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Zero-temperature thermodynamics of asymmetric Fermi gases at unitarity

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The equation of state of a dilute two-component asymmetric Fermi gas at unitarity is subject to strong constraints, which affect the spatial density profiles in atomic traps. These constraints require the existence of at least one nontrivial partially polarized (asymmetric) phase. We determine the relation between the structure of the spatial density profiles and the $T=0$ equation of state, based on the most accurate theoretical predictions available. We also show how the equation of state can be determined from experimental observations.

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We consider the $T=0$ thermodynamics of a dilute asymmetric Fermi gas comprising two species of equal mass with s-wave interactions at unitarity. This has been recently realized in ^{6}Li experiments [1–4]. We shall discuss the phase structure in the microcanonical and grand-canonical ensembles, and its manifestation in cold atomic traps using the local density approximation (LDA). The theoretical treatment of the grand-canonical ensemble is much simpler than the microcanonical ensemble as it consists of only pure phases. We discuss here the most general model-independent equation of state satisfying known constraints. For model-dependent analyses see [5–7].

Phase structure. We show the main defining features of a grand-canonical phase diagram in Fig. 1. The two species are labeled "a" and "b." The symmetry $a \leftrightarrow b$ allows us to consider only the region below the $\mu_a=\mu_b$ line where the locally averaged number densities and chemical potentials satisfy $n_b \leqslant n_a$ and $\mu_b \leqslant \mu_a$, respectively. The asymmetry of the system may thus be characterized by the dimensionless ratios:

$$x = n_b/n_a \leqslant 1, \quad y = \mu_b/\mu_a \leqslant 1. \tag{1}$$

Note that only x measures a physical asymmetry. There are four distinct regions: Vac—the vacuum, N_a—the fully polarized phases ($x=0$) comprising only species "a," PP$_a$—partially polarized phase(s) ($0<x<1$), and SF—the fully paired symmetric superfluid phase ($x=1$).

We shall discuss only two phase transitions: one between the fully polarized phase N_a (where $x=0$) and a partially polarized phase PP$_a$ ($0<n_b<n_a$), and another between a (possibly different) partially polarized phase and the symmetric fully paired phase SF (where $x=1$). At unitarity, phase transitions occur along rays characterized solely by their slope y_x. The two transitions we shall discuss are thus described by the two universal parameters y_0 and y_1, which naturally satisfy $y_0 \leqslant y_1$. A major point of this paper is to place an upper bound Y_0 on y_0 ($y_0 \leqslant Y_0$), a lower bound Y_1 on y_1 ($Y_1 \leqslant y_1$), and to show $Y_0 < Y_1$, which implies that the inequality $y_0 < y_1$ is strict. This directly implies the existence and stability of one or more partially polarized phase(s) PP$_a$. Possible phases in the region PP$_a$ include LOFF states [10], states with deformed Fermi surfaces [11], and p-wave superfluid states [12]. If several of these states exist and are stable, the corresponding phase transitions will be characterized by additional universal parameters y_x.

Functional forms of thermodynamic potentials. At unitarity, the energy density $\mathcal{E}(n_a,n_b)$ and the pressure $\mathcal{P}(\mu_a,\mu_b)$ have the form

$$\mathcal{E}(n_a,n_b) = \tfrac{3}{5}\alpha[n_a g(x)]^{5/3}, \quad \alpha = \frac{(6\pi^2)^{2/3}\hbar^2}{2m}, \tag{2a}$$

$$\mathcal{P}(\mu_a,\mu_b) = \tfrac{2}{5}\beta[\mu_a h(y)]^{5/2}, \quad \beta = \frac{1}{6\pi^2}\left[\frac{2m}{\hbar^2}\right]^{3/2}. \tag{2b}$$

Note that $g(x)=f^{3/5}(x)$, where $f(x)$ was introduced in [8]: The use of $g(x)$ rather than $f(x)$ significantly simplifies the formalism [9]. The $T=0$ thermodynamic properties of the system are completely determined by the functional form of $g(x)$ or $h(y)$. The number densities and chemical potentials are simply $n_{a,b}=\partial\mathcal{P}/\partial\mu_{a,b}$ and $\mu_{a,b}=\partial\mathcal{E}/\partial n_{a,b}$, respectively. As we show here, the functions $h(y)$ and $g(x)$ are tightly constrained by current Monte Carlo simulations, analytic calculations, and experimental results. The energy density and pressure are related via the Legendre transform [9]:

$$\mathcal{P}(\mu_a,\mu_b) = \mu_a n_a + \mu_b n_b - \mathcal{E}(n_a,n_b) = \tfrac{2}{3}\mathcal{E}(n_a,n_b). \tag{3}$$

