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Levinson's theorem and the second virial coefficient in one, two, and three dimensions

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The second virial coefficient $B(T)$ can be expressed in terms of two-body phase shifts and bound-state energies. The fact that $B(T)$ must remain continuous as the potential strength is varied is used to deduce the relationship between the phase shifts at zero energy and the number of bound states supported by the potential (Levinson's theorem). There still remains an ambiguity due to the possibility of zero-energy resonances; in one and three dimensions this can be removed by the additional information of whether the tangent of the phase shift goes to zero or to infinity at zero energy. In two dimensions, the problem is more subtle and a difficulty is encountered if the potential strength is such that a p-wave zero-energy resonance is present; the expression for $B(T)$ as the inverse Laplace transform of the Jost function gives the correct contribution from this resonance, but the phase-shift formula derived using asymptotic wave functions fails to include it, and hence is in disagreement with Levinson's theorem. The origin of this disagreement is traced to a noncommutivity in the wave function between the limits of large distance and low energy; this occurs only in the two-dimensional case, and needs to be handled carefully.

I. INTRODUCTION

Levinson's theorem, in its simplest form, relates the zero-energy behavior of the two-body scattering phase shifts to the number of bound states supported by the potential. In three dimensions the relation is[1-3]

$$\delta_l(0)=N_{B,l}\pi+q \ , \tag{1.1}$$

where $\delta_l(0)$ is the zero-energy phase shift for the lth partial wave and $N_{B,l}$ is the number of bound states of angular momentum l. q equals $\pi/2$ if $l=0$ and there is an s-wave zero-energy resonance; otherwise it is zero.

Although Levinson's theorem has been known for a long time, and is now treated as a matter of course in books on scattering theory,[1,2] nevertheless it is still a topic of current research interest, both in its basic form[4] and in various generalizations.[4-6] Recently, there has been considerable interest in scattering in one and two dimensions, and the corresponding forms of Levinson's theorem have been investigated.[7-11] It is found that there is still a connection between the zero-energy value of the phase shift and the number of bound states, but the detailed form of the relationship alters for different dimensions.

In this paper, we discuss the relation between Levinson's theorem and the second virial coefficient of a monatomic gas. The virial coefficients provide a measure of the deviation of thermodynamic functions from their ideal gas values.[12-14] For the pressure p, they are simply the coefficients in a power series in the number density ρ:

$$\beta p=\rho+B(T)\rho^2+C(T)\rho^3+\cdots \ . \tag{1.2}$$

$\beta=1/kT$ where k is Boltzmann's constant and T is the absolute temperature.

The second virial coefficient $B(T)$ depends only on binary collisions in the gas, and can be expressed in terms of two-body scattering parameters and bound-state energies. For the case where the two-body interaction is spherically symmetric, it can be expressed in terms of the phase shifts and bound-state energies of the two-body system.[12-15] We investigate the restrictions which this formula places on the zero-energy behavior of the phase shifts $\delta_\alpha(k)$. ($\alpha\equiv l$, m, and $\pm$, for three, two, and one dimensions, respectively.) First, we find that the expression for $B(T)$ is divergent unless $\delta_\alpha(0)$ takes certain values. Second, the requirement that $B(T)$ be a continuous function of the two-body potential strength further restricts these values. There still remains an ambiguity, due to the possibility of zero-energy resonances. This cannot be resolved purely on the basis of virial-coefficient considerations, and we have to invoke further information. In the three- and one-dimensional cases it turns out to be sufficient to know whether $\tan\delta_\alpha(k)$ goes to zero or diverges as $k\to 0$; we then have the complete form of Levinson's theorem. The two-dimensional case is not so straightforward. The phase-shift expression for $B(T)$, derived by exact analogy with the three-dimensional case, fails to include any contribution from a possible p-wave zero-energy resonance, and leads to an incorrect Levinson's theorem in this case. The investigation of this discrepancy leads us to look carefully at the asymptotic wave functions used in the derivation of the phase-shift formula for $B(T)$. We find that there is a fundamental noncommutivity between the limits of large distance ($r\to\infty$) and low energy ($k\to 0$). In the critical case of the p-wave zero-energy resonance this shows up as a divergence at $k=0$ in the integral defining $B(T)$. This divergence can be avoided by using the formalism for $B(T)$ based on the inverse Laplace transform of the logarithmic derivative of the Jost function, and this is presented in Sec. III A and Appendix E.

The derivations in this paper do not pretend in any way to be mathematically rigorous. We think that the interest of the present investigation lies in the way in which some very general properties of a macroscopic quantity, $B(T)$, almost uniquely constrain the behavior of a microscopic quantity $\delta_\alpha(0)$. The other special feature is the unification of the forms of Levinson's theorem in three, two, and one dimension: Here they emerge naturally as the result of parallel treatments.

II. THREE DIMENSIONS

A. Jost-function formulation

As mentioned above, $B(T)$ can be expressed in terms of the bound-state energies and phase shifts of the two-body system. Let us start, however, from the more general and elegant formulation in terms of the Jost function of scattering theory:[16]

$$B(T) = -\sqrt{2}\lambda^3 \sum_{l=0}^{\infty} (2l+1) \times \left[-\frac{1}{2\pi} \int_{c-i\infty}^{c+i\infty} d\gamma\, e^{\beta\gamma^2} \frac{f_l'(-i\gamma)}{f_l(-i\gamma)} \right] . \tag{2.1}$$

$\lambda = \sqrt{(2\pi\beta)}$ is the thermal wavelength. (We use units where $\hbar = 1$ and the particle mass is also unity.) $f_l(k)$ is the Jost function, as defined by Newton,[3] $f_l'(k) \equiv df_l(k)/dk$, and the integration contour is a vertical straight line to the right of all singularities of the integrand. Equation (2.1) is for the case of Boltzmann statistics; that is, we have not included the exchange effects which arise from Bose-Einstein or Fermi-Dirac statistics. There are easily included,[16] but are not necessary for the present discussion.

We now wish to express $B(T)$ in terms of phase shifts and bound-state energies. To do this, we use the following properties of $f_l(k)$:[3]

(i) $f_l(k)$ is analytic in the lower half k plane, with simple zeros at $k = -ik_{B,l}$, $k_{B,l}$ real and non-negative, corresponding to bound states of energies $E_{B,l} = -k_{B,l}^2$.

(ii)

$$f_l(k)/f_l(-k) = \exp[2i\delta_l(k)] , \tag{2.2}$$

where $\delta_l(k)$ is the phase shift for the lth partial wave.

(iii) As $k \to 0$,

$$\begin{aligned} f_l(k) &\sim \alpha_l + \beta_l k^2, \quad l \geq 1 \\ f_0(k) &\sim \alpha_0 + \beta_0 k , \end{aligned} \tag{2.3}$$

where $\alpha_l = 0$ only if there is a zero-energy bound state (or zero-energy resonance if $l = 0$), and in this case $\beta_l \neq 0$.

