Virial coefficients of trapped and untrapped three-component fermions with three-body forces in arbitrary spatial dimensions

A. J. Czejdo, J. E. Drut,* Y. Hou, J. R. McKenney, and K. J. Morrell
Department of Physics and Astronomy, University of North Carolina, Chapel Hill, North Carolina 27599, USA

(Received 30 March 2020; accepted 12 June 2020; published 29 June 2020)

Using a coarse temporal lattice approximation, we calculate the first few terms of the virial expansion of a three-species fermion system with a three-body contact interaction in d spatial dimensions, both in homogeneous space and in a harmonic trapping potential of frequency ω. Using the three-body problem to renormalize, we report analytic results for the change in the fourth- and fifth-order virial coefficients Δb_4 and Δb_5 as functions of Δb_3. Additionally, we argue that in the $\omega \to 0$ limit the relationship $b_n^{\mathrm{T}} = n^{-d/2} b_n$ holds between the trapped (T) and the homogeneous coefficients for *arbitrary* temperature and coupling strength (not merely in scale-invariant regimes). Finally, we point out an exact, universal (coupling- and frequency-independent) relationship between Δb_3^{T} in one dimension with three-body forces and Δb_2^{T} in two dimensions with two-body forces.

DOI: 10.1103/PhysRevA.101.063630

I. INTRODUCTION

Motivated by the recent interest in one-dimensional (1D) Fermi and Bose gases in the fine-tuned situation where only three-body interactions are present [1–9], we explore here the thermodynamics of fermions with a contact three-body interaction in the region of low fugacity (which corresponds to a dilute regime and therefore high temperatures in units of the energy scale set by the density). We focus on the fermionic case but explore the problem in arbitrary dimension d. To that end, we implement a semiclassical lattice approximation (SCLA) to calculate the virial coefficients b_n and carry out their evaluation up to $n = 5$ at leading order (LO) in that approximation.

The LO-SCLA was introduced in Ref. [10] as a way to estimate virial coefficients in two-component Fermi gases. The approximation seems crude in its definition but performs surprisingly well when the lowest nontrivial order in the virial expansion is used as a renormalized coupling constant (b_2 for two-body forces, for example, and b_3 in this work). Not surprisingly, the approximation was seen to work better at weak coupling, which makes sense, as the radius of convergence of the virial expansion was found to be quickly reduced as a result of the interaction. In Ref. [11] the next-to-leading-order SCLA was explored up to b_7, displaying the convergence properties up to the unitary point (in three dimensions), and in Ref. [12] the LO-SCLA was used for systems in a harmonic trap, showing that the approximation can capture the dependence on the trap frequency ω. In both cases, the analytic dependence of virial coefficients on the dimension was obtained, as is the case here. This is to be contrasted with conventional methods to calculate virial coefficients, which can be very precise but are limited to specific situations (coupling strength, dimension, etc.) and are typically unable to provide analytic insight, as they are entirely numerical.

Our analytic formulas for the virial coefficients, although approximate, support and shed light on the relationship $b_n^{\mathrm{T}} \to n^{-d/2} b_n$ in the $\omega \to 0$ limit, where the superindex T indicates the harmonically trapped situation. This connection is well known to be valid in the noninteracting limit and in the so-called unitary limit of spin-1/2 fermions in three dimensions, both of which feature temperature-independent coefficients b_n. As we argue, that relationship is actually valid for all temperatures and coupling constants and holds for three-body interactions just as well as for two-body interactions. Finally, we point out an exact, coupling- and frequency-independent relationship between Δb_3^{T} in one dimension with three-body forces and Δb_2^{T} in two dimensions with two-body forces.

II. HAMILTONIAN AND VIRIAL EXPANSION

We focus on a nonrelativistic Fermi system with a three-body contact interaction, such that the Hamiltonian for three flavors 1, 2, 3 is $\hat{H} = \hat{T} + \hat{V}$, where

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

and

$$\hat{V} = -g_d \int d^d x\, \hat{n}_1(\mathbf{x}) \hat{n}_2(\mathbf{x}) \hat{n}_3(\mathbf{x}), \tag{2}$$

where the field operators $\hat{\psi}_s$ and $\hat{\psi}_s^{\dagger}$ are fermionic fields for particles of types 1, 2, 3 (summed over s above), and $\hat{n}_s(\mathbf{x})$ are the coordinate-space densities. In the remainder of this work, we take $\hbar = k_{\mathrm{B}} = m = 1$. Besides the above, we also consider the case in which an external trapping potential term is added to the Hamiltonian, of the form

$$\hat{V}_{\mathrm{ext}} = \frac{1}{2} m \omega^2 \int d^d x\, \mathbf{x}^2 [\hat{n}_1(\mathbf{x}) + \hat{n}_2(\mathbf{x}) + \hat{n}_3(\mathbf{x})]. \tag{3}$$

