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Virial coefficients in the presence of an infinite number of bound states and strongly repulsive potentials: Application to the Efimov point

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Extending some previous work of Bollé [Phys. Rev. A **36**, 3259 (1987)], we construct expressions for the n-particle cluster coefficients that remedy difficulties associated with the presence of both an infinite number of bound states and strongly repulsive potentials. Applying the existence theorems for cluster coefficients implicit in the work of Ginibre [J. Math. Phys. **6**, 238 (1965); **6**, 252 (1965); **6**, 1432 (1965)], we demonstrate the validity of these expressions. We apply the formalism to obtain a well-behaved expression for b_3 at the Efimov point. As a by-product we are able to directly observe the divergence in b_3 due to the continuum part of the three-body resolvent together with the counterterms that render it convergent.

I. INTRODUCTION

The incorporation of bound-state effects in the equation of state of an imperfect gas is usually a reasonably straightforward matter. The equation of state is given parametrically by the Mayer equations[1]

$$\frac{P}{kT}=\sum_{n=1}^{\infty} b_n z^n , \tag{1a}$$

$$\rho=z\frac{d}{dz}\left[\frac{P}{kT}\right] , \tag{1b}$$

where the cluster coefficients b_n are defined as

$$b_n=\frac{1}{Vn!}\mathrm{Tr}(e^{-\beta H_n})_c . \tag{2}$$

The subscript c denotes that only the connected parts of the Boltzmann operator are taken. H_n denotes the n-body Hamiltonian of the system. In these equations, Boltzmann statistics are assumed and the notation for thermodynamic variables is that of Huang.[1] The contribution of bound states (if any) to b_n can be seen explicitly by evaluating the trace using a basis of eigenfunctions. Such an evaluation yields

$$b_n=\frac{1}{n!}\frac{1}{V}\left[\frac{Vn^{3/2}}{\lambda^3}\sum_m e^{-\beta E_m^n}+\mathrm{Tr}_n^{\mathrm{cont}}(e^{-\beta H_n})_c\right] , \tag{3}$$

where the trace over the bound states has been done explicitly and the sum over the continuum eigenfunctions is represented symbolically by the second term. E_m^n are the n-body bound-state energies. The standard Beth-Uhlenbeck expression for b_2 is of this form.[1] As well as explicitly displaying the bound-state contributions to b_n, the Beth-Uhlenbeck form, Eq. (3), also provides a convenient starting point for its exact evaluation.

In most cases the Beth-Uhlenbeck form is perfectly well defined and each term can be evaluated separately. Our concern here is in the instance where this form is not well defined by virtue of the fact that the bound-state sum is divergent. Such a divergence occurs when the bound-state spectrum of the n-body problem has an infinite number of bound states that accumulate at zero energy. We know of two examples of this: the three-body problem when the pair potential is at the Efimov point[2] (a pair potential is said to be "at the Efimov point" when it has a zero-energy bound state) and the Coulomb n-body problem.

The question that immediately arises is whether the divergence in the bound-state sum causes the cluster coefficients to diverge. If the cluster coefficients turn out to be convergent, then we have the further task of finding a representation for b_n to replace the Beth-Uhlenbeck form. Let us first consider the case of the Efimov point, where the strongest results will be determined, outlining previous work carried out by other authors and then the contribution to be made in this paper. In the case of the Efimov point, this question was first examined by Hoogeveen and Tjon[3] for some simplified models of binary-gas mixtures. They concluded that the divergence of the bound-state sum is canceled by an equal but opposite divergence in the continuum contribution and that the resulting b_3 is actually finite. This result was partially extended by Bollé[4] to the more realistic case of a one-component gas of particles interacting via bounded short-range potentials. Bollé achieved this as a by-product of the derivation of an alternative expression for b_3, the so-called Planck-Larkin structure,

$$b_3=\frac{1}{3!}\frac{1}{V}\left[\frac{V3^{3/2}}{\lambda^3}\sum_m (e^{-\beta E_m^n}-1)+C_3+D_3\right] . \tag{4}$$

Here, C_3 is an integral over configuration space of a polynomial in the potential and its derivatives. D_3 is defined in terms of a multiple integral over energy of an integrand that consists of the three-particle resolvent with various counterterms. In this expression one can see explicitly that the bound-state sum is convergent at the Efimov point. This expression, however, cannot be used to determine whether b_3 is convergent under realistic conditions. This is because of two limitations. Firstly, realistic systems interact via potentials that are strongly repulsive at short range (e.g., the Lennard-Jones form). Evaluation of C_3 with such potentials yields a divergent expression. This limitation can be overcome via a straightforward extension of Bollé's arguments. This extension occupies the main body of this paper. In Sec. II we shall present the formalism we shall be working with together with a rough outline of the derivation. In Sec. III we illustrate our procedure by deriving the Planck-Larkin structures for b_2. In Sec. IV we derive the analogous results for b_3 and state the results for general b_n. The resulting generalized Planck-Larkin structures, like Bollé's original expressions, have a further limitation. When applied to the Efimov point there are no manifest divergences in these expressions. However, it cannot be claimed from this that b_3 is finite at the Efimov point unless it can be established that the D_3 term is also well behaved. That this is indeed the case is established in Sec. V. We do not do this by direct examination as this would require knowledge of the behavior of the three-particle resolvent at the Efimov point, which, as far as we know, is not available in the literature. To derive this knowledge would be a considerably involved task, requiring a separate study. Instead we adopt a different, somewhat indirect, approach. It was our belief that the established existence theorems for quantum cluster coefficients would exclude the case of the Efimov point due to the unusual nature of the Efimov effect. It came then as a surprise to find that some results of Ginibre[5] on the infinite-volume limit of the fugacity expansion of the reduced density matrices do indeed imply that b_3 is well behaved at the Efimov point. This result only establishes the existence of b_3 at the Efimov point. It does not provide a well-behaved replacement for the Beth-Uhlenbeck form. However, we can use this result to show that D_3 is well behaved. We do this in Sec. V. This establishes the main result of this paper: a representation for b_3 that can be evaluated at the Efimov point. As we stated above, information about the behavior of the three-particle resolvent would determine whether D_3 is well behaved. We can turn this argument around. Since we can indirectly determine that D_3 is well behaved, we can then use this to yield information concerning the three-particle resolvent at the Efimov point. This is done in Sec. VI, where we also conclude with some comments.

The case of the Coulomb interaction is more complicated. Previous attempts to remove the divergence in the bound-state sum, to the best of our knowledge, have fallen into two categories. Firstly, it has been argued by Jackson and Klein[6] that in the many-body system the Coulomb potential is screened and that therefore the potential used in the evaluation of the cluster coefficients should be the screened Coulomb potential. Here there are, of course, a finite number of bound states and so the problem of the divergence of the bound-state sum does not arise. However, the arguments for using the screened Coulomb potential, although plausible, are heuristic. (A similar construction to that used by us in some work on the enhancement of the Efimov effect[7] could put this notion on a firm foundation.) In the second approach Bollé[4] also considers this problem as the prime application of the Planck-Larkin structures. In this case Eq. (4) is not appropriate as the bound-state sums are still divergent. Bollé overcomes this by deriving the following form for b_n, $n=2,3$, also referred to as a Planck-Larkin structure:

$$b_n=\frac{1}{n!}\frac{1}{V}\left[\frac{Vn^{3/2}}{\lambda^3}\sum_m (e^{-\beta E_m^n}-1+\beta E_m^n)+C_n'+D_n'\right] . \tag{5}$$

C_n' and D_n' are similar to the analogous terms in Eq. (4). In this expression the bound-state sums are convergent. C_n', however, is divergent. Our contribution to the Coulomb case is the generalization of Eq. (5). This is found in Secs. III and IV. Although the potential terms in our generalization are convergent for strongly repulsive potentials, we find that they continue to diverge for the Coulomb potential. Furthermore, to the best of our knowledge, there are no existence theorems for Coulomb cluster coefficients. As such our methods are of limited validity for the Coulomb case. Our results, however, will permit us to make some comments. These are included in Sec. VI.

Before we begin, let us first make some comments concerning our motivations. We have carried out some work[7] in which medium effects in a gas are partially taken into account via density-dependent potentials. This allows us to tune the density to the Efimov point. Our ultimate aim is to apply this formalism to a gas of helium atoms and to predict the behavior of this gas at the density corresponding to the Efimov point. This would constitute a means to display the full extent of the Efimov effect in a real system. In order to do this we require a representation for b_3 which is not only valid at the Efimov point, but can also accommodate the strongly repulsive core of the helium-helium interaction.

II. FORMALISM

We concentrate in this and the following two sections on b_2 and b_3 (we shall simply state the final results for general b_n at the end of Sec. IV),

$$b_2=\frac{1}{2!}\frac{2^{3/2}}{\lambda^3}\mathrm{Tr}_2(e^{-\beta H_2}-e^{-\beta K_2}) , \tag{6}$$

$$b_3=\frac{1}{3!}\frac{3^{3/2}}{\lambda^3}\mathrm{Tr}_3\left[e^{-\beta H_3}-e^{-\beta K_3}-\sum_{1\le i<j\le 3}(e^{-\beta(K_3+v_{ij})}-e^{-\beta K_3})\right] . \tag{7}$$

Here $\lambda=(2\pi\hbar^2\beta/m)^{1/2}$, $\beta=1/kT$, and $H_n=K_n+V_n$, where K_n is the n-body kinetic energy and V_n is the n-body potential energy. In this work we shall assume that the potential energy V_n is a pairwise sum of pair potentials v_{ij} between particles i and j (inclusion of many-body potentials in our work is straightforward). Note that in expressions (6) and (7) the center-of-mass integrations have been explicitly carried out. Thus Tr_n here and henceforth shall denote the trace over the remaining $3(n-1)$ relative degrees of freedom.

We begin by using the Watson representation[8] of the Boltzmann factor to write Eqs. (6) and (7) as

$$b_2=\frac{1}{2!}\frac{2^{3/2}}{\lambda^3}\mathrm{Tr}_2\left[\frac{1}{2\pi i}\int_c dz\, e^{-\beta z}R_2^c(z)\right], \tag{8}$$

$$b_3=\frac{1}{3!}\frac{3^{3/2}}{\lambda^3}\mathrm{Tr}_3\left[\frac{1}{2\pi i}\int_c dz\, e^{-\beta z}R_3^c(z)\right], \tag{9}$$

where $R_n^c(z)$ are the connected contributions of the n-particle resolvent (Green's function). In particular,

$$R_2^c(z)=\frac{1}{H_2-z}-\frac{1}{K_2-z}, \tag{10}$$

$$R_3^c(z)=\frac{1}{H_3-z}-\frac{1}{K_3-z}-\sum_{1\le i<j\le 3}\left[\frac{1}{K_3+v_{ij}-z}-\frac{1}{K_3-z}\right]. \tag{11}$$

The contour in both cases is clockwise around the spectrum of the respective resolvents (see Fig. 1). Note that the singularities of each resolvent are at the eigenvalues of the related Hamiltonian.

By deforming the contours as in Fig. 2 we can derive Beth-Uhlenbeck forms for b_2 and b_3:

$$b_2=\frac{1}{2!}\frac{2^{3/2}}{\lambda^3}\left[\sum_{m=1}^{N_2}e^{-\beta E_m^2}+\mathrm{Tr}_2\left[\frac{1}{2\pi i}\int_{c'} dz\, e^{-\beta z}R_2^c(z)\right]\right], \tag{12}$$

$$b_3=\frac{1}{3!}\frac{3^{3/2}}{\lambda^3}\left[\sum_{m=1}^{N_3}e^{-\beta E_m^3}+\mathrm{Tr}_3\left[\frac{1}{2\pi i}\int_{c'} dz\, e^{-\beta z}R_3^c(z)\right]\right], \tag{13}$$

where N_n is the number of n-body bound states. E_m^n is the mth n-body bound-state energy. (If $N_n=\infty$, then we must, strictly speaking, take a sequence of contours c_n', where c_n' encloses all but n of the bound-state poles and then take $n\to\infty$ at the end of the calculation. An alternative approach would be to regulate the potential with some parameter μ, which is zero for the actual potential, to ensure a finite number of bound states. μ is then taken to zero at the end of the calculation. Here we simply manipulate the expressions formally.)