Property (i) enables us to move the integration contour in (2.1) to the left, picking up the residues at the bound-state poles as we go, until the contour lies along the imaginary axis, indented around a possible singularity at the origin. Using (ii) and (iii), we then find

$$B(T) = -\sqrt{2}\lambda^3 \sum_{l=0}^{\infty} (2l+1) \left[\sum_B e^{-\beta E_{B,l}} + \frac{1}{\pi} \int_0^\infty dk\, e^{-\beta k^2} \frac{d\delta_l}{dk} + \xi \right] . \tag{2.4}$$

ξ is the contribution from the origin and is

$$\xi = \begin{cases} \frac{1}{2} & s\text{-wave zero-energy resonance,} \\ 0 & \text{otherwise.} \end{cases} \tag{2.5}$$

We note that (2.4) is the standard Uhlenbeck-Beth expression for the second virial coefficient,[12,13] with an extra term ξ. To our knowledge, Mishima and Tanaka[17] were the first to point our explicitly that such a term should be added to the Uhlenbeck-Beth formula. (They also add another term m_l, equal to the number of zero-energy bound states for $l \geq 1$. This is unnecessary in our formula, as we allow $E_{B,l}$ to be zero.) The same result was obtained in a rather different way by Bollé and Wilk.[18] The above is not to say that previous authors were unaware of how to correctly incorporate a zero-energy resonance into the usual Uhlenbeck-Beth formula; see, for example, Ref. 19, Sec. II β.

To bring out the connection between $B(T)$ and Levinson's theorem, we preform a partial integration on (2.4), giving

$$B(T) = -\sqrt{2}\lambda^3 \sum_{l=0}^{\infty} (2l+1) \left[\left[\sum_B e^{-\beta E_{B,l}} - \frac{1}{\pi}\delta_l(0) + \xi \right] + \frac{2\beta}{\pi} \int_0^\infty k\, dk\, e^{-\beta k^2} \delta_l(k) \right] . \tag{2.6}$$

Application of Levinson's theorem (1.1) allows us to write the terms in the large parentheses as

$$\begin{aligned} \sum_B e^{-\beta E_{B,l}} - \frac{1}{\pi}\delta_l(0) + \xi &= \sum_B e^{-\beta E_{B,l}} - N_{B,l} \\ &= \sum_B (e^{-\beta E_{B,l}} - 1) . \end{aligned} \tag{2.7}$$

Now consider what happens to the terms in $B(T)$ as the potential strength is changed continuously. To be precise, let the two-body potential be $gv(r)$, $g > 0$, and suppose it supports $N_{B,l}$ bound states of angular momentum l and energies $E_{B,l} \leq 0$. As g decreases, these bound states move into the continuum, and as each passes through zero the term $\sum_B \exp(-\beta E_{B,l})$ decreases discontinuously by unity. However, this does not mean that $B(T)$ also changes discontinuously; as is evident from (2.6) and (2.7), there is a compensating jump in $\delta_l(0)$. The term

$$\sum_B e^{-\beta E_{B,l}} - \frac{1}{\pi}\delta_l(0) + \xi \tag{2.8}$$

remains continuous as bound states move into the continuum, and the integral

$$\int_0^\infty k\,dk\,e^{-\beta k^2}\delta_l(k) \tag{2.9}$$

is also a continuous function of the potential strength.

This phenomenon of compensation between bound-state and continuum contributions to $B(T)$ was first explicitly pointed out by Rogers *et al.*[20] They used Levinson's theorem, as we have done above. Subsequently, other authors demonstrated this continuity without specifically invoking Levinson's theorem.[21,22] [The demonstrations in Ref. 21 are based on the Jost-function formula—Eq. (2.1) above.]

In this paper, we wish to show that the above procedure can be reversed; the assumption that $B(T)$ is a continuous function of the potential strength can be used to infer the form of Levinson's theorem. This is not a circular argument, since the continuity of $B(T)$ is necessary on physical grounds: any discontinuities in $B(T)$ would be reflected in the thermodynamic properties of the system. Also, as mentioned above, there are alternative expressions for $B(T)$ in three dimensions which demonstrate continuity without explicitly using Levinson's theorem.

However, we do not which to start from (2.4); this equation was derived using properties of the Jost function, and if we are going to assume these properties, then we should prove Levinson's theorem directly by evaluating the contour integral

$$\oint_C d\ln f_l(k)\ , \tag{2.10}$$

where C consists of a large semicircle in the lower half k plane, together with the real axis indented below at the origin.[3] [In fact, the steps one goes through in doing this are very similar to the steps involved in going from (2.1) to (2.4).]

B. Phase-shift formulation

There are many derivations in the literature of the phase-shift formula for $B(T)$. However, these seem to fall into one of two categories. The first type uses elementary scattering theory, but imposes the artificial boundary condition that the wave function of relative motion is zero for intermolecular separations greater than $r=R$.[12–14] Subsequently, the limit $R\to\infty$ is taken. The second type does not enclose the system, but uses more sophisticated concepts, such as analytic properties of scattering functions,[16,17] (for example, the Jost-function formulation given above) or the mathematical apparatus of formal scattering theory.[5,23,24] (We should mention two further derivations which do not fall into either of these categories: that of Larsen and Poll for anisotropic interactions,[25] and the very general one of Servadio.[26] However, neither of these are suitable for our purposes, since they either treat a more complicated case,[25] or do not use a partial-wave expansion.[26])

In Appendix A we give a derivation which uses only simple partial-wave scattering theory, but does not impose artificial boundary conditions. We find the expression

$$B(T)=-\sqrt{2}\lambda^3\sum_{l=0}^{\infty}(2l+1)\left[\sum_B e^{-\beta E_{B,l}} + \frac{1}{\pi}\int_0^\infty dk\,e^{-\beta k^2}\frac{d\delta_l}{dk} + (-1)^l\tfrac{1}{2}\sin^2\delta_l(0)\right]. \tag{2.11}$$

In deriving this, we have made the assumption that $\delta_l(k)$ is differentiable, and also that

$$\delta_l(0)=n\pi/2,\quad n=0,\pm1,\ldots\ . \tag{2.12}$$

This latter assumption is necessary in order that the integral over k converge (see Appendix A) and is thus necessary for the existence of $B(T)$.

Performing a partial integration on (2.11) gives

$$B(T)=-\sqrt{2}\lambda^3\sum_{l=0}^{\infty}(2l+1)\left[\left[\sum_B e^{-\beta E_{B,l}}-\frac{1}{\pi}\delta_l(0) + (-1)^l\tfrac{1}{2}\sin^2\delta_l(0)\right] + \frac{2\beta}{\pi}\int_0^\infty k\,dk\,e^{-\beta k^2}\delta_l(k)\right]. \tag{2.13}$$

We now assume that $B(T)$ and $\delta_l(k)$ for $k\neq0$ are continuous functions of the coupling parameter g. Then decreasing g continuously shows that $\delta_l(0)/\pi$ must decrease by unity each time a bound state disappears. This, coupled with the restriction (2.12), leads to the conclusion that

$$\delta_l(0)=N_{B,l}\pi+q\ , \tag{2.14}$$

where $q=n\pi/2$, $n=0,\pm1,\ldots$. Now consider the quantity

$$Q=-\frac{1}{\pi}\delta_l(0)+(-1)^l\tfrac{1}{2}\sin^2\delta_l(0)\ . \tag{2.15}$$

As g decreases, Q changes discontinuously as $\delta_l(0)$ decreases discontinuously according to (2.14). However, when g has decreased to the point where the potential $gv(r)$ no longer supports any bound states, then Q must remain constant, and, since $Q=0$ when $g=0$, this constant must be zero. The only values of $\delta_l(0)$ satisfying $Q=0$ are 0 and $(-1)^l\pi/2$. Thus we conclude that, in (2.14), q equals 0 or $(-1)^l\pi/2$.

