Semiclassical approximation to virial coefficients beyond the leading order

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We extend the calculation of virial coefficients of Fermi gases in the semiclassical approximation to next-to- and next-to-next-to-leading orders for \( b_2, b_3, b_4, \) and \( b_5 \). Our results feature relationships between interaction-induced changes \( \Delta b_3, \Delta b_4, \) and \( \Delta b_5 \) in terms of \( \Delta b_2 \), the latter being exactly known in many cases by virtue of the Beth-Uhlenbeck formula, and which we use as a renormalization condition. We compare our results in \( d = 1, 2, 3 \) spatial dimensions with known answers from Monte Carlo calculations and diagrammatic approaches. In particular, we find good agreement for \( \Delta b_3 \) with previous calculations in all dimensions and we formulate predictions for \( \Delta b_4 \) and \( \Delta b_5 \) for attractive interactions.

I. INTRODUCTION

The thermodynamics of interacting fermions at finite density is largely (though not only) controlled by the value of the temperature \( T \) relative to the Fermi energy scale \( \varepsilon_F \) or alternatively the chemical potential \( \mu \). For systems with attractive interactions, the regime \( \beta \mu \gg 1 \), where \( \beta = 1/(k_B T) \), often contains the onset of a superfluid or superconducting transition, while in the region \( \beta \mu \approx 0 \) a crossover regime between quantum and classical physics takes place. When \( z = e^{\beta \mu} \ll 1 \), systems are in a dilute, high-temperature regime whose thermodynamics is captured by the virial expansion, i.e. an expansion in powers of \( z \). Such an expansion encodes, at a given order \( n \), the physics of the \( n \)-body problem in the form of virial coefficients. The simplest form of the virial expansion is that of the pressure (which is naturally inherited by the density and the compressibility), with corresponding coefficients usually denoted by \( b_n \).

The applications of the virial expansion in quantum many-body physics have mushroomed in recent years with the equally widespread multiplication of ultracold-atom laboratories around the world (see e.g. [1–5]). Indeed, as the density is among the easiest thermodynamic observables to determine experimentally [6–9], the virial expansion has served as a natural non-perturbative ansatz to employ for the results of a variety of theoretical approaches in a dilute limit \( z \to 0 \), where \( z = e^{\beta \mu} \). For \( n \) \( > 1 \) the calculation two steps further in the semiclassical expansion, i.e. at next-to- and next-to-next-to-leading order (NLO and N2LO, respectively), and up to \( \Delta b_5 \).

II. HAMILTONIAN AND VIRIAL EXPANSION

We will focus on the simplest kind of interacting effective theory one can write for nonrelativistic fermionic matter in \( d \) spatial dimensions. The Hamiltonian for two species \( \uparrow, \downarrow \) is \( H = \hat{T} + \hat{V} \), where

\[
\hat{T} = \sum_{s=\uparrow,\downarrow} \int d^d x \, \hat{\psi}_{s}^\dagger(x) \left( -\frac{\hbar^2 \nabla^2}{2m} \right) \hat{\psi}_{s}(x),
\]

and

\[
\hat{V} = -g_{4D} \int d^d x \, \hat{n}_{\uparrow}(x) \hat{n}_{\downarrow}(x),
\]

where the field operators \( \hat{\psi}_s, \hat{\psi}_s^\dagger \) are fermionic fields for particles of spin \( s = \uparrow, \downarrow \), and \( \hat{n}_s(x) \) are the coordinate-space densities. In the remainder of this work, we will take \( \hbar = k_B = m = 1 \). Moreover, we will put the above Hamiltonian on a spatial lattice of spacing \( \ell \), whose calibration will be determined by our renormalization condition, as explained below.

