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S-matrix theory of reacting plasmas*

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The S-matrix formulation of quantum statistics, due to Dashen, Ma, and Bernstein, is extended to a multicomponent system and is then applied to a two-component nonrelativistic system of charged particles. A summation of terms corresponding to ring diagrams leads, in the high-temperature low-density limit, to the Debye-Hückel equation of state. Finally, the second virial coefficients for a system of reacting charged particles are derived, the reactions being described by multichannel scattering theory. The application of these results to deuterium plasma undergoing fusion is discussed.

I. INTRODUCTION

The thermodynamic properties of plasma undergoing fusion are of considerable practical value and theoretical interest. In the traditional approach to understand these properties, one uses the interparticle interactions and perturbation theory to calculate the approximate equation of state. One form of the equation of state is in terms of the virial expansion.[1] In the case that the existence of the interparticle potential is questionable (for instance, a system undergoing nuclear reactions), the usual approach is not applicable. In order to determine the thermodynamic behavior of this system, some new approach is necessary. Such an approach has been worked out by Dashen, Ma, and Bernstein.[2,3]

Dashen, Ma, and Bernstein[2] have formulated quantum statistical mechanics in terms of the many-particle on-shell S matrix which describes the scattering processes of the particles in the system. They treat the virial coefficients systematically to all orders, and their final mathematical forms for the virial coefficients are very compact and elegant. Only the S matrix is needed in this formalism; thus, when the interaction potential is unknown, but the S matrix can somehow be determined, one can use the S-matrix approach to treat such problems. The Dashen, Ma, and Bernstein (DMB) theory for a single-component system obeying Boltzmann statistics is reviewed in the Appendix of this paper.

The motivation for the work described in this paper was the study of the thermodynamic properties of deuterium plasma undergoing fusion. Hence, our discussion will focus on a deuterium plasma. The results of this paper can be applied or extended readily to many other problems—for example, systems undergoing chemical reactions. In order to simplify the notation and discussion, we restrict our discussion to the system which we describe next.

We are interested in a nonrelativistic deuterium plasma which is slightly exothermic[4]; the plasma is assumed to be fully ionized, electrically neutral, and in thermal equilibrium. The system is assumed to possess a high temperature and low density and can, therefore, be described by Boltzmann statistics. The constitutents of the system are e, D, p, n, T, and ^{3}He (electrons, deuterons, protons, neutrons, tritons, and ^{3}He nuclei). The electron, proton, and neutron are considered to be stable point particles with no internal degrees of freedom (we refer to these particles as elementary particles), while D, T, and ^{3}He are treated as stable point particles with internal degrees of freedom (these are composite particles). The plasma is assumed to be in its early stages of formation so that the densities of e and D are many orders of magnitude larger than those of p, n, T, and ^{3}He; to be specific, we assume that the densities of e and D are in the range 10^{12}–10^{16} particles per cm^3, while the densities of p, n, T, and ^{3}He are smaller than these by a factor of 10^{-6}, and that the temperature range is 10^4–5×10^5 eV.[5]

Because of their charge, the charged elementary particles scatter elastically via the Coulomb force (in this paper, we do not include radiation processes); contrast this with the D-D collisions which produce the following reactions[4]:

$$\mathrm{D}+\mathrm{D}\to\begin{cases}\mathrm{D}+\mathrm{D}\,,\\ p+\mathrm{T}+Q_1\,,\\ n+{}^3\mathrm{He}+Q_2\,,\end{cases}\tag{1.1}$$

where $Q_1=4.00$ MeV and $Q_2=3.25$ MeV. The reaction rates in the inelastic channels in Eq. (1.1) are extremely small compared to those in the elastic channel; thus, we can assume that the system is in thermal equilibrium, provided the energy Q_1+Q_2 is removed continually.

In the early stages of the plasma development, the only important exoergic reactions are those in Eq. (1.1). In the later stages of plasma development, other exothermic reactions can occur; the most prominent of these are

$$\begin{aligned} &D+T \to n + {}^4He + Q_3 , \\ &D + {}^3He \to p + {}^4He + Q_4 . \end{aligned} \tag{1.2}$$

In the newly formed plasma, because of the low densities of T and ^{3}He compared to D, the reactions in Eq. (1.2) will contribute negligibly to the equation of state (this is discussed further at the end of Sec. II); hence, we can treat this as a two-component system and need to concentrate only on the e-e, the e-D, and the D-D interactions, which we describe qualitatively below. More general problems can be treated by suitable generalizations of the methods we develop here.

The electron is an elementary particle with charge e and spin $\frac{1}{2}$. The deuteron consists of one proton and one neutron bound by 2.22 MeV; it has spin 1 and possesses no excited bound states. (Throughout, we shall neglect spin interactions.) We assume that the e-e and e-D interactions are described by the Coulomb potential. Because of the low thermal energies considered in this paper, the elastic D-D scattering takes place, on the average, well below the Coulomb barrier, which has a height of about 1 MeV; thus, it will be assumed that the nuclear force contributes negligibly to the elastic D-D scattering and that the elastic D-D scattering can be described by the Coulomb potential. A description of the inelastic processes in Eq. (1.1) which is tractable can be based on the simple model in which the deuterons penetrate the Coulomb barrier to be captured in a potential well (corresponding to the mutual attraction of the deuterons via the nuclear force). This will be the subject of the next paper in this series.

The problem is now well defined: We must adapt the DMB formalism so that it applies to a multicomponent system of particles which interact elastically via Coulomb forces and inelastically via nuclear forces which are unknown but whose S-matrix elements are known. In Sec. II of this paper, we develop the notation for a multicomponent system; then, in Sec. III, we demonstrate that the long-range Coulomb force can be treated within the framework of the DMB theory to obtain the Debye-Hueckel equation of state for a two-component system. Section IV is concerned with the theory of the equation of state for systems in which the occurrence of inelastic reactions requires a multichannel description of the scattering processes. Finally, in Sec. V, we summarize, discuss the limitations of, and suggest extensions of the results in this paper.

II. THE EQUATION OF STATE FOR A MULTICOMPONENT SYSTEM

In this section, we extend the DMB formalism to a multicomponent system of particles. We will be concerned primarily with the development of the notation.

We use letters s, t, ... to indicate the particle species; the particle densities are denoted by n_s, n_t, ..., where $\sum_s n_s = n$ is the total particle density (s as a free index runs over all species). Let z_s denote the fugacity for particles of species s and $b_{\{N_s\}}$ represent the cluster coefficient for the set of particles $\{N_s\}$ with $\sum_s N_s = N$. The equation of state for a multicomponent system can then be expressed in the following parametric forms:

$$\beta P = \sum_{N=1}^{\infty} \sum_{\{N_s\}} b_{\{N_s\}} \prod_s z_s^{N_s} , \tag{2.1}$$

$$n_s = \sum_{N=1}^{\infty} \sum_{\{N_s\}} b_{\{N_s\}} N_s \prod_s z_s^{N_s} , \tag{2.2}$$

$$\beta P = \sum_{N=1}^{\infty} \sum_{\{N_s\}} a_{\{N_s\}} \prod_s n_s^{N_s} , \tag{2.3}$$

where P is the pressure, n_s is the number density of particles of species s, $\beta = (\kappa T)^{-1}$, κ is the Boltzmann constant, T is the temperature, $\sum_s N_s = N$ in the internal sums in Eqs. (2.1)–(2.3), and N_s is any number of the set 0, 1, ..., N with $\sum_s N_s = N$. The cluster coefficient $b_{\{N_s\}}$ is given now by Eq. (A15).

