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Effective interactions in imperfect gases and enhancement of the Efimov effect

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In this paper we present a realization of the concept, first put forth by V. Efimov [*Few Body Dynamics,* edited by A. N. Mitra *et al.* (North-Holland, Amsterdam, 1976)], of enhancing the Efimov effect by placing the three particles in a medium whose parameters vary. We do this in the context of equilibrium statistical mechanics by incorporating three-body potentials and subsequently writing their contribution to the cluster series in terms of effective, density-dependent, two-body potentials. We then perform approximate partial summations of the cluster series expressing the sums in terms of cluster coefficients involving the effective potentials. From the high-temperature expansion of the corresponding equation of state for a model system, we find that, at the Efimov point, behavior resembling that of a first-order phase transition appears.

I. INTRODUCTION

When it was first discovered, the Efimov effect caused considerable surprise. It was quite unexpected that, under any circumstances, one could have a system in which an infinite number of bound states was generated through short-range forces (results on the number of two-body bound states can be found in Ref. 1). Efimov,[2] however, showed that in the case of three identical spinless particles interacting pairwise through short-range forces, there exists a family of approximately

$$N=\frac{1}{\pi}\ln\left[\frac{|a|}{r_0}\right] \tag{1}$$

bound states, where r_0 is the range and a is the scattering length of the pair potential. (This result has been subsequently confirmed by a number of authors.[3]) If $|a|$ is infinite or, equivalently, if the pair potential has a zero-energy two-body bound state, then this family contains an infinite number of three-body bound states.

Evidence of these levels in nature has, however, been somewhat elusive. Clearly, Efimov's family appears only if $|a|/r_0>e^{\pi}$. This condition is satisfied by relatively few systems: α particles,[4] spin-polarized ^{3}H atoms,[5] ^{4}He atoms,[6] and a few others.[7] In fact, in these systems the condition is only just satisfied, indicating that there is at most one Efimov level. Numerical integration of Faddeev's equations [recall that Eq. (1) is only approximate] has uncovered the presence of one (or possibly two) Efimov levels only in the case of the ^{4}He trimer.[6] Thus, even though the laws of quantum mechanics permit the generation of an infinite number of three-body bound states through short-range forces, it appears that nature has chosen not to endow any real system with this property.

Efimov,[7] however, has conceived of a situation where the full extent of his mechanism may be realized. He suggests that the three particles should be placed in some sort of "medium." The medium has properties (e.g., density) which vary. Because the medium modifies the pair interaction there exists the possibility of tuning the medium parameters so that the effective two-body interaction will have $|a|=\infty$. If the "bare" scattering length is already large, then perhaps even small-medium effects may be sufficient. In this paper we attempt to demonstrate that Efimov's program is realizable. We believe that no such demonstration has been attempted. (The papers of Ghassib[8] and Cornelius and Glockle[6] also indicate this.)

The first question we must address is the constitution of our medium. What we would like is something static and inert which only changes the pair interaction and does not interfere with the dynamics of the three particles. This way the problem is simply a three-body problem with an adjustable potential. In reality any medium cannot satisfy these conditions as it must consist of other particles. As such, from the beginning, we must consider a many-particle system. We now have the problem of considering how to relate the properties of many-particle systems to those of its three-particle subsystems. Such relations appear in the form of cluster expansions for the properties of many-particle systems.

In Sec. II we present the starting point of our calculation, the cluster expansion for the logarithm of the grand partition function. The nth coefficient in this expansion depends on the trace of the n-particle Hamiltonian. In particular, Efimov's family of bound states will give contributions to the third coefficient. In this formulation we represent the n-body potential energy as a pairwise sum over two-body potentials plus a triplet sum over three-body potentials. Not only does this provide a more realistic representation of the n-body potential[9] but it also provides us with a means to realize Efimov's program. We do this in Sec. III where we express some of the contributions to the cluster series which involve the three-body interaction in terms of an effective, density-dependent, two-body interaction. Using this we find that we can then approximately sum a certain class of diagrams to infinite order, expressing the result in terms of a second-cluster coefficient where the original two-body interaction is supplemented by a density-dependent two-body interaction.

In Sec. IV we consider an analogous construction where the summation is expressed approximately by a third-cluster coefficient with the same density-dependent effective potential. It is in this result that Efimov's program is realized. In the evaluation of this effective third-cluster coefficient we require the solution of the three-body problem, where the potential energy is a pairwise sum of a two-body interaction which varies with changes in density. We can thus tune the potential to yield an infinite number of three-body bound states. We refer to the density at which this occurs as the "Efimov point," ρ_e. We can thus conceive of obtaining a many-body system at some temperature and varying the density through the Efimov point. We then address the question as to how the bulk properties of the system reflect the unusual three-body behavior at ρ_e by obtaining the equation of state for our partially summed cluster series. This is done in Sec. V. In Sec. VI we obtain the high-temperature expansion of this equation of state. The expression obtained is valid only for bounded, short-range, two-body interactions. In Sec. VII we consider the high-temperature thermodynamic behavior at ρ_e implied by this equation of state. Finally, in Sec. VIII we conclude with a discussion of the limitations of our construction and discuss avenues where further investigation may be undertaken.

II. FEW-BODY DYNAMICS IN A MANY-PARTICLE SYSTEM

There are a number of intuitive ways in which one may account for contributions of the three-body force in terms of an effective two-body force. One may, for instance, use mean-field arguments. Alternatively, one may follow the procedures used in the classical statistical mechanics of liquids such as those of Sinanoglu[10] [whose techniques have been applied by Blaisten-Barojas *et al.* to ^{4}He (Ref. 11)]. Such techniques, although they provide some insight into how to handle our problem, cannot include the bound-state effects which we wish to study. On the other hand, these classical techniques could motivate a phenomenological approach. This, however, requires some support and some guidance from experimental data. Since we do not have these data we prefer to approach the problem on a microscopic, quantum-mechanical basis using a formulation of the many-body problem where the influence of three-body dynamics can be viewed directly. With this in mind the most simple and most obvious way to tackle the many-body problem is through the virial expansion in quantum statistical mechanics.

The virial expansion of the equation of state is given parametrically in terms of the Mayer equations[12]

$$\frac{PV}{kT}=\sum_{n=1}^{\infty}\frac{z^n}{n!}b_n\ , \tag{2a}$$

$$N=\sum_{n=1}^{\infty}\frac{z^n}{(n-1)!}b_n\ . \tag{2b}$$

The notation for the thermodynamic variables is that of Huang.[12] Equation (2a) is referred to as the cluster expansion, where b_n is the nth cluster coefficient which is defined as

$$b_n=\mathrm{Tr}_n(e^{-\beta H_n})_c\ , \tag{3}$$

where

$$H_n=K_{1,\ldots,n}+\sum_{i<j=1}^{n}V_{ij}+\sum_{i<j<k=1}^{n}V_{ijk},\ \ \beta=\frac{1}{kT}\ ,$$

Boltzmann statistics are assumed,

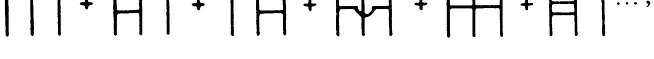
$$K_{1,\ldots,n}=\sum_{i=1}^{n}\frac{p_i^2}{2m}$$

and V_{ij} is referred to as the bare two-body interaction. H_n is simply the n-particle Hamiltonian. Our representation of the potential neglects four- and higher-body forces, but the formalism to be developed can be easily extended to include these if need be. The subscript c denotes that only the connected parts of the Boltzmann operator are to be included when taking the n-particle trace. The notion of a connected contribution derives, of course, from the diagrammatic representation of the operator. Since we will be using diagrammatic methods extensively, we briefly illustrate these. Further details may be found in the original paper of Lee and Yang[13] and other more recent contributions.[14,15]

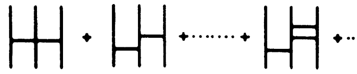
As an illustration of the diagrammatic representation we consider the three-body Boltzmann operator. It is well known that one can write the following perturbation expansion for this:

$$\begin{aligned} e^{-\beta H_3}&=e^{-\beta(K_{123}+V_{12}+V_{23}+V_{31}+V_{123})}\\ &=e^{-\beta K_{123}}+\int_0^\beta d\tau\, e^{-(\beta-\tau)K_{123}}(-V_{12}-V_{23}-V_{31}-V_{123})e^{-\tau K_{123}}\\ &\quad+\int_0^\beta d\tau\int_0^\tau d\tau'\, e^{-(\beta-\tau)K_{123}}(-V_{12}-V_{23}-V_{31}-V_{123})\\ &\qquad\times e^{-(\tau-\tau')K_{123}}(-V_{12}-V_{23}-V_{31}-V_{123})e^{-\tau' K_{123}}+\cdots\ . \end{aligned} \tag{4}$$

This can be expressed diagrammatically as

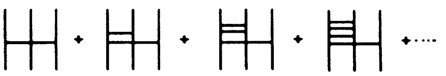

(5)

where each component in the diagram represents a certain operator in the above expansion, in the usual manner. The connected part of the Boltzmann operator is thus



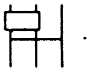
$$=e^{-\beta(K_{123}+V_{12}+V_{23}+V_{31}+V_{123})}-e^{-\beta K_{123}}+\sum_{i<j=1}^{3}\left(e^{-\beta(K_{123}+V_{ij})}-e^{-\beta K_{123}}\right) . \tag{6}$$

In this paper we shall supplement this notation with a few more definitions. We shall refer to single diagrams or sums of diagrams as "primitive." When we express contributions of three-body interactions by effective two-body interactions primitive diagrams with three-body interactions will be replaced by diagrams containing effective two-body interactions and fewer particle lines. The diagrams so derived will be referred to as "effective" diagrams to distinguish them from the primitive ones. Also we represent ladder sums by a box. For example,



(7a)

is represented by the more succinct notation,



(7b)

This notation may, in future use, imply the inclusion of disconnected diagrams. We shall, of course, regard it as implicit that these are excluded.

This formulation of the many-body problem provides a microscopic basis for our calculation. The only approximation made is in neglecting four- and higher-body forces in our representation of the n-body potential. We also, of course, assume conditions of thermodynamic equilibrium.

It is clear that three-body dynamics has a direct input into the many-body problem, when it is formulated this way. The simplest place to see this is the third-cluster coefficient. This can be written as follows:[14,16]

$$\mathrm{Tr}_3(e^{-\beta H_3})_c=\sum_{j=1}^{N_b}e^{-\beta E_j}-\lim_{\epsilon\to 0}\int_{-\chi_\alpha^2}^{\infty}\frac{dE}{2\pi i}e^{-\beta E}[R_c(E+i\epsilon)-R_c(E-i\epsilon)] , \tag{8}$$

where

$$R_c(E)=\mathrm{Tr}_3\left[\frac{1}{E-H_3}-\frac{1}{E-K_{123}}-\sum_{i<j=1}^{3}\left[\frac{1}{E-K_{123}-V_{ij}}-\frac{1}{E-K_{123}}\right]\right]$$

is the trace of the connected resolvent difference, N_b is the number of three-body bound states, and $-\chi_\alpha^2$ is the two-body threshold. In obtaining this expression the usual contour has been deformed so that the bound-state contributions (and thus the potential Efimov bound-state contributions) are explicitly shown. The three-body dynamics given in $R_c(E)$ must also, in some way, reflect Efimov's mechanism.

In Eq. (8) the input from the three-body problem is made explicit. However, one also notes a possible problem. From Eq. (8) one can see that when Efimov's mechanism generates an infinite number of bound states, then the bound-state sum diverges. This is because the bound states accumulate at zero energy. This may call into question the validity of the virial expansion in the presence of the Efimov Effect. Bollé,[16] however, has shown that as one approaches the Efimov point from either side, the third-cluster coefficient remains finite. This is the result of a cancellation of the divergence in the bound-state sum by a divergence in the continuum integration. (This result was shown earlier in a simplified model by Hoogeveen and Tjon.[17]) We thus have reason to believe that the cluster expansion may be used even when the potential strength is at the Efimov point. Having established our formalism, and having noted how this formalism reflects the contribution of the Efimov effect in a many-particle system, we now proceed to describe our program.

III. CONSTRUCTION OF AN EFFECTIVE SECOND-CLUSTER COEFFICIENT

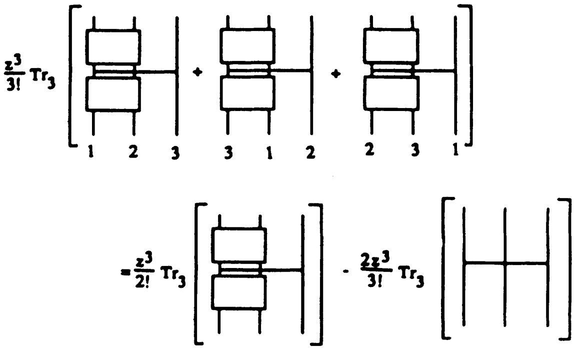
Our aim is to express the contributions of the three-body interactions in the Mayer equations in terms of effective two-body interactions. That is, we aim to transform the Mayer equations (2a), and (2b) into the form

$$\frac{PV}{kT}=\sum_{n=1}^{\infty}\frac{z^n}{n!}b_n^{\mathrm{eff}} , \tag{9a}$$

$$N=\sum_{n=1}^{\infty}\frac{z^n}{(n-1)!}b_n^{\text{eff}}\,, \tag{9b}$$

where b_n^{eff} is a cluster coefficient as before except that the potential in the n-body Hamiltonian here consists of a pairwise sum of density-dependent two-body forces. Although the enhancement of the Efimov contribution with varying density is contained in b_3^{eff}, we shall first illustrate our procedure in the construction of b_2^{eff}.

