Ground State Energy of Bose Particle System

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The ground state energy of the Bose particle system at low densities is investigated by using the method which is based on summing up the terms of the conventional perturbation series giving rise to the lowest order with respect to the density. The summation is shown to be greatly simplified if the scattering matrix is introduced, and a simple example is demonstrated for the repulsive square well potential by calculating a few terms of the series first directly and secondly with the aid of scattering matrix. The final result is shown to be valid both for weak and strong interactions and the calculation is carried out analytically for some types of potential function. The connection of the present method with the pseudopotential method and with the Brueckner theory is investigated and some problems associated with the attractive interactions are discussed.

§ 1. Introduction

In some problems of quantum mechanics or statistical mechanics a method is employed which is based on the summation of the important diagrams in the perturbation series\(^1\). In this paper we wish to investigate the ground state energy \(\varepsilon_0\) per particle of the Bose system along this line.

The quantity \(\varepsilon_0\) naturally depends on the density \(\rho\) of the system, on parameters characteristic of interatomic potential, etc. Now, let us imagine to plot \(\varepsilon_0\) versus \(\rho\) curve and seek the behaviours of the curve near at \(\rho = 0\). At \(\rho = 0\) the system is essentially assembly of free particles and it follows \(\varepsilon_0(\rho = 0) = 0\). Therefore it is sufficient to calculate \((\partial \varepsilon_0 / \partial \rho)_{\rho = 0}\) for our purpose. In other words, our problem is the idealized one to calculate the term linear in \(\rho\) when \(\varepsilon_0\) is expanded in terms of \(\rho\).

In § 2 the formal perturbation series in powers of the interatomic potential is discussed and the diagrams giving rise to the lowest order term of the ground state energy are identified to be those corresponding to the virtual processes in which the pair creations and annihilations take place successively. In § 3 the summation of the diagrams is carried out with the aid of the free-particle scattering matrix. A simple example of this procedure is demonstrated for the repulsive square well potential; first, a few terms of the series are calculated by direct integrations in § 2 and secondly by the use of scattering matrix in § 3. Both methods yield the same result for the terms of the series up to the order investigated in this paper. The lowest order term of the energy is calculated analytically for some types of the interatomic potential, and the problem associated with the presence of the bound states is discussed. In § 4 the perturbation series in terms of the
interatomic potential is transformed into the one in terms of the scattering matrix and it is shown that the diagrams summed up in § 2 do not appear in the new series and that an application to the hard-sphere potential leads to an expression obtained by pseudo-potential method. The alteration of the energy denominator proposed by Brueckner and Sawada\(^4\) is interpreted in an elementary way from the viewpoint of the present paper. It is suggested that an appropriate variational procedure is necessary to deal with the Bose system with attractive but saturating interactions.

§ 2. Perturbation series for the Bose system

Let us discuss in this section the behaviour of the formal perturbation series in powers of the interatomic potential for the Bose system. We assume that the unperturbed Hamiltonian is

\[ \mathcal{H}_0 = \hbar^2 / 2m \cdot \sum_a k_a^2 a_a^* a_a \]  

and the perturbing Hamiltonian is

\[ \mathcal{H}' = \hbar^2 / 2m \cdot V \cdot \sum_{\alpha \beta} v(\alpha \beta, \gamma \gamma') a_{\alpha}^* a_{\beta} a_{\gamma} a_{\gamma'} . \]  

The operators \(a^*\) and \(a\) are the usual creation and annihilation operators for the Bose particles. The matrix elements \(v(\alpha \beta, \gamma \gamma')\) are taken in the momentum representation, i.e.,

\[ v(\alpha \beta, \gamma \gamma') = \frac{1}{V} \int \exp (-ik_{\alpha} \cdot x - ik_{\beta} \cdot x) v(1,2) \exp (ik_{\gamma} \cdot x + ik_{\gamma'} \cdot x) dx_1 dx_2 \]

\[ = \delta (k_{\alpha} + k_{\beta} - k_{\gamma} - k_{\gamma'}) v(k_{\gamma}, k_{\gamma'}) \]  

where \(V\) is the normalization volume, \(\hbar^2 / 2m \cdot v(1,2)\) the two-body potential, \(k_{\alpha} = (k_{\alpha} - k_{\beta}) / 2, k_{\gamma} = (k_{\gamma} - k_{\gamma'}) / 2\), and \(v(q, q')\) is defined by

\[ v(q, q') = \int \exp (-i q \cdot x) v(x) \exp (i q' \cdot x) dx. \]

In the following we shall consider the non-singular two-body potentials so that the perturbation method can be applied. To deal with the case of a singular potential such as a hard-sphere one, it is still convenient to work directly with the matrix elements \(v(\alpha \beta, \gamma \gamma')\) by adopting some appropriate cutoff procedure. We shall prove later on that the final result is independent of the choice of such procedures.