As mentioned above, the virial expansion is an expansion around the dilute limit \( z \to 0 \), where \( z = e^{\beta \mu} \) is the fugacity, \( \beta \) is the inverse temperature, and \( \mu \) the chemical potential coupled to the total particle number operator \( \hat{N} \). The coefficient accompanying the \( n \)-th power of \( z \) in the expansion of the grand-canonical potential \( \Omega \) is the virial coefficient \( b_n \):

\[
-\beta \Omega = \ln \mathcal{Z} = Q_1 \sum_{n=1}^{\infty} b_n z^n,
\]

where

\[
\mathcal{Z} = \text{tr} \left[ e^{-\beta (\hat{H} - \mu \hat{N})} \right] = \sum_{N=0}^{\infty} z^N Q_N,
\]
is the grand-canonical partition function. $Q_N$ is the $N$-body partition function, $b_1 = 1$, and the higher-order coefficients are given by
\begin{align}
Q_1 b_2 &= Q_2 - \frac{Q_1^2}{2!}, \\
Q_1 b_3 &= Q_3 - b_2 Q_1^2 - \frac{Q_1^3}{3!}, \\
Q_1 b_4 &= Q_4 - \left( b_3 + \frac{b_2^2}{2} \right) Q_1^2 - b_2 Q_1^3 - \frac{Q_1^4}{4!}, \\
Q_1 b_5 &= Q_5 - (b_4 + b_2 b_3) Q_1^2 - \left( b_3^2 + b_3 \right) \frac{Q_1^3}{2} - b_2^2 \frac{Q_1^4}{3!} - \frac{Q_1^5}{5!}.
\end{align}

etcetera. The noninteracting virial coefficients for non-relativistic fermions in $d$ spatial dimensions are $b_n^{(0)} = (-1)^{n+1} n^{-(d+2)/2}$.

The highest power of $Q_1$ does not involve the interaction and therefore always disappears in the interaction change $\Delta b_n$:
\begin{align}
Q_1 \Delta b_2 &= \Delta Q_2, \\
Q_1 \Delta b_3 &= \Delta Q_3 - Q_1^2 \Delta b_2, \\
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, \\
Q_1 \Delta b_5 &= \Delta Q_5 - \Delta (b_4 + b_2 b_3) Q_1^2 - \frac{\Delta b_2}{2} Q_1^3 - \frac{\Delta b_2}{3!} Q_1^4.
\end{align}

Furthermore, in terms of the partition functions $Q_{MN}$ of $M$ particles of one type and $N$ of the other type, we have
\begin{align}
\Delta Q_2 &= \Delta Q_{11}, \\
\Delta Q_3 &= 2 \Delta Q_{21}, \\
\Delta Q_4 &= 2 \Delta Q_{31} + \Delta Q_{22}, \\
\Delta Q_5 &= 2 \Delta Q_{32} + 2 \Delta Q_{41}.
\end{align}

Therefore, the main complexity in the calculations presented below is in computing the few $\Delta Q_{MN}$ shown above within the semiclassical approximation.

### III. THE SEMICLASSICAL APPROXIMATION AT NEXT-TO-LEADING ORDER AND BEYOND

#### A. Trotter-Suzuki factorizations

We introduce a Trotter-Suzuki factorization of the Boltzmann weight, such that
\begin{equation}
\begin{aligned}
e^{-\beta (\hat{T} + \hat{V})} &= \left( e^{-\beta \hat{T}/n} e^{-\beta \hat{V}/n} \right)^n + \mathcal{O}(1/n), \\
e^{-\beta (\hat{T} + \hat{V})} &\approx e^{-\beta \hat{T}} e^{-\beta \hat{V}},
\end{aligned}
\end{equation}

which is equivalent to neglecting $[\hat{T}, \hat{V}]$ and higher-order commutators; for that reason we call this a semiclassical expansion. We define the NLO by setting $n = 2$ in the factorization, such that
\begin{equation}
e^{-\beta (\hat{T} + \hat{V})} \approx e^{-\beta \hat{T}/2} e^{-\beta \hat{V}/2} e^{-\beta \hat{T}/2} e^{-\beta \hat{V}/2}.
\end{equation}

