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N-BODY FADDEEV EQUATIONS AND THE CLUSTER EXPANSION

Willy Bierter

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Submitted to Journal of
Mathematical Physics

UCRL-18102
Preprint

UNIVERSITY OF CALIFORNIA

Lawrence Radiation Laboratory
Berkeley, California

AEC Contract No. W-7405-eng-48

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ABSTRACT

We derive a set of integral equations of the Faddeev type for the N-particle scattering amplitude. This Faddeev theory for the N-body scattering problem then provides a closed theory for the cluster coefficients of an arbitrary quantum gas, which is free of convergence difficulties encountered in former series expansions.

I. INTRODUCTION

For a dilute, imperfect gas the equations of state for the pressure P and the density ρ are given by the following expansions in terms of the fugacity z:[1]

$$P\beta = \sum_{N=1}^{\infty} b_N z^N ,$$

$$\rho = \sum_{N=1}^{\infty} N b_N z^N , \tag{1}$$

where $\beta = (kT)^{-1}$.

In the limit $V \to \infty$ the coefficients $b_N(V,\beta)$ tend to the volume-independent cluster coefficients $b_N(\beta)$:

$$b_N(\beta) = \lim_{V\to\infty} b_N(V,\beta) . \tag{2}$$

The virial expansion of the equation of state is defined to be

$$P\beta = \sum_{N=1}^{\infty} a_N(\beta) \rho^N , \tag{3}$$

where $a_N(\beta)$ is called the Nth virial coefficient. We can find the relationship between the virial coefficients a_N and the cluster coefficients b_N by substituting (3) into (1) and requiring that the

resulting equation be satisfied for every z. By equating the coefficient of each power of z we obtain

$$a_1 = b_1 = 1,$$

$$a_2 = -b_2,$$

$$a_3 = 4b_2^2 - 2b_3,$$

$$a_4 = -4b_2^3 + 10b_2b_3 - 3b_4. \tag{4}$$

Therefore, in order to know the virial coefficients a_N, which are a measure of the dynamical and statistical correlations, we have to calculate the corresponding cluster coefficients. This calculation, however, requires the solution of the N-body problem.

With the exception of the expression for the second virial coefficient given by Beth and Uhlenbeck,[2] for a long time no method for the actual calculation of cluster coefficients for a given interparticle interaction was known. Then Lee and Yang[3] made a step forward in a systematic approximation of higher cluster coefficients. These authors assume that only pair interactions are present in the N-body Hamiltonian H_N and expand the $\underline{N}$th cluster coefficient in terms of the binary collision operator

$$B_{ij}(\beta) = -V_{ij} \exp(-\beta H_{ij}) ,$$

where H_{ij} is the total Hamiltonian of the isolated pair (ij). This theory was applied to a calculation of the third virial coefficient by Pais and Uhlenbeck.[4]

Later it was recognized by Reiner[5] that, with the help of the Laplace transform relation between the Green's function $G^{(N)}(z) = (z - H_N)^{-1}$ and the statistical density operator $W_N(\beta) = \exp(-\beta H_N)$, it is possible to translate the Lee-Yang series expansion in terms of the binary collision operators into Watson's multiple scattering expansion of $G^{(N)}(z)$ in terms of the off-the-energy-shell two-particle scattering matrix.

Both formulations, however, are only applicable if no two- or many-body bound states are present, since whenever the kernel $G^{0(2)}V_{ij}$ has an eigenvalue outside the unit circle, both series expansions fail to converge. This divergence can be cured with the quasiparticle-method of Weinberg.[6]

But only since Faddeev[7] proposed his three-particle scattering theory has it become possible to circumvent the dubious series expansions and give a concise formulation of the third virial coefficient.

The aim of this work is to derive the Faddeev equations for any number N of particles interacting by pairs only and thus to give a completely consistent theory of the $\underline{N}$th cluster coefficient for an arbitrary quantum gas.

In Chapter II we review briefly the relation between the $\underline{N}$th cluster coefficient and the Green's function $G^{(N)}(z)$ for N

interacting particles. In Chapter III we derive the N-body Faddeev equations and in Chapter IV we give the general expression for the Nth cluster coefficient and write down explicitly the third cluster coefficient using the three-particle Faddeev equations.

II. CLUSTER COEFFICIENTS AND GREEN'S FUNCTIONS

The cluster coefficients (2) are related to dynamics through the statistical density operator

$$W_N(\beta) = \exp(-\beta H_N) \, . \tag{5}$$

H_N is the Hamiltonian for N interacting particles of the form

$$H_N = \sum_{i=1}^{N} p_i^{\,2} + \sum_{i<j}^{N} V_{ij} \, , \tag{6}$$

where $\vec{p}_i$ is the momentum of the ith particle and $V_{ij} = V(|\vec{r}_i - \vec{r}_j|)$ is the potential energy of interaction between the ith and jth particle. The units $\hbar = 2m = 1$ are used throughout.

The partition function of a system of N interacting particles is

$$Z_N(\beta) = \mathrm{Tr}_N \, W_N(\beta) = \mathrm{Tr}_N \exp(-\beta H_N) \, . \tag{7}$$

The index N at the trace symbol indicates that the trace has to be taken only in the space of N particles.

