Virial Expansion for a Strongly Correlated Fermi Gas

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Using a high temperature virial expansion, we present a controllable study of the thermodynamics of strongly correlated Fermi gases near the BEC-BCS crossover region. We propose a practical way to determine the expansion coefficients for both harmonically trapped and homogeneous cases, and calculate the third order coefficient $b_3(T)$ at finite temperatures T. At resonance, a T-independent coefficient $b_{3,\infty}^{\rm hom} \approx -0.290\,952\,95$ is determined in free space. These results are compared with a recent thermodynamic measurement of ^{6}Li atoms, at temperatures below the degeneracy temperature, and with Monte Carlo simulations.

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Strongly correlated Fermi gases are of wide interest and underlie many unanswered problems in quantum many-body systems, ranging from neutron stars, hadrons, and quark matter through to high T_c superconductors [1]. Recent investigations of Feshbach resonances in ultracold atomic Fermi gases have opened new, quantitative opportunities to address these challenges [1]. A great deal of theoretical work has been carried out for this simple, well-controlled case of a strongly interacting yet low-density Fermi gas, which is known as the unitarity limit. However, a profound understanding is plagued by the large interaction strength, for which the use of perturbation theory requires infinite order expansions. Numerically exact quantum Monte Carlo simulations are also less helpful than one might expect [2–4]. Because of the Fermi sign problem [2], computer simulations are often restricted to small samples, and are therefore difficult to extrapolate to the thermodynamic limit.

In this Letter, we approach this problem by using a *controllable* virial expansion study of *trapped* strongly interacting Fermi gases at high temperatures. We focus on the low-density physics which is described by an effective S-wave contact potential. Our expansion has a small parameter. The fugacity

$$z = \exp(\mu/k_B T) \ll 1$$

is small because the chemical potential μ diverges logarithmically to $-\infty$ at large temperatures T. The virial expansion up to the second virial coefficient was applied by Ho and Mueller to explore the universal thermodynamics of a homogeneous Fermi gas at unitarity [5]. Here we extend this to the third order coefficient. Most importantly, we present a practical theoretical strategy which can even be extended beyond third order. Surprisingly, we find that the simplest theoretical route to calculating these higher-order coefficients is via the use of exact solutions for the energy eigenstates of harmonically trapped clusters. This gives a unified approach to calculating virial coefficients in both trapped and untrapped cases.

In reality, the strongly interacting spin-1/2 ^{6}Li and ^{40}K fermionic gases were realized by tuning a magnetic field across a resonance [1]. Extensive experiments have studied the crossover from the BCS limit (Cooper pairing of atoms) to the BEC limit (Bose-Einstein condensation of diatomic dimers). The most interesting region lies at the middle of crossover, where the two-body S-wave scattering length a becomes much larger in magnitude than the inverse Fermi vector $1/k_F$ [6]. Fascinating phenomena may occur in this "unitarity limit" [7,8], such as the observed scale-invariant, universal thermodynamic behavior [9–11]. Accurate, high-order virial coefficients provide an extremely useful tool in analyzing these experimental results above the superfluid transition. At the same time,

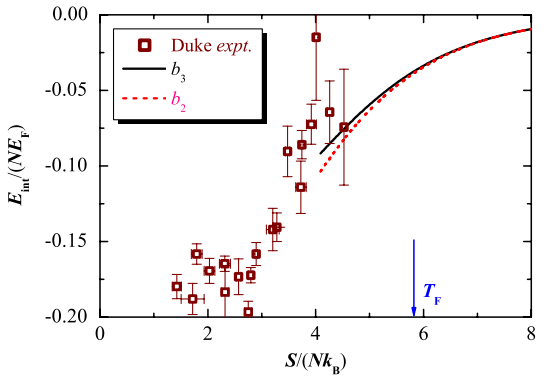

FIG. 1 (color online). Predicted interaction energy as a function of entropy at unitarity, compared with experimental data from Duke University [10]. The solid (dashed) line shows the contribution up to the third (second) order virial coefficient. The arrow indicates the degeneracy point.

the methods given here may have general applicability to other strongly interacting systems.

