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Ground State Energy of a Many-Particle Boson System

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Abstract

A trial expression for the ground state energy of a system of many bosons interacting with strong forces is studied. Using an approximate expression for the pair-distribution function and applying the variational principle in an appropriate way, we obtain a non-linear integrodifferential equation for the correlation function $f(r)$. This equation is subsequently linearised and its behaviour for large separations is studied. It is also shown that for large separations an effective reduced mass of the pair can be defined. This is given by $\mu^* = 2\mu$, where $\mu = m/2$ is the reduced mass of the pair.

1. *Introduction*

The study of many-particle boson systems has been the subject of theoretical investigations by a considerable number of people during the past years (Aviles, 1958; Jastrow, 1955; Feynman, 1953; Feenberg & Wu, 1961; Jackson & Feenberg, 1961; Feenberg, 1969; Gross, 1966; Enderby *et al.*, 1965; Reatto & Chester, 1967).

As is well known, systems of this sort, like liquid He^4, have also aroused the interest of experimentalists, and their properties have been studied in detail.

The starting-point of the present investigation is the work of Aviles (1958), in which some very interesting remarks were made about determination of the correlation function and evaluation of the ground state energy of a system of many bosons interacting with strong forces. The work of Aviles was based on that of Jastrow, who used cluster expansion techniques, known from the theory of classical imperfect gases, in order to calculate the ground state energy of many-particle boson and fermion systems.

In the next section the notation used is specified and the expression of the expectation value of the Hamiltonian which is derived by means of a

Jastrow-type trial function for the many-particle boson system is given.

In Section 3 an approximate expression is given for the function $G(\mathbf{r}_{12})$ which is defined by Aviles (1958) and is closely related to the pair-distribution function of statistical mechanics.

The trial expression of the energy obtained with the approximate expression for $G(\mathbf{r}_{12})$ is varied (without use of any *ad hoc* integral constraint) in Section 4. The interesting result obtained is a new, non-linear, equation for the correlation function f.

In the final section we linearise the above integrodifferential equation and study its asymptotic behaviour.

2. *The Trial Expectation Value for the Hamiltonian*

We consider a system of bosons in its ground state. The number of particles is assumed to be very large and the volume in which the system is enclosed is also assumed to be large, such that the density is constant:

$$\rho = \frac{N}{\Omega} \tag{2.1}$$

The Jastrow-type trial many-body wave function is therefore

$$\Psi^{tr}(\mathbf{r}_1, \ldots, \mathbf{r}_N) = \prod_{i<j=1}^{N} f(\mathbf{r}_i - \mathbf{r}_j) \tag{2.2}$$

The correlation functions $f(\mathbf{r}_i - \mathbf{r}_j) \equiv f(\mathbf{r}_{ij})$ are taken to have the following properties:

First, they are symmetric:

$$f(\mathbf{r}_{ij}) = f(\mathbf{r}_{ji}) \tag{2.3}$$

so that Ψ^{tr} is symmetric, as must be the case for the exact wave function for a Bose system.

Secondly, they are zero for distances less than or equal to the hard core radius of the interparticle (short-range) potential V_{ij}

$$f(\mathbf{r}_{ij}) = 0 \qquad \text{for} \qquad r_{ij} \leqslant c \tag{2.4}$$

so that Ψ^{tr} vanishes whenever r_{ij} is less than or equal to the hard core radius of the potential. Note that if there is a soft core potential then $c \to 0$ and the f's should be suppressed for small r_{ij}.

Obviously, the functions f allow also for correlations due to strong forces outside the hard core.

Thirdly, the correlation functions tend to unity for large inter-particle distances:

$$\lim_{r_{ij} \to \infty} f(\mathbf{r}_{ij}) = 1 \tag{2.5}$$

so that Ψ^{tr} goes over to the uncorrelated function when the particles are very far away from each other, in accordance with the asymptotic separability of the exact wave function.

