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Third- and Fourth-Order Virial Coefficients of Harmonically Trapped Fermions in a Semiclassical Approximation

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Third- and fourth-order virial coefficients of harmonically trapped fermions in a semiclassical approximation

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Using a leading-order semiclassical approximation, we calculate the third- and fourth-order virial coefficients of nonrelativistic spin-$1/2$ fermions in a harmonic trapping potential in arbitrary spatial dimensions, and as functions of temperature, trapping frequency, and coupling strength. Our simple, analytic results for the interaction-induced changes Δb_3 and Δb_4 agree qualitatively, and in some regimes quantitatively, with previous numerical calculations for the unitary limit of three-dimensional Fermi gases.

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I. INTRODUCTION

The properties of fermions at finite temperature and density are in part governed by the dimensionless product $\beta\mu$, where $\beta = 1/(k_B T)$ is the inverse temperature and μ is the chemical potential. Typically, the region $\beta\mu \simeq 0$ displays a crossover between quantum and classical physics, while $z = e^{\beta\mu} \ll 1$ indicates a dilute limit where the thermodynamics is given by the virial expansion, which expands a given physical quantity in powers of z. Since μ is coupled to the particle number N, the virial expansion at order N contains the physics of the N-body problem. In the simplest case, the coefficients b_n of the virial expansion determine the pressure, density, and compressibility, as well as other elementary thermodynamic quantities such as energy and entropy. The change in b_n due to interactions is usually denoted Δb_n.

The previous work of Ref. [1] calculated the third- and fourth-order virial coefficients Δb_3 and Δb_4, respectively, at leading order (LO) in a semiclassical lattice approximation (SCLA), of homogeneous spin-$1/2$ fermions in arbitrary dimension. The follow-up work of Ref. [2] extended those results up to Δb_7, while Ref. [3] carried out calculations up to next-to-next-to-leading order in the SCLA for up to Δb_5. In this article we provide another piece of the puzzle by generalizing the calculations of Ref. [1] to systems in a harmonic trap of frequency ω. We present our derivations with intermediate steps in detail and give analytic formulas for Δb_3 and Δb_4 as functions of $\beta\omega$ in arbitrary spatial dimension d. Our results, which will be given in terms of Δb_2, are thus also functions of the coupling strength.

II. HAMILTONIAN AND FORMALISM

As our focus is on systems with short-range interactions, such as dilute atomic gases or dilute neutron matter, the Hamiltonian reads

$$\hat{H} = \hat{H}_0 + \hat{V}_{\text{int}}, \tag{1}$$

where

$$\hat{H}_0 = \hat{T} + \hat{V}_{\text{ext}}, \tag{2}$$

and

$$\hat{T} = \sum_{s=1,2} \int d^d x\, \hat{\psi}_s^\dagger(\mathbf{x}) \left(-\frac{\hbar^2 \nabla^2}{2m} \right) \hat{\psi}_s(\mathbf{x}) \tag{3}$$

is the kinetic energy,

$$\hat{V}_{\text{ext}} = \frac{1}{2} m\omega^2 \int d^d x\, \mathbf{x}^2 [\hat{n}_1(\mathbf{x}) + \hat{n}_2(\mathbf{x})], \tag{4}$$

is the spherically symmetric external trapping potential, and

$$\hat{V}_{\text{int}} = -g_d \int d^d x\, \hat{n}_1(\mathbf{x}) \hat{n}_2(\mathbf{x}), \tag{5}$$

is the interaction.

In the above equations, the field operators $\hat{\psi}_s, \hat{\psi}_s^\dagger$ correspond to particles of species $s = 1, 2$, and $\hat{n}_s(\mathbf{x})$ are the coordinate-space densities. For the remainder of this work, we will set $\hbar = k_B = m = 1$.

A. Thermodynamics and the virial expansion

The equilibrium thermodynamics of our quantum many-body system can be captured by the grand-canonical partition function, namely,

$$\mathcal{Z} = \text{tr}[e^{-\beta(\hat{H} - \mu\hat{N})}] = e^{-\beta\Omega}, \tag{6}$$

where β is the inverse temperature, Ω is the grand thermodynamic potential, $\hat{N}$ is the total particle number operator, and μ is the overall chemical potential (we will not consider polarized systems in this work).

