Spectral density, Levinson's theorem, and the extra term in the second virial coefficient for the one-dimensional δ-function potential

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In contrast with the three-dimensional result, the Beth-Uhlenbeck (BU) formula in one dimension contains an extra $-1/2$ term. The origin of this $-1/2$ term is explained using a spectral density approach. To be explicit, a δ-function potential is used to show that the correction term arises from a pole of the density of states at zero energy. The spectral density method shows that this term is actually an artifact of the non-normalizability of the scattering states and an infrared cutoff regularization scheme has to be used to get the correct result in one dimension. The formal derivation of the BU formula would miss this term since it ignores the effects of the boundary terms. While the result is shown for the δ-function potential, the method and result are valid for more general potentials. Additionally, the one-dimensional Levinson theorem can be extracted from the spectral density method using the asymptotic form of general potentials. The importance of the result lies in the fact that all these correction terms in one dimension have a universal source: a pole at zero energy. Similar calculations using quantum field-theoretical approaches (without explicit infrared cutoff regularization schemes) also show the same subtleties with the correction term originating from the zero energy scattering states (Appendix A).

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I. INTRODUCTION

The virial expansion was developed in the beginning of the 20th century [1] to provide an estimate of the deviation of the behavior of real gases from the ideal gas equation. Since then, the second virial coefficient b_2 has been studied in great detail because it can be calculated analytically and gives the leading-order correction for real gases. The virial coefficients reflect, order by order, the effects of interactions on the n-body problem: the nth-order virial coefficient is determined by solving the n-body problem. Therefore, one can obtain the shift in b_2 from the free particle case *analytically* by solving the two-body Schrödinger equation with an interaction potential. Beth and Uhlenbeck, in their famous paper [2], showed that this shift δb_2 is related to the scattering phase shift in three dimensions. Since then the result has been generalized in lower dimensions as well [3–5]. Recently, it was proven that δb_2 is the imprint of the quantum scale anomaly in dilute quantum gases in one dimension with three-body local interactions and two dimensions with two-body local interactions [6,7] using a many-body path-integral formalism [8]. In an effort to extend this work with a one-dimensional (1D) local derivative-δ interaction, it was demonstrated that the derivative-δ potential shares a number of properties with the δ-function potential [9]. One of them is that a straightforward application of the Beth-Uhlenbeck (BU) formula misses a $-1/2$ term to give a nonzero result in the limit $E_B \to 0$ ($E = -E_B$, $E_B > 0$ is the bound-state energy). It has been previously shown that in one dimension the correct BU formula has an additional $-1/2$ term which produces the correct result for the 1D δ function in the limit $E_B \to 0$. The origin of this mysterious term in one dimension has been mentioned in several works [10–13].

The present paper is an effort to make the formalism more understandable and to connect different contexts that share the same property with regards to the $-1/2$ term. In this note, we use the spectral density approach to show in detail that this term is due to the non-normalizability of the scattering states and the contribution of the zero energy state of the system. We have used an infrared (large volume, length in one dimension) cutoff regularization method to systematically control the divergences in the calculation, which gives us the desired $-1/2$ term. For simplicity, and for the sake of better understanding, we have used the results of scattering from a δ-function potential, but the method can be implemented for general potentials as well. In addition to providing the correction term in the BU formula, the spectral density approach can also be used to derive the 1D Levinson theorem [14]. We have also investigated similar subtleties using different methods based on quantum field-theoretical treatments of the partition function [15]. These methods also give the correct $-1/2$ term, but in some its appearance seems simpler than others. We have chosen to give a sketch of the calculation using the method of [16] in Appendix A, since the subtleties there appear to be closely related to the ones in the spectral density method investigated here. A more comprehensive and detailed review of these issues will appear elsewhere [15].

This paper is organized as follows. In Sec. II we show how a naive application of the BU formula gives an incorrect

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result for the 1D δ-function interaction. In Sec. III we use the spectral density method to find the correction term to the BU formula. Finally, we discuss the relation between Levinson's theorem and the spectral density method in Sec. IV followed by a brief discussion of the whole topic in Sec. V.

II. BETH-UHLENBECK FORMULA

The BU formula [2] connects the shift of the second virial coefficient from the free case (δb_2) to the scattering phase shift of the potential. For a phase shift $\delta_l(k)$ corresponding to the lth partial wave, the BU formula in one dimension is given by (see Appendix B)

$$\delta b_2 = \sum_B e^{\beta E_B} + \frac{1}{\pi}\sum_{l=0,1}\int_0^\infty dk\, e^{-\beta k^2}\frac{d\delta_l(k)}{dk}, \tag{1}$$

where $E = -E_B$ ($E_B > 0$) is a bound-state energy and $\beta = 1/k_B T$. For the 1D δ-function potential, there is only a s-wave scattering phase shift, and hence the only possible value of l is zero. The scattering phase shift for this potential is given by $\delta_0(k) = \arctan\left(\frac{\sqrt{E_B}}{k}\right)$ in the units of reduced mass $\mu = 1/2$ [17]. From here on we will omit the l subscript on the phase shift and just denote it by $\delta(k)$. Using the BU formula given in Eq. (1), and plugging in the phase shift of the δ function one obtains

$$\delta b_2 = e^{\beta E_B} - \tfrac{1}{2}e^{\beta E_B}(1 - \mathrm{erf}[\sqrt{\beta E_B}]). \tag{2}$$

It is easy to see that this expression is incorrect by checking the limit $E_B \to 0$. When the potential strength goes to zero, one should expect that the shift in the second virial coefficient vanishes. In this case, instead of obtaining zero, we get $\delta b_2 = 1/2$ in the $E_B \to 0$ limit. Clearly, this is incorrect and Eq. (1) is missing terms. To determine the missing terms, we evaluate the quantity δb_2 using the spectral density method.

III. SPECTRAL DENSITY METHOD

Green's functions have extensive use in quantum mechanics [18]. One of them is the usage of the spectral representation of the retarded Green's function to find out the spectral function. The spectral function denotes the probability that a certain state with momentum k has energy E. This is exactly what the local density of states is. The local density of states can then be integrated with respect to real space to give the global density of states, a quantity which is related to scattering phase shifts. In this section, we are going to exploit this relation between the density of states and the retarded Green's function to find the missing term in the BU formula.