It does not seem possible to decide which of these values of q is appropriate solely on the basis of arguments involving the virial-coefficient formula. Thus we invoke a minimum of additional information about the zero-energy behavior of phase shifts. Specifically, we use the result[1,27] that $\tan\delta_l(k)\to0$ as $k\to0$ for $l\geq1$, and so $q=0$ for this case. The s-wave case is more complicated.[1,27] We now have

$$k \cot\delta_0(k) = -1/a + O(k^2), \quad k \to 0 \tag{2.16}$$

where a is the scattering length. If a is finite, then $\tan\delta_0(0)=0$ as before. The exceptional case occurs when a is infinite, and this happens whenever the potential strength is just sufficient to introduce a new discrete level at zero energy. In this case $\cot\delta_0(k) \to 0$ as $k \to 0$, so we must choose $q=\pi/2$. In fact, this case does not correspond to a true bound state, since the wave function is not normalizable. Instead, it is usually referred to as a "zero-energy resonance" or a "half-bound state."[1] Thus we have

$$q = \begin{cases} \pi/2 & s\text{-wave zero-energy resonance,} \\ 0 & \text{all other cases.} \end{cases} \tag{2.17}$$

There is an alternative way of extracting Levinson's theorem from (2.11), and that is to argue that the virial coefficient will vanish in the limit of infinite temperature. (We expect this to be true for potentials which do not contain a hard core.) Then, assuming that each partial-wave contribution must vanish separately, we get

$$0 = \sum_B 1 + \frac{1}{\pi} \int_0^\infty dk \frac{d\delta_l}{dk} + (-1)^l \tfrac{1}{2} \sin^2\delta_l(0) , \tag{2.18}$$

or

$$N_{B,l} + \frac{1}{\pi}[\delta_l(\infty) - \delta_l(0)] + (-1)^l \tfrac{1}{2} \sin^2\delta_l(0) = 0 . \tag{2.19}$$

(An argument of this type was used by Dashen *et al.*[5] to obtain a generalization of Levinson's theorem for N-body scattering.) If we can set $\delta_l(\infty)=0$, then we are back to the expression we obtained previously. Now, $\delta_l(\infty)=0$ if the potential is regular (i.e., if $r^2 v(r) \to 0$ as $r \to 0$), so for this class of potentials the two versions coincide. But the form (2.14) is also valid for singular potentials (provided they are repulsive at the origin), whereas (2.19) fails because $\delta_l(k)$ diverges as $k \to \infty$. (See Ref. 2 for a discussion of Levinson's theorem for singular potentials.) We note that this corresponds to two different ways of removing the mod π ambiguity from the phase shift. The more restrictive way is to set $\delta_l(\infty)=0$ and to invoke continuity in k to get $\delta_l(0)$; the more general way is to require δ_l to be a continuous function of the coupling parameter g, and require it to vanish when $g=0$.

III. TWO DIMENSIONS

In two dimensions, Levinson's theorem takes the form

$$\delta_m(0) = N_{B,m}\pi + q , \tag{3.1}$$

where $\delta_m(0)$ is the zero-energy phase shift for the mth partial wave and $N_{B,m}$ is the number of bound states of angular momentum m. q equals π if $m=1$ and there is a p-wave zero-energy resonance; otherwise, it is zero. (We note that in two dimensions both the s-wave and the p-wave zero-energy states are resonances; that is, they are not normalizable. See, e.g., Ref. 28, p. 266.) When no zero-energy resonances are present, (3.1) has the same form as in three dimensions. Levinson's theorem for this restricted case was assumed some time ago,[29] but only recently rigorously proved.[10] The extension to the general case is very recent,[11] and the result is unexpected: An s-wave zero-energy resonance contributes nothing, but a p-wave one contributes π. This result is most readily understood in relation to the low-energy behavior of the two-dimensional Jost function.[30]

We now find expressions for $B(T)$ in two dimensions, following the methods used In Sec. II for the three-dimensional case.

A. Jost-function formulation

The Schrödinger equation for the two-dimensional radial wave function can be written as (using units where $\hbar=1$ and the particle mass is also unity)

$$\left[-\frac{d^2}{dr^2} + v(r) + \frac{m^2 - \frac{1}{4}}{r^2} - k^2 \right] \chi_m(k,r) = 0 . \tag{3.2}$$

In complete analogy with the three-dimensional case[3] we introduce the regular solution $\varphi_m(k,r)$ satisfying the boundary condition

$$\lim_{r \to 0} (2/\pi)^{1/2} 2^m m! r^{-m-1/2} \varphi_m(k,r) = 1 , \tag{3.3}$$

and the irregular solution $f_m(k,r)$ satisfying the boundary condition

$$\lim_{r \to \infty} e^{ikr} f_m(k,r) = i^m e^{-i\pi/4} . \tag{3.4}$$

The Jost function $f_m(k)$ is then defined by

$$f_m(k) = k^{m-1/2} W[f_m(k,r), \varphi_m(k,r)] , \tag{3.5}$$

where $W[\ ]$ denotes the Wronskian of the two solutions.

The second virial coefficient can now be expressed in terms of the Jost function. The derivation is exactly parallel to that for the three-dimensional case (Ref. 16, Appendix A), so we do not repeat it here. The result is [compare (2.1) above]

$$B(T) = -\lambda^2 \sum_{m=-\infty}^{\infty} \left[-\frac{1}{2\pi} \int_{c-i\infty}^{c+i\infty} d\gamma\, e^{\beta\gamma^2} \frac{f_m'(-i\gamma)}{f_m(-i\gamma)} \right] . \tag{3.6}$$

The properties of $f_m(k)$ are for the most part the straightforward analogues of those of $f_l(k)$. The exception that concerns us is the behavior near the origin; property (iii) of Sec. II A must be replaced by the following.[30]

(iii)′ As $k \to 0$,

$$\begin{aligned} & f_m(k) \sim \alpha_m + \beta_m k^2, \quad m \geq 2 \\ & f_1(k) \sim \alpha_1 + \beta_1 k^2 \ln k , \\ & f_0(k) \sim \alpha_0 \ln k + \beta_0 , \end{aligned} \tag{3.7}$$

where $\alpha_m = 0$ only if there is a zero-energy bound state (or resonance if $m=0$ or 1), and in this case $\beta_m \neq 0$.

We now shift the contour to lie along the imaginary axis, and find

$$B(T)=-\lambda^2 \sum_{m=-\infty}^{\infty} \left[\sum_B e^{-\beta E_{B,m}} + \frac{1}{\pi}\int_0^\infty dk\, e^{-\beta k^2}\frac{d\delta_m}{dk} + \xi \right] . \tag{3.8}$$

ξ is the contribution from the origin, and is

$$\xi=\begin{cases} 1 & p\text{-wave zero-energy resonance,} \\ 0 & \text{all other cases.} \end{cases} \tag{3.9}$$

This term is new; previous expressions for $B(T)$ in two dimensions did not include ξ.[29,31] In exactly the same way as in Sec. II A, we can perform an integration by parts and use Levinson's theorem (3.1) to show that $B(T)$ as given by (3.8) has the required continuity property as the potential strength is varied. Note that the term ξ is necessary; if it were absent, $B(T)$ would change abruptly at potential strengths which give a zero-energy p-wave resonance.