The expectation value of the Hamiltonian of the system with the trial many-body wave function (2.2) is:

$$\langle H\rangle^{\text{tr}} = \frac{\displaystyle\int \prod_{i<j=1}^{N} f(\mathbf{r}_{ij}) \left[-\frac{\hbar^2}{2m}\sum_{k=1}^{N}\nabla_k^2 + \sum_{l<n=1}^{N} V_{ln}\right] \prod_{i<j=1}^{N} f(\mathbf{r}_{ij})\, d\mathbf{r}_1 \ldots d\mathbf{r}_N}{\displaystyle\int \prod_{i<j=1}^{N} f^2(\mathbf{r}_{ij})\, d\mathbf{r}_1 \ldots d\mathbf{r}_N} \tag{2.6}$$

One can now proceed to evaluate separately the potential and kinetic energy contributions to it. This is done by noting that the integrals in equation (2.6) are equal.

We give here the final result, since the details have been given by Aviles (1958). One finds

$$\frac{\langle H\rangle^{\text{tr}}}{N} = \tfrac{1}{2}\rho \int \left[\frac{\hbar^2}{2m}((\nabla f(\mathbf{r}_{12}))^2 - f(\mathbf{r}_{12})\nabla^2 f(\mathbf{r}_{12})) + V_{12} f^2(\mathbf{r}_{12})\right] G(\mathbf{r}_{12})\, d\mathbf{r}_{12} \tag{2.7}$$

where the function $G(\mathbf{r}_{12})$ is defined by

$$G(\mathbf{r}_{12}) = \frac{N(N-1)}{\rho^2} \frac{\displaystyle\int \prod_{\substack{i<j=1\\(ij)\neq(12)}}^{N} f^2(\mathbf{r}_{ij})\, d\mathbf{r}_3 \ldots d\mathbf{r}_N}{\displaystyle\int \prod_{i<j=1}^{N} f^2(\mathbf{r}_{ij})\, d\mathbf{r}_1 \ldots d\mathbf{r}_N} \tag{2.8}$$

This function is closely related to the better known pair-distribution function of statistical mechanics. One has the relations

$$G(\mathbf{r}_{12}) = \frac{Z_2(\mathbf{r}_{12})}{f^2(\mathbf{r}_{12})}, \qquad Z_2(\mathbf{r}_{12}) = \frac{\eta_2(\mathbf{r}_{12})}{\rho^2} \tag{2.9}$$

where

$$\eta_2(\mathbf{r}_{12}) = N(N-1). \frac{\int |\Psi|^2\, d\mathbf{r}_3 \ldots d\mathbf{r}_N}{\int |\Psi|^2\, d\mathbf{r}_1 \ldots d\mathbf{r}_N} \tag{2.10}$$

according to the notation of de Boer (1948). Here, of course, $\Psi = \Psi^{\text{tr}}$.

As pointed out by Aviles, the following cluster expansion, known from the classical theory of imperfect gases (Mayer & Montroll, 1941; Van Kampen, 1961), can be used for $G(\mathbf{r}_{12})$:

$$G(\mathbf{r}_{12}) = \sum_{m=0}^{\infty} \rho^m \gamma_m(\mathbf{r}_{12}) = 1 + \sum_{m=1}^{\infty} \rho^m \gamma_m(\mathbf{r}_{12}) \tag{2.11}$$

where

$$\gamma_m(\mathbf{r}_{12}) = \frac{1}{m!}\int \sum \prod h(\mathbf{r}_{ij})\, d\mathbf{r}^m, \qquad r^m = \{\mathbf{r}_3, \ldots, \mathbf{r}_{m+2}\} \tag{2.12}$$

Here, however, the function $h(\mathbf{r}_{ij})$ which is defined by

$$h(\mathbf{r}_{ij}) = f^2(\mathbf{r}_{ij}) - 1 \tag{2.13}$$

is different from $\exp\{-V(\mathbf{r}_{ij})/KT\} - 1$.