The global density of states in the spectral density method is given by [19]

$$\frac{dN}{dE} = -\frac{1}{\pi}\int_{-\infty}^{\infty} dx\, \mathrm{Im}[G(x,x)], \tag{3}$$

where $G(x,x')$ is the retarded Green's function of the system. For an attractive 1D δ-function potential we have exactly one bound state and a continuum of scattering states. So, the Hilbert space can be separated into two parts. One part includes the bound states and the other includes the scattering states. With this structure, the Green's function can be written as

$$G(x,x') = \lim_{\epsilon\to 0}\frac{\psi_B(x)\psi_B^*(x')}{E + E_B + i\epsilon} + \int_{-\infty}^{\infty}\frac{dk}{2\pi}\frac{\psi_k(x)\psi_k^*(x')}{E - k^2 + i\epsilon}, \tag{4}$$

where the first term corresponds to the bound state [$\psi_B(x)$] and the integral is over the momentum of scattering states [$\psi_k(x)$]. In Eq. (4) it is implicitly understood that the scattering states are defined only for positive energy of the system ($E > 0$) and bound states are defined for negative energy of the system ($E < 0$).

The density of states changes when the interaction is turned on. Without the interaction potential, we will only have a free particle with a continuous energy spectrum. The appearance of the bound states when the interaction is nonzero indicates the change in density of states. This change can be written in terms of Eq. (3):

$$\frac{d\Delta N}{dE} = -\frac{1}{\pi}\int_{-\infty}^{\infty} dx\, \mathrm{Im}[G(x,x)] + \frac{1}{\pi}\int_{-\infty}^{\infty} dx\, \mathrm{Im}[G_0(x,x)]. \tag{5}$$

$G_0(x,x')$ is the Green's function for the noninteracting case (free particle). The change in the density of states is related to the difference between the classical and quantum calculation of the second virial coefficient δb_2 by (see Appendix B)

$$\delta b_2 = \int_{-\infty}^{\infty} dE\, e^{-\beta E}\frac{d\Delta N}{dE}. \tag{6}$$

Writing out the whole expression explicitly we get

$$\delta b_2 = \int_{-\infty}^{\infty} dE\, e^{-\beta E}\left(-\frac{1}{\pi}\right)\int_{-\infty}^{\infty} dx\, \mathrm{Im}[G(x,x) - G_0(x,x)] \tag{7}$$

$$= \int_{-\infty}^{\infty} dE\, e^{-\beta E}\left(-\frac{1}{\pi}\right)\int_{-\infty}^{\infty} dx\, \mathrm{Im}\left[\frac{|\psi_B(x)|^2}{E + E_B + i\epsilon} + \int_{-\infty}^{\infty}\frac{dk}{2\pi}\frac{|\psi_k(x)|^2 - |\psi_0(x)|^2}{E - k^2 + i\epsilon}\right], \tag{8}$$

where $\psi_0(x)$ is the free particle wave function [it is still dependent on k, but we use $\psi_0(x)$ for notational convenience]. In Appendix C we verify that this form of writing the second virial coefficient using the spectral density function is equivalent to the BU formula. So, it may seem that this method of calculating the shift in the second virial coefficient will yield the same incorrect result for δb_2 in the case of a δ-function potential. Indeed, with a naive straightforward calculation one would end up with the same result. However, a careful consideration of divergent quantities (like the normalization of scattering states), which can explicitly be recognized in this method, yields the correct expression for δb_2 and provides a modification of the BU formula.

To arrive at the BU formula involving phase shift from the expression with density of states, we have used a certain approximation (see Appendix B). First, we evaluated the number of states in a large box of volume L and then took the limit $L \to \infty$. Even though the error in following this argument is usually negligible, in certain cases this boundary condition can contribute significantly. We will see in the following discussion how this approximation contributes to the evaluation of δb_2 in the spectral density formalism.

From Eq. (8), the calculation of the bound-state energy part is rather straightforward and gives a contribution of $e^{\beta E_B}$ (see Appendix C). So, here we consider the scattering part of δb_2 and denote it by $\delta b_2^{\rm sc}$, which is given by

$$\delta b_2^{\rm sc} = \int_0^\infty dE\, e^{-\beta E}\left(-\frac{1}{\pi}\right) \times \int_{-\infty}^{\infty} dx\, \mathrm{Im}\left[\int_{-\infty}^{\infty}\frac{dk}{2\pi}\frac{|\psi_k(x)|^2-|\psi_0(x)|^2}{E-k^2+i\epsilon}\right]. \quad (9)$$

The imaginary part of the denominator in the limit $\epsilon \to 0$ gives a δ function in k (Sokhotski-Plemelj theorem), yielding

$$\delta b_2^{\rm sc} = \int_0^\infty dE\, e^{-\beta E}\int_{-\infty}^{\infty} dx \times \int_{-\infty}^{\infty}\frac{dk}{2\pi}[|\psi_k(x)|^2-|\psi_0(x)|^2]\delta(E-k^2). \quad (10)$$

We can write the scattering states for a δ-function potential as [20]

$$\psi_k(x) = e^{ikx} + R(|k|)e^{i|k||x|}, \quad R(|k|) = -\frac{\kappa}{\kappa+i|k|}, \quad (11)$$

where $\kappa = \sqrt{E_B}$ is the wave vector corresponding to the bound-state energy. After performing the integration over k—using $\delta[f(x)] = \sum_{x_0}\frac{\delta(x-x_0)}{|f'(x_0)|}$, where $f(x_0)=0$—we get

$$\delta b_2^{\rm sc} = -\int_0^\infty dE\, e^{-\beta E}\int_{-\infty}^{\infty} dx \frac{\sqrt{E_B}}{\pi\sqrt{E}(E+E_B)} \times \left\{\sqrt{E_B}\cos[\sqrt{E}(|x|-x)] + \sqrt{E}\sin[\sqrt{E}(|x|-x)] - \frac{\sqrt{E_B}}{2}\right\}. \quad (12)$$