The manipulations carried out to yield Eqs. (12) and (13) from Eqs. (8) and (9) provide a clue as to the origin of the divergences in the bound-state sum for the cases of interest. Let us illustrate these manipulations for general b_n:

$$b_n=\frac{1}{n!}\frac{n^{3/2}}{\lambda^3}\mathrm{Tr}_n\left[\frac{1}{2\pi i}\int_c dz\, e^{-\beta z}R_n^c(z)\right]$$

$$=\frac{1}{n!}\frac{n^{3/2}}{\lambda^3}\mathrm{Tr}_n\left[\sum_{m=1}^{N_n}e^{-\beta E_m^n}|\Psi_m\rangle\langle\Psi_m|+\frac{1}{2\pi i}\int_{c'} dz\, e^{-\beta z}R_n^c(z)\right] \tag{14}$$

$$=\frac{1}{n!}\frac{n^{3/2}}{\lambda^3}\left[\sum_{m=1}^{N_n}e^{-\beta E_m^n}+\mathrm{Tr}_n\left[\frac{1}{2\pi i}\int_{c'} dz\, e^{-\beta z}R_n^c(z)\right]\right], \tag{15}$$

where $|\Psi_m\rangle$ are the n-body bound-state eigenvectors. In going from Eq. (14) to Eq. (15) one implicitly assumes that the trace of a sum is the sum of the traces. This is true only if each of the latter traces exist. This is clearly not the case if the bound-state sum diverges. As such our starting point in the calculation of b_n must be Eq. (14). (This argument is, of course, formal in that it assumes the convergence of b_n. We shall give conditions when this

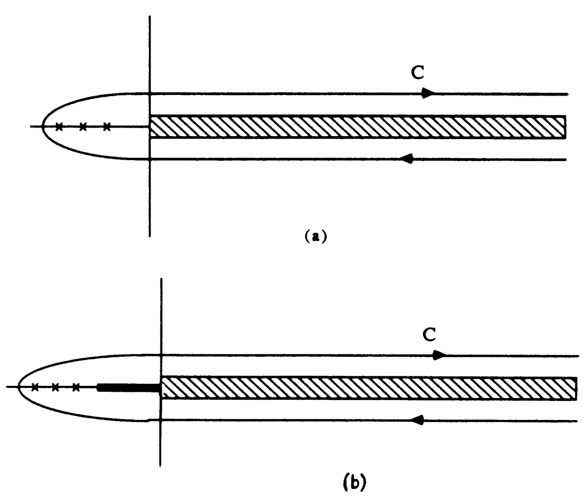

FIG. 1. (a) Contour for the Watson representation, Eq. (8). (b) Contour for the Watson representation, Eq. (9).

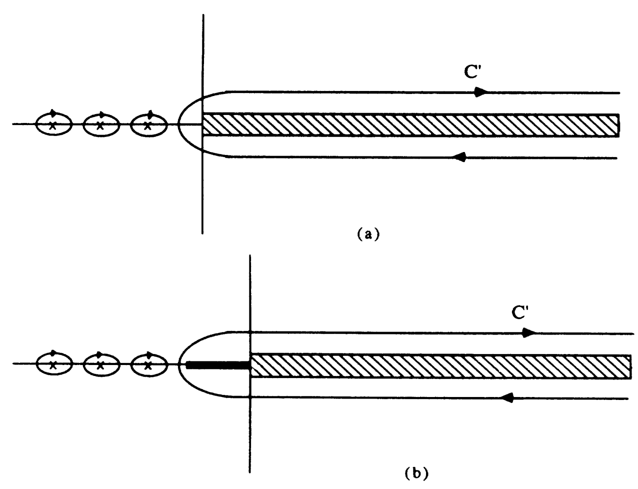

FIG. 2. (a) Deformation of contour in Fig. 1(a), which yields Eq. (12). (b) Deformation of contour in Fig. 1(b), which yields Eq. (13).

assumption is justified in Sec. V.)

Equation (14) is difficult to calculate with. It would be preferable to have an expression with the calculational advantages of the Beth-Uhlenbeck form. This form permits the evaluation of b_n with a knowledge solely of the bound-state energies and the continuum density of states. Equation (14) requires not only the eigenfunctions, but also requires that the bound-state and continuum contributions be combined before the trace can be evaluated. To derive a representation for b_n that is valid in the cases of interest and has essentially the calculational advantages of the Beth-Uhlenbeck form we follow a procedure originally due to Bollé.[4] However, in doing this we shall differ from Bollé's derivation in a number of regards.

Firstly, like Bollé, we manipulate the contour integral over C' in Eq. (14), essentially by adding and subtracting certain terms, to obtain an alternative expression. We then use the analytic and high-energy properties of the resolvent to rewrite the C' integration. This results in an expression for the argument of the trace in b_n (henceforth denoted as B_n) of the form

$$B_n = S_n + I_n ,$$

where S_n (I_n) is a modified bound-state (continuum) sum (integration). As Bollé has shown, the modification of the bound-state sum can be arranged to ensure that $\mathrm{Tr}_n(S_n)$ is convergent for the cases of interest. Bollé's use of the analytic and high-energy properties of the resolvent is somewhat indirect. Bollé, in a paper with Osborn,[9] used these properties to derive certain sum rules. Bollé's derivation of the Planck-Larkin structures is an application of these sum rules. We use the analytic and high-energy properties directly. In this respect, we differ with Bollé in only a cosmetic manner.

Another, more substantial point where we differ with Bollé is that we begin with a different representation for the high-energy series of the resolvent. It is this difference that renders our Planck-Larkin structures valid for strongly repulsive potentials. Working in a coordinate-space representation we calculate the high-energy expansion of the resolvent, as does Bollé, by evaluating the Laplace transform of a high-temperature expansion for the Boltzmann operator (the inverse of the Watson representation):

$$\langle \mathbf{x}|R_n(z)|\mathbf{x}'\rangle = \int_0^\infty e^{z\beta}\langle \mathbf{x}|e^{-\beta H_n}|\mathbf{x}'\rangle d\beta , \qquad \mathrm{Re}(z) < \inf\phi(H_n) \tag{16}$$

where $\phi(H_n)$ is the spectrum of H_n and $\mathbf{x}$ denotes the $3(n-1)$ relative coordinates.

The high-temperature expansion of $\langle \mathbf{x}|e^{-\beta H_n}|\mathbf{x}'\rangle$ that we use is essentially a renormalized version of the one Bollé uses. Bollé uses the asymptotic series derived by Wilk, Fujiwara, and Osborn[10]

$$\langle \mathbf{x}|e^{-\beta H_n}|\mathbf{x}'\rangle = \langle \mathbf{x}|e^{-\beta K_n}|\mathbf{x}'\rangle \sum_{m=0}^{\infty} \frac{(-\beta)^m}{m!} P_m^n(\mathbf{x},\mathbf{x}';q) , \tag{17}$$

where $q = \hbar^2/2m$ and the P_m^n are polynomials in the potential and its derivatives (as we shall not need these here, we refer the reader to the original work for the explicit form of these). We begin with a renormalized form of Eq. (17), derived in a another paper, also by Fujiwara, Osborn, and Wilk:[11]

$$\langle \mathbf{x}|e^{-\beta H_n}|\mathbf{x}'\rangle = \langle \mathbf{x}|e^{-\beta K_n}|\mathbf{x}'\rangle F_n(\mathbf{x},\mathbf{x}';\beta,q) , \tag{18}$$

where

$$\ln F_n(\mathbf{x},\mathbf{x}';\beta,q) = \sum_{m=1}^{\infty} \frac{(-\beta)^m}{m!} W_m^n(\mathbf{x},\mathbf{x}';q) ,$$

K_n is the n-body kinetic energy and the W_m^n are polynomials in the n-body potential energy and its derivatives. The evaluation of (16) with this for the Boltzmann factor is intractable. The evaluation can, however, be made if we use the expansion

$$F_n(\mathbf{x},\mathbf{x}';\beta,q) = e^{-\beta W_1^n(\mathbf{x},\mathbf{x}';q)} \sum_{m=0}^{\infty} \frac{(-\beta)^m}{m!} Q_m^n(\mathbf{x},\mathbf{x}';q) . \tag{19}$$

As we shall only need the diagonal elements, we write down the first few of these for reference:

$$\begin{aligned}
&W_1^n(\mathbf{x},\mathbf{x}';q) = V_n(\mathbf{x}) ,\\
&Q_0^n(\mathbf{x},\mathbf{x}';q) = 1 ,\\
&Q_1^n(\mathbf{x},\mathbf{x}';q) = 0 ,\\
&Q_2^n(\mathbf{x},\mathbf{x}';q) = -\tfrac{1}{3} q \Delta V_n(\mathbf{x}) ,\\
&Q_3^n(\mathbf{x},\mathbf{x}';q) = -\tfrac{1}{2} q [\nabla V_n(\mathbf{x})]^2 + \tfrac{1}{10} q^2 \Delta^2 V_n(\mathbf{x}) .
\end{aligned} \tag{20}$$

We refer the reader to the original papers for further details.

Substituting (19) into (16) we obtain

$$\langle \mathbf{x}|R_n(z)|\mathbf{x}'\rangle = \sum_{m=0}^{\infty} \frac{(-1)^m}{m!} Q_m^n(\mathbf{x},\mathbf{x}';q) \times \int_0^\infty e^{\beta(z - W_1^n)} \beta^m \langle \mathbf{x}|e^{-\beta K_n}|\mathbf{x}'\rangle d\beta . \tag{21}$$

Using the result

$$\langle \mathbf{x}|e^{-\beta K_n}|\mathbf{x}'\rangle = \frac{1}{(4\pi\beta q)^{d/2}} \exp\left[-\frac{(\mathbf{x}-\mathbf{x}')^2}{4\beta q} \right] , \tag{22}$$

where d is the dimension of the Laplacian [which is $3(n-1)$ here], we find that the β integral is identical to that in Eqs. (2.1)–(2.4) and (3.4) of Wilk, Fujiwara, and Osborn[10] except that z in their paper is replaced by $z - W_1^n$ to obtain the integral required here. With their result (which incorporates an analytic continuation) Eq. (21) becomes

$$\langle \mathbf{x}|R_n(z)|\mathbf{x}'\rangle = \frac{i\pi}{(4\pi q)^{d/2}}(z-W_1^n)^{d/2-1}\sum_{m=0}^{\infty}\frac{(-1)^m}{m!}Q_m^n(\mathbf{x},\mathbf{x}';q)\frac{1}{(z-W_1^n)^m}\left[\frac{\varepsilon_{W_1^n}}{2}\right]^{m+1-d/2}H^{(1)}_{d/2-1-m}(\varepsilon_{W_1^n}) , \tag{23}$$

where $\varepsilon_{W_1^n}=q^{-1/2}(z-W_1^n)^{1/2}|\mathbf{x}-\mathbf{x}'|$ and $H_i^{(1)}$ denotes the ith order Bessel function of the third kind.[12] This high-energy series is our starting point and it is here that the essential difference with the analysis of Bollé lies. Knowledge of the large-z behavior and the qualitative behavior of the singularity spectrum for the resolvents is all that we require. Let us now go on to derive the generalized Planck-Larkin structures.