As the calculation of $\mathcal{Z}$ is a formidable problem in the presence of interactions, we resort to approximations or numerical evaluations in order to access the thermodynamics. To that end, in this work we will use the virial expansion, which is an expansion around the dilute limit $z \to 0$, where $z = e^{\beta\mu}$ is the fugacity, i.e., it is a low-fugacity expansion (see Ref. [4] for a review on recent applications of the virial expansion to ultracold atoms). The coefficients accompanying the powers of z in the expansion Ω are the virial coefficients b_n,

$$-\beta\Omega = \ln \mathcal{Z} = Q_1 \sum_{n=1}^{\infty} b_n z^n, \tag{7}$$

where Q_1 is the one-body partition function. Using the fact that $\mathcal{Z}$ is itself a sum over canonical partition functions Q_N of all possible particle numbers N, namely,

$$\mathcal{Z} = \sum_{N=0}^{\infty} z^N Q_N, \tag{8}$$

we obtain expressions for the virial coefficients

$$b_1 = 1, \tag{9}$$

$$b_2 = \frac{Q_2}{Q_1} - \frac{Q_1}{2!}, \tag{10}$$

$$b_3 = \frac{Q_3}{Q_1} - b_2 Q_1 - \frac{Q_1^2}{3!}, \tag{11}$$

$$b_4 = \frac{Q_4}{Q_1} - \left(b_3 + \frac{b_2^2}{2}\right)Q_1 - b_2\frac{Q_1^2}{2!} - \frac{Q_1^3}{4!}, \tag{12}$$

and so on. In this work we will not pursue the virial expansion beyond b_4. The Q_N can themselves be written in terms of the partition functions $Q_{a,b}$ for a particles of type 1 and b particles of type 2,

$$Q_1 = 2Q_{1,0}, \tag{13}$$

$$Q_2 = 2Q_{2,0} + Q_{1,1}, \tag{14}$$

$$Q_3 = 2Q_{3,0} + 2Q_{2,1}, \tag{15}$$

$$Q_4 = 2Q_{4,0} + 2Q_{3,1} + Q_{2,2}, \tag{16}$$

and so on for higher orders. In the absence of intraspecies interactions, only $Q_{1,1}$, $Q_{2,1}$, $Q_{3,1}$, and $Q_{2,2}$ are affected, such that the change in b_2, b_3, and b_4 due to interactions is entirely given by

$$\Delta b_2 = \frac{\Delta Q_{1,1}}{Q_1}, \tag{17}$$

$$\Delta b_3 = \frac{2\Delta Q_{2,1}}{Q_1} - \Delta b_2 Q_1, \tag{18}$$

$$\Delta b_4 = \frac{2\Delta Q_{3,1} + \Delta Q_{2,2}}{Q_1} - \Delta\left(b_3 + \frac{b_2^2}{2}\right)Q_1 - \frac{\Delta b_2}{2}Q_1^2. \tag{19}$$

To calculate $\Delta Q_{m,n}$, we implement a semiclassical approximation, as described in the next section. Once we obtain the virial coefficients, one may rebuild the grand-canonical potential Ω to access the thermodynamics of the system as a function of the various parameters.

In order to connect to the *physical* parameters of the systems at hand, we will use the value of Δb_2 as a renormalization condition by relying on the exact answers as functions of $\beta\omega$ and the physical coupling λ. These exact answers are not always known analytically, but they can easily be obtained numerically by solving the two-body problem of interest.

Although in this work we will focus on systems in a harmonic trap, thus far the identities presented in this section are more general. As a reference for the trapped case, we present here the calculation of the noninteracting virial coefficients for arbitrary $\beta\omega$. (We note that such a calculation, while simple, does not appear in the literature.) Starting from the logarithm of the noninteracting partition function in d spatial dimensions, we have, for two fermion species,

$$\ln \mathcal{Z} = 2\sum_{\mathbf{n}} \ln\left(1 + z e^{-\beta\omega d/2}\prod_{i=1}^{d} e^{-\beta\omega n_i}\right). \tag{20}$$

Expanding in powers of z on both sides, and switching the order of the sums, we obtain

$$\begin{aligned} Q_1 \sum_{k=1}^{\infty} b_k^0 z^k &= 2\sum_{k=1}^{\infty} z^k \frac{(-1)^{k+1}}{k} e^{-\beta\omega dk/2}\left(\sum_{n=0}^{\infty} e^{-\beta\omega kn}\right)^d \\ &= 2\sum_{k=1}^{\infty} z^k \frac{(-1)^{k+1}}{2^d k}\left(\frac{1}{\sinh(\beta\omega k/2)}\right)^d. \end{aligned} \tag{21}$$