The x integrals of the oscillating terms are divergent. The physical origin of this divergence is the non-normalizability of the scattering states. To make our way around this divergence, we introduce an infrared cutoff regularization procedure. In this process we change the limit of integration $\int_{-\infty}^{\infty} dx \to \int_{-a}^{a} dx$ with $a \to \infty$. This is conceptually the same as considering a box of length $2a$ and then taking the boundaries to infinity. We only take the limit $a \to \infty$ after performing the E integral and hope that the divergences disappear. The quantity with the cutoff regularization becomes

$$\delta b_2^{\rm sc} = -\lim_{a\to\infty}\int_0^\infty dE\, e^{-\beta E}\int_{-a}^{a} dx \frac{\sqrt{E_B}}{\pi\sqrt{E}(E+E_B)} \times \left\{\sqrt{E_B}\cos[\sqrt{E}(|x|-x)] + \sqrt{E}\sin[\sqrt{E}(|x|-x)] - \frac{\sqrt{E_B}}{2}\right\}. \quad (13)$$

The integration over x is now finite and can be carried out to yield

$$-\lim_{a\to\infty}\int_0^\infty dE\, e^{-\beta E}\frac{\sqrt{E_B}}{2\pi\sqrt{E}(E+E_B)} \times \left[1-\cos(2\sqrt{E}a)+\frac{\sqrt{E_B}}{\sqrt{E}}\sin(2\sqrt{E}a)\right]. \quad (14)$$

The first term in the bracket is independent of the cutoff parameter a, and produces the same result as the BU formula:

$$-\int_0^\infty dE\, e^{-\beta E}\frac{\sqrt{E_B}}{2\pi\sqrt{E}(E+E_B)} = -\frac{1}{2}e^{\beta E_B}(1-\mathrm{erf}[\sqrt{\beta E_B}]). \quad (15)$$

So, the correction term to the BU formula appears from the cutoff regularization and needs to be evaluated explicitly. With the substitution of $E=k^2$, the term involving the cutoff parameter becomes

$$\lim_{a\to\infty}\int_0^\infty dk\, e^{-\beta k^2}\frac{\sqrt{E_B}}{\pi(k^2+E_B)}\left[\cos(2ka)-\frac{\sqrt{E_B}}{k}\sin(2ka)\right]. \quad (16)$$

The first term within the brackets can be rewritten as

$$\lim_{a\to\infty}\frac{1}{2\pi}\int_{-\infty}^{\infty} dk\, e^{-\beta k^2}\frac{\sqrt{E_B}}{(k^2+E_B)}e^{2ika} = 0. \quad (17)$$

The integration can be done by considering a semicircular contour in the upper half plane because $a>0$ [Fig. 1(a)]. The pole $k=+i\sqrt{E_B}$ contributes to the residue, and in the limit $a\to\infty$ the residue vanishes. The second term in Eq. (16), however, has three poles, at $k=\pm i\sqrt{E_B}$ and 0. We consider a similar semicircular contour in the upper half plane but now there is another pole on the real axis $k=0$ [Fig. 1(b)]. To avoid this, we take an infinitesimal semicircular detour around it (with radius $\epsilon\to 0$). The contribution from the pole inside the contour gives a zero contribution in the limit $a\to\infty$ as before but the small infinitesimal arc contributes a $-\frac{1}{2}$ term:

$$-\lim_{a\to\infty}\frac{1}{2\pi i}\int_{-\infty}^{\infty} dk\, e^{-\beta k^2}\frac{E_B}{k(k^2+E_B)}e^{2ika} = -\frac{1}{2}. \quad (18)$$

Combining Eq. (17), Eq. (18), and the contribution from the bound state part we now have the complete result:

$$\delta b_2 = e^{\beta E_B} - \tfrac{1}{2}e^{\beta E_B}(1-\mathrm{erf}[\sqrt{\beta E_B}]) - \tfrac{1}{2}. \quad (19)$$

We see that in the limit $E_B\to 0$ this now gives the correct answer, which is $\delta b_2 = 0$. The $-1/2$ term came from the residue of the pole at $k=0$, which is equivalent to the contribution of the zero energy state. This shows that we must be careful while dealing with the boundary terms that produces a divergence (taking the limit that the box length goes to infinity).

IV. CORRECTION TO THE BU FORMULA IN ONE DIMENSION AND LEVINSON'S THEOREM

In the previous section we found that there are subtle correction terms to the BU formula appearing from the infrared regularization procedure and carefully taking the length of the box to infinity. So, where did it go wrong in the BU formula derivation? As shown in Appendix C, the scattering part of Eq. (8) can also be rewritten as

$$\delta b_2^{\rm sc} = \int_0^\infty \frac{dk}{\pi}\, e^{-\beta k^2}\int_{-\infty}^{\infty} dx[|\psi_k(x)|^2-|\psi_0(x)|^2]. \quad (20)$$