*drut@email.unc.edu

One way to characterize the thermodynamics of the above system is through the virial expansion [13], 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, where β is the inverse temperature and μ the chemical potential coupled to the total particle number operator $\hat{N}$. The coefficients accompanying the powers of z in the expansion of the grand-canonical potential Ω are the virial coefficients; specifically,

$$-\beta\Omega = \ln \mathcal{Z} = Q_1 \sum_{n=1}^{\infty} b_n z^n, \tag{4}$$

where

$$\mathcal{Z} = \mathrm{Tr}[e^{-\beta(\hat{H}-\mu\hat{N})}] = \sum_{N=0}^{\infty} z^N Q_N \tag{5}$$

is the grand-canonical partition function, Q_1 is the one-body partition function, $b_1 = 1$, and the higher-order coefficients require solving the corresponding few-body problems,

$$Q_1 b_2 = Q_2 - \frac{Q_1^2}{2!}, \tag{6}$$

$$Q_1 b_3 = Q_3 - b_2 Q_1^2 - \frac{Q_1^3}{3!}, \tag{7}$$

$$Q_1 b_4 = Q_4 - \left(b_3 + \frac{b_2^2}{2}\right) Q_1^2 - b_2 \frac{Q_1^3}{2!} - \frac{Q_1^4}{4!}, \tag{8}$$

$$Q_1 b_5 = Q_5 - (b_4 + b_2 b_3) Q_1^2 - \left(b_2^2 + b_3\right)\frac{Q_1^3}{2} - b_2 \frac{Q_1^4}{3!} - \frac{Q_1^5}{5!}, \tag{9}$$

and so forth.

Since $Q_1 \propto V$, the above expressions display precisely how the volume dependence cancels out in each b_n. In particular, the highest power of Q_1 will always involve single-particle (i.e., noninteracting) physics and will therefore cancel in the change due to interactions Δb_n, such that

$$Q_1 \Delta b_2 = \Delta Q_2, \tag{10}$$

$$Q_1 \Delta b_3 = \Delta Q_3 - \Delta b_2 Q_1^2, \tag{11}$$

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

$$Q_1 \Delta b_5 = \Delta Q_5 - \Delta(b_4 + b_2 b_3) Q_1^2 - \frac{1}{2}\Delta\left(b_2^2 + b_3\right) Q_1^3 - \frac{\Delta b_2}{3!} Q_1^4, \tag{13}$$

and so on. Note that, when only three-body interactions are present, as in the case we consider here, there is no change in the two-body spectrum, i.e., $\Delta b_2 = 0$. Therefore, the above expressions simplify to

$$Q_1 \Delta b_3 = \Delta Q_3, \tag{14}$$

$$Q_1 \Delta b_4 = \Delta Q_4 - \Delta b_3 Q_1^2, \tag{15}$$

$$Q_1 \Delta b_5 = \Delta Q_5 - (\Delta b_4 + b_2 \Delta b_3) Q_1^2 - \frac{\Delta b_3}{2} Q_1^3. \tag{16}$$

In terms of the partition functions Q_{MNL} of M particles of type 1, N of type 2, and L of type 3, we have

$$\Delta Q_3 = \Delta Q_{111}, \tag{17}$$

$$\Delta Q_4 = 3\Delta Q_{211}, \tag{18}$$

$$\Delta Q_5 = 3\Delta Q_{311} + 3\Delta Q_{221}. \tag{19}$$

From the above equations we see that there is only a small number of nontrivial contributions to each virial coefficient. The main task is calculating each of these terms and for that purpose we use a coarse lattice (or semiclassical) approximation, as explained next.

III. THE SEMICLASSICAL APPROXIMATION AT LEADING ORDER

To carry out our calculations of virial coefficients we introduce a Trotter-Suzuki factorization of the Boltzmann weight. At the lowest possible order, the Trotter-Suzuki factorization amounts to keeping only the leading term in the formula

$$e^{-\beta(\hat{T}+\hat{V})} = e^{-\beta\hat{T}} e^{-\beta\hat{V}} \times e^{-\frac{\beta^2}{2}[\hat{T},\hat{V}]} \times \dots, \tag{20}$$

where higher orders involve exponentials of nested commutators of $\hat{T}$ with $\hat{V}$. Taking the leading order in this expansion is equivalent to setting $[\hat{T}, \hat{V}] = 0$, which is why we refer to it as a semiclassical approximation. As Refs. [10–12] have shown, this seemingly crude approximation provides surprisingly good answers, especially at weak coupling, and is therefore useful toward examining the virial expansion in an analytic fashion. Below, we give two explicit examples of the application of our approximation to the calculation of virial coefficients.

A. A simple example: Δb_3

As the simplest example, we consider Q_{111},

$$Q_{111} = \sum_{\mathbf{p}_j} \langle \mathbf{P}| e^{-\beta\hat{T}} e^{-\beta\hat{V}} |\mathbf{P}\rangle \tag{21}$$

$$= \sum_{\mathbf{p}_j} e^{-\beta(p_1^2+p_2^2+p_3^2)/2m} \langle \mathbf{P}| e^{-\beta\hat{V}} |\mathbf{P}\rangle, \tag{22}$$

where we have used a collective momentum index $\mathbf{P} = (\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3)$. Inserting a coordinate-space completeness relation to evaluate the potential energy factor, we obtain

$$\begin{aligned} e^{-\beta\hat{V}}|\mathbf{X}\rangle &= \prod_{\mathbf{z}} (1 + C\hat{n}_1(\mathbf{z})\hat{n}_2(\mathbf{z})\hat{n}_3(\mathbf{z}))|\mathbf{X}\rangle \\ &= |\mathbf{X}\rangle + C\sum_{\mathbf{z}} \delta(\mathbf{x}_1 - \mathbf{z})\delta(\mathbf{x}_2 - \mathbf{z})\delta(\mathbf{x}_3 - \mathbf{z})|\mathbf{X}\rangle \\ &= [1 + C\delta(\mathbf{x}_1 - \mathbf{x}_3)\delta(\mathbf{x}_2 - \mathbf{x}_3)]|\mathbf{X}\rangle, \end{aligned} \tag{23}$$