III. PLANCK-LARKIN STRUCTURE FOR b_2

We begin with the coordinate representation of Eq. (14) for $n=2$:

$$b_2=\frac{1}{2!}\frac{2^{3/2}}{\lambda^3}\mathrm{Tr}_2\left[\sum_{m=1}^{N_2}e^{-\beta E_m}|\Psi_m(\mathbf{x})|^2+\frac{1}{2\pi i}\int_{c'}dz\, e^{-\beta z}\langle \mathbf{x}|R_2^c(z)|\mathbf{x}\rangle\right] \tag{24}$$

[Tr_n here and in similar contexts later denotes integration over the $3(n-1)$ dimensional configuration space]. The high-energy series for $R_2^c(z)$ is

$$\begin{aligned}\langle \mathbf{x}|R_2^c(z)|\mathbf{x}\rangle &= \langle \mathbf{x}|R_2(z)-R_0(z)|\mathbf{x}\rangle\\ &=\lim_{\Delta\to 0}\left\{\frac{i\pi}{(4\pi q)^{3/2}}\left[(z-W_1)^{1/2}\left[\frac{\varepsilon_{W_1}}{2}\right]^{-1/2}H^{(1)}_{1/2}(\varepsilon_{W_1})-z^{1/2}\left[\frac{\varepsilon_0}{2}\right]^{-1/2}H^{(1)}_{1/2}(\varepsilon_0)\right]\right.\\ &\quad\left.+\frac{\pi}{(4\pi q)^{3/2}}\sum_{m=2}^{\infty}\frac{1}{m!}\frac{Q_m(\mathbf{x},\mathbf{x}';q)}{(z-W_1)^{m-1/2}}\left[\frac{\varepsilon_{W_1}}{2}\right]^{m-1/2}H^{(1)}_{m-1/2}(\varepsilon_{W_1})\right\} ,\end{aligned} \tag{25}$$

where $\Delta=|\mathbf{x}-\mathbf{x}'|$ and on the $m\geq 2$ terms we have used the result

$$H^{(1)}_{-\nu}(z)=e^{i\pi\nu}H^{(1)}_{\nu}(z) . \tag{26}$$

In these expressions we have dropped superscripts from the Q's, W's, and E_m's as it is clear from the context that the two-body version of these quantities are being used. We shall follow this practice whenever confusion is unlikely to arise.

Anticipating the ultimate use of the high-energy series we construct the following auxiliary function:

$$\begin{aligned}F_N^{(2)}(z;\mathbf{x},q)=z^N&\left\{\langle \mathbf{x}|R_2^c(z)|\mathbf{x}\rangle-\lim_{\Delta\to 0}\frac{i\pi}{(4\pi q)^{3/2}}\left[(z-W_1)^{1/2}\left[\frac{\varepsilon_{W_1}}{2}\right]^{-1/2}H^{(1)}_{1/2}(\varepsilon_{W_1})-z^{1/2}\left[\frac{\varepsilon_0}{2}\right]^{-1/2}H^{(1)}_{1/2}(\varepsilon_0)\right]\right.\\ &\left.-\frac{\pi}{(4\pi q)^{3/2}}\sum_{m=2}^{N+1}\frac{1}{m!}\frac{Q_m(\mathbf{x},q)}{(z-V)^{m-1/2}}\frac{\Gamma(m-\frac{1}{2})}{i\pi}\right\} .\end{aligned} \tag{27}$$

Using Eq. (25), it is apparent that

$$|F_N^{(2)}|\underset{z\to\infty}{=}O\left[\frac{1}{|z|^{3/2}}\right] . \tag{28}$$

The analytic structure of $F_N^{(2)}$ is readily apparent from its defining expression. It has poles and cuts corresponding to those of the resolvent, square-root branch cuts from the arguments of the Hankel functions and the analytic structure of the $(z-V)^{-m+1/2}$ terms. These singularities all lie on the real axis. We define a contour C which encloses these singularities in a clockwise direction. Note that the $(z-V)^{1/2}$ cut will overtake the bound states for various configurations. The contour C thus goes beyond a value σ where $\sigma=\inf[V_2(\mathbf{x})]$. Henceforth we shall assume that all contours, unless stated otherwise, are over the contour C. With this change of contour Eq. (24) becomes

$$b_2=\frac{1}{2!}\frac{2^{3/2}}{\lambda^3}\mathrm{Tr}_2\left[\sum_{m=1}^{N_2}e^{-\beta E_m}|\Psi_m(\mathbf{x})|^2+\frac{1}{2\pi i}\int_c dz\, e^{-\beta z}\left[\langle \mathbf{x}|R_2^c(z)|\mathbf{x}\rangle-\sum_i\frac{|\Psi_i(\mathbf{x})|^2}{E_i-z}\right]\right] , \tag{29}$$

where the extension of the contour requires the subtraction of the pole terms. For future reference, we denote B_2 here schematically as

$$B_2=S_0+E_0 ,$$

where S_0 (E_0) denotes the sum (integral) in the argument of the trace in Eq. (29). Using our knowledge of $F_N^{(2)}$ we can now derive the Planck-Larkin structure for b_2.

From (27) we have

$$\langle \mathbf{x}|R_2^c(z)|\mathbf{x}\rangle = F_0^{(2)}(z;\mathbf{x},q) + \lim_{\Delta\to 0}\frac{i\pi}{(4\pi q)^{3/2}}\left[(z-W_1)^{1/2}\left[\frac{\varepsilon_{W_1}}{2}\right]^{-1/2} H_{1/2}^{(1)}(\varepsilon_{W_1}) - z^{1/2}\left[\frac{\varepsilon_0}{2}\right]^{-1/2} H_{1/2}^{(1)}(\varepsilon_0)\right]. \quad (30)$$

Substituting this into the argument of the trace in Eq. (29) we obtain

$$B_2 = \sum_{m=1}^{N_2} e^{-\beta E_m}|\Psi_m(\mathbf{x})|^2 + \frac{1}{2\pi i}\int_c dz\, e^{-\beta z}\left[F_0^{(2)}(z;\mathbf{x},q) - \sum_i \frac{|\Psi_i(\mathbf{x})|^2}{E_i - z}\right]$$
$$+\frac{1}{2\pi i}\int_c dz\, e^{-\beta z}\lim_{\Delta\to 0}\frac{i\pi}{(4\pi q)^{3/2}}\left[(z-W_1)^{1/2}\left[\frac{\varepsilon_{W_1}}{2}\right]^{-1/2} H_{1/2}^{(1)}(\varepsilon_{W_1}) - z^{1/2}\left[\frac{\varepsilon_0}{2}\right]^{-1/2} H_{1/2}^{(1)}(\varepsilon_0)\right]. \quad (31)$$

The second integral can be evaluated explicitly and this is done in Appendix A. With some further manipulation of the third term Eq. (31) becomes

$$B_2 = \sum_{m=1}^{N_2} e^{-\beta E_m}|\Psi_m(\mathbf{x})|^2 + \frac{1}{2^{3/2}}\frac{1}{\lambda^3}(e^{-\beta v_{12}}-1)$$
$$+\frac{1}{2\pi i}\int_c dz\, F_0^{(2)}(z;\mathbf{x},q) - \frac{1}{2\pi i}\int_c dz \sum_i \frac{|\Psi_i(\mathbf{x})|^2}{E_i - z}$$
$$+\frac{1}{2\pi i}\int_c dz(e^{-\beta z}-1)\left[F_0^{(2)}(z;\mathbf{x},q) - \sum_i \frac{|\Psi_i(\mathbf{x})|^2}{E_i - z}\right] \quad (32)$$
$$= \sum_{m=1}^{N_2}(e^{-\beta E_m}-1)|\Psi_m(\mathbf{x})|^2 + \frac{1}{2^{3/2}}\frac{1}{\lambda^3}(e^{-\beta v_{12}}-1)$$
$$+\frac{1}{2\pi i}\int_c dz(e^{-\beta z}-1)$$
$$\times\left[F_0^{(2)}(z;\mathbf{x},q) - \sum_i \frac{|\Psi_i(\mathbf{x})|^2}{E_i - z}\right], \quad (33)$$

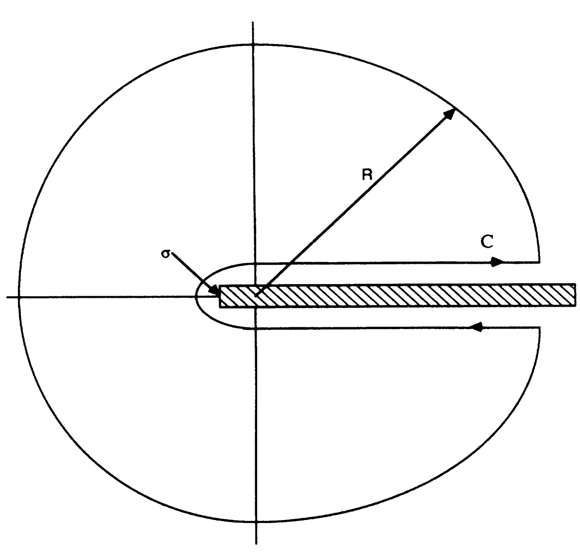

FIG. 3. Contour used to establish Eq. (34).

where the pole integrations in the fourth term are straightforward and we have used the result

$$\frac{1}{2\pi i}\int_c dz\, F_0^{(2)}(z;\mathbf{x},q) = 0 . \quad (34)$$

This result, which is essentially a restatement of one of the sum rules derived by Bollé and Osborn,[9] is readily verified by evaluating $F_0^{(2)}$ on the contour shown in Fig. 3 and taking $R\to\infty$. The contour over the arc vanishes in this limit by Eq. (28) yielding the result. Let us denote Eq. (33) in the following, schematic manner:

$$B_2 = S_1 + C_1 + E_1 .$$

If the trace of each individual term exists we can express b_2 as

$$b_2 = \frac{2^{3/2}}{2!\lambda^3}\sum_{m=1}^{N_2}(e^{-\beta E_m}-1) + \frac{1}{2!}\frac{1}{\lambda^6}\int d^3x\,(e^{-\beta v_{12}}-1)$$
$$+\frac{2^{3/2}}{2!\lambda^3}\mathrm{Tr}_2\left[\frac{1}{2\pi i}\int_c dz(e^{-\beta z}-1)\right.$$
$$\times\left[F_0^{(2)}(z;\mathbf{x},q)\right.$$
$$\left.\left.-\sum_i \frac{|\Psi_i(\mathbf{x})|^2}{E_i - z}\right]\right]. \quad (35)$$

We refer to Eq. (35) as the first-order Planck-Larkin structure for b_2. The second term here is precisely the classical expression for b_2.[1] As $\beta\to 0$, the classical term will dominate so that for sufficiently high temperature the bound-state sum, and the remainder term (i.e., E_1) will be negligible. In this expression the classical terms are convergent for potentials with strongly repulsive cores, unlike the expressions of Bollé. Note also that our treatment differs from that of Bollé in that it avoids the appearance of factors containing σ. Such factors hinder the usefulness of resulting Planck-Larkin expressions.

