International Journal of Theoretical Physics, Vol. 14. No. 3 (1975), pp. 211-216

Functional Derivative for the Distribution Function of a Λ-Nucleon Pair in Nuclear Matter

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Received: 27 *February* 1975

Abstract

An "exact" expression for the functional derivative of the distribution function of a Λ-nucleon pair in nuclear matter is derived. An approximate expression is also derived by means of the Kirkwood superposition approximation. The latter expression is subsequently used to obtain the Euler equation for the correlation function $f(r_{1\Lambda})$ of a Λ-nucleon pair in nuclear matter.

1. *Introduction*

J. C. Lee & A. Broyles (1966) have developed a variational method for the ground state of a many-particle spinless Bose system, using a Bijl (1940)-Dingle (1949) wave function

$$\Psi = \exp\left[\frac{1}{2} \sum_{i<j} u(r_{ij})\right]$$

They gave first an exact expression for the functional derivative of the pair-distribution function $p^{(2)}$. This functional derivative is given in terms of $p^{(2)}$ and also in terms of $p^{(3)}$ and $p^{(4)}$. By using subsequently the superposition approximation they obtained an approximate expression for the radial distribution function g and also an Euler-Lagrange equation for this function. The Euler equation is similar to a result derived by Hiroike (1962), who, however, considered an arbitrary variation of δg instead of $\delta\Psi$.

Becker (1969) and Pokrant & Stevens (1973) have adopted, more recently, the technique of Lee & Broyles in their treatment of the electron gas.

In the present paper a variational approach for a system, consisting of many identical particles, to which an "impurity" has been added will be developed. A typical example of such a system is the infinitely and uniformly extended nuclear matter ($A \to \infty$, $\Omega \to \infty$, in such a way that $A/\Omega = \rho$ = constant), to which a Λ-particle has been attached. In the present treatment this system of "(infinite) hypernuclear matter" will be considered, although the formalism may be applied equally well to other impure similar systems. The problem of impure nuclear matter has also been studied (Grypeos, 1971; 1974) by using the "closed form" approximate expression (Westhaus, 1966) for the Λ-nucleon pair distribution function $p_{N\Lambda}^{(2)}$. In the recent development of this study, Edelen's (1969) formalism, which involves "nonlocal" Euler-Lagrange operators, was found appropriate to be used. In the present approach no approximate expression for $p_{N\Lambda}^{(2)}$ is initially employed.

In the following section the energy functional, which is derived if a Jastrow (1955) type many-body wave function is used for the "impure system" (hypernuclear matter), will be considered, and "exact" expressions for the functional derivative of the distribution function of a Λ-nucleon pair: $p_{N\Lambda}^{(2)}$ and related functions will be obtained. In the last section approximate expressions for these functions will be given, and the corresponding Euler-Lagrange equation for the Λ-nucleon correlation function $f(r_{1\Lambda})$ will be derived.

2. *The Energy Functional and the Exact Expression for the Functional Derivative of* $p_{N\Lambda}^{(2)}$

The following trial many-body wave function will be used, for the total system (hypernuclear matter):

$$\Psi_{A+\Lambda} = \Psi_A \prod_{i=1}^{A} f(r_{i\Lambda}) \tag{2.1}$$

where Ψ_A is the exact ground-state wave function of the "pure system" (nuclear matter) and $f(r_{i\Lambda})$ is the Jastrow correlation function between the ith nucleon of nuclear matter and the impurity particle (Λ particle).

The Hamiltonian operator of hypernuclear matter is

$$\hat{H}_{A+\Lambda} = \hat{H}_A + \hat{H}_\Lambda \tag{2.2}$$

where $\hat{H}_A$ and $\hat{H}_\Lambda$ are the Hamiltonian operators of nuclear matter and of the Λ particle, respectively.

Use of (2.1) and (2.2) leads to an expression for the binding (or separation) energy B_Λ of the Λ particle upon which either a cluster expansion may be immediately performed (Downs and Grypeos, 1966) or integration by parts may be applied in such a way that B_Λ is written in the form (for spin and i spin independent central potentials, which are assumed) (Westhaus 1966; Westhaus and Clark 1966; Clark and Mueller 1969)

$$B_\Lambda = -\int d\mathbf{r}_1 \int d\mathbf{r}_\Lambda W_{N\Lambda}(r_{1\Lambda}) p_{N\Lambda}^{(2)}(\mathbf{r}_1, \mathbf{r}_\Lambda) \tag{2.3}$$

where $W_{N\Lambda}$ is the "effective potential"

$$W_{N\Lambda}(r_{1\Lambda}) = \frac{\hbar^2}{2\mu}\left[\frac{\nabla f(r_{1\Lambda})}{f(r_{1\Lambda})}\right]^2 - \frac{\hbar^2}{4M_\Lambda}\left\{\frac{\nabla^2 f(r_{1\Lambda})}{f(r_{1\Lambda})} + \left[\frac{\nabla f(r_{1\Lambda})}{f(r_{1\Lambda})}\right]^2\right\} + V_{N\Lambda}(r_{1\Lambda}) \tag{2.4}$$