where $C = (e^{\beta g_d} - 1)\ell^{2d}$, ℓ is an ultraviolet regulator in the form of a spatial lattice spacing, and we have used the fermionic relation $\hat{n}_s^2 = \hat{n}_s$. We have also introduced a collective index $\mathbf{X} = (\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3)$. The C-independent term yields the noninteracting result, such that we may write

$$\Delta Q_{111} = C \sum_{\mathbf{p}_j, \mathbf{x}_k} e^{-\beta(p_1^2+p_2^2+p_3^2)/2m} \times \delta(\mathbf{x}_1 - \mathbf{x}_3)\delta(\mathbf{x}_2 - \mathbf{x}_3)|\langle \mathbf{X}|\mathbf{P}\rangle|^2, \tag{24}$$

which simplifies substantially when using a plane-wave basis since $|\langle \mathbf{X}|\mathbf{P}\rangle|^2 = 1/V^3$, where V is the d-dimensional volume of the system. We then find

$$\Delta Q_{111} = C\frac{Q_{100}^3}{V^2}, \tag{25}$$

where

$$Q_{100} = \sum_{\mathbf{p}_1} e^{-\beta p_1^2/2m}. \tag{26}$$

Thus,

$$\Delta b_3 = C\frac{Q_{100}^3}{V^2 Q_1} = C\frac{Q_1^2}{27V^2} = \frac{1}{3}\frac{C}{\lambda_T^{2d}}, \tag{27}$$

where $Q_1 = 3Q_{100} = 3V/\lambda_T^d$, $\lambda_T = \sqrt{2\pi\beta}$ is the thermal wavelength, and V is the system's spatial volume. This relationship between the bare coupling constant C and the physical quantity Δb_3 provides a way to renormalize the problem. In other words, Δb_3 will play the role of the renormalized dimensionless coupling constant.

The general form of the change ΔQ_{MNL} in the partition function for M type 1 particles, N type 2 particles, and L type 3 particles, with a contact interaction, is given by

$$\Delta Q_{MNL} = \sum_{\bar{\mathbf{P}},\bar{\mathbf{X}}} e^{-\beta\bar{\mathbf{P}}^2/2m}|\langle\bar{\mathbf{X}}|\bar{\mathbf{P}}\rangle|^2(Cf_a(\bar{\mathbf{X}}) + C^2 f_b(\bar{\mathbf{X}}) + \cdots), \tag{28}$$

where $\bar{\mathbf{P}}$ and $\bar{\mathbf{X}}$ represent all momenta and positions of the $M+N+L$ particles, and the functions f_a, f_b, …, which encode the matrix element of $e^{-\beta\hat{V}}$, depend on the specific MNL case being considered. The wave function $\langle\bar{\mathbf{X}}|\bar{\mathbf{P}}\rangle$ is a product of three Slater determinants which, using a plane-wave single-particle basis, leads to Gaussian integrals over the momenta $\bar{\mathbf{P}}$.

B. Another example: Δb_4 in a harmonic trap

In this section we consider the case in which the system is held in a harmonic trapping potential of frequency ω. As the expressions for the virial coefficients in terms of the canonical partition functions carry over to this case, we simply add the superindex 'T' to denote quantities in the trapped system. To calculate Δb_4^{T} we need Δb_3^{T} and Q_1^{T}. The latter is of course trivial, as there is no interaction in that case (see Ref. [12]),

$$Q_1^{\mathrm{T}} = 3\sum_{\mathbf{n}} e^{-\beta E_{\mathbf{n}}} = 3e^{-\beta\omega d/2}\left(\frac{1}{1-e^{-\beta\omega}}\right)^d \tag{29}$$

$$= 3\left(\frac{1}{2\sinh(\beta\omega/2)}\right)^d, \tag{30}$$

where $E_{\mathbf{n}}$ is the single-particle energy level of the harmonic oscillator (separated in d-dimensional Cartesian coordinates such that $\mathbf{n}$ represents a d-dimensional vector of harmonic oscillator quantum numbers).

To obtain Δb_3^{T}, we proceed as in the previous example to obtain the analog of Eq. (25) for the trapped case:

$$\Delta Q_{111}^{\mathrm{T}} = C\sum_{\mathbf{n}_j,\mathbf{x}_k} e^{-\beta(E_{\mathbf{n}_1}+E_{\mathbf{n}_2}+E_{\mathbf{n}_3})} \times \delta(\mathbf{x}_1-\mathbf{x}_3)\delta(\mathbf{x}_2-\mathbf{x}_3)|\langle\mathbf{x}_1\mathbf{x}_2\mathbf{x}_3|\mathbf{n}_1\mathbf{n}_2\mathbf{n}_3\rangle|^2. \tag{31}$$

The sums over $\mathbf{x}_3$ and $\mathbf{x}_2$ can be carried out right away, and moreover,

$$|\langle\mathbf{x}_1\mathbf{x}_2\mathbf{x}_3|\mathbf{n}_1\mathbf{n}_2\mathbf{n}_3\rangle|^2 = |\phi_{\mathbf{n}_1}(\mathbf{x}_1)|^2|\phi_{\mathbf{n}_2}(\mathbf{x}_2)|^2|\phi_{\mathbf{n}_3}(\mathbf{x}_3)|^2, \tag{32}$$

where $\phi_{\mathbf{n}}(\mathbf{x})$ is the single-particle harmonic oscillator wave function in d-dimensional Cartesian coordinates. Using the above, we obtain

$$\Delta Q_{111}^{\mathrm{T}} = C\sum_{\mathbf{x}} \rho^3(\mathbf{x};\beta\omega), \tag{33}$$

where

$$\rho(\mathbf{x};\beta\omega) = \sum_{\mathbf{n}} e^{-\beta E_{\mathbf{n}}}|\phi_{\mathbf{n}}(\mathbf{x})|^2. \tag{34}$$

Note that $\sum_{\mathbf{x}}\rho(\mathbf{x};\beta\omega) = Q_1^{\mathrm{T}}/3$.