By $\sum \prod h(\mathbf{r}_{ij})$ we denote the sum of all connected products for which each particle of the set m is connected to particles 1 and 2 by an independent path. Diagrams can then be easily drawn to represent the various terms of expression (2.11).

3. *The Approximate Expression for* $G(\mathbf{r}_{12})$

The basic problem which one faces in calculating the ground state energy per particle of the many-body boson system from expression (2.7) is the determination of the correlation function f. Unlike the situation in the classical theory of imperfect gases, the shape of the f is unknown and must be determined for a given potential. The determination of the f will be done in the present study by means of functional variation. This is not, however, a straightforward task. Particular care is necessary when the variational principle is applied to expressions resulting from cluster expansions.

In this section we derive an approximate expression for $G(\mathbf{r}_{12})$ which is very suitable to be used when we vary $\langle H\rangle^{\text{tr}}/N$, as the analysis of the following section will show. In deriving this expression we have used previous experience in the impure nuclear matter problem (Westhaus, 1966; Grypeos, 1970, 1971).

We write expression (2.8) in the form

$$G(\mathbf{r}_{12}) = \frac{N(N-1)}{\rho^2} \frac{\displaystyle\int \prod_{\substack{i<j=1 \\ (ij)\neq(12)}}^{N} f^2(\mathbf{r}_{ij})\, d\mathbf{r}_3 \ldots d\mathbf{r}_N}{\displaystyle\int f^2(\mathbf{r}_{12})\, d\mathbf{r}_1\, d\mathbf{r}_2 \int \prod_{\substack{i<j=1 \\ (ij)\neq(12)}}^{N} f^2(\mathbf{r}_{ij})\, d\mathbf{r}_3 \ldots d\mathbf{r}_N} \tag{3.1}$$

The product

$$\prod_{\substack{i<j=1 \\ (ij)\neq(12)}}^{N} f^2(\mathbf{r}_{ij})$$

which appears both in the numerator and the denominator of this expression can be written

$$\prod_{\substack{i<j=1 \\ (ij)\neq(12)}}^{N} f^2(\mathbf{r}_{ij}) = \left[\prod_{i=3}^{N} f^2(\mathbf{r}_{1i})\right] \cdot \left[\prod_{j=3}^{N} f^2(\mathbf{r}_{2j})\right] \cdot \left[\prod_{\substack{i<j \\ (ij)\neq(1k) \\ (ij)\neq(2l)}}^{N} f^2(\mathbf{r}_{ij})\right] \tag{3.2}$$

The approximation which is made is to replace all the f's appearing in the last product of the above expression by unity. This amounts to taking into account the correlations between each of the 'interacting particles' (1.2) and all the other particles in the system, but neglecting the correlations between these remaining particles.

Taking into account expression (2.13), we write

$$\prod_{\substack{i<j=1\\(ij)\neq(12)}}^{N} f^2(\mathbf{r}_{ij}) \approx \left[\prod_{i=3}^{N} f^2(\mathbf{r}_{1i})\right]\cdot\left[\prod_{j=3}^{N} f^2(\mathbf{r}_{2j})\right] = \prod_{i=3}^{N} (1+h(\mathbf{r}_{1i}))(1+h(\mathbf{r}_{2i})) \tag{3.3}$$

Substituting this into expression (3.1) we observe that the integrals in the numerator and denominator factorise:

$$G(\mathbf{r}_{12}) = \frac{N(N-1)}{\rho^2}\frac{\left[\int (1+h(\mathbf{r}_{13}))(1+h(\mathbf{r}_{23}))\,d\mathbf{r}_3\right]^{N-2}}{\int f^2(\mathbf{r}_{12})\,d\mathbf{r}_1\,d\mathbf{r}_2\left[\int (1+h(\mathbf{r}_{13}))(1+h(\mathbf{r}_{23}))\,d\mathbf{r}_3\right]^{N-2}} \tag{3.4}$$