For low particle densities cluster expansions are useful perturbation approaches, since encounters of small numbers of particles dominate and account approximately for the thermodynamic properties of the N-particle system. Therefore, it is useful - in both classical and quantum statistical mechanics - to consider directly the expansion

of the partition function Z_N in terms of the cluster coefficients (2):

$$Z_N(\beta) = \sum_{\ell=1}^{N} \prod_{\{m_\ell\}} \frac{1}{m_\ell!} (Vb_\ell)^{m_\ell} , \tag{8}$$

where V is the volume occupied by the N-particle system. The combined sum and product in (8) has to be performed in the following way: The N particles are distributed according to some distribution of m_ℓ clusters of ℓ particles each. For this given partition one forms the product $\prod (Vb_\ell)^{m_\ell}/m_\ell!$ and sums over all possible partitions of N particles satisfying $\Sigma \ell m_\ell = N$.

There exists a relation between the probability operator W_N and the Green's function $G^{(N)}(z) = (z - H_N)^{-1}$, which is given by means of the inverse Laplace transform:[8]

$$W_N(\beta) = L^{-1} G^{(N)}(z) = \frac{1}{2\pi i} \int_\gamma dz\, e^{-\beta z}\, G^{(N)}(z) , \tag{9}$$

where the path of integration γ passes from $\infty + i\epsilon$ around the leftmost singularity of the integrand to $\infty - i\epsilon$.

The Green's function $G^{(N)}(z)$ is related to the scattering operator $T^{(N)}(z)$ for N interacting particles:

$$G^{(N)}(z) = G^{0(N)}(z) + G^{0(N)}(z)\, T^{(N)}(z)\, G^{0(N)}(z) , \tag{10}$$

with

$$G^{0(N)}(z) = \left(z - \sum_{i=1}^{N} p_i^{\,2}\right)^{-1} . \tag{11}$$

Bloch and De Dominicis[9] have shown in their proof of the linked-cluster expansion that the partition function Z_N can be written in the form

$$Z_N = \sum_{\ell=1}^{N} \prod_{\{m_\ell\}} \frac{1}{m_\ell!} \left(Z_\ell^{(c)}\right)^{m_\ell} , \tag{12}$$

where $Z_\ell^{(c)}$ is the partition function stemming from all connected ℓ-particle diagrams.

A comparison of (12) with (8) yields the cluster coefficients as the total contribution of all connected N-particle diagrams:

$$b_N(\beta) = \lim_{V\to\infty} V^{-1} Z_N^{(c)} = \lim_{V\to\infty} V^{-1} L^{-1} \langle \operatorname{Tr} G^{(N)}(z) \rangle_c . \tag{13}$$

All connected diagrams appearing in (13) are understood to acquire their meaning through the different terms in the respective representation of $G^{(N)}(z)$.

In (13) the specific statistics enters through the symmetry of the states used in the trace calculation. Therefore, $Z_N^{(c)}$ has the following form for Bose-Einstein and Fermi-Dirac statistics, respectively:

$$\text{BE} : Z_N^{(c)} = \frac{1}{N!} \int dp_1 \cdots dp_N \frac{1}{2\pi i} \int_\gamma dz\, e^{-\beta z} \sum_P \langle P(p_1 \cdots p_N)$$

$$\times \; |G^{(N)}(z)| p_1 \cdots p_N \rangle_c , \qquad (14)$$

$$\text{FD} : Z_N^{(c)} = \frac{1}{N!} \int dp_1 \cdots dp_N \frac{1}{2\pi i} \int_\gamma dz\, e^{-\beta z} \sum_P \epsilon_P \langle P(p_1 \cdots p_N)$$

$$\times \; |G^{(N)}(z)| p_1 \cdots p_N \rangle_c , \qquad (15)$$

where P denotes the permutation operator and ϵ_P is $+1$ (-1) for an even (odd) permutation of $(p_1 \cdots p_N)$.

We recognize from the relation (13) between the Nth cluster coefficient and the total Green's function $G^{(N)}$ on the one hand and the connection (10) between this total Green's function $G^{(N)}$ and the scattering operator $T^{(N)}$ on the other hand that we immediately have a consistent theory for all cluster coefficients once we can write down a coupled set of integral equations for the scattering amplitudes $T^{(N)}$ for N interacting particles.

For $N = 2$, $T^{(2)}$ satisfies the Lippmann-Schwinger equation

$$T^{(2)} = V + VG^{0(2)} T^{(2)}, \qquad (16)$$

and for $N = 3$, $T^{(3)}$ satisfies the three-particle Faddeev equations. Therefore, we have to find a generalization of these Faddeev equations to any number of particles interacting by pairs.

III. N-BODY FADDEEV EQUATIONS

In this chapter we will give a general procedure for writing down a set of integral equations for the N-particle scattering amplitude. This set turns out to be a generalization of the Faddeev equations for three-particle scattering. Like the Faddeev equations these equations will be linear integral equations of the Fredholm type for the off-the-energy-shell scattering amplitude of N particles, whose kernels depend only upon the scattering amplitudes for a lesser number of particles.