Using the Mehler kernel (see Ref. [12]) evaluated at equal spatial arguments, we find that

$$\rho(\mathbf{x};\beta\omega) = \omega^{\frac{d}{2}}\frac{e^{-\omega\tanh(\beta\omega/2)\mathbf{x}^2}}{(2\pi\,\sinh(\beta\omega))^{\frac{d}{2}}}, \tag{35}$$

where we note that $\tanh(\beta\omega/2) > 0$ for all $\beta\omega > 0$. Carrying out the resulting Gaussian integrals and simplifying,

$$\Delta b_3^{\mathrm{T}} = \frac{\Delta Q_{111}^{T}}{Q_1^{\mathrm{T}}} = \frac{1}{3^{\frac{d}{2}+1}}\left(\frac{\beta\omega}{\sinh(\beta\omega)}\right)^d\frac{C}{\lambda_T^{2d}}, \tag{36}$$

where $\lambda_T = \sqrt{2\pi\beta}$.

Note that, as $\beta\omega\to 0$, we obtain

$$\Delta b_3^{\mathrm{T}} = \frac{1}{3^{\frac{d}{2}+1}}\frac{C}{\lambda_T^{2d}} = \frac{1}{3^{\frac{d}{2}}}\Delta b_3, \tag{37}$$

where in the latter equality we have used Eq. (28).

For Δb_4^{T}, we need $\Delta Q_{211}^{\mathrm{T}}$, which is easily seen to be given by

$$\begin{aligned}\Delta Q_{211}^{\mathrm{T}} &= C\sum_{\mathbf{x},\mathbf{x}'}\rho^2(\mathbf{x};\beta\omega)[\rho(\mathbf{x};\beta\omega)\rho(\mathbf{x}';\beta\omega) - \rho^2(\mathbf{x},\mathbf{x}';\beta\omega)]\\ &= \Delta Q_{111}^{\mathrm{T}}Q_1^{\mathrm{T}}/3 - C\sum_{\mathbf{x},\mathbf{x}'}\rho^2(\mathbf{x};\beta\omega)\rho^2(\mathbf{x},\mathbf{x}';\beta\omega),\end{aligned} \tag{38}$$

where

$$\rho(\mathbf{x},\mathbf{x}';\beta\omega) = \sum_{\mathbf{n}} e^{-\beta E_{\mathbf{n}}}\phi_{\mathbf{n}}(\mathbf{x})\phi_{\mathbf{n}}(\mathbf{x}'), \tag{39}$$

which, using the Mehler kernel, becomes

$$\rho(\mathbf{x},\mathbf{x}';\beta\omega) = \frac{\omega^{\frac{d}{2}}e^{-\omega\coth(\beta\omega)(\mathbf{x}^2+\mathbf{x}'^2)/2+\omega\,\mathrm{csch}(\beta\omega)\mathbf{x}\cdot\mathbf{x}'}}{(2\pi\,\sinh(\beta\omega))^{\frac{d}{2}}}. \tag{40}$$

Thus, in the continuum limit,

$$\begin{aligned}\Delta b_4^{\mathrm{T}} &= 3\frac{\Delta Q_{211}^{T}}{Q_1^{\mathrm{T}}} - \Delta b_3^{\mathrm{T}}Q_1^{\mathrm{T}}\\ &= -\frac{3C}{Q_1^{\mathrm{T}}}\sum_{\mathbf{x},\mathbf{x}'}\rho^2(\mathbf{x};\beta\omega)\rho^2(\mathbf{x},\mathbf{x}';\beta\omega)\\ &= -\frac{C}{\lambda_T^{2d}}\frac{1}{2^{\frac{d}{2}}}\left[\frac{\beta\omega}{\sinh(\beta\omega)}\frac{1}{(1+3\cosh(\beta\omega))^{\frac{1}{2}}}\right]^d \qquad (41)\\ &= -\frac{3^{\frac{d}{2}+1}}{2^{\frac{d}{2}}}\frac{1}{(1+3\cosh(\beta\omega))^{\frac{d}{2}}}\Delta b_3^{\mathrm{T}}. \qquad (42)\end{aligned}$$

Note that, in the $\beta\omega \to 0$ limit, our approximation yields

$$\Delta b_4^{\mathrm{T}} = -\frac{3^{\frac{d}{2}}}{2^d}\frac{3}{2^{\frac{d}{2}}}\Delta b_3^{\mathrm{T}} = -\frac{1}{2^d}\frac{3}{2^{\frac{d}{2}}}\Delta b_3, \tag{43}$$

which we use below.