Both Eq. (18) and Eq. (19) approximate the true Boltzmann weight up to the same order in powers of $\beta$: the error is $\mathcal{O}(\beta^3)$. However, in all cases of interest here, the expressions will appear inside a trace, such that the error is pushed to $\mathcal{O}(\beta^3)$. Indeed, as far as the trace is concerned, Eq. (18) is equivalent to the more accurate, symmetric decomposition
\begin{equation}
e^{-\beta (\hat{T} + \hat{V})} \approx e^{-\beta \hat{T}/2} e^{-\beta \hat{V}} e^{-\beta \hat{T}/2},
\end{equation}

whose error is $\mathcal{O}(\beta^3)$, and similarly for Eq. (19). For the same reason, the error is actually $\mathcal{O}(1/n^2)$ rather than $\mathcal{O}(1/n)$ in Eq. (17).

#### B. A simple example at NLO

As the simplest nontrivial example of the NLO-SCLA, we consider $Q_{11}$, whose calculation begins as follows:
\begin{equation}
\begin{aligned}
Q_{11} &= \sum_{p_1 p_2} \langle p_1 p_2 | e^{-\beta \hat{T}/2} e^{-\beta \hat{V}} e^{-\beta \hat{T}/2} | p_1 p_2 \rangle \\
&= \sum_{p_1 p_2} \delta \left( |p_1^2 + p_2^2|/4m - \beta |p_1^2 + p_2^2|/4m \right) \\
&\times \langle p_1 p_2 | e^{-\beta \hat{V}/2} | p_3 p_4 \rangle \langle p_3 p_4 | e^{-\beta \hat{V}/2} | p_1 p_2 \rangle.
\end{aligned}
\end{equation}

The next step is to insert a coordinate-space completeness relation and use the following identity:
\begin{equation}
\begin{aligned}
e^{-\beta \hat{V}/2} |x_1 x_2 \rangle &= \prod_z \left( 1 + C n_z \langle z | n_z \rangle |x_1 x_2 \rangle \\
&= |x_1 x_2 \rangle + C \delta_{x_1, x_2} \sum_z \delta_{x_2, z} |x_1 x_2 \rangle \\
&= [1 + C \delta_{x_1, x_2}] |x_1 x_2 \rangle,
\end{aligned}
\end{equation}

where $C = (e^{\beta \delta d/2} - 1) \ell^d$ and we used the fermionic relation $\n_z^2 = \hat{n}_z$. Note that the series in powers of $C$ terminates at linear order for this particular state in which there is only one particle for one of the species (regardless of how many particles of the other species are present). The C-independent term yields the noninteracting result, such that
\begin{equation}
\begin{aligned}
\Delta Q_{11} &= \sum_{p^1 p^2 p^3 p^4} \langle p | X \rangle \langle X | p' \rangle \langle p' | X' \rangle \langle X' | p \rangle \\
&\times \left[ C \left( \delta_{x_1, x_2} + \delta_{x'_1, x'_2} \right) + C^2 \left( \delta_{x_1, x_2} \delta_{x'_1, x'_2} \right) \right]
\end{aligned}
\end{equation}

where $p$ is the shorthand for the set of momentum variables $p_1$ and $p_2$ and $p^2 = p_1^2 + p_2^2$, and similarly for $p'$, $X$, $X'$. 


Using a plane wave basis, \(|\langle \mathbf{x}_1 \mathbf{x}_2 | \mathbf{p}_1 \mathbf{p}_2 \rangle|^2 = 1/V^2\), where \(V = L^d\) in \(d\) spatial dimensions and \(L\) is the linear extent of the system, and we then find

\[
\Delta Q_{11} = C f_1/V + C^2 f_2/V^2, \tag{24}
\]

where \(f_1 = 2Q_{10}^2\), with

\[
Q_{10} = \sum_{\mathbf{p}_1} e^{-\beta \mathbf{p}_1^2/2m}, \tag{25}
\]

and

\[
f_1 = 2 \left( \frac{L}{\lambda_T} \right)^{2d}, \quad f_2 = \left( \frac{L}{\lambda_T} \right)^{3d/2}. \tag{28}
\]

where \(\lambda_T = \sqrt{2\pi \beta}\) is the thermal wavelength.