The procedure is based on a fundamental theorem of Hugenholtz with the following content:[10]

Let Γ_A and Γ_B be two disconnected graphs with N_A and N_B particle lines, respectively. The contribution of the graph Γ_A alone is denoted by $\langle p_A | (z - H_A)^{-1} | p_A' \rangle_{\Gamma_A}$. The same holds for Γ_B. The theorem then states that the contribution of all graphs $\Sigma\Gamma_{A+B}$ that can be obtained by combining Γ_A and Γ_B in such a way that the vertices of Γ_A and Γ_B appear in all possible relative orders amounts to

$$\begin{aligned}
&\langle p_A p_B \mid G_{A+B}(z) \mid p_A' p_B' \rangle \\
&= \langle p_A \mid G_A(z) \mid p_A' \rangle_{\Gamma_A} * \langle p_B \mid G_B(z) \mid p_B' \rangle_{\Gamma_B} \\
&\equiv \frac{1}{2\pi i} \int_C d\zeta \, \langle p_A \mid G_A(z - \zeta) \mid p_A' \rangle_{\Gamma_A} \langle p_B | G_B(\zeta) | p_B' \rangle_{\Gamma_B} .
\end{aligned} \tag{17}$$

In operator language (17) takes the form

$$G_{A+B}(z) = G_A(z) * G_B(z) = \frac{1}{2\pi i} \int_c d\zeta \; G_A(z - \zeta) \; G_B(\zeta), \qquad (18)$$

where

$$G_{A+B}(z) = (z - H_{A+B})^{-1}, \quad G_A(z) = (z - H_A)^{-1}, \; G_B(z) = (z - H_B)^{-1}.$$

The contour c of integration encircles the spectrum of $(\zeta - H_B)^{-1}$ in a counterclockwise way (or the spectrum of $(z - \zeta - H_A)^{-1}$ in a clockwise way).

We want to formulate the above theorem for the scattering operator T. To this end we introduce on both sides of (18) for the different Green's function $G(z)$ - according to (10) - the respective connected parts $G^0(z)\, T(z)\, G^0(z)$. After some operator algebra we obtain

$$\begin{aligned} T_{A+B}(z) &= T_A(z) * T_B(z) \\ &= G^{0\,-1}_{A+B}(z) \frac{1}{2\pi i} \int_c d\zeta \; G^0_A(z - \zeta) \; T_A(z - \zeta) \; G^0_A(z - \zeta) \\ &\qquad \times \; G_B{}^0(\zeta) \; T_B(\zeta) \; G_B{}^0(\zeta) \; G^{0\,-1}_{A+B}(z) \\ &= \frac{1}{2\pi i} \int_c d\zeta \left\{ G_A{}^0(z - \zeta) + G_B{}^0(\zeta) \right\} \\ &\qquad \times \; T_A(z - \zeta) \; T_B(\zeta) \left\{ G_A{}^0(z - \zeta) + G_B{}^0(\zeta) \right\}, \end{aligned} \qquad (19)$$

where

$$G_{A+B}{}^{0}(z) = (z - \Sigma p_A{}^2 - \Sigma p_B{}^2)^{-1}, \quad G_A{}^{0}(z) = (z - \Sigma p_A{}^2)^{-1},$$

$$G_B{}^{0}(z) = (z - \Sigma p_B{}^2)^{-1}.$$

If the N_B particles are noninteracting, we have to convolute the nonconnected part $G_B{}^0$ - instead of $G_B{}^0\, T_B\, G_B{}^0$ - with the connected part $G_A{}^0\, T_A\, G_A{}^0$ for the N_A particles. We find

$$T_A(z) * T_{p_1} * \ldots * T_{p_{N_B}}$$

$$= G_{A+B}^{0\,-1}(z)\, \frac{1}{2\pi i} \int_c d\zeta\, G_A{}^0(z - \zeta)\, T_A(z - \zeta)\, G_A{}^0(z - \zeta)\, G_B{}^0(\zeta)$$

$$\times\; G_{A+B}{}^{0\,-1}(z)$$

$$= \frac{1}{2\pi i} \int_c d\zeta\, T_A(z - \zeta)\, G_B{}^0(\zeta). \tag{20}$$

If both the N_A and the N_B particles are noninteracting, we have to convolute the two nonconnected parts $G_A{}^0$ and $G_B{}^0$, respectively. In this case we have

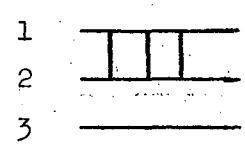
$$T_{\bar{p}_1} * \cdots * T_{\bar{p}_{N_A}} * T_{p_1} * \cdots * T_{p_{N_B}}$$

$$= G^{0\,-1}_{A+B}(z) \frac{1}{2\pi i} \int_c d\zeta \; G^0_A(z - \zeta)\, G^0_B(\zeta)\, G^{0\,-1}_{A+B}(z) = G^{0\,-1}_{A+B}(z) \; . \qquad (21)$$

These relations (19), (20) and (21), form the key point of our general procedure.

Before we discuss the derivation of the Faddeev equations for arbitrary N, we first exhibit the general procedure with the example of $N = 3$.