To identify the noninteracting virial coefficients b_n^0, we need Q_1,

$$Q_1 = 2\sum_{\mathbf{n}} e^{-\beta E_n} = 2e^{-\beta\omega d/2}\left(\frac{1}{1 - e^{-\beta\omega}}\right)^d \tag{22}$$

$$= 2\left(\frac{1}{2\sinh(\beta\omega/2)}\right)^d. \tag{23}$$

Thus, the virial coefficients of a trapped noninteracting spin-1/2 Fermi gas in d dimensions are

$$b_n^0 = \frac{(-1)^{n+1}}{n}\left(\frac{\sinh(\beta\omega/2)}{\sinh(\beta\omega n/2)}\right)^d. \tag{24}$$

Notably, in the limit $\beta\omega \ll 1$, we obtain

$$b_n^0 \to (-1)^{n+1}\left(\frac{1}{n}\right)^{d+1}, \tag{25}$$

which agrees in $d = 3$ with the local density approximation result quoted in Ref. [4]. The simple result of Eq. (24) should be a textbook calculation, but it does not appear elsewhere, to the best of our knowledge. Note that for the homogeneous (i.e., untrapped) system, the noninteracting virial coefficients in d dimensions are

$$b_n^{0,\text{hom}} = (-1)^{n+1}\left(\frac{1}{n}\right)^{\frac{d}{2}+1}, \tag{26}$$

such that $b_n^0 = b_n^{0,\text{hom}} n^{-\frac{d}{2}}$ for $\beta\omega \ll 1$.

B. Semiclassical lattice approximation

To calculate the interaction-induced change $\Delta Q_{m,n}$, we implement an approximation which consists in keeping the leading term in the commutator expansion,

$$e^{-\beta(\hat{H}_0 + \hat{V}_{\text{int}})} = e^{-\beta\hat{H}_0} e^{-\beta\hat{V}_{\text{int}}} \times e^{-\frac{\beta^2}{2}[\hat{H}_0, \hat{V}_{\text{int}}]} \times \cdots, \tag{27}$$

where the higher orders involve exponentials of nested commutators of $\hat{H}_0$ with $\hat{V}_{\text{int}}$. Thus, the leading order in this expansion consists in setting $[\hat{H}_0, \hat{V}_{\text{int}}] = 0$, which corresponds to a semiclassical approximation. Another way to see this approximation is in terms of a Trotter-Suzuki factorization, i.e.,

$$e^{-\beta(\hat{H}_0 + \hat{V}_{\text{int}})} = \lim_{n\to\infty} (e^{-\beta\hat{H}_0/n} e^{-\beta\hat{V}_{\text{int}}/n})^n, \tag{28}$$

where the $n = 1$ case is the leading order we pursue in this work and higher orders can be defined by increasing n.

C. Example: Calculation of $\Delta Q_{1,1}$ and Δb_2

In the approximation proposed above, the two-particle problem is analyzed as follows:

$$\begin{aligned} Q_{1,1} &= \mathrm{Tr}[e^{-\beta \hat{H}_0} e^{-\beta \hat{V}_{\mathrm{int}}}] \\ &= \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{x}_1,\mathbf{x}_2} \langle \mathbf{k}_1\mathbf{k}_2| e^{-\beta \hat{H}_0} |\mathbf{x}_1\mathbf{x}_2\rangle \langle \mathbf{x}_1\mathbf{x}_2| e^{-\beta \hat{V}_{\mathrm{int}}} |\mathbf{k}_1\mathbf{k}_2\rangle \\ &= \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{x}_1,\mathbf{x}_2} e^{-\beta(E_{\mathbf{k}_1}+E_{\mathbf{k}_2})} M_{\mathbf{x}_1,\mathbf{x}_2} |\langle \mathbf{k}_1\mathbf{k}_2|\mathbf{x}_1\mathbf{x}_2\rangle|^2, \end{aligned} \tag{29}$$

where we have inserted complete sets of states in coordinate space $\{|\mathbf{x}_1\mathbf{x}_2\rangle\}$ and in the basis $|\mathbf{k}_1\mathbf{k}_2\rangle$ of eigenstates of $\hat{H}_0$, whose single-particle eigenstates $|\mathbf{k}\rangle$ have eigenvalues $E_{\mathbf{k}}$. We have also made use of the fact that $\hat{V}_{\mathrm{int}}$ is diagonal in coordinate space, such that