B. Phase-shift formulation

In Appendix B we derive a phase-shift formula for $B(T)$, using the two-dimensional analogue of the three-dimensional derivation of Appendix A. the result is (3.8), *but with the term ξ missing.* This is incorrect for the case where a p-wave zero-energy resonance is present; continuity arguments analogous to those used in Sec. II B then lead to Levinson's theorem (3.1), but with the term q missing. This result is disturbing, since on the surface there appears to be nothing wrong with the working in Appendix B.

The derivation in Appendix B depends on the asymptotic form of the wave function. A clue as to the reason for the erroneous result may be obtain by looking carefully at this form for the cases where zero-energy resonances are present. Solving the Schrödinger equation (3.2), with k set equal to zero, in the region where r is large and the potential can be neglected, gives the following asymptotic forms for the s-wave and p-wave resonance wave functions:

$$\chi_0^{\rm res}(0,r)\sim c_0 r^{1/2}, \quad r\to\infty \tag{3.10}$$

$$\chi_1^{\rm res}(0,r)\sim c_1 r^{-1/2}, \quad r\to\infty \tag{3.11}$$

where c_0 and c_1 are constants. But using the asymptotic form

$$\chi_m(k,r)\sim(2/\pi)^{1/2}\cos\left[kr-(m+\tfrac{1}{2})\frac{\pi}{2}+\delta_m(k)\right], \quad r\to\infty \tag{3.12}$$

gives

$$\chi_m(0,r)\sim\text{const.}, \quad r\to\infty . \tag{3.13}$$

This is to be contrasted with the three-dimensional case, where the s-wave zero-energy wave function at resonance behaves asymptotically as a constant, and this is in accord with the zero-energy limit of the phase-shift form (A6). (It can also be verified that there is agreement in the one-dimensional case.) But in two dimensions the asymptotic form (3.13) is not compatible with the forms (3.10) and (3.11), and this would appear to be the reason why we are not getting the desired contribution from the p-wave resonance: Evaluating the trace formula for $B(T)$ [see Eq. (B6)] using the asymptotic form (3.12) simply omits all wave functions corresponding to zero-energy resonances.

The underlying cause is a noncommutivity in the limits $k\to 0$ and $r\to\infty$. This suggests that we repeat the derivations of Appendix B, but using a less extreme asymptotic form for $\chi_m(k,r)$. Specifically, we use

$$\chi_m(k,r)\sim(kr)^{1/2}[\cos\delta_m(k)J_m(kr) - \sin\delta_m(k)N_m(kr)], \quad r\to\infty . \tag{3.14}$$

[Inserting the leading asymptotic behavior of the Bessel functions $J_m(kr)$ and $N_m(kr)$ recovers (3.12).] The details are given in Appendix C. The result is exactly the same as before, except when there is a p-wave zero-energy resonance: In this case (and in no other), we obtain an integral which diverges at $k=0$. This now provides a clear indication that here the asymptotic-wave-function approach is not satisfactory, and it is not surprising that we obtain the wrong result in Appendix B. Clearly, it is far preferable to use the Jost-function method of Sec. III A; in that treatment, k is kept off the real axis and divergencies do not occur.

In the three-dimensional treatment, we found that the extra quantity ξ which had to be included in $B(T)$ could be expressed in terms of the zero-energy phase shift. [Compare (2.4) and (2.11).] We have not been able to find the analogous two-dimensional result from the on-shell treatment of Appendix C; however, Jost-function considerations lead to (we give only the p-wave case, since all other partial waves give zero contribution)

$$\xi=\lim_{k\to 0}\frac{1}{\pi}\ln k\,\sin[2\delta_1(k)] . \tag{3.15}$$

The details are given in Appendix E. Inserting the $k\to 0$ behavior of the phase shift (see Appendix D) then gives the desired result (3.9).

IV. ONE DIMENSION

Although $B(T)$ in one dimension has been calculated for some specific interactions (hard rods,[32] δ-function interaction[33]), a general phase-shift formula does not seem to have been given. In Appendix F we show that

$$B(T)=-2^{-1/2}\lambda\left[\sum_B e^{-\beta E_B}+\frac{1}{\pi}\int_0^\infty dk\, e^{-\beta k^2}\left[\frac{d\delta_-}{dk}+\frac{d\delta_+}{dk}\right]+\tfrac{1}{2}[\sin^2\delta_-(0)-\sin^2\delta_+(0)]\right] , \tag{4.1}$$

where $\delta_-(k)$ and $\delta_+(k)$ are the phase shifts for wave functions of odd and even parity, respectively. (See Appendix F.) In order for the k integral to exist, we have had to assume that

$$\delta_\pm(0)=n_\pm\pi/2,\quad n_\pm=0,\pm1,\ldots\ . \tag{4.2}$$

A partial integration gives

$$B(T)=-2^{-1/2}\lambda\left[\left[\sum_B e^{-\beta E_B^-}-\frac{1}{\pi}\delta_-(0)+\tfrac{1}{2}\sin^2\delta_-(0)\right]+\left[\sum_B e^{-\beta E_B^+}-\frac{1}{\pi}\delta_+(0)-\tfrac{1}{2}\sin^2\delta_+(0)\right]\right.$$
$$\left.+\frac{2\beta}{\pi}\int_0^\infty k\,dk\,e^{-\beta k^2}[\delta_-(k)+\delta_+(k)]\right]\ . \tag{4.3}$$

Here, we have divided the bound-state contributions into those associated with odd- and even-parity states. Applying the same continuity arguments as for the two- and three-dimensional cases, and taking into account (4.2), leads to the conclusion that

$$\delta_\pm(0)=N_{B\pm}\pi\mp q_\pm\ , \tag{4.4}$$

where $q_\pm$ is 0 or $\pi/2$. Again, as in the three-dimensional case, it does not seem possible to decide which value of $q_\pm$ is appropriate purely on virial-coefficient considerations. Thus we need some additional information on the low-energy behavior of $\delta_\pm(k)$. In Appendix G we show that the usual behavior is

$$\tan\delta_-(k)\to0,\quad k\to0 \tag{4.5}$$

$$\tan\delta_+(k)\to\pm\infty,\quad k\to0\ . \tag{4.6}$$

Hence (4.4) takes the form

$$\delta_-(0)=N_{B-}\pi\ , \tag{4.7}$$

$$\delta_+(0)=N_{B+}\pi-\pi/2\ . \tag{4.8}$$

The value for $\delta_-(0)$ is no surprise, since the antisymmetric one-dimensional wave function, for $x>0$, coincides with the usual three-dimensional s-wave radial wave function. But the value of $\delta_+(0)$ is unexpected and has only recently been given in the literature.[7–9] Thus it is pleasing that it comes naturally out of virial-coefficient considerations, with only a minimum of additional information in the form of (4.5) and (4.6).

