957 (1961), who gives a derivation of the Landau theory of a Fermi fluid in which he invokes the adiabatic hypothesis in a time-dependent perturbation formalism at $T \neq 0\,°\mathrm{K}$.

[22] Equation (A6) is the same as Eq. (16) in MII if we set $n_1(-p)$ and the last term in Eq. (A6) equal to zero.

[23] Details of the derivations of these identities are given in Appendix C of D. W. J. Shea, Ph.D. thesis, University of Colorado, 1968 (unpublished).

[24] See Eq. (C.27) of Ref. 23. This identity was given earlier as Eqs. (39) of MI.

[25] F. London, *Superfluids*, Vol. II (Wiley, New York, 1954), p. 45. See also F. Mohling, Phys. Rev. 135, A876 (1964), Sec. 6, for the case of a dilute hard-sphere Bose gas at very low temperatures.

[26] See Eq. (C.38) of Ref. 23. This identity was given earlier as the first of Eqs. (40) in MI.

[27] To derive this result, Eqs. (C.19), (C.22), and (C.26) of Ref. 23 must be used.

[28] See Appendix H of Ref. 2.

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Quantum-Mechanical Third Virial Coefficient and Three-Body Phase Shifts*

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A formalism is presented for the calculation of the quantum-mechanical third virial coefficient in terms of two- and three-body phase shifts. This is done for Boltzmann statistics and in the absence of bound states. The method is based on the expansion of three-body wave functions in terms of hyperspherical harmonics in six-dimensional space. Basic scattering equations are set down, including expressions for three-particle S, T, and R matrices and for the three-body phase shifts. Connection is then made with statistical mechanics and an expression proposed for the evaluation of the Boltzmann three-body cluster in terms of these three-body phase shifts. Using this method, the behavior of the third virial coefficient of a gas subject to binary square-well interactions is studied in the limit when T approaches zero.

INTRODUCTION

One of the earliest continuing and important concerns of statistical mechanics has been its application to the calculation of the equation of state of simple fluids. For moderately dense gases, we associate the names of Boltzmann, Ornstein,[1] Ursell,[2] Mayer,[3] as well as many others with the successful effort to develop methods and to calculate virial coefficients in classical statistical mechanics. The problem was reduced, at least in principle, to the evaluation of integrals of products of functions of two-body potentials and steady progress is being made in calculating increasingly complex coefficients.

For quantum fluids the situation is very much more intractable. Instead of evaluating integrals, one is faced, for the lth virial, with the need to calculate traces of statistical operators involving the lth-body Hamiltonian as well as lower ones. An elegant method was proposed for the second virial coefficient, involving only the two-body problem, by Uhlenbeck and Beth,[4] and by Gropper,[5] and has been used for a number of calculations. For the third virial coefficient the first attempts date only from the late 1950's and so far a number of distinct approaches have been used. The first, which was also the original method, has been the use of the binary-collision expansion by Pais and Uhlenbeck[6] and by Larsen.[7] This approach suffers from shortcomings relating to the convergence of the series expansion in the vicinity of bound states (which is the case for He^4) and from the exceeding difficulty in calculating any but the simplest terms. The second approach represents attempts to use the Watson-Faddeev[8] equations to obtain the third virial. Though the connection has been worked out by Gibson[9] and by Reiner[10] no explicit calculations have been made due to the difficulty of solving the Watson-Faddeev equations. Approximations involving a variational method and an assumption of a separable two-body scattering matrix have been proposed.[11] A somewhat related work is that of Baumgartl[12] who derives an approximate expression for the third virial coefficient which involves the two-particle scattering amplitude. It is very hard to understand the consequences of this approximation or its domain of validity. Finally, a most interesting method has been the use of numerical Monte Carlo path-integral techniques by Jordan and Fosdick[13] to obtain the three-body density-dependent terms of the pair-correlation function and then the third virial. The method may perhaps be characterized as a super Wigner-Kirkwood method in that contrary to the latter (which has also been used by Kihara[14] and by Larsen and Lieberman[15]) it faces no fundamental limitations to its domain of applicability but, nevertheless, it is especially suited for high temperatures. As the temperature decreases the calculations become increasingly laborious and good accuracy is difficult to achieve.

Comparison of the previous approaches with the treatment of Uhlenbeck and Beth for the second virial coefficient underlines the following facts.

(i) While in all of the foregoing methods one obtains position or momentum matrix elements of $e^{-\beta H}$ which are then integrated to obtain the trace, this is not found to be necessary for the second virial. In this case we take advantage of the fact that in the limit of infinite volume all positive energies are allowed and since what we wish to know are the partition-function sums $\sum_\nu e^{-\beta E_\nu}$, our need can be narrowed to knowing the energies of the bound states and the density of states (number of states per energy interval) for the particles with and without interaction. The latter is found to be related to the asymptotic behavior of the wave function (and to its phase shift). Calculations are then much simpler than those for the corresponding density-independent pair-correlation function which was only obtained recently.

(ii) The solution for the second virial coefficient is obtained in terms of the contribution of partial waves. This is especially convenient at low temperatures where the quantum-mechanical effects are strong. The lower the temperature, the smaller the span of energy sampled by the Boltzmann factor in the partition-function sums and the smaller the number of partial waves required.

(iii) The phase-shift formalism usually (depending on the model interaction) makes it possible to develop expansions at low temperatures to supplement and check the numerical results.

We see from this that for the second virial coefficient important conceptual simplifications have been made which free us from the brute-force evaluation of traces and vastly extend our powers of calculations. We believe that we can generalize these important features to apply to the third and higher virials.

In our method we expand the continuum wave functions of the three-body Schrödinger equation in six-dimensional spherical harmonics. This parallels a procedure used for the bound-state problem by Badalyan and Simonov[16] and we draw upon many of their results in our work. The main reason for following this approach is that it allows us to define and make use of a radial coordinate r, changing values of which correspond to scaling of the three-body system, without otherwise altering the configuration. For large values of r the three particles will then be far apart and we expect that a radial wave function will reach an asymptotic state allowing for the definition of a phase shift.

Inserting the wave function in a Schrödinger equation yields an infinite set of coupled differential equations for the radial amplitudes, in general to be solved numerically. For large values of the scaling distance r, the differential equations uncouple and each individual equation takes the form of Bessel's equation. This permits the association of a phase shift to each amplitude. However, and this is very important, by choosing our solutions to be eigenstates for the scattering[17,18] (a notion well known in the theory of two-body scattering with tensor forces) we can require all of the amplitudes of a given solution to have a common phase shift, and therefore are able to ascribe a unique phase shift to our continuum wave functions. This phase shift is then identical with the phase appearing in the elements of the diagonalized S matrix, and we take advantage of this relationship.

Accordingly, in this first paper, we devote the initial sections to establishing our general framework and to writing basic scattering equations for the three-body problem as they appear when making expansions in hyperspherical harmonics. This includes expressions for the three-particle S matrix (and the R matrix) and for the phase shifts.

We then propose a formula for the third virial coefficient in terms of these phase shifts (in a generalization of the formula of Uhlenbeck and Beth for the second virial coefficient) and, using the first and second Born approximation,[18] study the limiting behavior of the third virial as $T \to 0$.

BASIC FRAMEWORK

The quantum specification of a system of three particles requires nine operators and its associated quantum numbers.

If we call $\vec{r}_i$ and $\vec{p}_i$, $i = 1, 2, 3$, the position and momentum of each of the particles of equal mass m, we find that the following canonical transformations:

$$\begin{aligned}
&\vec{P} = \vec{p}_1 + \vec{p}_2 + \vec{p}_3, \quad \vec{R} = \tfrac{1}{3}(\vec{r}_1 + \vec{r}_2 + \vec{r}_3),\\
&\vec{p}_\xi = (\tfrac{2}{3})^{1/2}[\tfrac{1}{2}(\vec{p}_1 + \vec{p}_2) - \vec{p}_3],\\
&\vec{\xi} = (\tfrac{2}{3})^{1/2}[\tfrac{1}{2}(\vec{r}_1 + \vec{r}_2) - \vec{r}_3],\\
&\vec{p}_\eta = 2^{-1/2}(\vec{p}_1 - \vec{p}_2), \quad \vec{\eta} = 2^{-1/2}(\vec{r}_1 - \vec{r}_2),\\
&[\xi_i, (p_\xi)_j] = i\hbar\,\delta_{ij}, [\eta_i, (p_n)_j] = i\hbar\,\delta_{ij},\\
&[\vec{\eta}, \vec{p}_\xi] = [\vec{\xi}, \vec{p}_\eta] = 0
\end{aligned} \tag{1}$$

reduce the Schrödinger equation in the center-of-mass coordinate system to

$$\left(\frac{p_\xi^2}{2m}+\frac{p_\eta^2}{2m}+V(\vec{\xi},\vec{\eta})\right)\psi(\vec{\xi},\vec{\eta})=E\psi(\vec{\xi},\vec{\eta}), \tag{2}$$

where $\vec{p}_\xi=-i\hbar\vec{\nabla}_\xi$, $\vec{p}_\eta=-i\hbar\vec{\nabla}_\eta$.

We will be interested in applying our calculations to helium, the paradigm of a quantum-mechanical gas. We assume that our potential is the sum of short-ranged everywhere-finite spin-independent potentials and that these do not allow the existence of any two- or three-body bound states. These restrictions allow us to simplify considerably our formulation, although eventually we shall wish to relax some of them, especially the stricture on the existence of bound states.

Our next step is to define a six-dimensional coordinate system where the new variables have as components the canonical variables defined in (1), i.e.,

$$\vec{p}=(\vec{p}_\xi,\vec{p}_\eta),\quad \vec{r}=(\vec{\xi},\vec{\eta}). \tag{3a}$$

These six vectors $\vec{p}$ and $\vec{r}$ may then be labeled by specifying their moduli and a set of polar angles. The moduli obviously should be defined by

$$p^2=p_\xi^2+p_\eta^2,\quad r^2=\xi^2+\eta^2. \tag{3b}$$

The set of angles may be chosen in a great variety of ways. In order to use calculations already done elsewhere we adopt the following notation:

$$\begin{aligned}
p_1&=p_{\xi_1}=p\sin\vartheta_p\sin\phi_{1p}\cos\phi_{2p},\\
r_1&=r\sin\vartheta_r\sin\phi_{1r}\cos\phi_{2r},\\
p_2&=p_{\xi_2}=p\sin\vartheta_p\sin\phi_{1p}\sin\phi_{2p},\\
r_2&=r\sin\vartheta_r\sin\phi_{1r}\sin\phi_{2r},\\
p_3&=p_{\xi_3}=p\sin\vartheta_p\cos\phi_{1p},\\
r_3&=r\sin\vartheta_r\cos\phi_{1r},\\
p_4&=p_{\eta_1}=p\cos\vartheta_p\sin\phi_{3p}\cos\phi_{4p},\\
r_4&=r\cos\vartheta_r\sin\phi_{3r}\cos\phi_{4r},\\
p_5&=p_{\eta_2}=p\cos\vartheta_p\sin\phi_{3p}\sin\phi_{4p},\\
r_5&=r\cos\vartheta_r\sin\phi_{3r}\sin\phi_{4r},\\
p_6&=p_{\eta_3}=p\cos\vartheta_p\cos\phi_{3p},\\
r_6&=r\cos\vartheta_r\cos\phi_{3r}.
\end{aligned} \tag{3c}$$

Written in terms of the six-dimensional vectors the Schrödinger equation reads

$$[p^2/2m+V(\vec{r})]\psi(\vec{r})=E\psi(\vec{r}), \tag{4a}$$

where $\vec{p}=-i\hbar\vec{\nabla}_6$.

Using, then, the identity

$$p^2=p_r^2-5i\,p_r/r+K^2/r^2,$$

where we have defined

$$K^2=\frac{1}{2}\sum_{i,j=1}^{6}(r_ip_j-r_jp_i)^2$$

expressed in terms of the new $\vec{r}$'s and $\vec{p}$'s, and $p_r=\hat{r}\cdot\vec{p}$, we find that we can write the kinetic energy as the sum of a radial and an angular part. We have

$$\nabla_6^2=\nabla_r^2+\nabla_\theta^2/r^2, \tag{4b}$$

where $-\hbar^2\nabla_\theta^2=K^2$, $-\hbar^2\nabla_r^2=p_r^2-(5i/r)p_r$.

