Zero Temperature Thermodynamics of Asymmetric Fermi Gases at Unitarity

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(Dated: 27 March 2007)

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 non-trivial 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.

PACS numbers: 03.75.Ss

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].

a. Phase structure: We show the main defining features of a grand-canonical phase diagram in Fig. 1. The two species are labelled “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 $n_b \leq n_a$ and $\mu_b \leq \mu_a$ respectively. The asymmetry of the system may thus be characterized by the dimensionless ratios:

\[ x = n_b/n_a \leq 1, \quad y = \mu_b/\mu_a \leq 1. \]

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 $y_0 \leq y_1$. A major point of this paper is to place an upper bound $Y_0$ on $y_0$ ($y_0 \leq Y_0$), a lower bound $Y_1$ on $y_1$ ($Y_1 \leq y_1$), 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 exists and are stable, the corresponding phase transitions will be characterized by additional universal parameters $y_x$.

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

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

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

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 $n_{a,b} = \partial P/\partial \mu_{a,b}$ and $\mu_{a,b} = \partial E/\partial n_{a,b}$ 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]:

\[ P(\mu_a, \mu_b) = \mu_a n_a + \mu_b n_b - E(n_a, n_b) = \frac{2}{5} E(n_a, n_b). \quad (3) \]
c. Physical constraints: The thermodynamics of three phases are known. The vacuum has vanishing pressure $P_{\text{Vac}} = 0$, the fully polarized phase $N_a$ is a free Fermi gas,

$$P_{\text{FG}}(\mu_a) = \frac{2}{5} \beta \mu_a^{5/2},$$

and the pressure of the fully paired phase SF is symmetric in $\mu_a$ and $\mu_b$, and is described by a single parameter $\xi$,

$$P_{\text{SF}}(\mu_+) = \frac{4}{5} \beta \xi^{5/2} \mu_+^{5/2} \quad \text{where} \quad \mu_+ = \frac{\mu_a + \mu_b}{2}. \quad (5)$$

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 $\mu_b$ must be negative $y_0 < 0$. We will provide an upper bound $Y_0$ ($y_0 \lesssim Y_0$).

Note that $P_{\text{SF}}(\mu_+)$ depends only on the average chemical potential $\mu_+$. This insensitivity to the chemical potential difference $\mu_-$ is due to the existence of an energy gap $\Delta$ in the spectrum. The phase transition at $y = y_1$ marks the line where $\mu_-$ becomes large enough to break the superfluid pairs. In the phase SF, $\mu_-$ is constrained by the size of the physical gap $\mu_- \lesssim \Delta$ [8]. This provides a lower bound $Y_1 \leq y_1$, see below and [9]. (Recall from Eq. (1) that we are only considering regions where $0 \leq \mu_- = |\mu_-|$).

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 $P_{\text{FG}}(\mu_a) = P_{\text{SF}}(\mu_+)$ [6, 8]. This would occur at $y = y_c = (2\xi)^{3/5} - 1 \equiv y_0 = y_1$, and would imply that $Y_0 \equiv Y_1$. We argue below that $Y_1$ 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

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

$$h''(y) \geq 0, \quad \text{and} \quad y_0 \leq y_c \leq Y_1 \leq y_1. \quad (6b)$$

The corresponding constraints on $g(x)$ are

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

$$g''(x) \geq 0, \quad \text{and} \quad g'(0) \leq y_0, \quad g'(1) \in [g(1)(1 + Y_1^{-1})^{-1}, g(1)/2]. \quad (7c)$$

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

We obtain estimates for $Y_1$ and $\xi$ from Monte Carlo data [13–15]. The latest Monte Carlo estimates for the symmetric systems give $\xi = 0.42(1)$ [14, 15] and $\Delta/\varepsilon_F = 0.504(24)$ [15], where $\varepsilon_F$ is the Fermi energy of the free gas with the same density. This gives $y_c \approx -0.099(15)$, and the constraint $\mu_- \leq \Delta$ gives $Y_1 = (\xi - \Delta/\varepsilon_F)/(\xi + \Delta/\varepsilon_F) = -0.093(8, 9)$. 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].