For exceptional potential strengths, we can get zero-energy resonances. In the odd-parity case, $\tan\delta_-(k)$ diverges as $k\to0$; in the even-parity case, $\tan\delta_+(k)$ goes to zero as $k\to0$. (See Appendix G.) Thus we have the complete one-dimensional form of Levinson's theorem:

$$\delta_-(0)=N_{B-}\pi+q_-\ , \tag{4.9}$$

$$\delta_+(0)=N_{B+}\pi-\pi/2+q_+\ , \tag{4.10}$$

where

$$q_-=\begin{cases}\pi/2 & \text{zero-energy odd-parity resonance,}\\ 0 & \text{all other cases,}\end{cases} \tag{4.11}$$

$$q_+=\begin{cases}\pi/2 & \text{zero-energy even-parity resonance,}\\ 0 & \text{all other cases.}\end{cases} \tag{4.12}$$

We note that the effect of a zero-energy resonance is the same in each case: the phase shift is increased by $\pi/2$.

Results (4.7) and (4.8) are in agreement with Barton;[9] he did not consider the exceptional cases where there are zero-energy levels. Newton[8] and Bollé *et al.*[7] use a phase shift defined by

$$\det S=e^{2i\delta}\ , \tag{4.13}$$

where S is the S matrix. The connection with our odd- and even-parity phase shifts is simply

$$\delta=\delta_-+\delta_+\ , \tag{4.14}$$

so (4.9)–(4.12) give

$$\delta(0)=N_B\pi+q\ , \tag{4.15}$$

where

$$q=\begin{cases}0 & \text{zero-energy resonance,}\\ -\pi/2 & \text{all other cases,}\end{cases} \tag{4.16}$$

and N_B is the total number of bound states. This is in complete agreement with the above authors.

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APPENDIX A: SECOND VIRIAL COEFFICIENT IN THREE DIMENSIONS

We give a derivation of the phase-shift formula for $B(T)$, using only elementary scattering theory and not imposing artificial boundary conditions. A derivation along these lines was given some time ago by Blatt,[34] but unfortunately there is an error of detail in his calculation [a multiplicative factor of $1/k$ is missing in the integrand of the last integral in his equation (2.11)], and as a consequence he does not obtain a term which is important for our purposes. The following may be looked upon as a corrected version of Blatt's calculation.

Our starting point is the expression[13]

$$B(T)=-\lim_{V\to\infty}\frac{\lambda^6}{2V}\mathrm{Tr}(e^{-\beta H_2}-e^{-\beta H_2^0}) , \tag{A1}$$

where V is the volume of the container, H_2 is the Hamiltonian for two interacting particles, and H_2^0 is the corresponding quantity for two free particles. After separation of the center-of-mass motion, the limit $V\to\infty$ can be taken and we find

$$B(T)=-\sqrt{2}\lambda^3\mathrm{Tr}_{\mathrm{c.m.}}(e^{-\beta h_2}-e^{-\beta h_2^0}) , \tag{A2}$$

where h_2,h_2^0 are the Hamiltonians for the relative motion of the particles.

The trace is evaluated using complete sets of energy eigenstates for the interacting and noninteracting systems. Separating the discrete states, and performing a partial-wave expansion leads to

$$B(T)=-\sqrt{2}\lambda^3\sum_{l=0}^{\infty}(2l+1)\left[\sum_B e^{-\beta E_{B,l}}+\int_0^\infty dr\int_0^\infty dk\, e^{-\beta k^2}\{[\chi_l(k,r)]^2-[\chi_l^0(k,r)]^2\}\right] , \tag{A3}$$

where $E_{B,l}$ (≤ 0) are the bound-state energies corresponding to angular momentum l, and $\chi_l(k,r)$ is the radial wave function satisfying the Schrödinger equation

$$\left[-\frac{d^2}{dr^2}+v(r)+\frac{l(l+1)}{r^2}-k^2\right]\chi_l(k,r)=0 , \tag{A4}$$

with the boundary conditions

$$\chi_l(k,r)=0,\quad r=0 \tag{A5}$$

$$\chi_l(k,r)\sim(2/\pi)^{1/2}\sin\left[kr-\frac{l\pi}{2}+\delta_l(k)\right],\quad r\to\infty \tag{A6}$$

where $\delta_l(k)$ is the phase shift for the lth partial wave at wave number k. $\chi_l^0(k,r)$ is the corresponding solution for the noninteracting system, and has the asymptotic form

$$\chi_l^0(k,r)\sim(2/\pi)^{1/2}\sin\left[kr-\frac{l\pi}{2}\right],\quad r\to\infty . \tag{A7}$$

By taking solutions of (A4) at k and k' and letting $k'\to k$, we derive the formula

$$\int_0^R[\chi_l(k,r)]^2dr=\frac{1}{2k}\left[\frac{\partial\chi_l}{\partial k}\frac{\partial\chi_l}{\partial r}-\frac{\partial^2\chi_l}{\partial k\,\partial r}\chi_l\right]_0^R . \tag{A8}$$

The boundary condition (A5) ensures no contribution from the lower limit. At the upper limit we let $R\to\infty$ and use (A6) to obtain

$$\int_0^R[\chi_l(k,r)]^2dr\sim-\frac{1}{\pi k}\left[\tfrac{1}{2}\sin[2kR-l\pi+2\delta_l(k)]-k\left[R+\frac{\partial\delta_l}{\partial k}\right]\right],\quad R\to\infty . \tag{A9}$$

Similarly, we find

$$\int_0^R[\chi_l^0(k,r)]^2dr\sim-\frac{1}{\pi k}[\tfrac{1}{2}\sin(2kR-l\pi)-kR] ,\quad R\to\infty . \tag{A10}$$

Using these in (A3) gives

$$B(T)=-\sqrt{2}\lambda^3\sum_{l=0}^{\infty}(2l+1)\left[\sum_B e^{-\beta E_{B,l}}+\frac{1}{\pi}\int_0^\infty dk\,e^{-\beta k^2}\frac{d\delta_l}{dk}+\xi_l\right] , \tag{A11}$$

where

$$\xi_l=-\frac{1}{2\pi}\lim_{R\to\infty}\int_0^\infty dk\,e^{-\beta k^2}\frac{1}{k}\{\sin[2kR-l\pi+2\delta_l(k)]-\sin(2kR-l\pi)\} . \tag{A12}$$

This can be written as

$$\xi_l=-\frac{1}{2\pi}(-1)^l\lim_{R\to\infty}\int_0^\infty dk\,e^{-\beta k^2}\left[\frac{1}{k}\cos(2kR)\sin[2\delta_l(k)]-\frac{2}{k}\sin(2kR)\sin^2\delta_l(k)\right] . \tag{A13}$$

The first thing to note about this integral is that is necessarily diverges unless $\sin[2\delta_l(k)]$ vanishes at $k=0$. Thus we do not get a finite expression for the second virial coefficient unless $\delta_l(0)$ is a multiple of $\pi/2$. In fact, we can go further and conclude that at worst $k^{-1}\sin[2\delta_l(k)]$ has an integrable singularity at $k=0$. With this assumption, we can apply the Riemann-Lebesgue lemma[35] to the first term in (A13) and conclude that

$$\lim_{R\to\infty}\int_0^\infty dk\, e^{-\beta k^2}\frac{1}{k}\cos(2kR)\sin[2\delta_l(k)]=0\ . \tag{A14}$$

However, we must be more careful with the second term, since

$$\int_0^\infty dk\, e^{-\beta k^2}\frac{1}{k}\sin^2\delta_l(k) \tag{A15}$$

will diverge (and hence the Riemann-Lebesgue lemma will not apply), unless we make the stronger assumption that $k^{-1}\sin^2\delta_l(k)$ is integrable at $k=0$ [and this would imply that $\delta_l(0)$ is a multiple of π]. Rather than do this, we use

$$\lim_{R\to\infty}\frac{\sin(2kR)}{k}=\pi\delta(k)\ , \tag{A16}$$

where $\delta(k)$ is a Dirac delta function, and obtain

$$\xi_l=(-1)^l\tfrac{1}{2}\sin^2\delta_l(0)\ . \tag{A17}$$

At this point we have derived the expressions needed in Sec. II A above. Note that if we do invoke Levinson's theorem (1.1), then ξ_l is just the quantity ξ in (2.4).