Thus,

\[
\Delta Q_{11} = 2 \left( \frac{L}{\lambda_T} \right)^d \left[ \frac{C}{\lambda_T^d} + 2^{d+1} \left( \frac{C}{\lambda_T^d} \right)^2 \right], \tag{29}
\]

such that

\[
\Delta b_2 = \frac{\Delta Q_{11}}{Q_1} = \frac{C}{\lambda_T^d} + 2^{d+1} \left( \frac{C}{\lambda_T^d} \right)^2, \tag{30}
\]

where we have used \(Q_1 = 2Q_{10}\).

IV. RESULTS

A. Canonical partition functions at NLO

As explained in the introduction, the main partition functions involved in \(\Delta b_2\), \(\Delta b_3\), and \(\Delta b_4\) are \(\Delta Q_{11}\), derived in the previous section, as well as \(\Delta Q_{21}\), \(\Delta Q_{31}\), and \(\Delta Q_{22}\). Of these, the last one is the most mathematically demanding, as it involves contributions up to order \(C^4\). Below we present a sample of our results in the NLO-SCLA for these selected partition functions in the continuum limit.

Calculating \(\Delta b_3\) requires \(\Delta b_2\) and the following result:

\[
\frac{2\Delta Q_{21}}{Q_1} = \frac{C}{\lambda_T^{3d}} \left[ -2^{1-\frac{d}{2}} + \left( \frac{L}{\lambda_T} \right)^d \right] + \left( \frac{C}{\lambda_T^d} \right)^2 \left[ \left( 1 - \frac{2^{d+1}}{5^2} \right) \left( \frac{L}{\lambda_T} \right)^d + \frac{1}{2^{d}} \left( \frac{L}{\lambda_T} \right)^{2d} \right]. \tag{31}
\]

Both of the contributions displaying explicit dependence on \(L/\lambda_T\) will cancel out in the final expression for \(\Delta b_3\), giving a volume-independent result.

Calculating \(\Delta b_4\) requires \(\Delta b_2\), \(\Delta b_3\), and the following two results:

\[
\frac{2\Delta Q_{31}}{Q_1} = \frac{C}{\lambda_T^d} \left[ \frac{2}{3^2} - \frac{3}{2^2} \left( \frac{L}{\lambda_T} \right)^d + \left( \frac{L}{\lambda_T} \right)^{2d} \right] + \left( \frac{C}{\lambda_T^d} \right)^2 \left[ \frac{1}{3^2} + \left( \frac{2^{d+1}}{5^2} \right) \left( \frac{L}{\lambda_T} \right)^d + \frac{1}{2^{d}} \left( \frac{L}{\lambda_T} \right)^{2d} \right], \tag{32}
\]

\[
\frac{\Delta Q_{22}}{Q_1} = \frac{C}{\lambda_T^d} \left[ 2^{1-d} - 2^{1-\frac{d}{2}} \left( \frac{L}{\lambda_T} \right)^d + \left( \frac{L}{\lambda_T} \right)^{2d} \right] + \left( \frac{C}{\lambda_T^d} \right)^2 \left[ 2^{1-d} - 1 + \left( \frac{L}{\lambda_T} \right)^d + 2^{d-1} \left( \frac{L}{\lambda_T} \right)^{2d} \right] + \left( \frac{C}{\lambda_T^d} \right)^3 \left[ 1 + 2^{1-\frac{d}{2}} - \frac{2^{2d}}{5^2} \right] + \left( \frac{C}{\lambda_T^d} \right)^4 \left[ \left( 1 + \left( \frac{L}{\lambda_T} \right)^d + 2^{d-1} \left( \frac{L}{\lambda_T} \right)^{2d} \right] \tag{33}
\]

As mentioned above, also in this case, the explicit dependence on \(L/\lambda_T\) will be cancelled in the final expression for \(\Delta b_4\). Only the constant terms will remain.

