Finite-size and confinement effects in spin-polarized trapped Fermi gases

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We calculate the energy of a single fermion interacting resonantly with a Fermi sea of different-species fermions in anisotropic traps, and show that finite particle numbers and the trap geometry impact the phase structure and the critical polarization. Our findings contribute to understanding some experimental discrepancies in spin-polarized Fermi gases as finite-size and confinement effects.

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Experiments with spin-polarized Fermi gases [1, 2, 3, 4, 5, 6, 7] enable a unique exploration of superfluidity and universal properties in strongly-interacting asymmetric Fermi systems. There are very exciting experimental results of the MIT [1, 3, 4] and Rice University [2, 5] groups, however with differences in the observed phase structure and the critical polarization. In this Letter, we provide a first microscopic explanation of the MIT-Rice differences: The particle number and the trap geometry affect the interaction energy in the normal polarized phase and this impacts the limit of superfluidity in traps.

The MIT experiment [1, 3, 4] observed phase separation in the trap, with equal densities in the core, surrounded by a partially-polarized shell and an outer region of normal majority fermions. The study of vortices [1], in-situ density distributions [2], and the condensate fraction [1, 4] established a critical polarization $P_c = (N_\uparrow - N_\downarrow)/N_{\text{tot}} = 0.70(3)$ for the superfluid phase to exist. These results were obtained in a harmonic trap with cylindrical symmetry ($\omega_x = \omega_y = \alpha \omega$; $\omega_z = \omega$), with aspect ratio $\alpha \sim 5$, and total particle numbers $N_{\text{tot}} = N_\uparrow + N_\downarrow \sim 10^6 - 10^7$. The Rice experiment [2, 5] also observed phase separation, with a fully-paired core surrounded by normal majority fermions, but with a sharp phase boundary and extremely thin partially-polarized shell for low temperatures, and the unpolarized core exists to high polarization $P_c \gtrsim 0.9$. These experiments are in a highly elongated trap, with aspect ratio $\alpha \sim 35 - 45$, and for lower $N_{\text{tot}} \sim 10^5$. For these conditions, the core deformation and the double-peak structure in the axial density imply a breakdown of the local-density approximation (LDA) in Refs. [2, 3].

The critical polarization is influenced by the energy of the competing normal polarized phase. For large asymmetries, this is governed by the energy of a spin-down fermion interacting resonantly with a spin-up Fermi sea, which is a universal function of $\alpha$ and $N$. We study the energy of this spin-down fermion, the so-called Fermi polaron, in anisotropic traps for different particle numbers and show that the experimental differences can be understood partially based on our microscopic results.

This strongly-interacting Fermi polaron provides insights to problems in condensed-matter systems, with lower dimensions playing the role of trap-geometry effects, as well as to nuclear physics, where neutron-rich nuclei exhibit neutron skins [8], with neutron/proton densities similar to the spin densities in resonantly-interacting cold atoms.

Uniform system. The polaron energy $E$ was calculated variationally for the uniform system including one-particle–one-hole excitations (1p1h) [9, 10] and estimated in Ref. [11]. This leads to a Schwinger-Dyson equation, $G^{-1}(E) = 0$, or diagrammatically:

$$
E = G_0^{-1}(E, \mathbf{p} = 0) = (\cdots)^{-1}
$$

where $G$ ($G_0$) is the full (noninteracting) spin-down propagator with momentum $\mathbf{p} = 0$. For large S-wave scattering lengths, $1/\alpha_s = 0$, the energy is universal, $E = \mu_1 - \eta p_F^2/(2m)$, with Fermi momentum $p_F$. The self-consistent solution to Eq. (1) yields $\eta = -0.607$ [3].

This energy gain constrains the equation of state for large asymmetries, and thus the existence of partially-polarized phases and the critical polarization: The variational $\eta$ is lower than the maximal stress (from $\mu_1 - \mu_1 \lesssim 2\Delta$) for stability of the superfluid phase, $\mu_1/\mu_1 \gtrsim -0.09(3)$, and this requires the existence of at least one non-trivial partially-polarized phase in the uniform system [3, 11]. In LDA with Eq. (13), $\eta = -0.607$ leads to $P_c = 0.74$ and a critical density ratio $x_c = n_\uparrow/n_\downarrow = 0.47$ [12], which are in good agreement with $P_c$ of the MIT experiment [1, 3, 4] and with a tomography measurement of $x_c \approx 0.47$ [7]. Finally, the variational 1p1h $\eta$ value agrees very well with Monte-Carlo (MC) results [12, 13, 14, 15], and 2p2h contributions were shown to be small [10].