$$M_{\mathbf{x}_1,\mathbf{x}_2} = 1 + C\delta_{\mathbf{x}_1,\mathbf{x}_2}, \tag{30}$$

where

$$C = (e^{\beta g_d} - 1)\ell^d. \tag{31}$$

Here [5], we treated the interaction by placing the system on a spatial lattice of spacing ℓ, as in Ref. [2], which will set the scale for all the dimensionful quantities from this point on. We therefore assume from this point on that any remaining powers of ℓ have been absorbed into g_d, which now represents a lattice coupling, such that the combination βg_d is dimensionless.

Thus,

$$\Delta Q_{1,1} = C \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{x}} \ell^d\, e^{-\beta(E_{\mathbf{k}_1}+E_{\mathbf{k}_2})} |\phi_{\mathbf{k}_1}(\mathbf{x})|^2 |\phi_{\mathbf{k}_2}(\mathbf{x})|^2, \tag{32}$$

and we will use normalized single-particle wave functions in Cartesian coordinates which in one dimension (1D) take the form

$$\phi_n(x) = \frac{1}{\sqrt{2^n n!}} \left(\frac{\omega}{\pi}\right)^{1/4} e^{-\omega x^2/2} H_n(\sqrt{\omega}x), \tag{33}$$

where the H_n are Hermite polynomials. We note in passing that, in d dimensions, $\phi_{\mathbf{k}}(\mathbf{x})$ has units of $\ell^{-d/2}$, since ω has units of ℓ^{-2}; thus, $\Delta Q_{1,1}$ is dimensionless as expected.

The sums over $\mathbf{k}_1$ and $\mathbf{k}_2$ in Eq. (32) are independent and identical and take the form

$$\sum_{n=0}^{\infty} e^{-\beta E_n} |\phi_n(x)|^2 = \sqrt{\frac{\omega}{\pi}} e^{-\beta\omega/2 - \omega x^2} G(\beta\omega, \sqrt{\omega}x), \tag{34}$$

for each Cartesian dimension, where the function G can be calculated as a special case of Mehler's formula [6],

$$G(k, y) \equiv \sum_{n=0}^{\infty} \frac{e^{-kn}}{2^n n!} [H_n(y)]^2 = \frac{\exp[2y^2/(1+e^k)]}{\sqrt{1-e^{-2k}}}.$$

This formula encodes the finite-temperature, single-particle density matrix of a noninteracting, nonrelativistic system in a harmonic trapping potential, and therefore its use is essential in the calculations that follow.

Squaring the result, we obtain, in one spatial dimension,

$$\begin{aligned} \Delta Q_{11} &= 2C \int_0^{\infty} dx \frac{\omega}{2\pi \sinh(\beta\omega)} \exp[-2\omega x^2 \tanh(\beta\omega/2)] \\ &= C \frac{\sqrt{\omega}}{4} \frac{1}{\sqrt{\pi \sinh(\beta\omega)} \sinh(\beta\omega/2)}, \end{aligned} \tag{35}$$

where we have performed the last Gaussian integral along with some hyperbolic function simplifications. Note that ΔQ_{11} is a dimensionless quantity; we have, in the above equation, implicitly replaced a sum with an integral by taking the continuum limit. In doing so, notice that C has dimensions of ℓ^d [see Eqs. (30) and (31), and formulas below].

Generalizing to d spatial dimensions,

$$\Delta Q_{11} = C \left[\frac{\sqrt{\omega}}{4} \frac{1}{\sqrt{\pi \sinh(\beta\omega)} \sinh(\beta\omega/2)} \right]^d. \tag{36}$$

Using Eq. (22), we find that Q_1 cancels exactly in the final expression, as expected, such that

$$\Delta b_2 = \frac{C}{2} \left[\frac{\sqrt{\omega}}{2\sqrt{\pi \sinh(\beta\omega)}} \right]^d = \frac{C}{\lambda_T^d} \frac{1}{2} \left[\frac{\beta\omega}{2\sinh(\beta\omega)} \right]^{\frac{d}{2}}, \tag{37}$$

where we have used the thermal wavelength $\lambda_T = \sqrt{2\pi\beta}$ to write the result in as a function of $\beta\omega$.