Next, we wish to establish the connections between the virial coefficients $a_{\{N_s\}}$ and the cluster coefficients $b_{\{N_s\}}$. Because the relations become unwieldy for the general case, we give the results only for a two-component case of species s and t. Thus, we find for the first three sets of virial coefficients

$$\begin{aligned} &a_{10} = 1, \quad a_{01} = 1, \quad a_{11} = \frac{-b_{11}}{b_{01} b_{10}} , \\ &a_{20} = \frac{-b_{20}}{b_{10}^2} , \quad a_{02} = \frac{-b_{02}}{b_{01}^2} , \end{aligned} \tag{2.4}$$

$$\begin{aligned} &a_{21} = \frac{-2b_{21}}{b_{10}^2 b_{01}} + \left(\frac{4b_{11} b_{20}}{b_{10}^3 b_{01}} + \frac{b_{11}^2}{b_{10}^2 b_{01}^2} \right) , \\ &a_{12} = \frac{-2b_{12}}{b_{01}^2 b_{10}} + \left(\frac{4b_{11} b_{02}}{b_{01}^3 b_{10}} + \frac{b_{11}^2}{b_{10}^2 b_{01}^2} \right) , \\ &a_{30} = \frac{-2b_{30}}{b_{10}^3} + \left(\frac{4b_{20}^2}{b_{10}^4} \right) , \quad a_{03} = \frac{-2b_{03}}{b_{01}^3} + \left(\frac{4b_{02}^2}{b_{01}^4} \right) . \end{aligned} \tag{2.5}$$

Above, the first subscript refers to the species s and the second to the species t. In particular, for the problem under consideration,

$$b_{10} = \frac{1}{\lambda_s^3} , \quad b_{01} = \frac{1}{\lambda_t^3} , \tag{2.6}$$

where $\lambda_s = (2\pi\beta\hbar^2/m_s)^{1/2}$ is the thermal wavelength of particles of species s (m_s is the mass of a particle of species s).

The equation of state of a two-component system in terms of the virial coefficients is therefore

$$\beta P = a_{10}n_s + a_{01}n_t + a_{11}n_s n_t + a_{20}n_s^2 + a_{02}n_t^2 + a_{30}n_s^3 + a_{21}n_s^2 n_t + a_{12}n_s n_t^2 + a_{03}n_t^3 + \cdots . \tag{2.7}$$

With the relations in Eqs. (A15), (2.4), and (2.5), we have a method for evaluating explicitly the coefficients in Eq. (2.7).

Note in Eq. (2.7) that if $n_s \gg n_t$ and if all the virial coefficients for each order (in the density) are of the same order of magnitude, then the equation of state for a two-component system reduces to that for a one-component system. By an analogous argument based on Eq. (2.3), we can substantiate the claim made in the Introduction [see below Eq. (1.2)] that the newly formed deuterium plasma can be treated as a two-component system. Thus, in the following sections, we discuss the calculation of cluster coefficients for the two-component fully ionized gas.

III. SUMMATION OF RING DIAGRAMS AND THE DEBYE-HÜCKEL EQUATION OF STATE

In this section, we study the application of the DMB formalism to a high-temperature, low-density system of spinless charged particles with overall charge neutrality. Because of the high temperature and low density of the system, it can be described by Boltzmann statistics. Straightforward perturbation theory based on the Coulomb potential leads to a divergent expansion for the S matrix. Our approach is to develop an expansion for the T matrix which allows us to obtain expressions in such a form that the analysis by Dewitt[6,7] can be adopted. As a result of this analysis we can use the ring-sum technique of Mayer[8] to obtain finite results.

By using various relations in DMB, one can derive the expression

$$\mathrm{Tr}\left(S^{-1}\frac{\overleftrightarrow{\partial}}{\partial u}S\right) = 2\,\mathrm{Tr}[G_0^2 T - (G_0^\dagger)^2 T^\dagger] , \tag{3.1}$$

where S, T, and G_0 are many-body operators, as discussed in DMB. This identity can be used in Eq. (A15) to obtain a form for the cluster coefficient which is suitable for the analysis of this section (we do not consider bound states in this section):

$$\Omega N!\, b_{\{N_s\}} = \frac{1}{2\pi i}\oint du\, e^{-\beta u}[\mathrm{Tr}_{\{N_s\}}(G_0^2 T)]_c , \tag{3.2}$$

where Ω is the volume of the system and the contour goes from right to left in the upper-half plane, through the origin, and then from left to right in the lower-half plane.[2] It is desirable to express Eq. (3.2) in terms of the potential by means of the relation[9]

$$T = V + VG_0 T . \tag{3.3}$$

Throughout this section, V refers to the Coulomb potential; the nuclear interactions will be reinstated in the following section.

If the iterated form of Eq. (3.3) is substituted into Eq. (3.2), we obtain

$$\Omega N!\, b_{\{N_s\}} = \frac{1}{2\pi i}\oint du\, e^{-\beta u}\left(\mathrm{Tr}_{\{N_s\}}\sum_{l=1}^{\infty}[G_0(G_0 V)^l]\right)_c \equiv \Omega N! \sum_{l=1}^{\infty} b_{\{N_s\}}^{(l)} . \tag{3.4}$$

We concentrate on the first two terms in the trace in Eq. (3.4) and write

$$b_{\{N_s\}} \simeq (2\pi i \Omega N!)^{-1}\oint du\, e^{-\beta u}[\mathrm{Tr}_{\{N_s\}}(G_0 V G_0) + \mathrm{Tr}_{\{N_s\}}(G_0 V G_0 V G_0)]_c , \tag{3.5}$$

$$\equiv b_{\{N_s\}}^{(1)} + b_{\{N_s\}}^{(2)} , \tag{3.6}$$

where, in an obvious notation, V can be any of the following:

$$V_{ij} = \frac{Z_s Z_t e^2}{r_{ij}} , \quad V_{ij} = \frac{Z_s^2 e^2}{r_{ij}} , \quad V_{ij} = \frac{Z_t^2 e^2}{r_{ij}} , \tag{3.7}$$