We can continue this construction. To do this we manipulate the remainder term in Eq. (33) as follows:

$$E_1=\frac{1}{2\pi i}\int_c dz(e^{-\beta z}-1)\left[F_0^{(2)}(z;\mathbf{x},q)-\sum_i\frac{|\Psi_i(\mathbf{x})|^2}{E_i-z}\right] \tag{36}$$

$$=\frac{1}{2\pi i}\int_c dz(e^{-\beta z}-1)\left[\frac{1}{z}F_1^{(2)}(z;\mathbf{x},q)-\sum_i\frac{|\Psi_i(\mathbf{x})|^2}{E_i-z}+\frac{\pi}{(4\pi q)^{3/2}}\frac{1}{2!}\frac{Q_2(\mathbf{x};q)}{(z-W_1)^{3/2}}\frac{\Gamma(\frac{3}{2})}{i\pi}\right] \tag{37}$$

$$=\frac{1}{2\pi i}\frac{\pi}{(4\pi q)^{3/2}}\frac{1}{2!}Q_2(\mathbf{x};q)\frac{\Gamma(\frac{3}{2})}{i\pi}\int_c dz\frac{(e^{-\beta z}-1)}{(z-W_1)^{3/2}}-\beta\frac{1}{2\pi i}\int_c dz\,F_1^{(2)}(z;\mathbf{x},q)$$
$$+\frac{1}{2\pi i}\int_c dz\sum_i\beta z\frac{|\Psi_i(\mathbf{x})|^2}{E_i-z}+\frac{1}{2\pi i}\int_c dz(e^{-\beta z}-1+\beta z)\left[\frac{1}{z}F_1^{(2)}(z;\mathbf{x},q)-\sum_i\frac{|\Psi_i(\mathbf{x})|^2}{E_i-z}\right]. \tag{38}$$

The first term in Eq. (38) is evaluated in Appendix A. The second term is zero by construction, in direct analogy to Eq. (34). Evaluation of the third term is straightforward. Collecting this result with the other terms in Eq. (33) we obtain

$$B_2=\sum_{m=1}^{N_2}(e^{-\beta E_m}-1+\beta E_m)|\Psi_m(\mathbf{x})|^2+\frac{1}{2^{3/2}}\frac{1}{\lambda^3}(e^{-\beta v_{12}}-1)+\frac{1}{2^{3/2}}\frac{1}{\lambda^3}\beta^2\frac{1}{2!}Q_2(\mathbf{x};q)e^{-\beta v_{12}}$$
$$+\frac{1}{2\pi i}\int_c dz(e^{-\beta z}-1+\beta z)\left[\frac{1}{z}F_1^{(2)}(z;\mathbf{x},q)-\sum_i\frac{|\Psi_i(\mathbf{x})|^2}{E_i-z}\right]. \tag{39}$$

We denote this schematically as

$$B_2=S_2+C_2+E_2\ .$$

If the trace of each individual term exists we can thus express b_2 as

$$b_2=\frac{2^{3/2}}{2!\lambda^3}\sum_{m=1}^{N_2}(e^{-\beta E_m}-1+\beta E_m)+\frac{1}{2!}\frac{1}{\lambda^6}\int d^3x(e^{-\beta v_{12}}-1)+\frac{1}{2!}\frac{1}{\lambda^6}\beta^2\frac{1}{2!}\int d^3x Q_2(\mathbf{x};q)e^{-\beta v_{12}}$$
$$+\frac{2^{3/2}}{2!\lambda^3}\frac{1}{2\pi i}\mathrm{Tr}_2\left[\int_c dz(e^{-\beta z}-1+\beta z)\left[\frac{1}{z}F_1^{(2)}(z;\mathbf{x},q)-\sum_i\frac{|\Psi_i(\mathbf{x})|^2}{E_i-z}\right]\right]. \tag{40a}$$

We refer to this expression as the second-order Planck-Larkin structure for b_2.

We can continue this construction. Using the result

$$\int_c dz\left[e^{-\beta z}-1+\beta z+\cdots-(-1)^{p-1}\frac{(\beta z)^{p-1}}{(p-1)!}\right](z-W_1)^{-p-1/2}=2e^{-\beta W_1}\beta^{p-1/2}\Gamma(\tfrac{1}{2}-p) \tag{40b}$$

(readily proven by induction from the $p=1$ case given in Appendix A) one can obtain by induction a pth-order representation for B_2

$$B_2=S_p+C_p+F_p\ .$$

If the individual traces exist we obtain

$$b_2=\frac{2^{3/2}}{2!\lambda^3}\sum_{m=1}^{N_2}\left[e^{-\beta E_m}-1+\beta E_m-\cdots-(-1)^{p-1}\frac{(\beta E_m)^{p-1}}{(p-1)!}\right]$$
$$+\frac{1}{2!}\frac{1}{\lambda^6}\int d^3x(e^{-\beta v_{12}}-1)+\frac{1}{2!}\frac{1}{\lambda^6}\sum_{m=2}^{p}\frac{(-\beta)^m}{m!}\int d^3x Q_m(\mathbf{x};q)e^{-\beta v_{12}}$$
$$+\frac{2^{3/2}}{2!\lambda^3}\frac{1}{2\pi i}\mathrm{Tr}_2\left[\int_c dz\left[e^{-\beta z}-1+\beta z+\cdots-(-1)^{p-1}\frac{(\beta z)^{p-1}}{(p-1)!}\right]\left[\frac{1}{z^{p-1}}F_{p-1}^{(2)}(z;\mathbf{x},q)-\sum_i\frac{|\Psi_i(\mathbf{x})|^2}{E_i-z}\right]\right], \tag{41}$$

which is referred to as the pth-order Planck-Larkin structure for b_2. If the remainder term tends to zero as $p\to\infty$, then in this limit

$$b_2=\frac{1}{2!}\frac{1}{\lambda^6}\int d^3x(e^{-\beta v_{12}}-1)$$
$$+\frac{1}{2!}\frac{1}{\lambda^6}\sum_{m=2}^{\infty}\frac{(-\beta)^m}{m!}\int d^3x Q_m(\mathbf{x};q)e^{-\beta v_{12}}\ . \tag{42}$$

This is the Wigner-Kirkwood series for b_2, which is directly obtainable from Eq. (19). The $p\to\infty$ limit thus provides a check on our procedure. If the remainder does not tend to zero, then the Wigner-Kirkwood series is asymptotic and our construction must be terminated at some optimally chosen p.

If we denote $C_0=0$, then this section has done nothing more than provide a class of representations for B_2

$$B_2 = S_p + C_p + E_p \ .$$

In the usual representation, $p=0$, $\mathrm{Tr}_2(S_0)$ does not exist for the cases of interest. The hope behind the construction of this class of representations is that for some p, the trace of each individual term will exist. This would establish the convergence of b_2 for the cases of interest and simultaneously provide a convenient representation of b_2 for calculational purposes.

For b_2 we have one example with which to test this program, the Coulomb interaction. In this case we readily observe that

$$\mathrm{Tr}_2(S_p) < \infty$$

for $p \geq 2$. Unfortunately, the trace of C_p for all $p \geq 2$ is still divergent due to the long-range nature of the Coulomb force. In the full, two-component, charge neutral theory, this infrared divergence is only reduced from quadratic to linear. The persistence of divergences in the Coulomb problem is not surprising. Such divergences also occur in the fully classical problem and are taken to be indicative of collective behavior such as screening.[13,14] They are removed by partial summation. The divergences here would appear then to correspond to the semiclassical corrections to this collective behavior. We shall have more to say about this in Sec. VI. Even if we could remove these divergences we would still have to determine the behavior of the trace of E_p. This would be most difficult and would take us far afield. Such a task thus requires a separate study. Thus the Planck-Larkin structure, although improving the situation for the Coulomb case by rendering the bound-state sum finite, does not shed any light on whether the Coulomb b_2 is convergent. With the experience of this section we go on now to find Planck-Larkin representations for b_3 and higher cluster coefficients.

IV. PLANCK-LARKIN STRUCTURE FOR b_3 AND HIGHER CLUSTER COEFFICIENTS

The calculation of the Planck-Larkin structure for b_3 is the calculation we are most interested in because of its applications to the case of the Efimov point. The construction follows analogously to that of Sec. III:

$$b_3 = \frac{1}{3!}\frac{3^{3/2}}{\lambda^3}\mathrm{Tr}_3\left[\sum_{m=1}^{N_3} e^{-\beta E_m}|\Psi_m(\mathbf{x})|^2 + \frac{1}{2\pi i}\int_{c'} dz\, e^{-\beta z}\langle \mathbf{x}|R_3^c(z)|\mathbf{x}\rangle\right], \tag{43}$$

where

$$\langle \mathbf{x}|R_3^c(z)|\mathbf{x}\rangle = \left\langle \mathbf{x}\left|\frac{1}{H_3-z}-\frac{1}{K_3-z}-\sum_{1\leq i<j\leq 3}\left[\frac{1}{K_3+v_{ij}-z}-\frac{1}{K_3-z}\right]\right|\mathbf{x}\right\rangle \tag{44}$$

$$\begin{aligned}
&= \lim_{z\to\infty}\lim_{\Delta\to 0}\frac{i\pi}{(4\pi q)^3}\left\{(z-W_1)^2\left[\frac{\varepsilon_{W_1}}{2}\right]^{-2}H_2^{(1)}(\varepsilon_{W_1}) - z^2\left[\frac{\varepsilon_0}{2}\right]^{-2}H_2^{(1)}(\varepsilon_0)\right.\\
&\qquad\left. -\sum_\alpha\left[(z-W_1^\alpha)^2\left[\frac{\varepsilon_{W_1^\alpha}}{2}\right]^{-2}H_2^{(1)}(\varepsilon_{W_1^\alpha}) - z^2\left[\frac{\varepsilon_0}{2}\right]^{-2}H_2^{(1)}(\varepsilon_0)\right]\right\}\\
&\quad+\lim_{\Delta\to 0}\frac{i\pi}{(4\pi q)^3}\sum_{m=2}^{\infty}\frac{1}{m!}\left[\frac{Q_m(\mathbf{x},\mathbf{x}';q)}{(z-W_1)^{m-2}}\left[\frac{\varepsilon_{W_1}}{2}\right]^{m-2}H_{m-2}^{(1)}(\varepsilon_{W_1})\right.\\
&\qquad\left.-\sum_\alpha\frac{Q_m^\alpha(\mathbf{x},\mathbf{x}';q)}{(z-W_1^\alpha)^{m-2}}\left[\frac{\varepsilon_{W_1^\alpha}}{2}\right]^{m-2}H_{m-2}^{(1)}(\varepsilon_{W_1^\alpha})\right]\ .
\end{aligned} \tag{45}$$

Here, as is standard in the three-body problem, we use the odd person out notation $v_1 = v_{23}$ and cyclic. Also the α sum is from 1 to 3. Q_m^α is the same as Q_m except that the full three-particle potential energy V_3 in the latter is replaced by v_α to obtain the former.

The auxiliary function for the derivation of the Planck-Larkin structure of b_3 is

$$F_N^{(3)}(z;\mathbf{x},q) = z^N\left[r(z;\mathbf{x},q) - \frac{1}{(4\pi q)^3}\sum_{m=3}^{N+3}\frac{\Gamma(m-2)}{m!}\left[\frac{Q_m(\mathbf{x},q)}{(z-W_1)^{m-2}} - \sum_\alpha\frac{Q_m^\alpha(\mathbf{x},q)}{(z-W_1^\alpha)^{m-2}}\right]\right], \tag{46}$$

where

$$r(z;\mathbf{x},q)=\lim_{\Delta\to 0}\Bigg[\langle \mathbf{x}|R_3^c(z)|\mathbf{x}'\rangle-\frac{i\pi}{(4\pi q)^3}\Bigg\{(z-W_1)^2\left[\frac{\varepsilon_{W_1}}{2}\right]^{-2}H_2^{(1)}(\varepsilon_{W_1})-z^2\left[\frac{\varepsilon_0}{2}\right]^{-2}H_2^{(1)}(\varepsilon_0)$$
$$-\sum_\alpha\left[(z-W_1^\alpha)^2\left[\frac{\varepsilon_{W_1^\alpha}}{2}\right]^{-2}H_2^{(1)}(\varepsilon_{W_1^\alpha})-z^2\left[\frac{\varepsilon_0}{2}\right]^{-2}H_2^{(1)}(\varepsilon_0)\right]\Bigg\}$$
$$-\frac{i\pi}{(4\pi q)^3}\frac{1}{2!}\left[Q_2(\mathbf{x},\mathbf{x}';q)H_0^{(1)}(\varepsilon_{W_1})-\sum_\alpha Q_2^\alpha(\mathbf{x},\mathbf{x}';q)H_0^{(1)}(\varepsilon_{W_1^\alpha})\right]\Bigg] \tag{47}$$

We have split $F_N^{(3)}$, Eq. (46), into two terms. The second term comes from the $m=3$ to $N+3$ terms in Eq. (45) in which the $\Delta\to 0$ can be explicitly taken. The other terms in $F_N^{(3)}$, $r(z;\mathbf{x},q)$, comprise those terms where the $\Delta\to 0$ limit is most readily taken after the contour integration we shall be doing.

By construction

$$|F_N^{(3)}|_{z\to\infty}=O\left[\frac{1}{|z|^2}\right]. \tag{48}$$

The analytic structure of $F_N^{(3)}$ comprises that of the three-body resolvent, the square-root branch cuts in the arguments of the Hankel functions in $r(z;\mathbf{x},q)$ and the poles at W_1 and W_1^α in Eq. (46). We define a contour C that wraps clockwise around the singularities of $F_N^{(3)}$. C goes beyond a value σ where now $\sigma=\inf V_3(\mathbf{x})$. Here $\mathbf{x}$ represents the six relative degrees of freedom in the three-body problem.