and $p_{N\Lambda}^{(2)}$ is the Λ-nucleon pair distribution function, defined by

$$p_{N\Lambda}^{(2)}(\mathbf{r}_1, \mathbf{r}_\Lambda) = \frac{A\int |\Psi_{A+\Lambda}|^2 d\mathbf{r}_2 \cdots d\mathbf{r}_A}{\int |\Psi_{A+\Lambda}|^2 d\mathbf{r}_1 \cdots d\mathbf{r}_A \cdot d\mathbf{r}_\Lambda} \tag{2.5}$$

Since the nuclear system is assumed to be expanded isotropically, the number of nucleons being increased proportionately to the volume, $p_{N\Lambda}^{(2)}(\mathbf{r}_1, \mathbf{r}_\Lambda)$ is a function only of the distance between nucleon 1 and the Λ particle: $p_{N\Lambda}^{(2)} = p_{N\Lambda}^{(2)}(r_{1\Lambda})$.

Formula (2.3) is suitable in deriving Westhaus' approximate expression in closed form for B_Λ and will be also adopted in the present analysis.

Application of the variational principle requires the calculation of the functional derivative of the pair distribution function $p_{N\Lambda}^{(2)}(\mathbf{r}_1, \mathbf{r}_\Lambda)$. At this point it is useful to define the jth $N\Lambda$ distribution function $p_{N\Lambda}^{(j)}(\mathbf{r}_1, \cdots, \mathbf{r}_{j-1}, \mathbf{r}_\Lambda)$ as follows:

$$p_{N\Lambda}^{(j)}(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_{j-1}, \mathbf{r}_\Lambda) = \frac{A!}{(A-j+1)!}\frac{\int |\Psi_{A+\Lambda}|^2 d\mathbf{r}_j \cdots d\mathbf{r}_A}{\int |\Psi_{A+\Lambda}|^2 d\mathbf{r}_1 \cdots d\mathbf{r}_A d\mathbf{r}_\Lambda} \tag{2.6}$$

For $j = 2$ we obtain the previously quoted expression for $p_{N\Lambda}^{(2)}(\mathbf{r}_1, \mathbf{r}_\Lambda)$. It should be noted that in the various expressions of the distribution functions that we are using, the symbol for integration implies also summation over all spin and isospin coordinates.

The distribution function $p_{N\Lambda}^{(j)}$, is obviously different from the usual distribution function $p^{(j)}$, which is defined as follows:

$$p^{(j)}(\mathbf{r}_1 \cdots \mathbf{r}_j) = \frac{A!}{(A-j)!}\frac{\int |\Psi_A|^2 d\mathbf{r}_{j+1} \cdots d\mathbf{r}_A}{\int |\Psi_A|^2 d\mathbf{r}_1 \cdots d\mathbf{r}_A} \tag{2.7}$$

By considering expression (2.5) we may easily calculate the first variation of $\delta p_{N\Lambda}^{(2)}$ in the usual way. We find

$$\delta p_{N\Lambda}^{(2)}(r_{1\Lambda}) = 2\left[\frac{\delta f(r_{1\Lambda})}{f(r_{1\Lambda})} p_{N\Lambda}^{(2)}(r_{1\Lambda}) + \int \frac{\delta f(r_{2\Lambda})}{f(r_{2\Lambda})} p_{N\Lambda}^{(3)}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_\Lambda)\, d\mathbf{r}_2 \right.$$
$$\left. - p_{N\Lambda}^{(2)}(r_{1\Lambda}) \int \frac{\delta f(r_{1\Lambda})}{f(r_{1\Lambda})} p_{N\Lambda}^{(2)}(r_{1\Lambda})\, d\mathbf{r}_1 d\mathbf{r}_\Lambda\right] \tag{2.8}$$

In order to obtain the expression for the functional derivative $[\delta p_{N\Lambda}^{(2)}(r)]/\delta f(r_{1\Lambda})$, we must write $\delta p_{N\Lambda}^{(2)}(r)$ as follows:

$$\delta p_{N\Lambda}^{(2)}(r) = \int \left(\frac{\delta p_{N\Lambda}^{(2)}(r)}{\delta f(r_{1\Lambda})} \right) \delta f(r_{1\Lambda})\, d\mathbf{r}_{1\Lambda} \tag{2.9}$$