where Z_s is the charge number of species s and e is the charge of the electron. It is straightforward, but tedious, to show that $b_{\{N_s\}}^{(1)}$ in Eq. (3.6) does not contribute to the equation of state, Eq. (2.7), in the case of a fully ionized gas (assumed to be electrically neutral). To see this, substitute Eqs. (2.4) and (2.5) into Eq. (2.7); then, one must observe that $b_{11}^{(1)}$, $b_{20}^{(1)}, \ldots, b_{03}^{(1)}$ produce appropriate factors of λ_s^3 and λ_t^3 which combine with $b_{10} = 1/\lambda_s^3$ and $b_{01} = 1/\lambda_t^3$ in such a way that various terms in Eq. (2.7) form groups. Each group of terms is proportional to sums of powers of Z_s, Z_t, e^2, n_s, and n_t. In every instance, one can identify the factor $(Z_s e n_s + Z_t e n_t)$ which is zero by charge neutrality. Finally, we note that when $b_{\{N_s\}}^{(2)}$ in Eq. (3.6) is substituted into Eq. (2.5), the terms in parentheses are of higher order in e^2 than the first terms. Thus, we can use the approximations

$$a_{21} \simeq \frac{-2b_{21}}{b_{10}^2 b_{01}} , \quad a_{12} \simeq \frac{-2b_{12}}{b_{01}^2 b_{10}} , \tag{3.8a}$$

$$a_{30} \simeq \frac{-2b_{30}}{b_{10}^3} , \quad a_{03} \simeq \frac{-2b_{03}}{b_{01}^3} , \tag{3.8b}$$

when we study the effects of the Coulomb interaction on a fully ionized gas. From Eqs. (2.4)–(2.7) and (3.8), we see that the equation of state is now simply related to the cluster coefficients. For notational convenience we continue to restrict our discussion to two-component systems.

The perturbation expansion of $b_{\{N_s\}}$ for the two-particle case can be easily developed; thus, we discuss this case next. Expanding the two-body T operator in powers of the two-body potential and the resolvent G_0 gives, according to Eq. (3.4),

$$\Omega 2!\, b_{\{2\}} = \frac{1}{2\pi i} \oint du\, e^{-\beta u} \sum_{l=1}^{\infty} [\mathrm{Tr}_{\{2\}} G_0 (G_0 V)^l]_c , \quad (3.9)$$

where the subscript $\{2\}$ indicates $\{N_s\}$ for $\sum_s N_s = 2$.

We next define a function $b_{\{2\}}^{(l)}$ as follows:

$$\Omega 2!\, b_{\{2\}}^{(l)} = \frac{1}{2\pi i} \oint du\, e^{-\beta u} [\mathrm{Tr}_{\{2\}} G_0 (G_0 V)^l]_c . \quad (3.10)$$

If we set $u = y + E$,

$$E = \frac{(\vec{p}^{\,s})^2}{2m_s} + \frac{(\vec{p}^{\,t})^2}{2m_t},$$

where $\vec{p}^{\,s}$ and $\vec{p}^{\,t}$ are the momenta of the particles of species s and t, respectively, then we can write for Eq. (3.10)

$$\Omega 2!\, b_{\{2\}}^{(l)} = \frac{\Omega^2}{(2\pi\hbar)^6} \int d^3p^s d^3p^t e^{-\beta E} \frac{1}{2\pi i} \oint \frac{dy}{y} e^{-\beta y} \left\langle \vec{p}^{\,s}\vec{p}^{\,t} \left| \left(\frac{1}{y - (H_0 - E)} V \right)^l \right| \vec{p}^{\,s}\vec{p}^{\,t} \right\rangle . \quad (3.11)$$

The operator product in Eq. (3.11) can be written out in momentum space to give

$$\Omega 2!\, b_{\{2\}}^{(l)} = \frac{\Omega^{2l}}{(2\pi\hbar)^{6l}} \int d^3p^s d^3p^t e^{-\beta E} \int d^3p_1^s d^3p_1^t \cdots d^3p_{l-1}^s d^3p_{l-1}^t$$
$$\times \langle \vec{p}^{\,s}\vec{p}^{\,t} | V | \vec{p}_1^{\,s}\vec{p}_1^{\,t} \rangle \langle \vec{p}_1^{\,s}\vec{p}_1^{\,t} | V | \vec{p}_2^{\,s}\vec{p}_2^{\,t} \rangle \cdots \langle \vec{p}_{l-1}^{\,s}\vec{p}_{l-1}^{\,t} | V | \vec{p}^{\,s}\vec{p}^{\,t} \rangle$$
$$\times \frac{1}{2\pi i} \oint \frac{dy}{y^2} e^{-\beta y} \prod_{j=1}^{l-1} [y - (E_j - E)]^{-1} , \quad (3.12)$$

where

$$E_j = \frac{(\vec{p}_j^{\,s})^2}{2m_s} + \frac{(\vec{p}_j^{\,t})^2}{2m_t}, \quad (3.13)$$

$$\langle \vec{p}_1^{\,s}\vec{p}_2^{\,t} | V | \vec{p}_3^{\,s}\vec{p}_4^{\,t} \rangle = \frac{2(2\pi)^4 Z_s Z_t e^2 \hbar^5}{\Omega^2 q^2} \, \delta(\vec{p}_1^{\,s} + \vec{p}_2^{\,t} - \vec{p}_3^{\,s} - \vec{p}_4^{\,t}) , \quad (3.14)$$

$$\vec{q} = \vec{p}_3^{\,s} - \vec{p}_1^{\,s} . \quad (3.15)$$

The contour integral in Eq. (3.12) can be evaluated and the result represented as

$$\frac{1}{2\pi i} \oint \frac{dy}{y^2} e^{-\beta y} \prod_{j=1}^{l-1} [y - (E_j - E)]^{-1}$$
$$= (-1)^l \int_0^{\beta} d\beta_l \int_0^{\beta_l} d\beta_{l-1} \cdots \int_0^{\beta_2} d\beta_1 \, \exp[-(\beta_l - \beta_{l-1})(E_{l-1} - E) + \cdots + (\beta_2 - \beta_1)(E_1 - E)] . \quad (3.16)$$

In the classical limit (high-temperature, low-density limit), the above integral was shown by Dewitt[6] to reduce to

$$\frac{1}{2\pi i} \oint \frac{dy}{y^2} e^{-\beta y} \prod_{j=1}^{l-1} [y - (E_j - E)]^{-1} \simeq \frac{(-\beta)^l}{l!} . \quad (3.17)$$

Therefore, in the classical limit, Eq. (3.10) becomes

$$\Omega 2!\, b_2^{(l)} \simeq \frac{(-\beta)^l}{l!} \frac{1}{(2\pi\hbar)^6} \int d^3p^s d^3p^t e^{-\beta E}\, \mathrm{Tr}_{\{2\}}(V^l) \simeq \frac{(-\beta)^l}{\lambda_s^3 \lambda_t^3 l!} \mathrm{Tr}_{\{2\}}(V^l) . \quad (3.18)$$

For the three-particle case, the sum over l will lead to (connected) terms of the following form:

$$(V_{12} G_0 V_{23} + \cdots) + (V_{12} G_0 V_{23} G_0 V_{12} + \cdots) + (V_{12} G_0 V_{23} G_0 V_{31} + \cdots) .$$