In what follows, we first introduce a practical way to calculate the nth virial coefficients $b_n(T)$ and, by solving exactly the two- and three-particle problems, determine the second and third virial coefficients in an isotropic harmonic trap at the BCS-BEC crossover. We then focus on the unitarity limit and calculate the energy and entropy of a trapped gas using the virial expansion method.

Our main result is summarized in Fig. 1, which shows the comparison of the virial expansion prediction to a recent measurement of the entropy dependence of the interaction energy $E_{\rm int}(S)$ at unitarity. The experiment was carried out for atomic gases of ^{6}Li atoms at a broad Feshbach resonance [10]. We find an excellent agreement at temperatures *below* the Fermi degeneracy temperature T_F. This remarkable result is opposite to the consensus that the virial expansion is valid at the classical Boltzmann regime with $T \gg T_F$. We suggest that it can be understood by the significant suppression of higher-order virial coefficients in a harmonic trap.

Even in the absence of a harmonic trap, our method can still be used to calculate the virial coefficients. We determine a universal coefficient $b_{3,\infty}^{\rm hom} \approx -0.290\,952\,95$ for a *homogeneous* Fermi gas at unitarity, in contrast to a recent calculation that obtained a result with the opposite sign [12]. Our resulting equation of state is in good agreement with existing Monte Carlo results, and may provide a useful benchmark for testing future quantum Monte Carlo simulations of strongly interacting Fermi systems at high temperatures.

Virial expansion.—Let us consider the thermodynamic potential $\Omega = -k_B T \ln \mathcal{Z}$, where $\mathcal{Z} = {\rm Tr}\exp[-(\mathcal{H} - \mu\mathcal{N})/k_B T]$ is the grand partition function. At high temperatures, we can rewrite $\mathcal{Z}$ in terms of the partition functions of clusters, i.e., $Q_n = {\rm Tr}_n[\exp(-\mathcal{H}_n/k_B T)]$ with n denoting the number of particles in the cluster and ${\rm Tr}_n$ denoting the trace over n-particle states of the proper symmetry; thus we find $\mathcal{Z} = 1 + zQ_1 + z^2 Q_2 + \cdots$. The thermodynamic potential can then be written as

$$\Omega = -k_B T Q_1 [z + b_2 z^2 + \cdots + b_n z^n + \cdots], \quad (1)$$

where the virial coefficients are given by

$$b_2 = (Q_2 - Q_1^2/2)/Q_1, \quad (2)$$

$$b_3 = (Q_3 - Q_1 Q_2 + Q_1^2/3)/Q_1, \ \text{etc.} \quad (3)$$

These equations present a general definition of virial expansion and are applicable to both homogeneous and trapped systems. The determination of the nth virial coefficient thus requires full solutions up to the n-body problem. It is convenient to focus on the interaction effects only and consider $\Delta b_n \equiv b_n - b_n^{(1)}$ and $\Delta Q_n \equiv Q_n - Q_n^{(1)}$, where the superscript "1" denotes the noninteracting systems. We shall calculate $\Delta b_2 = \Delta Q_2/Q_1$ and $\Delta b_3 = \Delta Q_3/Q_1 - \Delta Q_2$.

Second and third virial coefficients in traps.—By solving the few-body problem exactly, we now evaluate the virial coefficients in a three-dimensional isotropic harmonic potential $V(\mathbf{r}) = m\omega r^2/2$, with a trapping frequency ω and fermion mass m. The partition function Q_1 is easily obtained from the single-particle spectrum of the harmonic potential, $E_{nl} = (2n + l + 3/2)\hbar\omega$, and the single-particle wave function, $R_{nl}(r)Y_l^m(\theta, \varphi)$. We find that $Q_1 = 2\exp(-3\tilde{\omega}/2)/[1 - \exp(-\tilde{\omega})]^3$ with a dimensionless frequency $\tilde{\omega} = \hbar\omega/k_B T \ll 1$. The prefactor of 2 in Q_1 accounts for the two possible spins of each fermion.