We can easily see by noting that $\Omega = N/\rho$ and also by adding and subtracting $2/\rho$ that

$$\int (1+h(\mathbf{r}_{13}))(1+h(\mathbf{r}_{23})\,d\mathbf{r}_3 = \frac{N-2}{\rho}\left\{1+\frac{1}{(N-2)}\left[2+\rho\int (h(\mathbf{r}_{13})+h(\mathbf{r}_{23})+h(\mathbf{r}_{13})\,h(\mathbf{r}_{23})\,d\mathbf{r}_3\right]\right\} \tag{3.5}$$

Substituting this into expression (3.1) and using the well-known formula

$$\mathrm{e}^x = \lim_{n\to\infty}\left(1+\frac{x}{n}\right)^n \tag{3.6}$$

we obtain for $G(\mathbf{r}_{12})$

$$G(\mathbf{r}_{12}) = \frac{(N-1)}{\rho}\frac{\exp\left\{2+\rho\int [h(\mathbf{r}_{13})+h(\mathbf{r}_{23})+h(\mathbf{r}_{13})\,h(\mathbf{r}_{23})]\,d\mathbf{r}_3\right\}}{\int f^2(\mathbf{r}_{12})\exp\left\{2+\rho\int [h(\mathbf{r}_{13})+h(\mathbf{r}_{23})+h(\mathbf{r}_{13})\,h(\mathbf{r}_{23})]\,d\mathbf{r}_3\right\}d\mathbf{r}_{12}} \tag{3.7}$$

Therefore, the final result for $G(\mathbf{r}_{12})$ is

$$G(\mathbf{r}_{12}) = \frac{(N-1)}{\rho}\frac{\mathrm{e}^{R(\mathbf{r}_{12})}}{\int f^2(\mathbf{r}_{12})\,\mathrm{e}^{R(\mathbf{r}_{12})}\,d\mathbf{r}_{12}} \tag{3.8}$$

where

$$R(\mathbf{r}_{12}) = \rho\int h(\mathbf{r}_{13})\,h(\mathbf{r}_{23})\,d\mathbf{r}_3 \tag{3.9}$$

or

$$R(\mathbf{r}_{12}) = \rho\int (f^2(\mathbf{r}_{13}-\mathbf{r}_{12})-1)(f^2(\mathbf{r}_{13})-1)\,d\mathbf{r}_{13} \tag{3.10}$$

If we expand the exponential in the numerator of (3.8):

$$e^R = 1 + \frac{R}{1!} + \frac{R^2}{2!} + \dots \tag{3.11}$$

and compare with the terms resulting from the cluster expansion (2.12), we see that our approximate $G(\mathbf{r}_{12})$ (normalised to 1) contains the exact zeroth and first-order terms of the cluster expansion (that is, the terms with $m = 0$ and $m = 1$) and also part of the second- and higher-order terms. We can think therefore of expression (3.8) as resulting from a partial summation.

In Fig. 1 we plot the diagrams which correspond to the terms of the cluster expansion with $m = 0$, 1 and 2. Among the various second-order terms the term c has been included in the approximate expression for $G(\mathbf{r}_{12})$. This is the 'separable configuration' of Section IIB of Aviles (1958).

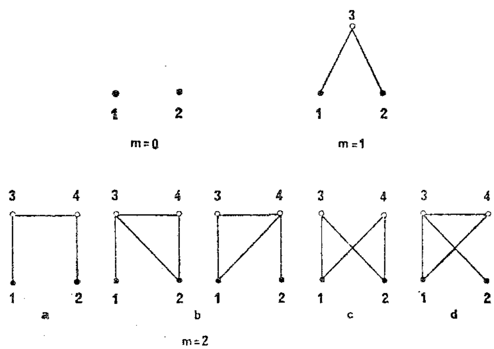

Figure 1.—Diagrams for $m = 0$, 1 and 2.