Hence, the three-particle cluster coefficient becomes

$$\Omega 3!\, b_{\{3\}} = \frac{1}{2\pi i} \oint du\, e^{-\beta u} \mathrm{Tr}_{\{3\}} [G_0 (G_0 V_{12} G_0 V_{23} + \cdots) + G_0 (G_0 V_{12} G_0 V_{23} G_0 V_{12} + \cdots) + G_0 (G_0 V_{12} G_0 V_{23} G_0 V_{31} + \cdots) + \cdots] .$$
$$(3.19)$$

We observe that Eq. (3.19) is of the same form as Eq. (3.9) except V in Eq. (3.9) is replaced by V_{12}, $V_{23}, \ldots$ in Eq. (3.19). Following the analysis used for the two-particle cluster coefficient in the classical limit, we find

$$\Omega 3!\, b_{\{3\}}^{(l)} \simeq \frac{(-\beta)^l}{\lambda_a^3 \lambda_b^3 \lambda_c^3} \frac{1}{l!} \mathrm{Tr}_{\{2\}}(V^l)\,, \tag{3.20}$$

where a, b, and c will run over the species labels s and t. Clearly, the above analysis holds for any $b_{\{N_s\}}^{(l)}$ (in the classical limit).

Next, we observe that the charge neutrality condition can be used to eliminate all terms in $b_{\{N_s\}}^{(l)}$ for $l<\sum_s N_s$. The argument is identical to that outlines below Eq. (3.7). The result is that the only nonzero terms are connected in such a manner that they can be represented graphically as a ring. The cluster coefficient for the lowest order (in terms of powers of e^2) will be denoted by $b_{\{N_s\}}$ (ring) and, as mentioned above, can be repre-
order (in terms of powers of e^2) will be denoted by $b_{\{N_s\}}$ (ring) and, as mentioned above, can be repre-
sented by a ring diagram.[8] According to the preceding discussion, we note that $b_{\{N_s\}}$ (ring) is the lowest-order term in $b_{\{N_s\}}^{(l)}$, where $l=\sum_s N_s$. Higher-order terms in $b_{\{N_s\}}^{(l)}$ have been analyzed by Mayer[8] and Abe.[10,11] Also, quantum-mechanical corrections to the cluster coefficients for a fully ionized gas have been calculated; a critical analysis of this problem is given by Ebeling *et al.*,[12] where additional references to the literature can also be found. We summarize here the results of the ring-sum analysis of Mayer.[8]

The lth cluster coefficient for the ring diagram in configuration space is, up to factors,

$$(\lambda_a^{-3}\lambda_b^{-3}\cdots\lambda_r^{-3}) \int d^3r_1 d^3r_2 \cdots d^3r_l\, V(r_{12})V(r_{23})\cdots V(r_{l1})\,, \tag{3.21}$$

where $l=\sum_s N_s$, $a, b, \ldots, r$ range over s and t, and there are l factors in the product $(\lambda_a^{-3}\lambda_b^{-3}\cdots\lambda_r^{-3})$. For V, Mayer uses

$$V_\epsilon(r_{ij}) = \frac{Z_s Z_t e^2 e^{-\epsilon r_{ij}}}{r_{ij}}\,,$$

where $r_{ij}=|\vec{r}_i-\vec{r}_j|$. After summing all ring diagrams, he sets $\epsilon\to 0$, and obtains for the contribution from all $b_{\{N_s\}}$(ring) to the equation of state the result

$$-(24\pi\lambda_{(D)}^3)^{-1}\,, \tag{3.22}$$

where the Debye length $\lambda_{(D)}$ is defined by

$$\lambda_{(D)} = [4\pi\beta e^2(Z_s^2 n_s + Z_t^2 n_t)]^{-1/2}\,. \tag{3.23}$$

Now, we clarify what is being summed and what terms are included in the equation of state.

Combining Eqs. (3.8), (2.4), (2.5), and the virial expansion of the equation of state, Eq. (2.7), shows that

$$\beta P \simeq (n_s+n_t) - \left[\left(\frac{b_{20}}{b_{10}^2}\right)n_s^2 + \left(\frac{b_{11}}{b_{10}b_{01}}\right)n_s n_t + \left(\frac{b_{02}}{b_{01}^2}\right)n_t^2\right]$$
$$-2\left[\left(\frac{b_{30}}{b_{10}^3}\right)n_s^3 + \left(\frac{b_{21}}{b_{10}^2 b_{01}}\right)n_s^2 n_t + \left(\frac{b_{12}}{b_{01}^2 b_{10}}\right)n_s n_t^2 + \left(\frac{b_{03}}{b_{01}^3}\right)n_t^3\right] + \cdots\,, \tag{3.24}$$

where the $b_{\{N_s\}}$ are to be approximated by $b_{\{N_s\}}$(ring) in Eq. (3.21) and $b_{10}=\lambda_s^{-3}$, $b_{01}=\lambda_t^{-3}$. Thus, with the approximation

$$b_{\{N_s\}}^{(l)} \simeq b_{\{N_s\}}(\text{ring})\,, \tag{3.25}$$

we obtain

$$\beta P \simeq (n_s+n_t) - \sum_{\substack{\{N_s\}\\ N=2}}^{\infty} (N-1)\, b_{\{N_s\}}(\text{ring}) \frac{N!}{N_s!\,N_t!} \times (n_s/\lambda_s^3)^{N_s}(n_t/\lambda_t^3)^{N_t}\,, \tag{3.26}$$

where $\sum_s N_s = N$. Now, if we set

$$\Lambda = \sum_{\substack{\{N_s\}\\ N=2}}^{\infty} b_{\{N_s\}}(\text{ring}) \frac{N!}{N_s!\,N_t!} (n_s/\lambda_s^3)^{N_s}(n_t/\lambda_t^3)^{N_t}\,, \tag{3.27}$$

then Eq. (3.26) becomes

$$\beta P \simeq (n_s+n_t) + \Lambda - \left(n_s\frac{\partial\Lambda}{\partial n_s} + n_t\frac{\partial\Lambda}{\partial n_t}\right). \tag{3.28}$$

Mayer[8] showed that

$$\Lambda = (12\pi\lambda_{(D)}^3)^{-1}\,. \tag{3.29}$$

Using Eqs. (3.23), (3.28), and (3.29), we finally obtain

$$\beta P \simeq (n_s+n_t) - (24\pi\lambda_{(D)}^3)^{-1}\,, \tag{3.30}$$

which is the Debye-Hueckel equation of state.

In this section, we have shown how the S-matrix formalism can be applied to a system of charged particles. There remains then the problem of treating a system of reacting charged particles; this is the subject of the next section.