Now, each term of the perturbation series can be written as an integral over various vectors \(q_i\), which are virtual momentum transfers. The successive terms of the series are:

\[ E_1 = \langle 0 | \mathcal{H}' | 0 \rangle = \hbar^2 / 2m \cdot N(N-1) / 2V \cdot v(00, 00) \]

\[ = \hbar^2 / 2m \cdot N(N-1) / 2V \cdot v(00, 00) \]  

where \(N\) is the total number of particles. The second-order energy is
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\[ E_2 = \langle 0 | \mathcal{H}' - \frac{1}{2} \mathcal{H} | 0 \rangle = \frac{\hbar^2}{2m} \frac{N(N-1)}{(2V)^2} \sum_{\mathbf{q} \neq \mathbf{0}} \nu(00,-\mathbf{q} \mathbf{q}) + \nu(00,\mathbf{q} - \mathbf{q}) \nu(\mathbf{q} - \mathbf{q},00) \]

\[ = \frac{\hbar^2}{2m} \frac{N(N-1)}{(2V)^2} \sum_{\mathbf{q} \neq \mathbf{0}} \nu(00,\mathbf{q}) \nu(\mathbf{q},00) \]

where use is made of eq. (3). In order to proceed to the higher order terms, it is convenient to introduce a graphical representation of the virtual processes as was used by Brueckner and Sawada. In Fig. 1, we give the diagram which represents a process giving rise to \( E_2 \).

Then, the diagrams corresponding to the processes that lead to the term linear in \( p \) are easily identified. Consider, for example, the diagram shown in Fig. 2. The process corresponding to this is characterized by the annihilation or creation of the unexcited particles in the intermediate states and therefore the energy term contains a factor \( \langle 0 | a_0^* a_0^* a_0^* a_0^* a_0^* a_0^* a_0^* a_0^* | 0 \rangle \sim N^4 \) in this case. Now the energy should be proportional to \( N \) and this suggests that the term under consideration has the form \( N \nu^2 \) and is of the higher orders with respect to \( \nu \) (the factor \( V^{-3} \) comes from \( \mathcal{H} ' \) and the sum over intermediate momentum states). We see from this argument that the lowest order term in \( \nu \) is such that the annihilation or creation of the unexcited particles must not occur except for the initial or final state. Then the diagrams having this character are easily written down. Since the annihilation of the unexcited particles does not occur in the intermediate states, in each stage of the virtual processes the pair with momenta \( \mathbf{q} \) and \( -\mathbf{q} \) should be destroyed and excited to the states \( (\mathbf{q}',-\mathbf{q}') \), etc., and finally returns to the ground state. Thus the diagrams interesting to us will be of the type shown in Fig. 3. Then the energy term in the \( n \)-th order corresponding to this process is easily shown to be

\[ \frac{\hbar^2 N(N-1)}{2m(2V)^n} \sum_{\mathbf{q}_{n-1}} \{ \nu(00,\mathbf{q}_{n-1} - \mathbf{q}_{n-1}) + \nu(00,-\mathbf{q}_{n-1} \mathbf{q}_{n-1}) \} \cdots \{ \nu(\mathbf{q}_2 - \mathbf{q}_2,\mathbf{q}_1 - \mathbf{q}_1) + \nu(\mathbf{q}_2 - \mathbf{q}_2, -\mathbf{q}_2 \mathbf{q}_1) \} v(\mathbf{q}_2 - \mathbf{q}_2, -\mathbf{q}_2 \mathbf{q}_1) v(\mathbf{q}_1 - \mathbf{q}_1,00) \]
where $\sum'$ means that $q_1 \neq 0$, $q_2 \neq 0$, ..., $q_{n-1} \neq 0$. Therefore, if we define $E_0$ to be the lowest order term of the energy, we have

$$E_0 = \frac{b^2 N (N - 1)}{4mV} \left\{ \nu(0, 0) - \frac{1}{(2V)} \sum \frac{\nu(0, q_i) \nu(q_i, 0)}{q_i^2} \right\} \left\{ \frac{1}{(2V)^2} \sum \frac{\nu(0, q_i) \nu(q_i, q_j) \nu(q_i, 0)}{q_i^2 q_j^2} \right\} \left\{ \frac{1}{(2V)^{n-1}} \sum \frac{\nu(0, q_{n-1}) \nu(q_{n-1}, q_{n-2}) \cdots \nu(q_2, q_1) \nu(q_1, 0)}{(-q_{n-1}^2) (-q_{n-2}^2) \cdots (-q_1^2)} \right\} + \ldots.$$  

(8)

Here we have carried out the change of variables $q_i \to q_i$, $q_j \to q_j$, etc., in eq. (7) and used eq. (3).

Before discussing the summation of (8), we wish to calculate by direct integrations a few terms of the series for the repulsive square well potential as an example.