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 $\mu_b$ and $g'(0) = y_0 \leq Y_0 = e_0/(\alpha n_a^{2/3})$.

Consider adding a single b fermion, with coordinate $r_0$, to a system of $N_a$ a fermions with coordinates $r_n$. Let $r_{nm} = |r_n - r_m|$. The wave function for the b fermion in the background of fixed a sources is

$$\phi(r_0; \{r_n\}) = \sum_n A_n \exp \left( \frac{-\kappa r_{0n}}{r_{0n}} \right). \quad (8)$$

FIG. 2: 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 (first-order phase transition) at $y = y_1$ in $h(y)$. Various other sample functions are lightly sketched within the allowed (dotted) triangular region.
and it satisfies the zero-range interaction boundary conditions if the following $N_a$ conditions are met:

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

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 $\kappa$ 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 $\kappa$ 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

$$\Psi(r_0; \{r_n\}) = \Phi_{\text{SD}}(\{r_n\})\phi(r_0; \{r_n\}), \quad (10)$$

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

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

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

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

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).

e. 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:

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

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 $2\mu_c = \lambda_0 - \lambda_1$ 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

$$(V(0) = 0)$$

is in the SF phase at the cross. The phase transitions will occur for $y = y_1$, $y = y_0$, and $y \to -\infty$ for $V(R_1) = V_1$, $V(R_0) = V_0$, and $V(R_{\text{vac}}) = V_{\text{vac}}$ respectively, with $R_0 < R_1 < R_{\text{vac}}$. As noted above, additional phase transitions may exist between $R_0$ and $R_1$.\n
f. Experiments: Accurate measurements of the density profiles would allow for a complete extraction of $h(y)$ and $g(x)$. For example, using $x = n_b(R)/n_a(R)$ and the expressions for $\mu_{a,b}$, we have

$$g^{2/3}(x) = [\lambda_0 - V(R)]/[\alpha n_a^{2/3}(R)]$$

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, $R_{\text{vac}} \propto \sqrt{V_{\text{vac}}}$, $R_0 \propto \sqrt{V_0}$, 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):

$$\gamma = \frac{1 - y_1}{1 - y_0} = \frac{R_{\text{vac}} - R_0}{R_{\text{vac}} - R_1} \approx 0.70(5). \quad (14)$$

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 $y_0 = 1$, then one obtains $P_c > 0.80...0.85$. 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 PF$_{x}$ region would be very thin, namely $(R_{x}^{2} - R_{0}^{2})/R_{vac}^{2} = 1 - \gamma = 0.107$, 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 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 both 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 novel phases.

The authors thank A. Schwenk and M. W. Zwierlein for comments, D. T. Son for many useful discussions, M. W. Zwierlein et al. for providing the data in Fig. 3, and the US Department of Energy for support under Grant No. DE-FG02-97ER41014.

*Notes 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, Lobo et al. [20] agree with our lower bound, obtaining $y_0 = -0.58(1) < y_c = -0.099(15)$, and 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 $g^{3/2}(x)$ (see [9]).

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In this appendix, we present some additional calculational details. We discuss the properties of the Legendre transformation, thermodynamic stability and convexity of thermodynamic potentials, and the Maxwell construction for mixed phases. We also provide details of the calculations whose results are presented in the main body.

1. Properties of the Legendre Transformation

Many of the thermodynamic constraints follow directly from properties of the Legendre transformation (3). We explain some of these properties here, because there has been some confusion in the literature.

The Legendre transform relates tangents in one ensemble to coordinates in the other. For example, a linear segment of \( g(x) \) over a finite interval in \( x \) will be mapped into a single point \( y \), where \( h(y) \) has a kink. Straight segments of \( g(x) \) arise from the Maxwell construction and indicate a phase coexistence (mixed phase). For this reason, the grand-canonical phase diagram is much simpler than other ensembles as it consists solely of pure phases.