To calculate the first-order Planck-Larkin structure, we proceed as in Sec. III. From Eq. (46) we have that

$$F_0^{(3)}(z;\mathbf{x},q)=r(z;\mathbf{x},q)-\frac{1}{(4\pi q)^3}\frac{1}{3!}\left[Q_3(\mathbf{x},q)\frac{1}{z-W_1}-\sum_\alpha Q_3^\alpha(\mathbf{x},q)\frac{1}{z-W_1^\alpha}\right]. \tag{49}$$

Thus the argument of the trace in Eq. (43) becomes

$$B_3=\sum_{m=1}^{N_3}e^{-\beta E_m}|\Psi_m(\mathbf{x})|^2+\frac{1}{2\pi i}\int_c dz\,e^{-\beta z}\left[\langle\mathbf{x}|R_3^c(z)|\mathbf{x}\rangle-\sum_i\frac{|\Psi_i(\mathbf{x})|^2}{E_i-z}\right]$$
$$=\sum_{m=1}^{N_3}e^{-\beta E_m}|\Psi_m(\mathbf{x})|^2+\frac{1}{2\pi i}\int_c dz\,e^{-\beta z}\left[F_0^{(3)}(z;\mathbf{x},q)-\sum_i\frac{|\Psi_i(\mathbf{x})|^2}{E_i-z}\right]$$
$$+\frac{1}{2\pi i}\lim_{\Delta\to 0}\frac{i\pi}{(4\pi q)^3}\int_c dz\,e^{-\beta z}\Bigg\{(z-W_1)^2\left[\frac{\varepsilon_{W_1}}{2}\right]^{-2}H_2^{(1)}(\varepsilon_{W_1})-z^2\left[\frac{\varepsilon_0}{2}\right]^{-2}H_2^{(1)}(\varepsilon_0)$$
$$-\sum_\alpha\left[(z-W_1^\alpha)^2\left[\frac{\varepsilon_{W_1^\alpha}}{2}\right]^{-2}H_2^{(1)}(\varepsilon_{W_1^\alpha})-z^2\left[\frac{\varepsilon_0}{2}\right]^{-2}H_2^{(1)}(\varepsilon_0)\right]\Bigg\}$$
$$+\frac{1}{2\pi i}\lim_{\Delta\to 0}\frac{i\pi}{(4\pi q)^3}\int_c dz\,e^{-\beta z}\frac{1}{2!}\left[Q_2(\mathbf{x},\mathbf{x}';q)H_0^{(1)}(\varepsilon_{W_1})-\sum_\alpha Q_2^\alpha(\mathbf{x},\mathbf{x}';q)H_0^{(1)}(\varepsilon_{W_1^\alpha})\right]$$
$$+\frac{1}{2\pi i}\frac{1}{(4\pi q)^3}\frac{1}{3!}\left[Q_3(\mathbf{x},q)\int_c dz\frac{e^{-\beta z}}{z-W_1}-\sum_\alpha Q_3^\alpha(\mathbf{x},q)\int_c dz\frac{e^{-\beta z}}{z-W_1^\alpha}\right]. \tag{50}$$

The $\Delta\to 0$ limits can be taken separately as each contour integral separately exists in this limit. The calculation of the third and fourth terms is outlined in Appendix A. The fifth term is trivially evaluated. We obtain

$$B_3=\sum_{m=1}^{N_3}e^{-\beta E_m}|\Psi_m(\mathbf{x})|^2+\frac{1}{2\pi i}\int_c dz\,e^{-\beta z}\left[F_0^{(3)}(z;\mathbf{x},q)-\sum_i\frac{|\Psi_i(\mathbf{x})|^2}{E_i-z}\right]$$
$$+\frac{1}{3^{3/2}}\frac{1}{\lambda^6}\left[e^{-\beta(v_{12}+v_{23}+v_{31})}-1-\sum_\alpha(e^{-\beta v_\alpha}-1)\right]+\frac{1}{2!}\frac{1}{3^{3/2}}\beta^2\frac{1}{\lambda^6}\left[Q_2(\mathbf{x},q)e^{-\beta(v_{12}+v_{23}+v_{31})}-\sum_\alpha Q_2^\alpha(\mathbf{x},q)e^{-\beta v_\alpha}\right]$$
$$-\frac{1}{3!}\frac{1}{3^{3/2}}\beta^3\frac{1}{\lambda^6}\left[Q_3(\mathbf{x},q)e^{-\beta(v_{12}+v_{23}+v_{31})}-\sum_\alpha Q_3^\alpha(\mathbf{x},q)e^{-\beta v_\alpha}\right]. \tag{51}$$

In (51)

$$\frac{1}{2\pi i}\int_c dz\, e^{-\beta z}\left[F_0^{(3)}(z;\mathbf{x},q)-\sum_i \frac{|\Psi_i(\mathbf{x})|^2}{E_i-z}\right]=-\sum_{m=1}^{N_3}|\Psi_m(\mathbf{x})|^2+\frac{1}{2\pi i}\int_c dz(e^{-\beta z}-1)\left[F_0^{(3)}(z;\mathbf{x},q)-\sum_i \frac{|\Psi_i(\mathbf{x})|^2}{E_i-z}\right] \tag{52}$$

as

$$\frac{1}{2\pi i}\int_c dz\, F_0^{(3)}(z;\mathbf{x},q)=0\ , \tag{53}$$

in direct analogy with Eq. (34). We now have a representation for B_3 of the form

$$B_3=S_1+C_1+E_1\ .$$

If we can take the trace term by term we obtain the first-order Planck-Larkin structure for b_3

$$b_3=\frac{3^{3/2}}{3!\lambda^3}\sum_{m=1}^{N_3}(e^{-\beta E_m}-1)+\frac{3^{3/2}}{3!\lambda^3}[\mathrm{Tr}_3(C_1)+\mathrm{Tr}_3(E_1)]\ , \tag{54}$$

where

$$\frac{3^{3/2}}{3!\lambda^3}\mathrm{Tr}_3(C_1)=\frac{1}{3!}\frac{1}{\lambda^9}\left[\mathrm{Tr}_3\left[e^{-\beta(v_{12}+v_{23}+v_{31})}-1-\sum_\alpha(e^{-\beta v_\alpha}-1)\right]\right.$$
$$\left.+\sum_{m=2}^{3}\frac{(-1)^m}{m!}\beta^m\mathrm{Tr}_3\left[Q_m(\mathbf{x},q)e^{-\beta(v_{12}+v_{23}+v_{31})}-\sum_\alpha Q_m^\alpha(\mathbf{x},q)e^{-\beta v_\alpha}\right]\right]\ . \tag{55}$$

Note that if we write $f_\alpha=e^{-\beta v_\alpha}-1$, then the first term on the right-hand side of Eq. (55) is the classical expression for b_3.[1] Also

$$\mathrm{Tr}_3(E_1)=\frac{1}{2\pi i}\int_c dz(e^{-\beta z}-1)\mathrm{Tr}_3\left[F_0^{(3)}(z;\mathbf{x},q)-\sum_i\frac{|\Psi_i(\mathbf{x})|^2}{E_i-z}\right]\ . \tag{56}$$

As with B_2 we can continue to get pth-order representations of B_3 and the corresponding pth-order Planck-Larkin structures. As the derivation is a straightforward generalization of Sec. III we simply quote the pth-order Planck-Larkin structures for b_3:

$$b_3=\frac{3^{3/2}}{3!\lambda^3}\sum_{m=1}^{N_3}\left[e^{-\beta E_m}-1+\beta E_m-\cdots-(-1)^{p-1}\frac{(\beta E_m)^{p-1}}{(p-1)!}\right]+\frac{3^{3/2}}{3!\lambda^3}[\mathrm{Tr}_3(C_p)+\mathrm{Tr}_3(E_p)]\ , \tag{57}$$

where

$$\frac{3^{3/2}}{3!\lambda^3}\mathrm{Tr}_3(C_p)=\frac{1}{3!}\frac{1}{\lambda^9}\left[\mathrm{Tr}_3\left[e^{-\beta(v_{12}+v_{23}+v_{31})}-1-\sum_\alpha(e^{-\beta v_\alpha}-1)\right]\right.$$
$$\left.+\sum_{m=2}^{p+2}\frac{(-1)^m}{m!}\beta^m\mathrm{Tr}_3\left[Q_m(\mathbf{x},q)e^{-\beta(v_{12}+v_{23}+v_{31})}-\sum_\alpha Q_m^\alpha(\mathbf{x},q)e^{-\beta v_\alpha}\right]\right]$$

and

$$\mathrm{Tr}_3(E_p)=\frac{1}{2\pi i}\int_c dz\left[e^{-\beta z}-1+\beta z-\cdots-(-1)^{p-1}\frac{(\beta z)^{p-1}}{(p-1)!}\right]\left[\frac{1}{z^{p-1}}F_{p-1}^{(3)}(z;\mathbf{x},q)-\sum_i\frac{|\Psi_i(\mathbf{x})|^2}{E_i-z}\right]\ . \tag{58}$$

Again we recover the Wigner-Kirkwood expansion in the $p\to\infty$ limit.

For the Coulomb problem this construction throws as much light on the convergence of b_3 as the analogous construction does for b_2. As such the comments made for the Coulomb b_2 apply here. For the case of the Efimov point, the picture is a little more rosy. Here we have both

$$\mathrm{Tr}_3(S_p)<\infty \quad \text{for } p\geq 1\ ,$$

$$\mathrm{Tr}_3(C_p)<\infty \quad \text{for all } p$$

(where the latter condition is not satisfied in Bollé's Planck-Larkin structures for strongly repulsive potentials). The manifest divergences, which previously caused concern, are thus absent in the generalized Planck-Larkin structures. The behavior of $\mathrm{Tr}_3(E_p)$, however, remains unknown. E_p involves the full three-particle resolvent at the Efimov point. This is a complicated object of which, to the best of our knowledge, little is known. As a consequence, the direct examination of $\mathrm{Tr}_3(E_p)$ is a difficult task whose pursual would take us far afield. However, without knowledge of its behavior, the application of the

Planck-Larkin structures is conditional. In Sec. V we shall take up the behavior of $\mathrm{Tr}_3(E_p)$ in a somewhat indirect manner, showing that b_3 is finite and that, as a consequence, the first-order Planck-Larkin structure is a valid representation of it. Before we do this we consider the results for general b_n.