Physical constraints. The thermodynamics of three phases are known. The vacuum has vanishing pressure $\mathcal{P}_{\text{Vac}}=0$, the fully polarized phase N_a is a free Fermi gas (FG),

$$\mathcal{P}_{\text{FG}}(\mu_a) = \tfrac{2}{5}\beta\mu_a^{5/2}, \tag{4}$$

and the pressure of the fully paired phase SF is symmetric in μ_a and μ_b, and is described by a single parameter ξ,

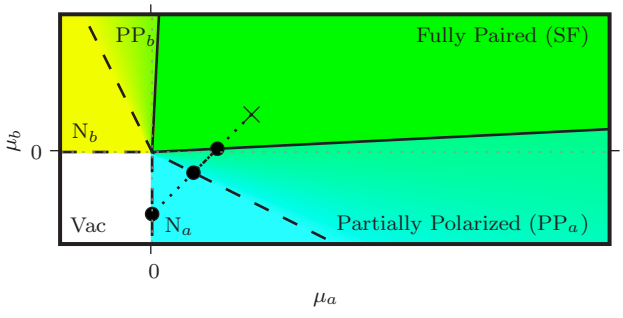

FIG. 1. (Color online) Grand-canonical phase diagram of a two-component Fermi gas at unitarity and $T=0$. Various phases are separated by phase transitions along the straight lines extending from the origin with constant slopes y_x. The dotted line follows the sequence of phases in a sample trap.

$$\mathcal{P}_{\mathrm{SF}}(\mu_+) = \frac{4}{5}\frac{\beta}{\xi^{3/2}}\mu_+^{5/2}, \quad \text{where } \mu_\pm = \frac{\mu_a \pm \mu_b}{2}. \tag{5}$$

These provide the limiting forms for $h(y)$ and limiting values of $g(x)$, [see Eqs. (6a) and (7a) below].

The phase transition at $y=y_0$ defines the border of the region where $\mu_b=y_0\mu_a$ is tuned to keep species "b" out of the system. Since the interspecies interaction is attractive, the critical μ_b must be negative $y_0<0$. We will provide an upper bound Y_0 ($y_0\leqslant Y_0$).

Note that $\mathcal{P}_{\mathrm{SF}}(\mu_+)$ depends only on the average chemical potential μ_+. This insensitivity to the chemical potential difference μ_- is due to the existence of an energy gap Δ in the spectrum. The phase transition at $y=y_1$ marks the line where μ_- becomes large enough to break the superfluid pairs. In the phase SF, μ_- is constrained by the size of the physical gap $\mu_-\leqslant\Delta$ [8]. This provides a lower bound $Y_1\leqslant y_1$, see below and [9].

[Recall from Eq. (1) that we are only considering regions where $0\leqslant\mu_-=|\mu_-|$].

If no stable partially polarized phase exists, then the region PP_a will vanish, being compressed into a single first-order transition line where pressure equilibrium is established $\mathcal{P}_{\mathrm{FG}}(\mu_a)=\mathcal{P}_{\mathrm{SF}}(\mu_+)$ [6,8]. This would occur at $y=y_c=(2\xi)^{3/5}-1\equiv y_0\equiv y_1$, and would imply that $Y_0\equiv Y_1$. We argue below that Y_0 is strictly less than Y_1, and therefore rule out this possibility.

Finally, thermodynamic stability requires that the pressure and energy density are convex functions, which implies that $g(x)$ and $h(y)$ are also convex [9]. The constraints on $h(y)$ are

$$h(y) = \begin{cases} 1, & \text{if } y \leqslant y_0, \\ (1+y)(2\xi)^{-3/5}, & \text{if } y \in [y_1, 1], \end{cases} \tag{6a}$$

$$h''(y) \geqslant 0, \tag{6b}$$

$$y_0 \leqslant Y_0 < y_c < Y_1 \leqslant y_1 \leqslant 1. \tag{6c}$$

The corresponding constraints on $g(x)$ are

$$g(0) = 1, \quad g(1) = (2\xi)^{3/5}, \tag{7a}$$

$$g''(x) \geqslant 0, \tag{7b}$$

$$g'(0) \leqslant Y_0, \quad g'(1) \in [g(1)(1+Y_1^{-1})^{-1}, g(1)/2]. \tag{7c}$$

Equations (6a) follow directly from Eqs. (2b), (4), and (5), Eq. (7a) from Eq. (2a), and the interval in Eq. (7c) from the properties of the Legendre transform and Eq. (6c) [9].