For the potential

$$v(x) = v_0 \ (v_0 > 0), \ r < a, \quad (r = |x|),$$

$$= 0, \quad r > a,$$

(9)

$v(q, q')$ is given by

$$v(q, q') = 4\pi r_0 a^2 j_1(ka)/k$$  

(10)

where $j_1(x)$ is the spherical Bessel function of order 1 and $k = |q - q'|$. Then we have

$$\nu(0, 0) = 4\pi r_0 a^3/3,$$

$$\frac{1}{(2V)} \sum \frac{\nu(0, q_i) \nu(q_i, 0)}{q_i^2} = 4\pi r_0 a^3 \int_0^\infty j_1(qa) dq = \frac{4\pi r_0 a^3}{15}$$

and

$$\frac{1}{(2V)^2} \sum \frac{\nu(0, q_i) \nu(q_i, q_j) \nu(q_i, 0)}{q_i^2 q_j^2} = \frac{2\pi}{\pi} \int_0^\infty \frac{j_1(qa)}{q_i^2} dq_i \int_0^\infty \frac{j_1(q'a)}{q_j^2} dq_j \frac{j_1(qa) \sin a(q_1 - q_2)}{q_i^2 (q_1 - q_2)} dq_i$$

$$= 4\pi r_0 a^3 \cdot 17/1260.$$  

Here we have used the Weber-Schafheitlin integral for the Bessel function. Using above equations, we have from eq. (8)

$$E_0 = \frac{2\pi b^2 r_0}{N} \left\{ \frac{v_0 a^2}{6} - \frac{v_0 a^2}{30} + \frac{17}{2520} v_0 a^2 \cdots \right\}$$  

(11)

up to the order of $v_0 a^2$. The further calculation is cumbersome and it is difficult to find the general term of the series. A convenient method to calculate the series will be given in the next section.
§ 3. Summation of the series

In order to sum up the series (8), it is convenient to replace the problem of summation by an equivalent and a simpler one. For this purpose we wish to proceed to the more general case where the unperturbed state is represented by the occupation numbers \( n_k \)'s, not necessarily corresponding to the ground state. Then it is easily verified that the energy term arising from the diagrams discussed in § 2 is given by

\[
E_0(n_k) = \frac{\hbar^2}{2m} \frac{1}{2V} \sum_{\alpha_1 \gamma_1} u(\alpha_\beta, \gamma) \langle n_k | a_\alpha^* a_\gamma | n_k \rangle
\]

where

\[
u(\alpha_\beta, \gamma) = v(\alpha_\beta, \gamma) + \frac{1}{V} \sum \frac{v(\alpha_\beta, \alpha_{\beta_1}, \gamma) v(\alpha_{\beta_1}, \gamma)}{k^2 + k_\gamma^2 - k_{\alpha_1}^2 - k_{\gamma_1}^2} + \frac{1}{V^2} \sum \frac{v(\alpha_\beta, \alpha_{\beta_2}, \alpha_{\beta_3}, \gamma) v(\alpha_{\beta_3}, \gamma)}{(k_\alpha^2 + k_\gamma^2 - k_{\alpha_1}^2 - k_{\alpha_3}^2) (k_\beta^2 + k_\gamma^2 - k_{\beta_1}^2 - k_{\beta_3}^2) + \ldots}.
\]

In eq. (13) \( \sum' \) means that the values of \( k_{\alpha_1}, k_{\beta_1}, \) etc., which make the energy denominator vanish, are excluded from the summation. One may verify that eq. (13) reduces to eq. (8) in the case of ground state, i.e. \( n_0 = N \) and \( n_k = 0 \) \( (k \neq 0) \).

Now, we note that the matrix elements \( u(\alpha_\beta, \gamma) \) satisfy the equation

\[
v(\alpha_\beta, \gamma) + \frac{1}{V} \sum \frac{u(\alpha_\beta, \sigma_\gamma)}{k^2 + k_\gamma^2 - k_{\alpha_1}^2 - k_{\gamma_1}^2} = u(\alpha_\beta, \gamma),
\]

which can be proved from the defining equation for \( u(\alpha_\beta, \gamma) \), eq. (13). This equation implies that \( u(\alpha_\beta, \gamma) \) is just the matrix element of the free-particle scattering operator. In order to transform this equation in the coordinate representation, we consider the wave function \( \Psi_{\alpha\gamma}(1, 2) \) defined by

\[
\Psi_{\alpha\gamma}(1, 2) = \exp(ik_{\alpha_1} \cdot x_1 + ik_{\gamma_1} \cdot x_2) + \frac{1}{V} \sum \frac{\exp(ik_{\alpha_1} \cdot x_1 + ik_{\gamma_1} \cdot x_2)}{k^2 + k_\gamma^2 - k_{\alpha_1}^2 - k_{\gamma_1}^2}
\times \int \exp(-ik_{\alpha} \cdot x_1' - ik_{\gamma} \cdot x_2') v(1', 2') \Psi_{\alpha\gamma}(1', 2') dx_1' dx_2'.
\]