Consider the following contribution to the cluster expansion:



(10)

by permutation symmetry. (The subtraction here is necessary because this diagram has been triple counted. We shall ignore this term for the present, including it again later.)

This diagram represents the following expression:

$$\frac{z^3}{2!}\text{Tr}_3\left[\int_0^{\beta}d\tau\, e^{-(\beta-\tau)(K_{123}+V_{12})}(-V_{123})e^{-\tau(K_{123}+V_{12})}\right]. \tag{11}$$

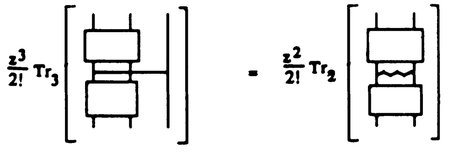
In the coordinate representation this becomes

$$\begin{aligned}\frac{z^3}{2!}\int_0^{\beta}d\tau\int d^3\mathbf{r}_1\,d^3\mathbf{r}_2\,d^3\mathbf{r}_3\,d^3\mathbf{r}_1'\,d^3\mathbf{r}_2'\,d^3\mathbf{r}_3'\langle\mathbf{r}_1\mathbf{r}_2|e^{-(\beta-\tau)(K_{12}+V_{12})}|\mathbf{r}_1'\mathbf{r}_2'\rangle&\\ \times\langle\mathbf{r}_3|e^{-(\beta-\tau)K_3}|\mathbf{r}_3'\rangle[-V_{123}(\mathbf{r}_1',\mathbf{r}_2',\mathbf{r}_3')]\langle\mathbf{r}_1'\mathbf{r}_2'|e^{-\tau(K_{12}+V_{12})}|\mathbf{r}_1\mathbf{r}_2\rangle\langle\mathbf{r}_3'|e^{-\tau K_3}|\mathbf{r}_3\rangle&\\ =\frac{z^2}{2!}\text{Tr}_2\left[\int_0^{\beta}d\tau\, e^{-(\beta-\tau)(K_{12}+V_{12})}[-V_{12}^{\text{eff}}(z;\beta,\tau)]e^{-\tau(K_{12}+V_{12})}\right],&\end{aligned} \tag{12}$$

where

$$V_{12}^{\text{eff}}(\mathbf{r}_1,\mathbf{r}_2;z;\beta,\tau)=z\int d^3\mathbf{r}_3'\,d^3\mathbf{r}_3\langle\mathbf{r}_3|e^{-(\beta-\tau)K_3}|\mathbf{r}_3'\rangle V_{123}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)\langle\mathbf{r}_3'|e^{-\tau K_3}|\mathbf{r}_3\rangle\ . \tag{13}$$

We have trivially rearranged the integral so that one of the integrations in the original trace is now in the definition of the effective potential, leaving the resulting expression as a two-particle trace instead of the original three-particle trace. We have thus expressed our original contribution in terms of an effective fugacity- and temperature-dependent two-body interaction. The net result is stated diagrammatically as follows:



, (14)

where

is the diagrammatic representation of the effective potential V_{12}^{eff}. The diagram on the right-hand side is an example of an effective diagram. Here we have an illustration of how we transform a primitive diagram into an effective one.

The summations which we eventually want to perform are difficult with this effective potential. This arises from its temperature dependence (we shall elaborate on this point later). We avoid these difficulties by performing a high-temperature expansion of the effective potential, i.e., given

$$\langle\mathbf{r}_3\,|\,e^{-\tau K_3}\,|\,\mathbf{r}_3'\rangle=\frac{1}{\lambda^3\left[\dfrac{\tau}{\beta}\right]^{3/2}}\exp\left[\frac{-\pi}{\lambda^2}\frac{(\mathbf{r}_3-\mathbf{r}_3')^2}{\dfrac{\tau}{\beta}}\right], \tag{15}$$

where $\lambda^2=[(2\pi\hbar^2/m)\beta]$ is the thermal wavelength, we can write

$$V_{12}^{\text{eff}}(\mathbf{r}_1,\mathbf{r}_2;z;\beta,\tau)=z\int d^3\mathbf{r}_3\,d^3\mathbf{r}_3'\frac{1}{\lambda^6}\frac{1}{\left[1-\dfrac{\tau}{\beta}\right]^{3/2}}\frac{1}{\left[\dfrac{\tau}{\beta}\right]^{3/2}}\exp\left[\frac{-\pi}{\lambda^2}\frac{(\mathbf{r}_3-\mathbf{r}_3')^2}{\dfrac{\tau}{\beta}\left[1-\dfrac{\tau}{\beta}\right]}\right]V_{123}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)\ . \tag{16}$$

Using Laplace's method to evaluate the $\mathbf{r}_3$ integration in the limit $\lambda\to 0$, we obtain the high-temperature series

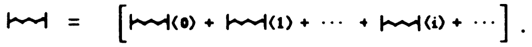
$$V_{12}^{\mathrm{eff}}(\mathbf{r}_1,\mathbf{r}_2;z;\beta,\tau)=\frac{z}{\lambda^3}\sum_{n=0}^{\infty}c_n a^{2n}V_{12;n}^{\mathrm{eff}}(\mathbf{r}_1,\mathbf{r}_2)\ , \tag{17}$$

where $a^2=\lambda^2(1-\tau/\beta)\tau/\beta$ and the first few c_n and $V_{12;n}^{\mathrm{eff}}$ are

$$\begin{gathered}c_0=1,\ \ c_1=\frac{1}{4\pi},\ \ c_2=\frac{1}{32\pi^2},\ \ V_{12;0}^{\mathrm{eff}}=\int d^3\mathbf{r}_3\,V_{123},\ \ V_{12;1}^{\mathrm{eff}}=\int d^3\mathbf{r}_3\,\nabla^2 V_{123}\ ,\\ V_{12;2}^{\mathrm{eff}}=\int d^3\mathbf{r}_3\,\nabla^2(\nabla^2 V_{123})\ .\end{gathered} \tag{18}$$

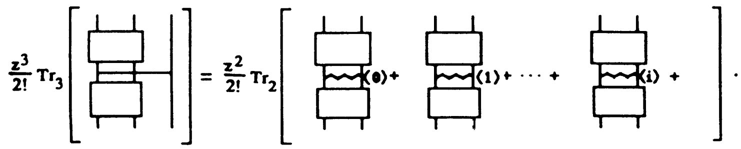
In performing this high-temperature expansion, we are essentially treating the third particle in Eqs. (10) and (11) semiclassically, while treating the other two particles fully quantum mechanically.

Let us denote the series representation, Eq. (17), diagrammatically in the following manner:



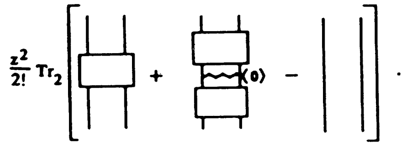
(19)

Substituting this into Eq. (14) we obtain



(20)

Let us group the first term in the expansion with the second-cluster coefficient. This is natural not only because our effective diagram is a two-particle trace, but also because it has the same prefactor as the second-cluster coefficient. [This latter fact is a consequence of two elements in our construction. First, the placement of a factor of z in the definition of the effective potential and, second, our use of permutation symmetry to get the factor of 3 in Eq. (10).] Let us also consider the low-density, high-temperature limit where $z/\lambda^3\rightarrow\rho$, the number density. Doing this we obtain



(21)

This is the diagrammatic representation of

$$\frac{z^2}{2!}\mathrm{Tr}_2\left[e^{-\beta(K_{12}+V_{12})}-e^{-\beta K_{12}}+\int_0^{\beta}d\tau\, e^{-(\beta-\tau)(K_{12}+V_{12})}(-\rho V_{12;0}^{\mathrm{eff}})e^{-\tau(K_{12}+V_{12})}\right]\ . \tag{22}$$

The operator in the brackets is the first two terms in the expansion of

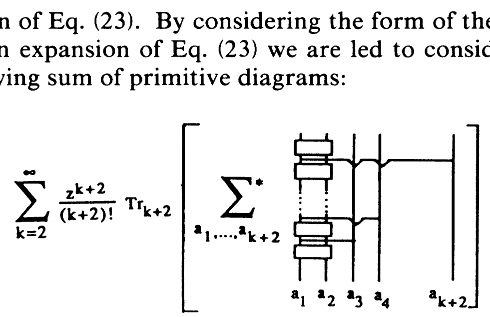
$$U_2(\beta,\rho)-e^{-\beta K_{12}}=e^{-\beta(K_{12}+V_{12}+\rho V_{12;0}^{\mathrm{eff}})}-e^{-\beta K_{12}}\ , \tag{23}$$

where $\rho V_{12;0}^{\mathrm{eff}}$ is taken as the perturbation. This result follows since (i) $U_2(0,\rho)=1$ for all ρ, and (ii) the first term in the expansion of the effective potential is independent of temperature. If we had retained any temperature dependence we would not have been able to make this identification. This is the difficulty inherent in the temperature dependence of the effective potential to which we alluded previously.

The definition of the effective second-cluster coefficient given at the beginning of this section is

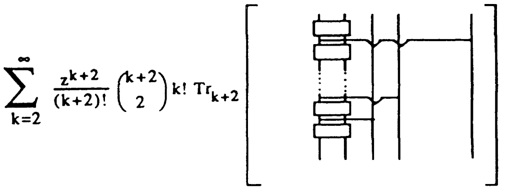
$$b_2^{\mathrm{eff}}=\frac{z^2}{2!}\mathrm{Tr}_2(e^{-\beta(K_{12}+V_{12}+\rho V_{12;0}^{\mathrm{eff}})}-e^{-\beta K_{12}})\ . \tag{24}$$

Thus we can fulfill our aim only if we can find primitive diagrams which yield the effective diagrams corresponding to the higher-order terms in the perturbation expansion of Eq. (23). By considering the form of the perturbation expansion of Eq. (23) we are led to consider the following sum of primitive diagrams:

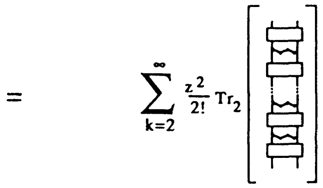


, (25)

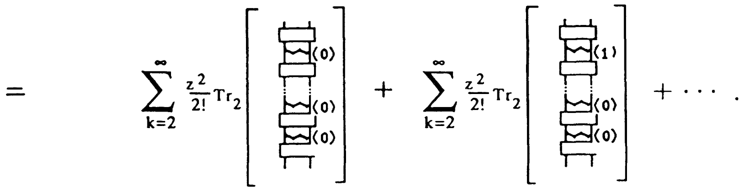
where the starred sum is a restricted one over different relabelings of the particle lines. The best way to describe the restrictions is to show how to construct relabelings which are included. [All such relabelings represent distinct contributions from the cluster series. Furthermore, there is no multiple counting of any diagram, so that the situation in Eq. (10) is exceptional.] First we choose two numbers (a_1,a_2) from $(1,2,\ldots,k+2)$. Hold these constant. Let $a_3,\ldots,a_{k+2}$ be a permutation of the remaining integers. Sum over all such permutations. Do this for all choices of (a_1,a_2). The first step corresponds to choosing which two particles contain the bare two-body interactions. The second step corresponds to the different temperature orderings of the three-body interactions. We now replace the three-body interactions by effective two-body interactions in much the same way as we did in Eqs. (10)–(14). Equation (25) becomes



(26)

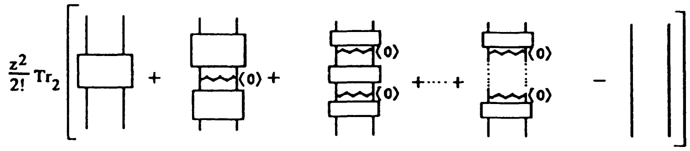


(27)



(28)

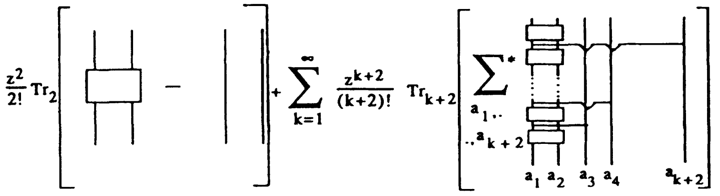
where we have used permutation symmetry in the first step, the definition of the effective potential in the second step and the high-temperature expansion of the effective potential in the third step. Here all terms except the first involve temperature-dependent parts of the effective potential. We now group the first sum in Eq. (28) with the second-cluster coefficient and the first term in Eq. (20). The result is



$$= \frac{z^2}{2!}\mathrm{Tr}_2\left(e^{-\beta(K_{12}+V_{12}+\rho V^{\mathrm{eff}}_{12;0})} - e^{-\beta K_{12}}\right) , \qquad (29)$$

where again we have taken the low-density high-temperature limit so that $z/\lambda^3 = \rho$. This contribution can be evaluated by calculating the density-dependent eigenvalues and eigenfunctions of $K_{12}+V_{12}+\rho V^{\mathrm{eff}}_{12;0}$ in the usual way.