Basic formalism. The strongly-interacting Fermi gas in a harmonic-oscillator trap is given by the Hamiltonian

$$
H = \sum_{n,\sigma} \varepsilon_n a^\dagger_{n,\sigma} a_{n,\sigma} +
\sum_{n_1, n_1', n_2, n_2'} \langle n_1', n_2' | V | n_1, n_2 \rangle a^\dagger_{n_1, 1} a^\dagger_{n_2, 1} a_{n_1', 1} a_{n_2', 1},
$$

where $\varepsilon_n = \alpha \omega (n_x + n_y + 1) + \omega (n_z + 1/2)$ are harmonic oscillator energies ($\hbar = 1$). The operator $a_{n,\sigma}$ annihilates...
a particle with spin \( \sigma = |, \downarrow \) in a state with quantum numbers \( n = (n_x, n_y, n_z) \). We use a contact interaction regulated by separable cutoff functions in momentum space,

\[
\langle p | V | p' \rangle = C(\Lambda) e^{-(p^2 + p'^2)/\Lambda^2} \text{ with } C(\Lambda) = \frac{4\pi/m}{\frac{1}{a_s} - \frac{\Lambda}{\sqrt{2} \pi}},
\]

where \( p, p' \) are incoming/outgoing relative momenta, \( m \) is the fermion mass and \( \Lambda \) a momentum cutoff. In this case, the harmonic-oscillator matrix elements can be expressed as a sum over separable functions \( F(n_1, n_2, S) \),

\[
\langle n_1, n_2 | V | n_3, n_4 \rangle = C(\Lambda) \sum_S F(n_1, n_2, S) F(n_3, n_4, S),
\]

with center-of-mass quantum numbers \( S, F(n_1, n_2, S) = \prod_{i=x,y,z} (m|\omega_i|)^{1/4} \tilde{F}(n_1, n_2, S), \lambda_i = \sqrt{m|\omega/\Lambda} \), and the dimensionless function \( \tilde{F} \) is given by

\[
\tilde{F}(n_1, n_2, S, \lambda_i) = (-1)^{n_2} \left( \frac{1}{2\pi} \right)^{\frac{1}{4}} 
\times \frac{(n_2 - 1)!}{n_1!} \frac{(1 - 2\lambda^2)^{n_1/2}}{(1 + 2\lambda^2)^{n_2/2}} f(n_i, S_i, n_2),
\]

where the relative quantum numbers \( n_i = n_{1i} + n_{2i} - S_i \) have to be even and positive, and one has for \( n_2 \leq n_i \)

\[
f(n_i, S_i, n_2) = \binom{n_2}{n_2} _2F_1(-n_{2i} - S_i, 1 - n_{2i} + n_{2i} - n_{2i}),
\]

with hypergeometric function \( _2F_1 \), and for \( n_2 > n_i \)

\[
f(n_i, S_i, n_2) = (-1)^{n_2 + n_i} \binom{S_i}{n_2 - n_i}
\times _2F_1(-n_{2i} - S_i, 1 + n_{2i} - n_{2i} - n_{2i} - 1).
\]

**Polaron energy.** Following the variational Ansatz of Refs. [9, 10], we calculate the energy \( E \) of the spin-down fermion, including 1p1h excitations in the wave function,

\[
|\psi\rangle = \phi_0 |\Omega\rangle + \sum_{m, h, p} \phi_{m, h, p} |m, h, p\rangle,
\]

where \( |\Omega\rangle \) denotes the Fermi sea with the spin-down particle in the \( n = 0 \) level [29], and \( |m, h, p\rangle \) consist of a spin-up fermion in \( h \) excited to a level \( p \) above the Fermi energy \( \varepsilon_F \), and the spin-down particle occupies the level \( m \). Therefore, the sum over \( h \) is restricted to occupied states, whereas \( p \) is over unoccupied states above \( \varepsilon_F \).

