

Virial coefficients of one-dimensional and two-dimensional Fermi gases by stochastic methods and a semiclassical lattice approximation

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We map out the interaction effects on the first six virial coefficients of one-dimensional Fermi gases with zero-range attractive and repulsive interactions and the first four virial coefficients of the two-dimensional analog with attractive interactions. To that end, we use two nonperturbative stochastic methods: projection by complex stochastic quantization, which allows us to determine high-order coefficients at weak coupling and estimate the radius of convergence of the virial expansion, and a path-integral representation of the virial coefficients. To complement our numerical calculations, we present leading-order results in a semiclassical lattice approximation, which we find to be surprisingly close to the expected answers.

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I. INTRODUCTION

The thermodynamics of strongly coupled matter is a topic of current interest in areas of physics that cover a wide range of scales, from quantum chromodynamics (QCD) [1] to ultracold atoms [2–4]. The finite temperature and density behavior of QCD is, in fact, one of the pressing challenges of that field as QCD at the finite baryon chemical potential is realized in relativistic heavy-ion collisions and deep inside neutron stars [1,5]. On the other hand, ultracold atoms have become an especially appealing laboratory to probe the properties of strongly coupled matter due to their purity and malleability and, in particular, due to the experimentalists' power to modify the interaction by dialing an external magnetic field across a Feshbach resonance [6]. Naturally, this amount of control on the experimental side poses a challenge to theoretical approaches. Indeed, strongly coupled atoms can be routinely studied, but their precise quantitative analysis on the theory side usually requires *ab initio* nonperturbative tools, such as the quantum Monte Carlo methods.

An alternative way to characterize the thermodynamics of a many-body system has historically been given by the virial expansion (VE), which is nonperturbative and valid in the dilute limit. The VE is an expansion in powers of the fugacity $z = e^{\beta\mu}$ (where β is the inverse temperature and μ is the chemical potential) such that the grand-canonical partition function is written as

$$\mathcal{Z} = \sum_{n=0}^{\infty} Q_n z^n, \quad (1)$$

where Q_n 's are the n -particle canonical partition functions. We arrive at the most common form of the VE by expanding the pressure P in powers of z ,

$$\beta PV = \ln \mathcal{Z} = Q_1 \sum_{n=1}^{\infty} b_n z^n, \quad (2)$$

where V is the (d -dimensional, spatial) volume and b_n are the virial coefficients. Other quantities of interest besides P

can also be expanded in powers of z (see, e.g., Ref. [7]). The appeal of the VE is that it encodes, at order n , how the two- through n -body problems govern the physics of the many-body system. Using Eq. (1) in Eq. (2) one sees this explicitly,

$$b_2 = \frac{Q_2}{Q_1} - \frac{Q_1}{2}, \quad (3)$$

$$b_3 = \frac{Q_3}{Q_1} - Q_2 + \frac{Q_1^2}{3}, \quad (4)$$

$$b_4 = \frac{Q_4}{Q_1} - Q_3 - \frac{Q_2^2}{2Q_1} + Q_2 Q_1 - \frac{Q_1^3}{4}, \quad (5)$$

and so forth. The above equations are entirely based on thermodynamics and valid for arbitrary interaction and spatial dimension.

The task of calculating b_n has typically been equated with solving the n -body problem, constructing the Q_n , and inserting those in the above equations. It is therefore not surprising that second-order calculations are easily carried out as all that is needed for b_2 is the solution to the two-body problem. In fact, formulas exist for b_2 for many cases, some of which we quote below, based on the celebrated Beth-Uhlenbeck result [8]. Obtaining b_3 and beyond, however, typically requires numerical methods (see, e.g., Refs. [9–11]). Although the b_n 's are a proxy for other quantities, their calculation has become an attractive challenge per se, especially in cases, such as the unitary limit [12] (the universal limit of zero interaction range and infinite scattering length), where the b_n 's represent universal constants of quantum many-body physics. For that reason, the calculation of the b_n 's has been vigorously pursued by several groups [11,13–18].