We can express our net result by the following equation:



$$= \frac{z^2}{2!}\mathrm{Tr}_2\left(e^{-\beta(K_{12}+V_{12}+\rho V^{\mathrm{eff}}_{12;0})} - e^{-\beta K_{12}}\right) + \text{“other terms .”} \qquad (30)$$

These other terms consist of diagrams each containing at least one of the temperature-dependent components of the effective potential. Also here are terms which were ignored in approximating z/λ^3 by ρ. We have thus approximately summed a certain class of diagrams involving three-body forces expressing the result in terms of an effective second-cluster coefficient.

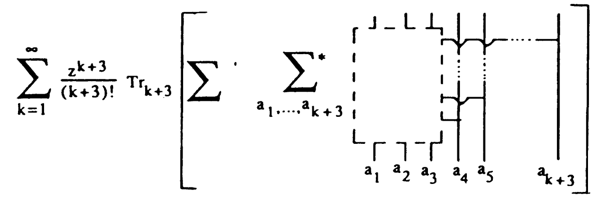
Note that because these other terms involve temperature-dependent components of the effective potential, these will not sum to give Boltzmann factors. We thus content ourselves, for the time being, with keeping track of these terms individually. Note also that since the "other terms" contain components of the effective potential which are of a higher order in β than $V^{\text{eff}}_{12;0}$ we expect that as the temperature increases the sum above is better and better approximated by the effective cluster coefficient.

IV. CONSTRUCTION OF THE THIRD-CLUSTER COEFFICIENT

We now proceed to generalize the construction of Sec. III. Our aim, of course, is to approximately sum some other class of diagrams, expressing the answer as an effective third-cluster coefficient. The means by which we may most readily do this is by considering the following procedure.

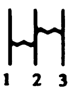
Consider the expansion of the effective third-cluster coefficient, where the density-dependent corrections to the two-body potentials are taken as perturbations. This series is represented as a sum of effective diagrams. Given the experience of Sec. III, each effective diagram should equal, in some approximation, a sum of primitive diagrams. We then select a particular effective diagram from this series. The form of this effective diagram should fairly readily suggest the sum of primitive diagrams from which it is derived. We then take this sum of primitive diagrams and express them in terms of effective diagrams, much as was done in Eqs. (25)–(28). The first term in the expansion of the effective diagram so obtained should, of course, be the particular effective diagram we initially selected from the effective third-cluster coefficient. We carry out this for all effective diagrams in the effective third-cluster coefficient.

We consider a general term from the effective third-cluster coefficient containing k effective interactions. Since there are many such terms we sum over all possible ones (we represent this by a dashed sum in all that follows). The experiences of Sec. III lead us to believe that this sum of effective diagrams derives from the following sum of primitive diagrams:

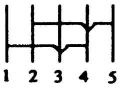


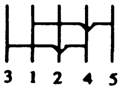
(31)

The starred sum is as before except that we initially choose three integers from $(1,2,\ldots,k+3)$, and we assign them to the variables a_1,a_2,a_3 so that $a_1<a_2<a_3$. The reason we need this condition is best illustrated by example. Let us consider the following effective diagram:



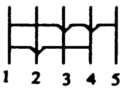
If we did not have this condition we would end up considering the following primitive diagrams, among others,





;

this second diagram equals

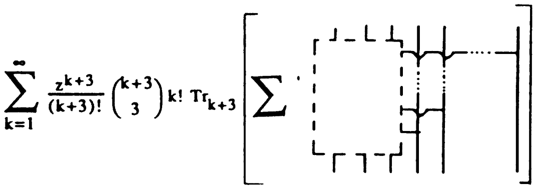


However, the effective diagram

also derives from this. However, this is an effective diagram distinct from the original one and already contained in the dashed sum. The condition $a_1<a_2<a_3$ thus allows us to avoid multiple counting.

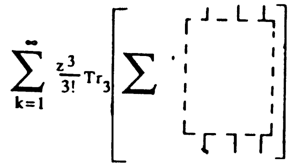
We construct the inside of the dotted box by inserting into it the original effective diagram. For each effective interaction here we insert a three-body interaction, where the third leg leads to one of the $a_4,\ldots,a_{k+3}$ particle lines (which one depends on where in the temperature order the original effective interaction lies.)

We now perform steps analogous to Eqs. (25)–(28) in Sec. III. By permutation symmetry Eq. (31) becomes



(32)

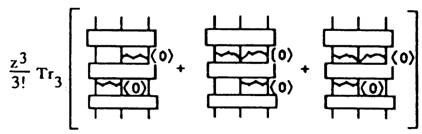
Using the definition of the effective potential this becomes



(33)

where the remaining two legs of the three-body interaction in the box are replaced by effective two-body interactions. If we then substitute the series (19) into Eq. (33), the first term yields our original sum of effective diagrams.

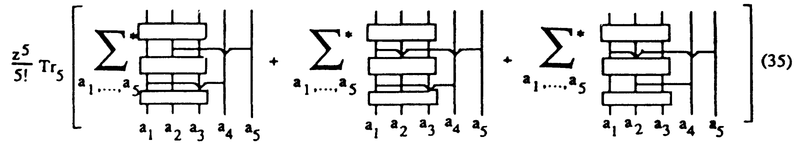
We provide a simple example of this construction. Let us consider the following contribution to b_3^{eff}:



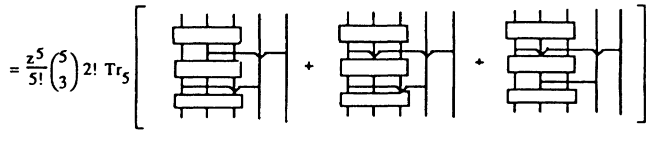
(34)

(The three terms here represent some of the terms in the dashed sum. There are six others which also have two effective interactions. Also the box notation is a simple generalization of the two-body case.)

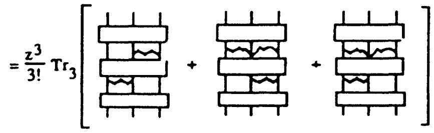
We are led to believe that these effective diagrams derive from the following sum of primitive diagrams:



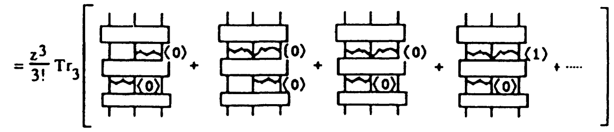
(35)



(36)



(37)

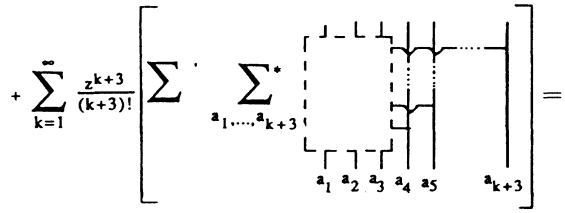


. (38)

The first three contributions are, as we expect, the original effective diagrams selected.

Our net result is thus

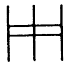
$$\frac{z^3}{3!}\mathrm{Tr}_3\left[e^{-\beta(K_{123}+V_{12}+V_{23}+V_{31})}-e^{-\beta K_{123}}-\sum_{i<j=1}^{3}\left(e^{-\beta(K_{123}+V_{ij})}-e^{\beta K_{123}}\right)\right]$$



$$=\frac{z^3}{3!}\mathrm{Tr}_3\left[e^{-\beta(K_{123}+V_{12}+\rho V^{\text{eff}}_{12;0}+V_{23}+\rho V^{\text{eff}}_{23;0}+V_{31}+\rho V^{\text{eff}}_{31;0})}-e^{-\beta K_{123}}\right.$$
$$\left.-\sum_{i<j=1}^{3}\left(e^{-\beta(K_{123}+V_{ij}+\rho V^{\text{eff}}_{ij;0})}-e^{-\beta K_{123}}\right)\right]+\text{other terms}\,.$$

(39)

The specification, other terms, is as in Eq. (30). Clearly we can similarly extend this procedure to express other approximate summations in terms of higher effective cluster coefficients b_n^{eff}, $n>3$. Carrying this out for all n would not exhaust all possible primitive diagrams. In fact, there would be many left over. For instance,



(40)

would not be included in any of the classes which we sum over. Furthermore, in approximating our sums by effective cluster coefficients we are neglecting many other terms. In inverting the cluster series to find the equation of state we need to take these neglected terms into account so that no significant terms are neglected in the resulting virial series. We do this in the evaluation of the equation of state which is presented in Sec. V.

Before we do this we present a simple model calculation to show how the number of Efimov states in our effective three-body problem changes with density. The effective third-cluster coefficient in Eq. (39) will contain

$$N=\frac{1}{\pi}\ln\frac{|a^{\text{eff}}(\rho)|}{r_0} \tag{41}$$

Efimov states, where a^{eff} is the scattering length of the two-body potential $V_{12}+\rho V^{\text{eff}}_{12;0}$ and is, of course, density dependent (we assume the range of the effective potential is similar to that of the bare potential). Since the ^{4}He gas is the system which will most readily show this enhancement of the Efimov effect, we consider potential parameters appropriate to ^{4}He.

The effective two-body force is defined to be

$$V^{\text{eff}}_{12;0}(\mathbf{r}_1,\mathbf{r}_2)=\int d^3\mathbf{r}_3\, V_{123}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)\,. \tag{42}$$

Let us assume that V_{12} and V_{123} take the forms shown in

Fig. 1. Here $V_b = C_6/R^6$, $U^3 = C_9/R^9$, C_6 and C_9 being the coefficients in the definition of the Van der Waals tail for these forces. Thus these latter expressions estimate, in order of magnitude, the scale of the true pair and three-body potentials. Note that we assume the three-body force to be predominantly repulsive, i.e., we assume it is dominated by the Axilrod-Teller tail. (For more details on the ^{4}He three-body force, see Refs. 9, 18, and 19).

At this stage we should also note that the true three-body force contains a hard core. In assuming that the three-body force can be taken as a perturbation, we have tacitly assumed that there is no hard core (as otherwise the effective potential is undefined; this dictates the use of the "square-wall" three-body potential in Fig. 1). This is a limitation inherent in our construction. However, it is not a serious one. There are two ways of seeing this. First, the presence of a hard core in the two-body force in our model means that the particles will never enter the region of configuration space where any particle is within b of another. As a result they never "feel" the short-range three-body force, and so we do no harm in ignoring the hard core in the true three-body force. Secondly, the model is realistic, provided there is some hard-core exclusion. Whether this is in the two-body force, the three-body force, or both does not qualitatively matter. In principle one could consider a Brueckner-type construction to moderate the hard-core problem. For our purposes we ignore this inessential complication.

Calculating the effective two-body force using Eq. (42) and the given form for the three-body interaction does not yield a square well. However, for simplicity, we approximate it as such. Using the fact that for helium $C_6 = 1.5e^2a_0^5$ and $C_9 = 1.5e^2a_0^8$ (Ref. 20), we readily find that the effective potential has the form of a square well, where the depth of the well is

$$V_{\text{eff}} = V_b\left[1 - \frac{2\pi}{3}\rho a_0^3\right] \tag{43}$$

and the range is R.

We wish to calculate the effective, density-dependent scattering length for this potential. Following Flugge's treatment[21] one can express V_{eff}, b, and R in terms of the effective scattering length and the effective, effective range r_{eff}. In the case $a_{\text{eff}}/R \gg 1$, which holds for ^{4}He, we obtain

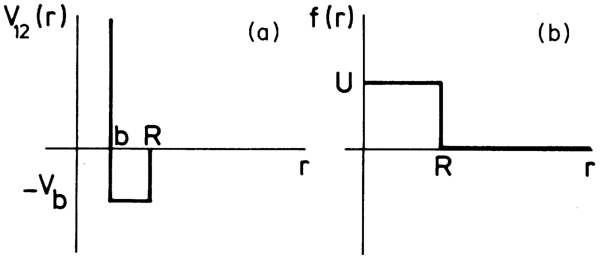


FIG. 1. Forms of potential for model calculation. (a) Bare pair potential. (b) Function used to construct bare three-body potential, where $V_{123} = f(r_{12})f(r_{23})f(r_{31})$.

$$R = r_{\text{eff}} - b\ ,$$

$$V_{\text{eff}} = \frac{\hbar^2}{m_{\text{He}}a_0^2}\left[\frac{a_0}{R}\right]^2\left[\left[\frac{\pi}{2}\right]^2\frac{1}{(1-b/R)^2} + \frac{2}{(1-b/R)a_{\text{eff}}/R}\right], \tag{44}$$

where $\hbar^2/m_{\text{He}}a_0^2 = 43K$.