IV. THE MULTICHANNEL PROBLEM FOR A SYSTEM OF REACTING CHARGED PARTICLES

So far, we have neglected the internal states of the composite particles (D, T, and ^{3}He). In order to take into account the reactions in deuterium plasma, it is necessary to reformulate the problem so that the S matrix includes inelastic scattering processes. As inferred in the Introduction, we shall neglect exchange effects and spin interactions and use Boltzmann statistics. Also, we have noted that the system can be treated as a two-component system consisting of electrons and deuterons. Before the deuterons undergo nuclear reactions, they are all in their ground state; moreover, we make the assumption that there are no bound states for pairs of these scattering particles.

At this point, we must develop the notation and define the reaction channels for this problem. The species label s is assigned values as follows:

$$\begin{aligned} &\text{for } e, \quad s=1\\ &\text{for D}, \quad s=2\\ &\text{for } p, \quad s=3\\ &\text{for } n, \quad s=4\\ &\text{for T}, \quad s=5\\ &\text{for } {}^3\text{He}, \quad s=6\,. \end{aligned} \tag{4.1}$$

A Greek letter (α, β, μ, ν) will be used to denote a channel; we use a notation in which $\alpha=1,2,\ldots$ or $\alpha=\alpha_1, \alpha_2, \ldots$. Taking into account all of the assumptions made thus far, we list below the pairs of particles which can interact and the associated channel numbers:

$$\begin{aligned} &e+e \quad (\alpha_1 \text{ or } \beta_1),\\ &e+\text{D} \quad (\alpha_2 \text{ or } \beta_2),\\ &\text{D}+\text{D} \quad (\alpha_3 \text{ or } \beta_3),\\ &p+\text{T} \quad (\alpha_4 \text{ or } \beta_4),\\ &n+{}^3\text{He} \quad (\alpha_5 \text{ or } \beta_5). \end{aligned} \tag{4.2}$$

Each α_i can label either an entrance channel or an exit channel—cf., Eq. (1.1). Next, we identify the potential v^α in each channel which is responsible for binding the composite particles in that channel:

$$\begin{aligned} &v^1=0,\\ &v^2=V_{34}=V_N(p,n),\\ &v^3=V_{34}+V_{34}=V_N(p,n)+V_N(p',n'),\\ &v^4=V_{24}=V_N(n,\text{D})=V_N(n,n,p),\\ &v^5=V_{23}=V_N(p,\text{D})=V_N(p,n,p). \end{aligned} \tag{4.3}$$

Here, $V_N(p,n)$ represents the nuclear potential[13] which binds one deuteron, $V_N(p',n')$ that of another deuteron, and so forth; recall that bound states of the scattering particles (for example, D + D) are not considered. The scattering potentials V^α in channel α are defined as follows:

$$\begin{aligned} &V^1=V_{11}=V_C(e,e),\\ &V^2=V_{12}=V_C(e,\text{D}),\\ &V^3=V_{22}=V_C(\text{D},\text{D}),\\ &V^4=V_{35}=V_C(p,\text{T}),\\ &V^5=V_{46}=V_N(n,{}^3\text{He}), \end{aligned} \tag{4.4}$$

where V_C represents the Coulomb potential (in elastic scattering, it is assumed that $V_C \gg V_N$). (Actually, the scattering potential V^α is an effective potential; for example, the more correct form for V^2 is $V_{12}=V_{en}+V_{ep}$.) Let H_0^α be the kinetic energy operator for the two freely moving particles in channel α; then, the channel-α Hamiltonian is defined by

$$H^\alpha = H_0^\alpha + v^\alpha\,. \tag{4.5}$$

In channel α, the total Hamiltonian $H(\alpha)$ is given by

$$H(\alpha)=H^\alpha+V^\alpha=H_0^\alpha+v^\alpha+V^\alpha\,. \tag{4.6}$$

We shall need also the operators[9]

$$\begin{aligned} &G^\alpha(u)=(u-H^\alpha)^{-1},\\ &T^{\beta\alpha}(u)=V^\alpha+V^\beta G^\beta(u)T^{\beta\alpha}(u), \end{aligned} \tag{4.7}$$

where $T^{\beta\alpha}$ is the T operator for scattering from channel α to channel β. Note also that state vectors must be characterized by a channel number.

We apply the notation and explain the new features of the multichannel problem, using the second-order cluster coefficients as a basis for our discussion. The multicomponent form of Eq. (A2) is

$$\Omega 2!\, b_{\{2\}} = (\mathrm{Tr}_{\{2\}} e^{-\beta H})_c = \mathrm{Tr}_{\{2\}}(e^{-\beta H} - e^{-\beta H_0})\,. \tag{4.8}$$

In the preceding section, the total Hamiltonian H did not include the internal potentials of composite particles. If one includes the internal potentials of the composite particles in the total Hamiltonian H, then the form of Eq. (4.8) does not change. However, the free particle Hamiltonian H_0 must be replaced by the channel-α Hamiltonian H^α, where H^α is the total Hamiltonian for both the free elementary particles and the free composite particles, as defined in Eq. (4.5). Next, we must express the trace of the cluster coefficient in Eq. (4.8) for two deuterons s and t in terms of the S matrix. If we introduce the operators H, V^α, and v^α, defined above, then the trace in Eq. (4.8) for the two deuterons can be expressed as follows[2,14]:

$$\Omega 2!\, b_{\{2\}}(\alpha_3) = \frac{1}{2\pi i}\int_C du\, e^{-\beta u} \sum_{\vec{p}^s,\vec{p}^t} \left\langle \vec{p}^s\vec{p}^t\psi^s\psi^t\alpha_3 \left| \left(\frac{1}{u-H} - \frac{1}{u-H^\alpha}\right) \right| \vec{p}^s\vec{p}^t\psi^s\psi^t\alpha_3 \right\rangle, \tag{4.9}$$

where the contour C runs just above the real axis from $+\infty$ to the left of the smallest pole of $(u-H^\alpha)^{-1}$ and returns to $+\infty$ just below the real axis. In Eq. (4.9), $\vec{p}^s$ and $\vec{p}^t$ are the center-of-mass momenta of the deuterons s and t, respectively, and $|\psi^s\rangle$ and $|\psi^t\rangle$ represent their internal state vectors. Now, Eq. (4.9) can be transformed into the form[2]

$$\Omega 2!\, b_{\{2\}}(\alpha_3) = \frac{1}{4\pi i}\sum_\mu \int_{2E_g}^\infty du\, e^{-\beta u} \sum_{\vec{p}^s,\vec{p}^t} \langle \vec{p}^s\vec{p}^t\psi^s\psi^t\alpha_3 | [S(\mu,\alpha_3)]^{-1} | \mu\rangle \frac{\overleftrightarrow{\partial}}{\partial u} \langle \mu | S(\mu,\alpha_3) | \vec{p}^s\vec{p}^t\psi^s\psi^t\alpha_3\rangle\,, \tag{4.10}$$

where $S(\mu,\alpha) = S^{\mu\alpha}$, $|\mu\rangle$ is a state in channel μ (all other labels are suppressed) and the sum over μ runs over all channels and over all state labels, and E_g is the ground-state energy of the deuteron ($E_g \simeq -2.22$ MeV).