Let us consider the nonconnected graph, in which the particles 1 and 2 are interacting, whereas particle 3 is free:



. (22)

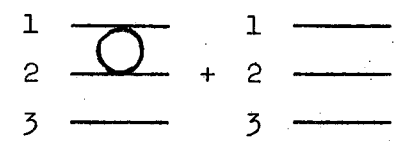
Moreover we specify in this graph the leftmost interaction, i.e., V_{12}. Then we write down the contribution to the three-particle scattering amplitude in the following way:

$$T_{12}^{(3)} = V_{12}\, G^{0(3)} \sum_{(\gamma)} M^{(\gamma)} \qquad (23)$$

We now introduce what we call "reduced graphs" (γ) over which one must sum in order to obtain the contribution (23) from the nonconnected diagram (22).

We define as "reduced graphs" all those graphs, which, when completed by the interaction V_{12}, essentially give again the graph (22). "Essentially" means that we do not care how many interaction lines follow the first one in these "reduced graphs." Therefore, there are two possible "reduced graphs" for the nonconnected diagram (22). The first "reduced graph" is connected, because several (at least one) interaction lines follow the first one and these are summed up by the Lippmann-Schwinger equation (16). The second one is nonconnected, because no interaction lines follow the first one, i.e., particles 1 and 2 move freely. Now we can give the prescription of how one finds $\sum_{(\gamma)} M^{(\gamma)}$:

Convolute the scattering amplitudes of all "reduced graphs" of (22) with the particle line 3 and sum up all these different contributions. In diagrammatical and algebraic form this reads as

$\sum_{(\gamma)} M^{(\gamma)} =$ 

$= T_{12}^{(2)} * T_3^{(1)}$

$$+ T_1^{(1)} * T_2^{(1)} * T_3^{(1)} \quad . \qquad (24)$$

The "scattering amplitude" of the "reduced graph", where particles 1 and 2 are free, is formally denoted by $T_1^{(1)} * T_2^{(1)}$ and is given by (21).

The first term in (24) is easily evaluated with the help of (20). We have

$$T_{12}^{(2)} * T_3^{(1)} = \frac{1}{2\pi i} \int_c d\zeta \langle p_3' | \frac{1}{\zeta - p_3^2} | p_3 \rangle \langle p_1' \, p_2' |$$

$$\times | T_{12}^{(2)} (z - \zeta) | p_1 \, p_2 \rangle$$

$$= \delta(p_3' - p_3) \langle p_1' \, p_2' | T_{12}^{(2)} (z - p_3^2) | p_1 \, p_2 \rangle . \tag{25}$$

In operator form this reads

$$T_{12}^{(2)} * T_3^{(1)} = T_{12}^{(2)} . \tag{26}$$

For the second term in (24) we find from (21)

$$T_1^{(1)} * T_2^{(1)} * T_3^{(1)} = G^{0(3)-1} . \tag{27}$$

Thus the total contribution of the two "reduced graphs" of the nonconnected diagram (22) to (23) is

$$T_{12}^{(3)} = V_{12} \, G^{0(3)} \, T_{12}^{(2)} + V_{12} = T_{12}^{(2)} , \tag{28}$$

where in the last step we used the Lippmann-Schwinger equation (16) for $T_{12}^{(2)}$ with the argument $(z - p_3^2)$.

Now we formulate the general procedure for finding the contribution of an arbitrary nonconnected graph consisting of p subgraphs (δ_p) to the scattering amplitude for N particles.

First we specify for any given nonconnected diagram its leftmost interaction V_{ij}. We assume that this leftmost V_{ij} lies in the subgraph (δ_1) consisting of $M < N$ particles. Then we draw all possible "reduced graphs" of (δ_1) which are defined in such a way as to essentially give again the given diagram, when completed by the interaction V_{ij}. These "reduced graphs" are either connected or nonconnected diagrams. In case they are connected they have again a leftmost interaction V_{ik}, and the corresponding scattering amplitude is $T_{ik}^{(M)}$. This scattering amplitude can in principle be obtained by summing up all interaction lines with the help of the Faddeev equations for $M < N$ particles. If the "reduced graph" is nonconnected it may have a connected "reduced subgraph" with $L < M$ particles and a leftmost interaction V_{ik}. Then the corresponding scattering amplitude is $T_{ik}^{(L)} \prod_{\nu=L+1}^{M} * T_{\nu}^{(1)}$. If the "reduced graph" is totally nonconnected the "scattering amplitude" is $\prod_{\nu=1}^{M} * T_{\nu}^{(1)}$. Finally we convolute the scattering amplitude of each "reduced graph" with the scattering amplitude of the subgraphs $\delta_2, \cdots, \delta_p$ and sum up all these contributions.

We can express this procedure as a theorem in the following way:

Theorem 1:

For any given nonconnected diagram consisting of p subgraphs (δ_p) with a leftmost interaction V_{ij} lying (supposedly) in (δ_1), its contribution to the scattering amplitude for N particles is

$$T_{ij}^{(N)} = V_{ij}\, G^{0(N)} \sum_{(\gamma)} T^{(\gamma)} * T^{(\delta_2)} * \ldots * T^{(\delta_p)}, \tag{29}$$

where the sum extends over all "reduced graphs" (γ) of (δ_1).