APPENDIX B: SECOND VIRIAL COEFFICIENT IN TWO DIMENSIONS

We now give a derivation of the phase-shift formula for $B(T)$ in two dimensions which parallels that for three dimensions given in Appendix A.

Our starting point is

$$B(T)=-\lim_{A\to\infty}\frac{\lambda^4}{2A}\mathrm{Tr}(e^{-\beta H_2}-e^{-\beta H_2^0})\ , \tag{B1}$$

where A is the area of the system, H_2 is the Hamiltonian for two interacting particles, and H_2^0 is the corresponding quantity for two free particles. Proceeding as in Appendix A, we find the analogue of (A3) to be

$$B(T)=-\lambda^2\sum_{m=-\infty}^{\infty}\left[\sum_B e^{-\beta E_{B,m}}+\int_0^\infty dr\int_0^\infty dk\, e^{-\beta k^2}\{[\chi_m(k,r)]^2-[\chi_m^0(k,r)]^2\}\right]\ , \tag{B2}$$

where $\chi_m(k,r)$ satisfies (3.2), with the boundary conditions

$$\chi_m(k,r)=0,\quad r=0 \tag{B3}$$

$$\chi_m(k,r)\sim(2/\pi)^{1/2}\cos\left[kr-(m+\tfrac{1}{2})\frac{\pi}{2}+\delta_m(k)\right]\ ,\quad r\to\infty\ . \tag{B4}$$

$\chi_m^0(k,r)$ satisfies (3.2) with $v(r)=0$, and has the asymptotic form

$$\chi_m^0(k,r)\sim(2/\pi)^{1/2}\cos\left[kr-(m+\tfrac{1}{2})\frac{\pi}{2}\right],\quad r\to\infty\ . \tag{B5}$$

Continuing as in Appendix A [(A8) holds unchanged], we arrive at

$$B(T)=-\lambda^2\sum_{m=-\infty}^{\infty}\left[\sum_B e^{-\beta E_{B,m}}+\frac{1}{\pi}\int_0^\infty dk\, e^{-\beta k^2}\frac{d\delta_m}{dk}+\xi_m\right]\ , \tag{B6}$$

where

$$\xi_m=\frac{1}{2\pi}\lim_{R\to\infty}\int_0^\infty dk\, e^{-\beta k^2}\frac{1}{k}\{\sin[2kR-(m+\tfrac{1}{2})\pi+2\delta_m(k)]-\sin[2kR-(m+\tfrac{1}{2})\pi]\}\ . \tag{B7}$$

This can be written as

$$\xi_m=\frac{1}{2\pi}(-1)^m\lim_{R\to\infty}\int_0^\infty dk\, e^{-\beta k^2}\left[\frac{1}{k}\sin(2kR)\sin[2\delta_m(k)]+\frac{2}{k}\cos(2kR)\sin^2\delta_m(k)\right]\ . \tag{B8}$$

This is very similar to (A13) for ξ_l, but there is an important difference. For the above integral to exist, we now require $k^{-1}\sin^2\delta_m(k)$ to be integrable at $k=0$, and hence $\delta_m(0)$ must be an integer multiple of π. Proceeding now as for the three-dimensional case, we find that the second term in (20) vanishes by the Riemann-Lebesque lemma,[35] and, upon using (A16), the first term also vanishes because $\sin[2\delta_m(0)]=0$. Thus we conclude that

$$\xi_m=0,\quad m\geq 0\ . \tag{B9}$$

However, this result is not correct; ξ_m should coincide with ξ as given by (3.9), and thus ξ_1 should be unity if there is a p-wave zero-energy resonance. The reason for this discrepancy is investigated in Sec. II B and Appendix C.

APPENDIX C: FURTHER INVESTIGATION OF $B(T)$ IN TWO DIMENSIONS

We wish to evaluate (B2) using the asymptotic wave function (3.14), rather than (3.12) which was used in Appendix B. Write (B2) as

$$B(T)=-\lambda^2\sum_{m=-\infty}^{\infty}\left[\sum_B e^{-\beta E_{B,m}}+B_m^c(T)\right], \quad \text{(C1)}$$

where

$$B_m^c(T)=\int_0^\infty dr\int_0^\infty dk\; e^{-\beta k^2}\{[\chi_m(k,r)]^2-[\chi_m^0(k,r)]^2\}\ . \quad \text{(C2)}$$

Introducing the notation

$$W_m(k,r)\equiv\frac{\partial\chi_m}{\partial k}\frac{\partial\chi_m}{\partial r}-\frac{\partial^2\chi_m}{\partial k\partial r}\chi_m\ , \quad \text{(C3)}$$

and using (A8) gives

$$B_m^c(T)=\lim_{R\to\infty}\int_0^\infty dk\, e^{-\beta k^2}\frac{1}{2k}[W_m(k,R)-W_m^0(k,R)]\ , \quad \text{(C4)}$$

where $W_m^0(k,r)$ means (C3) with χ_m replaced by the noninteracting wave function χ_m^0. Using (3.14) we find, after some simplification,

$$W_m(k,r)-W_m^0(k,r)\sim(2/\pi)k\delta_m'(k)+\sin^2\delta_m(k)[(kr)^2(-J'^2+N'^2+JJ''-NN'')+(kr)(JJ'-NN')] + \tfrac{1}{2}\sin[2\delta_m(k)][(kr)^2(JN''+NJ''-2J'N')+(kr)(JN'+NJ')],\quad r\to\infty \quad \text{(C5)}$$

where $J\equiv J_m(kr)$, $N\equiv N_m(kr)$, and primes denote differentiation with respect to the argument. This is now to be inserted in (C4) and the integral over k and the limit $R\to\infty$ to be performed. The order in which these are done is important: if $R\to\infty$ is taken first, then we are simply back to the treatment of Appendix B, and the same erroneous result (B9) will be obtained.