These can be given explicit representations. Using our spherical coordinate system we find

$$\begin{aligned}
\nabla_r^2&=\frac{1}{r^5}\frac{\partial}{\partial r}\left(r^5\frac{\partial}{\partial r}\right)=\frac{\partial^2}{\partial r^2}+\frac{5}{r}\frac{\partial}{\partial r},\\
\nabla_\theta^2&=\frac{1}{\sin^2\vartheta_r\cos^2\vartheta_r}\frac{\partial}{\partial\vartheta_r}\left(\sin^2\vartheta_r\cos^2\vartheta_r\frac{\partial}{\partial\vartheta_r}\right)\\
&\quad+\frac{1}{\cos^2\vartheta_r}\left[\frac{1}{\sin\phi_{3r}}\frac{\partial}{\partial\phi_{3r}}\left(\sin\phi_{3r}\frac{\partial}{\partial\phi_{3r}}\right)\right.\\
&\quad\left.+\frac{1}{\sin^2\phi_{3r}}\frac{\partial^2}{\partial\phi_{4r}^2}\right]+\frac{1}{\sin^2\vartheta_r}\left[\frac{1}{\sin\phi_{1r}}\frac{\partial}{\partial\phi_{1r}}\right.\\
&\quad\left.\times\left(\sin\phi_{1r}\frac{\partial}{\partial\phi_{1r}}\right)+\frac{1}{\sin^2\phi_{1r}}\frac{\partial^2}{\partial\phi_{2r}^2}\right].
\end{aligned} \tag{5}$$

The eigenfunctions of ∇_θ^2 are surface hyperspherical harmonic polynomials which satisfy

$$\nabla_\theta^2\mathcal{U}_K(\hat{r})=-K(K+4)\,\mathcal{U}_K(\hat{r}). \tag{6a}$$

It can be shown that K is an integer and at the same time the degree of the harmonic polynomial. These eigenfunctions are degenerate; in fact, for a given K we have $(K+3)!\,(K+2)/12K!$ of them. Included in the set of operators which removes this degeneracy we find the angular momentum and its projection over an axis such as z:

$$\vec{L}=\vec{r}_1\times\vec{p}_1+\vec{r}_2\times\vec{p}_2+\vec{r}_3\times\vec{p}_3,\quad M=\hat{z}\cdot\vec{L}.$$

Two other operators are necessary for a complete description of the system, but they are somewhat arbitrary and we shall not specify them here. The surface hyperspherical harmonics are then represented by

$$\mathcal{U}_{K\lambda}(\hat{r}). \tag{6b}$$

The vector $\hat{r}$ indicates a given direction in the six-dimensional space, and the index λ stands for the set of quantum numbers L, m, μ, ν. We identify L and m as the angular and the azimuthal quantum numbers.

For obvious reasons the surface harmonics are chosen to be orthonormal and will satisfy the completeness relations

$$\begin{aligned}
&\int\mathcal{U}^*_{K'\lambda'}(\hat{r})\,\mathcal{U}_{K\lambda}(\hat{r})\,d\Omega_{\hat{r}}=\delta_{K\lambda}^{K'\lambda'},\\
&\sum_{K\lambda}\mathcal{U}^*_{K\lambda}(\hat{r})\,\mathcal{U}_{K\lambda}(\hat{r}')=\delta(\hat{r}-\hat{r}').
\end{aligned} \tag{6c}$$

For the purposes of this paper we do not need to study in further detail these hyperspherical harmonics. As we will see, a great deal of our method is based on the use of very simple relations which suffice to outline the path to follow for the study of the first few quantum virial coefficients.

SCATTERING

We wish to represent three free particles in the center-of-mass coordinate system. In our six-dimensional space this is readily written as

$$\varphi=(2\pi)^{-3}e^{i\vec{k}\cdot\vec{r}}\,,\quad \hbar\vec{k}=\vec{p}\,.$$

We want to expand this in a series of surface hyperspherical harmonics. Using relations (4)–(6), we find that the radial part of the free-particle Schrödinger equation, associated with harmonics of degree K, reads

$$\left[\frac{\partial^2}{\partial r^2}+\frac{5}{r}\frac{\partial}{\partial r}-\frac{K(K+4)}{r^2}+k^2\right]u(k,r)=0 \tag{7}$$

and has as solutions Bessel functions of order $K+2$, divided by r^2. The general solution that is regular at $r=0$ can therefore be written as

$$\sum_{K\lambda}\tilde{A}_{K\lambda}\frac{J_{k+2}(kr)}{k^2r^2}\mathfrak{u}_{K\lambda}(\hat{r})\,.$$

Since a plane wave is a solution of the Schrödinger equation which is well behaved at the origin we expect that we can express it in this latter form. In Appendix A we show, using an addition theorem for the hyperspherical harmonics, that we can write the plane-wave expansion as

$$\frac{1}{(2\pi)^3}e^{i\vec{k}\cdot\vec{r}}=\sum_{K\lambda}A_{K\lambda}\frac{J_{K+2}(kr)}{k^2r^2}\mathfrak{u}^*_{K\lambda}(\hat{r})\mathfrak{u}_{K\lambda}(\hat{k})\,. \tag{8}$$

Using the orthonormality relations

$$\langle\vec{k}\,|\,\vec{q}\rangle=(2\pi)^{-6}\int d^3r\,e^{i(\vec{q}-\vec{k})\cdot\vec{r}}=\delta(k-q)\delta(\hat{k}-\hat{q})\,q^{-5}\,,$$

we readily obtain a condition for the constant $A_{K\lambda}$,

$$|A_{K\lambda}|^2=1\,. \tag{9}$$

Let us now introduce the Green's function which takes into account an "outgoing-wave" boundary condition for the scattering:

$$G^+(\vec{k};\vec{r})=\frac{2m}{\hbar^2}\int\frac{\exp[i(\vec{k}'_\xi\cdot\vec{\xi}+\vec{k}'_\eta\cdot\vec{\eta})]}{k^2+i\epsilon-k'^2_\xi-k'^2_\eta}\times k'^2_\xi\,k'^2_\eta\,dk'_\xi\,dk'_\eta\,\frac{d\Omega_{k'_\xi}}{(2\pi)^3}\,\frac{d\Omega_{k'_\eta}}{(2\pi)^3}\,.$$

Using the expression given by Eq. (8) for the ex-potentials we obtain a useful expansion

$$G^+(k;\vec{r}-\vec{r}\,')=\sum_{K\lambda}\left(\frac{2m}{\hbar^2}\right)\frac{G^+_K(k;r,r')}{r^2r'^2}\mathfrak{u}^*_{K\lambda}(\hat{r})\,\mathfrak{u}_{K\lambda}(\hat{r}')\,, \tag{10}$$

where

$$G^+_K(k;r,r')=\int_0^\infty\frac{J_{K+2}(k'r)J_{K+2}(k'r')}{k^2+i\epsilon-k'^2}\,k'\,dk'=-i\tfrac{1}{2}\pi J_{K+2}(kr_<)H^{(1)}_{K+2}(kr_>)\,.$$

The last expression for the radial part of the Green's function may be obtained using the general method outlined in Morse and Feshbach, or using the theory of Bessel functions.[19] Here we used the standard convention that $r_<$ ($r_>$) represent the smaller (larger) among r or r'.

The integral representation of the Schrödinger equation is then

$$\psi^+(\vec{k},\vec{r})=(2\pi)^{-3}e^{i\vec{k}\cdot\vec{r}}+\int d^6\vec{r}\,'\,G^+(\vec{k};\vec{r},\vec{r}\,')V(\vec{r}\,')\psi^+(\vec{k},\vec{r}\,')\,. \tag{11}$$

We can write the wave function as

$$\psi^+(\vec{k},\vec{r})=\sum_{K\lambda;K'\lambda'}\psi^{K'\lambda'}_{K\lambda}\mathfrak{u}^*_{K\lambda}(\hat{r})\mathfrak{u}_{K'\lambda'}(\hat{k})\,, \tag{12a}$$

where

$$\psi^{K'\lambda'}_{K\lambda}=\int\psi^+(\vec{k};\vec{r})\mathfrak{u}_{K\lambda}(\hat{r})\mathfrak{u}^*_{K'\lambda'}(\hat{k})\,d\Omega_{\hat{k}}\,d\Omega_{\hat{r}}\,. \tag{12b}$$

Equation (11) therefore implies that

$$\psi^{K'\lambda'}_{K\lambda}(k,r)=A_{K\lambda}\frac{J_{K+2}(kr)}{k^2r^2}\delta^{K'\lambda'}_{K\lambda}+\sum_{K''\lambda''}\int\frac{G^+_K(k;r,r')}{r^2r'^2}\times U^{K''\lambda''}_{K\lambda}(r')\psi^{K'\lambda'}_{K''\lambda''}(k,r')r'^5\,dr'\,, \tag{13}$$

where

$$U^{K''\lambda''}_{K\lambda}=(2m/\hbar^2)V^{K''\lambda''}_{K\lambda}(r)\,,$$
$$V^{K''\lambda''}_{K\lambda}(r)=\int\mathfrak{u}^*_{K''\lambda''}(\hat{r})\,V(\vec{r})\mathfrak{u}_{K\lambda}(\hat{r})\,d\Omega_{\hat{r}}\,. \tag{14}$$

If we apply ∇^2_6 to the terms of Eq. (13) we obtain a system of associated differential equations which we can write as

$$\left(\frac{d^2}{dr^2}+\frac{5}{r}\frac{d}{dr}-\frac{K(K+4)}{r^2}+k^2\right)\psi^{K'\lambda'}_{K\lambda}(k,r)=\sum_{K''\lambda''}U^{K''\lambda''}_{K\lambda}(r)\,\psi^{K'\lambda'}_{K''\lambda''}(k,r)\,, \tag{15}$$

or equivalently

$$\left(\frac{d^2}{dr^2}+\frac{1}{r}\frac{d}{dr}-\frac{(K+2)^2}{r^2}+k^2\right)\omega^{K'\lambda'}_{K\lambda}(k,r)=\sum_{K''\lambda''}U^{K''\lambda''}_{K\lambda}(r)\,\omega^{K'\lambda'}_{K''\lambda''}(k,r)\,, \tag{16}$$

where we have set

$$\omega^{K'\lambda'}_{K\lambda}(r)=(r^2k^2/A_{K\lambda})\,\psi^{K'\lambda'}_{K\lambda}\,.$$

Equations (15) and (16) represent the generalization of the radial equation of the two-body problem and, in a manner analogous to that development, we shall wish to solve them to obtain three-body phase shifts.

In order to study the scattering we must analyze the behavior of $\psi^{K'\lambda'}_{K\lambda}$ when $r\to\infty$. Using the asymptotic expansions

$$J_{K+2}(kr) \to (2/\pi kr)^{1/2} \cos(kr - \tfrac{1}{2}(K+2)\pi - \tfrac{1}{4}\pi),$$

$$H^{(1)}_{K+2}(kr) \to (2/\pi kr)^{1/2} \exp\{i\,[kr - \tfrac{1}{2}(K+2)\pi - \tfrac{1}{4}\pi]\},$$

we obtain

$$\begin{aligned}\psi^{K'\lambda'}_{K\lambda} = {} & \frac{1}{(kr)^{5/2}} A_{K\lambda} \exp\{-i[kr - \tfrac{1}{2}(K+2)\pi - \tfrac{1}{4}\pi]\}\, \delta^{K'\lambda'}_{K\lambda} \\ & + \frac{1}{(kr)^{5/2}} \frac{\exp\{i\,[kr - \tfrac{1}{2}(K+2)\pi - \tfrac{1}{4}\pi]\}}{(2\pi)^{1/2}} \\ & \times \left(\delta^{K'\lambda'}_{K\lambda} A_{K\lambda} + 2k^2 \frac{\pi}{2} \sum_{K''\lambda''} (-i) \int \frac{J_{K+2}(kr')}{r'^2} \right. \\ & \left. \times\, U^{K''\lambda''}_{K\lambda}(r')\, \psi^{K'\lambda'}_{K''\lambda''}(kr')\, r'^5\, dr' \right), \\ & \text{as } r \to \infty. \qquad (17)\end{aligned}$$

We wish to express this in terms of the scattering matrices T and S defined by[18]

$$\langle \vec{\mathrm{q}} |\, T\, | \vec{\mathrm{k}} \rangle = \langle \vec{\mathrm{q}} |\, V\, | \psi_{\vec{\mathrm{k}}} \rangle, \qquad (18a)$$

$$\langle \vec{\mathrm{q}} |\, S\, | \vec{\mathrm{k}} \rangle = \delta(\vec{\mathrm{q}} - \vec{\mathrm{k}}) - 2\pi i\, \delta(E_{\vec{\mathrm{q}}} - E_{\vec{\mathrm{k}}})\, \langle \vec{\mathrm{q}} |\, T\, | \vec{\mathrm{k}} \rangle\ . \qquad (18b)$$

Using Eqs. (8) and (12) we expand the first of the above equations to obtain

$$\langle \vec{\mathrm{q}} |\, T\, | \vec{\mathrm{k}} \rangle = \sum_{K\lambda;K'\lambda'} T^{K'\lambda'}_{K\lambda}(q,k)\, \mathcal{U}^*_{K\lambda}(\hat{q})\, \mathcal{U}_{K'\lambda'}(\hat{k}), \qquad (19)$$

where

$$\begin{aligned}T^{K'\lambda'}_{K\lambda}(q,k) = {} & \sum_{K''\lambda''} A^*_{K\lambda} \int \frac{J_{K+2}(qr)}{q^2 r^2} \\ & \times V^{K''\lambda''}_{K\lambda}(r)\, \psi^{K'\lambda'}_{K''\lambda''}(k,r)\, r^5\, dr\,.\end{aligned}$$

We see then that Eq. (17) can be written as

$$\begin{aligned}\psi^{K'\lambda'}_{K\lambda} = {} & (kr)^{-5/2} A_{K\lambda} \frac{\exp\{-i\,[kr - \tfrac{1}{2}(K+2)\pi - \tfrac{1}{4}\pi]\}}{(2\pi)^{1/2}} \\ & \times \delta^{K'\lambda'}_{K\lambda} + (kr)^{-5/2} A_{K\lambda} \frac{\exp\{i\,[kr - \tfrac{1}{2}(K+2)\pi - \tfrac{1}{4}\pi]\}}{(2\pi)^{1/2}} \\ & \times [\delta^{K'\lambda'}_{K\lambda} - (2\pi i k^4 m/\hbar^2)\, T^{K'\lambda'}_{K\lambda}(k,k)], \\ & \text{as } r \to \infty. \qquad (20)\end{aligned}$$

Furthermore, using for the definition of the density of states

$$q^5\, dq\, d\Omega_{\hat{q}} = \rho(E_q)\, dE_q\, d\Omega_{\hat{q}}\,,$$

we get $\rho(E_q) = mq^4/\hbar^2$.