Next we formulate the general procedure for finding the contribution of an arbitrary connected graph to the scattering amplitude for N particles as a theorem.

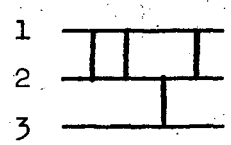
Theorem 2:

Cut any given connected diagram into two disconnected subdiagrams such that one of them is the nonconnected diagram (δ_1) with the leftmost interaction V_{ij} of Theorem 1. We denote the other subdiagram by (δ). Then apply Theorem 1, i.e., convolute the scattering amplitudes of all "reduced graphs" (γ) of (δ_1) with the scattering amplitude of (δ). Go on to the right with a free propagation $G^{0(N)}$ and finally connect (δ_1) and (δ) pairwise by $T_{\ell k}^{(N)}$ with $\ell \in (\delta_1)$, $k \in (\delta)$. In an algebraic form this reads

$$T_{ij}^{(N)} = V_{ij}\, G^{0(N)} \sum_{(\gamma)} T^{(\gamma)} * T^{(\delta)}\, G^{0(N)} \sum_{\substack{\ell \in (\delta_1) \\ k \in (\delta)}} T_{\ell k}^{(N)}. \tag{30}$$

Relations (29) and (30), summed up for all those different types of nonconnected and connected diagrams (with the leftmost interaction V_{ij}) which yield a different value for $\sum_{(\gamma)} M^{(\gamma)}$, constitute the equations which determine the N-particle scattering amplitude $T_{ij}^{(N)}$. Their kernels depend only upon the scattering amplitudes for less than N particles. Since the squares of these kernels have no δ-functions, these equations are of the Fredholm type.

We proceed with the example $N = 3$ and consider the following connected graph:



. (31)

According to Theorem 2 we cut the interaction line V_{23} and get back the nonconnected diagram (22). Then we apply Theorem 1 and use (30) to obtain the following contribution to the three-particle scattering amplitude:

$$T_{12}^{(3)} = V_{12}\, G^{0(3)}\, T_{12}^{(2)} * T_3^{(1)}\, G^{0(3)} \left(T_{13}^{(3)} + T_{23}^{(3)} \right)$$
$$+ V_{12}\, G^{0(3)}\, T_1^{(1)} * T_2^{(1)} * T_3^{(1)}\, G^{0(3)} \left(T_{13}^{(3)} + T_{23}^{(3)} \right) . \tag{32}$$

With the help of the operator relations (26) and (27) we obtain

$$T_{12}^{(3)} = T_{12}^{(2)}\, G^{0(3)} \left(T_{13}^{(3)} + T_{23}^{(3)} \right) . \tag{33}$$

The total contribution of the nonconnected and the connected diagrams (22) and (31) with the leftmost interaction V_{12} yields the well-known three-particle Faddeev equations:

$$T_{12}^{(3)} = T_{12}^{(2)} + T_{12}^{(2)} G^{0(3)} \left(T_{13}^{(3)} + T_{23}^{(3)} \right). \tag{34}$$

Two similar equations can be derived for the diagrams with a different leftmost interaction.

As an illustration of the general procedure, in the Appendix, we use Theorems 1 and 2 to derive the four-body Faddeev equations.

The total scattering amplitude for N interacting particles is the contribution of all nonconnected and connected diagrams with different leftmost interactions V_{ij}:

$$T^{(N)} = \sum_{i<j}^{N} T_{ij}^{(N)} . \tag{35}$$

IV. CLUSTER COEFFICIENTS FOR A BOSON GAS

The Faddeev theory for the N-body scattering problem thus provides a closed formulation of the dynamical correlation problem. We can now express the total Green's function $G^{(N)}(z)$, appearing in the expression (13) for the Nth cluster coefficient in terms of the scattering amplitudes $T_{ij}^{(N)}$ for N interacting particles, which satisfy the N-body Faddeev equations. Consequently, we have a completely consistent theory for the cluster coefficients, which is free of convergence difficulties encountered in series expansions in terms of a two-body scattering matrix or a binary collision matrix.

We can write (13) in the general form

$$b_N(\beta) = \lim_{V\to\infty} V^{-1}L^{-1} \left\langle \mathrm{Tr}\left\{G^{0(N)}(z) + G^{0(N)}(z)\sum_{i<j}^{N} T_{ij}^{(N)}(z)G^{0(N)}(z)\right\}\right\rangle_c, \tag{36}$$

where $T_{ij}^{(N)}$ is given by the remark after Theorem 2. The first term in (36),

$$b_N^{(0)}(\beta) = \lim_{V\to\infty} V^{-1} L^{-1} \left\langle \mathrm{Tr}\, G^{0(N)}(z) \right\rangle_c , \tag{37}$$

leads to the cluster coefficient of an ideal boson gas, since $G^{0(N)}$ does not contain the interaction. We have to select only connected diagrams. This is achieved by introducing $(n - 1)$ δ-functions in (37). This can be done in $(n - 1)!$ possible ways. By taking into

account the usual factor $V/(8\pi)^3$ we obtain the well-known result for a boson gas in terms of the thermal de Broglie wavelength $\lambda = (4\pi\beta)^{\frac{1}{2}}$:

$$b_N^{(0)}(\beta) = \lambda^{-3} N^{-5/2} . \tag{38}$$

With this result we can write our general expression (36) in the form

$$b_N(\beta) = b_N^{(0)}(\beta) + \lim_{V\to\infty} V^{-1} L^{-1} \langle \mathrm{Tr} \left\{ G^{0(N)}(z) \sum_{i<j}^{N} T_{ij}^{(N)}(z) G^{0(N)}(z) \right\} \rangle_c . \tag{39}$$