If we multiply this equation by \( \exp(-ik_{\alpha} \cdot x_1 - ik_{\gamma} \cdot x_2) v(1, 2) \) and integrate by \( x_1 \) and \( x_2 \) in the volume \( V \), we see that the resulting equation is just identical with eq. (14) provided that \( u(\alpha_\beta, \gamma) \) is given by

\[
u(\alpha_\beta, \gamma) = \frac{1}{V} \int \exp(-ik_{\alpha} \cdot x_1 - ik_{\gamma} \cdot x_2) v(1, 2) \Psi_{\alpha\gamma}(1, 2) dx_1 dx_2.
\]

Or, if we put

\[
\Psi_{\alpha\gamma}(1, 2) = \exp[i(k_{\alpha} + k_{\gamma}) \cdot X] \varphi_{\alpha\gamma}(x)
\]

where \( X \) is the center-of-mass coordinate \( \left[ = (x_1 + x_2)/2 \right] \) and \( x \) the relative coordinate.
\(\frac{d}{d\mathbf{x}}(\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_0 - \mathbf{k}_2) = \int \exp(-i\mathbf{k}_{a\mathbf{r}} \cdot \mathbf{x}) v(\mathbf{x}) \varphi_{\mathbf{k}_2}(\mathbf{x}) d\mathbf{x} \tag{17}\)

and

\[
\varphi_{\mathbf{k}_2}(\mathbf{x}) = \exp(i\mathbf{k}_{\mathbf{k}_2} \cdot \mathbf{x}) + \frac{1}{2V} \sum_{\mathbf{k}_{\mathbf{r}}} \frac{\exp(i\mathbf{k}_{a\mathbf{r}} \cdot \mathbf{x})}{k_{\mathbf{k}_2}^2 - k_{\mathbf{r}}^2} \int \exp(-i\mathbf{k}_{\mathbf{k}_2} \cdot \mathbf{x}') v(\mathbf{x'}) \varphi_{\mathbf{r}}(\mathbf{x}') d\mathbf{x}'. \tag{18}\]

If we operate \(\rho^2\) on eq. (18), we have

\[
\left[ -\rho^2 + \frac{v(\mathbf{x})}{2} \right] \varphi(\mathbf{x}) = k_{\mathbf{k}_2}^2 \varphi(\mathbf{x}) + \frac{1}{2V} \sum_{\mathbf{k}_{\mathbf{r}}} \int \exp[i\mathbf{q} \cdot (\mathbf{x}' - \mathbf{x})] v(\mathbf{x'}) \varphi(\mathbf{x'}) d\mathbf{x}'. \tag{19}\]

This is the Schrödinger equation for the scattering problem except for the second term on the right-hand side. The appearance of this term is due to the finite volume of the system and consistent with the periodic boundary condition imposed on \(\varphi(\mathbf{x})\). This will be seen in the following way; if we multiply eq. (19) by \(\exp(-i\mathbf{q}_0 \cdot \mathbf{x})\) with \(\mathbf{q}_0\) satisfying the periodic condition, we have

\[
(\mathbf{q}_0^2 - k_{\mathbf{k}_2}^2) \int \exp(-i\mathbf{q}_0 \cdot \mathbf{x}) \varphi(\mathbf{x}) d\mathbf{x} = 1/2 \cdot [\delta(\mathbf{k}_{\mathbf{k}_2}, \mathbf{q}_0) - 1] \int \exp(-i\mathbf{q}_0 \cdot \mathbf{x}) v(\mathbf{x}) \varphi(\mathbf{x}) d\mathbf{x}. \]

From this equation it follows that the appearance of the second term is consistent with the boundary condition, since, if this term is missing in eq. (19), then it follows \(\int \exp(-i\mathbf{q}_0 \cdot \mathbf{x}) v(\mathbf{x}) \varphi(\mathbf{x}) d\mathbf{x} = 0\), for \(\mathbf{q}_0 = k_{\mathbf{k}_2}\), which is not always valid for an arbitrary value of \(k_{\mathbf{k}_2}\) satisfying the periodic condition. In the limit \(V \to \infty\), however, this term may be neglected and eq. (19) reduces to the usual scattering equation.

Returning now to the summation of (8), we see that \(E_0\) is given by

\[
E_0/N = b^5/4m \cdot u(00,00). \tag{20}\]

In calculating \(u(00,00)\) it is sufficient to consider only the spherically symmetric solution of eq. (19). Also the solution should approach 1 for \(r = ||\mathbf{x}|| \to \infty\), for \(\varphi(\mathbf{x}) \to \exp(i\mathbf{k}_{\mathbf{k}_2} \cdot \mathbf{x})\) at large \(r\) and \(k_{\mathbf{k}_2} = 0\) in this case. Furthermore, the second term on the right-hand side of eq. (19) may be neglected as we have mentioned above.

From these considerations it follows that

\[
u (00,00) = 4\pi \int_0^\infty v(r) R(r) r^2 dr \tag{21}\]

where \(R(r)\) satisfies the equations

\[
[1/r^2 \cdot d/dr(r^2d/dr) - v(r)/2] R(r) = 0 \tag{22a}\]

and

\[R(r) \to 1, \quad (r \to \infty) \tag{22b}\]
Furthermore, $R(r)$ should be regular at $r=0$.