The arguments of this and the previous section are readily extended to general b_n. The calculation of the even cluster coefficients follows that of b_2, involving half-integer–order Hankel functions while the calculation of the odd cluster coefficients follows that of b_3, involving integer-order Hankel functions. The only portions of the expressions derived that differ nontrivially for different n are the number of classical terms in the pth-order Planck-Larkin structures and the form of the auxiliary function. We simply quote the results. The pth-order Planck-Larkin structure for b_n is

$$b_n=\frac{n^{3/2}}{n!\lambda^3}\sum_{m=1}^{N_n}\left[e^{-\beta E_m}-1+\beta E_m-\cdots-(-1)^{p-1}\frac{(\beta E_m)^{p-1}}{(p-1)!}\right]+\frac{n^{3/2}}{n!\lambda^3}\mathrm{Tr}_n(C_p)+\frac{n^{3/2}}{n!\lambda^3}\mathrm{Tr}_n(E_p)\ , \tag{59}$$

where

$$\frac{n^{3/2}}{n!\lambda^3}\mathrm{Tr}_n(C_p)=\frac{1}{n!}\frac{1}{\lambda^{3n}}\left[\mathrm{Tr}_n[e^{-\beta V}]_c+\sum_{m=2}^{p+s}\frac{(-1)^m}{m!}\beta^m\mathrm{Tr}_n[Q_m(\mathbf{x},q)e^{-\beta V}]_c\right] \tag{60}$$

and

$$E_p=\frac{1}{2\pi i}\int_c dz\left[e^{-\beta z}-1+\beta z-\cdots-(-1)^{p-1}\frac{(\beta z)^{p-1}}{(p-1)!}\right]\times\left[\frac{1}{z^{p-1}}F_{p-1}^{(n)}(z;\mathbf{x},q)-\sum_i\frac{|\Psi_i(\mathbf{x})|^2}{E_i-z}\right], \tag{61}$$

where $s=\frac{3}{2}n-3$ $(\frac{3}{2}n-\frac{5}{2})$ for n even (odd). $[A]_c$ denotes the connected part of A. The corresponding auxiliary function is

$$F_N^{(n)}(z;\mathbf{x},q)=z^N\left[r^n(z;\mathbf{x},q)-\frac{a}{(4\pi q)^{(3/2)(n-1)}}\sum_{m=b}^{N+b}\frac{\Gamma(m+1-d)}{m!}\left[\frac{Q_m(\mathbf{x},q)}{(z-W_1)^{m+1-d}}\right]_c\right], \tag{62}$$

where

$$a=(-1)^{(3/2)n-1/2}\quad\text{for } n \text{ odd}$$
$$=i(-1)^{(3/2)n}\quad\text{for } n \text{ even}\ ,$$
$$b=\tfrac{3}{2}(n-1)\quad\text{for } n \text{ odd}$$
$$=\tfrac{3}{2}n-2\quad\text{for } n \text{ even}\ ,$$
$$d=\tfrac{3}{2}(n-1)\ ,$$

and

$$r^n(z;\mathbf{x},q)=\lim_{\Delta\to 0}\left\{\langle\mathbf{x}|R_n^c(z)|\mathbf{x}'\rangle-\frac{i\pi}{(4\pi q)^{(3/2)(n-1)}}\sum_{m=0}^{b-1}\frac{(-1)^m}{m!}\left[Q_m(\mathbf{x},\mathbf{x}';q)\frac{1}{(z-W_1)^{m-(3/2)n+5/2}}\times\left[\frac{\varepsilon_{W_1}}{2}\right]^{m-(3/2)n+5/2}H^{(1)}_{(3/2)n-5/2-m}(\varepsilon_{W_1})\right]_c\right\}. \tag{63}$$

V. BEHAVIOR OF $\mathrm{Tr}_n(E_p)$

Sections III and IV have done nothing more than to derive a class of partitions for B_n of the form

$$B_n=S_p+C_p+E_p\ . \tag{64}$$

As we have seen, we have insufficient knowledge of E_p to determine, from this partition, the behavior of the cluster coefficients. The further information required, as we have pointed out, can be obtained only with considerable effort. Such effort demands a separate study. For the case of the Efimov point, however, we can obtain the further information required with only a little extra effort by using an alternative approach.

The idea is simple. The further information required in the case of the Efimov point is the behavior of $\mathrm{Tr}_3(E_p)$. Let us rearrange our usual expression for B_n

$$E_p=B_n-S_p-C_p\ . \tag{65}$$

It is clear from this that if we can establish the convergence of the trace of B_n independently, then $\mathrm{Tr}_3(E_p)$ is convergent for $p>0$. As a result, the trace of each term on the right-hand side of Eq. (64) is convergent. One can then take the trace of B_n term by term. It follows that the corresponding Planck-Larkin structure is well behaved. This alternative approach separates our two main issues. The original approach attempted to use the partitions of B_n to simultaneously establish the convergence of b_n as well as yield replacements for the ill-defined Beth-Uhlenbeck form. This alternative approach seeks to establish the convergence of b_n separately, without being concerned with explicit representations, and then use this to validate our Planck-Larkin expressions through the argument above. We were motivated to consider this alternative in the hope that the literature on rigorous results in statistical mechanics contained quantum analogs of the well-known theorems for the thermodynamic limit of the classical cluster coefficients. While we had some confidence that the quantum generalizations did exist, we felt that the unusual behavior of the cases of interest would result in their exclusion from these theorems. We have found that existence theorems for quantum cluster coefficients are implicit in some results of Ginibre.[5] Not surprisingly, the conditions on Ginibre's results are not satisfied for the Coulomb problem. Somewhat to our surprise, however, the conditions are satisfied in the case of the Efimov point. As a result of this and our argument above, the Planck-Larkin structures for $p>0$ provide well-defined expressions for the convergent third cluster coefficient at the Efimov point.

To demonstrate the assertions made above we consider Ginibre's results in some detail. The main result is given as a theorem (of which we refer the reader to Ginibre[5] for further details).

Theorem. Consider a system of particles interacting pairwise via a pair potential $\Phi(\mathbf{x})$. If $\Phi(\mathbf{x})$ satisfies the following conditions, (a) $\Phi(\mathbf{x})$ is continuous for all $\mathbf{x}$ (except perhaps at the origin) and $\Phi(\mathbf{x})=\Phi(-\mathbf{x})$; (b) (stability) $\sum_{1\le i<j\le m}\Phi(\mathbf{x}_i-\mathbf{x}_j)\ge -mB$ for some B; and (c) $\int_{|\mathbf{x}|>c}d^3x\,|\Phi(\mathbf{x})|<\infty$ for some $c>0$, then (i) the finite-volume reduced density matrices of the system are analytic functions of the fugacity for $|z|<R$ where $R>0$ and (ii) for $|z|<R$ the infinite-volume limit of the reduced density matrices exists. The convergence is uniform for $|z|<R'<R$ and thus the limit is analytic in this region.

Note that there is no explicit expression for R. In other versions of the theorem, which have somewhat stronger conditions on the potential, an explicit expression can be found. These conditions are not satisfied for the cases of interest here. Note also that the strongly repulsive intermolecular potentials with which we are concerned satisfy the above conditions. The Coulomb potential does not.

The diagonal part of the one-particle reduced density matrix (which is constant by translational invariance) is simply the average density. As such the power series in z, referred to in part (ii) of the theorem above, is simply the second Mayer equation [Eq. (1(b)]. As a result (ii) implies that the cluster coefficients are convergent. (We use the term "cluster coefficient" here to denote the infinite-volume limit of the finite-volume cluster coefficients as this is the meaning we have implicitly attached to this term in the sections prior to this one.) Actually, although it is not explicitly stated, Ginibre essentially proves the existence of the cluster coefficients in the process of establishing (ii). However, because Ginibre's proof is quite technical and involved, it is somewhat difficult to see this. To assist the interested reader we provide in Appendix B a guided tour of Ginibre's work, emphasizing the elements we require. The remarkable aspect of Ginibre's theorem is that its conditions are independent of properties of a quantum-mechanical nature. This is possible because the theorem is established using path integral representations for operators. As a result the presence of the Efimov effect does not spoil the result. (One of the motivations of the work of Hoogeveen and Tjon[3] was the concern that if a system was even near the Efimov point, let alone at it, that this may effect the convergence of the cluster expansion. Ginibre's results show that this is not the case.)

VI. DISCUSSION

We would like to conclude with some comments together with some discussion concerning further work to be done. In Sec. V we demonstrated that $\mathrm{Tr}_3(E_p)$ is convergent at the Efimov point for $p\ge 1$. As we have pointed out we can use this result to say something about the behavior of the three-particle resolvent at the Efimov point. This can be done by considering the $p=1$ and $p=0$ remainder terms. Let us first consider the $p=1$ term. We know that

$$\mathrm{Tr}_3\left[\frac{1}{2\pi i}\int_c dz(e^{-\beta z}-1)\left[F_0^{(3)}(z;\mathbf{x},q)-\sum_i\frac{|\Psi_i(\mathbf{x})|^2}{E_i-z}\right]\right]<\infty\ . \tag{66}$$

Since

$$\mathrm{Tr}_3\left[\frac{1}{2\pi i}\int_c dz\,F_0^{(3)}(z;\mathbf{x},q)\right]$$

and

$$\mathrm{Tr}_3\left[\frac{1}{2\pi i}\int_c dz\,e^{-\beta z}[F_0^{(3)}(z;\mathbf{x},q)-\langle\mathbf{x}|R_c^3(z)|\mathbf{x}\rangle]\right] \tag{67}$$

are both convergent (they have been explicitly calculated) Eq. (66) implies that

$$\mathrm{Tr}_3\left[\frac{1}{2\pi i}\int_{c'}dz\,e^{-\beta z}\langle\mathbf{x}|R_3^c(z)|\mathbf{x}\rangle+\sum_i|\Psi_i(\mathbf{x})|^2\right]<\infty\ , \tag{68}$$

where we have reverted to the contour used in Fig. 2. Comparing this to the $p=0$ case

$$\mathrm{Tr}_3\left[\frac{1}{2\pi i}\int_{c'} dz\, e^{-\beta z}\langle \mathbf{x}|R_3^c(z)|\mathbf{x}\rangle\right]=\infty \ , \tag{69}$$

we can explicitly observe the counterterm required to ensure the convergence of the continuum integration. Note that we have formally evaluated a contour integral to obtain the second term in the argument of the trace in Eq. (68). Strictly speaking, we cannot do this. The reason is that we do not know whether the divergence, which the counterterm removes, is in the trace or whether it is in the contour integral. If it is in the trace, then Eqs. (68) and (69) are the ones that illustrate the removal of the divergence. We are inclined to think, however, that the divergence is in the small-z behavior of the resolvent and that the counterterm to this divergence is the sum over the bound states in Eq. (66).

With regards to the Efimov point, as we have stated a number of times, our aim has been to (a) establish the behavior of b_3 and (b) if b_3 is convergent, to find a replacement for the Beth-Uhlenbeck form. We have followed the previous work of Bollé in order to pursue these aims. The reader may have noticed, however, that in the argument above the convergent terms in Eq. (67) exactly cancel the classical terms, resulting in

$$b_3=\frac{3^{3/2}}{3!\lambda^3}\left\{\sum_{m=1}^{N_3}(e^{-\beta E_m}-1)+\mathrm{Tr}_3\left[\frac{1}{2\pi i}\int_c dz\, e^{-\beta z}\left[\langle \mathbf{x}|R_3^c(z)|\mathbf{x}\rangle-\sum_i\frac{|\Psi_i(\mathbf{x})|^2}{E_i-z}\right]+\sum_i\frac{|\Psi_i(\mathbf{x})|^2}{E_i-z}\right]\right\} . \tag{70}$$

This expression actually fulfills our two aims. In fact, it can be obtained though a simple formal argument. Start with the zeroth-order representation of B_3. Adding and subtracting the bound-state part of the resolvent in the contour integral, followed by a simple contour integration, yields the following representation for B_3:

$$B_3=\sum_{m=1}^{N_3}(e^{-\beta E_m}-1)|\Psi_m(\mathbf{x})|^2+\frac{1}{2\pi i}\int_c dz\left[e^{-\beta z}\left[\langle \mathbf{x}|R_3^c(z)|\mathbf{x}\rangle-\sum_i\frac{|\Psi_i(\mathbf{x})|^2}{E_i-z}\right]+\sum_i\frac{|\Psi_i(\mathbf{x})|^2}{E_i-z}\right]=S+I \ . \tag{71}$$

$\mathrm{Tr}_3(S)$ is convergent by inspection. $\mathrm{Tr}_3(B_3)$ is convergent by Ginibre's theorem. It thus follows that $\mathrm{Tr}_3(I)$ is convergent and that Eq. (70) is well behaved. This simple argument satisfies both (a) and (b). At this stage we must enquire as to the relationship between the above expressions and the Planck-Larkin structures. The relationship is clear. The Planck-Larkin structures not only satisfy (a) and (b) above, but they also provide asymptotic expressions for the high-temperature limit. Such expressions can only be obtained from Eq. (70) via arguments essentially equivalent to our previous derivation. We might also point out that it is the high-temperature expressions that are required in our previous work.[7]

Of the cases of interest only that of the Efimov point has yielded to our techniques. We have already outlined why we cannot treat the Coulomb problem any further. We would, however, like to suggest a procedure that may remove the manifest divergences in the classical terms of the Coulomb case. This procedure is essentially a generalization of the well-known techniques used in the fully classical problem. Start with a two-component charge neutral system (our work can accommodate two-component systems with only a little further effort). Substitute the second-order Planck-Larkin structure for b_n into the Mayer equations (of course, any $p\geq 2$ may be used). The bound-state sums are convergent. Gather the so-called ring diagrams[13,14] in the fully classical parts of the Planck-Larkin structures. It is well known that while each individual diagram diverges, the sum is actually convergent. The need for this partial summation reflects the phenomenon of screening in the Coulomb problem. It is our proposition that all classical terms from the Planck-Larkin structures can be grouped into such series and that, after their summation divergences, no longer appear. This procedure would yield semiclassical corrections to the usual Debye-Hückel theory not only from the classical terms (these could be obtained using a Wigner-Kirkwood expansion), but also from the bound-state sums. It is evident that a considerable effort is required in order to carry out this suggestion. As such we present it here only as a conjecture. Its verification clearly requires a separate study. Before this study is carried out, however, we believe a further avenue should be explored.