For $N = 2$ the sum $\sum_{i<j}^{N} T_{ij}^{(N)}(z)$, is replaced by the two-particle scattering amplitude $T^{(2)}(z)$ and the result for the second term in (39) is the well-known Uhlenbeck-Beth expression in terms of the bound-state energies $\epsilon_{n\ell}$ and the phase shifts η_ℓ,

$$b_2^{(1)}(\beta) = (2)^{\frac{1}{2}} \lambda^{-3} \sum_{\ell=0}^{\infty} (2\ell + 1) \left\{ \sum_n \exp(-\beta\epsilon_{n\ell}) + \frac{1}{\pi} \int_0^\infty dk\, k^2 \frac{\partial\eta_\ell(k)}{\partial k} \exp(-2\beta k^2) \right\} , \tag{40}$$

where the sum extends only over even values of ℓ in the case of a boson gas.

The third cluster coefficient can be written with the help of the Faddeev equations (34) in the following form:

$$b_3(\beta) = b_3^{(0)}(\beta) + \lim_{V\to\infty} V^{-1} L^{-1} \langle \mathrm{Tr}\Big\{ G^{0(3)}(z) \sum_{i<j}^{3} T_{ij}^{(2)}(z)$$

$$\times\ G^{0(3)}(z) + G^{0(3)}(z) \sum_{\substack{i<j \\ k\neq i,j}}^{3} T_{ij}^{(2)}(z)\ G^{0(3)}(z)$$

$$\times \left(T_{ik}^{(3)} + T_{jk}^{(3)}\right) G^{0(3)}(z) \Big\} \rangle_c$$

$$= b_3^{(0)}(\beta) + b_3^{(1)}(\beta) + b_3^{(2)}(\beta)\ , \tag{41}$$

where $b_3^{(0)}(\beta)$ is given by (38).

The term $b_3^{(1)}(\beta)$ takes into account all correlations due to a single pair interaction and a third particle, being only statistically correlated to the pair. It is immaterial which term $T_{ij}^{(2)}$ we take in the sum for $b_3^{(1)}(\beta)$ in (41) provided we include a factor 3 to account for the three other equivalent choices. The connectedness of the diagram is insured by the introduction of a sum of two δ-functions. Together with the usual factor $V/(8\pi)^3$ we obtain

$$b_3^{(1)}(\beta) = \frac{1}{2(8\pi)^3} \int dp_1 dp_2 dp_3 \frac{1}{2\pi i} \int_c dz\ e^{-\beta z} [\delta(p_3 - p_1) + \delta(p_3 - p_2)]$$

$$\times \langle p_1 p_2 p_3 | T_{12}^{(2)}(z) | p_1 p_2 p_3 \rangle \left(z - \sum_{i=1}^{3} p_i^{\,2} \right)^{-2} . \tag{42}$$

Dynamical and statistical three-particle correlations are contained in $b_3^{(2)}$. Taking into account (14) and again the factor $V/(8\pi)^3$, we find

$$b_3^{(2)}(\beta) = \frac{1}{3!(8\pi)^3} \sum_P \int dp_1 dp_2 dp_3 \frac{1}{2\pi i} \int_c dz\, e^{-\beta z}$$

$$\times \langle P(p_1 p_2 p_3) \Big| \sum_{\substack{i<j \\ k\neq i,j}}^{3} T_{ij}^{(2)}(z) G^{0(3)}(z) \left(T_{ik}^{(3)} + T_{jk}^{(3)}\right) \Big|$$

$$\times\ p_1 p_2 p_3 \rangle_c \cdot \left(z - \sum_{i=1}^{3} p_i^2\right)^{-2}. \qquad (43)$$

We note that the correlation term $b_3^{(1)}(\beta)$ can be calculated without any approximation and is thus valid for any temperature. In order to know the correlation term $b_3^{(2)}(\beta)$ we have to solve the three-particle Faddeev equations, which can be done only approximately with the present computers.

We wish to outline briefly the necessary steps in an actual calculation of (43). Before solving the coupled set of integral equations, we have to choose first a reasonable representation of the two-particle scattering matrix associated with the interparticle potential. This choice is even more crucial here than in a description of nucleon-deuteron scattering, etc., since one has to perform as a

final step an integration over all energy variables. Therefore the chosen representation for $T_{ij}^{(2)}$ should be close to the exact one over a very large energy interval. Elsewhere we have discussed extensively the merits of the Weinberg-quasiparticle-representation[6] of $T_{ij}^{(2)}$ which we used in the Faddeev equations for deuteron-potential[11] and deuteron-nucleon[12] scattering. We believe that here also this representation gives a reasonable description for higher values of the energy parameters than the usual pole-approximation representation of $T_{ij}^{(2)}$,[13] and that the calculations for $b_3^{(2)}$ will be valid in a much wider temperature region.