4. *A Non-Linear Integrodifferential Equation for the Correlation Function*

With expression (3.8) for $G(\mathbf{r}_{12})$ the trial expectation value of the Hamiltonian takes the form

$$\frac{\langle H\rangle^{tr}}{N} = \frac{(\rho/2)(N-1)\int [f(\mathbf{r}_{12})\, W_{12} f(\mathbf{r}_{12})]\, e^{R(\mathbf{r}_{12})}\, d\mathbf{r}_{12}}{\rho \int f^2(\mathbf{r}_{12})\, e^{R(\mathbf{r}_{12})}\, d\mathbf{r}_{12}} \tag{4.1}$$

where the 'effective potential' W_{12} is given by

$$W_{12} = \frac{\hbar^2}{2m}\left[\left(\frac{\nabla f(\mathbf{r}_{12})}{f(\mathbf{r}_{12})}\right)^2 - \frac{\nabla^2 f(\mathbf{r}_{12})}{f(\mathbf{r}_{12})}\right] + V_{12} \tag{4.2}$$

We can write expression (4.1) as follows (since $N \to \infty$):

$$\frac{\langle H\rangle^{tr}}{N} = \frac{\rho}{2}\int f(\mathbf{r}_{12})\, W_{12} f(\mathbf{r}_{12})\, e^{R(\mathbf{r}_{12})}\, d\mathbf{r}_{12} \tag{4.3}$$

provided that we require

$$\rho \int (f^2(\mathbf{r}_{12})\, e^{R(\mathbf{r}_{12})} - 1)\, d\mathbf{r}_{12} = \text{finite} \tag{4.4}$$

In the following we assume central forces and we take the functions f and G as depending upon the relative distance $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$.

Variation of $\langle H \rangle^{\text{tr}}/N$ with constraint (4.4) is equivalent to

$$\delta \left(\frac{4\pi\rho}{2}\right) \int_c^\infty \mathscr{L}(r_{12}, f(r_{12}), f'(r_{12}), f''(r_{12}))\, dr_{12} = 0 \tag{4.5}$$

where

$$\mathscr{L} = \mathscr{L}_1 + \lambda \mathscr{L}_2 = r_{12}^2 \left[\frac{\hbar^2}{2m}\left[\left(\frac{df}{dr_{12}}\right)^2 - f\left(\frac{d^2 f}{dr_{12}^2} + \frac{2}{r_{12}}\frac{df}{dr_{12}}\right)\right] + V(r_{12}) f^2\right] e^{R(r_{12})}$$
$$+ \lambda(r_{12}^2(f^2\, e^{R(r_{12})} - 1)) \tag{4.6}$$

The functional variation leads to the following equation:

$$-\frac{\hbar^2}{2\mu}\left[\frac{d^2 f}{dr_{12}^2} + \left(\frac{2}{r_{12}} + \frac{dR}{dr_{12}}\right)\frac{df}{dr_{12}}\right]$$
$$+\left[-\frac{\hbar^2}{4m}\left(\frac{2}{r_{12}}\frac{dR}{dr_{12}} + \left(\frac{dR}{dr_{12}}\right)^2 + \frac{d^2 R}{dr_{12}^2}\right) + V(r_{12}) + \lambda\right] f$$
$$+\left[\frac{\hbar^2}{2m}\left(\left(\frac{df}{dr_{12}}\right)^2 - f\cdot\left(\frac{d^2 f}{dr_{12}^2} + \frac{2}{r_{12}}\frac{df}{dr_{12}}\right)\right) + (V(r_{12}) + \lambda) f^2\right]\cdot\frac{R_f}{2} = 0 \tag{4.7}$$

where $\mu = m/2$. The boundary conditions are

$$f(c) = 0, \qquad f(\infty) = 1 \tag{4.8}$$

Equation (4.7) is a non-linear integrodifferential equation for the unknown correlation function f.

The function R_f has its origin in the dependence of R on f through the integral expression (3.10). It is given by

$$R_f(r_{12}) = 4\rho \int f(r_{13})\, (f^2(|\mathbf{r}_{13} - \mathbf{r}_{12}|) - 1)\, d\mathbf{r}_{13} \tag{4.9}$$

The parameter λ is the Lagrange multiplier due to constraint (4.4).