It is implicit in the above that the Coulomb cluster coefficients are intrinsically divergent. We know of no proof that establishes this. It thus remains possible that the Coulomb cluster coefficients are actually finite. There can only be two ways for this to occur. The first is if our expressions are approximate in some way, and that compensating divergences have been thrown away in this approximation. The second case requires that the manifest divergences in the classical terms be compensated by opposite divergences in the remainder term. The difficulties encountered in examining this second case are apparent from our previous discussion. The first scenario is more interesting. Our expressions are approximate in that we have been assuming Boltzmann statistics throughout. It is well known that Fermi statistics are of considerable importance in maintaining the stability of the Coulomb n-body problem. It may be that they have some role to play in diminishing the remaining divergences. Unfortunately, generalizing our results to quantum statistics is not the simple matter is may seem. The problem arises right at the very first step, in the high-temperature series of Fujiwara, Osborn, and Wilk.[11] We illustrate the problem in the simple case of b_2. The exchange contribution to b_2 requires matrix elements of the form

$$\langle \mathbf{x}|e^{-\beta H_2}|-\mathbf{x}\rangle \ .$$

The high-temperature series for this matrix element involves various scalar functions W_n which are essentially averages of polynomials of the potential and its derivatives on a straight line from $-\mathbf{x}$ to $\mathbf{x}$. Since this line goes through the origin these functions are divergent. This divergence, if it were isolated to the Coulomb problem, would not cause any surprise. Unfortunately, the problem is much more serious as these divergences also occur in the Bose statistics correction at the Efimov point (actually they occur for all strongly repulsive potentials). However, Ginibre's theorem is true for both Boltzmann and quantum statistics. We know then that these divergences are a result of the means used to derive these series and are not intrinsic. To generalize our results so that we can calculate corrections due to quantum statistics, we thus need to derive an alternative high-temperature series for the exchange matrix elements. We are currently attempting such a derivation.

We would like to conclude with a general comment concerning the Planck-Larkin structures. If we observe these structures away from the present context they look somewhat strange. This is because we have, in the one expression, contributions that are usually associated with the low-temperature limit (i.e., the bound-states sums) and contributions usually associated with the high-temperature limit (the classical terms). It is clear that this peaceful coexistence arises because we have used analyticity to relate high- and low-energy properties. The hybrid nature of these expressions elicits the hope that various truncations of them may approximately represent the cluster coefficients over the full temperature range. This too is a subject for further work.

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APPENDIX A

Here we outline the evaluation of various integrals whose results are quoted in the text. Note that throughout this appendix the following definition of the square root is taken:

$$z=re^{i\Theta},\quad 0\le r<\infty,\quad 0\le\Theta<2\pi,\quad \sqrt{z}=r^{1/2}e^{i\Theta/2}\ ,$$

i.e., we select the square root with the positive imaginary part. This choice is dictated in the integral identity used in going from Eq. (21) to Eq. (23).

To obtain Eq. (32) we require the result

$$\frac{1}{2\pi i}\frac{\pi i}{(4\pi q)^{3/2}}\int_c dz\, e^{-\beta z}\lim_{\Delta\to 0}\left[(z-W_1)^{1/2}\left[\frac{\varepsilon_{W_1}}{2}\right]^{-1/2}H^{(1)}_{1/2}(\varepsilon_{W_1})-z^{1/2}\left[\frac{\varepsilon_0}{2}\right]^{-1/2}H^{(1)}_{1/2}(\varepsilon_0)\right]=\frac{1}{2^{3/2}}\frac{1}{\lambda^3}(e^{-\beta v_{12}}-1)\ . \tag{A1}$$

The integral in (A1) can be written

$$\frac{1}{2}\frac{1}{(4\pi q)^{3/2}}\lim_{\eta\to 0}\int_\sigma^\infty dE\, e^{-\beta E}\lim_{\Delta\to 0}\left\{\left[(E+i\eta-W_1)^{1/2}\left[\frac{\varepsilon^+_{W_1}}{2}\right]^{-1/2}H^{(1)}_{1/2}(\varepsilon^+_{W_1})\right.\right.$$
$$\left.-(E-i\eta-W_1)^{1/2}\left[\frac{\varepsilon^-_{W_1}}{2}\right]^{-1/2}H^{(1)}_{1/2}(\varepsilon^-_{W_1})\right]-\left[(E+i\eta)^{1/2}\left[\frac{\varepsilon^+_0}{2}\right]^{-1/2}H^{(1)}_{1/2}(\varepsilon^+_0)\right.$$
$$\left.\left.-(E-i\eta)^{1/2}\left[\frac{\varepsilon^-_0}{2}\right]^{-1/2}H^{(1)}_{1/2}(\varepsilon^-_0)\right]\right\}\ , \tag{A2}$$

where $\varepsilon^\pm_x=q^{-1/2}(E\pm i\eta-x)^{1/2}\Delta$. Note

$$(E+i\eta)^{1/2}\left[\frac{\varepsilon^+_0}{2}\right]^{-1/2}H^{(1)}_{1/2}(\varepsilon^+_0)-(E-i\eta)^{1/2}\left[\frac{\varepsilon^-_0}{2}\right]^{-1/2}H^{(1)}_{1/2}(\varepsilon^-_0)$$
$$=|E|^{1/2}\left[\frac{q^{-1/2}|E|^{1/2}\Delta}{2}\right]^{-1/2}H^{(1)}_{1/2}(q^{-1/2}|E|^{1/2}\Delta)$$
$$-i|E|^{1/2}\left[\frac{q^{-1/2}|E|^{1/2}\Delta}{2}\right]^{-1/2}H^{(1)}_{1/2}(-q^{-1/2}|E|^{1/2}\Delta)+O(\eta)\quad\text{for } E>0$$
$$=O(\eta)\quad\text{for } E<0\ [\text{as } (E\pm i\eta)^{1/2}=i|E|+O(\eta)\quad\text{for } E<0] \tag{A3}$$
$$=|E|^{1/2}\left[\frac{q^{-1/2}|E|^{1/2}\Delta}{2}\right]^{-1/2}2J_{1/2}(q^{-1/2}|E|^{1/2}\Delta)\Theta(E)+O(\eta) \tag{A4}$$
$$=\frac{2}{\Gamma(3/2)}E^{1/2}\Theta(E)+O(\Delta)+O(\eta)\ , \tag{A5}$$

where we have used the results

$$-iH^{(1)}_{1/2}(-\varepsilon)=H^{(2)}_{1/2}(\varepsilon),\quad H^{(1)}_\nu+H^{(2)}_\nu=2J_\nu\ ,$$

and the small argument expansion of J_ν. $\Theta(E)$ is a Heaviside step function. Similarly for the first difference. The integral in (A1) becomes

$$\frac{1}{\Gamma(\frac{3}{2})}\frac{1}{(4\pi q)^{3/2}}\int_\sigma^\infty dE\, e^{-\beta E}[\Theta(E-W_1)(E-W_1)^{1/2}-\Theta(E)E^{1/2}] \tag{A6}$$

$$=\frac{1}{2^{3/2}}\frac{1}{\lambda^3}(e^{-\beta v_{12}}-1)\ \text{ as } (4\pi q\beta)^{1/2}=\sqrt{2}\lambda \tag{A7}$$

as required.

Next we consider the integral in Eq. (38)

$$\int_c dz\,(e^{-\beta z}-1)(z-W_1)^{-3/2}$$
$$=-2\int_c dz\,\beta e^{-\beta z}(z-W_1)^{-1/2}$$
$$\text{using integration by parts}\ . \tag{A8}$$

$$=-4\beta\int_{W_1}^\infty dE\, e^{-\beta E}(E-W_1)^{-1/2}$$
$$=2\beta^{1/2}e^{-\beta W_1}\Gamma(-\tfrac{1}{2})\ . \tag{A9}$$

The result given in the text follows. The result in Eq. (40b) follows in a similar manner by induction.

The third term in Eq. (50) is evaluated as follows. We write the contour integral

$$\lim_{\Delta\to 0}\int_c dz\, e^{-\beta z}\left\{(z-W_1)^2\left[\frac{\varepsilon_{W_1}}{2}\right]^{-2}H^{(1)}_2(\varepsilon_{W_1})-z^2\left[\frac{\varepsilon_0}{2}\right]^{-2}H^{(1)}_2(\varepsilon_0)\right.$$
$$\left.-\sum_\alpha\left[(z-W_1^\alpha)^2\left[\frac{\varepsilon_{W_1^\alpha}}{2}\right]^{-2}H^{(1)}_2(\varepsilon_{W_1^\alpha})-z^2\left[\frac{\varepsilon_0}{2}\right]^{-2}H^{(1)}_2(\varepsilon_0)\right]\right\}$$

as

$$\int_\sigma^\infty dE\, e^{-\beta E}f(E)\ .$$

The contribution to the integrand $f(E)$ from the W_1 term

$$(E^+-W_1)^2\left[\frac{\varepsilon^+_{W_1}}{2}\right]^{-2}H^{(1)}_2(\varepsilon^+_{W_1})$$
$$-(E^--W_1)^2\left[\frac{\varepsilon^-_{W_1}}{2}\right]^{-2}H^{(1)}_2(\varepsilon^-_{W_1})\ , \tag{A10}$$

where

$$\varepsilon^\pm_x=q^{-1/2}(E^\pm-x)^{1/2}\Delta,\quad E^\pm=E\pm i\eta$$

now

$$\varepsilon^\pm_{W_1}=\pm q^{-1/2}(E-W_1)^{1/2}\Delta=\pm\varepsilon\ \text{ for } E>W_1$$
$$=iq^{-1/2}|E-W_1|^{1/2}\Delta\quad\text{for } E<W_1\ .$$

Thus (A10) becomes

$$(E-W_1)^2\left[\frac{\varepsilon}{2}\right]^{-2}[H^{(1)}_2(\varepsilon)-H^{(1)}_2(-\varepsilon)]$$
$$\times\Theta(E-W_1)+O(\eta) \tag{A11}$$
$$=(E-W_1)^2\left[\frac{\varepsilon}{2}\right]^{-2}2J_2(\varepsilon)\Theta(E-W_1)+O(\eta)$$
$$=(E-W_1)^2\Theta(E-W_1)+O(\eta)+O(\Delta)\ , \tag{A12}$$

similarly for the other expressions in the integrand. The integral in question becomes

$$\int_\sigma^\infty dE\, e^{-\beta E}\left[(E-W_1)^2\Theta(E-W_1)-E^2\Theta(E)\right.$$
$$\left.-\sum_\alpha[(E-W_1^\alpha)^2\Theta(E-W_1^\alpha)-E^2\Theta(E)]\right]\ , \tag{A13}$$

from which the answer given in the text follows readily. The other integral in Eq. (50) follows in a similar manner.

APPENDIX B

We present in this appendix an outline of Ginibre's proof, emphasizing the elements that imply the existence of the cluster coefficients. The interested reader can find full details in Refs. 5 and 15. Ginibre's theorem is essentially the quantum analog of a classical result due to Ruelle.[16] The analogy is a fairly direct one because of the use of path integral representations. We thus commend to the interested reader a prior examination of Ruelle's work.