In the next section, we use the above expressions to assemble the calculation of \(\Delta b_3\) and \(\Delta b_4\), using Eqs. 9 through 16 at NLO. We will, in fact, go beyond the above expressions and present results for \(\Delta b_5\) as well, and extend the whole analysis to N2LO. As the equations
in the latter case are much too long to be displayed in
the present format in a useful manner, we have made a
Python code available with all our results as part of our
Supplemental Material [16].

The above derivations where carried out on paper for
$\Delta b_3$ and using a specially designed computer-algebra
code for $\Delta b_4$ and $\Delta b_5$, involving a combination of
FORM [17], Python code, and Mathematica. As checks
for those automated derivations, we have verified that the
cancellations guaranteeing that $\Delta b_n$ does not depend
explicitly on $L/\lambda_T$ were satisfied.

B. Virial coefficients: Analytic results at LO and
NLO

Previous work [14] [15] calculated the virial coefficients
in the LO-SCLA, which yields, for a fermionic two-species
system with a contact interaction, in $d$ spatial dimen-
sions,

\begin{align*}
\Delta b_3 &= -2^{1-d} \Delta b_2, \\
\Delta b_4 &= 2(3^{1-d} + 2^{-d-1}) \Delta b_2 \\
&\quad + 2^{1-d} (2^{-d-1} - 1)(\Delta b_2)^2, \\
\end{align*}

(34)

where we have corrected the coefficient of $(\Delta b_2)^2$ relative
to Ref. [14]. Also at LO, but going beyond the work of
Ref. [14], Ref. [15] found

\begin{align*}
\Delta b_5 &= -(2^{-d} + 6^{-d}) \Delta b_2 \\
&\quad + 4(2^{-d} + 3^{-d} - 7^{-d})(\Delta b_2)^2,
\end{align*}

(35)

which we show here for completeness as we will calculate
$\Delta b_5$ at higher orders in the SCLA.

As our main results, we have extended the above calcula-
tions to NLO and N2LO for $\Delta b_3$, $\Delta b_4$, and $\Delta b_5$. At
NLO, we found

\begin{align*}
\Delta b_2 &= \tilde{C} + 2^{1-d} \tilde{C}^2, \\
\Delta b_3 &= -2^{1-d} \tilde{C} + \left(1 - \frac{2^{1-d}}{5^2}\right) \tilde{C}^2, \\
\Delta b_4 &= 2(3^{1-d} + 2^{-d-1}) \tilde{C} + \left(3^{1-d} + 2^{-d-1} - \frac{3}{2^{d}}\right) \tilde{C}^2 \\
&\quad + \left(1 + 2^{1-d} - \frac{2^{d+2}}{5^2}\right) \tilde{C}^3 + \left(\frac{3}{4} - \frac{2^{d}}{3^2}\right) \tilde{C}^4, \\
\Delta b_5 &= -\left(2^{1-d} + \frac{2^{1-d}}{3^2}\right) \tilde{C} \\
&\quad + \left(\frac{7}{2^d} - \frac{2^{1+d}}{3^2} + \frac{7}{3^2} - \frac{2}{7^2} - \frac{2^{1+d}}{11^2} - 3 \cdot \frac{2^{1+d}}{19^2}\right) \tilde{C}^2 \\
&\quad + \left[2^{1-d} - 2^{1-d} + 4 \cdot 3^{1-d} \\
&\quad - 2^{d+2} \left(\frac{2}{3^d} + \frac{5^d}{11^2} - \frac{7^{-d}}{19^2}\right)\right] \tilde{C}^3 \\
&\quad + \left(1 + 2^{1-d} - \frac{2^{1+d} 3^{1-d}}{3^d 5^2} - \frac{3}{7^2} + 3 \cdot \frac{2^{1+d}}{29^2}\right) \tilde{C}^4,
\end{align*}

(36)

where $\tilde{C} = (e^{3g_{ad}/2} - 1)^{d^2}/\lambda_T^2$.