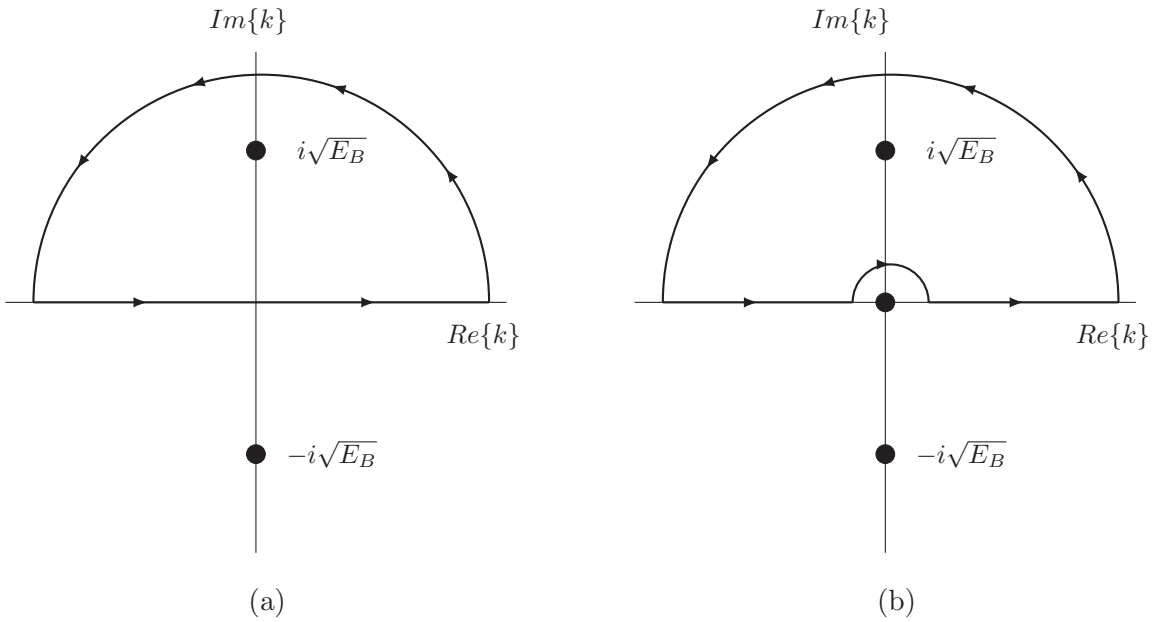

FIG. 1. (a) Contour for integration in Eq. (17). The poles are at $k = \pm i\sqrt{E_B}$ but there is no pole at $k = 0$. (b) Integration contour required in Eq. (18). The poles are at $k = \pm i\sqrt{E_B}$ and at $k = 0$. The small detour around $k = 0$ contributes the extra $-1/2$ term.

Looking closely at Eq. (20), one can recognize that the x integrals over the scattering states are divergent as well. Instead of treating this divergence carefully, we rewrote the probability density (density of states) in terms of phase shifts assuming that there is no consequence of ignoring the effects of taking the box boundaries to infinity. In fact, one can carry out the same cutoff regularization scheme starting from Eq. (20)—considering $\psi_k(x) = \cos[k|x| + \delta(k)]$—and get a more generalized correction term involving phase shifts equivalent to Eq. (16). This approach gives us the modification to the BU formula:

$$\delta b_2 = \sum_B e^{\beta E_B} + \int_0^\infty \frac{dk}{\pi}\frac{d\delta(k)}{dk}\, e^{-\beta k^2} + I, \tag{21}$$

where

$$I = \lim_{a\to\infty}\int_0^\infty dk\, \frac{e^{-\beta k^2}}{2\pi k}(\sin(2ka)\{\cos[2\delta(k)] - 1\} + \cos(2ka)\sin[2\delta(k)]). \tag{22}$$

One can check that Eqs. (22) and (16) are identical by plugging in the phase shift for the δ-function potential $\delta(k) = \arctan(\frac{\sqrt{E_B}}{k})$. The contribution of the correction term depends on the nature of the interacting system at $k = 0$. For a system with a bound state at zero energy ($k = 0$), the integral I vanishes in the limit $a \to \infty$ (because there is no pole anymore at $k = 0$). Otherwise it will contribute a nonzero correction to Eq. (21). This statement has a very close relation to Levinson's theorem [21–24]. Levinson's theorem relates the number of bound states for a symmetric potential to the phase shift at zero energy and infinite energy.

To see how the spectral density formalism relates to Levinson's theorem in one dimension, we refer back to Eq. (3). Instead of finding δb_2, now we want to calculate ΔN by integrating over all energy. Integrating over all energies should give $\Delta N = 0$ because the introduction of the potential only changes the density of states, but we still are within the same Hilbert space [25]. From Eq. (3), integrating both sides with respect to E, we obtain

$$\Delta N = \int_{-\infty}^{\infty} dE\left(-\frac{1}{\pi}\right)\int_{-\infty}^{\infty} dx\, \mathrm{Im}\left[\sum_B \frac{|\psi_B(x)|^2}{E + E_B + i\epsilon} + \int_{-\infty}^{\infty}\frac{dk}{2\pi}\frac{|\psi_k(x)|^2 - |\psi_0(x)|^2}{E - k^2 + i\epsilon}\right]. \tag{23}$$

Here, we have introduced a sum over the number of bound states in the expression of the Green's function. In case of the attractive δ-function potential there is just one bound state, but in general there can be more than one bound state for a given potential. In Eq. (23) the k and x integration can be carried out in the same way as in Sec. III to arrive at the result

$$\Delta N = \sum_B \int_{-\infty}^{0} dE\, \delta(E + E_B) + \frac{1}{\pi}\int_0^\infty dk\, \frac{d\delta}{dk} + I_1, \tag{24}$$

where

$$I_1 = \lim_{a\to\infty}\int_0^\infty dk\, \frac{1}{2\pi k}(\sin(2ka)\{\cos[2\delta(k)] - 1\} + \cos(2ka)\sin[2\delta(k)]). \tag{25}$$

Carrying out the E integral on the right-hand side now gives

$$\Delta N = N_B + \frac{\delta(\infty) - \delta(0)}{\pi} + I_1 \tag{26}$$

$$\Rightarrow N_B = \frac{\delta(0) - \delta(\infty)}{\pi} - I_1, \tag{27}$$

where N_B is the number of bound states. Equation (27) is precisely Levinson's theorem in one dimension for the even-parity case, which relates the number of bound states to the scattering phase shift. For a potential with $E_B > 0$ ($E = -E_B < 0$), I_1 is nonzero, otherwise for a half-bound state ($E_B = 0$) it is zero. In the case of the δ-function potential,

which does not support any half-bound state, $I_1 = -1/2$, and $\delta(0) = \pi/2$, giving $N_B = 1$, which is exactly the number of bound states supported by the potential.

One can show Levinson's theorem in one dimension by using a number of methods, including Sturm-Liouville theory, Jost functions, and the S-matrix method [12,13,26,27]. From those calculations one ends up with the following form of Levinson's theorem (in the even-parity case):

$$N_B = \begin{cases} \frac{\delta(0)-\delta(\infty)}{\pi} & \text{for the critical case} \\ \frac{\delta(0)-\delta(\infty)}{\pi} + \frac{1}{2} & \text{for the noncritical case,} \end{cases} \tag{28}$$

where by the critical case we mean the case with $E_B = 0$ (half-bound state) and the noncritical case means $E_B > 0$. So, we see that the value of the correction term I_1 is actually universal and is equal to $-1/2$ (for $E_B > 0$) irrespective of the exact form of the potential. We have used the even-parity, $\psi_k(x) = \cos[k|x| + \delta(k)]$, case to arrive at Levinson's theorem and the correction term to the BU formula using the spectral density method. One can similarly use an odd-parity scattering wave function and follow the same regularization procedure to arrive at the odd-parity results of Levinson's theorem as well. Finally, we note that the extra $-1/2$ term in the BU formula does not appear in three dimensions. In lower dimensions, an arbitrarily small attraction will produce a bound state, so that in the noninteracting limit the bound-state term in Eq. (1) must be kept. However, in three dimensions, the bound state does not appear immediately when the interactions are turned on, but at a nontrivial coupling strength (namely, at the so-called unitary point). Therefore the bound-state term does not appear below this point (the BCS side).