First we present some relations. Starting with the definitions of the thermodynamic potential densities \( \mathcal{E}(n_a, n_b) \) and \( -\mathcal{P}(\mu_a, \mu_b) \) defined in (2), we differentiate to find the densities

\[
\begin{align*}
n_a &= \frac{\partial \mathcal{P}}{\partial \mu_a} = \beta [\mu_a h(y)]^{3/2} [h(y) - y h'(y)], \quad (A1a) \\
n_b &= \frac{\partial \mathcal{P}}{\partial \mu_b} = \beta [\mu_b h(y)]^{3/2} h'(y), \quad (A1b)
\end{align*}
\]

and the chemical potentials

\[
\begin{align*}
\mu_a &= \frac{\partial \mathcal{E}}{\partial n_a} = \alpha [n_ag(x)]^{2/3} [g(x) - x g'(x)], \quad (A2a) \\
\mu_b &= \frac{\partial \mathcal{E}}{\partial n_b} = \alpha [n_ag(x)]^{2/3} g'(x). \quad (A2b)
\end{align*}
\]

From these relations and the definitions of the asymmetry parameters \( x = n_b/n_a \) and \( y = \mu_b/\mu_a \), we obtain the following dictionary. These relations may be used to express \( g(x) \) and \( x \) in terms of \( h(y) \) and \( y \) or vice versa:

\[
\begin{align*}
y &= \frac{g'(x)}{g(x) - x g'(x)}, \quad h(y) = \frac{1}{g(x) - x g'(x)}, \quad (A3a) \\
x &= \frac{h'(y)}{h(y) - y h'(y)}, \quad g(x) = \frac{1}{h(y) - y h'(y)}. \quad (A3b)
\end{align*}
\]

The important geometric property of the Legendre transformation is that it maps tangents in one space to points in the other. Consider the grand-canonical ensemble described by the function \( \mathcal{P}(\mu_a, \mu_b) \). The tangents \((\partial_{\mu_a} \mathcal{P}, \partial_{\mu_b} \mathcal{P}) = (n_a, n_b)\) to this function at a point \((\mu_a, \mu_b)\) in the grand-canonical ensemble map directly to the coordinate \((n_a, n_b)\) in the microcanonical ensemble. Note that the Legendre transformation is symmetric: tangents in the microcanonical ensemble map back to points in the grand-canonical ensemble.

2. Thermodynamic Stability: The Second Law

The thermodynamic potentials follow from a strict minimization procedure over all possible states. If this is properly carried out, the potentials will be convex functions of their arguments. This convexity is the geometric manifestation of the second law. Locally, the requirement is that the Hessian of the potentials—the matrix of second partial derivatives—be positive semi-definite. One can easily show that this requirement also implies that both density and concentration sound modes are stable with corresponding real sound velocities. We shall evaluate now the Hessians for the thermodynamic potential densities in the case of a two species at unitarity and \( T = 0 \). We thus find that

\[
H(\mathcal{P}_b) \propto \begin{bmatrix} 3(h - y h')^2 + 2 y h'' & 3(h h' - y h'^2) - 2 y h h'' \\ 3(h h' - y h'^2) - 2 y h h'' & 3h'^2 + 2h h'' \end{bmatrix},
\]

\[
H(\mathcal{E}_g) \propto \begin{bmatrix} 4(g - x g')^2 + 6x^2 g'' & 4(g g' - x g'^2) - 6x g g'' \\ 4(g g' - x g'^2) - 6x g g'' & 4g'^2 + 6g g'' \end{bmatrix},
\]

\[
H(\mathcal{E}_f) \propto \begin{bmatrix} 10f - 12x f' + 9x^2 f'' & 6f' - 9x f'' \\ 6f' - 9x f'' & 9f'' \end{bmatrix}.
\]

The corresponding determinants are:

\[
\det[H(\mathcal{P}_b)] \propto h^3 h'' \quad (A4) \\
\det[H(\mathcal{E}_g)] \propto g^3 g'' \quad (A5) \\
\det[H(\mathcal{E}_f)] \propto 5f f'' - 2f^2. \quad (A6)
\]