From eqs. (20), (21) and (22a) we have

$$E_0/N = 2\pi b^2 \rho /m \cdot (r^2dR/dr)_{r=\infty}. \tag{23}$$

We see that eqs. (22a), (22b) and (23) are applicable to the strong interactions and identical with those obtained in the previous paper. For the repulsive square well potential considered in § 2, the solution of eq. (22a) is

$$R=1+A/r, \ (r>a) \quad \text{and} \quad R=B \sqrt[3]{V_0/2} \cdot r/r, \ (r<a).$$

From the condition that $R(r)$ and $R'(r)$ should be continuous at $r=a$, we have

$$A=\sqrt[3][2]{V_0} \quad \text{th} \ a \sqrt[3][2]{V_0}/2 \quad -a.$$ \(\text{th} \ x = x - 1/3 \cdot x^3 + 2/15 \cdot x^5 - 17/315 \cdot x^7 + \ldots \)

Therefore from eq. (23), we have

$$E_0/N = 2\pi b^2 \rho /m \cdot \left[a - \sqrt[3][2]{V_0} \quad \text{th} \ a \sqrt[3][2]{V_0}/2 \right]. \tag{24}$$

If we expand $\text{th} \ x$ as

$$\text{th} \ x = x - 1/3 \cdot x^3 + 2/15 \cdot x^5 - 17/315 \cdot x^7 + \ldots$$

the result is easily shown to be identical with eq. (11) obtained by direct integrations.

It should be noted here that eq. (24) remains finite as $V_0 \to \infty$. On the other hand, if $\text{th} \ x$ is expanded in powers of $x$, each term of the series is divergent in this limit. This feature of the case of strong interaction implies that an appropriate procedure of summing up all the divergent terms of the conventional perturbation series is necessary to obtain a finite result. For the potential under consideration, the limiting case is just the hard-sphere one, and eq. (24) is naturally reduced to the formula obtained by Lenz.

We wish further to remark that the discussions developed in this paper are also applicable to the weak interactions for which $\nu(q, q')$ is finite. In this case, each term of the perturbation series may be finite. However, the result is meaningless if the series is terminated in the finite order terms as far as the density dependence of the energy is concerned. Therefore it follows that the summation of diagrams is necessary even for weak interactions if one wishes to investigate a correct functional relation of the energy with the density.

In conclusion we wish to calculate $E_0/N$ for some types of potential function.

(a) Attractive square well potential with the hard-core repulsion

In this case $\nu(x)$ is given by

$$\begin{cases} 
\nu(x) = \infty, & r < a, \\
\nu(x) = -v_0, & (v_0 > 0), \quad a < r < a + d, \\
\nu(x) = 0, & a + d < r.
\end{cases}$$

It is easy to see that

$$E_0/N = \frac{2\pi b^2 \rho}{m} \left[a + d - \sqrt[3][2]{V_0} \tan \sqrt[3][2]{V_0}/2 \cdot d \right]. \tag{25}$$
(b) Sutherland potential

Two-body potential \( V(r) \) is defined by

\[
V(r) = \begin{cases} 
\infty, & r < a, \\
-V_0 \left( \frac{a}{r} \right)^n, & r > a.
\end{cases}
\]

For this potential the solution of (22a) is given by the Bessel function for \( r > a \), and the boundary conditions at \( r = \infty \), eq. (22b), and at \( r = a \), \( R(a) = 0 \), uniquely determine the solution. Then we have

\[
\frac{E_0}{N} = \frac{2\pi \hbar^2}{m} \frac{\Gamma^{(n-3)/(n-2)}}{\Gamma^{(n-1)/(n-2)}} \left( \frac{k}{n-2} \right)^{2(n-2)} \frac{\int_{1/(n-2)}^{(2n-2)/n} \left( \frac{2ka^{(2n-2)/n}}{(n-2)} \right)}{\int_{1/(n-2)}^{(2n-2)/n} \left( \frac{2ka^{(2n-2)/n}}{(n-2)} \right)}.
\]

with \( k^2 = mV_0 \sigma^2 / \hbar^2 \).

In particular, for the van der Waals attraction, \( n = 6 \), eq. (26) reduces to

\[
\frac{E_0}{N} = \frac{2\pi \hbar^2}{m} \frac{\Gamma^{(3/4)}}{\Gamma^{(5/4)}} \frac{1}{2} \left( \frac{mV_0}{\hbar^2} \right)^{1/4} a^{3/4} \frac{\int_{1/4}^{1/4} \left( \frac{mV_0}{\hbar^2} \right)^{1/4} a/2b}{\int_{1/4}^{1/4} \left( \frac{mV_0}{\hbar^2} \right)^{1/4} a/2b}.
\]

In the limit \( V_0 \to 0 \), eq. (26a) reduces to Lenz's formula\(^9\) for the hard-sphere potential.