If we use the transformation

$$f(r_{12}) = 1 - \frac{c}{r_{12}}\, u(r_{12}) \tag{4.10}$$

we obtain, after some algebra, the following equation for the new correlation function u:

$$\left[\frac{\hbar^2}{2\mu}+\frac{\hbar^2}{2m}\cdot\frac{K}{2}+\frac{\hbar^2}{2m}\cdot\frac{R_f{}^0}{2}\right]\frac{d^2u}{dr_{12}^2}+\frac{\hbar^2}{2\mu}\frac{dR}{dr_{12}}\frac{du}{dr_{12}}+\left[-\frac{\hbar^2}{2m}\frac{1}{r_{12}}\frac{dR}{dr_{12}}\right.$$
$$\left.+\frac{\hbar^2}{4m}\left(\left(\frac{dR}{dr_{12}}\right)^2+\frac{d^2R}{dr_{12}^2}\right)-(V(r_{12})+\lambda)(K+1)-(V(r_{12})+\lambda)R_f{}^0\right]u$$
$$=\frac{r_{12}}{c}\left\{\frac{\hbar^2}{4m}\left(\frac{2}{r_{12}}\frac{dR}{dr_{12}}+\left(\frac{dR}{dr_{12}}\right)^2+\frac{d^2R}{dr_{12}^2}\right)-(V(r_{12})+\lambda)\left(1+\frac{K}{2}\right)\right.$$
$$-(V(r_{12})+\lambda)\frac{R_f{}^0}{2}-\frac{c^2}{r_{12}^2}\left[\frac{\hbar^2}{2m}\left(\frac{u^2}{r_{12}^2}-\frac{2u}{r_{12}}\frac{du}{dr_{12}}+\left(\frac{du}{dr_{12}}\right)^2\right)-\frac{\hbar^2}{2m}u.\frac{d^2u}{dr_{12}^2}\right.$$
$$\left.\left.+(V(r_{12})+\lambda)u^2\right].\left(\frac{K}{2}+\frac{R_f{}^0}{2}\right)\right\} \tag{4.11}$$

The boundary conditions for the $u(r)$ are

$$u(c)=1, \qquad u(\infty)=0 \tag{4.12}$$

The function R is given in terms of u by

$$R(r_{12})=\rho\int\left(\frac{c^2}{|\mathbf{r}_{13}-\mathbf{r}_{12}|^2}u^2(|\mathbf{r}_{13}-\mathbf{r}_{12}|)-\frac{2c}{|\mathbf{r}_{13}-\mathbf{r}_{12}|}u(|\mathbf{r}_{13}-\mathbf{r}_{12}|)\right)$$
$$\times\left(\frac{c^2}{r_{13}^2}u^2(r_{13})-\frac{2c}{r_{13}}u(r_{13})\right)d\mathbf{r}_{13} \tag{4.13}$$

For the function R_f we have written

$$R_f=K+R_f{}^0 \tag{4.14}$$

where K is a constant given by

$$K=4\xi \tag{4.15}$$

with

$$\xi=\rho\int(f^2(r)-1)\,d\mathbf{r} \tag{4.16}$$

The value of this constant is discussed in the next section. The function $R_f{}^0$ is given by

$$R_f{}^0(r_{12})=4\rho\int\left(\frac{c^2}{|\mathbf{r}_{13}-\mathbf{r}_{12}|^2}u^2(|\mathbf{r}_{13}\quad\mathbf{r}_{12}|)-\frac{2c}{|\mathbf{r}_{13}-\mathbf{r}_{12}|}u(|\mathbf{r}_{13}-\mathbf{r}_{12}|)\right)$$
$$\times\left(-\frac{c}{r_{13}}u(r_{13})\right)d\mathbf{r}_{13} \tag{4.17}$$

Note that the functions $R(r_{12})$ and $R_f{}^0(r_{12})$ tend to zero for large r_{12}, provided, of course, that they are calculated with u approaching zero for large r_{12} sufficiently rapidly. We should also expect that in such a case the $R(r_{12})$ and $R_f(r_{12})$ tend to zero for large r_{12} quite rapidly.