From these it is easy to see that the Hessians of \( \mathcal{P} \) and \( \mathcal{E} \) are positive definite if \( h'' > 0 \) and \( h \geq 0 \), or \( g'' > 0 \) and \( g \geq 0 \). If one were to use the parametrization of the

\[1\] Strictly speaking the grand-canonical potential is \( -\mathcal{V} \mathcal{P}(\mu_a, \mu_b) \), notice the minus sign, where \( \mathcal{V} \) is the volume.
energy density \( E \) through \( f \) as suggested by Cohen [8] the situation is more complicated, as one would have to satisfy the nonlinear differential constraint

\[
5f f'' - 2 f'^2 \geq 0, \quad \text{(A7)}
\]

cf. Eq. (6) in Ref. [8].

Though not related by a strict Legendre transformation, equations (A3) show that the universal functions \( g(x) \) and \( h(y) \) are similarly related, hence Fig. 2 exhibits the same Maxwell construction properties. Note that the linear Maxwell construction only works with the functions \( f(y) \) that saturate the inequality (A7) [8]:

\[
f(x) = (A + Bx)^{5/3}. \quad \text{(A8)}
\]

For this reason, the function \( g(x) \) is substantially simpler to discuss than \( f(x) \). By further requiring saturation of inequality (A7) throughout the entire interval, Cohen [8] obtained

\[
f(x) = \{1 + [(2x)^{3/5} - 1]x\}^{5/3}, \quad \text{(A9)}
\]

which describes the case of a vanishing partially polarized region \( \mathcal{P}_a \).

Finally, we discuss the physical significance of kinks in \( E(n) \) which translate to flat regions of \( \mathcal{P}(\mu) \) in the grand-canonical ensemble. A kink in \( E(n) \) means that, for a range of tangents (chemical potentials), the energy of the ground state does not change. In other words, the system is insensitive to a range of chemical potentials. For example, the superfluid phase SF is insensitive to a range of chemical potential splitting \( \mu_- \) because of the physical gap in the spectrum. The flat regions in the grand canonical ensemble represents the same physical state (same densities) that are stable over a range of chemical potentials due to this gap.

As discussed in the main text, the system may or may not respond to chemical potential differences strictly less than the gap \( \mu_- < \Delta \), but will definitely respond when \( \mu_- > \Delta \). This gave us the bound \( Y_1 \) on the transition parameter \( y_1 \) (see (A18) below).

3. Maxwell Construction

As an example, let us consider the Maxwell construction for phase coexistence in the microcanonical ensemble with a single species “a”. The Maxwell construction for the case of two species at unitarity is somewhat more complicated, but, as we discussed above, involves the same type of linear construction if the function \( g(x) \) is used. This ensemble is constructed by minimizing the energy density \( E(n) \) over all phases \( \rho \) with fixed total particle number \( N = nV \), and volume \( V \):

\[
E(n) = \min_\rho E_\rho(N/V). \quad \text{(A10)}
\]

In the microcanonical ensemble, this procedure is slightly complicated by the possibility of phase coexistence. Consider two distinct pure phases \( \rho \in \{1, 2\} \) with given energy densities \( E_1(n) \) and \( E_2(n) \); an example of two such phases is shown in Fig. 4. Minimizing (A10) over these phases separately produces an energy density \( E(n) \) that is not convex. The Maxwell construction proceeds by constructing a series of systems with fixed \( N \) by combining a physical fraction \( z \) of the system in phase \( \rho_1 \) with density \( n_1 \) and the remaining fraction \( 1 - z \) in phase \( \rho_2 \) with density \( n_2 \) subject to the constraint of fixed average density

\[
n = \frac{N}{V} = zn_1 + (1 - z)n_2. \quad \text{(A11)}
\]

This leaves two degrees of freedom and defines a series of two-component mixed phases that must also be considered in (A10) with energy density:

\[
E(n) = zE_\rho_1(n_1) + (1 - z)E_\rho_2(n_2). \quad \text{(A12)}
\]