V. DISCUSSION

Cutoff regularization schemes, both ultraviolet (high energy or high momentum) and infrared (large volume, small energy or small momentum), are highly used in quantum field theory to deal with infinities in the calculations. In this note we saw how using an infrared cutoff can yield the correction term in the original BU formula in one dimension, and leads to the unusual form of Levinson's theorem in this case. Compared to other methods, the spectral density method provides a rather straightforward and physically insightful way to derive the extra $-1/2$ correction term in the BU formula, as well as the corresponding Levinson theorem in one dimension. We also use a quantum field theory method that shows that it is only the zero energy behavior of the theory, regardless of the actual functional form of the potential, that dictates these correction terms, and hence we see an apparent surprising universality of the values of the integrals I and I_1.

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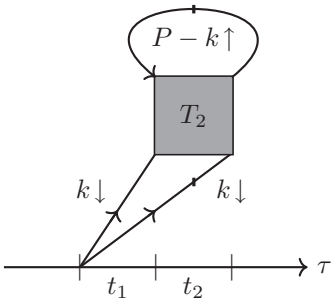

FIG. 2. Diagram corresponding to the calculation of δb_2. The tree-level contact coupling is replaced by the full 1PI two-body T matrix T_2, where T_2 is a function only of the center-of-mass momentum P flowing through the s channel. The tick marks represent $G^{(0,1)}$ propagators.

APPENDIX A: VIRIAL EXPANSION WITH FEYNMAN DIAGRAMS

Various techniques have been developed for perturbatively calculating virial coefficients from field theory [16,28–31]. In particular, we will employ the technique developed in [16], which expands the many-body propagator in powers of fugacity and works directly in imaginary time instead of frequency. One can also use the field-theoretic method described in [6,32] where the Hubbard-Stratonovich transformation has been used to get the $-1/2$ term. However, this following method includes some subtleties that resemble the spectral density method discussed in the main paper.

The noninteracting many-body time-ordered propagator is given by the well-known expression [33]

$$\begin{aligned} G^0(p,\tau) &= e^{-(\epsilon_p-\mu)\tau}[-\Theta(\tau) + n_F(\epsilon_p - \mu)] \\ &= e^{\mu\tau}\left[\sum_{n\geqslant 0} G^{(0,n)}(p,\tau) z^n\right], \end{aligned} \tag{A1}$$

where we have made a virial expansion of the Fermi distribution function $n_F(x) = (e^x + 1)^{-1}$ to define

$$\begin{aligned} G^{(0,0)}(p,\tau) &= -\Theta(\tau) e^{-\epsilon_p \tau}, \\ G^{(0,n\geqslant 1)}(p,\tau) &= (-1)^{n-1} e^{-\epsilon_p \tau} e^{-n\beta\epsilon_p}. \end{aligned} \tag{A2}$$

The basic procedure is to note that $n = \frac{\partial P}{\partial \mu}|_\beta = -\lim_{\eta\to 0-} \int \frac{dp}{2\pi} G(p,\eta)$, since

$$\begin{aligned} G(0,\eta) &= \langle \psi(x,\eta)\psi^\dagger(x,0)\rangle, \\ \lim_{\eta\to 0-} G(0,\eta) &= -\langle \psi^\dagger(x,0)\psi(x,0)\rangle = -n \\ &= \lim_{\eta\to 0-} \int \frac{dp}{2\pi} G(p,\eta). \end{aligned} \tag{A3}$$

Therefore knowledge of the exact two-point Green's function $G(p,\tau)$ gives the number density from which we can extract δb_2. The exact two-point Green's function is built perturbatively from the noninteracting two-point Green's function, so a controlled expansion in fugacity can be obtained. The contribution to δb_2 can be readily seen to be given by just a single diagram given in Fig. 2 [34], corresponding to the expression

$$\begin{aligned} \delta n_2 = -\int \frac{dP}{2\pi}\frac{dk}{2\pi} dt_1 dt_2\, \theta(t_1)\theta(t_2)\theta(\beta - t_1 - t_2) T_2(P,t_2) \\ \times e^{-(\beta-t_2)(\epsilon_k+\epsilon_{P-k})}, \end{aligned} \tag{A4}$$

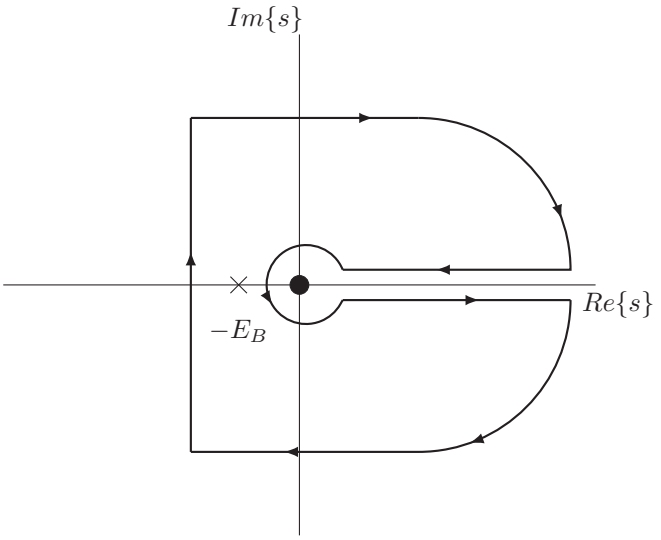

FIG. 3. Contour for evaluating the Bromwich integral. Besides the pole at the bound state $s = -E_B$ and the branch cut for $s > 0$, a singularity exists at the origin that goes as $1/s$, so that the infinitesimal circle surrounding the origin contributes to the integral.