Minimizing \( \langle \psi | H | \psi \rangle \) with respect to \( \phi_0, \phi_{m, h, p} \), we find the self-consistent equation for \( E \) in anisotropic traps,

\[
E - \varepsilon_0 = \sum_{\varepsilon_h \leq \varepsilon_F} \sum_{S, L} F(0, h, S) \left[ M^{-1}(\varepsilon_F, E + \varepsilon_h) \right]_{S, L} F(0, h, L),
\]

where \( \varepsilon_0 \) is measured from the energy of the Fermi sea, in weak coupling \( E \approx \varepsilon_0 \), and the matrix \( M \) is given by

\[
M(\varepsilon_F, E + \varepsilon_h)_{S, L} = \left[ \frac{1}{C(\Lambda)} - D(\alpha, \Delta \tilde{E}) \right] \delta_{S, L}
\times \sum_{\varepsilon_p \leq \varepsilon_F} \sum_{m} \frac{F(m, p, S)F(m, p, L)}{E + \varepsilon_h - (\varepsilon_p + \varepsilon_m)}.
\]

Here \( \Delta \tilde{E} = \alpha(S_x + S_y + 2) + S_z + 1 - (E + \varepsilon_h)/\omega \) and \( D(\alpha, \Delta \tilde{E}) \) is identical to the last term of Eq. (10) with unrestricted sum over \( p \) and \( |S, L\rangle \). For an isotropic trap, \( D(1, \Delta \tilde{E}) \) has the simple analytical form

\[
D(1, \Delta \tilde{E}) = \frac{m A}{2(2\pi)^{3/2}} + \left( \frac{m\omega}{2\pi} \right)^{3/2} \frac{\sqrt{\pi} \Gamma(\Delta \tilde{E}/2)}{\omega \Gamma((\Delta \tilde{E} - 1)/2)}.
\]

The cancellation of the first term in Eq. (11) with the cutoff in the \( 1/C(\Lambda) \) term in Eq. (10) demonstrates that \( E \) is cutoff independent for large \( \Lambda \). We have verified that this is the case for all studied \( \alpha \) and \( A > 10^4 \sqrt{m\omega}/2 \).

Moreover, we have found numerically that the diagonal matrix elements of \( M(\varepsilon_F, E + \varepsilon_h) \) depend only on the center-of-mass excitation \( \alpha(S_x + S_y) + S_z \).

For large scattering lengths, \( 1/a_s = 0 \), the energy is a universal function of the aspect ratio and the spin-up particle number \( N = N_1 \), and we generalize the scaling for the uniform system to anisotropic traps,

\[
E = \eta(\alpha, N) E_F(\alpha, N),
\]
where $E_F(\alpha, N) = (6\pi^2n_1(0))^{2/3}/(2m)$ is the local Fermi energy of spin-up particles at the center of the trap. In the upper panel of Fig. 1 we show $E_F(1, N)$ for an isotropic trap divided by the large-$N$ expression $E_F,\infty(1, N) = \omega(6N)^{1/3}$. The points are for alternating odd-even values of the Fermi level $\eta_F$, which defines the Fermi energy $\varepsilon_F = \omega(\alpha n_F + (2\alpha + 1)/2)$. The local Fermi energy approaches $E_{\omega,\infty}(1, N)$ from above (below) for odd (even) $n_F$. With increasing $\alpha$, this effect decreases and the envelopes approach the large-$N$ result faster.