IV. RESULTS IN HOMOGENEOUS SPACE

A. Virial coefficients

Using the steps outlined above, we have calculated Δb_4 and Δb_5 and obtained

$$\Delta b_4 = -C\frac{Q_1 Q_1(2\beta)}{9V^2} = -3\frac{Q_1(2\beta)}{Q_1}\Delta b_3, \tag{44}$$

$$\Delta b_5 = C\left(\frac{(Q_1(2\beta))^2}{9V^2} + \frac{Q_1 Q_1(3\beta)}{9V^2}\right) = \left(\frac{3(Q_1(2\beta))^2}{Q_1^2} + \frac{3Q_1(3\beta)}{Q_1}\right)\Delta b_3 \tag{45}$$

for the fermionic three-species system with a three-body contact interaction in d spatial dimensions. In the latter equation, the first term on the right-hand side represents the contribution of Q_{221}, and the second term that of Q_{311}.

In the continuum limit, it is easy to perform the resulting Gaussian integrals that determine Q_1 and obtain

$$\Delta b_4 = -\frac{3}{2^{\frac{d}{2}}}\Delta b_3, \tag{46}$$

$$\Delta b_5 = 3\left(\frac{1}{2^d} + \frac{1}{3^{\frac{d}{2}}}\right)\Delta b_3. \tag{47}$$

Using these results, one may calculate the pressure, density, compressibility, and even Tan's contact (with knowledge of Δb_3 as a function of the interaction strength, e.g., $\beta\epsilon_B$ in one or two dimensions, where ϵ_B is the trimer binding energy). To provide a description of the thermodynamics that is as universal as possible across spatial dimensions, we use Δb_3 as the measure of the interaction strength and display our results in terms of that parameter. Furthermore, one may also define a (dimensionless) contact density as

$$\mathcal{C} = \frac{\lambda_T^d}{V}\frac{\partial \ln \mathcal{Z}}{\partial \Delta b_3}, \tag{48}$$

which differs from the conventional definition by a chain-rule factor $\partial\Delta b_3/\partial\lambda$ (which in turn can be determined by solving the three-body scattering problem), where λ is the d-dimensional coupling constant. To make the expression dimensionless, we have used the thermal wavelength $\lambda_T = \sqrt{2\pi\beta}$.

B. Thermodynamics and contact across dimensions

The interaction-induced change in the pressure ΔP can be written in dimensionless form in arbitrary dimension as

$$\beta V \Delta P = Q_1 \sum_{k=1}^{\infty} \Delta b_k\, z^k. \tag{49}$$

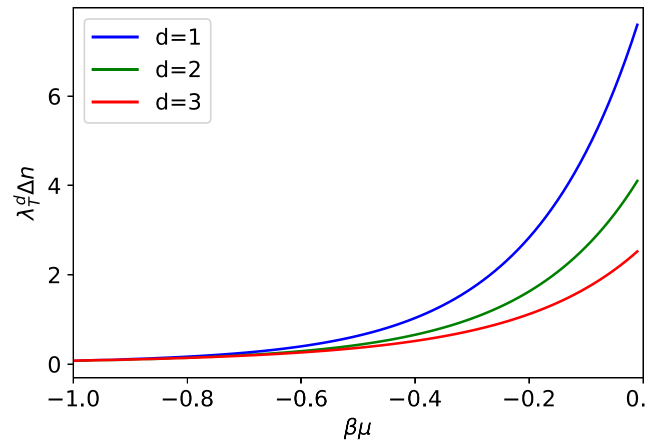

FIG. 1. Density, in units of $\lambda_T^d = (2\pi\beta)^{d/2}$, as a function of $\ln z = \beta\mu$, at $\Delta b_3 = 0.25$, for $d = 1$ (top, blue line), $d = 2$ (middle, green line), and $d = 3$ (bottom, red line).

Similarly, the interaction-induced change in the density can be written as

$$\lambda_T^d \Delta n = 3\sum_{k=1}^{\infty} k\, \Delta b_k\, z^k, \tag{50}$$

and, using our definition of the contact in Eq. (49),

$$\Delta\mathcal{C} = 3\sum_{k=1}^{\infty} \frac{\partial \Delta b_k}{\partial \Delta b_3} z^k. \tag{51}$$

Implementing our LO-SCLA results, we obtain

$$\beta\lambda_T^d \Delta P \simeq 3\Delta b_3\, z^3\left[1 - \frac{3}{2^{\frac{d}{2}}}z + 3\left(\frac{1}{2^d} + \frac{1}{3^{\frac{d}{2}}}\right)z^2\right], \tag{52}$$

$$\lambda_T^d \Delta n \simeq 9\,\Delta b_3\, z^3\left[1 - \frac{4}{2^{\frac{d}{2}}}z + 5\left(\frac{1}{2^d} + \frac{1}{3^{\frac{d}{2}}}\right)z^2\right], \tag{53}$$

$$\Delta\mathcal{C} \simeq 3z^3\left[1 - \frac{3}{2^{\frac{d}{2}}}z + 3\left(\frac{1}{2^d} + \frac{1}{3^{\frac{d}{2}}}\right)z^2\right]. \tag{54}$$

As an example, in Fig. 1 we display the density as a function of the logarithm of the fugacity $\ln z = \beta\mu$ for $\Delta b_3 = 0.25$ and for $d = 1, 2, 3$.

The behavior of Δn as a function of $\beta\mu$ in Fig. 1 is as expected for a system with attractive interactions, namely, the interaction-induced change in the density is positive and enhanced by increasing $\beta\mu$ (or, equivalently, washed out at low densities, i.e., for large and negative $\beta\mu$). Also as expected (and as observed in Refs. [10] and [11] for two-body interactions), interaction effects are more pronounced in lower dimensions at fixed Δb_3.