Note that, while the above expressions resemble truncated
power series in $\tilde{C}$, they actually display the full
answer at NLO, as defined by Eq. (19). Furthermore,
we note that as in the LO case, at NLO $\Delta b_2$ is always
positive and $\Delta b_3$ is always negative, for positive $\tilde{C}$ in
d = 1, 2, 3. The behavior of $\Delta b_4$ and $\Delta b_5$, however, is
less obvious.

Solving for $\tilde{C}$ in terms of $\Delta b_2$ at NLO, we find

\begin{equation}
\tilde{C} = 2^{-d} \left(\sqrt{1 + 2^{1-d} \Delta b_2} - 1\right),
\end{equation}

(41)

where we have chosen the solution that yields a real and
positive value for $\tilde{C}$, which corresponds to attractive in-
teractions and thus positive $\Delta b_2$. Using that result yields
$\Delta b_3 - \Delta b_5$ in terms of $\Delta b_2$.

C. Virial coefficients: Comparing LO, NLO, and
N2LO with previous results across dimensions

1D attractive Fermi gas. In Fig. 1, we compare our
LO, NLO, and N2LO results for $\Delta b_n$ for the 1D Fermi
gas with attractive interactions. We have in this case
used the exact result [18] [19]

\begin{equation}
\Delta b_2^{1D,\text{exact}} = -\frac{1}{2\sqrt{2}} + \frac{e^{\lambda^2/4}}{2\sqrt{2}} [1 + \text{erf}(\lambda/2)],
\end{equation}

(42)

into Eq. (41) to define $\tilde{C}$ as a function of the dimension-
less physical coupling $\lambda = 2\sqrt{3}/a_0$, where $a_0$ is the 1D
scattering length.
Our 1D calculations show excellent agreement with the quantum Monte Carlo data of Ref. [14] for $\Delta b_3$ and $\Delta b_4$. For the latter, the Monte Carlo calculations fail beyond $\lambda \approx 1$, but our analytic results do not show any particular feature in that region. $\Delta b_3$, $\Delta b_4$, and $\Delta b_5$ all show signs of convergence within the region of $\lambda$ shown in the figure.

2D attractive Fermi gas.- In Fig. 2 we compare our LO, NLO, and N2LO results for $\Delta b_n$ for the 2D Fermi gas with attractive interactions [20]. In this case, we have relied on the exact result given by [18, 21–26]

$$\Delta b_2^{2D,\text{exact}} = e^{\lambda^2} - \int_0^\infty \frac{dy}{\text{erf} \sqrt{2}} 2e^{-\lambda^2 y^2},$$

(43)

to define $\tilde{C}$ as a function of the physical coupling $\lambda_3 = \sqrt{\beta/\epsilon_B}$, where $\epsilon_B$ is the binding energy of the two-body problem.

Our 2D results display similarities to the 1D case: the agreement of our $\Delta b_3$ with the diagrammatic results of Ref. [23] is remarkable (see also Fig. 3), and the progression of $\Delta b_4$ and $\Delta b_5$ appears to show convergence in the region shown in Fig. 2.

3D attractive Fermi gas.- Finally, in 3D we have [18, 29]

$$\Delta b_2^{3D,\text{exact}} = \begin{cases} e^{\lambda_3^2}\left[1 - \text{erf}(-\lambda_3)\right], & \lambda_3 < 0, \\ \sqrt{2}\lambda_3^2 - \frac{\lambda_3^2}{\sqrt{2}}\left[1 - \text{erf}(\lambda_3)\right], & \lambda_3 > 0, \end{cases}$$

(44)

where $\lambda_3 = \sqrt{3}/a_0$, and $a_0$ is the s-wave scattering length. Note the unitarity limit corresponds to $\lambda_3 = 0$.