(c) Lennard-Jones (6-10) potential

This potential was discussed in the previous paper\(^7\), so that we only give the result:

\[
\frac{E_0}{N} = \frac{4\pi}{\Gamma(1/4)} \frac{2^{3/4} \Gamma^{(3/4)}}{\Gamma^{(5/4)}} \frac{1}{\Gamma^{(5/8)}} \frac{m^{-7/8} V_0^{1/8} \sigma^{3/4} \hbar^{7/4}}{\rho}.
\]

It should be noted here that the \( E_0/N \) becomes \(-\infty\) if the bound state with zero energy appears in the two-body system. For example, if \( \sqrt{(\sigma/2)d} \) is equal to \( \pi/2 \) in eq. (25), \( E_0/N = -\infty \). The above condition for \( \nu_0 \) and \( d \) just corresponds to the appearance of the bound state with zero energy. In this case \( E_0/N \) versus \( \rho \) curve coincides with the negative \( E_0/N \) axis near \( \rho = 0 \). The similar situation exists for the potential functions (b) and (c). In the case of (b), (we take \( n = 6 \) for simplicity), as \( V_0 \) increases from 0, \( E_0/N \) decreases from the positive value until it becomes \(-\infty\) when \( (mV_0)^{1/2} a/2b = \xi \), where \( \xi \) is the least positive root of \( J_1(\xi) = 0 \). Similarly, for the potential (c), \( E_0/N \) becomes \(-\infty\) at \( \gamma = 5/8 \). It seems, therefore, that the behaviour of the energy versus density curve is markedly dependent on the presence of the bound state in the two-body problem.

§ 4. Perturbation method in terms of scattering matrix

In the previous sections we have discussed the summation of the diagrams giving rise to the lowest order term of the energy. If one compares eq. (5) with eq. (20), one may easily see that \( E_0 \) is just the first order energy with \( u(\alpha \beta, \lambda \gamma) \) replaced by \( u(\alpha^2 \beta, \lambda^2 \gamma) \). This suggests that the potential function is effectively replaced by the scattering matrix. In this section we wish to discuss the pertubational treatment of the
scattering matrix.

Let us first consider the meaning of eq. (14). Originally this equation was introduced for the purpose of summing up the series (8) and u-matrix is explicitly expanded in terms of \( \nu(q', q) \) as in eq. (13). However, we may regard eq. (14) conversely as the defining equation for \( \nu(q', q) \) in terms of u-matrix. Then we have, writing \( u(\alpha, \beta, \gamma) = u(q', q) \) with \( k_{x, q} = q' \) and \( k_{x, q} = q \) [see eq. (17)],

\[
\nu(q', q) = u(q', q) + \frac{1}{2V} \sum_{q''} \frac{u(q', q'') u(q'', q)}{q''^2 - q^2} + \frac{1}{(2V)^2} \sum_{q'''} \frac{u(q', q''') u(q''', q''') u(q''', q) - \cdots}{(q''^2 - q^2) (q''''^2 - q''^2)}. \tag{28}
\]

If one substitutes this equation in the perturbation series in powers of \( \nu \)-matrix, the series will be transformed in the one in powers of scattering matrix. For example, if one retains only the first term in eq. (28), the first order energy will be given by eq. (20). As is well known, the scattering matrix does exist even for the strong interaction and therefore it may be expected that the series in terms of u-matrix is valid for such a case. Furthermore, the following feature of the series may be expected: since the diagrams, in which the creation or annihilation of the unexcited particles does not occur except for the initial or final state, are included already in the u-matrix, such diagrams will not appear in the u-matrix series. In other words, only the diagrams corresponding to the process of the creation or annihilation of the unexcited particles in the intermediate states will appear in the new series. That this is the case will be verified up to the third order in the following.

The first and the second order energy were given by eqs. (5) and (6) and the third order one is easily shown to be

\[
E_3 = \frac{h^2}{2m} \frac{N(N-1)}{2V} \left[ \sum_{q} \nu(0, q') \nu(q', q) \nu(q, 0) + \sum_{q} \nu(0, q) \nu(q, 0) \right] \times [2(N-2) \nu(q/2, q/2) + \nu(-q/2, q/2)] - (2N-3) \nu(0, 0) \]. \tag{29}

If we substitute eq. (28) in this expression and in eqs. (5) and (6) and express the perturbation series in terms u-matrix, we have

\[
E = \frac{h^2}{2m} \frac{N(N-1)}{2V} \left[ u(0, 0) + \frac{1}{(2V)^2} \sum_{q} \nu(0, q) u(q, 0) \right] \times [2(N-2) u(q/2, q/2) + u(-q/2, q/2)] - (2N-3) u(0, 0) \] \tag{30}

up to the third order. It should be noted here that the diagrams corresponding to Fig. 3 no longer appear in eq. (30), as we have expected. The similar feature of the new series may be true for any higher order terms.