In this paper we focus on the virial coefficients of the generic lattice Hamiltonian of two-species nonrelativistic fermions with zero-range interactions, i.e.,

$$\hat{H} = \sum_{\mathbf{p}} \frac{\mathbf{p}^2}{2m} \hat{n}_{\mathbf{p}} - g \sum_{\mathbf{x}} \hat{n}_{\uparrow}(\mathbf{x}) \hat{n}_{\downarrow}(\mathbf{x}), \quad (6)$$

where the total density operator in momentum space is $\hat{n}_{\mathbf{p}} = \hat{n}_{\uparrow,\mathbf{p}} + \hat{n}_{\downarrow,\mathbf{p}}$ and $\hat{n}_s(\mathbf{x})$ is the density for spin s at position \mathbf{x} . We will use units such that $\hbar = k_B = m = 1$.

For the above Hamiltonian, we obtain the first six virial coefficients of the one-dimensional (1D) case, i.e., the Gaudin-Yang model [19] and the first four virial coefficients of the two-dimensional (2D) case. Although the former is a classic problem that has been extensively studied (see, e.g., Ref. [20] for a recent review of 1D Fermi gases), its virial coefficients beyond b_2 are calculated here (see also a perturbative estimate in Ref. [21]). The 2D case, in contrast, has been under intense scrutiny in recent years as it has been realized experimentally with ultracold atoms by several groups [22–28]. Moreover, its thermal properties have been explored theoretically as well by various authors (see Ref. [29] for a review), and its virial coefficients b_2 and b_3 have been known for a few years.

To determine b_n , we developed two stochastic methods which bypass the direct solution of the n -body problem. One of our objectives is to show that it is possible to design methods that allow to calculate high-order virial coefficients without solving the n -body problem at the price of reduced precision. The first method is based on the idea of Fourier particle-number projection of nuclear physics [30] as applied to the auxiliary field path-integral representation of \mathcal{Z} . That approach naturally yields a complex measure, and for that reason we implement the complex Langevin algorithm to sample the field [31]. The resulting method is able to compute high-order virial coefficients at weak couplings and can estimate the radius of convergence α_0 of the VE as a function of the coupling strength. The second method consists in the stochastic evaluation of the *change* in the virial coefficients due to interaction effects Δb_n . This second method uses the definition of the b_n in their path-integral form derived from \mathcal{Z} , but it does not use \mathcal{Z} directly. Thus, it is able to evaluate b_n at stronger couplings than the projection method but gives no information about the radius of convergence. Besides those two stochastic methods, we implement a semiclassical lattice approximation (SCLA) at leading order (LO). In all cases we use the known results for Δb_2 as the renormalization condition that connects the bare lattice coupling to the physical coupling.

The generalization of our approaches to higher dimensions is straightforward. In fact, the generic system studied here (a nonrelativistic gas with zero-range interactions) has been under intense investigation both theoretically and experimentally in the past decade in 1D, 2D, and three dimensions (3D), and analytic results exist for b_2 in all dimensions based on the Beth-Uhlenbeck formula mentioned above [8,13,32–34].

II. FORMALISM

A. Stochastic methods

Using Eq. (2), b_n can be obtained by Fourier projection. Following that route, we define the function,

$$b_n(\alpha) \equiv \frac{1}{Q_1} \int_0^{2\pi} \frac{d\phi}{2\pi} e^{i\phi n} \ln \mathcal{Z}[z \rightarrow \alpha e^{-i\phi}] = b_n \alpha^n. \quad (7)$$

To proceed, we write \mathcal{Z} as a path integral over a Hubbard-Stratonovich (HS) field σ (see e.g., Refs. [35,36]), $\mathcal{Z} = \int \mathcal{D}\sigma \det^2 M[\sigma, z]$ where we focus on unpolarized systems, thus the power of 2. The matrix $M[\sigma, z]$ encodes the dynamics and parameters of the system of interest; in particular, the z dependence appears as $M[\sigma, z] = \mathbb{1} + zU[\sigma]$, where $U[\sigma]$ contains the kinetic energy and interaction information (see Ref. [35] for details on the specific forms of $M[\sigma, z]$ and $U[\sigma]$). Setting $z \rightarrow \alpha e^{-i\phi}$ and differentiating both sides with respect to α yields

$$b_n = \frac{1}{n\alpha^{n-1}} \frac{1}{Q_1} \int_0^{2\pi} \frac{d\phi}{2\pi} e^{i\phi n} \langle \text{tr}[2M^{-1} \partial M / \partial \alpha] \rangle_{\phi, \alpha}, \quad (8)$$