Hence we find

$$\delta(\vec{\mathrm{k}} - \vec{\mathrm{q}}) = \frac{\delta(k-q)}{q^5}\, \delta(\hat{k} - \hat{q}) = \frac{\delta(E_k - E_q)}{\rho(E_q)}\, \delta(\hat{k} - \hat{q}).$$

Taking advantage of this we factor a δ function expressing the conservation of energy and write

$$\begin{aligned}\langle \vec{\mathrm{q}} |\, S\, | \vec{\mathrm{k}} \rangle = {} & \frac{\delta(E_q - E_k)}{\rho(E_q)} \\ & \times \sum_{K\lambda;K'\lambda'} S^{K'\lambda'}_{K\lambda}(q)\, \mathcal{U}^*_{K\lambda}(\hat{q})\, \mathcal{U}_{K'\lambda'}(\hat{k})\,. \qquad (21)\end{aligned}$$

From Eq. (18), (19), and (21), we then readily arrive at

$$S^{K'\lambda'}_{K\lambda}(q) = \delta^{K'\lambda'}_{K\lambda} - 2\pi i\, \rho(E_q)\, T^{K'\lambda'}_{K\lambda}(q). \qquad (22)$$

Finally, Eq. (20) reads, with the help of (19) and (21),

$$\begin{aligned}\psi^{K'\lambda'}_{K\lambda}(k,r) = {} & \frac{A_{K\lambda}}{(kr)^{5/2}} \frac{\exp\{-i\,[kr - \tfrac{1}{2}(K+2)\pi - \tfrac{1}{4}\pi]\}}{(2\pi)^{1/2}}\, \delta^{K'\lambda'}_{K\lambda} \\ & + \frac{A_{K\lambda}}{(kr)^{5/2}} \frac{\exp\{i[kr - \tfrac{1}{2}(K+2)\pi - \tfrac{1}{4}\pi]\}}{(2\pi)^{1/2}}\, S^{K'\lambda'}_{K\lambda}(k), \\ & \text{as } r \to \infty\,. \qquad (23)\end{aligned}$$

This is a fundamental equation which, if we wish, may be generalized to accommodate a larger number of particles.

We recall that the S matrix is unitary:

$$\sum_{K''\lambda''} S^{K''\lambda''}_{K\lambda}\, S^{\dagger K\lambda}_{K''\lambda''} = \sum_{K''\lambda''} S^{\dagger K''\lambda''}_{K\lambda}\, S^{K'\lambda'}_{K''\lambda''} = \delta^{K'\lambda'}_{K\lambda}\,.$$

Furthermore, if we make the assumption that the potential is symmetric,

$$V^{K'\lambda'}_{K\lambda} = V^{K\lambda}_{K'\lambda'}\,, \qquad (24)$$

we can show (see Appendix B) that the S matrix is also symmetric,

$$S^{K'\lambda'}_{K\lambda} = S^{K\lambda}_{K'\lambda'}\,. \qquad (25)$$

Actually we feel that the hypothesis that the potential is symmetric does not imply a restriction on the kind of interaction that we are interested in considering, i.e., time-reversal-invariant potentials.

THREE-BODY PHASE SHIFTS

Since the S matrix is symmetric and also unitary we can diagonalize it by an orthogonal matrix, say U.[20]

If S^α_α are the resulting diagonal elements, i.e.,

$$S^\alpha_\alpha = e^{2i\delta_\alpha}\,, \qquad (26)$$

where δ_α is a real function which we may call the three-body eigenphase shift, then when S is not diagonal, we can write an arbitrary matrix element as

$$S^{K'\lambda'}_{K\lambda} = \textstyle\sum_\alpha U^\alpha_{K\lambda}\, e^{2i\delta_\alpha}\, U^{T\,(K'\lambda')}_\alpha\,, \qquad (27a)$$

$$\text{where} \quad \sum_{K'\lambda'} U^{K'\lambda'}_\alpha\, U^{T\beta}_{K'\lambda'} = \delta^\beta_\alpha\,. \qquad (27b)$$

The T matrix can be obtained from (22) and (27) and since S is symmetric $T(k) = T(k,k)$ is also. In its diagonal representation the diagonal matrix elements are

$$T^\alpha_\alpha = -(\hbar^2/\pi m k^4)\, e^{i\delta_\alpha} \sin\delta_\alpha\,. \qquad (28)$$

In order to discuss or calculate the phase shifts, it is often convenient to work with real quantities rather than complex ones. This is done by introducing the reaction matrix R,[18] defined by

$$\langle \vec{\mathrm{q}} |\, R\, | \vec{\mathrm{p}} \rangle = \langle \vec{\mathrm{q}} |\, V\, | \psi_{\vec{\mathrm{p}}} \rangle\,, \qquad (29a)$$

where $\psi_{\vec{p}}$ denotes a standing-wave function. R is then related to a Green's function by

$$R = V + VG(E)R\,, \tag{29b}$$

but now G is a standing-wave Green's function:

$$\begin{aligned}\langle \vec{r}\,|\,G(E)\,|\,\vec{r}\,'\rangle &= \frac{2m}{\hbar^2}\,\mathcal{P}\int \frac{\exp\{i\,[\vec{k}'_\xi\cdot(\vec{\xi}-\vec{\xi}\,')+\vec{k}_\eta\cdot(\vec{\eta}-\vec{\eta})]\}}{k^2-k_\xi'^2-k_\eta'^2}\\ &\quad\times k_\xi'^2\,k_\eta'^2\,dk'_\xi\,dk'_\eta\,\frac{d\Omega_{k'_\xi}}{(2\pi)^3}\frac{d\Omega_{k'_\eta}}{(2\pi)^3}\\ &= \tfrac{1}{2}\pi\,J_{K+2}(r<)N_{K+2}(r>)\,.\end{aligned}$$

The general relation between the T matrix and the R matrix[18] is

$$T(E) = R(E) - i\pi R(E)\,\delta(E-K)\,T(E),$$

where here K stands for the kinetic energy. It follows that in our formalism

$$\begin{aligned}T_{K\lambda}^{K'\lambda'}(q,k) &= R_{K\lambda}^{K'\lambda'}(q,k) - i\pi\rho(E_k)\\ &\quad\times\sum_{K''\lambda''} R_{K\lambda}^{K''\lambda''}(q,k)\,T_{K''\lambda''}^{K'\lambda'}(k,k)\,.\end{aligned}\tag{30}$$

In an analogous way to what we have done for the T matrix we obtain the following relations:

$$\begin{aligned}\psi_{K\lambda}^{K'\lambda'} &= A_{K\lambda}\frac{J_{K+2}}{(kr)^2}\,\delta_{K\lambda}^{K'\lambda'} + \sum_{K''\lambda''}\int\frac{G_K(k,r,r')}{r^2r'^2}\\ &\quad\times U_{K\lambda}^{K''\lambda''}(r')\,\psi_{K''\lambda''}^{K'\lambda'}(kr')\,r'^5\,dr'\,,\\ R_{K\lambda}^{K'\lambda'}(q,k) &= \sum_{K''\lambda''} A^*_{K\lambda}\int\frac{J_{K+2}(qr)}{q^2r^2}\,V_{K\lambda}^{K''\lambda''}(r)\\ &\quad\times\psi_{K''\lambda''}^{K'\lambda'}(kr)\,r^5\,dr\,.\end{aligned}\tag{31}$$

We also have

$$R_{K\lambda}^{K'\lambda'}(k) = -\sum_\alpha U_{K\lambda}^\alpha\,\frac{\tan\delta_\alpha}{\pi mk^4/\hbar^2}\,U_\alpha^{T\,K'\lambda'}\,. \tag{32}$$

This last relation may be obtained using (28) and (30).

The asymptotic behavior for the wave function is then

$$\begin{aligned}\psi_{K\lambda}^{K'\lambda'} &\rightarrow 2A_{K\lambda}/(kr)^{5/2}(2\pi)^{1/2}\\ &\quad\times\cos[kr-\tfrac{1}{2}(K+2)\pi-\tfrac{1}{4}\pi]\,\delta_{K\lambda}^{K'\lambda'}\\ &\quad+(\pi mk^4/\hbar^2)\sin[kr-\tfrac{1}{2}(K+2)\pi-\tfrac{1}{4}\pi]\,R_{K\lambda}^{K'\lambda'}\};\end{aligned}\tag{33a}$$

hence,

$$\begin{aligned}\psi_{K\lambda}^{K'\lambda'} &\rightarrow \frac{2A_{K\lambda}}{(kr)^{5/2}(2\pi)^{1/2}}\sum_\alpha U_{K\lambda}^\alpha\\ &\quad\times\frac{\cos[kr-\frac{1}{2}(K+2)\pi-\frac{1}{4}\pi+\delta_\alpha]}{\cos\delta_\alpha}\,U_\alpha^{T\,K'\lambda'}\,.\end{aligned}\tag{33b}$$

We can see that the linear combination

$$\phi_{K\lambda}^\alpha = \frac{(kr)^{5/2}}{A_{K\lambda}}\left(\frac{\pi}{2}\right)^{1/2}\sum_{K'\lambda'}\psi_{K\lambda}^{K'\lambda'}\,U_{K'\lambda'}^\alpha \tag{34a}$$

has the asymptotic behavior

$$\phi_{K\lambda}^\alpha \rightarrow (U_{K\lambda}^\alpha/\cos\delta_\alpha)\cos[kr-\tfrac{1}{2}(K+2)\pi-\tfrac{1}{4}\pi+\delta_\alpha]\,. \tag{34b}$$

That is to say, these solutions are characterized by the fact that for a given α, the wave functions having different indices K, λ have the same phase shifts. We will refer to each set as a scattering eigensolution of the problem and represent it as a column vector having as components the $\phi_{K\lambda}^\alpha$ with different K, λ, i.e.,

$$\phi^\alpha(kr) = \begin{bmatrix}\phi_{K_0\lambda_0}^\alpha\\ \phi_{K_1\lambda_1}^\alpha\\ \vdots\\ \phi_{K\lambda}^\alpha\\ \vdots\end{bmatrix}\,. \tag{34c}$$

It can be shown that the usual orthogonality properties for the scattering eigensolutions hold. In order to clarify the role of the index α and its relationship with the set K, λ we study the limit of ϕ^α as the potential V goes to zero. We do this in two steps. We first make the nondiagonal terms go to zero, i.e.,

$$V_{K'\lambda'}^{K\lambda} \rightarrow V_{K\lambda}^{K\lambda}\,\delta_{K'\lambda'}^{K\lambda}\,, \tag{35}$$

and then consider $V_{K\lambda}^{K\lambda}$ infinitesimal. In this limit, using Eqs. (31) and (35), we calculate the R matrix in the Born approximation

$$R_{K\lambda}^{K'\lambda'} = \delta_{K\lambda}^{K'\lambda'}\,k^{-4}\int_0^\infty J_{K+2}(kr)\,V_{K\lambda}^{K\lambda}\,J_{K+2}(kr)\,r\,dr\,. \tag{36}$$

We observe that for an infinitesimal interaction the first Born approximation is essentially exact.