From Eq. (43) we have

$$\rho = \frac{1}{\frac{2\pi}{3}a_0^3}\left[1 - \frac{V_{\text{eff}}}{V_b}\right] \tag{45}$$

which with Eq. (44) allows us to consider ρ as a function of a_{eff}. Then defining

$$\rho_e = \lim_{a_{\text{eff}}\to\infty}\rho\ ,$$

we see that

$$\rho_e = \frac{24}{2\pi^3}\frac{1}{a_0^3}\left[1 - \frac{b}{R}\right]\frac{R}{a_{\text{bare}}}\ ,$$

which gives

$$a_{\text{eff}} = \frac{a_{\text{bare}}}{\left[1 - \frac{\rho}{\rho_e}\right]}\ . \tag{46}$$

Note that only lowest order terms in R/a_{bare} have been retained.

Thus for our simple-model system the number of Efimov levels in the effective third-virial coefficient is

$$N = \frac{1}{\pi}\ln\left[\frac{|a_{\text{bare}}|}{r_0}\frac{1}{\left|1 - \frac{\rho}{\rho_e}\right|}\right]\ . \tag{47}$$

(Note, ρ is an average density and thus density fluctuations prevent us from getting more than eight Efimov levels on average. This is a result of logarithmic dependence of N.)

We show in Table I the value of ρ_e for various helium potentials. The potential parameters are taken from Huber's paper.[6] Note that the Efimov densities are quite high (for comparison, the density of liquid helium is 35 000 mol/m^3). Such densities still correspond to an imperfect gas, provided the temperature is high enough.

TABLE I. Potential parameters for various ^{4}He potentials together with the corresponding Efimov densities (Ref. 23).

Potential	r_0 (Å)	a_{bare} (Å)	ρ_e (mol/m^3)
Smith-Thakkar	6.81	50.5	247 000
MDD2	7.40	160	78 100
Beck	7.54	1080	11 600
Aziz	7.40	125	100 000
Lennard-Jones	8.0	−176	

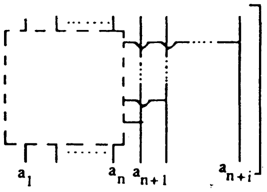
Note also that we only get enhancement if $a_{\text{bare}} > 0$. These points are elaborated on in subsequent discussion.

V. OBTAINING THE EQUATION OF STATE

Having approximately summed the cluster series, we now obtain the corresponding equation of state, so that we can observe how the enhancement of the Efimov effect in b_3^{eff} is reflected in the thermodynamic properties of our many-body system.

The effective nth-cluster coefficients originate from various types of diagrams. Let us denote these by $f_n(z)$, where

$$f_n(z) = \frac{n!}{z^n}\sum_{i=0}^{\infty}\frac{z^{n+i}}{(n+i)!}\mathrm{Tr}_{n+i}\left[\sum{}' \sum_{a_1,\ldots,a_{n+i}}^{*}\right.$$

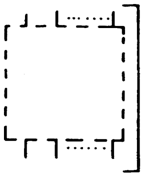


. (48)

For $i=0$ the operator in the trace is, by definition, the connected part of the n-particle Boltzmann operator with only bare pair interactions. The notation for the sums and for "filling the dotted box" is the obvious generalization of the rules given in Sec. IV.

We manipulate Eq. (48) in a manner similar to that in Secs. III and IV, replacing the three-body forces by effective two-body forces. We do not yet expand the effective potential. The result is that

$$\frac{f_n(z)}{Vn!} = g_n\left(\frac{z}{\lambda^3}\right) = \frac{1}{Vn!}\sum_{i=0}^{\infty}\left(\frac{z}{\lambda^3}\right)^i \mathrm{Tr}_{n+i}\left[\sum{}'\right.$$



, (49)

where the rules for filling the box are again simple generalizations of the rules in the preceding sections. Note, we differ here from preceding sections in the definition of the effective potential. Here

$$V_{12}^{\text{eff}}(\mathbf{r}_1,\mathbf{r}_2;z;\beta,\tau) = \sum_{n=0}^{\infty} c_n a^{2n} V_{12;n}^{\text{eff}}(\mathbf{r}_1,\mathbf{r}_2) \ . \tag{50}$$

We have simply taken the factor of z/λ^3 out of Eq. (17). This factor thus appears explicitly in Eq. (49). This redefinition is somewhat more convenient in what follows. As we will be using the definition (49) frequently, we shall define the following abbreviated notation:

$$g_n\left[\frac{z}{\lambda^3}\right] = \frac{1}{Vn!}\sum_{i=0}^{\infty}\left[\frac{z}{\lambda^3}\right]^i \mathrm{Tr}_n\,(i\text{eff}) \ , \tag{51}$$

where the rules for the construction of the operator in the trace are implicit. We only denote the fact that each operator has i effective two-body interactions. The Mayer equations thus assume the form

$$\frac{P}{kT} = \sum_{n=1}^{\infty} z^n g_n\left[\frac{z}{\lambda^3}\right] + \sum_{n=3}^{\infty}\frac{z^n}{Vn!}\mathrm{Tr}_n\,(\mathrm{DI}) \ , \tag{52a}$$

$$\begin{aligned} z\frac{\partial}{\partial z}\left[\frac{P}{kT}\right] = \rho = \frac{z}{\lambda^3} &+ \sum_{n=2}^{\infty} n z^n g_n\left[\frac{z}{\lambda^3}\right] \\ &+ \sum_{n=2}^{\infty} z^n\left[z\frac{\partial}{\partial z}g_n\left[\frac{z}{\lambda^3}\right]\right] \\ &+ \sum_{n=3}^{\infty}\frac{nz^n}{n!}\mathrm{Tr}_n\,(\mathrm{DI}) \ . \end{aligned} \tag{52b}$$

Tr_n (DI) denotes the trace over all n-particle diagrams which have not been included in any of the classes over which we have summed. DI denotes diagrams ignored. [We include here also the term we previously ignored in Eq. (10)]. Note that $g_1(z/\lambda^3) = b_1 = 1/\lambda^3$. The third term in (52b) results from the fact that the effective cluster coefficients, $g_n(z/\lambda^3)$, are now a function of z.

We now must eliminate z between (52a) and (52b) in order to obtain the equation of state. The standard way of doing this[12] consists of writing ρ as a power series in z and inverting this to get z as a power series in ρ. This requires a series expansion in z for $g_n(z/\lambda^3)$. This is given in the definition, Eq. (51). The resulting series for z in ρ would be substituted into the cluster series to obtain the equation of state. This method is inappropriate in our situation because our key result, the observation of an enhancement of the Efimov effect relies on the fact that in the low-density, high-temperature limit $g_3(z/\lambda^3) \to g_3(\rho)$ and that

$$g_3(\rho) = b_3^{\text{eff}}(\rho) + \text{other terms} \ . \tag{53}$$

Expanding $g_n(z/\lambda^3)$ in powers of z/λ^3 results in $b_3^{\text{eff}}(\rho)$ being expanded in powers of ρ. Since this would obscure our main result we must develop a way to obtain the equation of state while keeping these important summations intact. Rather than expand $g_n(z/\lambda^3)$ as a power series in z, we instead replace it by

$$g_n(\rho) + \left[g_n\left[\frac{z}{\lambda^3}\right] - g_n(\rho)\right] \ .$$

We expect the latter term to vanish in the low-density high-temperature limit faster than the former. We incorporate this in (52a) and (52b). Rearranging (52b) to a more convenient form, we obtain

$$\frac{z}{\lambda^3}=\rho\left\{1-\sum_{n=2}^{\infty}\frac{1}{\rho}nz^n g_n(\rho)-\sum_{n=2}^{\infty}\frac{1}{\rho}nz^n\left[g_n\left[\frac{z}{\lambda^3}\right]-g_n(\rho)\right]-\sum_{n=2}^{\infty}\frac{1}{\rho}z^n\left[z\frac{\partial}{\partial z}g_n\left[\frac{z}{\lambda^3}\right]\right]-\sum_{n=3}^{\infty}\frac{1}{\rho}\frac{nz^n}{n!}\mathrm{Tr}_n\,(\mathrm{DI})\right\}. \tag{54}$$

Using the definition of $g_n(z/\lambda^3)$, Eq. (51) in the third and forth terms on the right-hand side of (54), we obtain

$$\frac{z}{\lambda^3}=\rho\left[1-\sum_{n=2}^{\infty}\frac{1}{\rho}nz^n g_n(\rho)-\sum_{n=2}^{\infty}\frac{1}{\rho}z^n\sum_{i=1}^{\infty}\frac{1}{Vn!}\left\{\left[\left[\frac{z}{\lambda^3}\right]^i-\rho^i\right]n+i\left[\frac{z}{\lambda^3}\right]^i\right\}\mathrm{Tr}_n\,(i\mathrm{eff})-\sum_{n=3}^{\infty}\frac{1}{\rho}\frac{nz^n}{n!}\mathrm{Tr}_n\,(\mathrm{DI})\right]. \tag{55}$$

It is easy to see from this expression that $(z/\lambda^3)-\rho=O(\rho^2)$. Thus to first order in ρ, $z/\lambda^3=\rho$. Note also that Eq. (55) also gives $(z/\lambda^3)-\rho=2z^2g_2(\rho)+\cdots$. To lowest order in inverse temperature $g_2(\rho)$ behaves as $(\beta V_0)^{\alpha}$, where α is some number and V_0 is the energy scale of the two-body potential. [For bounded short-range potentials $\alpha=1$; see Sec. VI. For the more singular Lennard-Jones potential, $\alpha=\frac{1}{4}$ (Ref. 22)]. Thus the right-hand side is small for low density or high temperature. This is important for our later considerations. To denote both of these limits we write

$$\frac{z}{\lambda^3}=\rho[1+O(\epsilon)]\ , \tag{56}$$

where ϵ is a small parameter which may be either $\rho\sigma^3$ (σ is a characteristic length of the potential) or $(\beta V_0)^{\alpha}$. Our series is effectively a double series in these two parameters.

In order to obtain z/λ^3 as a function of ρ and β to a higher order in ϵ we iterate Eq. (55). That is, we write Eq. (55) as

$$\frac{z}{\lambda^3}=f\left[\rho,\frac{z}{\lambda^3}\right]$$

and calculate

$$\frac{z}{\lambda^3}=f\left[\rho,f\left[\rho,\frac{z}{\lambda^3}\right]\right].$$

For example, from Eq. (55) we have

$$\frac{z}{\lambda^3}=\rho\left[1-\frac{2}{\rho}\lambda^6\left[\frac{z}{\lambda^3}\right]^2 g_2(\rho)\right.$$
$$\left.-\lambda^6\left[\frac{z}{\lambda^3}\right]^2\frac{1}{\rho}\sum_{i=1}^{\infty}\frac{1}{2V}i\left[\frac{z}{\lambda^3}\right]^i\mathrm{Tr}_2\,(i\mathrm{eff})+O(z^3)\right] \tag{57}$$

in order to get z/λ^3 to second order we need to know z/λ^3 to first order on the right-hand side. This has already been obtained in Eq. (56). Substituting (56) into the right-hand side of Eq. (57), i.e., iterating once, we get

$$\frac{z}{\lambda^3}=\rho\left[1-2\lambda^6\rho g_2(\rho)\right.$$
$$\left.-\lambda^6\rho\sum_{i=1}^{\infty}\frac{1}{2V}i\rho^i\mathrm{Tr}_2\,(i\mathrm{eff})+O(\epsilon^2)\right]$$
$$=\rho\left[1-2\lambda^6\rho g_2(\rho)-\lambda^6\rho\rho\frac{\partial}{\partial\rho}g_2(\rho)+O(\epsilon^2)\right]. \tag{58}$$

We now have z/λ^3 to ϵ^2. This allows us, on the next iteration, to calculate z/λ^3 to order ϵ^3. We may continue this to any order we wish. The iteration is straightforward but tedious. We present the answer to order ϵ^4

$$\frac{z}{\lambda^3}=\rho[1+x_2+x_3+x_4+O(\epsilon^4)]\ , \tag{59}$$

where x_2 can be read from Eq. (58), and x_3 and x_4 are given in the Appendix.

In Eq. (58) we could expand $g_2(\rho)$ in ρ and β. This expansion would, of, course, contain terms of order ϵ^2 which could be grouped with the terms neglected. If we were to do this, however, we would be neglecting the physics we are aiming to investigate [particularly if we were to subsequently expand out $g_3(\rho)$]. Furthermore, there is no numerical inconsistency in not expanding $g_2(\rho)$, for the aim of any approximation is to control the size of the term neglected. What Eq. (58) says is

$$\left|\frac{z}{\lambda^3\rho}-1+2\lambda^6\rho g_2(\rho)+\lambda^6\rho\rho\frac{\partial}{\partial\rho}g_2(\rho)\right|<O(\epsilon^2)\ .$$

Similarly for Eq. (59). Our procedure thus corresponds to a particular partial summation of the ϵ series.