To solve the two- and three-fermion problems, we adopt a short-range S-wave pseudopotential for interatomic interactions, in accord with the experimental situation of broad Feshbach resonances. This can be replaced by the Bethe-Peierls contact conditions on the wave function $\psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_n)$: when any particles i and j with unlike spins close to each other, $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j| \to 0$, $r_{ij}\psi$ satisfies

$$\partial(r_{ij}\psi)/\partial r_{ij} = -(r_{ij}\psi)/a. \quad (4)$$

Otherwise, the wave function ψ obeys the noninteracting Schrödinger equation,

$$\sum_{i=1}^{n}\left[-\frac{\hbar^2}{2m}\nabla_{\mathbf{r}_i}^2 + \frac{1}{2}m\omega r_i^2\right]\psi = E\psi. \quad (5)$$

Unlike Bose gases, no additional many-particle interaction parameters are required. This is due to the absence of many-particle S-wave bound states (i.e., Efimov-like states) for these low-density Fermi gases, which has a physical origin in the Pauli exclusion principle.

The Hamiltonian of two fermions with different spins was solved by Busch *et al.* [13]. As the center of mass is separable for a harmonic trap, we may single out the (single-particle) center-of-mass energy $E_{\rm c.m.}$ and rewrite the total energy as $E = E_{\rm c.m.} + E_{\rm rel}$. Following Busch *et al.* [13], the relative energy $E_{\rm rel} = (2\nu + 3/2)\hbar\omega$ satisfies, $2\Gamma(-\nu)/\Gamma(-\nu - 1/2) = d/a$, where $d = \sqrt{2\hbar/m\omega}$ is the length scale of the trap, and the (un-normalized) two-body relative wave function is given by, $\psi_{2b}^{\rm rel}(\mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1; \nu) = \exp(-r^2/2d^2)\Gamma(-\nu)U(-\nu, 3/2, r^2/d^2)$. Here, the total angular momentum of $\psi_{2b}^{\rm rel}$ is strictly zero since only these states do not vanish at $r = 0$ and thus are influenced by the pseudopotential. Γ and U are the Gamma function and confluent hypergeometric function, respectively. It is readily shown that $b_2 - b_2^{(1)} = \Delta Q_2/Q_1$ is given by $b_2 - b_2^{(1)} = (1/2)\sum_{\nu_n}[e^{-(2\nu_n + 3/2)\tilde{\omega}} - e^{-(2\nu_n^{(1)} + 3/2)\tilde{\omega}}]$, where the summation over $E_{\rm c.m.}$ cancels Q_1 in the denominator, and $\nu_n^{(1)} = 0, 1, \ldots$ is the nth solution of the relative energy spectra in the noninteracting limit. At unitarity, the two-body solutions, $\nu_{n,\infty} = n - 1/2$, are known exactly [13], leading to

$$b_{2,\infty} - b_{2,\infty}^{(1)} = \frac{1}{2}\frac{\exp(-\tilde{\omega}/2)}{[1+\exp(-\tilde{\omega})]} = \frac{1}{4} - \frac{1}{32}\tilde{\omega}^2 + \cdots. \quad (6)$$