Minimizing \( E(n) - \mu n \), where \( \mu \) is a Lagrange multiplier, leads to the line segment shown in bold in Fig. 4, which is the convex hull of the energy densities. More specifically, by varying \( n_{1,2} \) and \( z \), (and assuming that all derivatives exists), one obtains the slope

\[
\mu_\pm = \frac{E_{\rho_1}(n_1) - E_{\rho_2}(n_2)}{n_1 - n_2} = \frac{\partial E_{\rho_1}(n_1)}{\partial n_1} = \frac{\partial E_{\rho_2}(n_2)}{\partial n_2}. \quad \text{(A13)}
\]

This is simultaneously the slope of the line segment defining the mixed phase, and the tangents to the two energy densities. In the case of the \( E_{\rho_2} \) shown in Fig. 4, the function has a cusp at the point of transition. In this case, \( \partial E_{\rho_2}(n_2) / \partial n_2 \) should be interpreted as the appropriate value in the interval defined by the corresponding derivatives computed to the left and to the right of the kink. In (A13) \( \partial E_{\rho_2}/\partial n_2 \) may assume any of these values to satisfy the equilibrium condition. This construction

FIG. 4: Maxwell construction for two competing phases in the microcanonical ensemble \( \rho \in \{1, 2\} \) with given energy densities \( E_1(n) \) and \( E_2(n) \). The right phase has a gap as signified by the kink. The left phase has no gap. A first-order phase transition connects the two phases. Minimizing (A10) produces the thin solid curve, but this is not convex. The Maxwell construction amounts to finding the convex hull—the thick solid line—which restores the convexity of \( E(n) \) required by the second law of thermodynamics.
guarantees that the potential $\mathcal{E}(n)$ will be convex as required by the second law of thermodynamics.

The conditions of minimization are equivalent to the conditions that the chemical potential and pressure of the two coexisting phases be equal. Note that phase coexistence occurs only along the linear segment. Along this entire segment, the tangent is the same. Thus, the entire region of phase coexistence is described by a single point $\mu_c$ representing the phase transition in the grand-canonical ensemble. Furthermore, since the density changes discontinuously from one side of the phase transition to the other, the pressure—though continuous—will have a kink at $\mu_c$, consistent with a first-order transition.

For this reason, phase structures are much simpler when considered in the grand-canonical ensemble. In this ensemble, the phase diagram consists of only pure phases: all phase coexistence (mixtures) occur along first-order phase transitions.

### 4. Constraints

Here we present a few more details about the extraction of the various constraints in the main text. We start with the bound $Y_0$. Recall that the transition is defined by chemical potential $\mu_b$ required to keep out species “b.” This is bounded by the energy gained by adding the single particle $\epsilon_0$ which we estimate: $\mu_b \leq \epsilon_0$. We must relate this to the chemical potential $\mu_a$ through the density of the free Fermi sea $n_a = \beta \mu_a^{3/2} \Rightarrow \mu_a = (n_a/\beta)^{2/3} = \alpha n_a^{2/3}$. We now express the constraint $\mu_b \leq \epsilon_0$ in terms of $y_0$:

$$y_0 = \frac{\mu_b}{\mu_a} \leq \frac{\epsilon_0}{\alpha n_a^{2/3}} = Y_0.$$  \hfill (A14)

The bound $Y_1$ follows from the constraint $\mu_- \leq \Delta$. To express this in terms of the data, we need to express the chemical potentials in terms of the normalization Fermi energy $\varepsilon_F = \mu_F^{SG}$ of a free gas of the same density $n_+ = n_a + n_b = 2(2m\mu_F^{SG})^{3/2}/(6\pi^2)$:

$$\varepsilon_F = \frac{1}{2m} [(3\pi^2)n_+]^{2/3}.$$  \hfill (A15)

The relationship between the density of the symmetric phase SF and the chemical potential $\mu_+$ is determined by the parameter $\xi$ from (5):

$$n_+ = \frac{\partial \mathcal{P}_{SF}(\mu_+)}{\partial \mu_+} = \frac{2\beta}{\xi^{3/2}} \mu_+^{3/2}.$$  \hfill (A16)