Having obtained z/λ^3 as a function of ρ, to any order we wish, we can subsequently find the equation of state by substituting this expression into the cluster series. Substituting Eq. (59) into the following form for the cluster series,

$$\frac{P}{kT}=\sum_{n=1}^{\infty}z^n g_n(\rho)$$
$$+\sum_{n=2}^{\infty}z^n\sum_{i=1}^{\infty}\frac{1}{Vn!}\left[\left[\frac{z}{\lambda^3}\right]^i-\rho^i\right]\mathrm{Tr}_n\,(i\mathrm{eff})$$
$$+\sum_{n=3}^{\infty}\frac{z^n}{Vn!}\mathrm{Tr}_n\,(\mathrm{DI})\ , \tag{60}$$

we find, by more straightforward but tedious algebra that

$$\frac{P}{kT}=\rho[1+a_2+a_3+a_4+O(\epsilon^4)] , \tag{61}$$

where a_2,a_3,a_4, are now effective virial coefficients. From the derivation it is apparent that each a_n is a partial summation of the ϵ series whose leading term is ϵ^{n-1}. The expressions for these are somewhat complicated and are given in the Appendix.

We now have an expression for the low-density and/or high-temperature properties of a Boltzmann gas, obtained by partial summation of the cluster series. The contributions of the effective three-body problem are given in terms involving g_3 in a_3 and a_4.

In order to evaluate this whole expression we need to solve the two-body, three-body, and four-body problem for the potential $V_{12}+\rho V_{12;0}^{\text{eff}}$ as well as evaluating the contributions of the other components of the effective potential (i.e., the so-called other terms). This is a daunting task. Here we satisfy ourselves with calculating a high-temperature series.

VI. THE HIGH-TEMPERATURE EXPANSION OF THE EQUATION OF STATE

In order to make use of our equation of state we need to consider a situation where the parameter ϵ is small enough so that the contributions of the terms neglected in Eq. (61) are negligible. Thus we need to consider low density and/or high temperature. We choose to consider the case of high temperature. That is, we allow the situation where $\rho\sigma^3$ can be of order 1. The reason for this is clear from our calculation in Sec. IV for the case of ^{4}He. Here it was shown, for a simplified model, that to reach the Efimov point, one requires a density $\rho_e \approx 10^5$ mol/m^3. This corresponds to $\rho_e\sigma^3=O(1)$. Thus in applying our results to ^{4}He at the Efimov point we must use the virial expansion not as a low-density expansion but as a high-temperature one.

Ideally we would like to continue in the vein of the calculation in Sec. IV, using an effective hard-core pair potential since that is what is appropriate to ^{4}He. We also require that few-body effects be incorporated properly, since we are interested in the Efimov effect. Unfortunately the high-temperature series that we require have not been calculated under both these conditions. The best result to date has been that of Bollé,[16] who calculates the high-temperature expansions of the second- and third-virial coefficients, incorporating few-body effects, but only considering bounded, short-range potentials. Bollé obtains

$$a_2=\frac{-b_2}{b_1^2}=-\tfrac{1}{2}\sum_{n=1}^{\infty}\frac{(-1)^n}{n!}\beta^n\int d^3\mathbf{x}\,P_n(\mathbf{x}) , \tag{62}$$

$$\begin{aligned}a_3=\frac{4b_2^2}{b_1^4}-\frac{2b_3}{b_1^3}=&\sum_{n=3}^{\infty}(-1)^n\beta^n\sum_{i=1}^{n-1}\frac{1}{(n-i)!i!}\int d^3\mathbf{x}\,P_{n-i}(\mathbf{x})\int d^3\mathbf{y}\,P_i(\mathbf{y})\\&-\tfrac{1}{3}\sum_{n=3}^{\infty}\tfrac{1}{2}\beta^n\left[\frac{(\chi_\alpha^2)^{n-2}}{(n-2)!}\int d^6\rho\,P_2^c(\rho)+\frac{(-1)^n}{n!}\int d^6\rho\,P_n^c(\rho)\right] ,\end{aligned} \tag{63}$$

where $-\chi_\alpha^2$ is the two-body threshold and P_n and P_n^c are polynomials in the potential and its derivatives. ρ as an integration variable denotes use of Jacobi coordinates. In a_2 (and thus in b_2) it seems likely that the series can be partially summed to give one which is defined for hard-core potentials. For example, the first term in $P_n(x)$ is the potential raised to the nth power, i.e., $P_n(\mathbf{x})=V^n(\mathbf{x})+Q_n(\mathbf{x})$, where $Q_n(\mathbf{x})$ represents the remaining terms. Thus

$$\begin{aligned}a_2=&-\tfrac{1}{2}\int d^3\mathbf{x}(e^{-\beta V}-1)\\&-\tfrac{1}{2}\sum_{n=1}^{\infty}\frac{(-1)^n}{n!}\beta^n\int d^3\mathbf{x}\,Q_n(\mathbf{x}) .\end{aligned} \tag{64}$$

One expects to be able to do other partial summations so that the whole series is defined for hard-core potentials. However, for a_3 (and thus b_3) there are terms involving $-\chi_\alpha^2$ which are associated only with P_2^c. In order to define an expression for a_3 which is valid for hard-core potentials this term will have to be grouped with other terms involving P_n^c, none of which has any dependence on $-\chi_\alpha^2$. The resulting summation will thus not be an exponential. Furthermore, it is not obvious that the sum can be explicitly done.

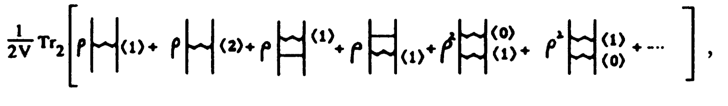
Even if we could resum Eqs. (62) and (63) so that they were defined for hard-core potentials, we would still have the further problem of treating the other terms in $g_n(\rho)$ which involve the temperature-dependent components of the effective potential. Each of these individual terms is undefined if $V_{12;i}^{\text{eff}}$, for $i\geq 0$, have hard cores. Again partial summations are needed. In view of these complications we satisfy ourselves for the present with the (unrealistic) model system involving bounded short-range pair potentials.

In obtaining our high-temperature expansion for the equation of state we require high-temperature expansions for $g_n(\rho)$. In fact, we will soon see that we require these expansions only to order β^3. Thus we need expansions of $g_n(\rho)$ only for $n=2,3,4$. We now outline the major steps in the calculation leaving the (considerable) detail to the reader.

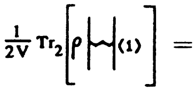
Let us first consider $g_2(\rho)$

$$g_2(\rho)=\frac{1}{2V}\mathrm{Tr}_2(e^{-\beta(K_{12}+V_{12}+\rho V^{\mathrm{eff}}_{12;0})}-e^{-\beta K_{12}})$$
$$+\sum_{i=1}^{\infty}\frac{1}{2V}\rho^i\mathrm{Tr}_2(i\mathrm{eff})\ . \tag{65}$$

The first term is of the form of a second-cluster coefficient. The high-temperature expansion for this is given in Eq. (62). (Note that density plays the role of an independent parameter in the equations of Bollé.) The remaining terms in $g_2(\rho)$ are


(66)

where the terms neglected are of order β^4 or higher. The high-temperature expansion for these terms is done in the standard way using Laplace's method. For completeness we present the calculation of the first term



$$=\frac{1}{2V}\int_0^\beta d\tau\int d^3\mathbf{r}_1\,d^3\mathbf{r}_2\,d^3\mathbf{r}'_1\,d^3\mathbf{r}'_2\frac{1}{\lambda^6}\left[\frac{1}{\lambda^3}\frac{1}{(1-\tau/\beta)^{3/2}}\frac{1}{(\tau/\beta)^{3/2}}\right]^2\exp\left[\frac{-\pi}{\lambda^2}\frac{(\mathbf{r}_1-\mathbf{r}'_1)^2}{(\tau/\beta)(1-\tau/\beta)}\right]$$
$$\times\exp\left[\frac{-\pi}{\lambda^2}\frac{(\mathbf{r}_2-\mathbf{r}'_2)^2}{(\tau/\beta)(1-\tau/\beta)}\right]\left[\frac{-1}{4\pi}\right]\lambda^2\left[1-\frac{\tau}{\beta}\right]\frac{\tau}{\beta}\rho V^{\mathrm{eff}}_{12;1}(\mathbf{r}'_1,\mathbf{r}'_2)\ . \tag{67}$$

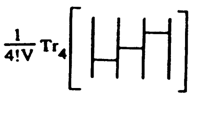
One then changes variables to $\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_1-\mathbf{r}'_1=\mathbf{x}$, $\mathbf{r}_2-\mathbf{r}'_2=\mathbf{y}$ and does the $\mathbf{x},\mathbf{y}$ integrals by Laplace's method. This involves expanding the potential as a Taylor series in $\mathbf{x},\mathbf{y}$. We keep terms up to and including quadratic. All higher terms in the Taylor series contribute terms of order β^4 or higher. We then simply evaluate the Gaussian integrals to obtain

$$-\frac{\hbar^2}{24m}\beta^2\frac{1}{\lambda^6}\int d^3\mathbf{r}\,\rho V^{\mathrm{eff}}_{12;1}$$
$$-\frac{1}{240}\left[\frac{\hbar^2}{m}\right]^2\beta^3\frac{1}{\lambda^6}\int d^3\mathbf{r}\,\nabla^2(\rho V^{\mathrm{eff}}_{12;1})\ . \tag{68}$$

The other terms are calculated in a similar manner. The high-temperature expansion for $g_3(\rho)$ can be done in an entirely analogous manner.

The lowest-order terms in the high-temperature expansion are always easy to calculate because the product of propagators tends to a product of δ functions (see Bloch's[15] discussion of the classical limit). With this in mind we can see that, for instance, to lowest order a_5 goes like β^4 because these must be at least four pair interactions since the diagrams contributing must be connected.

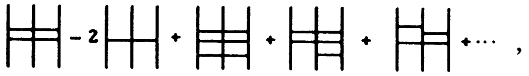
The calculation of $g_4(\rho)$ is somewhat different to the calculation of $g_2(\rho)$ and $g_3(\rho)$ because the high-temperature expansion for the effective fourth-cluster coefficient, taking into account few-body effects, is not available. We content ourselves with finding the high-temperature terms using Laplaces's method as above. For instance, $g_4(\rho)$ contains the following diagram:


(69)

Using the above method, we obtain, in a straightforward calculation

$$-\frac{1}{144}\frac{1}{\lambda^{12}}\beta^3\left[\int d^3\mathbf{x}\,V_{12}(\mathbf{x})\right]^3\ . \tag{70}$$

The expressions for a_3 and a_4 in the Appendix show that we also require, to order β^3, the high-temperature series of the contributions of the ignored diagrams. These are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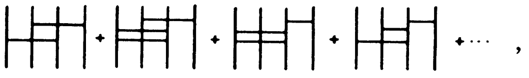
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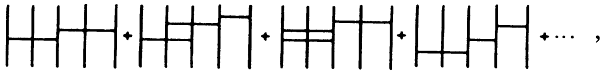
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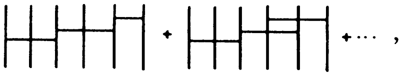
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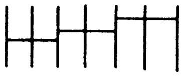
(75)

where we have listed only a representative subset of the terms needed in each trace. The high-temperature expansions of these are straightforward.

By grouping together high-temperature expansions of all components of a_2,a_3,a_4 we arrive (after more straightforward but tedious calculation) at the final form for the high-temperature series for the equation of state

$$\frac{P}{kT}=\rho[1+d_2\beta+d_3\beta^2+d_4\beta^3+O(\beta^4)]\ . \tag{76}$$

The coefficients d_2,d_3,d_4, are long expressions which are given in the Appendix. This expression, Eq. (76), is valid for arbitrary density, provided one is at a sufficiently high temperature.

VII. THERMODYNAMICS

The expression derived for the equation of state is typical of what one would expect for an imperfect gas. One interesting feature to note is that bound-state contributions do not appear in the high-temperature expansion of the second- and third-cluster coefficients. These are cancelled by equal and opposite contributions in the continuum integration. This can be seen explicitly in Bollé's derivation.[16] It thus appears that the full richness of the Efimov effect is not reflected in the high-temperature properties of the ^{4}He gas. This, however, is only partially true, for while the bound states make no contribution, the two-body continuum does. This contribution appears through the two-body threshold $-\chi_\alpha^2$ which appears in g_3. At the Efimov point $\chi_\alpha^2=0$. If we assume that the bare potential has a bound state and that the three-body force is predominantly repulsive, then, as a function of density, χ_α^2 has the form given in Fig. 2. For $\rho>\rho_e$ there is no two-body bound state; thus the threshold is zero. For $\rho<\rho_e$ the perturbation expansion of the two-body binding energy tells us that

$$\chi_\alpha^2=-(\rho-\rho_e)\langle\psi_e\,|\,V_{12;0}^{\mathrm{eff}}\,|\,\psi_e\rangle+O(\rho-\rho_e)^2\ , \qquad (77)$$

where $|\psi_e\rangle$ is the wave function of the zero-energy bound state. We thus observe that $\chi_\alpha^2(\rho)$ is a continuous function with a discontinuous first derivative at the Efimov point. This discontinuity, however, is small since the χ_α^2 contributions are of order β^3. (We now see why the expansions were carried out to order β^3.)