Ginibre begins with the definition of the configuration space m-particle reduced density matrices:

$$\bar{\rho}_\Lambda(\mathbf{x}_1,\ldots,\mathbf{x}_m,\mathbf{y}_1,\ldots,\mathbf{y}_m)=\frac{1}{\mathbf{Z}}\sum_{n=0}^{\infty}\frac{z^{m+n}}{n!}\int_\Lambda d^3u_1\cdots d^3u_n\langle\mathbf{x}_1,\ldots,\mathbf{x}_m,\mathbf{u}_1,\ldots,\mathbf{u}_n|e^{-\beta H}|\mathbf{y}_1,\ldots,\mathbf{y}_m,\mathbf{u}_1,\ldots,\mathbf{u}_n\rangle\ , \tag{B1}$$

where Λ is the volume of the system, $\mathbf{Z}$ is the grand partition function, and Boltzmann statistics are used. We refer the reader to Ginibre for the generalization to quantum statistics. Using the Feynman-Kac formula the Boltzmann factor is written as a path integral:

$$\langle\mathbf{x}_1,\ldots,\mathbf{x}_m|e^{-\beta H}|\mathbf{y}_1,\ldots,\mathbf{y}_m\rangle=\int P^\beta_{\mathbf{x}_1\mathbf{y}_1}(d\omega_1)\cdots P^\beta_{\mathbf{x}_m\mathbf{y}_m}(d\omega_m)e^{-U(\omega_1,\ldots,\omega_m)}\ , \tag{B2}$$

where $P^\beta_{\mathbf{x}_i\mathbf{y}_i}(d\omega_i)$ are Wiener measures on the trajectory space and

$$U(\omega_1,\ldots,\omega_m)=\int_0^\beta dt\sum_{1\le i<j\le m}\Phi[\omega_i(t)-\omega_j(t)]\ . \tag{B3}$$

The reduced density matrices are then written as

$$\bar{\rho}_\Lambda(\mathbf{x}_1,\ldots,\mathbf{x}_m,\mathbf{y}_1,\ldots,\mathbf{y}_m)=\int P^\beta_{\mathbf{x}_1\mathbf{y}_1}(d\omega_1)\cdots P^\beta_{\mathbf{x}_m\mathbf{y}_m}(d\omega_m)\rho_\Lambda(\omega_1,\ldots,\omega_m)\alpha(\omega_1)\cdots\alpha(\omega_m)\ , \tag{B4}$$

where

$$\alpha(\omega_i)=1 \quad \text{if } \omega_i\in\Lambda$$
$$=0 \quad \text{otherwise}\ ,$$

and the $\rho_\Lambda(\omega_1,\ldots,\omega_m)$ satisfy an infinite set of coupled integral equations, referred to as the Kirkwood-Salzburg equations:

$$\begin{aligned}\rho_\Lambda(\omega_1)&=z\alpha(\omega_1)\left[1+\sum_{s=1}^{\infty}\frac{1}{s!}\int d^3u_1P^\beta_{\mathbf{u}_1\mathbf{u}_1}(d\mu_1)\cdots d^3u_sP^\beta_{\mathbf{u}_s\mathbf{u}_s}(d\mu_s)K(\omega_1|\mu_1)\cdots K(\omega_1|\mu_s)\rho_\Lambda(\mu_1,\ldots,\mu_s)\right]\ ,\\ \rho_\Lambda(\omega_1,\ldots,\omega_m)&=z\alpha(\omega_1)\cdots\alpha(\omega_m)e^{-U(\omega_1,\ldots,\omega_m)}\\ &\times\left[\rho_\Lambda(\omega_2,\ldots,\omega_m)+\sum_{s=1}^{\infty}\frac{1}{s!}\int d^3u_1P^\beta_{\mathbf{u}_1\mathbf{u}_1}(d\mu_1)\cdots d^3u_sP^\beta_{\mathbf{u}_s\mathbf{u}_s}(d\mu_s)\right.\\ &\left.\times K(\omega_1|\mu_1)\cdots K(\omega_1|\mu_s)\rho_\Lambda(\omega_2,\ldots,\omega_m,\mu_1,\ldots,\mu_s)\right]\ .\end{aligned} \tag{B5}$$

Defining vectors

$$\Gamma_\Lambda=(\rho_\Lambda(\omega_1),\rho_\Lambda(\omega_1,\omega_2),\rho_\Lambda(\omega_1,\omega_2,\omega_3),\ldots,\rho_\Lambda(\omega_1,\ldots,\omega_s),\ldots)$$

and

$$\xi=(z,0,0,\ldots)$$

and defining the operator A_Λ by

$$A_\Lambda h=(\alpha(\omega_1)h(\omega_1),\alpha(\omega_1)\alpha(\omega_2)h(\omega_1,\omega_2),\alpha(\omega_1)\alpha(\omega_2)\alpha(\omega_3)h(\omega_1,\omega_2,\omega_3),\ldots,\alpha(\omega_1)\cdots\alpha(\omega_s)h(\omega_1,\ldots,\omega_s),\ldots)$$

the Kirkwood-Salzburg equations can be written as

$$\Gamma_\Lambda=A_\Lambda(\xi+K\Gamma_\Lambda)\ . \tag{B6}$$

Note that Ginibre's K is modified slightly from the one implied by (B5). This is done for technical reasons. The best explanation of this modification and the reason for it can be found in Ref. 17.

Γ_Λ is an element of a space whose general element is denoted

$$h=(h(\omega_1),h(\omega_1,\omega_2),h(\omega_1,\omega_2,\omega_3),\ldots,h(\omega_1,\ldots,\omega_s),\ldots)\ .$$

By defining a norm on this space, Ginibre constructs a Banach space. The definition of the norm depends on the conditions on the potential. For the conditions we have quoted in the text, the norm is

$$\|h\|=\sup_m\sup_{(\omega_1,\ldots,\omega_m)}\frac{|h(\omega_1,\ldots,\omega_m)|}{\prod_{i=1}^{m}\Delta(\omega_i)}\ , \tag{B7}$$

where $\Delta(\omega_i)$ is an auxiliary function, satisfying various conditions (see p. 382 of the first entry in Ref. 15) and whose functional form is constrained to ensure that the operator K is bounded. [Ginibre also considers the case of absolutely integrable potentials, i.e., $c=0$ in condition (c) in Sec. V. In this case one can ensure that K is bounded by choosing Δ as a suitably constrained constant. The $c=0$ case, of course, does not cover the potentials of interest to us. However, we found that going through the $c=0$ case first provided a valuable guide to the more complicated $c>0$ case, which is the one of interest.] The norm (B7) induces a corresponding operator norm. Ginibre shows that for $|z|<R$, $\|K\|<1$. It then follows[18] that

$$\Gamma_\Lambda = A_\Lambda\xi + A_\Lambda(KA_\Lambda)\xi + A_\Lambda(KA_\Lambda)^2\xi + \cdots \tag{B8}$$

converges. As z appears linearly in K, this result establishes the analyticity of Γ_Λ. Using (B4), the analyticity in z of the reduced density matrices follow, proving part (i) of Ginibre's theorem.

Ginibre proves his second result with the aid of the following lemma.

Lemma. Without loss of generality, let Λ be a sphere of radius L centered on the origin. Let $m'>m>0$. Then

$$\| A_L K A_{L+m'} - A_L K A_{L+m} \| \le \eta(m) , \tag{B9}$$

where $\eta(m)$ tends to zero as $m\to\infty$. Ginibre uses this lemma to show that

$$\| A_L \Gamma_{L+m'} - A_L \Gamma_{L+m} \| < \varepsilon(m) \tag{B10}$$

for $m'>m>0$. This is a Cauchy criterion for $A_L\Gamma_{L+m}$ as $m\to\infty$. As a result each element of the vector $A_L\Gamma_{L+m}$ tends to a limit as $m\to\infty$ (recall that $A_L\Gamma_{L+m}$ are elements of a Banach space which, by definition, is complete). This limit is denoted by $A_L\Gamma$ and one has

$$\| A_L\Gamma - A_L\Gamma_{L+m} \| < \varepsilon(m) . \tag{B11}$$

From this result Ginibre proves part (ii) of the theorem: if $\mathbf{x}_i,\mathbf{y}_i\in D$, where D is a compact subset of the sphere of radius L, then $\bar\rho_L(\mathbf{x}_1,\ldots,\mathbf{x}_m,\mathbf{y}_1,\ldots,\mathbf{y}_m)$ tends to a limit, denoted $\bar\rho(\mathbf{x}_1,\ldots,\mathbf{x}_m,\mathbf{y}_1,\ldots,\mathbf{y}_m)$ as $L\to\infty$. This limit is uniform in z for $|z|\le R'<R$. The results for the cluster coefficients are clearly contained in this result. To see this explicitly, consider the definition of the cluster coefficients:

$$nb_n(\mathbf{x}) = \lim_{L\to\infty} \frac{1}{z^n}\int P^\beta_{\mathbf{xx}}(d\omega)[A_L(KA_L)^{n-1}\xi]_1 . \tag{B12}$$

The subscript 1 denotes the first element of the vector inside the brackets. To establish the existence of the limit consider, for $m'>m>0$,

$$\begin{aligned} |nb_n^{L+m'}(\mathbf{x}) - nb_n^{L+m}(\mathbf{x})| &= \frac{1}{|z|^n}\int P^\beta_{\mathbf{xx}}(d\omega)|[A_{L+m'}(KA_{L+m'})^{n-1}\xi]_1 - [A_{L+m}(KA_{L+m})^{n-1}\xi]_1| \\ &\le \frac{1}{|z|^{n-1}}\frac{1}{\inf\Delta(\omega)}\int P^\beta_{\mathbf{xx}}(d\omega)\| A_{L+m'}(KA_{L+m'})^{n-1} - A_{L+m}(KA_{L+m})^{n-1}\|\Delta(\omega) , \end{aligned} \tag{B13}$$

where $\mathbf{x}\in D$. Let D be contained in a sphere of radius $L-r$. The integration over ω in Eq. (B14) is split into two subdomains A and B. In A, ω is contained completely in the sphere of radius L. For this part of the integration we have

$$\begin{aligned} &\| A_{L+m'}(KA_{L+m'})^{n-1} - A_{L+m}(KA_{L+m})^{n-1}\| \\ &\quad = \| A_L(KA_{L+m'})^{n-1} - A_L(KA_{L+m})^{n-1}\| . \end{aligned} \tag{B14}$$

The lemma can be used to bound (B14) via simple manipulations. The path integration over A is then bounded by

$$k\eta(m)\int_A P^\beta_{\mathbf{xx}}(d\omega)\Delta(\omega) , \tag{B15}$$

where k is some constant. Since $\Delta(\omega)$ is integrable, the integration over the A domain can be made arbitrarily small by making m sufficiently large. For the integration over the B domain the trajectory ω must travel at least a distance r in a "time" β. Since the integrand can be bounded by some constant k' this integration can be estimated by

$$k'\int_B P^\beta_{\mathbf{xx}}(d\omega)\Delta(\omega) .$$

Ginibre has some estimates that show that this integral can be made arbitrarily small by letting r become sufficiently large (with an adjustment of L if necessary). This establishes a Cauchy criterion for $nb_n^L(\mathbf{x})$. As a result the limit exists as $L\to\infty$ provided $\mathbf{x}$ is in D (as D is arbitrary this is not a restriction). We denote this limit by $nb_n(\mathbf{x})$. By considering the explicit integral representation, Eq. (B12), we can see that for $\mathbf{x},\mathbf{x}'\in D$, translational invariance implies that $nb_n(\mathbf{x})=nb_n(\mathbf{x}')$. As D is arbitrary, it follows that $nb_n(\mathbf{x})$ is independent of $\mathbf{x}$.

The argument above provides an outline of the explicit demonstration that Ginibre's results imply the existence of the cluster coefficients. The reader interested in a more detailed demonstration can supplement this outline with a detailed study of Ginibre's original work.

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