When the matrix R is diagonal, Eqs. (27b) and (32) enable us to define a way to correlate the index α with K, λ. Since R is diagonal,

$$R_{K\lambda}^{K\lambda} = -\hbar^2\tan\delta_\alpha/\pi mk^4\,,$$

then U is also diagonal, and in fact simply

$$U_\alpha^{K\lambda} = \delta_\alpha^{K\lambda}\,, \tag{37}$$

and this in turn implies that any scattering eigensolution has only one component different from zero and we shall refer to the eigensolution by this index $K\lambda$.

In the limit when V goes to zero we clearly have

$$\phi^{K\lambda}(k,r)\to\phi^{0K\lambda}=\begin{bmatrix}0\\0\\ \vdots\\ \phi^{K\lambda}_{K\lambda}=\left(\dfrac{\pi}{2}\right)^{1/2}\dfrac{(kr)^{5/2}}{A_{K\lambda}}\;J_{K+2}(kr)\\ \vdots\\0\\0\end{bmatrix}.$$

As we turn on the interaction other components of the eigensolution vector become different from zero. However, we can expect (and we shall see this in an actual example later in this paper) that there will be regimes for which these new components are small compared to the dominant component associated with the index K.

In any case, and quite generally, given an expression for ψ (or some analytical numerical approximation for it) we can evaluate the left-hand side of Eq. (32) by using (31). Equation (32) with (27b) then clearly represent a system of algebraic equations to be solved for the eigenphase shifts and for the matrix elements of U. If we assume that the number of components which are effectively coupled is equal to N, then due to the symmetry of R we have $(N^2+N)/2$ algebraic equations from (32) and the same number from (27b). The number of equations and of unknowns, i.e., N phase shifts and N^2 matrix elements for U, are then the same and the system should have a solution provided $\det|R|\neq 0$.

THIRD CLUSTER AND THREE-BODY SHIFTS

We recall that the third virial coefficient can be expressed in terms of the coefficients b_1, b_2, and b_3 which appear in the expansion of the pressure and the number density in powers of the fugacity. If we write

$$p/kT=\textstyle\sum_1^\infty b_l z^l\,,\quad N/V=\sum_1^\infty l\,b_l z^l\,, \tag{38}$$

then by elimination of the fugacity z we obtain

$$\begin{aligned}B&=-N\,b_2/b_1^2\,,\\ C&=N^2(4b_2^2/b_1^4-2b_3/b_1^3)=4B^2-2N^2b_3/b_1^3\,.\end{aligned} \tag{39}$$

N is, of course, the number of particles in a box of volume V and here k is Boltzmann's constant. The fugacity coefficients b_l become volume independent in the limit of large volume. To evaluate them we proceed in two ways, related in that they represent two approaches to the calculation of Thiele semi-invariants. In our first procedure we express the b_l's as l particle-cluster integrals

$$b_l^{\pm}(V)=(1/l!\,V)\textstyle\sum_\mu\int d^{3l}r$$
$$\times\langle\vec{r}_1\mu_1\vec{r}_2\mu_2\cdots\vec{r}_l\mu_l\,|\,U_l^{\pm}\,|\vec{r}_1\mu_1\cdots\vec{r}_l\mu_l\rangle\,, \tag{40}$$

where μ_i is the z component of the spin coordinate of the ith particle, $\vec{r}_i$ is its space coordinates. The integrands are the generalized Ursell functions devised by Lee and Yang.[21] The volume V is taken to be large and, in fact, we intend later in our discussion to let it go to infinity.

The N-particle Ursell functions $U_N^{\pm}$, appropriate to symmetric (+) or antisymmetric statistics, are in turn related to the matrix elements of the N-body operators $W_N=\exp(-\beta H_N)$ where $\beta=1/kT$ and H_N is the Hamiltonian. We also label these matrix elements by a plus or minus to indicate that the basic states, with respect to which we evaluate these matrix elements, are symmetrized or antisymmetrized, i.e., these states are

$$|\vec{1}\,\vec{2}\,\vec{3}\cdots\vec{N}\rangle^{\pm}=(\vec{N}!)^{-1/2}\textstyle\sum_{\mathcal{P}}(\pm)^{\mathcal{P}}\,|\,\mathcal{P}(\vec{1},\vec{2},\cdots,\vec{N})\rangle\,, \tag{41}$$

where we sum over all permutations and have let $1\cdots N$ refer to the coordinates and spin. For the cases $l=1$, $l=2$, and $l=3$ we have the relations

$$\begin{aligned}\langle\vec{1}'\,|\,U_1^{\pm}\,|\,\vec{1}\rangle&=\langle\vec{1}'\,|\,W_1^{\pm}\,|\,\vec{1}\rangle\,,\\ \langle\vec{1}',\vec{2}'\,|\,U_2^{\pm}\,|\,\vec{1},\vec{2}\rangle&=\langle\vec{1}'\vec{2}'\,|\,W_2^{\pm}|\vec{1},\vec{2}\rangle\\ &\quad-\langle\vec{1}'\,|\,W_1^{\pm}\,|\,\vec{1}\rangle\langle\vec{2}'\,|\,W_1^{\pm}|\,\vec{2}\rangle\,,\\ \langle\vec{1}'\vec{2}'\vec{3}'\,|\,U_3^{\pm}\,|\,\vec{1}\,\vec{2}\,\vec{3}\rangle&=\langle 1'\,2'\,3'\,|\,W_3^{\pm}\,|\,1\,2\,3\rangle\\ &\quad-\langle\vec{1}'\,\vec{2}'\,|\,W_2^{\pm}\,|\,\vec{1}\,\vec{2}\rangle\langle\vec{3}'\,|\,W_1^{\pm}\,|\,\vec{3}\rangle\\ &\quad-\langle\vec{2}'\,\vec{3}'\,|\,W_2^{\pm}\,|\,\vec{2}\,\vec{3}\rangle\langle\vec{1}'\,|\,W_1^{\pm}\,|\,\vec{1}\rangle\\ &\quad-\langle\vec{3}'\,\vec{1}'\,|\,W_2^{\pm}\,|\,\vec{3}\,\vec{1}\rangle\langle\vec{2}'\,|\,W_1^{\pm}\,|\,2\rangle\\ &\quad+2\langle\vec{1}'\,|\,W_1^{\pm}\,|\,\vec{1}\rangle\langle\vec{2}'\,|\,W_1^{\pm}\,|\,\vec{2}\rangle\langle\vec{3}'\,|\,W_1^{\pm}\,|\,\vec{3}\rangle\,.\end{aligned} \tag{42}$$

To express the Ursell functions in terms of nonsymmetrized Boltzmann matrix elements it is convenient to use a result due to Feynman:

$$\begin{aligned}\langle\vec{1}'\cdots\vec{N}'\,|\,W_N^{\pm}\,|\,\vec{1}\cdots\vec{N}\rangle\\ =\textstyle\sum_{\mathcal{P}}(\pm)^{\mathcal{P}}\langle\mathcal{P}(\vec{1}'\cdots\vec{N}')|\,W_N\,|\,\vec{1}\cdots\vec{N}\rangle\,.\end{aligned} \tag{43}$$

Since we assume a spin-independent Hamiltonian we can sum over the spins and then, separating the results into the Boltzmann contribution and that due to exchange (to the non-Boltzmann statistics), we readily obtain after some rearrangement the following expressions for b_1 and b_3 which we require:

$$b_1=(2s+1)/\lambda_T^3\,,\quad b_3=b_3^{\mathrm{Boltz}}+b_3^{\mathrm{exch}}\,, \tag{44}$$

where

$$b_3^{\mathrm{Boltz}} = \frac{(2s+1)^3}{3!\,V} \int d\vec{r}_1\, d\vec{r}_2\, d\vec{r}_3 \times \{\langle \vec{r}_1 \vec{r}_2 \vec{r}_3 | e^{-\beta H_3} - e^{-\beta T_3} | \vec{r}_1 \vec{r}_2 \vec{r}_3 \rangle - 3 \langle \vec{r}_1 \vec{r}_2 | e^{-\beta H_2} - e^{-\beta T_2} | \vec{r}_1 \vec{r}_2 \rangle \langle \vec{r}_3 | e^{-\beta T_1} | \tilde{r}_3 \rangle\} \tag{45}$$

and

$$b_3^{\mathrm{exch}} = \frac{2s+1}{3V} \int d\vec{r}_1\, d\vec{r}_2\, d\vec{r}_3 \times \langle \vec{r}_2 \vec{r}_3 \vec{r}_1 | e^{-\beta H_3} | \vec{r}_1 \vec{r}_2 \vec{r}_3 \rangle + \langle \vec{r}_3 \vec{r}_1 \vec{r}_2 | e^{-\beta H_3} | \vec{r}_1 \vec{r}_2 \vec{r}_3 \rangle \pm \frac{(2s+1)^2}{2!\,V} \int d\vec{r}_1\, d\vec{r}_2\, d\vec{r}_3 \langle \vec{r}_2 \vec{r}_1 \vec{r}_3 | e^{-\beta H_3} - e^{-\beta(H_2+T_1)} | \vec{r}_1 \vec{r}_2 \vec{r}_3 \rangle\,. \tag{46}$$

The upper sign holds for bosons and the lower one for fermions. The spin is denoted by s, and λ_T is the thermal wavelength, equal to $h/(2\pi mkT)^{1/2}$.

Let us now concentrate on the Boltzmann part of b_3. For very large volume we can, with negligible error, separate and evaluate the contribution of the center of mass. Using the set of canonical variables previously defined we obtain

$$b_3^{\mathrm{Boltz}} = [(2S+1)^3/3!](3^{3/2}/\lambda_T^3) \times \int d\vec{\xi}\, d\vec{\eta}\, \{\langle \vec{\xi} \vec{\eta} | e^{-\beta H_{\mathrm{rel}}(123)} - e^{-\beta T_{\mathrm{rel}}(123)} | \vec{\xi} \vec{\eta} \rangle \times - 3 \langle \vec{\xi} \vec{\eta} | e^{-\beta H_{\mathrm{rel}}(123)} - e^{-\beta T_{\mathrm{rel}}(123)} | \vec{\xi} \vec{\eta} \rangle\}, \tag{47}$$

where

$$H_{\mathrm{rel}}(123) = (p_\xi^2/2m) + (p_\eta^2/2m) + V_{12}(\vec{\xi}, \vec{\eta}) + V_{13}(\vec{\xi}, \vec{\eta}) + V_{23}(\vec{\xi}, \vec{\eta}),$$

$$H_{\mathrm{rel}}(12/3) = (p_\xi^2/2m) + (p_\eta^2/2m) + V_{12}(\vec{\xi}, \vec{\eta}),$$

$$T_{\mathrm{rel}}(123) = (p_\xi^2/2m) + (p_\eta^2/2m).$$

A term $V_{123}(\vec{\xi}, \vec{\eta})$ could, if we wished, be added to $H_{\mathrm{rel}}(123)$. This expression for b_3^{Boltz} can now be rewritten as

$$b_3^{\mathrm{Boltz}} = (2S+1)^3 (3^{1/2}/2) \lambda_T^{-3} \sum_{k, K, \lambda} \{(e^{-\beta \epsilon_{kK\lambda}^{123}} - e^{-\beta \epsilon_{kK\lambda}^{0}}) - 3(e^{-\beta \epsilon_{kK\lambda}^{12/3}} - e^{-\beta \epsilon_{kK\lambda}^{0}})\}, \tag{48}$$

where $\epsilon_{kK\lambda}^{123}$, $\epsilon_{kK\lambda}^{12/3}$, $\epsilon_{kK\lambda}^{0}$ are the eigenvalues of $H_{\mathrm{rel}}(123)$, $H_{\mathrm{rel}}(12/3)$, and $T_{\mathrm{rel}}(123)$.