V. RESULTS IN A HARMONIC TRAP

A. Fourth- and fifth-order virial coefficients

We have generalized our example of Δb_4^{T}, discussed in a previous section, to Δb_5^{T}. For future reference, we show both results:

$$\Delta b_4^{\mathrm{T}} = -\frac{3^{\frac{d}{2}+1}}{2^{\frac{d}{2}}}\frac{1}{(1+3\cosh(\beta\omega))^{\frac{d}{2}}}\Delta b_3^{\mathrm{T}}, \tag{55}$$

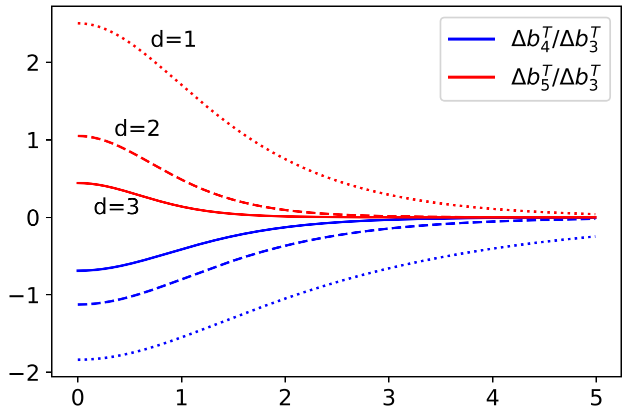

FIG. 2. Δb_4^T (lower three, blue lines) and Δb_5^T (upper three, red lines), in units of Δb_3^T, as a function of $\beta\omega$ in the LO-SCLA. Results are shown in $d = 1$ (dotted lines), $d = 2$ (dashed lines), and $d = 3$ (solid lines).

$$\Delta b_5^{\rm T} = 3^{\frac{d}{2}+1}\left(\left[\frac{1}{12\cosh^2(\beta\omega)+4\cosh(\beta\omega)-1}\right]^{\frac{d}{2}} + \left[\frac{1}{12\cosh^2(\beta\omega)+8\cosh(\beta\omega)}\right]^{\frac{d}{2}}\right)\Delta b_3^{\rm T}. \quad (56)$$

In Fig. 2 we show these results in $d = 1, 2, 3$ as a function of $\beta\omega$. In contrast to the behavior of Δb_4^T for the case of two-body interactions, explored in Refs. [12] and [14], here both $\Delta b_4^{\rm T}$ and $\Delta b_5^{\rm T}$ display monotonic behavior. Furthermore, at this order in the SCLA, both $\Delta b_4^{\rm T}$ and $\Delta b_5^{\rm T}$ are proportional to $\Delta b_3^{\rm T}$, such that the results in Fig. 2 are universal predictions in the sense of being coupling independent.

B. A universal relation in the $\beta\omega \to 0$ limit

Note that, in the $\beta\omega \to 0$ limit, where the homogeneous system is recovered,

$$\Delta b_5^{\rm T} \to 3^{\frac{d}{2}+1}\frac{1}{5^{\frac{d}{2}}}\left(\frac{1}{2^d}+\frac{1}{3^{\frac{d}{2}}}\right)\Delta b_3^{\rm T} = \frac{3}{5^{\frac{d}{2}}}\left(\frac{1}{2^d}+\frac{1}{3^{\frac{d}{2}}}\right)\Delta b_3. \quad (57)$$

Using Eqs. (44), (47), and (58), we find that trapped and untrapped virial coefficients are related, in the $\beta\omega \to 0$ limit, as follows:

$$\Delta b_3^{\rm T} = 3^{-\frac{d}{2}}\Delta b_3, \quad (58)$$

$$\Delta b_4^{\rm T} = 4^{-\frac{d}{2}}\Delta b_4, \quad (59)$$

$$\Delta b_5^{\rm T} = 5^{-\frac{d}{2}}\Delta b_5. \quad (60)$$

Although we have only explored $\Delta b_n^{\rm T}$ for $n = 3, 4$, and 5 here (the cases $n = 1$ and 2 are trivially satisfied as well), the fact that the above relationship holds points us to conjecture that the relation

$$b_n^{\rm T}\big|_{\beta\omega\to 0} = n^{-\frac{d}{2}} b_n \quad (61)$$

is universally valid for all n, couplings, and temperatures (it is well known to be satisfied by noninteracting gases). Other authors (see, e.g., [13,15,16]) have noted (and proven using the local density approximation) that this relationship is satisfied in the unitary limit (where the b_n are temperature independent), and the same connection was found for $n = 3, 4$ in systems with two-body forces in Ref. [12] for arbitrary couplings (within the LO-SCLA). In principle, there is no special reason why $b_n^{\rm T}$ should not approach b_n when the trapping potential is removed. That there is a d- and n-dependent factor connecting these two quantities in the noninteracting case is merely a geometrical artifact of the choice of basis in which the calculations are performed (namely, the harmonic oscillator basis in the trapped case and plane waves in the homogeneous case), which has no impact on physical quantities. Based entirely on dimensional analysis, however, the natural guess is that $b_n^{\rm T}$ may approach b_n times a dimensionless function of temperature and other dynamical scales. (That would actually change the partition function in a nontrivial way, in particular, concerning Tan's contact, but let us put that aside for the moment.) Such a dimensionless function could only result from the interplay between the trapping potential $\hat{V}_{\rm ext}$ and the interaction $\hat{V}$, possibly leading to subtleties in the $\omega \to 0$ limit (similar to those arising from degenerate perturbation theory). However, the fact that $[\hat{V}_{\rm ext}, \hat{V}] = 0$ suggests that there should be no such subtlety and therefore no residual dependence on interaction-related scales in the relationship between $b_n^{\rm T}$ and b_n as $\beta\omega \to 0$. In that limit, the dimensionless quantities $b_n^{\rm T}$ and b_n should be related by a coupling- and temperature-independent function; their connection should be entirely geometrical and fully determined by the noninteracting case, for which $b_n^{\rm T} = n^{-\frac{d}{2}} b_n$ when $\beta\omega \to 0$. We therefore conclude that the conjecture is true for all n, coupling strengths, and temperatures.