Parameters. For Fig. 2 we used

$$\xi = 0.42(1), \quad Y_0 \approx -0.5, \quad Y_1 = -0.09(3), \quad y_1 = 0.05.$$

We obtain estimates for Y_1 and ξ from Monte Carlo data [13–15]. The latest Monte Carlo estimates for the symmetric systems give $\xi=0.42(1)$ [14,15] and $\Delta/\epsilon_{\mathrm{F}}=0.504(24)$ [15], where ϵ_{F} is the Fermi energy of the free gas with the same density. This gives $y_c\approx-0.099(15)$, and the constraint $\mu_-\leqslant\Delta$ gives $Y_1=(\xi-\Delta/\epsilon_{\mathrm{F}})/(\xi+\Delta/\epsilon_{\mathrm{F}})=-0.09(3)$ [8,9]. Since within the statistical errors $Y_1\approx y_c$, the possibility of an empty PP_a region at unitarity cannot yet be ruled out by this value of Y_1, as was noted earlier by Cohen [8].

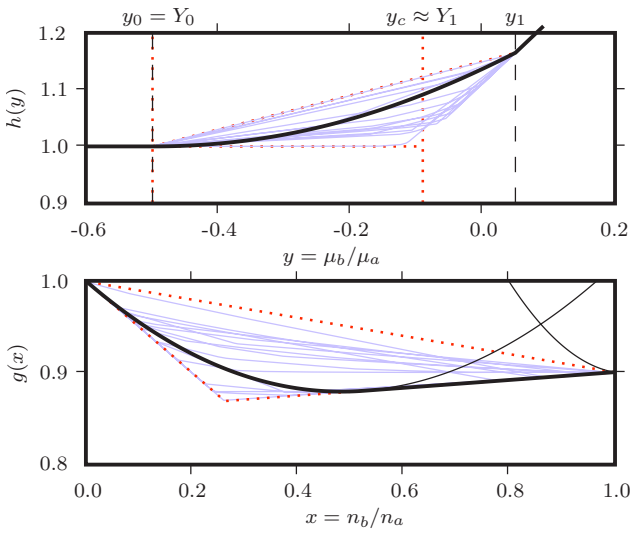

FIG. 2. (Color online) Example of a function $h(y)$ and the corresponding function $g(x)$ shown as thick lines. Maxwell's construction for phase coexistence leads to a linear $g(x)$ for $x\in(0.5,1.0)$, interpolating between the two pure phases shown with lighter lines. This corresponds to the kink and/or first-order phase transition at $y=y_1$ in $h(y)$. Various other sample functions are lightly sketched within the allowed (dotted) triangular region.

We now estimate Y_0. Let e_0 be the energy required to add one particle b to a fully polarized gas of density n_a. Consider adding a large, but infinitesimal amount of b, $1\ll N_b\ll N_a$. In the thermodynamic limit, the required energy per particle will be the critical chemical potential $\mu_b=\alpha n_a^{2/3}g'(0)$ defining the transition y_0. If the added particles repel, the energy will be $N_b e_0$, and $\mu_b=e_0$. If they bind, the additional binding energy must be included, giving $\mu_b<e_0$. In this way, e_0 provides a bound for μ_b and $g'(0)=y_0\leqslant Y_0=e_0/(\alpha n_a^{2/3})$.

Consider adding a single b fermion, with coordinate $\mathbf{r}_0$, to a system of N_a a fermions with coordinates $\mathbf{r}_n$. Let $r_{nm}=|\mathbf{r}_n-\mathbf{r}_m|$. The wave function for the b fermion in the background of fixed a sources is

$$\phi(\mathbf{r}_0;\{\mathbf{r}_n\}) = \sum_n A_n \frac{\exp(-\kappa r_{0n})}{r_{0n}}, \tag{8}$$

and it satisfies the zero-range interaction boundary conditions if the following N_a conditions are met:

$$\left(-\kappa+\frac{1}{a}\right)A_n + \sum_{m\neq n} A_m \frac{\exp(-\kappa r_{nm})}{r_{nm}} = 0. \tag{9}$$