where $P[\sigma, z] \equiv \det^2 M[\sigma, z] / \mathcal{Z}[z]$ and we have used angle brackets as a shorthand notation for the expectation value with $P[\sigma, \alpha e^{i\phi}]$ as a weight. In practice, we use a discrete Fourier transform such that

$$\frac{\partial b_n(\alpha)}{\partial \alpha} = \frac{1}{Q_1} \frac{1}{N_k} \sum_{k=0}^{N_k-1} e^{i\phi_k n} \langle \text{tr}[2M^{-1} \partial M / \partial \alpha] \rangle_{\phi_k, \alpha}, \quad (9)$$

where $\phi_k = 2\pi k / N_k$, $k = 0, \dots, N_k - 1$, and N_k is the number of discretization points. This is the fundamental equation of the proposed approach. Calculating the expectation values inside the sum in Eq. (9) for N_k values of ϕ_k and carrying out the Fourier sum for different values of n , one obtains the desired b_n . As long as N_k is large enough, the same stochastic calculation of said expectation values over N_k points is used for obtaining b_n for *all* the desired values of n up to statistical effects. In such a calculation, the results for b_n must be independent of α such that that variable can be used as a measure of the reliability of the method. In practice we plot

$$b_n = \frac{1}{n\alpha^{n-1}} \frac{\partial b_n(\alpha)}{\partial \alpha}, \quad (10)$$

as a function of α and fit a constant. The α^n dependence of the n th order term is the main limiting factor in extracting high-order virial coefficients. To overcome that limitation, it is desirable to make α as large as possible but less than unity to remain in the virial region. Thus, deviations in Eq. (10) from constant behavior as α is *decreased* are indicative of uncertainties due to statistical noise or insufficient Fourier points. On the other hand, nonconstant behavior as α is *increased* indicates the appearance of roots of \mathcal{Z} in the complex- z plane, which yield branch-cut singularities in $\ln \mathcal{Z}$ and point to the radius of convergence of the VE (see below).

Evaluating the expectation values in Eq. (9) involves calculations that suffer from a phase problem as $P[\sigma, \alpha e^{-i\phi}]$ will generally be a complex weight. To address that issue, we turn to complex stochastic quantization via the complex Langevin (CL) method, which has recently been applied to the characterization of other aspects of nonrelativistic fermions [21,37–39]. We employ the CL method in the same way described in Ref. [21] (where it was applied to address repulsive interactions), setting the fugacity to $z \rightarrow \alpha e^{-i\phi}$. The quantity in the expectation value appearing in Eq. (9), namely, $\text{tr}[M^{-1} \partial M / \partial \alpha]$, corresponds to the density of the system. Thus, the proposed approach effectively consists in the Fourier projection of the virial coefficients from the

density equation of state, which is reminiscent of other approaches, such as those of Refs. [15,16,18,34].

Our second method calculates the interaction effects on b_n using their definition in terms of path integrals, derived analytically from the path-integral form of \mathcal{Z} . In that formalism, the change in b_n due to interactions is

$$\begin{aligned}\Delta b_2 &= \frac{\Delta Q_{1,1}}{Q_1}, & \Delta b_3 &= \frac{2 \Delta Q_{2,1}}{Q_1} - Q_1 \Delta b_2, \\ \Delta b_4 &= \frac{2 \Delta Q_{3,1} + \Delta Q_{2,2}}{Q_1} - \frac{Q_1^2}{2} \Delta b_2 - \frac{Q_1}{2} (\Delta b_2^2 + 2 \Delta b_3),\end{aligned}$$

where $Q_{m,n}$ is the partition function for m particles of one species and n of the other and $\Delta Q_{m,0} = 0$ because we only have contact interactions. The VE of the fermion determinant yields

$$\begin{aligned}Q_{1,1} &= \int \mathcal{D}\sigma \operatorname{tr}^2 U[\sigma], \\ 2Q_{2,1} &= \int \mathcal{D}\sigma \operatorname{tr}^3 U[\sigma] \left(1 - \frac{\operatorname{tr} U^2[\sigma]}{\operatorname{tr}^2 U[\sigma]}\right), \\ 2Q_{3,1} &= \frac{1}{3} \int \mathcal{D}\sigma \operatorname{tr}^4 U[\sigma] \left(1 - \frac{3 \operatorname{tr} U^2[\sigma]}{\operatorname{tr}^2 U[\sigma]} + \frac{2 \operatorname{tr} U^3[\sigma]}{\operatorname{tr}^3 U[\sigma]}\right), \\ Q_{2,2} &= \frac{1}{4} \int \mathcal{D}\sigma \operatorname{tr}^4 U[\sigma] \left(1 - \frac{\operatorname{tr} U^2[\sigma]}{\operatorname{tr}^2 U[\sigma]}\right)^2,\end{aligned}\quad (11)$$