Results. Using Eq. (12), we solve Eq. (9) iteratively for $\eta(\alpha, N)$, with a numerical precision better than 1%. To this end, we take the matrix $M(\varepsilon_F, E + c_0)$ to be diagonal. This is correct in the large-$N$ limit, and we have checked numerically that the off-diagonal matrix elements are considerably smaller than the diagonal ones for all studied values of $N$. In the lower panel of Fig. 1 we show $\eta(1, N)$ for an isotropic trap as a function of $N$. The effects due to finite particle numbers and confinement of the trap are clearly present: The odd-even systematics seen in the local Fermi energy $E_F(1, N)$ is small compared to the decrease of $\eta(1, N)$ with particle number. Therefore, the decrease is not due to the change in the local Fermi energy. For one spin-up fermion, the exact ground-state energy in a trap is $E(1, 1) = \omega/2 > 0$, thus $\eta(1, 1) = (36\pi)^{-1/3} = 0.207$ [21]. With increasing $N$, $\eta(1, N)$ decreases and saturates. Using the Ansatz, $\eta(\alpha, N) = a(\alpha)(1 + b(\alpha)N^{-c(\alpha)})$, we fit our numerical results for odd (even) $n_F$ separately and find $a(1) \approx -0.61$ and $c(1) \approx 0.34$ (0.32). This is in very good agreement with $\eta = -0.607$ for the uniform system [9] and natural large-$N$ corrections of $1/E_{\omega,\infty}(1, N) \sim N^{-1/3}$. Therefore, $\sim 10\%$ changes of $\eta$ are natural for $N \sim 10^4$.

In Fig. 2 we show the dependence of $\eta(\alpha, N)$ on trap geometry, for various aspect ratios from $\alpha = 1$ to $\alpha = 35$, as a function of the spin-up particle number. The single-particle energy depends significantly on the aspect ratio, while the odd-even Fermi level effect decreases with increasing $N, \alpha$ and is negligible for $\alpha \gtrsim 10$. For fixed $N$, $\eta(\alpha, N)$ increases with increasing $\alpha$. In addition, for larger aspect ratios, the dependence on $N$ is stronger. For each $\alpha$, we fit our combined results (including odd and even $n_F$) with the power-law Ansatz and show the fits in Fig. 2. We find $a(\alpha) \approx -0.61(1)$, consistent with the uniform result for all studied aspect ratios, and $c(\alpha)$ ranges from $c(1) \approx 0.36$ to $c(35) \approx 0.31$.

Critical polarization. We now explore the impact of the calculated finite-size and confinement (trap) effects on the phase structure. We consider an unpolarized superfluid phase and a partially-polarized normal Fermi liquid. Following Ref. [19], the free energy is given by

$$E_{\text{tot}} = 2 \int_{|r| < R_S} \left[ c_s(n_s(r)) + V(r) - \mu_s \right] n_s(r) \, dr + \int_{R_S < |r| < R_{\text{tot}}} \left[ c_n(x(r)) n_\uparrow(r) + V(r)(n_\uparrow(r) + n_\downarrow(r)) - \mu_\uparrow n_\uparrow(r) - \mu_\downarrow n_\downarrow(r) \right] \, dr,$$

where $x = n_\uparrow/n_\downarrow \leq 1$, $R_S^2 = \alpha(R_x^2 + R_y^2) + R_z^2$ defines the
boundary of the superfluid phase, and the excess spin-up density vanishes at $R_\tau$. As discussed, the LDA of Eq. (13) breaks down for the Rice experiment [2,5]. We only use this here to explore the impact of $\eta(\alpha, N)$ on the critical polarization. In a full density-functional calculation, this can also be combined with surface tension [18] or gradient terms. For the uniform system at unitarity, the energy density of the superfluid $\epsilon_s$ and of the partially-polarized normal Fermi liquid $\epsilon_n$ are given by [19]

$$\epsilon_s(n_a) = \frac{3}{5} \left( \frac{6\pi^2 n_a}{2m} \right)^{2/3} \text{ and } \epsilon_n(x) = \frac{3}{5} \left( \frac{6\pi^2 n}{2m} \right)^{2/3} (\epsilon(x)), $$

(14)

with superfluid density $n_a$ and universal energy $\xi = 0.42$ of the symmetric system [13, 15], which is consistent with $\xi = 0.46 \pm 0.05$ of Ref. [2]. Assuming $x \ll 1$, the energy of adding spin-down fermions to the normal phase is determined by $\eta(\alpha, N)$, with corrections due to a spin-down quasiparticle effective mass $m^*$ and due to quasiparticle interactions $B$ [19]:

$$\epsilon(x) = 1 + \frac{3}{5} \eta(\alpha, N) x + \frac{m}{m^*} x^{5/3} + B x^2. $$

(15)

We take $\eta(\alpha, N)$ from Fig. [2] but for simplicity consider two cases for the quasiparticle spectrum: $m^*/m = 1$, $B = 0$, as well as the MC values $m^*/m = 1.09$, $B = 0.14$ [13], which show these are corrections to the leading effects from $\eta$. This however does not include the effects of Fermi statistics of the minority particles on $\eta$.