As was already pointed out in the introduction, Reiner[5] obtained a theory for the Nth cluster coefficient - equivalent to the binary collision expansion of Lee and Yang - by using Watson's multiple scattering expansion of $G^{(N)}(z)$ in (13):

$$G^{(N)}(z) = G^{0(N)}(z) \sum_{\mu=0}^{\infty} \left(\sum_{i<j}^{N}{}' \, T_{ij}^{(2)}(z) \, G^{0(N)}(z) \right)^{\mu} , \qquad (44)$$

where the prime at the summation over pairs (ij) forbids the occurrence of two consecutive identical indices in the expansion. In our formulation we get this multiple scattering expansion result for the Nth cluster coefficient directly from (41) by repeatedly iterating the Faddeev equations and replacing all indices 3 by N.

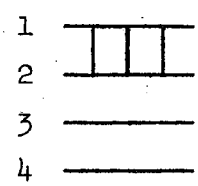
ACKNOWLEDGMENT

The author is indebted to Dr. Geoffrey Chew for the kind hospitality extended to him by the Theoretical Group of the Lawrence Radiation Laboratory. A research fellowship from the "Swiss National Fund" is gratefully acknowledged.

APPENDIX

In this appendix we derive the four-body Faddeev equations with the procedure outlined in Chapter III. For convenience we write all relations in operator form.

First we consider all nonconnected diagrams with the leftmost interaction V_{12} and evaluate them according to Theorem 1:

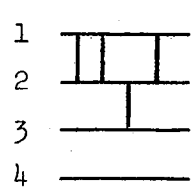


(A1)

$$T_{12}^{(4)} = V_{12}\, G^{0(4)} \left\{ T_{12}^{(2)} * T_3^{(1)} * T_4^{(1)} + T_1^{(1)} * T_2^{(1)} * T_3^{(1)} * T_4^{(1)} \right\} . \tag{A2}$$

With the help of relations (20) and (21) we find

$$T_{12}^{(4)} = T_{12}^{(2)} . \tag{A3}$$



(A4)

$$T_{12}^{(4)} = V_{12}\, G^{0(4)} \Big\{ T_{12;4}^{(3)} * T_4^{(1)} + T_{13;4}^{(3)} * T_4^{(1)}$$

$$+ T_{23;4}^{(3)} * T_4^{(1)} + T_{23}^{(2)} * T_1^{(1)} * T_4^{(1)}$$

$$+ T_{13}^{(2)} * T_2^{(1)} * T_4^{(1)} \Big\} . \qquad \text{(A5)}$$

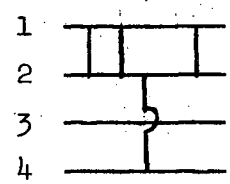
The index after the semicolon in the three-particle scattering amplitudes $T^{(3)}$ denotes the spectator particle. All the three-particle scattering amplitudes are given by the homogeneous Faddeev equations (33). Using (34) and (20), we obtain for (A5)

$$T_{12}^{(4)} = V_{12}\, G^{0(4)} \Big\{ T_{12;4}^{(3)} - T_{12}^{(2)} + T_{13;4}^{(3)} - T_{13}^{(2)}$$

$$+ T_{23;4}^{(3)} - T_{23}^{(2)} + T_{23}^{(2)} + T_{13}^{(2)} \Big\} . \qquad \text{(A6)}$$

Using once more the Faddeev equations (34) for $T_{12;4}^{(3)}$ and the Lippmann-Schwinger equation for $T_{12}^{(2)}$, we finally have

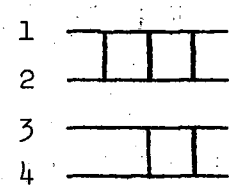
$$T_{12}^{(4)} = T_{12;4}^{(3)} - T_{12}^{(2)} . \qquad \text{(A7)}$$



(A8)

This diagram has the same structure as (A4) except that particle 3 is now the spectator particle. In analogy to (A7) we get the contribution

$$T_{12}^{(4)} = T_{12;3}^{(3)} - T_{12}^{(2)} . \tag{A9}$$



(A10)

$$T_{12}^{(4)} = V_{12}\, G^{0(4)} \left\{ T_{12}^{(2)} * T_{34}^{(2)} + T_1^{(1)} * T_2^{(1)} * T_{34}^{(2)} \right\} . \tag{A11}$$