5. *Linearisation of the Non-Linear Equation and Investigation of its Asymptotic Behaviour*

The non-linear equation (4.7) of the previous section can be reduced to a linear integrodifferential equation if we write

$$f = f_1 + f_2 \tag{5.1}$$

and neglect terms of second and higher order in f_2. In the above expression f_1 is a given first approximation to f.

The linear integrodifferential equation which we obtain for the f_2 is the following:

$$\begin{aligned}
&-\left[\frac{\hbar^2}{2\mu}+\frac{\hbar^2}{4m}f_1 R_f^{(1)}\right]\frac{d^2 f_2}{dr_{12}^2}-\left[\frac{\hbar^2}{2\mu}\left(\frac{2}{r_{12}}+\frac{dR^{(1)}}{dr_{12}}\right)+\left(\frac{\hbar^2}{2m}\left(\frac{f_1}{r_{12}}-\frac{df_1}{dr_{12}}\right)\right).R_f^{(1)}\right]\frac{df_2}{dr_{12}}\\
&+\left[(V(r_{12})+\lambda)(1+f_1 R_f^{(1)})-\frac{\hbar^2}{4m}\left(\frac{2}{r_{12}}\frac{dR^{(1)}}{dr_{12}}+\left(\frac{dR^{(1)}}{dr_{12}}\right)^2+\left(\frac{d^2R^{(1)}}{dr_{12}^2}\right)+R_f^{(1)}\right.\right.\\
&\times\left.\left.\frac{d^2 f_1}{dr_{12}^2}+\frac{2}{r_{12}}R_f^{(1)}\frac{df_1}{dr_{12}}\right)\right]f_2=\frac{\hbar^2}{2\mu}\left[\frac{d^2 f_1}{dr_{12}^2}+\left(\frac{2}{r_{12}}+\frac{d(R^{(1)}+R^{(2)})}{dr_{12}}\right)\frac{df_1}{dr_{12}}\right]\\
&+\left[-(V(r_{12})+\lambda)+\frac{\hbar^2}{4m}\left(\frac{2}{r_{12}}\frac{d(R^{(1)}+R^{(2)})}{dr_{12}}+\left(\frac{dR^{(1)}}{dr_{12}}\right)^2+2\left(\frac{dR^{(1)}}{dr_{12}}\right)\left(\frac{dR^{(2)}}{dr_{12}}\right)\right.\right.\\
&\left.\left.+\frac{d^2(R^{(1)}+R^{(2)})}{dr_{12}^2}\right]f_1-\left[(V(r_{12})+\lambda)f_1{}^2+\frac{\hbar^2}{2m}\left(\left(\frac{df_1}{dr_{12}}\right)^2-f_1\left(\frac{d^2 f_1}{dr_{12}^2}+\frac{2}{r_{12}}\right.\right.\right.\\
&\left.\left.\left.\times\frac{df_1}{dr_{12}}\right)\right)\right]\left(\frac{R_f^{(1)}+R_f^{(2)}}{2}\right)
\end{aligned}\tag{5.2}$$

with boundary conditions

$$f_2(c)=0, \qquad f_2(\infty)=0 \tag{5.3}$$

The functions $R^{(1)}$, $R^{(2)}$, $R_f^{(1)}$ and $R_f^{(2)}$ are defined as follows:

$$R^{(1)}(r_{12})=\rho\int(f_1{}^2(|\mathbf{r}_{13}-\mathbf{r}_{12}|)-1)(f_1{}^2(r_{13})-1)\,d\mathbf{r}_{13} \tag{5.4}$$