Thus, we have simply $\varepsilon_F = \mu_+/\xi$. We now express the constraint:

$$\frac{\mu_-}{\varepsilon_F} = \frac{\mu_-}{\mu_+} = \frac{1 - y_1}{1 + y_1} \leq \frac{\Delta}{\varepsilon_F}. $$  \hfill (A17)

Solving for $y_1$ gives the constraint

$$y_1 \geq Y_1 = \frac{\xi - \Delta/\varepsilon_F}{\xi + \Delta/\varepsilon_F}.$$  \hfill (A18)

These constraints transform directly into constraints on the derivatives of $g(x)$ through the dictionary (A3). For example, when $x = 0$ we have

$$y_0 \leq Y_0 \quad \Rightarrow \quad \frac{g'(0)}{g(0)} = g'(0) \leq Y_0,$$  \hfill (A19)

where we have used the fact that $g(0) = 1$. Likewise at $x = 1$ we have

$$y_1 \geq Y_1 \quad \Rightarrow \quad \frac{g'(1)}{g(1) + g'(1)} \geq Y_1,$$  \hfill (A20)

which gives a lower bound on $g'(1)$. The upper bound on $g'(1)$ is simply the condition that $y_1 \leq 1$ which we may impose by symmetry:

$$y_1 \leq 1 \quad \Rightarrow \quad \frac{g'(1)}{g(1) + g'(1)} \leq 1.$$  \hfill (A21)

### 5. Density Profiles

We consider the following functional form for $g(x)$:

$$g(x) = \begin{cases} y_0 + y_0' x + x^2 & \text{where } x \in [0, x_T], \\ c + dx & \text{where } x \in [x_T, 1]. \end{cases}$$  \hfill (A22)

The form of the function has been arbitrarily chosen between 0 and $x_T$ (for simplicity, we chose a quadratic polynomial) with the correct intercept $g(0) = 1$ and slope $g'(0) = y_0$. From this curve, we proceed with the Maxwell construction by finding the line that passes through $(x, g(x)) = (1, g(1))$ and that is tangent to the given curve $g(x_T)$ at the point $x_T$. The resulting $g(x)$ is shown with solid thick line in Fig. 2 and Fig. 7.

Once this curve is established, one can extract $h(y)$ using Eqs. (A3). The only complication arises when there are kinks or linear segments. In this case, there is a linear segment of $g(x)$ for $x \in [x_T, 1]$. From (A3) we see that, throughout this region, $y$ and $h(y)$ take on only a single value: this is the first-order phase transition $y_1$. This will result in a kink in the function $h(y)$ at this location.

To compute the density profiles in a trap, we first parametrize the trap so as to establish the spatial variations of the chemical potential. Let us consider a spherical harmonic trap $V(r) \propto r^2$ and consider the coordinate $\tilde{R} = R/R_{\text{vac}}$ where $R_{\text{vac}}$ is the radius of the cloud. The effective chemical potentials are established by (13) once the Lagrange multipliers $\lambda_{a,b}$ are chosen. Once this is done, the functional form of $h(y)$ can be used to directly map the position $\tilde{R}$ to the densities using Eq. (A1). In Fig. 5 we show several trap density profiles with the sample function (A22).

### 6. Extracting $g(x)$ from Experiment

In principle, once the radial density profiles have been measured to sufficient accuracy, one can extract the func-
This first-order differential equation may be integrated with the boundary condition $g(0) = 1$ to find the function $g(x)$. Finally, $\lambda_0$ will have to be fit to the trap profile. Note, there are many other ways to extract the same information: we have simply chosen a simple method. Other methods may be less sensitive to experimental errors for example. We leave it to future work to perform this extraction and the accompanying error analysis.