We now argue in a way patterned after the discussion of the second virial coefficient by Uhlenbeck and Beth. As we make the volume of the box very large these eigenvalues become very dense and essentially span all positive energies. We are then able to replace the sums by integrals:

$$\sum_n e^{-\beta E_n} \to \int dk \left(\frac{dn}{dk}\right) \exp\left(-\frac{\hbar}{2m} \beta k^2\right). \tag{49}$$

The density of states dn/dk is then different for the system with or without interaction and we determine this difference. We chose the relative volume to be a spherical box of radius R_0 much larger than any length involved in the problem. The wave function must vanish at the wall of the box and this implies for a component K' of the eigenfunction $\phi^{K\lambda}$ the relations

$$k R_0 + \tfrac{1}{2}(K'+2)\pi - \tfrac{1}{4}\pi + \delta_{K\lambda} = \tfrac{1}{2}(2n+1)\pi\,, \qquad k R_0 + \tfrac{1}{2}(K'+2)\pi - \tfrac{1}{4}\pi = \tfrac{1}{2}(2n+1)\pi, \quad n = 0, 1, 2, \ldots \tag{50}$$

for the case with and without interaction. In the limit of infinite volume we then obtain for the difference between the density of states of a system with and without interaction,

$$\left(\frac{dn}{dk}\right)_{K\lambda} - \left(\frac{dn}{dk}\right)_{K\lambda}^{0} = \frac{1}{\pi} \frac{d}{dk} \delta_{K\lambda}. \tag{51}$$

Our formula for b_3^{Boltz} then becomes

$$(2S+1)^3 (3^{1/2}/2) \lambda_T^{-3} \frac{1}{\pi} \int_0^\infty dk \sum_{K\lambda} \frac{d}{dk} \times (\delta_{K\lambda}^{(123)} - 3\delta_{K\lambda}^{(12/3)}) \exp\left(-\frac{\hbar^2}{2m} \beta k^2\right), \tag{52}$$

where we sum over all possible values of the quantum numbers $K\lambda$.

Another way of establishing a phase-shift formula is to follow the point of view of Watson (for the second virial coefficient). For a finite but large spherical box of radius R_0 we calculate the shift in the eigenvalues of the energy caused by the presence of the interaction. These changes are reflected in slight shifts in the eigenwave vectors. We have for the K' component of the solution

$$k R_0 + \tfrac{1}{2}(K'+2)\pi - \tfrac{1}{4}\pi + \delta_{K\lambda} = \tfrac{1}{2}(2n+1)\pi,$$

$$k_0 R_0 + \tfrac{1}{2}(K'+2)\pi - \tfrac{1}{4}\pi = \tfrac{1}{2}(2n+1)\pi, \quad n = 0, 1, 2, \ldots .$$

Keeping terms to first order in $1/R_0$ it follows that

$$\delta k = k - k_0 = -\delta_{K\lambda}/R_0$$

and

$$\delta\epsilon_{k, K\lambda} = \frac{\hbar^2}{2m}(k^2 - k_0^2) = \frac{\hbar^2 k}{m} \delta k = -\frac{\hbar^2}{m R_0} k \delta_{K\lambda}. \tag{53}$$

Possible slight differences in R_0 for different components would only manifest themselves in higher order of R_0^{-1}. We now observe that

$$e^{-\beta \epsilon_{K\lambda}^{123}} \sim e^{-\beta \epsilon_{K\lambda}^{0}} \left(1 + \frac{\hbar^2}{m} \beta \frac{k_0}{R_0} \delta_{K\lambda}^{(123)} + \cdots\right); \tag{54}$$

letting $\dfrac{dn_{K\lambda}}{dk} = \dfrac{R_0}{\pi}$,

we can write

$$b_3^{\mathrm{Boltz}} = (2S+1)^3 \frac{\sqrt{3}}{(2\pi)^2} \frac{1}{\lambda_T}$$

$$\times \sum_{K\lambda} \int_0^\infty [\delta_{K\lambda}^{(123)}(k) - 3\delta_{K\lambda}^{(12/3)}(k)]$$

$$\times \exp \; -\frac{\hbar^2}{2m}\beta k^2 \;\; k dk , \qquad (55)$$

which in the case of no-bound states, which we have assumed, is related to our previous formula by a simple partial integration.

The two formulas for b_3 represent one of the most important results of this paper; to show the difficulty in extending it to non-Boltzmann statistics as well as to clarify some of the features and assumptions of the present derivation we back up a bit and then proceed from a somewhat different tack than we have so far. Instead of relying on the Ursell expansion let us simply take the logarithm of the grand partition function.[22] If

$$\Xi = 1 + z \,\mathrm{Tr} e^{-\beta T_1} + z^2 \,\mathrm{Tr} e^{-\beta H_2} + z^3 \,\mathrm{Tr} e^{-\beta H_3} + \cdots , \qquad (56)$$

then

$$\begin{aligned} \ln\Xi &= V \sum b_l z^l \\ &= z \,\mathrm{Tr} e^{-\beta T_1} + z^2[\mathrm{Tr} e^{-\beta H_2} - \tfrac{1}{2}(\mathrm{Tr} e^{-\beta T_1})^2] \\ &\quad + z^3[\mathrm{Tr} e^{-\beta H_3} - \mathrm{Tr} e^{-\beta T_1} \,\mathrm{Tr} e^{-\beta H_2} \\ &\quad + \tfrac{1}{3}(\mathrm{Tr} e^{-\beta T_1})^3] + \cdots . \end{aligned} \qquad (57)$$

Using then relations such as

$$\mathrm{Tr} e^{-\beta H_3} = (1/3!)\,\mathrm{Tr}^B e^{-\beta H_3} + (1/3!) \int d\vec{1}\, d\vec{2}\, d\vec{3}$$

$$\times \sum_{\mathcal{P} \neq I} (\pm)^{\mathcal{P}} \langle \mathcal{P}(\vec{1}\,\vec{2}\,\vec{3}) | e^{-\beta H_3} | \vec{1}\,\vec{2}\,\vec{3} \rangle , \qquad (58)$$

where we denote with a B traces which involve all states irrespective of symmetry and where the matrix element, above, is taken with unsymmetrized basic states. We can separate the traces into a Boltzmann part and an exchange part. We obtain for the Boltzmann contribution of each cluster,

$$\begin{aligned} b_1 &= (1/\lambda_T^3)(2S+1), \\ b_2^{\mathrm{Boltz}} &= \frac{1}{V}\frac{1}{2!}[\mathrm{Tr}^B e^{-\beta H_2} - (\mathrm{Tr}^B e^{-\beta T_1})^2], \\ b_3^{\mathrm{Boltz}} &= (1/V)(1/3!)[\mathrm{Tr}^B e^{-\beta H_3} - 3\,\mathrm{Tr}^B e^{-\beta T_1} \\ &\quad \times \mathrm{Tr}^B e^{-\beta H_2} + 2(\mathrm{Tr}^B e^{-\beta T_1})^3]. \end{aligned} \qquad (59)$$

As we know from the Ursell development the b_l's are volume independent (in the limit of large volume) but the individual traces appearing in the expression above are not, i.e., the trace $\mathrm{Tr} e^{-\beta H_3} \to O(V^3)$, the trace $\mathrm{Tr} e^{-\beta H_2} \to O(V^2)$, etc. It is then very important to regroup these terms into quantities which can be calculated but which have lower volume dependence. Thus we write

$$\begin{aligned} b_3^{\mathrm{Boltz}} &= (1/V)(1/3!)[\mathrm{Tr}(e^{-\beta H_3} - e^{-\beta T_3}) \\ &\quad - 3\,\mathrm{Tr} e^{-\beta T_1}\,\mathrm{Tr}(e^{-\beta H_2} - e^{-\beta T_2})]. \end{aligned} \qquad (60)$$

The possibility of writing

$$(\mathrm{Tr} e^{-\beta T_1})^3 = \mathrm{Tr} e^{-\beta T_3}$$

only holds for Boltzmann statistics. Now

$$(1/V)\,\mathrm{Tr}(e^{-\beta H_3} - e^{-\beta T_3})$$

and $(3/V)\,\mathrm{Tr} e^{-\beta T_1}\,\mathrm{Tr}(e^{-\beta H_2} - e^{-\beta T_2})$

both still go as the volume, thus preventing us from usefully writing a neat formula in terms of three- and two-body phase shifts. We find that we must write our answer as the trace of a three-body operator, which we do,

$$\begin{aligned} b_3^{\mathrm{Boltz}} &= (1/3!V)\,\mathrm{Tr}^B[(e^{-\beta H_3} - e^{-\beta T_3}) \\ &\quad - 3(e^{-\beta(H_2 + T_1)} - e^{-\beta T_3})], \end{aligned} \qquad (61)$$

and this, as we have seen, can be written as an integral involving phase-shift sums or their derivative. We should emphasize that in the phase-shift expression

$$\sum (\delta_{K\lambda}^{(123)} - 3\delta_{K\lambda}^{(12/3)}),$$

the phase shifts (or partial sums of phase shifts) must be subtracted before the sums are performed since each separate sum $\sum \delta_{K\lambda}^{(123)}$ and $\sum_{K\lambda}^{(12/3)}$ is divergent in the limit of infinite volume.

The difficulty in extending our results to non-Boltzmann statistics stems from the fact that the product of one- and two-body traces involves far fewer permutations than three-body traces (if we express them as we have done earlier as integrals involving basic states and their permutations), and we have yet not succeeded in writing a useful phase-shift expression for the exchange. We hope that a detailed examination of the properties of the hyperspherical harmonics, which we chose to form a representation of the permutation group as well as the rotation group, will help us to do this.

LOW-TEMPERATURE BEHAVIOR

In the preceding sections we have set up a formalism which allows us to calculate the Boltzmann part of the third virial coefficient at arbitrary temperatures. To summarize the required procedure: We have to evaluate hyperspherical harmonics and the coupling matrix elements for our chosen potential. We must then solve, in general numerically, the set of differential equations (16) or a truncated set for possibly unnormalized solutions which then yield the desired phase shifts. Finally, we use these phase shifts in integrals which involve a Boltzmann factor. We evaluate formulas for the cluster b_3 or an equation such as

$$C_{\mathrm{Boltz}} = 4B_{\mathrm{Boltz}}^2 - N^2 \frac{\sqrt{3}}{\pi} \lambda_T^6 \int_0^\infty dk\, e^{-\lambda_T^2 (k^2/4\pi)}$$

$$\times \frac{d}{dk} \sum_{K\lambda} (\delta_{K\lambda}^{(123)} - 3\delta_{K\lambda}^{(12/3)}). \qquad (62)$$

Two very important features of such a calculation must be emphasized, both of which mirror the situation which holds for the second virial coefficient. First, for any given T, the presence of the Boltzmann factor in the equation above acts as a cutoff on the energy or wave-number range for which one must calculate phase shifts in order to evaluate the contribution of the cluster to a prescribed accuracy.

Second, for any wave number k for which we are interested we find that the bulk of the contribution comes from the consideration of polynomials of order extending roughly up to kR, where R is a length which describes the extent of the three-body cluster. The argument is an adaptation of that used by Badalyan and Simonov for the bound-state problem. To describe a change of the wave function over an angle θ_{eff} requires K's such that $K\theta_{\text{eff}} \sim 1$. The effective angular parameter θ_{eff} is then determined by the ratio of the distance over which the wave function changes significantly, $1/k$, to the radial distance in six-dimensional space

$$r = \frac{1}{3}\left(\sum_{i<j}^{3} r_{ij}^2\right)^{1/2},$$

which is of the order of the three-dimensional extension R, and the estimate follows. From another point of view, as shown by Smith,[23] K^2 measures how closely three bodies simultaneously approach each other. One finds classically that if R is a three-body impact parameter describing with a value of the parameter r the distance of closest approach, then again $K = kR$, which implies the result we need.

A key point in the application of the above analysis to our situation is that thanks to our being interested in the contribution of the partial waves to a three-body cluster we also have this finite distance R. The cluster is so constructed as to contribute only when the particles are involved in a genuine three-body event.

Even with these simplifications the calculation of the third virial up to temperatures of a few degrees Kelvin is clearly nontrivial and still lies ahead of us. In the limit of very low temperatures, however, we see from our discussion that we only need to know the behavior of the phase shifts at very low energies and for small K. This behavior can be determined analytically for a model such as a square well and we show the details of such a calculation in Appendices C and D.

By specifically using a square well we are able to draw upon explicit calculations of the angular matrix elements of the potential for $L = 0$ (total angular momentum) by Badalyan and Simonov and this is, or course, very useful! The results, however, are not narrowly restricted to the square well as it turns out that for any finite short-ranged intermolecular potential the matrix elements behave as $1/r^3$ for large distance r, and the low-energy behavior of the phase shifts reflects the shape of this tail. Thus, consideration of another potential would simply change the numerical coefficients of our answer.

We do make approximations. The most serious of these is that we only evaluate phase shifts corresponding to the total angular momentum of zero. This does, however, include $K = 0$; it also enables us to study the convergence of the phase-shift contribution for higher K (albeit for only one angular momentum), and the approximation only affects a numerical coefficient of the phase shifts. This is also true of another approximation which we make and which states that the phase shifts are given by the diagonal elements of the R matrix instead of by the elements of the diagonalized matrix. In both cases the leading wave-number dependence of the phase shifts is not affected and therefore the approximations do not affect the limiting temperature dependence of the third cluster.