$$R^{(2)}(r_{12})=4\rho\int(f_1{}^2(|\mathbf{r}_{13}-\mathbf{r}_{12}|)-1)f_1(r_{13})f_2(r_{13})\,d\mathbf{r}_{13} \tag{5.5}$$

$$R_f^{(1)}(r_{12}) = K + 4\rho \int (f_1^2(|\mathbf{r}_{13} - \mathbf{r}_{12}|) - 1)(f_1(r_{13}) - 1)\, d\mathbf{r}_{13} \quad (5.6)$$

$$R_f^{(2)}(r_{12}) = 4\rho \int [(f_1(|\mathbf{r}_{13} - \mathbf{r}_{12}|) - 1).2f_1(r_{13}) + (f_1^2(|\mathbf{r}_{13} - \mathbf{r}_{12}|) - 1)] f_2(r_{13})\, d\mathbf{r}_{13} \quad (5.7)$$

We should note that it seems preferable in practice to integrate numerically, instead of equation (5.2), the equation which results by linearising equation (4.11). The appropriate procedure would be, of course, to integrate numerically equation (4.11) itself. These numerical integrations, although complicated, should be feasible with a modern computer (provided, of course, that a solution exists).

Having obtained the correlation function, the trial energy per particle can easily be calculated from expression (4.3).

We discuss finally the asymptotic behaviour of the non-linear equation.

By virtue of the remark made at the end of the previous section, equation (4.11) takes in general the following form for large separations:

$$\left[\frac{\hbar^2}{2\mu} + \frac{\hbar^2}{2m}\frac{K}{2}\right]\frac{d^2u}{dr_{12}^2} + [-(V(r_{12}) + \lambda)(K+1)]u$$
$$= \frac{r_{12}}{c}\left[\frac{\hbar^2}{4m}\left(\frac{2}{r_{12}}\frac{dR}{dr_{12}} + \frac{d^2R}{dr_{12}^2}\right) - (V(r_{12}) + \lambda)\left(1 + \frac{K}{2}\right) - (V(r_{12}) + \lambda)\frac{R_f^{\,0}}{2}\right] \quad (5.8)$$

Therefore, in order that u tends to zero for $r_{12} \to \infty$ we must choose the value of λ such that $K = -2$. So the following condition must be satisfied:

$$2\rho \int (1 - f^2(r))\, d\mathbf{r} = 1 \quad (5.9)$$

In addition, λ should be negative.

From equation (5.8) and the value of K it is also clear that for large r_{12} we can define an 'effective' reduced mass μ^* of the pair. This is given in terms of the actual reduced mass by $\mu^* = 2\mu$.

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References

Aviles, J. B. (1958). *Annals of Physics, New York*, **5**, 251.
de Boer, J. (1948). *Reports on Progress in Physics*, **12**, 305.
Enderby, J., Gaskell, J. and March, N. (1965). *Proceedings of the Physical Society (London)*, **85**, 217.

Feenberg, E. (1969). *Theory of Quantum Fluids*. Academic Press, London.
Feenberg, E. and Wu, F. (1961). *Physical Review*, **122**, 739.
Feynman, R. (1953). *Physical Review*, **91**, 1291.
Gross, E. (1966). Dynamics of interacting bosons, in *Physics of Many-Particle Systems* (Ed. E. Meeron). Gordon & Breach, New York. (See also other references cited in this article.)
Grypeos, M. E. (1970). *Lettere al Nuovo Cimento*, **4**, 973.
Grypeos, M. E. (1971). *Nuovo Cimento*, **6**, 245.
Jackson, H. W. and Feenberg, E. (1961). *Annals of Physics, New York*, **15**, 266.
Jastrow, R. (1955). *Physical Review*, **98**, 1479.
Mayer, J. and Montroll, E. (1941). *Journal of Chemical Physics*, **9**, 2, 626.
Reatto, L. and Chester, G. (1967). *Physical Review*, **155**, 88.
Van Kampen, N. G. (1961). *Physica*, **27**, 783.
Westhaus, P. (1966). Ph.D. thesis, unpublished.