What are the consequences of this discontinuity for the thermodynamic behavior? At this stage some care must be taken. The equation of state, as given in the Appendix, contains a term which has a factor $(\partial/\partial\rho)\chi_\alpha^2$. This implies that at the Efimov point the pressure exhibits a discontinuity as a function of density. This, however, is not the case because density is not an independent variable. The independent variable is the fugacity z, and the density is given by the second Mayer equation. In order to examine the thermodynamic behavior we must thus return to the Mayer equations.

Using the expansions of Bollé in $g_3(z/\lambda^3)$ we readily see that there is a term in Eq. (52a) here which contains a factor $\chi_\alpha^2(z/\lambda^3)$. With Fig. 2 in mind (where the independent variable is now z/λ^3 and not the density) we see that the pressure, as a function of z/λ^3, for constant temperature, has the form given in Fig. 3(a). The density subsequently has the form given in Fig. 3(b). Thus at the Efimov point we find that the gas exhibits behavior characteristic of a first-order phase transition. [In Sec. IV we used a high-temperature approximation $z/\lambda^3=\rho$ and defined the Efimov point as the density for which $V_{12}+\rho V_{12;0}^{\mathrm{eff}}$ had a zero-energy two-body bound state. Our discussion here shows that we must examine the fugacity dependence of the pressure rather than the density dependence. As a result we must now define the Efimov point to be the value of z/λ^3 where $V_{12}+(z/\lambda^3)V_{12;0}^{\mathrm{eff}}$ has a zero-energy bound state. We denote this value as $(z/\lambda^3)_e$.]

The discontinuity in the density can be readily calculated and is found to be

$$\frac{\rho\left[\left[\frac{z}{\lambda^3}\right]_e^+,T\right]-\rho\left[\left[\frac{z}{\lambda^3}\right]_e^-,T\right]}{\rho\left[\left[\frac{z}{\lambda^3}\right]_e^+,T\right]}=\frac{\beta^3}{2}\left[\frac{z}{\lambda^3}\right]_e^2\left[\int d^3\mathbf{r}\left[V_{12}+\left[\frac{z}{\lambda^3}\right]_e V_{12;0}^{\mathrm{eff}}\right)\right]^2\left\langle\psi_e\left|\left[\frac{z}{\lambda^3}\right]_e V_{12;0}^{\mathrm{eff}}\right|\psi_e\right\rangle+O(\beta^4)$$

$$=k(\beta V_0)^2(\beta V')\left[\left[\frac{z}{\lambda^3}\right]_e\sigma^3\right]^2, \qquad (78)$$

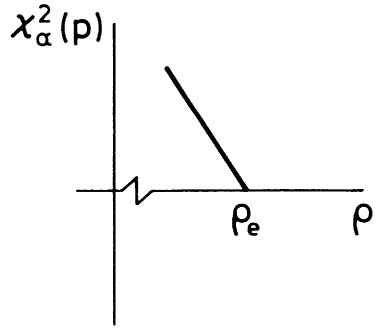

FIG. 2. Behavior of two-body threshold in the vicinity of the Efimov point.

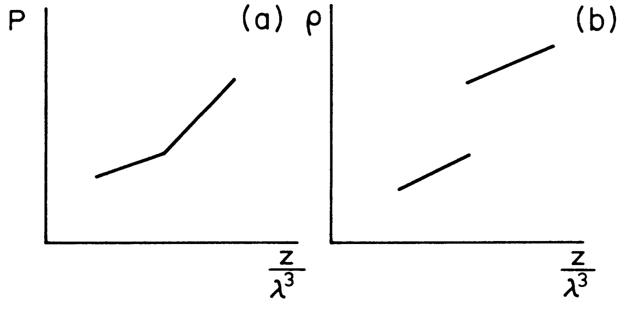

FIG. 3. Qualitative behavior of the Mayer equations in the vicinity of the Efimov point. (a) Pressure and (b) density.

where k is a number of order 1, σ is of the order of the range of the effective potential, V_0 is of the order of the depth of the effective well, and $V'=V_0-V_b$, where V_b is of the order of the depth of the bare well. At 100 K we find that the fractional density discontinuity is roughly of the order of 10^{-6}. Note that unlike the gas-liquid phase transition, there is no critical point here.

VIII. DISCUSSION

If our aim is to model a ^{4}He gas at densities sufficiently close to the Efimov point and at temperatures sufficiently high so that a virial expansion is an accurate representation of the equation of state, then our approach has limitations. First, as we have previously discussed, the three-body force in the helium system contains a hard core. Our expression for the effective potential diverges if the three-body potential possesses a hard core. We need to improve our construction to handle this more realistic case. We know, however, what to expect from a more proper treatment, for we are guided by the use of effective potentials to represent three-body forces in other situations (e.g., by Sinanoglu[10] in the classical theory of liquids and in nuclear-matter calculations[23]). In these cases one finds the following form for the effective potential:

$$V_{12}^{\text{eff}}(\mathbf{r}_1,\mathbf{r}_2)=\rho\int d^3\mathbf{r}_3\, g^{(3)}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)V_{123}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)\;, \tag{79}$$

where $g^{(3)}$ is a three-particle correlation function. The form of this function expresses the obvious face that, because of the hard cores, there is little probability of finding the particles close to each other. Thus they only rarely "feel" the short-range component of the three-body potential. This correlation function counteracts any hard-core component in V_{123} so that the effective potential is finite. Our treatment thus ignores the strong short-range correlations which exist in the system.

A more serious problem exists in the fact that to calculate thermodynamic properties one requires the calculation of various quantum-mechanical traces. To calculate the part of $g_3(\rho)$ which has the form of a third-cluster coefficient requires a solution of the three-body problem. On top of this, $g_2(\rho)$ and $g_3(\rho)$ have contributions which cannot be written as cluster coefficients, i.e., the terms involving the temperature-dependent effective potentials. The prospects of calculating the thermodynamic properties explicitly, even numerically, constitute a difficult problem. With this in mind we have considered the less ambitious case of calculating high-temperature expansions for the equation of state, using the series of Bollé. These, however, are only valid for bounded, short-range potentials. In order to evaluate the high-temperature properties of a realistic system, we thus need to generalize the results of Bollé to include hard-core potentials as well as needing to write the other terms so that they too are defined for hard-core potentials. A low-temperature expansion should also be considered.

Another limitation is the use of Boltzmann statistics. Helium is a Bose system (in fact the Efimov effect relies on this). The Mayer equations are well known for the case of Bose statistics.[13] The generalization of our construction is then rather straightforward, and we expect only slight quantitative differences to the results given here. This is not surprising given that we are considering the high-temperature case. We feel it best to present the full Bose result when other limitations have been overcome.

A further limitation lies in our assumptions when applying our formalism to the ^{4}He system. It has not been established whether the dimer of helium is slightly bound or slightly unbound. All that is known is that it is close to zero energy. We have assumed the dimer is bound. The reason for this is that in the gas the long-range van der Waals tail of the three-body interaction is dominant in the effective potential, and this tends to be repulsive. Thus the energy of the effective dimer can only be greater than the bare dimer. If we had an unbound dimer, density effects would lead to an effective dimer which was even more unbound. This does not mean that ^{4}He will not show the enhancement of the Efimov effect if the potential has an unbound dimer. The reason is the following. For intermediate ranges the three-body force is attractive. For lower temperatures and higher densities the effective potential will tend to increase binding, because under these conditions the correlation function has more probability in these intermediate ranges. Thus one gets more of a contribution to the effective potential from the attractive portion of the three-body force. How low in temperature or how high in density one needs to go to make the effective potential attractive is a subject for further investigation. These qualitative considerations are given quantitative support by the calculations of Blaisten-Barojas *et al.*[11] who calculate these effective potentials for use in the classical theory of liquids.

Clearly some obstacles need to be overcome in order to model a realistic system. Work aiming to overcome these is in progress. In the meantime our simplified model has shown that there exists the prospect for microscopic few-body dynamics to induce interesting macroscopic properties. In concluding we would like to point out that a more realistic model will show qualitatively similar thermodynamics to our simple model. Also, as outlined above, this behavior will occur whether helium has a bound or virtual dimer. As a result, the thermodynamic behavior outlined above is expected to occur in a real gas. The Efimov point, where the interesting behavior lies is, however, somewhat ill determined by the theory at present.

Note added in proof. In the process of generalizing Bollé's work on the high-temperature expansion of b_3 to include the case of hard-core potentials we came across an element of Bollé's derivation which cast doubt on the presence of the χ_α^2 term in the series, Eq. (63). Professor Bollé has confirmed in correspondance that the term in χ_α^2 is absent from Eq. (63) and that he has provided details in an erratum [Phys. Rev. A **39**, 2753 (1989)]. A result of the removal of the χ_α^2 terms is that the phase transitionlike behavior outlined in Sec. VII does not occur. Consequently the appearance of bound-state effects at high temperature depends on whether Bollé's series are convergent or asymptotic. We will discuss this question and our generalization of Bollé's work in a future paper.

ACKNOWLEDGMENTS

One of us (C.P.) would like to acknowledge stimulating discussions with Mark Thomson and Geoff Adam. He also acknowledges the financial assistance of the Australian Government.

APPENDIX

In this Appendix we detail the various series defined in the text by Eqs. (59), (61), and (76). We begin with Eq. (59)

$$
\begin{aligned}
\frac{z}{\lambda^3} &= \rho[1+x_2+x_3+x_4+O(\epsilon^4)]\ ,\\
x_2 &= -2\lambda^6\rho g_2(\rho) - \lambda^6\rho\rho\frac{\partial}{\partial\rho}g_2(\rho)\ ,\\
x_3 &= -4\lambda^6\rho x_2 g_2(\rho) - 3\lambda^9\rho^2 g_3(\rho) - 4\lambda^6\rho x_2\rho\frac{\partial}{\partial\rho}g_2(\rho) - \lambda^6\rho x_2\rho\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}g_2(\rho)\\
&\quad -\lambda^9\rho^2\rho\frac{\partial}{\partial\rho}g_3(\rho) - \lambda^9\rho^2\frac{1}{2V}\mathrm{Tr}_3(\mathrm{DI}) - \lambda^{12}\rho^3\frac{1}{6V}\mathrm{Tr}_4(\mathrm{DI}) - \lambda^{15}\rho^4\frac{1}{24V}\mathrm{Tr}_5(\mathrm{DI})\ ,\\
x_4 &= -2\lambda^6\rho x_2^2 g_2(\rho) - 4\lambda^6\rho x_3 g_2(\rho) - 9\lambda^9\rho^2 x_2 g_3(\rho) - 4\lambda^{12}\rho^3 g_4(\rho)\\
&\quad -2\lambda^6\rho x_3\rho\frac{\partial}{\partial\rho}g_2(\rho) - \tfrac{5}{2}\lambda^6\rho x_2^2\rho\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}g_2(\rho) - 4\lambda^6\rho x_2^2\rho\frac{\partial}{\partial\rho}g_2(\rho) - \lambda^6\rho x_3\rho\frac{\partial}{\partial p}\rho\frac{\partial}{\partial p}g_2(\rho)\\
&\quad -\tfrac{1}{2}\lambda^6\rho x_2^2\rho\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}g_2(\rho) - 6\lambda^9\rho^2 x_2\rho\frac{\partial}{\partial\rho}g_3(\rho) - \lambda^9\rho^2 x_2\rho\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}g_3(\rho) - \lambda^{12}\rho^3\rho\frac{\partial}{\partial\rho}g_4(\rho)\\
&\quad -3\lambda^9\rho^2 x_2\frac{1}{2V}\mathrm{Tr}_3(\mathrm{DI}) - 4\lambda^{12}\rho^3 x_2\frac{1}{6V}\mathrm{Tr}_4(\mathrm{DI}) - 5\lambda^{15}\rho^4 x_2\frac{1}{24V}\mathrm{Tr}_5(\mathrm{DI})\\
&\quad -\lambda^{18}\rho^5\frac{1}{5!V}\mathrm{Tr}_6(\mathrm{DI}) - \lambda^{21}\rho^6\frac{1}{6!V}\mathrm{Tr}_7(\mathrm{DI})\ .
\end{aligned}
$$