For uniform distributions where the lowest state has constant $A_m=A$, approximating the sum as an integral gives $\kappa-a^{-1}=4\pi n_a/\kappa^2$. This continuum approximation is not very accurate in the unitary limit, since κ is comparable to the inverse interparticle spacing and $\kappa^3/n_a\approx 4\pi$. To estimate corrections, the equations can be solved for various lattice configurations. We find that κ deviates from the continuum result by a factor of 0.84(3) for simple lattice configurations and perturbations (see [9] for details). We now estimate the

energy of the system using the wave function

$$\Psi(\mathbf{r}_0;\{\mathbf{r}_n\}) = \Phi_{\mathrm{SD}}(\{\mathbf{r}_n\})\phi(\mathbf{r}_0;\{\mathbf{r}_n\}), \tag{10}$$

where Φ_{SD} is a Slater determinant for a free Fermi gas and obtain $e_0 \approx -\hbar^2\kappa^2/m$ [9]:

$$e_0 \approx \begin{cases} 4\pi\hbar^2 n_a a/m, & \text{if } a \to 0^-, \\ -0.71(5)\hbar^2(4\pi n_a)^{2/3}/m, & \text{if } a \to \pm\infty, \\ -\hbar^2/(ma^2), & \text{if } a \to 0^+. \end{cases} \tag{11}$$

Note that this result interpolates between the correct leading order BEC and BCS results. This estimate assumes that the fluctuations of the number density $n_a(\mathbf{r})$ on a scale of the order $1/\kappa$ affect κ very little. The result is consistent with this assumption, as discussed in [9]. The constraint at unitarity is thus

$$Y_0 \approx -0.54(4) < y_c = -0.099(15). \tag{12}$$

If Y_0 is strictly less than y_c, then convexity in $g(x)$ and $h(y)$ implies $y_c < Y_1$ (see Fig. 2).

Trap profiles. For large systems with a slowly varying confining potential, gradient terms may be neglected, and the LDA employed to determine the density distribution by introducing spatially varying effective chemical potentials,

$$\mu_{a,b}(\mathbf{R}) = \lambda_{a,b} - V(\mathbf{R}). \tag{13}$$

Lagrange multipliers $\lambda_{a,b}$ fix the total particle numbers N_a and N_b. The LDA may be inaccurate near phase boundaries where the densities change rapidly. The gradient terms will smear out these transition regions and provide an additional surface tension proportional to the local curvature [16].

In the LDA, the density profile may be constructed from the local densities $n_{a,b}$ using Eq. (13) (explicit formulae are provided in [9]). The dotted line in Fig. 1 shows the sequence of phases contained in a sample trap. Since $2\mu_- = \lambda_a - \lambda_b$ is fixed, traps contain the sequence of phases encountered along a 45° line through such a diagram. In this example, the center of the cloud $[V(\mathbf{0})=0]$ is in the SF phase at the cross. The phase transitions will occur for $y=y_1$, $y=y_0$, and $y=-\infty$ for $V(\mathbf{R}_1)=V_1$, $V(\mathbf{R}_0)=V_0$, and $V(\mathbf{R}_{\mathrm{vac}})=V_{\mathrm{vac}}$, respectively, with $R_0 < R_1 < R_{\mathrm{vac}}$. As noted above, additional phase transitions may exist between R_0 and R_1.

Experiments. Accurate measurements of the density profiles would allow for a complete extraction of $h(y)$ and $g(x)$. For example, using $x = n_b(\mathbf{R})/n_a(\mathbf{R})$ and the expressions for $\mu_{a,b}$, we have $g^{2/3}(x)g'(x) = [\lambda_b - V(\mathbf{R})]/[\alpha n_a^{2/3}(\mathbf{R})]$ from which $g(x)$ may be extracted using the boundary condition $g(0)=1$ [9].

For harmonic traps, the locations of the main phase transitions, $R_{\mathrm{vac}} \propto \sqrt{V_{\mathrm{vac}}}$, $R_0 \propto \sqrt{V_0}$, and $R_1 \propto \sqrt{V_1}$, are completely determined by the Lagrange multipliers $\lambda_{a,b}$, and the universal numbers y_0 and y_1. Within the LDA, we obtain the following model independent relationship, to be compared with the recent MIT data [3] (see Fig. 3):