and so on at higher orders. Inserting these expressions in Eq. (11) (and their noninteracting versions) yields stochastic formulas for Δb_n . To evaluate those, we use the usual two-species action $S[\sigma, z] = -2 \ln \det M[\sigma, z]$ to sample σ and extrapolate the results to the $z = 0$ limit. This method is similar in spirit to that of Ref. [11] but employs a field integral representation instead of an integral over particle paths.

B. Semiclassical lattice approximation

Using the formulas of Eq. (11), it is possible to implement what we call the semiclassical lattice approximation in which we neglect the commutator of the kinetic-energy matrix T and the potential-energy matrix V at leading order. Thus, the matrix $U[\sigma]$ becomes simply $U[\sigma] = e^{-\beta T} \mathcal{V}[\sigma]$, where $\mathcal{V}[\sigma]$ encodes the specific form of the HS transformation. Such an approximation amounts to a coarse discretization of the imaginary-time direction, which nevertheless becomes exact in two different limits: $V \rightarrow 0$ and $T \rightarrow 0$. In between those limits, higher orders in the SCLA can be reached by using finer temporal meshes; we leave calculations beyond LO to future work. At LO, the path integrals can be carried out analytically,

$$\Delta b_3 = -2^{1-d/2} \Delta b_2, \quad (12)$$

$$\begin{aligned}\Delta b_4 &= 2(3^{-d/2} + 2^{-d-1}) \Delta b_2 \\ &\quad + 2^{1-d/2} (2^{-d-1} - 1) (\Delta b_2)^2,\end{aligned}\quad (13)$$

where we present our results in terms of Δb_2 because we will use the exact Δb_2 as a renormalization condition.

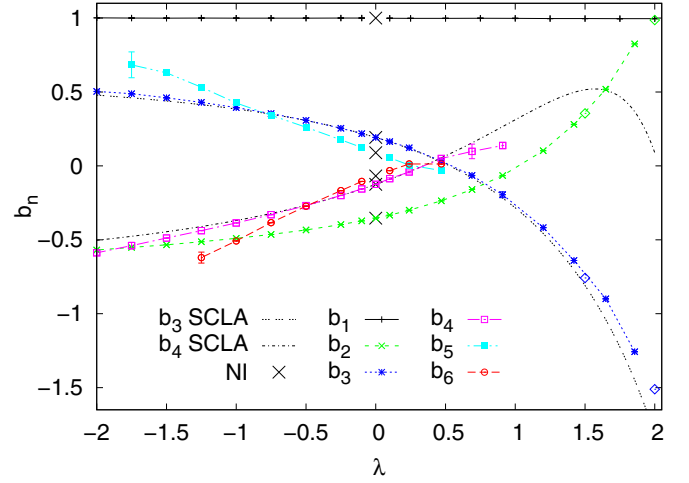


FIG. 1. Virial coefficients b_n for $n = 1-6$ for the 1D Fermi gas as a function of the dimensionless coupling λ as obtained with our projection method. Crosses on the y axis denote the noninteracting values of $b_n = (-1)^{n+1} n^{-3/2}$. The leading order of the semiclassical lattice approximation (LO-SCLA) is shown with a dashed-dotted line for Δb_3 and with a dashed line for Δb_4 . Green and blue diamonds show the results obtained with our second stochastic method for comparison.