A consequence of the $1/r^3$ tail of the coupling matrix elements is that there does not exist a scattering-length effective-range approximation for the low-energy behavior of the phase shifts.[24] The Born approximation does however apply and we have calculated the R matrix and the phase shifts in first and second Born. The contribution of the first Born vanishes identically because of the subtraction between $\delta^{(123)}$ and $-3\delta^{(12/3)}$. The second Born gives us to leading order in k,

$$\delta^{(123)}\,,\quad \delta^{(12/3)} \to O(k^2),$$

and inserting this in our formula for b_3 we obtain

$$b_3^{\text{Boltz}} = A(2mV_0/\hbar^2)^2(a^6/\lambda_T^5)(2S+1)^3, \tag{63}$$

where a is the range, V is the depth of the potential, and A is a constant which we evaluate in Appendix D.

The results of Pais and Uhlenbeck[6] for hard spheres, using the binary-collision expansion, reveal the same limiting temperature dependence for the third cluster. Since our results hold for a repulsive potential as well as for an attractive one, and since at the lowest thermal energies a finite repulsive well is very much like a hard core, this common temperature dependence is satisfactory.

The third virial is then

$$C_{\text{Boltz}} = 4B_{\text{Boltz}}^2 - 2N^2 b_3/b_1^3 = 4(-N^2\lambda_T^2\alpha)^2 - 2N^2\lambda_T^4[A(2mV_0/\hbar^2)^2 a^6], \tag{64}$$

since in the absence of bound states, at very low temperatures, we can write a scattering-length expression for B. The scattering length α is defined by $\delta^{(12)} \to k\alpha$ for small k. We thus find that unless there is an exact cancellation of this term the limiting behavior for C_{Boltz} is

$$C_{\text{Boltz}} \to 1/T^2 \tag{65}$$

at very low temperatures.

CONCLUSION

The methods that we have presented for the third virial can be generalized to apply to more numerous particles. For the four- or higher-body problems we can define new canonical variables, generate higher-order hyperspherical harmonics, and develop a scattering formalism. We can obtain phase shifts and in a straightforward extension of our present work, use them to evaluate Boltzmann clusters. Thus, at least from a conceptual point of view, the way to the calculation of an arbitrary virial coefficient is open to us!

Two restrictions remain. We have no phase-shift expressions for the exchange part of the clusters, and we have not allowed bound states. These limitations must be overcome, and these topics, together with the evaluation of more hyperspherical harmonics and the detailing of our program for the higher virial coefficients, will be the object of future work.

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APPENDIX A

We wish to show that

$$e^{i\vec{k}\cdot\vec{r}} = \sum_{K\lambda} A_{K\lambda} \frac{J_{K+2}(kr)}{k^2r^2} \mathcal{U}^{*}_{K\lambda}(\hat{r})\mathcal{U}_{K\lambda}(\hat{k}).$$

The argument relies heavily on the results presented in the Bateman manuscript project.[25]

From their Lemma (1)[26] we learn that there exists one and only one surface harmonic of degree K which is invariant under all those orthogonal transformations which leave one point of the unit sphere fixed, i.e., given our unit vector $\hat{k}$ there is only one harmonic of degree K such that $\mathcal{U}_K(\hat{r})$ depends only on r and $\hat{r}\cdot\hat{k}$, and $\mathrm{U}_K(\hat{k}) = 1$. This surface harmonic is given by $C_K^2(\hat{k}\cdot\hat{r})/C_K^2(1)$, where C_K^2 is a Gegenbauer polynomial of degree K and order 2.

It follows from this and from our remarks on the general solution of the free-particle Schrödinger equation that we can write

$$e^{i\vec{k}\cdot\vec{r}} = \sum_K a_K \frac{J_{K+2}(kr)}{k^2r^2} \frac{C_K^2(\hat{k}\cdot\hat{r})}{C_K^2(1)} .$$

We learn further from their theorem (4)[27] that if our $\mathcal{U}_{K\lambda}$'s are chosen real and orthonormal on the unit sphere then

$$C_K^2(\hat{k}\cdot\hat{r})/C_K^2(1) = (\omega/h)\textstyle\sum_\lambda \mathcal{U}_{K\lambda}(\hat{r})\mathcal{U}_{K\lambda}(\hat{k}),$$

where ω/h is a constant divided by the number of linearly independent polynomials of degree K. We thus have established our theorem when the surface harmonics are real. A modification of this argument supplies the proof when we allow complex surface harmonics. We find then that

$$\textstyle\sum_\lambda \mathcal{U}_{K\lambda}(\hat{r})\mathcal{U}^{*}_{K\lambda}(\hat{k})$$

is an orthogonal invariant and therefore can be equated to a multiple of $C_K^2(\hat{k}\cdot\hat{r})$. We note that the coefficient $A_{K\lambda}$ is in fact independent of λ.

APPENDIX B

We are interested in showing that if the potential is symmetric, the S matrix is also symmetric.

Let us write

$$\phi_{K\lambda}^{K'\lambda'} = (2\pi kr)^{1/2}\, \omega_{K\lambda}^{K'\lambda'} . \tag{B1}$$

Then Eq. (16) reads

$$\left(\frac{d^2}{dr^2} + k^2 - \frac{(K+2)^2 - \frac{1}{4}}{r^2}\right) \phi_{K\lambda}^{K'\lambda'} = \sum_{K''\lambda''} U_{K\lambda}^{K''\lambda''}\, \phi_{K''\lambda''}^{K'\lambda'} ; \tag{B2}$$

defining
$$L_K = \frac{d^2}{dr^2} + k^2 - \frac{(K+2)^2 - \frac{1}{4}}{r^2} ,$$

we have
$$L_K \phi_{K\lambda}^{K'\lambda'} = \sum_{K''\lambda''} U_{K\lambda}^{K''\lambda''}\, \phi_{K''\lambda''}^{K'\lambda'} ,$$

$$U_{K\lambda}^{K''\lambda''} = U_{K''\lambda''}^{K\lambda} .$$

Hence

$$\phi_{K\lambda}^{K'\lambda'} = e^{-i[kr - (K+2)\pi/2 - \pi/4]}\,\delta_{K\lambda}^{K'\lambda'} + S_{K\lambda}^{K'\lambda'}(k)\, e^{i[kr - (K+2)\pi/2 - \pi/4]} \quad \text{as } r \to \infty .$$

In order to define general "Wronskians" we consider first a set of interactions such that only four equations are coupled. We call this a four-level system. We will see that the generalization for any even number of levels follows at once. An odd number of levels produces some difficulties that we do not need to consider since we may always assume that the number of equations effectively coupled is even.

Because (B2) is of second order, the system is equivalent to eight first-order differential equations which, of course, can be reduced to one of the eighth order. Since we are interested in solutions that are not singular at the origin, we need only consider four solutions.

We can build six independent Wronskians. They are

$$\begin{aligned}
&W_1(\phi_\nu^{\nu'}, \phi_\mu^{\mu'})\\
&\quad= \phi_1^2 L_1 \phi_1^1 - \phi_1^1 L_1 \phi_1^2 + \phi_1^4 L_1 \phi_1^3 - \phi_1^3 L_1 \phi_1^4\\
&\qquad + \phi_2^2 L_2 \phi_2^1 - \phi_2^1 L_2 \phi_2^2 + \phi_2^4 L_2 \phi_2^3 - \phi_2^3 L_2 \phi_2^4\\
&\qquad + \phi_3^2 L_3 \phi_3^1 - \phi_3^1 L_2 \phi_3^2 + \phi_3^4 L_3 \phi_3^3 - \phi_3^3 L_3 \phi_3^4\\
&\qquad + \phi_4^2 L_4 \phi_4^1 - \phi_4^1 L_4 \phi_4^2 + \phi_4^4 L_4 \phi_4^3 - \phi_4^3 L_4 \phi_4^4 \equiv 0\ ,\\
&W_2(\phi_\nu^{\nu'}, \phi_\mu^{\mu'})\\
&\quad= \phi_1^3 L_1 \phi_1^1 + \phi_1^4 L_1 \phi_1^2 - \phi_1^1 L_1 \phi_1^3 - \phi_1^2 L_1 \phi_1^4\\
&\qquad + \phi_2^3 L_2 \phi_2^1 + \phi_2^4 L_2 \phi_2^2 - \phi_2^1 L_2 \phi_2^3 - \phi_2^2 L_2 \phi_2^4\\
&\qquad + \phi_3^3 L_3 \phi_3^1 + \phi_3^4 L_3 \phi_3^2 - \phi_3^1 L_3 \phi_3^3 - \phi_3^2 L_3 \phi_3^4\\
&\qquad + \phi_4^3 L_4 \phi_4^1 + \phi_4^4 L_4 \phi_4^2 - \phi_4^1 L_4 \phi_4^3 - \phi_4^2 L_2 \phi_4^4 \equiv 0,\\
&W_3(\phi_\nu^{\nu'}, \phi_\mu^{\mu'})\\
&\quad= \phi_1^4 L_1 \phi_1^1 - \phi_1^3 L_1 \phi_1^2 + \phi_1^2 L_1 \phi_1^3 - \phi_1^1 L_1 \phi_1^4\\
&\qquad + \phi_2^4 L_2 \phi_2^1 - \phi_2^3 L_2 \phi_2^2 + \phi_2^2 L_2 \phi_2^2 - \phi_2^1 L_2 \phi_2^4\\
&\qquad + \phi_3^4 L_3 \phi_3^1 - \phi_3^3 L_3 \phi_3^2 + \phi_3^2 L_3 \phi_3^3 - \phi_3^1 L_3 \phi_3^4\\
&\qquad + \phi_4^4 L_4 \phi_4^1 - \phi_4^1 L_4 \phi_4^2 + \phi_4^2 L_4 \phi_4^3 - \phi_4^1 L_4 \phi_4^4 \equiv 0.
\end{aligned}$$

The other three Wronskians appear as a result of a convenient change of sign in the first three. Then, we have

$$\begin{aligned}
W_4 = {}& \phi_1^2 L_1 \phi_1^1 - \phi_1^1 L_1 \phi_1^2 - \phi_1^4 L_1 \phi_1^3 + \phi_1^3 L_1 \phi_1^4\\
&+ \phi_2^2 L_2 \phi_2^1 - \phi_2^1 L_2 \phi_2^2 - \phi_2^4 L_2 \phi_2^3 - \phi_2^3 L_2 \phi_2^4\\
&+ \phi_3^2 L_3 \phi_3^1 - \phi_3^1 L_3 \phi_3^2 - \phi_3^4 L_3 \phi_3^3 + \phi_3^3 L_3 \phi_3^4\\
&+ \phi_4^1 L_4 \phi_4^1 - \phi_4^1 L_4 \phi_4^2 - \phi_4^4 L_4 \phi_4^3 + \phi_4^3 L_4 \phi_4^4 \equiv 0.
\end{aligned}$$

Here the change in sign is in the third and fourth term, seventh and eighth term, and so on, of W_1.

$$\begin{aligned}
W_5 = {}& \phi_1^3 L_1 \phi_1^1 - \phi_1^4 L_1 \phi_1^2 - \phi_1^1 L_1 \phi_1^3 + \phi_1^2 L_1 \phi_1^4\\
&+ \phi_2^3 L_2 \phi_2^1 - \phi_2^4 L_2 \phi_2^2 - \phi_2^1 L_2 \phi_2^3 + \phi_2^2 L_2 \phi_2^4\\
&+ \phi_3^3 L_3 \phi_3^1 - \phi_3^4 L_3 \phi_3^2 - \phi_3^1 L_3 \phi_3^3 + \phi_3^2 L_3 \phi_3^4\\
&+ \phi_4^3 L_4 \phi_4^1 - \phi_4^4 L_4 \phi_4^2 - \phi_4^1 L_4 \phi_4^3 + \phi_4^2 L_2 \phi_4^4 \equiv 0,
\end{aligned}$$

W_5 is obtained from W_2 if we change the sign of the second, fourth, sixth, eighth, etc., term in W_2, and

$$\begin{aligned}
W_6 = {}& \phi_1^4 L_1 \phi_1^1 + \phi_1^3 L_1 \phi_1^2 - \phi_1^2 L_1 \phi_1^3 - \phi_1^1 L_1 \phi_1^4\\
&+ \phi_2^4 L_2 \phi_2^1 + \phi_2^3 L_2 \phi_2^2 - \phi_2^2 L_2 \phi_2^3 - \phi_2^1 L_2 \phi_2^3\\
&+ \phi_3^4 L_3 \phi_3^1 + \phi_3^3 L_3 \phi_3^2 - \phi_3^2 L_3 \phi_3^3 - \phi_3^1 L_3 \phi_3^4\\
&+ \phi_4^4 L_4 \phi_4^1 + \phi_4^3 L_4 \phi_4^2 - \phi_4^2 L_4 \phi_4^3 - \phi_4^1 L_4 \phi_4^4 \equiv 0.
\end{aligned}$$