Equation (61) is

$$
\begin{aligned}
\frac{P}{kT} &= \rho[1+a_2+a_3+a_4+O(\epsilon^4)]\ ,\\
a_2 &= -\lambda^6\rho g_2(\rho) - \lambda^6\rho\rho\frac{\partial}{\partial\rho}g_2(\rho)\ ,\\
a_3 &= 4(\lambda^6\rho)^2[g_2(\rho)]^2 + 8(\lambda^6\rho)^2 g_2(\rho)\rho\frac{\partial}{\partial\rho}g_2(\rho) + 3(\lambda^6\rho)^2\left[\rho\frac{\partial}{\partial\rho}g_2(\rho)\right]^2\\
&\quad +2(\lambda^6\rho)^2 g_2(\rho)\rho\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}g_2(\rho) + (\lambda^6\rho)^2\left[\rho\frac{\partial}{\partial\rho}g_2(\rho)\right]\left[\rho\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}g_2(\rho)\right] - 2\lambda^9\rho^2 g_3(\rho)\\
&\quad -\lambda^9\rho^2\rho\frac{\partial}{\partial\rho}g_3(\rho) - \frac{1}{3V}\lambda^9\rho^2\mathrm{Tr}_3(\mathrm{DI}) - \frac{1}{8V}\lambda^{12}\rho^3\mathrm{Tr}_4(\mathrm{DI}) - \frac{1}{30V}\lambda^{15}\rho^4\mathrm{Tr}_5(\mathrm{DI})\ ,\\
a_4 &= -20(\lambda^6\rho)^3[g_2(\rho)]^3 - 46(\lambda^6\rho)^3[g_2(\rho)]^2\rho\frac{\partial}{\partial\rho}g_2(\rho)\\
&\quad +18(\lambda^6\rho)(\lambda^9\rho^2)g_2(\rho)g_3(\rho) - 31(\lambda^6\rho)^3 g_2(\rho)\left[\rho\frac{\partial}{\partial\rho}g_2(\rho)\right]^2\\
&\quad -20(\lambda^6\rho)^3[g_2(\rho)]^2\left[\rho\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}g_2(\rho)\right] - 24(\lambda^6\rho)^3[g_2(\rho)]\left[\rho\frac{\partial}{\partial\rho}g_2(\rho)\right]\left[\rho\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}g_2(\rho)\right]\\
&\quad +12(\lambda^6\rho)(\lambda^9\rho^2)g_2(\rho)\rho\frac{\partial}{\partial\rho}g_3(\rho) + 3(\lambda^6\rho)(\lambda^9\rho^2)g_2(\rho)\frac{1}{V}\mathrm{Tr}_3(\mathrm{DI})\\
&\quad +2(\lambda^6\rho)(\lambda^{12}\rho^3)g_2(\rho)\frac{4}{3V}\mathrm{Tr}_4(\mathrm{DI}) + 2(\lambda^6\rho)(\lambda^{15}\rho^4)g_2(\rho)\frac{5}{12V}\mathrm{Tr}_5(\mathrm{DI})\\
&\quad +9(\lambda^6\rho)(\lambda^9\rho^2)g_3(\rho)\rho\frac{\partial}{\partial\rho}g_2(\rho) - 3\lambda^{12}\rho^3 g_4(\rho)
\end{aligned}
$$

$$+6(\lambda^6\rho)(\lambda^9\rho^2)\left[\rho\frac{\partial}{\partial\rho}g_2(\rho)\right]\left[\rho\frac{\partial}{\partial\rho}g_3(\rho)\right]-\tfrac{13}{2}(\lambda^6\rho)^3\left[\rho\frac{\partial}{\partial\rho}g_2(\rho)\right]^3$$

$$-7(\lambda^6\rho)^3\left[\rho\frac{\partial}{\partial\rho}g_2(\rho)\right]^2\left[\rho\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}g_2(\rho)\right]+(\lambda^6\rho)(\lambda^9\rho^2)\rho\frac{\partial}{\partial\rho}g_2(\rho)\frac{3}{2V}\mathrm{Tr}_3(\mathrm{DI})$$

$$+(\lambda^6\rho)(\lambda^{12}\rho^3)\rho\frac{\partial}{\partial\rho}g_2(\rho)\frac{2}{3V}\mathrm{Tr}_4(\mathrm{DI})+(\lambda^6\rho)(\lambda^{15}\rho^4)\rho\frac{\partial}{\partial\rho}g_2(\rho)\frac{5}{24V}\mathrm{Tr}_5(\mathrm{DI})$$

$$+3(\lambda^6\rho)(\lambda^9\rho^2)g_3(\rho)\rho\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}g_2(\rho)-2(\lambda^6\rho)^3g_2(\rho)\left[\rho\frac{\partial}{\partial p}\rho\frac{\partial}{\partial\rho}g_2(\rho)\right]^2$$

$$-(\lambda^6\rho)^3\left[\rho\frac{\partial}{\partial\rho}g_2(\rho)\right]\left[\rho\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}g_2(\rho)\right]^2+(\lambda^6\rho)(\lambda^9\rho^2)\left[\rho\frac{\partial}{\partial\rho}g_3(\rho)\right]\left[\rho\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}g_2(\rho)\right]$$

$$+(\lambda^6\rho)(\lambda^9\rho^2)\rho\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}g_2(\rho)\frac{1}{2V}\mathrm{Tr}_3(\mathrm{DI})+(\lambda^6\rho)(\lambda^{12}\rho^3)\rho\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}g_2(\rho)\frac{1}{6V}\mathrm{Tr}_4(\mathrm{DI})$$

$$+(\lambda^6\rho)(\lambda^{15}\rho^4)\rho\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}g_2(\rho)\frac{1}{24V}\mathrm{Tr}_5(\mathrm{DI})-2(\lambda^6\rho)^3[g_2(\rho)]^2\rho\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}g_2(\rho)$$

$$-2(\lambda^6\rho)^3[g_2(\rho)]\left[\rho\frac{\partial}{\partial\rho}g_2(\rho)\right]\left[\rho\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}g_2(\rho)\right]-\tfrac{1}{2}(\lambda^6\rho)^3\left[\rho\frac{\partial}{\partial\rho}g_2(\rho)\right]^2\rho\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}g_2(\rho)$$

$$+2(\lambda^6\rho)(\lambda^9\rho^2)g_2(\rho)\rho\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}g_3(\rho)+(\lambda^6\rho)(\lambda^9\rho^2)\left[\rho\frac{\partial}{\partial\rho}g_2(\rho)\right]\left[\rho\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}g_3(\rho)\right]$$

$$-\lambda^{12}\rho^3\rho\frac{\partial}{\partial\rho}g_4(\rho)-\lambda^{18}\rho^5\frac{5}{6!V}\mathrm{Tr}_6(\mathrm{DI})-\lambda^{21}\rho^6\frac{6}{7!V}\mathrm{Tr}_7(\mathrm{DI})\ .$$

Equation (76) is

$$\frac{P}{kT}=\rho[1+d_2\beta+d_3\beta^2+d_4\beta^3+O(\beta^4)]\ ,$$

$$d_2=\rho\left[\frac{1}{2}\int d^3\mathbf{r}(V_{12}+\rho V^{\mathrm{eff}}_{12;0})+\frac{1}{2}\int d^3\mathbf{r}\,\rho V^{\mathrm{eff}}_{12;0}\right]-\tfrac{2}{3}\rho^2\int d^6\rho\, V_{123}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)\ ,$$

$$d_3=\rho\left[-\frac{1}{4}\int d^3\mathbf{r}\left[(V_{12}+\rho V^{\mathrm{eff}}_{12;0})^2-\frac{\hbar^2}{3m}\nabla^2(V_{12}+\rho V^{\mathrm{eff}}_{12;0})\right]\right.$$

$$\left.-\frac{1}{4}\int d^3\mathbf{r}\left[2(V_{12}+\rho V^{\mathrm{eff}}_{12;0})\rho V^{\mathrm{eff}}_{12;0}-\frac{\hbar^2}{3m}\nabla^2(\rho V^{\mathrm{eff}}_{12;0})\right]+\frac{1}{12}\frac{\hbar^2}{m}\int d^3\mathbf{r}\,\rho V^{\mathrm{eff}}_{12;1}\right]$$

$$+\rho^2\left[\frac{7}{3}\int d^3\mathbf{r}(V_{12}+\rho V^{\mathrm{eff}}_{12;0})\int d^3\mathbf{y}\rho V^{\mathrm{eff}}_{12;0}+\left[\int d^3\mathbf{y}\rho V^{\mathrm{eff}}_{12;0}\right]^2\right.$$

$$\left.-\frac{1}{3}\frac{\hbar^2}{m}\int d^6\rho\,\nabla^2_{\mathbf{x}}V_{123}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)-\frac{1}{6}\int d^6\rho[V_{123}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)]^2\right]$$

$$-\rho^3\frac{3}{8}\int d^9\rho\, V_{123}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)V_{123}(\mathbf{r}_2,\mathbf{r}_3,\mathbf{r}_4)-\rho^4\frac{1}{2}\int d^{12}\rho\, V_{123}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)V_{123}(\mathbf{r}_3,\mathbf{r}_4,\mathbf{r}_5)\ ,$$

$$d_4=\rho\left\{\frac{1}{12}\int d^3\mathbf{r}\left[(V_{12}+\rho V^{\mathrm{eff}}_{12;0})^3-\frac{\hbar^2}{m}(V_{12}+\rho V^{\mathrm{eff}}_{12;0})\nabla^2(V_{12}+\rho V^{\mathrm{eff}}_{12;0})\right.\right.$$

$$\left.-\frac{\hbar^2}{2m}[\nabla(V_{12}+\rho V^{\mathrm{eff}}_{12;0})]^2+\left[\frac{\hbar^2}{m}\right]^2\tfrac{1}{10}\nabla^4(V_{12}+\rho V^{\mathrm{eff}}_{12;0})\right]$$

$$+\frac{1}{12}\int d^3\mathbf{r}\left[3(V_{12}+\rho V^{\mathrm{eff}}_{12;0})^2(\rho V^{\mathrm{eff}}_{12;0})-\frac{\hbar^2}{m}\rho V^{\mathrm{eff}}_{12;0}\nabla^2(V_{12}+\rho V^{\mathrm{eff}}_{12;0})-\frac{\hbar^2}{m}(V_{12}+\rho V^{\mathrm{eff}}_{12;0})\nabla^2(\rho V^{\mathrm{eff}}_{12;0})\right.$$

$$\left.-\frac{\hbar^2}{m}\nabla(\rho V^{\mathrm{eff}}_{12;0})\nabla(V_{12}+\rho V^{\mathrm{eff}}_{12;0})+\left[\frac{\hbar^2}{m}\right]^2\frac{1}{10}\nabla^4(\rho V^{\mathrm{eff}}_{12;0})\right]$$