\section{Mean Field (Eagles-Leggett) Results}

In this section we consider the Eagles-Leggett mean-field model \cite{17}. In this model, one can easily calculate $\xi$ and $\Delta$ (see for example \cite{7}):

$$\xi_{MF} = 0.5906, \quad \frac{\Delta_{MF}}{\xi_{MF}} = 0.6864. \quad (A24)$$

These determine the properties of the superfluid phase SF. If we consider only homogeneous and isotropic phases, then there are three distinct phases: SF, $N_{a,b}$, and $\lambda_0$. The SF phase is the usual symmetric BCS-BEC crossover phase, the PP$_a$ phase is a partially polarized two-component Fermi liquid, and the N$_a$ phase is a fully polarized single-component Fermi liquid. One of the shortcomings of the mean-field crossover models is that they neglect the Hartree-Fock contributions.

These terms enter the energy density as $\mathcal{E}_{HF} \approx gn_an_b$ where $g$ is the coupling constant. In the limit of a short-range interaction, one takes the range of the interaction $r_0 \rightarrow 0$ to zero while holding the vacuum inverse s-wave scattering length $a^{-1}$ fixed.\textsuperscript{3} This requires that the interaction strength be taken to zero $g \sim \pi r_0/m \rightarrow 0$. The densities $n_{a,b}$ contain no singularities and so the Hartree-Fock contributions vanish. These contributions may be included in weak coupling by resumming particle-particle ladders to obtain $\mathcal{E}_{HF} \approx 4\pi \hbar^2 a n_an_b/m$, but this procedure may not be extrapolated to unitarity.

Thus, in mean-field, the partially polarized state simply has the pressure of two independent free Fermi gases:

$$P_{FG_2}(\mu_a, \mu_b) = \frac{2}{\xi} \beta \left( \mu_a^{5/2} + \mu_b^{5/2} \right). \quad (A25)$$

Pressure equilibrium thus determines the phase transitions in this model and we have the two conditions

$$P_{FG_2}(\mu_a, y_0^{MF} \mu_b) = P_{FG}(\mu_a), \quad (A26a)$$

$$P_{FG_2}(\mu_a, y_1^{MF} \mu_b) = P_{SF}(\mu_+). \quad (A26b)$$

These imply trivially that $y_0^{MF} = 0$. Since the Hartree-Fock terms vanish, there is no interaction energy and the phase transition between $N_a$ and PP$_a$ occurs for $\mu_b = 0$. The SF/PP$_a$ transition at $y_1$ is governed by condition (A26b). Using Eq. (5) and $\mu_b = y_0 \mu_a$, we have

$$2\xi_{MF}^{-3/2} \left( \frac{1 + y_1^{MF}}{2} \right)^{5/2} = 1 + (y_1^{MF})^{5/2}. \quad (A27)$$

This may be solved numerically using Eq. (A24) to obtain $y_1^{MF} = 0.1067$. To summarize: In the Eagles-Leggett mean-field crossover model with homogeneous and isotropic phases, we have:

$$y_0^{MF} = Y_0^{MF} = 0, \quad y_1^{MF} = 0.1051, \quad (A28a)$$

$$Y_1^{MF} = -0.0750, \quad y_1^{MF} = 0.1067. \quad (A28b)$$

\textsuperscript{2} There is the possibility that other phases, like LOFF, compete with the partially polarized phase $N_{a,b}$. In the mean-field model it is unlikely that these phases will drastically alter the locations of the phase transitions. The LOFF-like regions are always very thin, and we neglect these possibilities here.

\textsuperscript{3} The $a^{-1} = 0$ limit at unitarity does not represent a singularity.
Obviously the lower bound $Y_1^{MF}$ is useless for our purposes.