The three-fermion problem was studied analytically by Werner and Castin [14] at unitarity, and numerically by Kestner and Duan [15] for arbitrary scattering lengths. Although the calculations are more involved, the exact solution is intuitively understandable. Let us skip the trivial center-of-mass motion. Assuming a spin state $\downarrow\uparrow\downarrow$ and using the Jacobi coordinates $\mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1$ and $\rho = (2/\sqrt{3})[\mathbf{r}_3 - (\mathbf{r}_1/2 + \mathbf{r}_2/2)]$ as shown in the inset of Fig. 2, the three-body relative wave function $\psi_{3b}^{\mathrm{rel}}(\mathbf{r}, \rho)$ can be written as

$$\psi_{3b}^{\mathrm{rel}} = (1 - \mathcal{P}_{13})\sum_n a_n R_{nl}(\rho) Y_l^m(\hat{\rho}) \psi_{2b}^{\mathrm{rel}}(\mathbf{r}; \nu_n), \quad (7)$$

which is simply the summation of products of the eigenstate of the paired particles 1 and 2, $\psi_{2b}^{\mathrm{rel}}(\mathbf{r}; \nu_n)$, and of the eigenstate of particle 3 relative to the pair, $R_{nl}(\rho)Y_l^m(\hat{\rho})$. The value of ν_n for each index "n" is uniquely determined from energy conservation: $E_{\mathrm{rel}}/\hbar\omega = (2n + l + 3/2) + (2\nu_n + 3/2)$ and should not be confused with the solutions for the two-body relative energy. The relative wave function ψ_{3b}^{rel} has a *well-defined* total relative angular momentum of the 3 particles with quantum numbers l and m. The operator $\mathcal{P}_{13}$ ensures the correct exchange symmetry of the wave function. This introduces correlations between the 1–2 pair and the remaining particle 3 and thus a hybridization as parametrized by a_n. We solve the eigenstate "a_n" and eigenvalue E_{rel} by imposing the Bethe-Peierls boundary condition Eq. (4). We find

$$\frac{2\Gamma(-\nu_n)}{\Gamma(-\nu_n - 1/2)} a_n + C_{nm} a_m = \left(\frac{d}{a}\right) a_n, \quad (8)$$

where the (symmetric) matrix $C_{nm} \equiv [(-1)^l/\sqrt{\pi}] \times \int_0^\infty d\rho \rho^2 R_{nl}(\rho) R_{ml}(\rho/2) \psi_{2b}^{\mathrm{rel}}(\sqrt{3}\rho/2; \nu_m)$ arises from the exchange operator $\mathcal{P}_{13}$. Without C_{nm} we have a three-body problem of uncorrelated pair and single particle. We label the relative energy in this case as $\bar{E}_{\mathrm{rel}}$ and calculate it directly from the two-body relative energy.

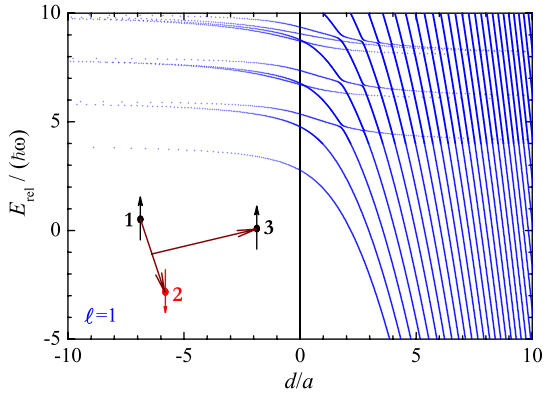

FIG. 2 (color online). Relative energy levels of a three-fermion system at the ground state section ($l = 1$).

We have solved Eq. (8) numerically for 10^4 energy levels E_{rel} at different relative angular momenta l and have checked that at unitarity our results agree exactly with the analytic spectrum in Ref. [14], with relative numerical errors typically $<10^{-6}$. Figure 2 shows how the relative energy spectrum evolves from the BCS to the BEC side in the subspace of $l = 1$.