where the only nonvanishing integration region is $t_1, t_2 > 0$ with $t_1 + t_2 < \beta$, T_2 is the off-shell two-body T matrix analytically continued to imaginary time, and $\theta(t)$ is the Heaviside step function. Integrating over t_1 gives

$$\begin{aligned}\delta n_2 &= -\int \frac{dP}{2\pi}\frac{dk}{2\pi} dt_2\, \theta(t_2) T_2(P, t_2)\theta(\beta - t_2)(\beta - t_2) \\ &\quad \times e^{-(\beta - t_2)(\epsilon_k + \epsilon_{P-k})} \\ &= -\int \frac{dP}{2\pi}\frac{dk}{2\pi}\frac{ds}{2\pi i} e^{-\beta s} T_2(s - P^2/4)\frac{1}{(s - \epsilon_k - \epsilon_{P-k})^2},\end{aligned} \tag{A5}$$

where we used that the inverse Laplace transform of a product is a convolution $\int dt\, g(t) f(\beta - t) = \int \frac{1}{2\pi i} e^{-\beta s} f(s) g(s)$, $\frac{1}{(s-\epsilon_k-\epsilon_{P-k})^2}$ is the Laplace transform of $te^{-t(\epsilon_k+\epsilon_{P-k})}$, $T_2(s - P^2/4) = \frac{C}{1+\frac{C}{2}\frac{1}{\sqrt{-(s-P^2/4)-i\epsilon}}}$ is the Euclidean two-body T matrix in the usual frequency space, and C is the coupling constant. It should be mentioned that the usual Bromwich-Mellin contour over which the integral over s is taken begins at $\mathrm{Re}[s] < 0$ as the sign of the exponential in the Laplace transform is taken opposite the standard convention in mathematics [35]. A consequence of this is that the integrand of (A5) is analytic to the left of the contour instead of the usual right of the contour, and in evaluating the integral we close the contour on the right instead of the left, as indicated in Fig. 3.

Using the substitution $k \to k + P/2$ followed by $s \to s + P^2/4$, the integrals over k and P become trivial and we get

$$\delta n_2 = \frac{i}{8\pi^{3/2}\sqrt{\beta}} \int ds\, e^{-\beta s} \frac{1}{(-s)^{3/2}} \frac{C}{1 + \frac{C}{2}\frac{1}{\sqrt{-s}}}. \tag{A6}$$

The analytic structure is such that $\frac{1}{1+\frac{C}{2}\frac{1}{\sqrt{-s}}}$ has a pole at the bound state $s = -C^2/4 = -E_b$ for $C < 0$ with residue $-\frac{C^2}{2}$, and $\frac{1}{(-s)^{3/2}}$ has a branch cut along the positive real axis $s > 0$. Therefore, closing the contour on the right half of the complex s plane, the pole gives the contribution

$$\begin{aligned}\delta n_2^{\text{bound}} &= (-2\pi i)\frac{i}{8\pi^{3/2}\sqrt{\beta}} \frac{1}{\left(\frac{|C|}{2}\right)^3} e^{\beta C^2/4} C\left(-\frac{C^2}{2}\right) \\ &= \frac{1}{\pi^{1/2}\sqrt{\beta}} e^{\beta E_b},\end{aligned} \tag{A7}$$

while the branch cut gives the contribution

$$\begin{aligned}\delta n_2^{\text{scattering}} &= \frac{i}{8\pi^{3/2}\sqrt{\beta}} \int_0^\infty dx\, e^{-\beta x} \mathrm{disc}\left[\frac{1}{(-x - i\epsilon)^{3/2}} \frac{C}{1 + \frac{C}{2}\frac{1}{\sqrt{-s-i\epsilon}}}\right] \\ &= \frac{i}{8\pi^{3/2}\sqrt{\beta}} \int_0^\infty dx\, e^{-\beta x} (2i)\, \mathrm{Im}\left[\frac{1}{(-x - i\epsilon)^{3/2}} \frac{C}{1 + \frac{C}{2}\frac{1}{\sqrt{-s-i\epsilon}}}\right] \\ &= \frac{i}{8\pi^{3/2}\sqrt{\beta}} \int_0^\infty dx\, e^{-\beta x} (2i)\left[-\frac{1}{x^{3/2}} \frac{C}{1 + \frac{C^2}{4x}}\right] = -\frac{1}{2\pi^{1/2}\sqrt{\beta}} e^{\beta E_b}[1 - \mathrm{erf}(\sqrt{\beta E_b})].\end{aligned} \tag{A8}$$

Additionally, the infinitesimal circle surrounding the origin does not vanish and contributes

$$\begin{aligned}\delta n_2^{\text{origin}} &= -\frac{i}{8\pi^{3/2}\sqrt{\beta}} \lim_{R\to 0} \int d(\mathrm{Re}^{i\theta})\, e^{-\beta(\mathrm{Re}^{i\theta})} \frac{1}{(-\mathrm{Re}^{i\theta})^{3/2}} \frac{C}{1 + \frac{C}{2}\frac{1}{\sqrt{-\mathrm{Re}^{i\theta}}}} \\ &= -\frac{i}{8\pi^{3/2}\sqrt{\beta}} \lim_{R\to 0} \int_0^{2\pi} (i\mathrm{Re}^{i\theta}) d\theta\, \frac{1}{(-\mathrm{Re}^{i\theta})^{3/2}} \frac{C}{\frac{C}{2}\frac{1}{\sqrt{-\mathrm{Re}^{i\theta}}}} = -\frac{1}{2\pi^{1/2}\sqrt{\beta}}.\end{aligned} \tag{A9}$$

Adding Eqs. (A7), (A8), and (A9), one can write

$$\delta b_2 = \tfrac{1}{2} e^{\beta E_b}[1 + \mathrm{erf}(\sqrt{\beta E_b})] - \tfrac{1}{2}. \tag{A10}$$

Note that if the circle around the origin were not included one would be missing a $1/2$. In two and three dimensions, this circle gives a vanishing contribution. The origin of the term

$-1/2$ in this method is very similar to the origin of the term spectral density method, both given by a contribution of the contour around the pole at zero energy in the complex plane.