Consider the contribution of the elastic exit channel β_3 to $b_{\{2\}}(\alpha_3)$ in Eq. (4.10). Let this contribution be denoted by $b_{\rm DD}(\alpha_3 \to \beta_3)$; then, we have

$$\Omega 2!\, b_{\rm DD}(\alpha_3\to\beta_3) = \frac{1}{4\pi i}\int_{2E_g}^\infty du\, e^{-\beta u} \sum_{\vec{p}^s,\vec{p}^t} \langle \vec{p}^s\vec{p}^t\psi^s\psi^t\alpha_3 | [S(\beta_3,\alpha_3)]^{-1} | \beta_3\rangle \frac{\overleftrightarrow{\partial}}{\partial u} \langle \beta_3 | S(\beta_3,\alpha_3) | \vec{p}^s\vec{p}^t\psi^s\psi^t\alpha_3\rangle\,, \tag{4.11}$$

where a sum over the intermediate states of channel β_3 is implied. We assume that the interaction between two deuterons can be resolved into a Coulomb interaction plus a nuclear interaction. In our simple model the potential will be approximated by an effective potential which consists of a potential well with a tail given by the Coulomb potential. From Eqs. (3.2), (4.9), and (4.11), we can write, dropping temporarily the channel numbers,

$$\Omega 2!\, b_{\rm DD}(\alpha_3\to\beta_3) = \frac{1}{2\pi i}\int_C du\, e^{-\beta u}\, {\rm Tr}[G_0^2(u) T(u)]\,. \tag{4.12}$$

We approximate T by $T \simeq T_C + T_N$, where T_C is the Coulomb T matrix and T_N is the nuclear T matrix, and set $y = u - 2E_g$ to obtain

$$\Omega 2!\, b_{\rm DD}(\alpha_3\to\beta_3) \simeq \frac{e^{-2\beta E_g}}{2\pi i}\int_C dy\, e^{-\beta y}\, {\rm Tr}\{G_0^2(y)[T_C(y) + T_N(y)]\}\,. \tag{4.13}$$

Thus, as one would expect, $b_{\rm DD}(\alpha_3\to\beta_3)$ can be separated approximately into two terms: the first term has been analyzed in Sec. III and the second is a new one. The contribution of $b_{\rm DD}(\alpha_3\to\beta_3)$ to the second virial coefficient is given by

$$a_{\rm DD}(\alpha_3\to\beta_3) = \frac{-b_{\rm DD}(\alpha_3\to\beta_3)}{b_{1\rm D}^2}, \tag{4.14}$$

where

$$b_{1\rm D} = \Omega^{-1}\, {\rm Tr}_{1\rm D}(e^{-\beta H^\alpha})\,, \tag{4.15}$$

and ${\rm Tr}_{1\rm D}$ means that the trace is to be taken in the one-particle space of the deuteron. Thus,

$$b_{1\rm D} = \frac{e^{-\beta E_g}}{\lambda_{\rm D}^3}, \tag{4.16}$$

where $\lambda_{\rm D}$ is the thermal wavelength of the deuteron. Therefore, we obtain

$$a_{\rm DD}(\alpha_3\to\beta_3) = \frac{-\lambda_{\rm D}^6}{2\pi i}\int_C dy\, e^{-\beta y}\, {\rm Tr}[G_0^2(y) T_C(y)] - \frac{\lambda_{\rm D}^6}{2\pi i}\int_C dy\, e^{-\beta y}\, {\rm Tr}[G_0^2(y) T_N(y)]\,. \tag{4.17}$$

As mentioned above, the first term of Eq. (4.17) is exactly the second virial coefficient due to the pure Coulomb interaction which was dealt with in Sec. III. As discussed previously, the second term of Eq. (4.17) is negligible in the deuterium plasma. The main point to note here is that the factor $e^{-2\beta E_g}$ in Eq. (4.13) does not appear in Eq. (4.17).

Finally, we come to the most interesting part of the multichannel problem. For the contributions of the inelastic channels to the second virial coefficient, we write [cf., Eq. (4.14)]

$$a_{\rm DD}(\alpha_3\to\beta_i) = -\frac{b_{\rm DD}(\alpha_3\to\beta_i)}{b_{1\rm D}^2}, \quad i = 4, 5\,. \tag{4.18}$$

We use Eqs. (A.10), (4.10), and (4.16) to obtain

$$a_{\rm DD}(\alpha_3\to\beta_4) = \frac{e^{2\beta E_g}\lambda_{\rm D}^6}{4\pi i}\int_{2E_g}^\infty dy\, e^{-\beta y} \sum_{\vec{p}^s,\vec{p}^t,\vec{p}^3,\vec{p}^5} \langle \vec{p}^s\vec{p}^t\psi^s\psi^t\alpha_3 | [2\pi i\delta(y - H^{\alpha_3}) T^\dagger(\alpha_3,\beta_4)] | \vec{p}^3\vec{p}^5\psi^5\beta_4\rangle \times \frac{\overleftrightarrow{\partial}}{\partial y} \langle \vec{p}^3\vec{p}^5\psi^5\beta_4 | [2\pi i\delta(y - H^{\beta_4}) T(\beta_4,\alpha_3)] | \vec{p}^s\vec{p}^t\psi^s\psi^t\alpha_3\rangle\,, \tag{4.19}$$

$$a_{\mathrm{DD}}(\alpha_3\to\beta_5)=\frac{e^{2\beta E_g}\lambda_{\mathrm{D}}^6}{4\pi i}\int_{2E_g}^{\infty}dy\,e^{-\beta y}\sum_{\vec{p}^s,\vec{p}^t,\vec{p}^4,\vec{p}^6}\langle\vec{p}^s\vec{p}^t\psi^s\psi^t\alpha_3|[2\pi i\delta(y-H^{\alpha_3})T^\dagger(\alpha_3,\beta_5)]|\vec{p}^4\vec{p}^6\psi^6\beta_5\rangle$$
$$\times\frac{\overleftrightarrow{\partial}}{\partial y}\langle\vec{p}^4\vec{p}^6\psi^6\beta_5|[2\pi i\delta(y-H^{\beta_5})T(\beta_5,\alpha_3)]|\vec{p}^s\vec{p}^t\psi^s\psi^t\alpha_3\rangle\,. \qquad (4.20)$$

In Eq. (4.19), $\vec{p}^3$ is the proton momentum, and $\vec{p}^s$ is the center-of-mass momentum of T; $|\psi^5\rangle$ is the internal (ground) state of T. In Eq. (4.20), $\vec{p}^4$ is the neutron momentum, and $\vec{p}^6$ is the center-of-mass momentum of ^{3}He; $|\psi^6\rangle$ represents the ground state of ^{3}He. The T matrices in Eqs. (4.19) and (4.20) correspond to the nuclear forces responsible for the nuclear reactions (actually, both are stripping reactions). With these results, we have for the equation of state

$$\frac{P}{\kappa T}\simeq[(n_e+n_{\mathrm{D}})-(24\pi\lambda_{(D)}^3)^{-1}]$$
$$-[a_{\mathrm{DD}}(\alpha_3\to\beta_4)+a_{\mathrm{DD}}(\alpha_3\to\beta_5)]n_{\mathrm{D}}^2\,, \qquad (4.21)$$

where $\lambda_{(D)}$ is the Debye wavelength defined in Eq. (3.23).