To calculate the third virial coefficient using $b_3 - b_3^{(1)} = \Delta Q_3/Q_1 - \Delta Q_2$, we notice that the spin states of $\downarrow\uparrow\downarrow$ and $\uparrow\downarrow\uparrow$ contribute equally to Q_3. Also, Q_1 in the denominator is canceled by the summation over $E_{\mathrm{c.m.}}$, and the term $-\Delta Q_2$ is canceled by the difference between $\bar{E}_{\mathrm{rel}}$ and the non-interacting energy $E_{\mathrm{rel}}^{(1)}$. Thus, the third virial coefficient is determined solely by the exchange correlation, so that $b_3 - b_3^{(1)} = \sum \exp(-E_{\mathrm{rel}}/k_B T) - \sum \exp(-\bar{E}_{\mathrm{rel}}/k_B T)$, where the summation is performed over all possible three-body states that are affected by interactions. At unitarity, we obtain

$$b_{3,\infty} - b_{3,\infty}^{(1)} = -0.06833960 + 0.038867\tilde{\omega}^2 + \cdots. \quad (9)$$

The second and third virial coefficients through the crossover is given in Fig. 3 at three typical temperatures. Here we consider a gas with $N = 100$ atoms and scale the inverse scattering length using the Fermi vector at the trap center, $k_F = (24N)^{1/6}/(d/\sqrt{2})$. The temperature is given in units of Fermi temperature $T_F = E_F/k_B = (3N)^{1/3} \times (\hbar\omega/k_B)$. All the curves with distinct temperatures cross at $a \to \pm\infty$. This is the manifestation of universal behavior anticipated if there is no any intrinsic length scale. However, the characteristic length scale d of harmonic traps brings a small (nonuniversal) temperature dependence that decreases as $N^{-2/3}$, shown by the terms $\tilde{\omega}^2$ in Eqs. (6) and (9).

High-T thermodynamics in traps.—We are ready to investigate the thermodynamics of a strongly interacting Fermi gas at high temperatures. At unitarity, the energy

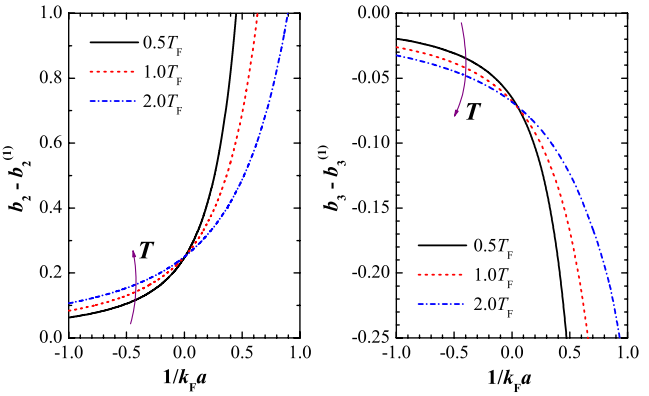

FIG. 3 (color online). The second and third virial coefficients as a function of the interaction parameter $1/k_F a$. We have used a total number of atoms $N = 100$, leading to $\tilde{\omega} = (3N)^{-1/3} \approx 0.15$ at $T = T_F$.

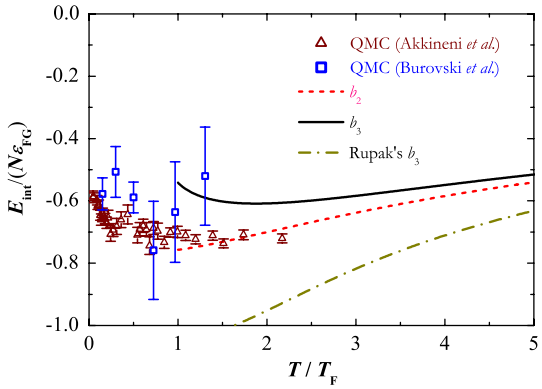

FIG. 4 (color online). Temperature dependence of interaction energy of a homogeneous gas at unitarity, obtained using different virial coefficients. For comparison, two quantum Monte Carlo data reported in Refs. [2,4] are shown. A finite range of interactions has been used in Ref. [2], which may lead to a systematic downshift in energies. We list also the result calculated by using Rupak's $b_{3,\infty}^{\rm hom} \approx 1.11$.