For the evaluation of the first term in (A11) we have to use relation (19):

$$T_{12}^{(2)} * T_{34}^{(2)} = \frac{1}{2\pi i} \int_c d\zeta \left[(z - \zeta - H_{12}^{0})^{-1} + (\zeta - H_{34}^{0})^{-1} \right]$$

$$\times\ T_{12}^{(2)}(z - \zeta)\, T_{34}^{(2)}(\zeta) \left[(z - \zeta - H_{12}^{0})^{-1} + (\zeta - H_{34}^{0})^{-1} \right] , \tag{A12}$$

where

$$H_{12}^{0} = \sum_{i=1}^{2} p_i^2, \quad H_{34}^{0} = \sum_{i=3}^{4} p_i^2 .$$

We define the following amplitudes $U_{ij}^{(4)}$ in terms of the two-particle scattering amplitudes $T_{ij}^{(2)}$:

$$U_{ij}^{(4)} = T_{ij}^{(2)} + \frac{1}{2\pi i} \int_c d\zeta \left\{ T_{ij}^{(2)}(\zeta)\,(z - \zeta - H_{k\ell}^{0})^{-1} \right.$$

$$\times\; T_{k\ell}^{(2)}(z - \zeta)(z - \zeta - H_{k\ell}^{0})^{-1} + T_{ij}^{(2)}(\zeta)(\zeta - H_{ij}^{0})^{-1}$$

$$\left. \times\; (z - \zeta - H_{k\ell}^{0})^{-1}\, T_{k\ell}^{(2)}(z - \zeta) \right\} . \tag{A13}$$

One can easily show that these amplitudes $U_{ij}^{(4)}$ obey the following set of equations:

$$U_{ij}^{(4)} = T_{ij}^{(2)} + T_{ij}^{(2)}\, G^{0(4)}\, U_{k\ell}^{(4)}$$

$$U_{k\ell}^{(4)} = T_{k\ell}^{(2)} + T_{k\ell}^{(2)}\, G^{0(4)}\, U_{ij}^{(4)} . \tag{A14}$$

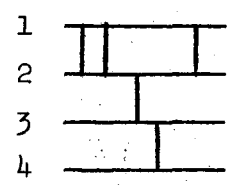
Using the definition (A13) for $U_{ij}^{(4)}$ and the fact that therein the pairs of indices (ij) and $(k\ell)$ are interchangeable, we find for (A11)

$$T_{12}^{(4)} = V_{12}\, G^{0(4)} \left\{ U_{12}^{(4)} - T_{12}^{(2)} + U_{34}^{(4)} - T_{34}^{(2)} + T_{34}^{(2)} \right\} . \tag{A15}$$

Using the above equations (A14) for $U_{12}^{(4)}$ and the Lippmann-Schwinger equation for $T_{12}^{(2)}$, we finally have

$$T_{12}^{(4)} = U_{12}^{(4)} - T_{12} . \tag{A16}$$

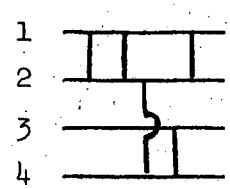
Now we consider all connected diagrams and make use of Theorem 2.



(A17)

We cut the interaction line V_{34} and then we have again the nonconnected diagram (A4). Applying Theorem 1, with the result (A7), and using the relation (30), we find

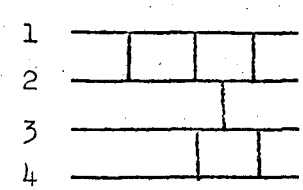
$$T_{12}^{(4)} = \left(T_{12;4}^{(3)} - T_{12}^{(2)} \right) G^{0(4)} \left(T_{14}^{(4)} + T_{24}^{(4)} + T_{34}^{(4)} \right) . \tag{A18}$$



(A19)

The same procedure as for (A17) - except that we use the result (A9) - leads to

$$T_{12}^{(4)} = \left(T_{12;3}^{(3)} - T_{12}^{(2)}\right) G^{0(4)} \left(T_{13}^{(4)} + T_{23}^{(4)} + T_{34}^{(4)}\right). \tag{A20}$$



(A21)

Cutting the interaction line V_{23} and using the result (A16), we get

$$T_{12}^{(4)} = \left(U_{12}^{(4)} - T_{12}^{(2)}\right) G^{0(4)} \left(T_{13}^{(4)} + T_{14}^{(4)} + T_{23}^{(4)} + T_{24}^{(4)}\right). \tag{A22}$$

The total contribution of all nonconnected and connected diagrams yields the four-body Faddeev equations (see the remark after Theorem 2). In a general form, they read

$$\begin{aligned} T_{ij}^{(4)} = {} & T_{ij}^{(2)} + T_{ij;k}^{(3)} - T_{ij}^{(2)} + T_{ij;\ell}^{(3)} - T_{ij}^{(2)} + U_{ij}^{(4)} \\ & - T_{ij}^{(2)} + \left(T_{ij;k}^{(3)} - T_{ij}^{(2)}\right) G^{0(4)} \left(T_{ik}^{(4)} + T_{jk}^{(4)} + T_{k\ell}^{(4)}\right) \\ & + \left(T_{ij;\ell}^{(3)} - T_{ij}^{(2)}\right) G^{0(4)} \left(T_{i\ell}^{(4)} + T_{j\ell}^{(4)} + T_{k\ell}^{(4)}\right) \\ & + \left(U_{ij}^{(4)} - T_{ij}^{(2)}\right) G^{0(4)} \left(T_{ik}^{(4)} + T_{i\ell}^{(4)} + T_{jk}^{(4)} + T_{j\ell}^{(4)}\right). \end{aligned} \tag{A23}$$

The same set of equations (A23) was also derived by Alessandrini,[14] using complicated operator algebra.

FOOTNOTES AND REFERENCES

* This work was supported in part by the U.S. Atomic Energy Commission.

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