Now we integrate the Wronskians from zero to infinity. Hence, for example, we have

$$\begin{aligned}
&\int_0^\infty W_2 dr\\
&\quad= \lim_{r\to\infty} \phi_1^3 \frac{d}{dr}\ \phi_1^1 + \phi_1^4 \frac{d}{dr}\ \phi_1^2 - \phi_1^1 \frac{d}{dr}\ \phi_1^3 - \phi_1^2 \frac{d}{dr}\ \phi_1^4\\
&\qquad + \phi_2^3 \frac{d}{dr}\ \phi_2^1 + \phi_2^4 \frac{d}{dr}\ \phi_2^2 - \phi_2^1 \frac{d}{dr}\ \phi_2^3 - \phi_2^2 \frac{d}{dr}\ \phi_2^4\\
&\qquad + \phi_3^3 \frac{d}{dr}\ \phi_3^1 + \phi_3^4 \frac{d}{dr}\ \phi_3^2 - \phi_3^1 \frac{d}{dr}\ \phi_3^3 - \phi_3^2 \frac{d}{dr}\ \phi_3^4\\
&\qquad + \phi_4^3 \frac{d}{dr}\ \phi_4^1 + \phi_4^4 \frac{d}{dr}\ \phi_4^2 - \phi_4^1 \frac{d}{dr}\ \phi_4^3 - \phi_4^2 \frac{d}{dr}\ \phi_4^4 \equiv 0, \text{ etc.}
\end{aligned}$$

We see that if we replace L_k by d/dr in the expression for W_2, we obtain the above expression. Now, taking advantage of the asymptotic behavior of the wave function we readily obtain

$$\int_0^\infty W_2 dr = 2ik(-S_1^3 - S_2^4 + S_3^1 + S_4^2) = 0\ .$$

Hence $S_1^3 + S_2^4 - S_3^1 - S_4^2 = 0$.

Analogously, using W_1 and W_3 we get

$$S_1^2 - S_2^1 + S_3^4 - S_4^3 = 0, \quad S_1^4 - S_2^3 + S_3^2 - S_4^1 = 0.$$

From W_4, W_5, W_6 we get

$$S_1^2 - S_2^1 - S_3^4 + S_4^3 = 0\ , \quad S_1^3 - S_2^4 - S_3^1 + S_4^2 = 0\ ,$$
$$S_1^4 + S_2^3 - S_3^2 - S_4^1 = 0\ .$$

Therefore,

$$S_1^2 = S_2^1, \quad S_3^4 = S_4^3, \quad S_1^3 = S_3^1\ ,$$
$$S_2^3 = S_3^2, \quad S_1^4 = S_4^1, \quad S_2^4 = S_4^2\ .$$

Obviously we can generalize this proof and obtain

$$S_{K\lambda}^{K'\lambda'} = S_{K'\lambda'}^{K\lambda}.$$

APPENDIX C: EXAMPLES AND APPROXIMATIONS

TWO-LEVEL SYSTEM

In order to clarify the formalism and state a relevant approximation concerning the R matrix, we will study the case when the number of levels is limited to two. The general form for the orthogonal matrix in two dimensions is

$$U = \begin{pmatrix} \cos\epsilon & \sin\epsilon \\ -\sin\epsilon & \cos\epsilon \end{pmatrix}.$$

Hence using Eq. (32) we obtain

$$\tan\delta_1 \cos^2\epsilon + \sin^2\epsilon \tan\delta_2 = -\tilde{R}_1^1 ,$$
$$\tfrac{1}{2}\sin 2\epsilon(\tan\delta_1 - \tan\delta_2) = -\tilde{R}_1^2 ,$$
$$\sin^2\epsilon \tan\delta_1 + \cos^2\epsilon \tan\delta_2 = -\tilde{R}_2^2 ,$$

where $\tilde{R}_i^j = (\pi m k^4/\hbar^2) R_i^j$. (C1)

If in some approximation we calculate the matrix elements of the reaction matrix, then the equations above allow the calculation of ϵ, δ_1, and δ_2. We can observe that this is due to the symmetry of the R matrix.

Making use of the fact that the trace and the determinant are invariants we readily obtain

$$-(\tilde{R}_1^1 + \tilde{R}_1^2) = \tan\delta_1 + \tan\delta_2 ,$$
$$-2\tilde{R}_1^2/\sin(2\epsilon) = \tan\delta_1 - \tan\delta_2 .$$

Hence the solution is

$$-\tan\delta_1 = -\tfrac{1}{2}(\tilde{R}_1^1 + \tilde{R}_2^2) + \tfrac{1}{2}[(\tilde{R}_1^1 + \tilde{R}_2^2)^2 - 4(\tilde{R}_1^1\tilde{R}_2^2 - \tilde{R}_1^2)^2]^{1/2} ,$$
$$-\tan\delta_2 = -\tfrac{1}{2}(\tilde{R}_1^1 + \tilde{R}_2^2) - \tfrac{1}{2}[(\tilde{R}_1^1 + \tilde{R}_2^2)^2 - 4(\tilde{R}_1^1\tilde{R}_2^2 - \tilde{R}_1^2)^2]^{1/2} ,$$
$$-\sin 2\epsilon = 2\tilde{R}_1^2/(\tan\delta_1 - \tan\delta_2) .$$

If we now assume that the following approximation holds,

$$\tilde{R}_2^2\tilde{R}_1^1 \gg (\tilde{R}_1^2)^2 , \qquad \text{(C2)}$$

then, using Eq. (C2) in the equation for δ_1, δ_2, and ϵ we obtain

$$\tan\delta_1 = -\tilde{R}_1^1, \quad \tan\delta_2 = -\tilde{R}_2^2,$$
$$\sin 2\epsilon = -\tilde{R}_1^2/(\tilde{R}_1^1 - \tilde{R}_2^2) .$$

That is to say that the phase shifts are determined in this approximation merely by the diagonal matrix elements of the R matrix.

Square-Well Interparticle Potential

As we have already stated, we are interested in applying our formalism to a kind of potential that is finite everywhere, short ranged and without bound states. It is clear that this interaction can be approximated by an appropriate summation of square-well potentials.

With the goal of studying the behavior of the matrix elements $R_{K\lambda}^{K'\lambda'}$ and of b_3 as $T \to 0$, it is, in principle, enough to study just one term in that representation, the square-well potential.

We then have

$$V(\vec{r}) = V_{12}(\sqrt{2}\vec{\eta}) + V_{13}[(\sqrt{\tfrac{3}{2}})\vec{\xi} + \vec{\eta}/\sqrt{2}]$$
$$+ V_{23}[(\sqrt{\tfrac{3}{2}})\vec{\xi} - \vec{\eta}/\sqrt{2}] ,$$

where $V_{ij}(\vec{r}_{ij}) = V_0$ if $|\vec{r}_{ij}| < a$

$= 0$ if $|\vec{r}_{ij}| > a$,

and $\vec{r}_{ij}$ is a function of $\vec{\xi}$ and $\vec{\eta}$ which can easily be obtained using Eq. (3).

If we know the hyperspherical harmonics [Eq. (6)] we can obtain the matrix elements Eq. (14). As stated in the body of the paper, in this illustrative example we restrict ourselves to a total angular momentum of zero.

Calculations done by Simonov show that in this case the harmonic polynomials are totally specified by two quantum numbers, namely, K, the degree of the polynomial, and ν, the symmetry quantum number. A representation in terms of the Jacobi polynomials is

$$\mathcal{U}_{K,0,\nu} = (K + 2/2\pi^3)^{1/2} e^{-i\beta\nu}$$
$$\times A^{|\nu|} P^{|\nu|,0}_{1/2(K/2-|\nu|)}(1 - 2A^2) ,$$
$$A^2 = \cos^2 2\theta + \sin^2 2\theta \cos^2(\hat{\xi}\cdot\hat{\eta}) ,$$
$$\tan\beta = \tan 2\theta \cos(\hat{\xi}\cdot\hat{\eta}) ,$$
$$\nu = -\tfrac{1}{2}K, \quad -\tfrac{1}{2}K + 2, \quad \ldots, \quad \tfrac{1}{2}K; \quad L = 0 ,$$
$$K = 2n, \quad n = 0, 1, 2, \ldots, \quad \text{etc.}$$

Hence, we have $\frac{1}{2}K + 1$ polynomials of degree K with $L = 0$. When $\nu = 3m$, $m = 0, 1, 2, \ldots$, the state is symmetric under permutation of particles. If $m = -1, -2, -3, \ldots$, the state is antisymmetric. All the other states belong to a two-dimensional representation of the permutation group.

Using this representation, Badalyan and Simonov calculated the following expressions for the matrix elements of the square well:

$$V_{000}^{000} = 3V_0 \frac{2}{\pi}\left[\arcsin\frac{a}{\sqrt{2}r} - \tfrac{1}{4}\sin\left(4\arcsin\frac{a}{\sqrt{2}r}\right)\right] ,$$
$$r \geq \frac{a}{\sqrt{2}} ,$$
$$V_{000}^{000} = 3V_0 , \quad r \leq \frac{a}{\sqrt{2}}$$
$$V_{K,0,\nu}^{000} = \frac{2(-1)^{K/4-\nu/2}}{(K+2)^{1/2}}\{V_K^{(12)}(r)$$
$$+ \cos\tfrac{2}{3}\pi\nu[V_K^{(13)}(r) + V_K^{(23)}(r)]\}\begin{cases}1, & \nu > 0\\ 2^{-1/2}, & \nu = 0\end{cases} \qquad \text{(C3)}$$

$$V_{K,0,\nu}^{000} = \frac{-2(-1)^{K/4-|\nu|/2}}{(K+2)^{1/2}}$$
$$\times [V_K^{(23)}(r) + V_K^{(13)}(r)] \sin\tfrac{2}{3}\pi|\nu| , \qquad \nu < 0$$

$$V_K^{(i,j)} = -\frac{16}{\pi} V_0 \frac{(a/r)^3[2 - (a/r)^2]^{3/2}}{K(K+4)}$$
$$\times C_{K/2+1}^2\left(\frac{a^2}{r^2} - 1\right)\Theta\left(r - \frac{a}{\sqrt{2}}\right), \text{for } K > 0$$

where $C_{K/2+1}^2(a^2/r^2 - 1)$ is a Gegenbauer polynomial, $\Theta(r - a/\sqrt{2})$ is a step function, and V_0 and a are the height and range of the well, respectively. Recurrence relations exist for the $V_{K\nu}^{K'\nu'}$ which allow them to be expressed in terms of $V_{K\nu}^{00}$. However, for our numerical estimate we will use the property

$$V_{K'0\nu'}^{K0\nu} \simeq V_{|K-K'|,0,|\nu-\nu'|}^{0,0,0} \quad , \tag{C4}$$

which holds for large quantum numbers, i.e., for

$$K \gg 1, \quad K' \gg 1, \quad t = K - K' \ll K \, ,$$

$$\tfrac{1}{2}K - \nu \gg 1, \quad \tfrac{1}{2}K' - \nu' \gg 1 \, .$$

When the quantum numbers are small, (C4) gives the order of magnitude. For the sake of simplicity, we will use it for calculating all the matrix elements.