E and entropy S in the limit of small $\tilde{\omega}$ or large N can be calculated according to the universal relations [7,8],

$$E = -3\alpha\Omega/2, \tag{10}$$

$$S = -(3\alpha/2 + 1)\Omega/T - k_B N \ln z, \tag{11}$$

together with Eq. (1) for Ω and the number identity $N = -(\partial\Omega/\partial\mu) = Q_1[z + 2b_2 z^2 + \cdots]$, and the virial coefficients shown in Eqs. (6) and (9). Here, $\alpha = 2$ for a harmonically trapped gas. We also calculate the equation of state $E_{\rm IG}(S)$ of an ideal noninteracting Fermi gas, using $b_n^{(1)} = (-1)^{n+1}[1/n^4 - \tilde{\omega}^2/(8n^2) + \cdots]$.

Figure 1 shows the predicted interaction energy $E_{\rm int} = E - E_{\rm IG}$ as a function of entropy, compared to the experimental data reported by Luo *et al.* [10]. We find a rapid convergence of expansion, even below the degeneracy temperature T_F, with excellent agreement between theory and experiment: the virial expansion is applicable to a trapped Fermi gas even at $T < T_F$.

This remarkable observation is counterintuitive, as the virial expansion is generally believed to be useful at the Boltzmann regime with $T \gg T_F$. This occurs because there is a significant reduction of higher-order virial coefficients in harmonic traps. Consider the thermodynamic potential of a harmonically trapped gas in the local density approximation, $\Omega = \int \Omega(\mathbf{r}) d\mathbf{r} \propto \int d\mathbf{r}[z(\mathbf{r}) + b_{2,\infty}^{\rm hom} z^2(\mathbf{r}) + \cdots + b_{n,\infty}^{\rm hom} z^n(\mathbf{r}) + \cdots]$, where $z(\mathbf{r}) = z\exp[-V(\mathbf{r})/k_B T]$ is a local fugacity with the local chemical potential $\mu(\mathbf{r}) = \mu - V(\mathbf{r})$. It is readily seen on spatial integration that the universal (T-independent) part of the trapped virial coefficient is,

$$b_{n,\infty}(\text{universal}) = \left(\frac{1}{n^{3/2}}\right) b_{n,\infty}^{\rm hom}. \tag{12}$$

Therefore, the higher density of states in traps suppresses the higher-order virial coefficients, leading to an improved convergence of the expansion at low temperatures.

High-T thermodynamics in free space.—Using relation (12), we may determine the third virial coefficient in free space: $b_{3,\infty}^{\rm hom} \approx -0.290\,952\,95$. This does not agree with a previous field-theoretic calculation reported by Rupak [12], $b_{3,\infty}^{\rm hom} \approx 1.11$. As well, we may calculate the high-T thermodynamics in free space, by taking $\alpha = 1$ and $Q_1 = 2V(mk_B T/2\pi\hbar^2)^{3/2}$ in Eqs. (10) and (11). Figure 4 presents the interaction energy $E_{\rm int}$ of a homogeneous Fermi gas at unitarity as a function of temperature. For comparison, we also show the results of two quantum Monte Carlo simulations. The virial expansion in free space seems to converge at $T > 2T_F$.

In conclusion, we have shown that the virial expansion converges rapidly for a degenerate, resonant Fermi gas in a harmonic trap. This allows us to investigate the thermodynamics in a controllable way. We have proposed a practical method to obtain the third virial coefficient throughout BCS-BEC crossover. Higher-order coefficients are calculable in a similar manner, and may hold the prospect of revealing the exact thermodynamics of resonant Fermi gases in the deep degenerate regime. The current work provides a useful benchmark on testing future experiments and quantum Monte Carlo simulations on strongly interacting Fermi gases.

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