C. An exact relation across systems and dimensions

Finally, we point out a coupling-independent relationship between the 1D case with a three-body interaction (i.e., the 1D case of the system studied in this work) and the 2D case with only two-body interactions (denoted below by the superindex "2b2D"). As pointed out in Ref. [17], there exists an exact relationship between the three-body problem of the former situation and the two-body problem of the latter. That relationship yields a simple proportionality rule between the corresponding virial coefficients, given by

$$\Delta b_3 = \frac{Q_{111}^{\rm c.m.}}{Q_{11}^{\rm c.m.,\,2b2D}}\frac{Q_1^{\rm 2b2D}}{Q_1}\Delta b_2^{\rm 2b2D}, \quad (62)$$

where the superscript "c.m." indicates the partition function associated with the center-of-mass motion, which is not affected by the interactions and completely factorizes (both in the spatially homogeneous and in the harmonically trapped case). In the spatially homogeneous case, the proportionality factor between Δb_3 and $\Delta b_2^{\rm 2b2D}$ is $1/\sqrt{3}$, as shown in Ref. [17]. On the other hand, in the harmonically trapped case, the relationship becomes

$$\Delta b_3^{\rm T} = \tfrac{2}{3}\Delta b_2^{\rm T,2b2D}. \quad (63)$$

We stress that while this relationship is restricted to the 1D values of $\Delta b_3^{\rm T}$ and $\Delta b_2^{\rm T,2b2D}$, it is valid for all couplings and all values of $\beta\omega$ and in that sense it is universal.

For completeness and future reference, we provide here details on the origin of this correspondence for the trapped case, which first appeared in Ref. [5], based on the 2D solution in Ref. [18]. The Schrödinger equation for this system takes the form

$$\left[-\frac{\nabla_{\mathbf{r}}^2}{2m}+g\delta(x-y)\delta(y-z)+\frac{1}{2}m\omega^2\mathbf{r}^2\right]\psi(\mathbf{r})=E\psi(\mathbf{r}), \tag{64}$$

where x, y, and z again indicate the different-flavor particles, $\mathbf{r}=(x,y,z)$, and

$$\nabla_{\mathbf{r}}^2=\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}. \tag{65}$$

Factoring out the center-of-mass motion by defining $Q=\frac{1}{\sqrt{3}}(x+y+z)$, $q_1=\frac{1}{\sqrt{2}}(y-x)$, $q_2=\frac{1}{\sqrt{6}}(x+y-2z)$, and $\psi(x,y,z)=\Phi(Q)\phi(\mathbf{q})$, with $\mathbf{q}=(q_1,q_2)$, we obtain

$$\left[-\frac{1}{2m}\frac{\partial^2}{\partial Q^2}+\frac{1}{2}m\omega^2Q^2\right]\Phi(Q)=E_{\text{c.m.}}\Phi(Q), \tag{66}$$

for the c.m. motion, and

$$\left[-\frac{\nabla_{\mathbf{q}}^2}{2m}+\tilde{g}\delta(\mathbf{q})+\frac{1}{2}m\omega^2\mathbf{q}^2\right]\phi(\mathbf{q})=E_r\phi(\mathbf{q}), \tag{67}$$

where $\tilde{g}=g/\sqrt{3}$ is the effective coupling and E_r is the energy of relative motion, which is identical to that of a single particle in a 2D harmonic oscillator potential with a δ potential at the origin. This establishes the exact relationship between our three-body 1D problem and its two-body 2D counterpart with two-body interactions.

As in the spatially homogeneous case, the eigenvalues $\epsilon_\omega=E_r/\omega$ of the harmonically trapped system are determined implicitly, in this case as solutions to

$$\frac{1}{\tilde{g}}=\frac{m}{\pi}\sum_{n=0}^{\Lambda_\omega}\frac{1}{\epsilon_\omega-(2n+1)}\to\frac{m}{2\pi}\left[\psi_0\left(\frac{1-\epsilon_\omega}{2}\right)-\ln\Lambda_\omega\right], \tag{68}$$

where $\psi_0(z)$ is the digamma function, where Λ_ω is a UV cutoff. Unlike in the untrapped problem, with its unique bound state, the trapped problem admits an infinite set of discrete excited states (all with positive energy). The problem is renormalized by relating the bare coupling to the ϵ_ω occurring in the lowest-energy branch.