III. RESULTS

A. Virial coefficients in 1D

To analyze the 1D case, our calculations used a lattice of spatial size $N_x = 30$ and temporal size $N_\tau = 120-200$. We otherwise used the same lattice parameters as those of Ref. [21]. The number of Fourier points was set to $N_k = 30$ for the main results with explorations covering $N_k = 20-100$ showing no significant variation. By definition, $b_1 = 1$ and, for the 1D contact interaction studied here (see Ref. [32]),

$$b_2^{(1D)} = -\frac{1}{\sqrt{2}} + \frac{e^{\lambda^2/4}}{2\sqrt{2}} [1 + \operatorname{erf}(\lambda/2)], \quad (14)$$

where erf is the error function and λ is the dimensionless coupling. The noninteracting limit is $b_2^{(1D)} \rightarrow -\frac{1}{2\sqrt{2}}$. We will use the analytic form of Eq. (14) as a renormalization condition, i.e., to define the coupling λ from our lattice determination of b_2 . As a consequence, our plots of b_2 below will be exact by definition. Our first result appears in Fig. 1 where we map out the λ dependence of the first six b_n 's. The smoothness of the results gives confidence that the method works as expected. Perhaps the most prominent feature in Fig. 1 is the monotonicity of the stochastic data for each b_n : Besides the constant $b_1 = 1$, the even n coefficients increase as a function of λ , whereas the odd ones decrease. More specifically, toward the repulsive side ($\lambda < 0$), the b_n 's grow in magnitude and maintain their signs: The even ones which start out negative at $\lambda = 0$, become more negative, and the odd ones which start out positive grow as well. Toward the attractive side, the monotonic behavior implies that in a wide region $0 < \lambda < 1$ many of the coefficients cross the $b_n = 0$ line, which suggests the VE may be useful up to $z \simeq 0.5$ (see, however, our results below for the radius of convergence). Beyond that point, the coefficients grow in magnitude and eventually

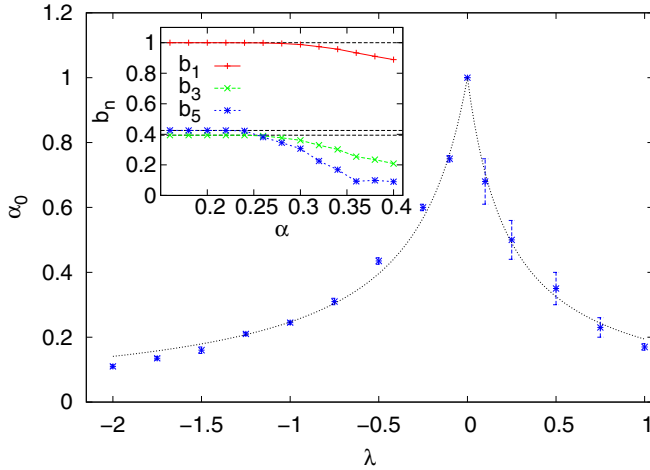


FIG. 2. Estimate of the radius of convergence α_0 of the virial expansion as a function of the coupling λ . The inset: b_n for $n = 1, 3, 5$ for $\lambda = -1$. Constant behavior as a function of α is expected when the coefficient of the n th power of z is extracted successfully. Deviation from such a constant as α is increased shows the appearance of roots of \mathcal{Z} on the complex- z plane, which yields the estimate α_0 for the radius of convergence shown in the main plot.

change sign relative to their noninteracting values. Using the second stochastic method (applied below in 2D), we checked the above results of Fig. 1 for b_2 and b_3 .

B. Radius of convergence via the projection method

In the inset of Fig. 2 we show b_n as a function of α . As anticipated, for each virial order n there is a region around $\alpha = 0$ for which b_n does not vary, which allows us to extract the value of b_n itself. Beyond a λ -dependent value of α , however, the calculation runs into the roots of \mathcal{Z} on the complex plane and the constant behavior is lost. We stress that this is not due to systematic or statistical effects but rather a feature of the calculation that represents the radius of convergence α_0 of the virial expansion. The main plot of Fig. 2 shows our results for α_0 as a function of λ , obtained by locating the point where the constant behavior as a function of α is lost. Our results are consistent with the expected value of $\alpha_0 = 1$ for the noninteracting case, which is easily derived by noting that the noninteracting partition function has a root at $z = -1$. The dashed line in the main plot of Fig. 2 shows a fit $\alpha_0(\lambda) = 1/(1 + C|\lambda|)$, where $C \simeq 3.05(5)$ on the repulsive side ($\lambda < 0$) and $C \simeq 4.15(5)$ on the attractive side ($\lambda > 0$). Although the fit is merely descriptive, it does point to a nontrivial feature, namely, the nonanalyticity of α_0 around the maximum at $\lambda = 0$: The data appear to display a cusp.