It is not at all clear how the second term in braces in Eq. (4.21) compares in magnitude to the last two. Indeed, it would be of considerable interest to understand the qualitative behavior of these new terms to identify conditions under which they become important. From Eqs. (4.18)–(4.20), it is clear that we need to evaluate the multichannel T matrices. This problem is currently under investigation.

V. SUMMARY AND OUTLOOK

In this paper, we have been concerned with a nonrelativistic deuterium plasma which is exothermic, fully ionized, electrically neutral, and in thermal equilibrium. In order to treat this system, it was necessary to make certain extensions of the DMB formalism to allow for the long-range Coulomb force and the multichannel aspect of the reactions of charged particles. First, we presented the virial equation of state for a multicomponent system, treated the problem of notation, and derived relations between cluster and virial coefficients for the two-component case. Then, we cast the DMB formalism into a new form such that the analysis by Dewitt[6,7] could be used. As a result of this analysis, the ring sum was performed in a conventional manner.[8] Finally, we derived expressions to describe the contributions of nuclear reactions to the equation of state for a two-component plasma undergoing fusion. These preliminary results are subject to some limitations and are in need of specific extensions which we discuss next.

The second virial coefficient is related to the two-body *on-shell* T matrix; the third virial coefficient involves three-particle S-matrix elements. The state-of-the-art analysis of the three-body problem proceeds by means of the Faddeev equations[15-17] and this is completely appropriate for this problem. However, a price is exacted for using the Faddeev equations, namely *off-shell* (or half-off-shell) two-body T matrices are introduced. This is a problem because there is no general method for converting cross-section data into off-shell T-matrix elements. The multichannel effective-range theory of Ross and Shaw[18] and the K-matrix formalism of de Swart *et al.*[19] can be used as a starting point in this problem. Alternatively, one can develop a model potential and fit it to the experimental data. For example, the D-D scattering can be described, for present purposes, by means of square-well potentials with Coulomb tails; such barrier-penetration problems are discussed in detail by Blatt and Weisskopf,[20] but there remain difficulties with the low-energy case (which is of interest here). Another problem with three-particle scattering amplitudes is discussed and solved by Dashen and Ma.[21]

The neglect of spin interactions and particle statistics is of little consequence in the present case. However, we have ignored photons in a system of charged particles at high temperature; this represents an undesirable deficiency of the formalism in this paper, and work is in progress to eliminate this deficiency. Next, we discuss briefly how one can take into account the transverse electromagnetic interactions between the charged particles (the radiative corrections to the nuclear reactions are more subtle and difficult, but are probably unimportant in the problem under study).

The Nth cluster coefficient involves the T operator, $T(u)$ [cf., Eq. (A15) and the first line of Eq. (A10)]. One then resolves $T(u)$ into two parts: $T(u)=T_\gamma(u)+T'(u)$; here, $T_\gamma(u)$ represents the contribution from photons, while $T'(u)$ describes the Coulomb and nuclear interactions (in the presence of radiation). Next, one assumes that the $T_\gamma(u)$ and $T'(u)$ are approximately independent, so that the representation of $T_\gamma(u)$ in terms of the iterations of the Lippmann-Schwinger equation

$$T_\gamma(u)=V_\gamma+V_\gamma G_0(u)T_\gamma(u)$$

allows us to include the effects of photons in terms of the electromagnetic interaction potentials V_γ. As usual, the electromagnetic interactions will lead to various divergences which must be eliminated by renormalization procedures.

In order to describe thermonuclear plasmas, many other extensions of the DMB theory will be necessary. In particular, the formalism must be generalized so that it can be applied to anisotropic, inhomogeneous, finite, and nonequilibrium systems in the presence of external fields. Such extensions as suggested here will require a great deal of work. Techniques for treating the nonequilibrium aspect of the problem are reviewed by Grandy,[22] and scattering in external fields is the subject of two papers by Prugovecki and Tip.[23]

We have made no mention of the work of others on the equation of state of reacting plasmas. Development of a physical-cluster theory for a multispecies reactive gas was undertaken earlier by Lawson and Dahler; they applied their results to a model of interest in physical chemistry.[24] A multispecies virial expansion based on the time-delay operator has been given and its relation to the work of DMB has been established by Osborn.[25] Our results could have been derived on the basis of Osborn's virial expansion. There have been other related investigations reported in the literature.[12,26,27] Our approach here differs from the earlier work in two respects.

(1) We have used the S-matrix formalism of DMB as the basis for the computations of the equation of state (see Sec. I for a discussion of the desirability of using the S-matrix theory).

(2) We focus our attention on developing methods for including the nuclear contributions to the equation of state for a plasma.

This paper is the first of two. In the next paper, we estimate the nuclear contributions to the equation of state on the basis of model potentials with repulsive Coulomb tails and on the basis of the effective-range and K-matrix theories.[18,19]

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APPENDIX: S-MATRIX FORMULATION OF QUANTUM STATISTICS

In this appendix we summarize the basic relations which relate the Nth cluster coefficient b_N to the scattering operator S. We discuss only the case of Boltzmann statistics (the cases of Bose-Einstein and Fermi-Dirac statistics treated in DMB are not of interest in this paper).

The grand potential f for a single-component system of N particles is given, in statistical mechanics, by

$$\Omega f(\beta, g, \Omega) = \ln \operatorname{Tr}\{\exp[\beta(G-H)]\},$$

where G is the Gibbs potential, with $G = gN$ and $z = \exp(\beta g)$, g is the chemical potential, and H is the complete Hamiltonian of the system—our notation differs slightly from that of DMB. This can be transformed into[2]

$$\Omega f = \Omega f_0 + \Omega \sum_{N=2}^{\infty} z^N b_N , \tag{A1}$$

where f_0 is the free-particle grand potential,

$$\Omega b_N = \frac{1}{N!} (\operatorname{Tr}_N e^{-\beta H})_c$$

is the Nth cluster coefficient, and the subscript c indicates that only the connected terms in the trace are to be used.[2,3]