As mentioned above, we will use this result to connect to the physical coupling λ of a given system, as a renormalization condition at a given value of $\beta\omega$. To that end, we first solve for C/λ_T^d,

$$\frac{C}{\lambda_T^d} = 2\Delta b_2 \left[\frac{2\sinh(\beta\omega)}{\beta\omega} \right]^{\frac{d}{2}}. \tag{38}$$

In the unitary limit of the 3D Fermi gas [7], for instance, the exact answer for Δb_2 is known [4],

$$\Delta b_2 = \frac{1}{2} \left(\frac{e^{-\beta\omega/2}}{1 + e^{-\beta\omega}} \right) = \frac{1}{4\cosh(\beta\omega/2)}. \tag{39}$$

Using that result in Eq. (38) yields

$$\frac{C}{\lambda_T^3} = \frac{e^{-\beta\omega/2}}{1 + e^{-\beta\omega}} \left[\frac{2\sinh(\beta\omega)}{\beta\omega} \right]^{3/2}. \tag{40}$$

As we will show below, this type of renormalization is very practical as our results for Δb_3 and Δb_4 are simple quadratic functions of C/λ_T^d with $\beta\omega$-dependent coefficients.

III. RESULTS

Following the steps outlined above in the example calculation of Δb_2, we have calculated the various contributions to Δb_3 and Δb_4, which we present in this section. In all cases, the central component of the calculation is the use of the analytic form of Mehler's kernel, which effectively reduces the calculation to a small number of Gaussian integrals.

A. Result for $\Delta Q_{2,1}$ and Δb_3

With small modifications to the example for Δb_2, it is straightforward to show that

$$\begin{aligned} \Delta Q_{2,1} = & \frac{C}{\lambda_T^d} \left[\frac{\beta\omega}{4\sinh^3(\beta\omega)} \right]^{\frac{d}{2}} \\ & \times \left[\frac{1}{2^{\frac{d}{2}} \tanh^d(\beta\omega/2)} - \left(\frac{2\cosh^2(\beta\omega/2)}{4\cosh^2(\beta\omega/2) - 1} \right)^{\frac{d}{2}} \right], \end{aligned} \tag{41}$$

and using the results of the previous section, it is easy to assemble the final answer for Δb_3 in our approximation using

$$\Delta b_3 = \frac{2\Delta Q_{2,1}}{Q_1} - \Delta b_2 Q_1. \tag{42}$$

Note that Q_1 diverges in the $\beta\omega \to 0$ limit, but that divergence will cancel out in the final expression for Δb_3. Indeed, after simplifications, we obtain

$$\Delta b_3 = -\frac{C}{\lambda_T^d}\left[\frac{\beta\omega}{2\sinh(\beta\omega)}\right]^{\frac{d}{2}}\left(\frac{1}{4\cosh^2(\beta\omega/2)-1}\right)^{\frac{d}{2}}, \tag{43}$$

which is manifestly finite in the $\beta\omega \to 0$ limit. In that limit,

$$\Delta b_3 \to -\frac{C}{\lambda_T^d}\frac{1}{6^{\frac{d}{2}}}. \tag{44}$$

We recall the result of Ref. [1] for the homogeneous case, namely,

$$\Delta b_3^{\text{hom}} = -\frac{C}{\lambda_T^d}\frac{1}{2^{\frac{d}{2}}}, \tag{45}$$

which shows that the relationship between the homogeneous and trapped cases, pointed out in the Introduction, is also satisfied once interactions are turned on.

B. Result for $\Delta Q_{3,1}$, $\Delta Q_{2,2}$, and Δb_4

Again following the steps outlined above, we obtain

$$\begin{aligned}\frac{2\Delta Q_{3,1}}{Q_1} = \frac{C}{2\lambda_T^d}\left[\frac{\sqrt{2\beta\omega}\sinh(\beta\omega/2)}{2\sinh^2(\beta\omega)}\right]^d\Bigg\{&\left(\frac{1}{2\tanh^3(\beta\omega/2)}\right)^{\frac{d}{2}} + 2\tanh^{\frac{d}{2}}(\beta\omega)\left(\frac{\cosh(\beta\omega)+1}{2\cosh(\beta\omega)+1}\right)^{\frac{d}{2}} \\ &- 2\coth^{\frac{d}{2}}(\beta\omega/2)\left(\frac{\cosh(\beta\omega)+1}{2\cosh(\beta\omega)+1}\right)^{\frac{d}{2}} - \left(\frac{1}{2\tanh(\beta\omega/2)}\right)^{\frac{d}{2}}\Bigg\},\end{aligned} \tag{46}$$

