally, to explore the stability and structure of the polarized superfluid, and to determine its evolution with mass ratio.

In summary, we performed QMC studies of heavy-light fermion mixtures at unitarity. We find that the ground-state energy of the superfluid and the average quasi-particle dispersion agrees closely with the superfluid with equal masses and the same reduced mass $m$, as predicted by BCS theory. In contrast, the system at finite polarization is very different from the equal-mass case, resulting in significantly different profiles of trapped systems, even for the case of equal numbers of heavy and light particles. Polarized superfluids are very near to stability for more light than heavy particles. In the majority heavy case, we find an energy minimum at approximately a 3:1 heavy to light ratio which evolves rapidly with mass ratio and interaction strength. The extra scale made available by the mass ratio produces a variety of fascinating new physical effects in cold Fermi atoms near unitarity.

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Note added in proof—An analysis of the phase diagram of Fermi mixtures at unitarity was recently published [28]. It would be interesting to see this calculation repeated for the equation of state that we have obtained.

[1] S. Giorgini, L. P. Pitaevskii, and S. Stringari, Rev. Mod. Phys. 80, 1215 (2008).
[2] W. Ketterle and M. W. Zwierlein, in Ultracold Fermi Gases, Proceedings of the International School of Physics “Enrico Fermi,” Course CLXIV, edited by M. Inguscio, W. Ketterle, and C. Salomon (IOS Press, Amsterdam, 2008). [arXiv:0801.2500]
[3] A. Gezerlis and J. Carlson, Phys. Rev. C, 77 032801 (2008).
[4] S. Gandolfi et al., Phys. Rev. Lett. 101, 132501 (2008)
[5] M. G. Alford et al., Rev. Mod. Phys. 80, 1455 (2008).
[6] J. Carlson et al., Phys. Rev. Lett. 91, 050401 (2003).
[7] G. E. Astrakharchik et al., Phys. Rev. Lett. 93, 200404 (2004).
[8] J. Carlson and S. Reddy, Phys. Rev. Lett. 95, 060401 (2005).
[9] J. Carlson and S. Reddy, Phys. Rev. Lett. 100, 150403 (2008).
[10] C. Lobo et al., Phys. Rev. Lett. 97, 200403 (2006).
[11] A. Bulgac and M. M. Forbes, Phys. Rev. A 75, 031605 (2007).
[12] S. Pilati and S. Giorgini, Phys. Rev. Lett. 100, 030401 (2008).
[13] L. Luo and J. E. Thomas, J. Low Temp. Phys. 154, 1 (2009).
[14] A. Schirotzek et al., Phys. Rev. Lett. 101, 140403 (2008).
[15] Y. Shin et al., Nature 451, 689 (2008).
[16] M. Taglieber et al., Phys. Rev. Lett. 100, 010401 (2008).
[17] E. Wille et al., Phys. Rev. Lett. 100, 053201 (2008).
[18] W. V. Liu and F. Wilczek, Phys. Rev. Lett. 90 047002 (2003).
[19] E. Braaten and H.-W. Hammer, Phys. Rept. 428, 259 (2006).
[20] S.T. Wu, C.-H. Pao, and S.-K. Yip, Phys. Rev. B 74, 224504 (2006).
[21] J. von Stecher, C. H. Greene, and D. Blume, Phys. Rev. A 76, 053613 (2007).
[22] R. Combescot et al., Phys. Rev. Lett. 98, 180402 (2007).
[23] M. A. Baranov, C. Lobo, and G. V. Shlyapnikov, Phys. Rev. A 78, 033620 (2008).
[24] Y. Nishida, D. T. Son, and S. Tan, Phys. Rev. Lett. 100, 090405 (2008).
[25] Y. Nishida, Phys. Rev. A 79, 013629 (2009).
[26] H. Guo et al., Phys. Rev. A 80, 011601(R) (2009).
[27] A. Bulgac and M. M. Forbes, Phys. Rev. Lett. 101, 215301 (2008).
[28] I. Bausmerth, A. Recati, and S. Stringari, Phys. Rev. A 79, 043622 (2009).