Next, we express the second and third cluster coefficients in terms of S instead of H. The explicit forms of these coefficients are

$$\Omega 2!\, b_2 = (\operatorname{Tr}_2 e^{-\beta H})_c = \operatorname{Tr}_2(e^{-\beta H} - e^{-\beta H_0}) , \tag{A2}$$

$$\Omega 3!\, b_3 = (\operatorname{Tr}_3 e^{-\beta H})_c = \operatorname{Tr}_3\Big(e^{-\beta H} - e^{-\beta H_0} - \sum_{i<j} (e^{-\beta(H_0+V_{ij})} - e^{-\beta H_0})\Big), \tag{A3}$$

where V_{ij} is the interaction potential between the ith and jth particles, H_0 is the free-particle Hamiltonian, and

$$H = H_0 + \sum_{i<j} V_{ij} .$$

If we define the resolvents

$$G(u) = (u-H)^{-1}, \quad G_0(u) = (u-H_0)^{-1},$$
$$G_{ij}(u) = (u - H_0 - V_{ij})^{-1}, \tag{A4}$$

then we can express the second and third cluster coefficients in the form

$$\Omega 2!\, b_2 = \frac{1}{2\pi i} \oint du\, e^{-\beta u} \operatorname{Tr}_2 [G(u) - G_0(u)] , \tag{A5}$$

$$\Omega 3!\, b_3 = \frac{1}{2\pi i} \oint du\, e^{-\beta u} \operatorname{Tr}_3 \Big(G(u) - G_0(u) - \sum_{i<j} [G_{ij}(u) - G_0(u)]\Big), \tag{A6}$$

where the contour integral is taken along a counterclockwise path. Note in Eq. (A6) that in $G_{ij}(u)$, H_0 is the Hamiltonian for three free particles. We see that $G(u)$ may have poles along both the positive and negative real axes. The poles along the negative real axis correspond to bound states. For the case when there are no bound states, Eqs. (A5) and (A6) can be written in the form

$$\Omega 2!\, b_2 = -\frac{1}{\pi}\int_0^\infty du\, e^{-\beta u}\, \mathrm{Im}\,\mathrm{Tr}_2\,[G(u) - G_0(u)]\,, \tag{A7}$$

$$\Omega 3!\, b_3 = -\frac{1}{\pi}\int_0^\infty du\, e^{-\beta u}\, \mathrm{Im}\,\mathrm{Tr}_3\Big(G(u) - G_0(u) - \sum_{i<j}\,[G_{ij}(u) - G_0(u)]\Big)\,, \tag{A8}$$

where Im stands for the imaginary part, and now in $G(u)$, $G_0(u)$, and $G_{ij}(u)$ it is understood that u stands for $u + i\eta$ ($\eta \to 0^+$ as a final step).

In order to express Eqs. (A5) and (A6) in terms of the scattering operator, we define the operators T, Ω_s, and S as follows[2,9]:

$$T(u) = V + VG(u)V\,, \quad \Omega_s(u) = G(u)G_0^{-1}(u)\,, \quad S(u) = \Omega_s^{-1}(u^*)\,\Omega_s(u)\,, \tag{A9}$$

where $V = H - H_0$. These operators satisfy the relations[2]

$$\begin{aligned} &S(u) = 1 + (G_0 - G_0^\dagger)T(u) = 1 - 2\pi i\, \delta(u - H_0)T(u)\,, \\ &S^{-1} = 1 - (G_0 - G_0^\dagger)T^\dagger = 1 + 2\pi i \delta(u - H_0)T^\dagger\,, \\ &T - T^\dagger = T^\dagger(G_0 - G_0^\dagger)T = T(G_0 - G_0^\dagger)T^\dagger\,. \end{aligned} \tag{A10}$$

Utilizing the above identities, one can show that

$$\mathrm{Im}\,\mathrm{Tr}_2(G - G_0) = -\frac{1}{4i}\,\mathrm{Tr}_2\Big(S^{-1}\frac{\overleftrightarrow{\partial}}{\partial u}S\Big)\,, \quad \mathrm{Im}\,\mathrm{Tr}_3\sum_{i<j}\,(G_{ij} - G_0) = -\frac{1}{4i}\,\mathrm{Tr}_3\Big(\sum_{i<j} S_{ij}^{-1}\frac{\overleftrightarrow{\partial}}{\partial u}S_{ij}\Big)\,, \tag{A11}$$

where

$$S^{-1}\frac{\overleftrightarrow{\partial}}{\partial u}S = S^{-1}\frac{\partial S}{\partial u} - \frac{\partial S^{-1}}{\partial u}S\,, \quad S_{ij}^{-1}\frac{\overleftrightarrow{\partial}}{\partial u}S_{ij} = S_{ij}^{-1}\frac{\partial S}{\partial u} - \frac{\partial S_{ij}^{-1}}{\partial u}S_{ij}\,. \tag{A12}$$

Hence,

$$\Omega 2!\, b_2 = \frac{1}{4\pi i}\int_0^\infty du\, e^{-\beta u}\,\mathrm{Tr}_2\Big(S^{-1}(u)\frac{\overleftrightarrow{\partial}}{\partial u}S(u)\Big)\,, \tag{A13}$$

$$\Omega 3!\, b_3 = \frac{1}{4\pi i}\int_0^\infty du\, e^{-\beta u}\,\mathrm{Tr}_3\Big(S^{-1}(u)\frac{\overleftrightarrow{\partial}}{\partial u}S(u) - \sum_{i<j} S_{ij}^{-1}(u)\frac{\overleftrightarrow{\partial}}{\partial u}S_{ij}(u)\Big)\,. \tag{A14}$$

Above, S_{ij} corresponds to the scattering of particles i and j, while the third particle moves freely.

In Eq. (A13) only connected terms appear. In Eq. (A14) both connected and disconnected terms occur; however, Eq. (A14) involves the difference of two quantities, the second of which consists entirely of disconnected terms which cancel all disconnected terms in the first quantity. This means that only connected T-matrix elements contribute to b_3. This rule can be generalized to more complicated cases when more than three particles are considered. Therefore, the Nth cluster coefficient becomes

$$\Omega N!\, b_N = \frac{1}{4\pi i}\int_0^\infty du\, e^{-\beta u}\Big(\mathrm{Tr}_N S^{-1}(u)\frac{\overleftrightarrow{\partial}}{\partial u}S(u)\Big)_c\,, \tag{A15}$$

where the subscript c denotes connected part. For the case when there are bound states, this expression is to be replaced by[2]

$$\Omega N!\, b_N = \sum_\alpha\,(\Omega N!\, b_{N\alpha})e^{-\beta B_{N\alpha}}\lambda_N^{-3}\,,$$

where

$$b_{N\alpha} = \int_0^\infty du\, e^{-\beta u}\Big(\mathrm{Tr}_{N\alpha}S^{-1}\frac{\overleftrightarrow{\partial}}{\partial u}S(u)\Big)_c \tag{A17}$$

and

$$\lambda_N^{-3} = \Big(\frac{Nm}{2\pi\beta\hbar^2}\Big)^{3/2}\,. \tag{A18}$$

The quantity $B_{N\alpha}$ in (A16) is the total binding energy in channel α. The trace $\mathrm{Tr}_{N\alpha}$ in Eq. (A17) is restricted to the channel $N\alpha$ in the center-of-mass frame.

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