8. Calculation of $\epsilon_0$

The Hamiltonian describing a system of $N_n$ species “a” fermions interacting with one additional species “b” fermion is:

$$\hat{H} = \hat{H}_a + \hat{H}_0 = \left( \sum_{n=1}^{N_n} \hat{T}_n \right) + \left( \hat{T}_0 + \sum_{n=1}^{N_n} \hat{V}_{n,0} \right), \quad (A29)$$

where $\hat{T}_k$ are the corresponding kinetic energy operators and $\hat{V}_{n,0}$ is the potential between the fermion of species “a” with coordinate $r_n$ with the fermion of species “b” with coordinate $r_0$. Recall that we use the variational wave function (10)

$$\Psi(r_0; \{r_n\}) = \Phi_{SD}(\{r_n\})\phi(r_0; \{r_n\}), \quad (A30)$$

where (8)

$$\phi(r_0; \{r_n\}) = \sum_n A_n \exp \left(-\frac{\kappa r_{0n}}{r_{0n}}\right) \quad (A31)$$

is an eigenfunction of the operator $\hat{H}_0$:

$$\hat{H}_0\phi(r_0; \{r_n\}) = -\frac{\hbar^2 \kappa^2 \langle \{r_n\} \rangle}{2m} \phi(r_0; \{r_n\}). \quad (A32)$$

The Slater determinant is of course an eigenfunction of $\hat{H}_a$:

$$\hat{H}_a\Phi_{SD}(\{r_n\}) = E_{FG}\Phi_{SD}(\{r_n\}). \quad (A33)$$

Two additional terms arise from $\hat{H}_a$ acting on the product wave function. The first term is a cross-derivative which arises from applying $\hat{H}_a$ to both the Slater determinant and $\phi(r_0; \{r_n\})$. This gives a vanishing contribution, since the integral over momenta

$$\frac{\hbar^2}{m} \int_{k<k_F} \frac{dk}{(2\pi)^3} \int_{j=0}^{N_n} \sum_{l=1}^{N_n} (ik \cdot \nabla_l)\phi^2(r_0; \{r_n\}) \quad (A34)$$

is identically zero because of the symmetry of the Fermi sea. The second kind of term is due to $\hat{H}_a$ acting on $\phi(r_0; \{r_n\})$ and which pulls down derivatives of $\kappa(\{r_n\})$ and $A_n(\{r_n\})$:

$$\hat{H}_a\phi(r_0; \{r_n\}) = -\frac{\hbar^2 \kappa^2 \langle \{r_n\} \rangle}{2m} \phi(r_0; \{r_n\}) + \text{derivative corrections}. \quad (A35)$$

In what follows, we neglect the derivative corrections, but, as we discuss below, we expect these to be small. Within this approximation, the expectation value of this Hamiltonian is

$$\langle \Psi | \hat{H} | \Psi \rangle = E_{FG} + \epsilon_0 = E_{FG} - \frac{\hbar^2 \kappa^2}{m} \quad (A36)$$

where $E_{FG}$ is the ground state energy of the system of $N_n$ fermions alone. This contribution arises by applying $\sum_{n=1}^{N_n} T_n$ to the Slater determinant alone. It is implied here that $\phi(r_0; \{r_n\})$ is normalized.

We have checked explicitly that at unitarity for several simple lattice configurations (fcc, bcc) and for configurations in which the positions of all the fermion species “a” were randomly changed from the ideal lattice configurations within the Fermi hole, the values of $\kappa$ varied by a few percent at most, see Fig. 6. This analysis thus confirms our assumption that the fluctuations in a free Fermi gas of the number density $n_a(r)$ do not affect in a noticeable manner the value of $\kappa$.

For comparison, we replot the function $g(x)$ from Fig. 2 and include the Monte Carlo data from [20]. The authors of Ref. [20] simulated a two-component polarized normal Fermi gas, which provides a variational bound on the energy. We thank S. Giorgini for sending us their numerical results [20].
FIG. 7: Monte Carlo variational upper bound on $g(x)$ from [20] plotted on top of the function $g(x)$ from our Figure 2. Note the agreement from small polarizations indicating that our estimate for $Y_0$ is consistent with their proper variational bound. For larger polarizations, the true curve will lie below the results of Ref. [20] for two reasons: 1) The Maxwell construction for $g(x)$ (see Fig. (2) of [20]) and 2) The authors of Ref. [20] considered only normal Fermi partially polarized states. As shown in [12], at $T = 0$, partially polarized states will be superfluid. This could noticeably lower the energy for substantial polarizations at unitarity.