In Fig. 4 we compare our LO, NLO, and N2LO results for $\Delta b_n$ for the 3D Fermi gas with attractive interactions.
V. SUMMARY AND CONCLUSIONS

In this work we calculated the interaction-induced change in the third to fifth virial coefficients, \( \Delta b_3 - \Delta b_5 \), of spin-1/2 fermions with attractive interactions at NLO and N2LO in a semiclassical lattice approximation. Using a renormalization prescription based on matching \( \Delta b_2 \) to the known exact results, we obtained analytic relationships between \( \Delta b_n \) and \( \Delta b_2 \), for \( n = 3, 4, 5 \), valid in the SCLA for arbitrary spatial dimension. In particular, we showed our results for 1D, 2D, and 3D.

Our NLO and N2LO results in 1D show a clear improvement over the LO results of Ref. [14] for \( b_3 \) and \( b_5 \), and predict \( b_5 \) (in fact, the latter could not be calculated reliably in the Monte Carlo approach of Ref. [14]). Similarly, our calculations in 2D at NLO and N2LO for \( \Delta b_3 \) are a dramatic improvement over the LO result of Ref. [14], and predict \( \Delta b_4 \) and \( \Delta b_5 \) in a wide range of couplings.

| Reference  | \( \Delta b_2 \) | \( \Delta b_3 \) | \( \Delta b_4 \) | \( \Delta b_5 \) |
|------------|-----------------|-----------------|-----------------|-----------------|
| \( 1/\sqrt{2} \) | -0.355          | 0.078(18)       | -               | -               |
| LO         | -0.53           | 0.0695          | 0.254           | -               |
| NLO        | -0.391          | 0.0173          | 0.158           | -               |
| N2LO       | -0.364          | 0.0179          | 0.128           | -               |

This behavior shows that, barring lattice artifacts that will likely modify the final (i.e. converged) answer, studies at even higher order will be needed to establish the convergence properties of the SCLA.

In this case, the behavior of our approximation seems somewhat more promising than in 1D and 2D. First, we find excellent agreement with the exact result for \( \Delta b_3 \) of Ref. [30] in the strongly coupled regime, shown in more detail in Fig. 4 (see also Refs. [31–34]). Moreover, our results for \( \Delta b_4 \) and \( \Delta b_5 \) appear to be converged at N2LO, at least within the scale of our plots.

A closer look at the unitary point [28] at \( \lambda_3 = 0 \) is shown in Table I, revealing that the alleged convergence seen in the plots is not necessarily uniform, as shown by \( \Delta b_4 \). For that case, our results are still far from the expected reference value (path-integral Monte Carlo result from Ref. [27]). This behavior shows that, barring lattice artifacts that will likely modify the final (i.e. converged) answer, studies at even higher order will be needed to establish the convergence properties of the SCLA.
Our 3D results show remarkable agreement with the exact result of Ref. [30] for $\Delta b_3$, even as far as the unitary point. On the other hand, discrepancies in the case of $\Delta b_4$ at unitarity, which was calculated in Ref. [27], remain to be resolved. Regardless, we expect our results to be accurate at least at weak coupling (i.e. around $1/\lambda_3 = 0$). Additionally, our calculations for $\Delta b_5$ in 3D are also a prediction, with the caveat that their validity at strong coupling (in particular at unitarity, in spite of the seemingly convergent behavior) should be further studied.

Finally, it should be pointed that, although we have shown results for a variety of attractively interacting Fermi gases, our analytic results apply to repulsively interacting cases as well. To facilitate the application of our results to those and other cases, we have made our results available in a Python code as Supplemental Material [16].

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