APPENDIX B: SECOND VIRIAL COEFFICIENT AND DENSITY OF STATES

The asymptotic form for a scattering wave function in one dimension is

$$\psi_{\mathbf{k}}(x) = e^{i\mathbf{k}x} + ie^{ik|x|} f(\mathrm{sgn}(x), k), \tag{B1}$$

which has a partial wave decomposition [27]

$$\psi_{\mathbf{k}}(x) = \sum_{\ell=0,1} (-i)^{\ell} [\mathrm{sgn}(x)]^{\ell} e^{i\delta_{\ell}} \cos(k|x| + \zeta_{\ell} + \delta_{\ell}), \tag{B2}$$

where $\zeta_{\ell} = \pi\ell/2$, $f(\mathrm{sgn}(x), k) = \sum_{\ell=0,1} [\mathrm{sgn}(x)]^{\ell} e^{i\delta_{\ell}} \sin\delta_{\ell}$.

Imposing hard-wall boundary conditions at $|x| = R$ quantizes k:

$$k_n R + \zeta_{\ell} + \delta_{\ell}(k_n) = (n + 1/2)\pi, \tag{B3}$$

and assuming that, for large R, the phase shift becomes a smooth function of k then

$$\begin{aligned} (k_{n+1} - k_n)R + (k_{n+1} - k_n)\delta'_{\ell}(k_n) &= \pi, \\ \frac{dN_{\ell}}{dk} &= \frac{R + \delta'_{\ell}(k)}{\pi}, \\ \frac{d\Delta N_{\ell}}{dk} &= \frac{\delta'_{\ell}(k)}{\pi}. \end{aligned} \tag{B4}$$

The definition of the relative two-body partition function in terms of the density of states $g(E)$ is

$$Z_2 = \int dE\, g(E) e^{-\beta E}. \tag{B5}$$

Therefore,

$$\begin{aligned} \Delta Z_2 = Z_2 - Z_2^0 &= \sum_{\ell=0}^{1} \sum_{i=0}^{n_{\ell}} e^{\beta E_{b,\ell,i}} + \sum_{\ell=0}^{1} \int dE \frac{d\Delta N_{\ell}}{dE} e^{-\beta E} \\ &= \sum_{\ell=0}^{1} \sum_{i=0}^{n_{\ell}} e^{\beta E_{b,\ell,i}} + \frac{1}{\pi} \sum_{\ell=0}^{1} \int_0^{\infty} dk \frac{d\delta_{\ell}}{dk} e^{-\beta k^2}, \end{aligned} \tag{B6}$$

where we used the bound-state part $g_{\mathrm{bound}}(E) = \sum_{\ell=0}^{1} \sum_{i=0}^{n_{\ell}} \delta(E - E_{b,\ell,i})$ and defined n_{ℓ} to be the number of bound states of parity ℓ.

In this paper we take as our convention for Δb_2

$$\Delta b_2 = \Delta Z_2 = \sum_{\ell=0}^{1} \sum_{i=0}^{n_{\ell}} e^{\beta E_{b,\ell,i}} + \frac{1}{\pi} \sum_{\ell=0}^{1} \int_0^{\infty} dk \frac{d\delta_{\ell}}{dk} e^{-\beta k^2}. \tag{B7}$$

APPENDIX C: FROM THE SPECTRAL DENSITY METHOD TO THE BU FORMULA

In this Appendix we verify that using the retarded Green's function to find the density of states is equivalent to the BU formula. To show this, we start from Eq. (8):

$$\begin{aligned} \delta b_2 = \int_{-\infty}^{\infty} dE\, e^{-\beta E} \left(-\frac{1}{\pi}\right) \int_{-\infty}^{\infty} dx\, \mathrm{Im}\Bigg[\sum_B \frac{|\psi_B(x)|^2}{E + E_B + i\epsilon} \\ + \int_{-\infty}^{\infty} \frac{dk}{2\pi} \frac{|\psi_k(x)|^2 - |\psi_0(x)|^2}{E - k^2 + i\epsilon} \Bigg]. \end{aligned} \tag{C1}$$

Here we have introduced a sum over bound states as well since for a more general potential there can be more than one bound state. Now we will rearrange the orders of integration. Since the continuum part displays some complexity, we will come back to it after we compute the contribution of the discrete bound-states part first.

The integral over the bound states is

$$\int_{-\infty}^{0} dE\, e^{-\beta E} \left(-\frac{1}{\pi}\right) \int_{-\infty}^{\infty} dx\, \mathrm{Im}\left[\sum_B \frac{|\psi_B(x)|^2}{E + E_B + i\epsilon} \right] \tag{C2}$$

$$= \int_{-\infty}^{0} dE\, e^{-\beta E} \left(-\frac{1}{\pi}\right) (-\pi) \sum_B \delta(E + E_B) \tag{C3}$$

$$= \sum_B e^{\beta E_B}. \tag{C4}$$

The limit of the integration is $-\infty$ to zero because the bound states are only defined for negative energy. To arrive at the second line we have used the normalization of the bound states $\int_{-\infty}^{\infty} |\psi_B(x)|^2 dx = 1$ and the δ function appears due to the Sokhotski-Plemelj theorem. The appearance of the factor $\delta(E + E_B)$ can also be visualized by the fact that the imaginary part of the factor inside the bracket is zero everywhere except only when $E = -E_B$ and at $E = -E_B$ the factor is infinite, which mimics the definition of the δ function.

Coming back to the continuum part of Eq. (8), we can integrate with respect to E first to get

$$\left(-\frac{1}{\pi}\right) \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} \frac{dk}{2\pi} (|\psi_k(x)|^2 - |\psi_0(x)|^2) \times \mathrm{Im}\left[\int_0^{\infty} dE\, \frac{e^{-\beta E}}{E - k^2 + i\epsilon} \right] \tag{C5}$$

$$= \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} \frac{dk}{2\pi} [|\psi_k(x)|^2 - |\psi_0(x)|^2] e^{-\beta k^2} \tag{C6}$$

$$= \int_0^{\infty} \frac{dk}{\pi} e^{-\beta k^2} \int_{-\infty}^{\infty} dx [|\psi_k(x)|^2 - |\psi_0(x)|^2]. \tag{C7}$$

The x integral gives the change in probability density for a particular momentum k, which is nothing but the density of states $g(k)$. Recognizing this reduces Eq. (C7) to the familiar form of the BU formula derivation [Eq. (C8)], which can subsequently be rewritten in terms of the scattering phase shifts, giving the celebrated BU formula:

$$\delta b_2 = \sum_B e^{\beta E_B} + \int_0^{\infty} \frac{dk}{\pi} e^{-\beta k^2} [g(k) - g_0(k)] \tag{C8}$$

$$= \sum_B e^{\beta E_B} + \int_0^{\infty} \frac{dk}{\pi} \frac{d\delta(k)}{dk} e^{-\beta k^2}. \tag{C9}$$

Here in writing the second line we have used the result from Appendix B.