Thus we investigate the possibility of doing the k integral first. We start by looking at the behavior of the integrand of (C4) near $k=0$. Inserting the standard expansions of the Bessel functions[36] into (C5) gives

$$(1/2k)[W_m(k,R)-W_m^0(k,R)]\sim(1/\pi)\{\delta_m'(k)+\sin^2\delta_m(k)[O(k^{-2m+1})]+\sin[2\delta_m(k)][-mk^{-1}+O(k)]\},\quad m\ge 2 \quad \text{(C6)}$$

$$(1/2k)[W_1(k,R)-W_0^0(k,R)]\sim(1/\pi)\{\delta_1'(k)+\sin^2\delta_1(k)[(2/\pi)(1+2\gamma)k^{-1}+O(k\ln k)]+\sin[2\delta_1(k)][-k^{-1}+O(k)]\}\ , \quad \text{(C7)}$$

$$(1/2k)[W_0(k,R)-W_1^0(k,R)]\sim(1/\pi)\{\delta_0'(k)+\sin^2\delta_0(k)[(2/\pi)k^{-1}+O(k\ln k)]+\sin[2\delta_0(k)][O(k)]\}\ . \quad \text{(C8)}$$

In (C7) γ is Euler's constant. In (C6)–(C8) we are assuming that R is fixed and large enough so that (C5) is valid.

To investigate this further, we need the $k\to 0$ behavior of the terms involving the phase shifts $\delta_0(k)$ and $\delta_1(k)$. This is given in Appendix D. For $m\ge 2$ we find

$$\sin^2\delta_m(k)\sim\alpha^{-2}k^{2\nu},\quad \sin[2\delta_m(k)]\sim 2\alpha^{-1}k^{\nu},\quad k\to 0 \quad \text{(C9)}$$

where $\nu=2m$ unless there is a zero-energy level, in which case $\nu=2m-2$. Thus for $m\ge 2$ there are no problems: the right-hand side of (C6) behaves at worst like k as $k\to 0$. For $m=1$ the usual behavior is

$$\sin^2\delta_1(k)\sim a_1^2k^4,\quad \sin[2\delta_1(k)]\sim -2a_1k^2,\quad k\to 0 \quad \text{(C10)}$$

where a_1 is a constant, and this causes no problems in (C7). The interesting case is when there is a zero-energy resonance; the behavior is now

$$\sin^2\delta_1^{\rm res}(k)\sim\pi^2/(2\ln k)^2\ ,\qquad \sin[2\delta_1^{\rm res}(k)]\sim\pi/\ln k,\quad k\to 0 \quad \text{(C11)}$$

and inserting this in (C7) gives rise to the nonintegrable singularity $(k\ln k)^{-1}$. Thus straightforward substitution of (C5) into (C4) gives a divergent result in the case where there is a zero-energy p-wave resonance. For $m=0$ we find

$$\sin^2\delta_0(k)\sim\pi^2/(2\ln k)^2\ ,\qquad \sin[2\delta_0(k)]\sim\pi/\ln k, k\to 0\ . \quad \text{(C12)}$$

The only effect of a zero-energy resonance is to cause $\delta_0(0)$ to pass through a multiple of π (see Appendix D); the approach to $k=0$ is still dominated by the logarithmic term as given in (C12). Insertion of (C12) into (C8) shows that the right-hand side is integrable at $k=0$. We have also performed the analogous calculation for the three-dimensional case, and there are no divergencies for any value of l.[37]

APPENDIX D: LOW-ENERGY BEHAVIOR OF $\cot\delta_m(k)$

The low-energy behavior of $\cot\delta_\alpha(k)$ in two dimensions is somewhat more complicated than that in three dimensions or in one dimension. This is mainly due to the presence of logarithmic terms in the small-z expansion of the irregular Bessel function $N_m(z)$.

To simplify our analysis, we assume that the potential is effectively zero for r greater than some distance R_c. For $m\ge 2$ there are no complications, and a treatment parallel to that used in the three-dimensional case[27] gives

$$\cot\delta_m(k)\sim\alpha k^{-\nu},\quad k\to 0,\ m\ge 2 \quad \text{(D1)}$$

where α is a constant, $\nu=2m$ in the normal case, and $\nu=2m-2$ if there is a zero-energy bound state.

For the s-wave case, the low-energy expansion takes the form[38,39]

$$\frac{\pi}{2}\cot\delta_0(k)=\gamma+\ln\frac{k}{2}-\frac{1}{a_0}+O(k^2)\ , \tag{D2}$$

where a_0 is the scattering length and γ is Euler's constant. (We remark that there are other definitions of the scattering length in two dimensions—see Refs. 39 and 40.) For $a_0\neq 0$, the logarithm dominates and so

$$\cot\delta_0(k)\sim(2/\pi)\ln k,\quad k\rightarrow 0\ . \tag{D3}$$

As a new bound state appears, a_0 changes sign, being zero at the critical potential strength which gives a zero-energy resonance. (This behavior is different from that of the three-dimensional s-wave scattering length, which becomes infinite under these circumstances. See Ref. 39 for a discussion of this point.) This means that the cotangent changes to a new branch, and so $\delta_0(0)$ must pass through a multiple of π.

For the p-wave case, the corresponding expansion is[38,39]

$$\cot\delta_1(k)=-\frac{1}{a_1}\frac{1}{k^2}+\frac{2}{\pi}\ln k+O(1),\quad k\rightarrow 0\ . \tag{D4}$$

a_1 is the p-wave scattering length, and its behavior is similar to that of its three-dimensional counterpart. For $|a_1|\neq\infty$ the first term dominates, and the behavior is the same as that given by (D1) with $\nu=2m$. But for $|a_1|=\infty$, which corresponds to a zero-energy resonance, the first term vanishes and

$$\cot\delta_1^{\rm res}(k)\sim(2/\pi)\ln k,\quad k\rightarrow 0\ . \tag{D5}$$

APPENDIX E: ADDITIONAL TERM IN PHASE-SHIFT EXPRESSION FOR $B(T)$ IN TWO DIMENSIONS

We wish to justify (3.15); that is, we wish to show that the quantity which must be added to the phase-shift term in the expression for $B(T)$ is

$$\xi=\lim_{k\rightarrow 0}\frac{1}{\pi}\ln k\,\sin[2\delta_1(k)]\ . \tag{E1}$$

From Sec. II A, we see that ξ is the contribution from the origin to the contour integral in (3.6):

$$\xi=\frac{1}{2}\lim_{k\rightarrow 0}k\frac{f_1'(k)}{f_1(k)}\ . \tag{E2}$$

The use of (3.7) gives (3.9). However, we wish to relate ξ to the zero-energy phase shift $\delta_1(0)$.