$$\begin{aligned}\frac{\Delta Q_{2,2}}{Q_1} = \frac{C}{2\lambda_T^d}\left[\frac{\sqrt{2\beta\omega}\sinh(\beta\omega/2)}{2\sinh^2(\beta\omega)}\right]^d\Bigg\{&\left(\frac{1}{2\tanh^3(\beta\omega/2)}\right)^{\frac{d}{2}} - 2\coth^{\frac{d}{2}}(\beta\omega/2)\left(\frac{\cosh(\beta\omega)+1}{2\cosh(\beta\omega)+1}\right)^{\frac{d}{2}} + \left(\frac{\tanh(\beta\omega)}{2}\right)^{\frac{d}{2}} \\ &+ \left(\frac{C}{2\lambda_T^d}\right)\frac{(2\beta\omega)^{\frac{d}{2}}}{2^d}\left[\frac{1}{\tanh^d(\beta\omega/2)} + 1 - 2[\operatorname{sech}(\beta\omega)+1]^{\frac{d}{2}}\right]\Bigg\}.\end{aligned} \tag{47}$$

Combining these with results from the previous sections, the final answer for Δb_4 can be assembled using

$$\Delta b_4 = \frac{2\Delta Q_{3,1} + \Delta Q_{2,2}}{Q_1} - \Delta\left(b_3 + \frac{b_2^2}{2}\right)Q_1 - \frac{\Delta b_2}{2}Q_1^2. \tag{48}$$

After several simplifications and cancellations (which can be tracked by their degree of divergence as $\beta\omega \to 0$, while the final result for Δb_4 is finite), we obtain

$$\begin{aligned}\Delta b_4 = &\frac{C}{2\lambda_T^d}\left[\frac{\sqrt{2\beta\omega}\sinh(\beta\omega/2)}{2\sinh^2(\beta\omega)}\right]^d \\ &\times\Bigg\{2\tanh^{\frac{d}{2}}(\beta\omega)\left(\frac{\cosh(\beta\omega)+1}{2\cosh(\beta\omega)+1}\right)^{\frac{d}{2}} + \left(\frac{\tanh(\beta\omega)}{2}\right)^{\frac{d}{2}} \\ &+ \left(\frac{C}{2\lambda_T^d}\right)\frac{(2\beta\omega)^{\frac{d}{2}}}{2^d}[1-2[\operatorname{sech}(\beta\omega)+1]^{\frac{d}{2}}]\Bigg\}.\end{aligned} \tag{49}$$

In this case, the limit $\beta\omega \to 0$ yields

$$\Delta b_4 \to \frac{C}{\lambda_T^d}4^{-\frac{d}{2}}(3^{-\frac{d}{2}} + 2^{-d-1}) + \left(\frac{C}{\lambda_T^d}\right)^2 4^{-d-1}(1-2^{\frac{d}{2}+1}). \tag{50}$$

Once again, we recall the homogeneous result

$$\Delta b_4^{\text{hom}} = \frac{C}{\lambda_T^d}\left(3^{-\frac{d}{2}} + 2^{-d-1}\right) + \left(\frac{C}{\lambda_T^d}\right)^2 4^{-\frac{d}{2}-1}\left(1-2^{\frac{d}{2}+1}\right), \tag{51}$$

and find that $\Delta b_4 = \Delta b_4^{\text{hom}} 4^{-\frac{d}{2}}$, as expected.

C. Results in terms of Δb_2

Finally, collecting our results for Δb_3 and Δb_4 and expressing them in terms of Δb_2 [via Eq. (38)], we obtain

$$\Delta b_3 = -2\left(\frac{1}{4\cosh^2(\beta\omega/2)-1}\right)^{\frac{d}{2}}\Delta b_2, \tag{52}$$

and

$$\Delta b_4 = \left(\frac{1}{2\cosh(\beta\omega)}\right)^{\frac{d}{2}} f_1(\beta\omega, d)\Delta b_2 + f_2(\beta\omega, d)(\Delta b_2)^2, \tag{53}$$

where

$$f_1(\beta\omega, d) = \left(\frac{1}{2\cosh(\beta\omega/2)}\right)^d + 2\left(\frac{1}{4\cosh^2(\beta\omega/2)-1}\right)^{\frac{d}{2}}, \tag{54}$$

and

$$f_2(\beta\omega, d) = \left(\frac{1}{2\cosh(\beta\omega/2)}\right)^d - 2\left(\frac{1}{4\cosh^2(\beta\omega/2)-2}\right)^{\frac{d}{2}}. \tag{55}$$