$$
\begin{aligned}
&+\frac{1}{120}\left[\frac{\hbar^2}{m}\right]^2\int d^3\mathbf{r}\,\nabla^2(\rho V^{\mathrm{eff}}_{12;1})-\frac{1}{12}\frac{\hbar^2}{m}\int d^3\mathbf{r}(V_{12}+\rho V^{\mathrm{eff}}_{12;0})\rho V^{\mathrm{eff}}_{12;1}\\
&-\frac{1}{24}\frac{\hbar^2}{m}\int d^3\mathbf{r}(\rho V^{\mathrm{eff}}_{12;0})(\rho V^{\mathrm{eff}}_{12;1})+\frac{1}{240}\frac{\hbar^2}{m}\int d^3\mathbf{r}(\rho V^{\mathrm{eff}}_{12;2})\Bigg\}\\
&+\rho^2\Bigg[-\frac{7}{2}\int d^3\mathbf{r}(V_{12}+\rho V^{\mathrm{eff}}_{12;0})\int d^3\mathbf{y}(V_{12}+\rho V^{\mathrm{eff}}_{12;0})\rho V^{\mathrm{eff}}_{12;0}\\
&\quad+\frac{2}{3}\frac{\hbar^2}{m}\int d^3\mathbf{r}(V_{12}+\rho V^{\mathrm{eff}}_{12;0})\int d^3\mathbf{y}\,\nabla^2(\rho V^{\mathrm{eff}}_{12;0})+\frac{1}{24}\frac{\hbar^2}{m}\int d^3\mathbf{r}(V_{12}+\rho V^{\mathrm{eff}}_{12;0})\int d^3\mathbf{y}(\rho V^{\mathrm{eff}}_{12;1})\\
&\quad-\frac{7}{4}\int d^3\mathbf{r}(\rho V^{\mathrm{eff}}_{12;0})\int d^3\mathbf{y}(V_{12}+\rho V^{\mathrm{eff}}_{12;0})^2+\frac{1}{4}\frac{\hbar^2}{m}\int d^3\mathbf{r}(\rho V^{\mathrm{eff}}_{12;0})\int d^3\mathbf{y}\,\nabla^2(V_{12}+\rho V^{\mathrm{eff}}_{12;0})\\
&\quad+\frac{13}{48}\frac{\hbar^2}{m}\int d^3\mathbf{r}(\rho V^{\mathrm{eff}}_{12;0})\int d^3\mathbf{y}(\rho V^{\mathrm{eff}}_{12;1})-2\int d^3\mathbf{r}(\rho V^{\mathrm{eff}}_{12;0})\int d^3\mathbf{y}(V_{12}+\rho V^{\mathrm{eff}}_{12;0})\rho V^{\mathrm{eff}}_{12;0}\\
&\quad+\frac{7}{12}\frac{\hbar^2}{m}\int d^3\mathbf{r}\,\rho V^{\mathrm{eff}}_{12;0}\int d^3\mathbf{y}\,\nabla^2(\rho V^{\mathrm{eff}}_{12;0})-\frac{1}{2}\int d^3\mathbf{r}(\rho V^{\mathrm{eff}}_{12;0})^2\int d^3\mathbf{y}(V_{12}+\rho V^{\mathrm{eff}}_{12;0})\\
&\quad-\frac{1}{4}\int d^3\mathbf{r}\,\rho V^{\mathrm{eff}}_{12;0}\int d^3\mathbf{y}(\rho V^{\mathrm{eff}}_{12;0})^2-\chi^2_\alpha\left[\int d^3\mathbf{r}(V_{12}+\rho V^{\mathrm{eff}}_{12;0})\right]^2-\frac{1}{12}\left[\rho\frac{\partial}{\partial\rho}\chi^2_\alpha\right]\left[\int d^3\mathbf{r}(V_{12}+\rho V^{\mathrm{eff}}_{12;0})\right]\\
&\quad+\frac{1}{3}\int d^3\rho(V_{12}+\rho V^{\mathrm{eff}}_{12;0})(\mathbf{r}_{12})(V_{12}+\rho V^{\mathrm{eff}}_{12;0})(\mathbf{r}_{23})(V_{12}+\rho V^{\mathrm{eff}}_{12;0})(\mathbf{r}_{31})\\
&\quad+\frac{1}{12}\frac{\hbar^2}{m}\left[\int d^3\mathbf{r}\,\nabla(V_{12}+\rho V^{\mathrm{eff}}_{12;0})\right]^2-\frac{1}{6}\chi^2_\alpha\int d^3\mathbf{r}(V_{12}+\rho V^{\mathrm{eff}}_{12;0})\int d^3\mathbf{y}\,\rho V^{\mathrm{eff}}_{12;0}\\
&\quad+\frac{1}{2}\int d^3\rho(V_{12}+\rho V^{\mathrm{eff}}_{12;0})(\mathbf{r}_{12})(V_{12}+\rho V^{\mathrm{eff}}_{12;0})(\mathbf{r}_{23})\rho V^{\mathrm{eff}}_{12;0}(\mathbf{r}_{31})\\
&\quad+\frac{1}{6}\frac{\hbar^2}{m}\left[\int d^3\mathbf{r}\,\nabla(\rho V^{\mathrm{eff}}_{12;0})\right]\left[\int d^3\mathbf{y}\,\nabla(V_{12}+\rho V^{\mathrm{eff}}_{12;0})\right]\\
&\quad-\frac{1}{5}\left[\frac{\hbar^2}{m}\right]^2\int d^6\rho\,\nabla^4_{\mathbf{x}}V_{123}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)-\frac{4}{5}\left[\frac{\hbar^2}{m}\right]^2\int d^6\rho\,\nabla^2_{\mathbf{x}}\nabla^2_{\mathbf{y}+\mathbf{x}}V_{123}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)\\
&\quad-\frac{1}{6}\left[\frac{\hbar^2}{m}\right]\int d^6\rho\,V_{123}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)\nabla^2_{\mathbf{x}}V_{123}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)\\
&\quad-\frac{1}{24}\left[\frac{\hbar^2}{m}\right]\int d^6\rho[\nabla_{\mathbf{x}}V_{123}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)]^2+\frac{1}{18}\int d^6\rho[V_{123}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)]^3\\
&\quad+\frac{1}{2}\int d^6\rho[V_{123}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)]^2V_{12}(\mathbf{r}_1,\mathbf{r}_2)+\int d^6\rho\,V_{123}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)V_{12}(\mathbf{r}_1,\mathbf{r}_2)V_{12}(\mathbf{r}_2,\mathbf{r}_3)\Bigg]\\
&+\rho^3\Bigg[\frac{1}{4}\left[\int d^3\mathbf{r}(V_{12}+\rho V^{\mathrm{eff}}_{12;0})\right]^2\left[\int d^3\mathbf{y}\,\rho V^{\mathrm{eff}}_{12;0}\right]\\
&\quad+\frac{23}{8}\int d^3\mathbf{r}(V_{12}+\rho V^{\mathrm{eff}}_{12;0})\left[\int d^3\mathbf{y}\,\rho V^{\mathrm{eff}}_{12;0}\right]^2+\frac{13}{8}\left[\int d^3\mathbf{r}\,\rho V^{\mathrm{eff}}_{12;0}\right]^3\\
&\quad-\frac{1}{12}\int d^3\mathbf{r}(V_{12}+\rho V^{\mathrm{eff}}_{12;0})\left[\int d^3\rho[V_{123}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)]^2\right]-\frac{1}{12}\left[\int d^3\mathbf{r}\,\rho V^{\mathrm{eff}}_{12;0}\right]\left[\int d^3\rho[V_{123}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)]^2\right]\\
&\quad-\frac{3}{8}\left[\frac{\hbar^2}{m}\right]\int d^9\rho\,V_{123}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)\nabla^2_{\mathbf{x}}V_{123}(\mathbf{r}_2,\mathbf{r}_3,\mathbf{r}_4)\\
&\quad-\frac{1}{16}\left[\frac{\hbar^2}{m}\right]\int d^9\rho[\nabla_{\mathbf{x}}V_{123}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)\cdot\nabla_{\mathbf{x}}V_{123}(\mathbf{r}_2,\mathbf{r}_3,\mathbf{r}_4)]+\frac{3}{4}\int d^9\rho[V_{123}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)]^2V_{123}(\mathbf{r}_2,\mathbf{r}_3,\mathbf{r}_4)\\
&\quad+\frac{1}{2}\int d^9\rho\,V_{123}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)V_{123}(\mathbf{r}_2,\mathbf{r}_3,\mathbf{r}_4)V_{123}(\mathbf{r}_1,\mathbf{r}_3,\mathbf{r}_4)+\frac{3}{4}\int d^9\rho[V_{123}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)]^2V_{12}(\mathbf{r}_3,\mathbf{r}_4)
\end{aligned}
$$

$$
\begin{aligned}
&+3\int d^9\rho\, V_{123}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)V_{123}(\mathbf{r}_2,\mathbf{r}_3,\mathbf{r}_4)V_{12}(\mathbf{r}_3,\mathbf{r}_4)+\frac{3}{4}\int d^9\rho\, V_{123}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)V_{123}(\mathbf{r}_2,\mathbf{r}_3,\mathbf{r}_4)V_{12}(\mathbf{r}_2,\mathbf{r}_3)\\
&+\frac{3}{4}\int d^9\rho V_{123}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)V_{123}(\mathbf{r}_2,\mathbf{r}_3,\mathbf{r}_4)V_{12}(\mathbf{r}_1,\mathbf{r}_3)+\frac{3}{2}\int d^9\rho V_{123}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)V_{12}(\mathbf{r}_3,\mathbf{r}_4)V_{12}(\mathbf{r}_2,\mathbf{r}_3)\\
&+\frac{3}{2}\int d^9\rho\, V_{123}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)V_{12}(\mathbf{r}_3,\mathbf{r}_4)V_{12}(\mathbf{r}_2,\mathbf{r}_4)\\
&+\frac{3}{4}\int d^9\rho\, V_{123}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)[V_{12}(\mathbf{r}_3,\mathbf{r}_4)]^2\\
&+\frac{3}{4}\int d^9\rho\, V_{123}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)V_{12}(\mathbf{r}_1,\mathbf{r}_2)V_{12}(\mathbf{r}_3,\mathbf{r}_4)\\
&+\frac{1}{2}\int d^9\rho\, V_{123}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)V_{12}(\mathbf{r}_2,\mathbf{r}_3)V_{12}(\mathbf{r}_3,\mathbf{r}_4)\\
&+\frac{1}{4}\int d^9\rho\, V_{123}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)V_{12}(\mathbf{r}_2,\mathbf{r}_3)V_{12}(\mathbf{r}_1,\mathbf{r}_4)\Bigg]\\
+\rho^4\Bigg[&-\frac{1}{4}\int d^3\mathbf{r}(V_{12}+\rho V^{\mathrm{eff}}_{12;0})\left[\int d^9\rho\, V_{123}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)V_{123}(\mathbf{r}_2,\mathbf{r}_3,\mathbf{r}_4)\right]\\
&-\frac{1}{4}\int d^3\mathbf{r}\,\rho V^{\mathrm{eff}}_{12;0}\left[\int d^6\rho\, V_{123}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)V_{123}(\mathbf{r}_2,\mathbf{r}_3,\mathbf{r}_4)\right]-\frac{1}{2}\left[\frac{\hbar^2}{m}\right]\int d^{12}\rho\, V_{123}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)\nabla^2_{\mathrm{x}}V_{123}(\mathbf{r}_3,\mathbf{r}_4,\mathbf{r}_5)\\
&-\frac{1}{24}\left[\frac{\hbar^2}{m}\right]\int d^{12}\rho[\nabla_{\mathrm{x}}V_{123}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)\cdot\nabla_{\mathrm{x}}V_{123}(\mathbf{r}_3,\mathbf{r}_4,\mathbf{r}_5)]\\
&+\frac{1}{30}\int d^{12}\rho\sum{}^{*}\, V_{123}(\mathbf{r}_i,\mathbf{r}_j,\mathbf{r}_{\mathrm{k}})V_{123}(\mathbf{r}_{\mathrm{l}},\mathbf{r}_{\mathrm{m}},\mathbf{r}_{\mathrm{n}})V_{123}(\mathbf{r}_{\mathrm{o}},\mathbf{r}_{\mathrm{p}},\mathbf{r}_{\mathrm{q}})\\
&+\frac{1}{30}\int d^{12}\rho\sum{}^{*}\, V_{123}(\mathbf{r}_{\mathrm{i}},\mathbf{r}_{\mathrm{j}},\mathbf{r}_{\mathrm{k}})V_{123}(\mathbf{r}_{\mathrm{l}},\mathbf{r}_{\mathrm{m}},\mathbf{r}_{\mathrm{n}})V_{12}(\mathbf{r}_{\mathrm{o}},\mathbf{r}_{\mathrm{p}})\\
&+\frac{1}{30}\int d^{12}\rho\sum{}^{*}\, V_{123}(\mathbf{r}_{\mathrm{i}},\mathbf{r}_{\mathrm{j}},\mathbf{r}_{\mathrm{k}})V_{12}(\mathbf{r}_{\mathrm{l}},\mathbf{r}_{\mathrm{m}})V_{12}(\mathbf{r}_{\mathrm{n}},\mathbf{r}_{\mathrm{o}})\Bigg]\\
+\rho^5\Bigg[&-\frac{1}{8}\int d^3\mathbf{r}(V_{12}+\rho V^{\mathrm{eff}}_{12;0})\left[\int d^{12}\rho\, V_{123}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)V_{123}(\mathbf{r}_3,\mathbf{r}_4,\mathbf{r}_5)\right]\\
&-\frac{1}{8}\int d^3\mathbf{r}\,\rho V^{\mathrm{eff}}_{12;0}\int d^{12}\rho\, V_{123}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)V_{123}(\mathbf{r}_3,\mathbf{r}_4,\mathbf{r}_5)\\
&+\frac{5}{6!}\int d^{15}\rho\sum{}^{*}\, V_{123}(\mathbf{r}_{\mathrm{i}},\mathbf{r}_{\mathrm{j}},\mathbf{r}_{\mathrm{k}})V_{123}(\mathbf{r}_{\mathrm{l}},\mathbf{r}_{\mathrm{m}},\mathbf{r}_{\mathrm{n}})V_{123}(\mathbf{r}_{\mathrm{o}},\mathbf{r}_{\mathrm{p}},\mathbf{r}_{\mathrm{q}})\\
&+\frac{5}{6!}\int d^{15}\rho\sum{}^{*}\, V_{123}(\mathbf{r}_{\mathrm{i}},\mathbf{r}_{\mathrm{j}},\mathbf{r}_{\mathrm{k}})V_{123}(\mathbf{r}_{\mathrm{l}},\mathbf{r}_{\mathrm{m}},\mathbf{r}_{\mathrm{n}})V_{12}(\mathbf{r}_{\mathrm{o}},\mathbf{r}_{\mathrm{p}})\\
&+\frac{6}{7!}\int d^{18}\rho\sum{}^{*}\, V_{123}(\mathbf{r}_i,\mathbf{r}_{\mathrm{j}},\mathbf{r}_{\mathrm{k}})V_{123}(\mathbf{r}_{\mathrm{l}},\mathbf{r}_{\mathrm{m}},\mathbf{r}_{\mathrm{n}})V_{123}(\mathbf{r}_{\mathrm{o}},\mathbf{r}_{\mathrm{p}},\mathbf{r}_{\mathrm{q}})\Bigg]\ ,
\end{aligned}
$$

where the symbol ρ as an integration variable denotes, in this expression, the use of generalized Jacobi coordinates and the starred sums denote that only connected contributions, which do not appear in the partial summations, are included in the sums.

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