If we consider the hard-sphere system and set \( u(0, 0) \) to be \( 8 \pi a \), neglecting the dependence of u-matrix on \( q \), we have from eq. (30)
\[ E = \frac{2\pi a^2 \rho}{m} \left[ 1 + \frac{a^2}{\pi^2 L^2} (2N - 5) \sum_{l=1}^{N'} \frac{1}{(l^2 + m^2 + n^2)^2} \right] \]

\((V = L^3)\), which is consistent with the result obtained by Huang and Yang\(^{10}\) with the aid of pseudopotential method. Therefore we are able to conclude that the pseudopotential method is equivalent to the perturbation theoretical treatment of the free-particle scattering matrix. However, as was pointed out by Brueckner and Sawada\(^{4}\), the perturbation method is not appropriate in this case, for the energy term corresponding to the diagram shown in Fig. 4 is divergent. To avoid this difficulty they have summed up the diagrams of this type up to infinite order. This process seems to be quite reasonable if the \(\nu\)-matrix formalism is employed, since the diagrams appearing in the new series must at least once create or annihilate the unexcited particles in the intermediate states. Indeed, as we have shown previously\(^{10}\), this formalism leads to the exact formula obtained by Lee, Huang and Yang\(^{11}\) which is appropriate for the low density limits. Therefore one may conclude that the free-particle scattering matrix formalism is exact as long as the density of the system is sufficiently low.

At higher densities, however, the free-particle scattering theory will become poor, since, in this case, the many-body effects of the unexcited particles on the virtual pair will not be neglected. In order to deal with these effects, Brueckner and Sawada\(^{4}\) have altered the energy denominator so that the Green function describes the propagation in the presence of the unexcited particles. This propagator alteration may be interpreted in the following way. Also this procedure will provide a clue to solving the difficulties associated with the attractive interactions.

As we have done in § 2, we start from the weak interaction, i.e., we consider the Hamiltonian

\[ \mathcal{H} = \frac{\hbar^2}{2m} \sum_{\alpha} k_\alpha^2 a_\alpha^* a_\alpha + \frac{\hbar^2}{2m} \sum_{\alpha \neq \beta} \psi(\alpha \beta, \alpha \gamma) a_\alpha^* a_\beta^* a_\gamma a_\alpha, \]  

where \(\psi(\alpha \beta, \alpha \gamma)\) is assumed to have a definite value. In § 2, the first term (kinetic energy) was considered as the unperturbed Hamiltonian and the second term as the perturbing one, and the multiple interaction of a pair of particles excited from the ground state was treated. Then we were led to the concept of free-particle scattering matrix. Hence, it will be necessary to choose another way of separation of the Hamiltonian into the unperturbed and the perturbing one, if one wishes to take into account the effects of the unexcited particles on the propagator. The simplest way of this separation will be such that the parts of the interaction Hamiltonian which are diagonal in the number representation are included in the unperturbed system. That is to say, the unperturbed Hamiltonian is considered to be

\[ \mathcal{H}_0 = \frac{\hbar^2}{2m} \sum_{\alpha} k_\alpha^2 a_\alpha^* a_\alpha + \frac{1}{2\mathcal{V}} \sum_{\alpha \neq \beta} \left\{ \psi(\alpha \beta, \alpha \beta) + \psi(\alpha \beta, \beta \alpha) \right\} a_\alpha^* a_\beta^* a_\alpha a_\beta \]
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\[ + \frac{1}{2V} \sum_{a} v(\alpha \alpha, \alpha \beta) a_{a}^{*} a_{a}^{*} a_{\beta} a_{\beta} \]  

(32)

and the remaining part is assumed to be the perturbing one.

Now consider the unperturbed wave vector \( |n_{0}, n_{1}, \ldots, n_{b}, \ldots> \). The unperturbed energy corresponding to this is

\[ E_{0}(n_{0}) = \frac{\hbar^{2}}{2m} \left[ \sum_{a} k_{a}^{2} n_{a} + \frac{1}{2V} \sum_{\alpha \neq \beta} \{ v(\alpha \beta, \alpha \beta) + v(\alpha \beta, \beta \alpha) \} n_{\alpha} n_{\beta} + \frac{1}{2V} \sum_{a} v(\alpha \alpha, \alpha \alpha) n_{a} (n_{a} - 1) \right] \]  

(33)

Therefore if one repeats the procedure discussed in § 2 and § 3, the energy denominator in eq. (13) will be altered in the following way:

\[ \frac{\hbar^{2}}{2m} \cdot (k_{0}^{2} + k_{1}^{2} - k_{0}^{2} - k_{0}^{2}) \rightarrow E_{0}(n_{0}, n_{1}, \ldots) - E_{0}(n_{0}, \ldots n_{a} + 1, n_{a} + 1, n_{a} - 1, n_{a} - 1) \]

\[ = \frac{\hbar^{2}}{2m} \{ \varepsilon(\lambda) + \varepsilon(\gamma) - \varepsilon(\alpha) - \varepsilon(\beta) \} \]  