The critical polarization $P_c(\alpha, N_{\text{tot}})$ is obtained, when the phase boundary reaches the trap center $R_S \to 0$. In chemical equilibrium, $\mu_S = (\mu_\uparrow + \mu_\downarrow)/2$, the ground state of the system is determined by requiring that the energy functional, Eq. (13), is stationary with respect to variations of the densities and of the phase boundary $R_S$, so that the pressure between the two phases is equal: $2n_\uparrow^2 (\partial \epsilon_s/\partial n_\uparrow) = n_\downarrow^2 (\partial \epsilon_n/\partial n_\downarrow) + n_\uparrow n_\downarrow (\partial \epsilon_s/\partial n_\downarrow)$. This leads to an equation for the critical density ratio at the center of the trap, $x_c(\alpha, N_{\text{tot}}) = x(R_S = 0, \alpha, N_{\text{tot}})$ [13]:

$$\epsilon(x_c) + \frac{3}{5} (1 - x_c) \partial_x \epsilon(x_c) - (2x_c^{5/3} \epsilon(x_c)^2)^{1/3} = 0. $$

Given $N_{\text{tot}}$ and $x_c$, the spin-up/spin-down densities and particle numbers are determined from the variation of $E_{\text{tot}}$.

In Fig. 3 we show the dependence of the critical polarization $P_c(\alpha, N_{\text{tot}})$ and the critical density ratio $x_c(\alpha, N_{\text{tot}})$ as a function of aspect ratio, for total particle numbers $N_{\text{tot}} = 10^4$ and $N_{\text{tot}} = 10^5$, where the experimental differences from the uniform system exists. For $\alpha = 1$, $N_{\text{tot}} = 10^7$ and the MC $m^*$, $B$ values, we reach the uniform system $P_c = 0.74$ and $x_c = 0.47$. For fixed $N_{\text{tot}} = 10^4$ and increasing $\alpha$ from 1 to 35, $P_c$ increases from 0.82 to 0.89 and $x_c$ decreases from 0.40 to 0.31 (for the MC $m^*$, $B$ values). For fixed $\alpha = 35$, $P_c$ increases with decreasing $N_{\text{tot}} = 10^5, 10^4, 10^3$ from 0.82, 0.89, 0.96 and $x_c$ decreases from 0.39, 0.31, 0.18 (for the MC $m^*$, $B$ values; results for $N_{\text{tot}} = 10^3$ not shown in Fig. 3). In addition, we show in Fig. 3 the dependence on the quasiparticle spectrum (through $m^*$) and interaction $B$. For given $\alpha$ and $N_{\text{tot}}$, $P_c$ is larger and $x_c$ smaller for the MC $m^*$, $B$ values, compared to $m^*/m = 1$, $B = 0$, but as expected, the uncertainty due to $m^*$, $B$ is smaller than the variation of $P_c$ and $x_c$ with $\alpha$, $N_{\text{tot}}$. This dependence also becomes weaker with increasing $\alpha$ and decreasing $N_{\text{tot}}$.

In summary, for lower particle numbers and more elongated traps, the energy of the normal polarized phase increases and the superfluid extends to larger population imbalances. This provides a microscopic understanding of the MIT-Rice differences due to the dependence of the polaron energy on the particle number and the trap geometry. Finite-size effects are stronger in highly-elongated systems as the dimensionality of the problem is continuously reduced with increasing aspect ratio. The $N + 1$-body problem is a natural first step towards general asymmetries and contributions to the total energy beyond $\eta(\alpha, N)$. In addition, effects from a full density-functional calculation need to be studied.

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[21] The exact two-body ground-state energy [17] is reproduced, if we generalize the first term in Eq. (15) to include a sum over the spin-down particle in level $n$, $\sum_n \delta n |n\rangle$. 