[1] H. K. Onnes, Expression of the equation of state of gases and liquids by means of series, in *Through Measurement to Knowledge* (Springer, Dordrecht, 1991), pp. 146–163.

[2] E. Beth and G. E. Uhlenbeck, The quantum theory of the non-ideal gas. II. Behaviour at low temperatures, Physica **4**, 915 (1937).

[3] M. E. Portnoi and I. Galbraith, Levinson's theorem and scattering phase-shift contributions to the partition function of interacting gases in two dimensions, Phys. Rev. B **58**, 3963 (1998).

[4] T. Kristensen, X. Leyronas, and L. Pricoupenko, Second-order virial expansion for an atomic gas in a harmonic waveguide, Phys. Rev. A **93**, 063636 (2016).

[5] X. Cui, Quasi-one-dimensional atomic gases across wide and narrow confinement-induced resonances, Phys. Rev. A **86**, 012705 (2012).

[6] W. S. Daza, J. E. Drut, C. L. Lin, and C. R. Ordóñez, Virial expansion for the Tan contact and Beth-Uhlenbeck formula from two-dimensional SO(2, 1) anomalies, Phys. Rev. A **97**, 033630 (2018).

[7] 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).

[8] C. R. Ordóñez, Path-integral Fujikawa's approach to anomalous virial theorems and equations of state for systems with SO(2, 1) symmetry, Physica A **446**, 64 (2016).

[9] H. E. Camblong, A. Chakraborty, W. S. Daza, J. E. Drut, C. L. Lin, and C. R. Ordóñez, Quantum anomaly and thermodynamics of one-dimensional fermions with antisymmetric two-body interactions, arXiv:1908.05210 (2019).

[10] A. Amaya-Tapia, S. Y. Larsen, and M. Lassaut, Second virial coefficient in one dimension as a function of asymptotic quantities, Mol. Phys. **103**, 1301 (2005).

[11] L. R. Dodd and A. M. Gibbs, Cluster coefficients for the one-dimensional Bose gas with point interactions, J. Math. Phys. **15**, 41 (1974).

[12] M. S. de Bianchi, Levinson's theorem, zero-energy resonances, and time delay in one-dimensional scattering systems, J. Math. Phys. **35**, 2719 (1994).

[13] G. Barton, Levinson's theorem in one dimension: Heuristics, J. Phys. A **18**, 479 (1985).

[14] L. J. Boya and J. Casahorrán, Theorem of Levinson via the spectral density, Int. J. Theor. Phys. **46**, 1998 (2007).

[15] H. Camblong *et al.* (unpublished).

[16] X. Leyronas, Virial expansion with Feynman diagrams, Phys. Rev. A **84**, 053633 (2011).

[17] I. R. Lapidus, Phase shifts for scattering by a one-dimensional delta-function potential, Am. J. Phys. **37**, 930 (1969).

[18] E. N. Economou, *Green's Functions in Quantum Physics* (Springer, New York, 1983), Vol. 3.

[19] V. Gasparian, T. Christen, and M. Büttiker, Partial densities of states, scattering matrices, and Green's functions, Phys. Rev. A **54**, 4022 (1996).

[20] D. J. Griffiths and D. F. Schroeter, *Introduction to Quantum Mechanics* (Cambridge University, Cambridge, England, 2018).

[21] N. Levinson, Determination of the potential from the asymptotic phase, Phys. Rev. **75**, 1445 (1949).

[22] N. Levinson, On the uniqueness of the potential in a Schrödinger equation for a given asymptotic phase, Danske Vid. Selsk. Mat.-Fys. Medd. **25**, 29 (1949).

[23] R. G. Newton, Noncentral potentials: The generalized Levinson theorem and the structure of the spectrum, J. Math. Phys. **18**, 1348 (1977).

[24] M. Wellner, Levinson's theorem (an elementary derivation), Am. J. Phys. **32**, 787 (1964).

[25] S. Weinberg, *Lectures on Quantum Mechanics* (Cambridge University, Cambridge, England, 2015).

[26] S. H. Dong and Z. Q. Ma, Levinson's theorem for the Schrödinger equation in one dimension, Int. J. Theor. Phys. **39**, 469 (2000).

[27] J. H. Eberly, Quantum scattering theory in one dimension, Am. J. Phys. **33**, 771 (1965).

[28] R. Dashen, S. K. Ma, and H. J. Bernstein, *S*-matrix formulation of statistical mechanics, Phys. Rev. **187**, 345 (1969).

[29] D. B. Kaplan and S. Sun, New Field-Theoretic Method for the Virial Expansion, Phys. Rev. Lett. **107**, 030601 (2011).

[30] V. Ngampruetikorn, M. M. Parish, and J. Levinsen, High-temperature limit of the resonant fermi gas, Phys. Rev. A **91**, 013606 (2015).

[31] M. Barth and J. Hofmann, Efimov correlations in strongly interacting Bose gases, Phys. Rev. A **92**, 062716 (2015).

[32] C. Chafin and T. Schäfer, Scale breaking and fluid dynamics in a dilute two-dimensional Fermi gas, Phys. Rev. A **88**, 043636 (2013).

[33] A. A. Abrikosov, L. P. Gorkov, and I. E. Dzialoshinski, *Methods of Quantum Field Theory in Statistical Physics*, Dover Books on Physics Series (Dover, New York, 1975).

[34] M. Barth and J. Hofmann, Pairing effects in the nondegenerate limit of the two-dimensional Fermi gas, Phys. Rev. A **89**, 013614 (2014).

[35] G. B. Arfken, H. J. Weber, and F. E. Harris, *Mathematical Methods for Physicists: A Comprehensive Guide* (Elsevier, Amsterdam, 2013).