The above formulas for Δb_3 and Δb_4 are the main result of this work. In the following, we explore their behavior as a function of d and $\beta\omega$, focusing in particular on the unitary limit of the 3D Fermi gas. While numerical results exist for

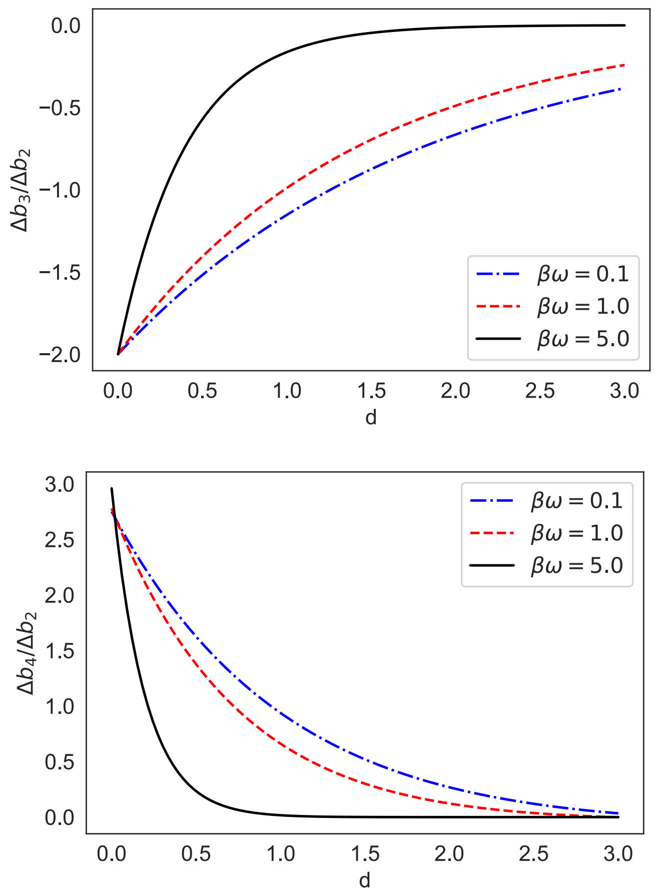

FIG. 1. $\Delta b_3/\Delta b_2$ (top) and $\Delta b_4/\Delta b_2$ (bottom) as functions of the spatial dimension d at fixed $\beta\omega = 0.1$, 1.0, and 5.0, for Δb_2 corresponding to the unitary limit in $d = 3$, Eq. (39).

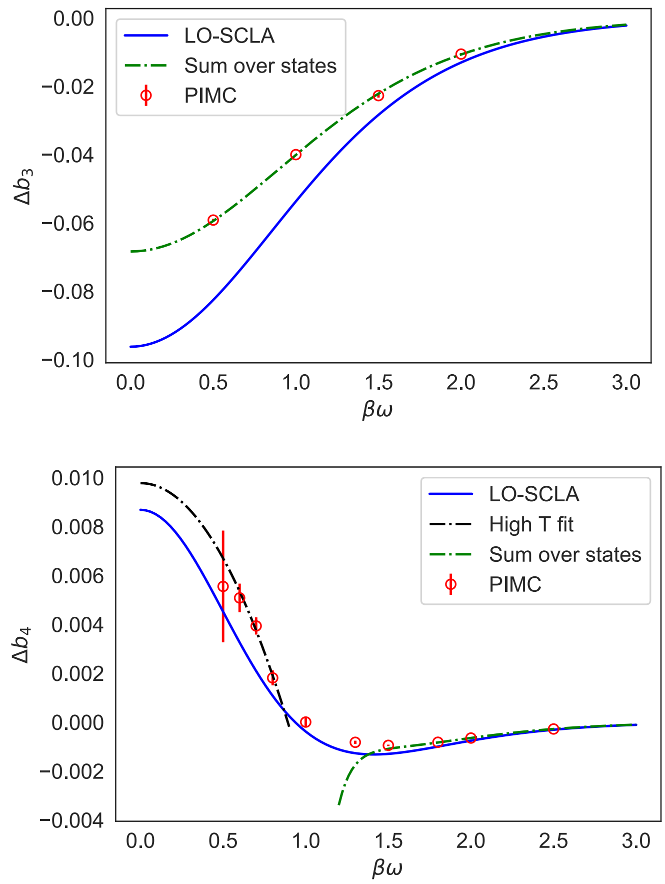

FIG. 2. Comparison of our LO-SCLA results for Δb_3 (top) and Δb_4 (bottom) as a function of $\beta\omega$. The high-temperature fits and PIMC results are from Ref. [20]; the sum-over-states results are from Ref. [21].