C. Virial coefficients in 2D

Besides the 1D case above, we applied the second method to the 2D analog, which was studied up to second order in the VE in Refs. [33,34,40] and up to third order in Refs. [9,10]. The Hamiltonian is essentially identical to that of Eq. (6), generalized to 2D. In that case, the coupling g becomes simply a bare parameter, and the physical coupling is given by $\lambda_2 = \sqrt{\beta \varepsilon_B}$, where ε_B is the binding energy of the

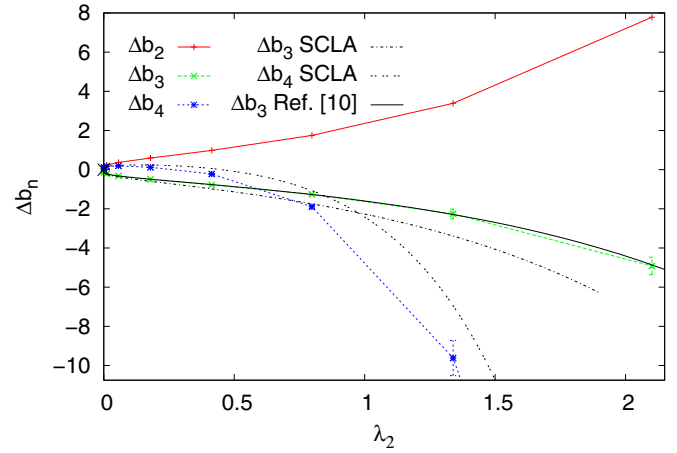


FIG. 3. Interaction change in the virial coefficients Δb_n for $n = 2-4$ for the 2D Fermi gas as a function of the dimensionless coupling λ_2 . The solid red line connects the data for Δb_2 , the green line shows Δb_3 , and the blue line shows Δb_4 . The LO-SCLA is shown with a dashed-dotted line for Δb_3 and with a dashed line for Δb_4 . The solid black line shows the result for Δb_3 of Ref. [10]. Note that the data for Δb_2 reproduce the exact result of Eq. (15) by virtue of the renormalization condition (see the text).

two-body system. The second-order virial coefficient in 2D is known [33,34,41] and given by

$$b_2^{(2D)} = -\frac{1}{4} + e^{\lambda_2^2} - \int_0^\infty \frac{dy}{y} \frac{2e^{-\lambda_2^2 y^2}}{\pi^2 + 4 \ln^2 y}. \quad (15)$$

The noninteracting limit yields $b_2^{(2D)} \rightarrow -\frac{1}{4}$. As in our 1D calculations, we used Eq. (15) to define λ_2 by calculating b_2 on the lattice. In Fig. 3 we show our results for b_2 , b_3 , and b_4 . By definition, b_2 is reproduced exactly, and the output of the calculation is b_3 and b_4 .

D. Semiclassical lattice approximation

The predictions of the LO-SCLA are compared with those of our stochastic methods in Figs. 1 and 3. The LO-SCLA predicts in 1D: $\Delta b_3 = -\sqrt{2}\Delta b_2$ and $\Delta b_4 = (4\sqrt{3} + 3)/6 \Delta b_2 - 3\sqrt{2}/4(\Delta b_2)^2$ and in 2D: $\Delta b_3 = -\Delta b_2$ and $\Delta b_4 = 11/12 \Delta b_2 - 7/8(\Delta b_2)^2$. As is clear in Figs. 1 and 3, there are differences between those predictions and the stochastic results. However, it is remarkable that at LO the SCLA predicts not only the correct sign of Δb_3 , but also a deviation smaller than 10% in 1D and close to 20% in 2D, at least, for the regime of couplings that is studied here. Such results encourage higher-order studies of the SCLA, which will be carried out elsewhere.

A few comments are in order regarding the observed behavior of the b_n 's, some of which can be understood analytically. For instance, b_2 is dominated at strong coupling by an anti-Gaussian term [see Eqs. (14) and (15)]. That term is due to the appearance of a bound state, which happens in 1D and 2D as soon as the attractive coupling is turned on. Thus, b_2 diverges very strongly as the coupling is increased on the attractive side. As for b_3 , within the LO-SCLA, it will inherit the behavior of b_2 , which is supported by our data.