To continue, we shall calculate the phase shifts in first and second Born approximation. Since at low energy the phase shifts are small, we have

$$\delta_{K\lambda}(k) \simeq -\tilde{R}_{K\lambda}^{K\lambda}(k) \, .$$

To calculate $\tilde{R}_{K\nu}^{K\nu}(k)$ in the first Born approximation we set

$$\psi_{K',L'=0,\nu'}^{K'',L''=0,\nu''} = \frac{A_{K',0,\nu'} J_{K''+2}}{k^2 r^2} \, \delta_{K'\nu'}^{K''\nu''} \tag{C5}$$

in Eq. (31). In general, we then need to evaluate the integral

$$I_{K\lambda}^{K'\lambda'} = \int_0^\infty J_{K+2}(kr) V_{K\lambda}^{K'\lambda'}(r) J_{K'+2}(kr) r \, dr \quad . \tag{C6}$$

Recalling the behavior of the Bessel function for small values of the argument, we are led to evaluate the above integral at low energy using the asymptotic behavior of the potential

$$V_{K\nu}^{K''\nu''} \to V_0 C_{K\nu}^{K''\nu''} a^3/r^3 \quad , \tag{C7a}$$

where $C_{K\nu}^{K''\nu''}$ is a constant which can be easily evaluated using Eqs. (C3) and (C4):

$$C_{K,\nu}^{K+t,\nu+s} = (-1)^{3|t|/4-s/2} \left(\frac{8}{3\pi\sqrt{2}} \right) \times \frac{(|t|+6)(|t|+8)}{|t|(|t|+2)^{1/2}} \left(1 + 2\cos\tfrac{1}{3}2\pi s\right) ,$$

$$s > 0, \quad s \leqslant \tfrac{1}{2}|t| \, , \quad t \neq 0 \tag{C7b}$$

$$C_{K,\nu}^{K+t,\nu+s} = (8/\pi\sqrt{2}), \quad t = 0, \quad s = 0$$

$$C_{K,\nu}^{K+t,\nu+s} = (-1)^{3|t|/4+s/2} \left(\frac{8}{3\pi\sqrt{2}} \right) \times \frac{(|t|+6)(|t|+8)}{|t|(|t|+2)^{1/2}} \left(2\sin\tfrac{1}{3}2\pi s\right), \quad s < 0.$$

We then write the following approximation:

$$I_{K,\lambda}^{K+t,\lambda} \simeq C_{K,\lambda}^{K+t,\lambda} \int_0^\infty J_{K+2}(kr) J_{K+t+2}(kr) \frac{dr}{r^2}$$

$$= \frac{k}{\pi} \frac{(-1)^{t/2} C_{K,\lambda}^{K+t,\lambda'}}{(1-t^2)(K+\frac{1}{2}t+\frac{5}{2})(K+\frac{1}{2}t+\frac{3}{2})} \, , \tag{C8}$$

where we have used the fact that t is an even integer. Thus, using Eq. (31), we get for the modulus

$$\left| R_{K\nu}^{K'\nu'} \right| = \left| V_0 a^3 I_{K\nu}^{K'\nu'} / k^4 \right| \quad .$$

We then can easily see that

$$(R_{K\nu}^{K+t,\nu+s})^2 / R_{K\nu}^{K\nu} R_{K+t,\nu+s}^{K+t,\nu+s} \propto 1/t^3 \, ,$$

for large t and thus becomes quite small. In our illustrative example we ignore the nondiagonal terms in computing the eigenphase shifts for the square well. Using Eqs. (32) and (C6) the solution then reads

$$\tilde{R}_{K\nu}^{K\nu} \simeq \pi[(mV_0/\hbar^2)a^3] I_{K\nu}^{K\nu} \quad , \tag{C9}$$

where $\tilde{R}_{K\nu}^{K\nu}$ was already defined in Eq. (C1).

Using the formulas above, we may write for the phase shift in first Born approximation,

$$\delta_{K,0,\nu}^{(123)} \simeq a_{K\nu;1}^{(123)} k \quad ,$$

$$a_{K\nu;1}^{(123)} = -\frac{mV_0 a^3}{\hbar^2} \frac{8}{\pi\sqrt{2}} \frac{1}{(K+\frac{5}{2})(K+\frac{3}{2})} \, . \tag{C10}$$

To calculate the phase shift in the second Born, we start with the wave function

$$\psi_{K''\lambda''}^{K'\lambda'} = (1/k^2 r^2)[A_{K''\lambda''} J_{K''+2} \delta_{K''\lambda''}^{K'\lambda'} + A_{K'\lambda'} \tfrac{1}{2}\pi \times (2m/\hbar^2) \int J_{K''+2}(kr<) N_{K''+2}(kr>) \times V_{K''\lambda''}^{K'\lambda'} J_{K'+2}(kr') r' dr'] \, .$$

After replacing this in Eq. (31), we obtain

$$R_{K0\nu}^{K'0\nu'} = R_{K\nu}^{(1)K'\nu'} + R_{K\nu}^{(2)K'\nu'} \quad ,$$

where

$$R_{K\nu}^{(1)K'\nu'} = A_{K\nu}^{*} A_{K'\nu'} (1/k^4) \int_0^\infty J_{K+2}(kr) \times V_{K\nu}^{K'\nu'}(r) J_{K'+2}(kr) r \, dr \quad ,$$

$$R_{K\nu}^{(2)K'\nu'} = A_{K\nu}^{*} A_{K'\nu'} \frac{\pi}{2k^4} \times \sum_{K''\lambda''} \left\{ \int_0^\infty J_{K+2}(kr) V_{K\nu}^{K''\lambda''}(r) r \, dr \times \int_0^\infty J_{K''+2}(kr<) N_{K''+2}(kr>) \frac{2m}{\hbar^2} \times V_{K''\lambda''}^{K'\nu'}(r') J_{K'+2}(kr') r' \, dr' \right\} . \tag{C11}$$

The summation over intermediate states should be done using all of the states. Nevertheless, in the spirit of our approximations we sum only over $L = 0$ states, and we can verify that this procedure will modify only the estimate of the constant A in the final formula.

We therefore find

$$\tilde{R}_K^{(2)K'} = \left(\frac{\pi m}{\hbar^2} V_0 a^3 \right)^2 A_{K\lambda}^{*} A_{K'\lambda'} k^2 \times \sum_{K''\nu''} C_{K\nu}^{K''\nu''} C_{K''\nu''}^{K'\nu'} I_{K,K'',K'} \quad , \tag{C12}$$

where

$$I_{K,K'',K'} = \int_0^\infty du \left[J_{K+2}(u)/u^2 \right]$$

$$\times \int_0^\infty dv\, J_{K''+2}(r<) N_{K''+2}(r>) J_{K'+2}(v) \quad ,$$

and thus in the diagonal approximation

$$\delta_{K\nu}^{(123)} = a_{K\nu;1}^{(123)} k - \left(\frac{\pi m}{\hbar^2} V_0 a^3\right)^2 k^2$$

$$\times \sum_{K''\nu''} C_{K\nu}^{K''\nu''} C_{K''\nu''}^{K\nu} I_{K,K'',K} \quad . \tag{C13}$$

We find

$$I_{K,K'',K} = 2\int_0^\infty du\,[J_{K+2}(u) N_{K''+2}(u)/u^2]$$

$$\times \int_0^u J_{K''+2}(v) J_{K+2}(v)\, dv/v^2$$

and show in Appendix E that for $K''=K$ we obtain

$$I_{K,K,K} = (12/\pi)\,[\Gamma(2K+2)/\Gamma(2K+7)] \quad .$$

We have not been able to evaluate the more general integral $I_{K,K'',K'}$. Using our methods this would require a generalization of Eq. (E3). We expect, however, that in analogy to the integral given by Eq. (C8), the contribution of $I_{K,K'',K'}$ for K'' much different from K or K' would be very much smaller than that of $I_{K,K,K}$.

We can then write

$$\delta_{K\nu}^{(123)} \simeq a_{K\nu;1}^{(123)} k + a_{K\nu;2}^{(123)} k^2 \quad , \tag{C14a}$$

where, using (C13), we have for $a_{K\nu;2}^{(123)}$,

$$a_{K\nu;2}^{(123)} = -\left(\frac{\pi}{2}\right)^2 \left(\frac{2m V_0}{\hbar^2}\right)^2 a^6\, \frac{12}{\pi}\, \frac{\Gamma(2K+2)}{\Gamma(2K+7)}\, (C_{K\nu}^{K\nu})^2 \quad . \tag{C14b}$$

We readily estimate $(C)^2$ using Eq. (C7b),

$$(C_{K\nu}^{K\nu})^2 \simeq 64/2\pi^2 \quad . \tag{C14c}$$

For computing the third cluster integral we must calculate the phase shifts when we turn on only the interaction between two particles, say, 1 and 2. In this case, we set $V^{23} = V^{13} = 0$, and use the same procedure already outlined. We can easily see that

$$\delta_{K\nu}^{12/3} = \tfrac{1}{3} a_{K\nu;1}^{(123)} k + a_{K\nu;2}^{(12/3)} k^2 \quad , \tag{C15a}$$

$$\text{where} \quad a_{K\nu;2}^{(12/3)} \simeq \tfrac{1}{9}\, a_{K\nu;2}^{(123)} \quad . \tag{C15b}$$

APPENDIX D: CALCULATION OF b_3 WHEN $T \to 0$

Our Born development yields a power series in k for the phase shifts

$$\delta_{K\lambda} = \textstyle\sum_n a_{K\lambda,n} k^n \quad .$$

It then follows using Eq. (55) that

$$b_3^{\text{Boltz}} = [(2S+1)^3 \sqrt{3}/2\pi]\, \mathcal{S}/\lambda_T^3 \quad ,$$

where

$$\mathcal{S} = \sum_{K,\lambda,n} \left(\frac{4\pi}{\lambda_T^2}\right)^{n/2} [a_{K\lambda,n}^{(123)} - 3a_{K\lambda,n}^{(12/3)}]\, \Gamma(1+n/2) \quad .$$

Using our results from Appendix C and Eqs. (C14a) and (C15a) we obtain a null contribution in first Born ($n=1$). The leading term as $T \to 0$ is from the second Born. After some algebra we obtain

$$b_3^{\text{Boltz}} \sim (2S+1)^3 A (1/\lambda_T^5)(2mV_0/\hbar^2)^2 a^6 \quad ,$$

where $A \sim -3^{1/2}(8/45\pi)$.

At this point a further remark is in order. It is clear that the extension of our Born formulas to include nonzero L would not change the wave-number dependence of our results since it follows from essentially dimensional considerations. Would a more careful diagonalization alter this k dependence? The answer is negative. This follows from the fact that in the first Born approximation we have

$$(R^{123})_{K\lambda}^{K'\lambda'} - 3(R^{12/3})_{K\lambda}^{K'\lambda'} = 0 \quad ,$$

together with an expansion of the respective U matrices (i.e, $U^{(123)}$ and $U^{(12/3)}$) in powers of k. We find then zero contribution to order k but that both first and second Born contribute in order k^2.

APPENDIX E

We have to evaluate

$$I = \int_0^\infty J_p(x) N_p(x) \frac{dx}{x^2} \int_0^x J_p(y) J_p(y) \frac{dy}{y^2} \quad . \tag{E1}$$

Making the transformation

$$x = x, \quad y = x\tan\theta,$$

with the Jacobian

$$\frac{\partial(x,y)}{\partial(x,\theta)} = \frac{x}{\cos^2\theta} \quad ,$$

we can write

$$I = \int_0^\infty \frac{dx}{x^3} \int_0^{\pi/4} J_p(x) N_p(x)\, \frac{J_p(x\tan\theta) J_p(x\tan\theta)\, d\theta}{\sin^2\theta} \quad . \tag{E2}$$

Using the integral representations[25]

$$J_p(x) N_p(x) = -(2/\pi)\int_0^\infty J_{2p}(2x\cosh t)\, dt, \quad x>0 \tag{E3}$$

$$J_p(x\tan\theta) J_p(x\tan\theta)$$

$$= (2/\pi)\int_0^{\pi/2} J_{2p}(2x\tan\theta\cos\phi)\, d\phi, \quad \operatorname{Re} 2p > -1 \tag{E4}$$

we obtain

$$I = -\left(\frac{2}{\pi}\right)^2 \int_0^\infty \frac{dx}{x^3} \int_0^{\pi/4} \frac{d\theta}{\sin^2\theta} \int_0^\infty dt \int_0^{\pi/2} d\phi$$

$$\times J_{2p}(2x\tan\theta\cos\phi) J_{2p}(2x\cosh t) \quad , \tag{E5}$$

with $0 \leqslant \tan\theta\cos\phi \leqslant \cosh t$.

Now[25] we have

$$\int_0^\infty t^{-3} J_{2p}(at) J_{2p}(bt)\, dt$$

$$= [a^{2p} 2^{-3} b^{2-2p} \Gamma(2p-1)/\Gamma(2)\,\Gamma(2p+1)]$$

$$\times\, {}_2F_1(2p-1,\, -1;\, 2p+1;\, a^2/b^2)\,,$$

$$\mathrm{Re}(2p-2)>0,\quad 0<a<b \tag{E6}$$

where

$${}_2F_1(2p-1,\, -1,\, 2p+1,\, \tan^2\theta\cos^2\phi/\cosh^2 t) = 1-\frac{2p-1}{2p+1}\,\frac{\tan^2\theta\cos^2\phi}{\cosh^2 t}\ .$$

We, therefore, can integrate over each variable. Using

$$\int_0^\infty dt/(\cosh t)^{2m} = 2^{2m-2}[\Gamma(m)/\Gamma(2m)]\ ,$$

$$\int_0^{\pi/2}(\cos\phi)^K\, d\phi = \frac{\pi}{2^{K+1}}\,\frac{\Gamma(K+1)}{\Gamma(\frac{1}{2}K+1)\,\Gamma(\frac{1}{2}K+1)}\ ,$$

we obtain after some algebra

$$I=(6/\pi)[\Gamma(2p-2)/\Gamma(2p+3)]\ . \tag{E7}$$

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