The S matrix can be expressed in terms of the regular solution $\varphi_m(k,r)$ and the Jost function $f_m(k)$ by [cf. Ref. 3, Eq. (5.17)]

$$S_m(k)=1-\left[i(2\pi)^{1/2}k^m\int_0^\infty dr\,r^{1/2}J_m(kr)v(r)\varphi_m(k,r)\right]\Big/f_m(-k)\ . \tag{E3}$$

Since $\varphi_m(k,r)$ is an entire analytic function of k^2 we have

$$S_1(k)-1=\left[-i(\pi/2)^{1/2}k^2\int_0^\infty dr\,r^{3/2}v(r)\varphi_1(o,r)+O(k^4)\right]\Big/f_1(-k),\quad k\rightarrow 0\ . \tag{E4}$$

The Jost function satisfies [cf. Ref. 3, Eq. (4.4)]

$$f_m(k)=1-i(\pi/2)^{1/2}k^m\int_0^\infty dr\,r^{1/2}\times H_m^{(2)}(kr)v(r)\varphi_m(k,r)\ , \tag{E5}$$

from which one can derive

$$f_1'(-k)=\left[(2/\pi)^{1/2}\int_0^\infty dr\,r^{3/2}v(r)\varphi_1(O,r)\right]k\ln k+O(k),\quad k\rightarrow 0\ . \tag{E6}$$

From (E4) and (E6) we derive

$$\lim_{k\rightarrow 0}(-k)\frac{f_1'(-k)}{f_1(-k)}=-\frac{2i}{\pi}\lim_{k\rightarrow 0}\ln k[S_1(k)-1]\ . \tag{E7}$$

From (E2), (E7), and the relation $S_1(k)=\exp[2i\delta_1(k)]$, we find

$$\xi=\frac{1}{\pi}\lim_{k\rightarrow 0}\ln k\{2i\sin^2\delta_1(k)+\sin[2\delta_1(k)]\}\ . \tag{E8}$$

From (C10) and (C11),

$$\lim_{k\rightarrow 0}\ln k\sin^2\delta_1(k)=0\ . \tag{E9}$$

Alternatively, (E9) follows from the requirement that $B(T)$, and hence ξ, must be real. Thus (E8) reduces to (E1).

APPENDIX F: SECOND VIRIAL COEFFICIENT IN ONE DIMENSION

We derive a phase-shift expression for $B(T)$ in one dimension, using methods which parallel those used for three dimensions in Appendix A. We start from

$$B(T)=-\lim_{L\rightarrow\infty}\frac{\lambda^2}{2L}{\rm Tr}(e^{-\beta H_2}-e^{-\beta H_2^0})\ , \tag{F1}$$

where L is the length of the line containing the system. Removal of the center-of-mass motion gives

$$B(T)=-2^{-1/2}\lambda{\rm Tr}_{\rm c.m.}(e^{-\beta h_2}-e^{-\beta h_2^0})\ . \tag{F2}$$

The trace is evaluated using states of odd and even parity. We find

$$B(T)=-2^{-1/2}\lambda\left[\sum_B e^{-\beta E_B}+\int_0^\infty dx\int_0^\infty dk\, e^{-\beta k^2}\{[\chi_+(k,x)]^2-[\chi_+^0(k,x)]^2+[\chi_-(k,x)]^2-[\chi_-^0(k,x)]^2\}\right], \tag{F3}$$

where E_B are the bound-state energies and $\chi_\pm(k,x)$ satisfy the Schrödinger equation

$$\left[-\frac{d^2}{dx^2}+v(x)-k^2\right]\chi_\pm(k,x)=0, \tag{F4}$$

with the boundary conditions

$$\chi_-(k,x)\sim\pi^{-1/2}\sin[kx\pm\delta_-(k)],\quad x\to\pm\infty \tag{F5}$$

$$\chi_+(k,x)\sim\pi^{-1/2}\cos[kx\pm\delta_+(k)],\quad x\to\pm\infty. \tag{F6}$$

These define the odd- and even-parity phase shifts, $\delta_-(k)$ and $\delta_+(k)$, respectively.[41] The free wave functions are simply

$$\chi_-^0(k,x)=\pi^{-1/2}\sin(kx),\quad \chi_+^0(k,x)=\pi^{-1/2}\cos(kx). \tag{F7}$$

Proceeding as in Appendix A, we establish the formulas

$$\int_{-\infty}^{\infty}\{[\chi_\pm(k,x)]^2-[\chi_\pm^0(k,x)]^2\}dx =\frac{1}{\pi}\frac{\partial\delta_\pm}{\partial k}\pm\lim_{X\to\infty}\frac{1}{2\pi k}\{\sin[2kX+2\delta_\pm(k)]-\sin(2kX)\}. \tag{F8}$$

These are now used in (F3). In order for the k integral to exist, we require $\delta_\pm(0)$ to be integer multiples of $\pi/2$. Continuing as in Appendix A, we obtain finally

$$B(T)=-2^{-1/2}\lambda\left[\sum_B e^{-\beta E_B}+\frac{1}{\pi}\int_0^\infty dk\, e^{-\beta k^2}\left[\frac{d\delta_-}{dk}+\frac{d\delta_+}{dk}\right]+\xi\right], \tag{F9}$$

where

$$\xi=\tfrac{1}{2}[\sin^2\delta_-(0)-\sin^2\delta_+(0)]. \tag{F10}$$

APPENDIX G: LOW-ENERGY BEHAVIOR OF $\tan\delta_\pm(k)$

The phase shifts have the following integral representations:[41]

$$\tan[\delta_-(k)]=-\frac{1}{k}\int_0^\infty \sin(kx)v(x)\varphi_-(k,x)dx, \tag{G1}$$

$$\tan[\delta_+(k)]=-\frac{1}{k}\int_0^\infty \cos(kx)v(x)\varphi_+(k,x)dx, \tag{G2}$$

where $\varphi_\pm(k,x)$ satisfy the integral equations

$$\varphi_-(k,x)=\sin(kx)+\int_0^\infty K_-(k;x,x')v(x')\varphi_-(k,x')dx', \tag{G3}$$

$$\varphi_+(k,x)=\cos(kx)+\int_0^\infty K_+(k;x,x')v(x')\varphi_+(k,x')dx'. \tag{G4}$$

The Green's functions are

$$K_-(k;x,x')=-\frac{1}{k}\cos(kx_>)\sin(kx_<), \tag{G5}$$

$$K_+(k;x,x')=-\frac{1}{k}\sin(kx_>)\cos(kx_<), \tag{G6}$$

where $x_>$ ($x_<$) is the greater (lesser) of x and x'.

Consider first the odd-parity case. As $k\to 0$, $K_-(k;x,x')\sim -x_<$, and using this in (G3) gives $\varphi_-(k,x)\sim kc_-(x)$, where $c_-(x)$ is independent of k. Thus from (G1),

$$\tan\delta_-(k)\sim -k\int_0^\infty xv(x)c_-(x)dx,\quad k\to 0. \tag{G7}$$

Thus, provided this integral (which is just the scattering length) is finite, we have

$$\tan\delta_-(k)\to 0 \text{ as } k\to 0. \tag{G8}$$

In the exceptional case of a zero-energy resonance, $c_-(x)$ becomes infinite and so $\delta_-(0)$ will be an integral multiple of $\pi/2$. This is all exactly as expected, since the odd-parity one-dimensional wave function is identical (for $x=r\geq 0$) to the s-wave radial wave function for three-dimensional scattering.

For the even-parity case, we find $\varphi_+(k,x)\sim c_+(x)$ as $k\to 0$, leading to

$$\tan\delta_+(k)\sim -\frac{1}{k}\int_0^\infty v(x)c_+(x)dx,\quad k\to 0. \tag{G9}$$

Thus, provided the integral does not vanish, we have

$$\tan\delta_+(k)\to\pm\infty,\quad k\to 0. \tag{G10}$$

The exceptional case, this time corresponding to an even-parity zero-energy resonance, occurs when the integral in (G9) is zero, and so $\delta_+(0)$ must now be an integral multiple of π.

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