As far as b_4 , the LO-SCLA involves a Δb_2 term with a positive coefficient and a $(\Delta b_2)^2$ term with a negative coefficient; that is the reason for the nonmonotonic behavior: The $(\Delta b_2)^2$ term eventually takes over. The origin of these linear and quadratic terms is similar to those in perturbation theory: The linear term comes from a single diagram, whereas the quadratic term comes from two diagrams, one with an odd and one with an even number of fermion loops such that their prefactors have different signs (and the negative one dominates).

Although we focus here on 1D and 2D, it is also interesting to test the predictions of the LO-SCLA for the 3D Fermi gas at unitarity. There, known results (see, e.g., Refs. [14–18]) give $\Delta b_2 = 1/\sqrt{2}$ and $\Delta b_3 = -0.35505\dots$ such that $\Delta b_3/\Delta b_2 \simeq -0.50\dots$, whereas the LO-SCLA yields $\Delta b_3/\Delta b_2 = -1/\sqrt{2} \simeq -0.707$, thus matching the sign of Δb_3 but overshooting its magnitude by about 40%. Similarly, the most accurate result at unitarity [11] is $b_4 = 0.078(18)$, which yields $\Delta b_4 = 0.109(18)$, whereas the LO-SCLA yields $\Delta b_4 = 0.029\dots$, which matches the sign of the expected result but undershoots its magnitude by roughly a factor of 3. Nevertheless, these results are encouraging when considering that they come from a mere leading-order approximation.

IV. SUMMARY AND CONCLUSIONS

We have calculated the first few virial coefficients b_n of two systems: fermions in 1D and 2D both with a contact interaction. In 1D, we evaluated the first six b_n 's as a function of the coupling strength λ in both attractive and repulsive regimes. In the 2D case, we calculated Δb_3 and Δb_4 for attractive interactions. To carry out our calculations, we implemented two different stochastic lattice methods. The first method relied on projecting the b_n 's out of the path-integral form of the density equation of state. The second approach used a path-integral representation of the virial coefficients as derived from the path-integral form of \mathcal{Z} . The latter method enables calculations in a way that requires neither matrix inversion nor determinants but which is sensitive to statistical noise as n is increased due to the various volume-scaling cancellations required to resolve each b_n from the canonical partition functions. However, that noise can, at least, partially be addressed by obtaining more samples, a task that can be carried out in a perfectly scalable fashion. The stochastic approaches proposed here are not as precise as exact diagonalization but provide a systematic way to high-order coefficients without solving the n -body problem. Finally, we used a semiclassical approximation which at leading order compares remarkably well with our stochastic results for the coupling strengths studied.

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APPENDIX A: SEMICLASSICAL APPROXIMATION

From the equations in main text it is easy to see that

$$\Delta b_2 = \frac{\Delta Q_{1,1}}{Q_1} = \frac{1}{Q_1} \int \mathcal{D}\sigma (\text{tr}^2 U[\sigma] - \text{tr}^2 U_0), \quad (\text{A1})$$

where $U_0 = e^{-\beta T}$ is the noninteracting transfer matrix (T being the kinetic-energy matrix) and $U[\sigma] = e^{-\beta T} \mathcal{V}[\sigma]$ (\mathcal{V} being the chosen HS representation of the interaction). Carrying out the path integrals, it is straightforward to find

$$\Delta b_2 = (e^{\beta g} - 1) \frac{V}{Q_1} \left(\frac{\text{tr} U_0}{V} \right)^2, \quad (\text{A2})$$

where $Q_1/V \rightarrow 2/\lambda_T^d$ in the continuum limit in d spatial dimensions and all lengths are in units of the lattice spacing $\ell = 1$. Moreover, $\text{tr} U_0 = Q_1/2$ such that, in the continuum