VI. SUMMARY AND CONCLUSIONS

In this work we have calculated the high-temperature thermodynamics of three-flavored Fermi gases with a contact three-body interaction in d spatial dimensions, as determined by the virial expansion. We carried out calculations in homogeneous space as well as in a harmonic trapping potential of frequency ω. To that end, we implemented a coarse temporal lattice approximation at leading order (the LO-SCLA) and calculated the change in the virial coefficients Δb_n due to interaction effects. In this context, we established a relation between the first two nontrivial virial coefficients, namely, Δb_4 and Δb_5, as functions of Δb_3. In addition, we argued that in the $\beta\omega\to 0$ limit, the relationship $\Delta b_n^{\mathrm{T}}=n^{-d/2}\Delta b_n$ holds between the trapped and the homogeneous coefficients for arbitrary n, coupling strengths, and temperatures; furthermore, it is valid for systems with two- and three-body interactions. We showed that our calculations reproduce that relationship for $n=3,4,5$. Finally, we showed a relationship between the harmonically trapped case in one dimension with three-body interactions and its analog in two dimensions with two-body interactions, namely, $\Delta b_3^{\mathrm{T}}=\frac{2}{3}\Delta b_2^{\mathrm{T,2b2D}}$. In closing, a comment is in order regarding the nature of purely contact (i.e., nonderivative) three-body interactions for $d>1$. The dimension of the coupling constant for such an n-body interaction is $L^{d(n-1)-2}$ (where L has units of length), which is always positive for $n=3$ and $d>1$, indicating that the three-body interaction is an irrelevant operator in $d>1$. Therefore, renormalizing to a nontrivial interaction effect will likely require the systematic inclusion of a two-body interaction. The effect of not including the latter would appear when calculating at higher orders in the temporal lattice approximation, where it would manifest as a progressive shrinkage of the range of values of Δb_3 for which renormalization is possible with just a three-body coupling.

ACKNOWLEDGMENT

This material is based upon work supported by the National Science Foundation under Grant No. PHY1452635 (Computational Physics Program).

[1] Y. Nishida, Universal bound states of one-dimensional bosons with two- and three-body attractions, Phys. Rev. A **97**, 061603(R) (2018).

[2] L. Pricoupenko, Pure confinement-induced trimer in one-dimensional atomic waveguides, Phys. Rev. A **97**, 061604(R) (2018).

[3] G. Guijarro, A. Pricoupenko, G. E. Astrakharchik, J. Boronat, and D. S. Petrov, One-dimensional three-boson problem with two- and three-body interactions, Phys. Rev. A **97**, 061605(R) (2018).

[4] Y. Sekino and Y. Nishida, Quantum droplet of one-dimensional bosons with a three-body attraction, Phys. Rev. A **97**, 011602(R) (2018).

[5] M. Valiente and V. Pastukhov, Anomalous frequency shifts in a one-dimensional trapped Bose gas, Phys. Rev. A **99**, 053607 (2019).

[6] J. R. McKenney and J. E. Drut, Fermi-Fermi crossover in the ground state of one-dimensional few-body systems with anomalous three-body interactions, Phys. Rev. A **99**, 013615 (2019).

[7] M. Valiente, Three-body repulsive forces among identical bosons in one dimension, Phys. Rev. A **100**, 013614 (2019).

[8] J. Maki and C. R. Ordóñez, Virial expansion for a three-component Fermi gas in one dimension: The quantum anomaly correspondence, Phys. Rev. A **100**, 063604 (2019).

[9] W. S. Daza, J. E. Drut, C. L. Lin, and Carlos R. Ordóñez, A quantum field-theoretical perspective on scale anomalies in 1D systems with three-body interactions, Mod. Phys. Lett. A **34**, 1950291 (2019).

[10] C. R. Shill and J. E. Drut, Virial coefficients of one-dimensional and two-dimensional Fermi gases by stochastic methods and a semiclassical lattice approximation, Phys. Rev. A **98**, 053615 (2018).

[11] Y. Hou, A. J. Czejdo, J. DeChant, C. R. Shill, and J. E. Drut, Leading- and next-to-leading-order semiclassical approximation to the first seven virial coefficients of spin-1/2 fermions across spatial dimensions, Phys. Rev. A **100**, 063627 (2019).

[12] K. J. Morrell, C. E. Berger, and J. E. Drut, Third- and fourth-order virial coefficients of harmonically trapped fermions in a semiclassical approximation, Phys. Rev. A **100**, 063626 (2019).

[13] X.-J. Liu, Virial expansion for a strongly correlated Fermi system and its application to ultracold atomic Fermi gases, Phys. Rep. **524**, 37 (2013).

[14] Y. Yan and D. Blume, Path-Integral Monte Carlo Determination of the Fourth-Order Virial Coefficient for a Unitary Two-Component Fermi Gas with Zero-Range Interactions, Phys. Rev. Lett. **116**, 230401 (2016).

[15] X.-J. Liu, H. Hu, and P. D. Drummond, Virial Expansion for a Strongly Correlated Fermi Gas, Phys. Rev. Lett. **102**, 160401 (2009).

[16] X.-J. Liu, H. Hu, and P. D. Drummond, Three attractively interacting fermions in a harmonic trap: Exact solution, ferromagnetism, and high-temperature thermodynamics, Phys. Rev. A **82**, 023619 (2010).

[17] J. E. Drut, J. R. McKenney, W. S. Daza, C. L. Lin, and C. R. Ordóñez, Quantum Anomaly and Thermodynamics of One-Dimensional Fermions with Three-Body Interactions, Phys. Rev. Lett. **120**, 243002 (2018).

[18] T. Busch, B.-G. Englert, K. Rzażewski, and M. Wilkens, Two cold atoms in a harmonic trap, Found. Phys. **28**, 549 (1998).