(34)

where

\[ \varepsilon(\lambda) = k_{\lambda}^{2} + \frac{1}{V} \sum_{\mu} \{ v(\lambda \mu', \lambda \mu') + v(\lambda' \mu, \lambda' \mu') \} n_{\lambda}, - \frac{1}{V} v(\lambda \lambda, \lambda \lambda) n_{\lambda}. \]  

(35)

As we have remarked in the previous sections, the matrix elements \( v(\alpha \beta, \gamma \gamma) \) can be replaced by \( u(\alpha \beta, \gamma \gamma) \) in the case of strong interactions. Therefore, if we replace \( v 's \) in eq. (35) by \( u 's \), using eq. (14) we have

\[ v(\alpha \beta, \gamma \gamma) + \frac{1}{V} \sum_{\tau} v(\alpha \beta, \sigma \tau) \frac{u(\sigma \tau, \gamma \gamma)}{\varepsilon(\lambda) + \varepsilon(\gamma) - \varepsilon(\sigma) - \varepsilon(\tau)} = u(\alpha \beta, \gamma \gamma) \]  

(36)

as an equation to determine the \( u \)-matrix. Here \( \varepsilon(\lambda) \) corresponds to the energy of a particle interacting with the unexcited particles and is given by

\[ \varepsilon(\lambda) = k_{\lambda}^{2} + \frac{1}{V} \sum_{\mu} \{ u(\lambda \mu', \lambda \mu') + u(\lambda' \mu, \lambda' \mu') \} n_{\lambda}, - \frac{1}{V} u(\lambda \lambda, \lambda \lambda) n_{\lambda}. \]

For the ground state, i.e., for \( n_{0} = N \) and \( n_{k} = 0 \) (\( k \neq 0 \)), the energy denominator is given by

\[ G(\sigma, \tau) = \{ \varepsilon(0) - \varepsilon(\sigma) + \varepsilon(0) - \varepsilon(\tau) \}^{-1} \]

\[ = - \{ k_{0}^{2} + \rho[u(\sigma 0, \tau 0) + u(\sigma 0, 0 \tau) - u(0 0, 0 0)] \]

\[ + k_{\tau}^{2} + \rho[u(\tau 0, \tau 0) + u(\tau 0, 0 \tau) - u(0 0, 0 0)] \}^{-1}. \]  

(37)

It should be noted here that this Green function together with eq. (36) is just the fundamental equation for the ground state of the Bose system in Brueckner and Sawada’s theory [see eqs. (2) and (3) of reference 4), p. 1128].

We have shown above that the propagator alteration is carried out by a proper choice
of the separation of the total Hamiltonian. This viewpoint is also useful to see how the situation is in the case of attractive interactions. By the attractive interactions we mean that the \( u(00,00) \) is negative. In this case the sound velocity becomes imaginary if one formally applies the formula for the excitation energy spectrum\(^4\)

\[
b_{\omega_\eta} = \left( \frac{b^2}{2m} \right) \left\{ \frac{q^2}{\rho} + \rho \left[ u(0q,00) - u(00,00) \right] + \rho^2 u^2(00,q0) - u(00,00) \right\} \frac{1}{2}.
\]

For in the limit \( q \rightarrow 0 \), eq. (38) becomes

\[
b_{\omega_\eta} = \left( \frac{b^2}{2m} \right) q \left\{ 2 \rho \left[ u(00,00) \right] \right\} \frac{1}{2}.
\]

Thus, the excitation energy becomes imaginary if \( u(00,00) < 0 \). Such a feature is, of course, physically meaningless, hence it represents a breakdown in the approximation employed rather than a physical effect. In order to clarify this point, we first note that the assumption that nearly all the particles are in the single particle state with momentum 0 was used in deriving the excitation energy spectrum\(^4,12\). This assumption may be valid for the purely repulsive potentials but is entirely misleading for the attractive potentials under consideration. This may be seen as follows.

From eq. (37) it follows that the Green function \( G(\sigma, \tau) \) becomes positive for the small momentum transfer, since in the limit \( \sigma, \tau \rightarrow 0 \), \( G(\sigma, \tau) \) approaches \( -\{2\rho u(00,00)\}^{-1} \) which is positive. Now the energy denominator represents the energy difference between the ground and excited states, and the above argument indicates that the energy value for the state in which two particles are excited is smaller than that of the ground state in which \( n_k = N \) and \( n_k = 0 \) \( (k \neq 0) \), provided that the momenta of excited particles are small. Thus, the latter state is no longer stable and does not represent the true ground state. One of the way to find this will be the variational procedure in which the energy given by eq. (33) (with \( v \)'s replaced by \( u \)'s) becomes minimum with respect to the variation of the occupation numbers. After the occupation numbers are determined, the usual procedure may be applied to the determination of excitation energy. We do not enter into this problem here, but we wish only to remark that the variation procedure in the configurational space has already been employed by various workers\(^10\).

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