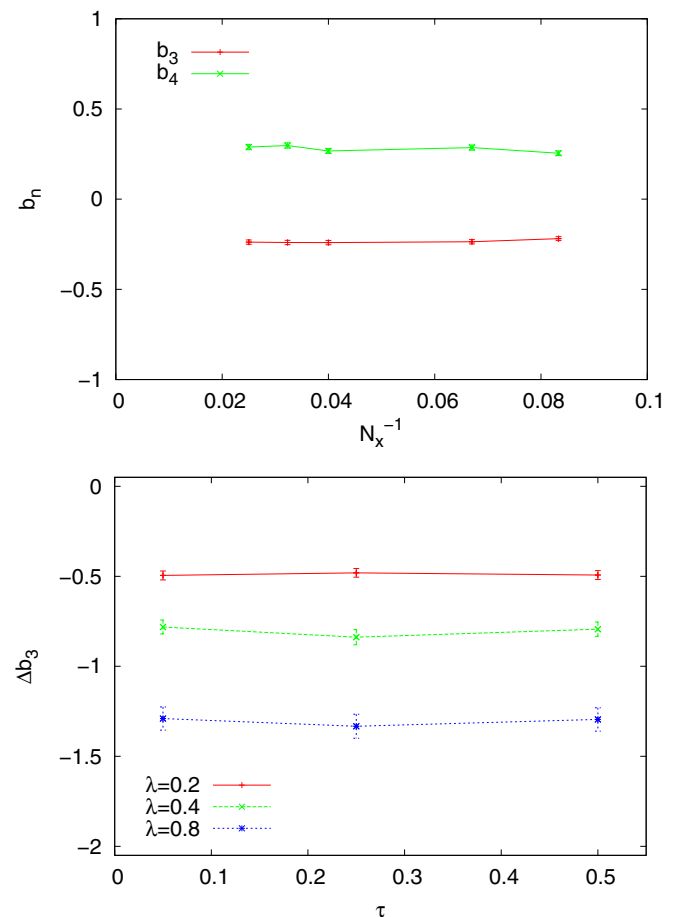


FIG. 4. Top: Illustration of the size of the finite- N_x effects on b_3 and b_4 in 1D at $\lambda = 1$. The error bars show statistical effects. Bottom: Illustration of the size of the finite- τ effects on Δb_3 in 2D for varying λ .

limit,

$$\Delta b_2 = \frac{1}{\lambda_T^d} \frac{e^{\beta g} - 1}{2}. \quad (\text{A3})$$

The calculation of Δb_3 is only slightly more tedious and yields

$$\Delta b_3 = \frac{2 \Delta Q_{2,1}}{Q_1} - Q_1 \Delta b_2 = -\frac{1}{\lambda_T^d} \frac{e^{\beta g} - 1}{2^{d/2}}. \quad (\text{A4})$$

We thus obtain the result advertised in the main text, namely,

$$\Delta b_3 = -2^{1-d/2} \Delta b_2. \quad (\text{A5})$$

The calculation of Δb_4 follows the same steps but yields a contribution that is quadratic in Δb_2 :

$$\Delta b_4 = 2(3^{-d/2} + 2^{-d-1}) \Delta b_2 \quad (\text{A6})$$

$$+ 2^{1-d/2} (2^{-d-1} - 1) (\Delta b_2)^2. \quad (\text{A7})$$

APPENDIX B: SYSTEMATIC EFFECTS

Because we chose a lattice regularization to carry out our calculations, there are a few systematic effects that need to be taken into account. First of all, we have put the system on

a lattice and must describe how to take the continuum limit. That amounts to enlarging the window $\ell \ll \lambda_T \ll L$, where $\ell = 1$, $L = N_x \ell$, and $\lambda_T = \sqrt{2\pi\beta}$ is the thermal wavelength.

Our main results correspond to $N_x = 30$ and $\lambda_T \simeq 7$ such that the above window is well satisfied. As an illustration of the size of the finite- N_x effects, we show results for varying N_x in Fig. 4 (top). The variation is appreciable but small on the scale of the corresponding plot in the main text.

The second systematic effect to account for is the number of Fourier points N_k used for the projection. Relying on Nyquist's theorem, taking N_k at least twice as large as the highest desired virial coefficient n_{\max} should be sufficient. However, that lower bound turns out to be much too optimistic in practice. As a conservative choice, we set $N_k = 30$ and find that it enables projections up to $n = 6$ with up to two decimal places. Note that the computation time scales linearly with N_k and is perfectly parallelizable in that variable.

The third systematic effect is the dependence on the temporal lattice spacing τ . We have tested $\tau = 0.05, 0.25$, and 0.5 as shown in Fig. 4 (bottom). Remarkably, the variation is small on the scale of the plot in the main figure (somewhat zoomed in here).

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