these quantities in some cases, in particular in 2D [8–11] (see also Refs. [12–14]) and in 3D at unitarity [15–19], most of those correspond to homogeneous systems and do not feature explicit, analytic dependence on the dimension nor on $\beta\omega$, as shown here. Our results are therefore useful in that they are able to provide analytic insight into the behavior of virial coefficients across dimensions, and as a function of the temperature (or trapping frequency) as well as the coupling strength. Below, we evaluate our formulas and discuss the resulting answers.

D. Qualitative behavior

To illustrate our analytic results, in Fig. 1 we show $\Delta b_3/\Delta b_2$ and $\Delta b_4/\Delta b_2$ as a function of the spatial dimension d, at various $\beta\omega$, fixing Δb_2 to its value in the unitary limit (as a reference point). We find that, as d increases, the magnitude of the interaction-induced change Δb_n decreases. This suggests that, using Δb_2 as the fixed, dimension-independent coupling, the radius of convergence of the virial expansion increases with d. This is consistent with the idea that, in higher dimensions, the kinetic energy dominates over the interactions and mean-field type of approaches capture the behavior of the system correctly.

As a comparison with previous calculations, we show in Fig. 2 our results in 3D at unitarity as a function of $\beta\omega$, superimposed with the data from Ref. [20]. While we do not expect, *a priori*, good quantitative agreement in this strong-coupling regime, we find at least qualitative agreement for both Δb_3 and Δb_4, and surprisingly good agreement at the quantitative level for Δb_4. Clearly, the LO-SCLA is able to capture more than just the shape of the $\beta\omega$ dependence of the virial coefficients.

IV. SUMMARY AND CONCLUSIONS

In this article we have implemented a semiclassical approximation, at leading order, to calculate the virial coefficients Δb_3 and Δb_4 of harmonically trapped Fermi gases. Our calculations yield analytic answers as functions of $\beta\omega$ and, by defining the lattice coupling C so as to match Δb_2 to the known exact result, we also obtain the dependence on the physical coupling strength. Notably, our results are also analytic functions of the spatial dimension d, allowing us to study the behavior of the virial expansion across dimensions. We find that, at fixed Δb_2, the magnitude of Δb_n decreases as d increases, for all $\beta\omega$.

Although there have been many (and very precise) determinations of virial coefficients in the literature, they are mostly numerical and focus on specific dimensions or couplings (and most of them are for homogeneous systems). Our approach and results are, in that sense, complementary: We do not expect high precision from the LO-SCLA, but through it we are able to study, explicitly, the variations with the parameters of the problem, which yield qualitative analytic insight into the properties of the virial expansion. We have demonstrated the quality of our leading-order results for Δb_3 and Δb_4 in the unitary limit by showing that they qualitatively follow the expected answers, which is an encouraging sign to proceed to next-to-leading order in future work. Furthermore, the approximate agreement with prior results at unitarity suggests that, between the noninteracting regime and the unitary point, that agreement should be even better than shown here.

We would like to stress that the calculation presented here is nonperturbative in the same sense as in lattice Monte Carlo approaches, except that we have implemented a very coarse temporal lattice. Increasing the order of the approximation (beyond LO-SCLA studied here) amounts to reducing the temporal lattice spacing effects. Those effects disappear in the limit where either $\hat{H}_0$ or $\hat{V}_{\rm int}$ appear on their own. When both are present, the regime of validity of the SCLA at a given order is controlled by the magnitude of the commutator $[\hat{H}_0, \hat{V}_{\rm int}]$, i.e., it will depend on the coupling strength.

Finally, it should be pointed out that the renormalization of the lattice theory based on Δb_2 does not by itself eliminate all the lattice artifacts. Future studies should explore the use of improved actions (see, e.g., Refs. [22,23]), potentially making use of prior knowledge of Δb_3 where available, to enhance the quality of the expansion.

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