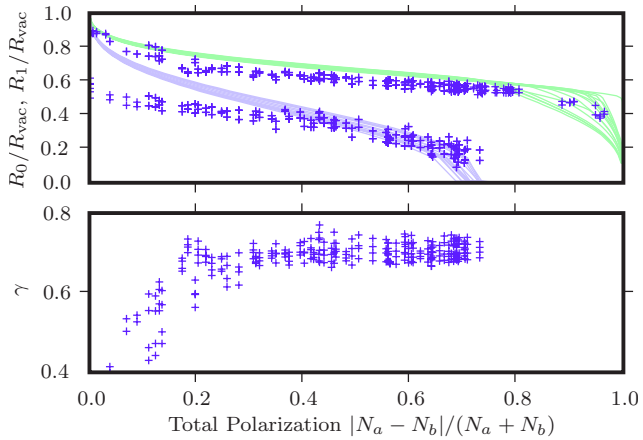

FIG. 3. (Color online) Measured transition radii from Ref. [3]. The upper plot shows the normalized data (crosses) on top of data generated from several randomly generated functions $h(y)$. The lower plot shows the parameter γ defined in Eq. (14).

$$\gamma = \frac{1-y_1}{1-y_0} = \frac{R_{\mathrm{vac}}^2 - R_0^2}{R_{\mathrm{vac}}^2 - R_1^2} \approx 0.70(5). \tag{14}$$

To extract more information, one must consider a specific functional form for $h(y)$ and $g(x)$. We have analyzed a large sample of allowed functions $h(y)$ and $g(x)$, a few of which are sketched in Figs. 2 and 3. We find that the total polarization $P=(N_a-N_b)/(N_a+N_b)$ is quite insensitive to the functional form. However, the critical polarization P_c—where the innermost phase transition approaches the center of the trap $R_1=0$—is quite sensitive to y_1. The MIT experiments [1,3] measure $P_c=0.70(5)$. If $y_1=0$, then one obtains $P_c > 0.80\ldots0.85$. However, if one considers $y_1 \approx 0.05$ $[g'(1)\approx 0.04]$, then values of $P_c \approx 0.7$ and smaller emerge, compatible with those measured in [1,3]. Using Eq. (14), this gives a value of $y_0 = g'(0) \approx -0.4$. Our estimate for $Y_0 \approx -0.54(4)$ is consistent with this extracted experimental value within existing uncertainties.

Within the Eagles-Leggett extension of the BCS model [17], one obtains the values $y_0=0$, $y_c=0.105$, and $y_1=0.107$ (see [7,9]), which would correspond to a parameter $\gamma=0.893$, as opposed to the $\gamma=0.70(5)$ extracted from experiment. At the same time, the spatial layer for the PP_a region would be very thin, namely $(R_0^2-R_1^2)/(R_{\mathrm{vac}}^2-R_1^2) = 1-\gamma = 0.107$, compared with our estimate $1-\gamma \approx 0.30(5)$.

Our analysis is strictly valid only at $T=0$. The deviations in Fig. 3 are most likely finite temperature effects. The regions of the phase diagram most sensitive to $T \neq 0$ are those with small μ, thus, the transition radii in traps with small asymmetry will be most affected. For large polarizations, the temperature should not affect the SF phase which is gapped, but will affect phases with zero or small gap excitations. This could alter the values of y_1 slightly and y_0 significantly. We thus caution against taking the extracted numbers in this section too seriously until a similar finite temperature analysis is presented.

Since $Y_1 < 0$ (as determined from the value of the pairing gap), a positive y_1 suggests a first-order phase transition out

of the SF phase for a critical $\mu_- < \Delta$. This conclusion is also consistent with the form of the quasiparticle spectrum computed in [15], which has a minimum at a finite momentum.

In conclusion, we have shown that thermodynamic constraints, accurate Monte Carlo simulations, analytic estimates, and experimental data place tight constraints on the equation of state of the asymmetric $T=0$ unitary gas. These constraints imply that there exists a region where *one or more nontrivial partially polarized phases exist*. These phases likely exhibit very interesting microscopic physics. In particular, any ungapped polarized phase is unstable towards the formation of a state with two symbiotic superfluids at $T=0$ [12]. The tight constraints on the forms of $g(x)$ and $h(y)$ we present will help locate these phases.

Note added. Chevy [18] independently arrived at similar conclusions. The latest MIT analysis [19] agrees with our conclusion that the SF phase occupies the center of the trap and shows that the LDA is applicable. In a recent variational Monte Carlo study, the results of Lobo *et al.* [20] agree with our lower bound obtaining $Y_0 = -0.58(1) < y_c = -0.099(15)$, and Lobo *et al.* concluded that the transition at y_1 is first order. This is consistent with our results: their function $f(x)$ is very similar to our $g^{5/3}(x)$ (see [9]).

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