The result is

$$\frac{\delta p_{N\Lambda}^{(2)}(r)}{\delta f(r_{1\Lambda})} = \frac{2}{f(r_{1\Lambda})} [p_{N\Lambda}^{(2)}(r_{1\Lambda})\delta(\mathbf{r}_{1\Lambda} - \mathbf{r}) + p_{N\Lambda}^{(3)}(\mathbf{r} + \mathbf{r}_\Lambda, \mathbf{r}_{1\Lambda} + \mathbf{r}_\Lambda, \mathbf{r}_\Lambda) - \Omega p_{N\Lambda}^{(2)}(r_{1\Lambda}) p_{N\Lambda}^{(2)}(r)] \tag{2.10}$$

We see that $[\delta p_{N\Lambda}^{(2)}(r)]/\delta f(r_{1\Lambda})$ is expressed in terms of $f(r_{1\Lambda})$ and the distribution functions $p_{N\Lambda}^{(2)}$ and $p_{N\Lambda}^{(3)}$. If we compare the above result for the functional derivative of $p_{N\Lambda}^{(2)}$ with the corresponding result for the pair distribution function of the Bose system, we observe that in the present case the expression for the functional derivative is simpler.

In the case of a system consisting of identical particles, it is customary to define the so-called g-distribution functions, which are closely related to the p:

$$g^{(j)}(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_j) = \frac{A!}{\rho^j (A-j)!} \frac{\int |\Psi_A|^2 d\mathbf{r}_{j+1} \cdots d\mathbf{r}_A}{\int |\Psi_A|^2 d\mathbf{r}_1 \cdots d\mathbf{r}_A} = \rho^{-j} p^{(j)}(\mathbf{r}_1, \cdots \mathbf{r}_j) \tag{2.11}$$

In the case of the system, with the impurity, which we are discussing, we may define the following $g_{N\Lambda}^{(j)}$ distribution functions:

$$g_{N\Lambda}^{(j)}(\mathbf{r}_1, \ldots, \mathbf{r}_{j-1}, \mathbf{r}_\Lambda) = \frac{\Omega \cdot A!}{\rho^{j-1}(A-j+1)!} \frac{\int |\Psi_{A+\Lambda}|^2 d\mathbf{r}_j \cdots d\mathbf{r}_A}{\int |\Psi_{A+\Lambda}|^2 d\mathbf{r}_1 \cdots d\mathbf{r}_A \cdot d\mathbf{r}_\Lambda} = \frac{\Omega}{\rho^{j-1}} p_{N\Lambda}^{(j)}(\mathbf{r}_1, \ldots, \mathbf{r}_{j-1}, \mathbf{r}_\Lambda) \tag{2.12}$$

The function $g_{N\Lambda}^{(2)}$ is the radial distribution function $g_{N\Lambda}(r_{1\Lambda})$. We may further define the related $G_{N\Lambda}$-distribution function as follows:

$$g_{N\Lambda}(r_{1\Lambda}) = f^2(r_{1\Lambda}) G_{N\Lambda}(r_{1\Lambda}) \tag{2.13}$$

The "exact" expressions for the functional derivatives of $g_{N\Lambda}$ and $G_{N\Lambda}$ are easily obtained from the formula (2.10). We find

$$\frac{\delta g_{N\Lambda}(r)}{\delta f(r_{1\Lambda})} = \frac{2}{f(r_{1\Lambda})} [g_{N\Lambda}(r_{1\Lambda})\delta(\mathbf{r}_{1\Lambda} - r) + \rho g_{N\Lambda}^{(3)}(\mathbf{r} + \mathbf{r}_\Lambda, \mathbf{r}_{1\Lambda} + \mathbf{r}_\Lambda, \mathbf{r}_\Lambda) - \rho g_{N\Lambda}(r_{1\Lambda}) g_{N\Lambda}(r)] \tag{2.14}$$

and

$$\frac{\delta G_{N\Lambda}(r)}{\delta f(r_{1\Lambda})} = \frac{2\rho}{f^2(r)f(r_{1\Lambda})} [g^{(3)}(\mathbf{r}+\mathbf{r}_\Lambda, \mathbf{r}_{1\Lambda}+\mathbf{r}_\Lambda, \mathbf{r}_\Lambda) - f^2(r_{1\Lambda})G_{N\Lambda}(\mathbf{r}_{1\Lambda})f^2(r)G_{N\Lambda}(r)] \tag{2.15}$$

3. *Approximate Expressions for the Functional Derivatives and the Euler Equation for the Correlation Function* $f(r_{1\Lambda})$

It is advisable, for practical purposes, to obtain approximate expressions of the functional derivatives of the distribution functions $g_{N\Lambda}$ and $G_{N\Lambda}$, which were derived in the previous section

We shall use the Kirkwood superposition approximation, which is written in the present case as follows:

$$g^{(3)}_{N\Lambda}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_\Lambda) \approx g(\Lambda)(r_{12})g_{N\Lambda}(r_{1\Lambda})g_{N\Lambda}(r_{2\Lambda}) \tag{3.1}$$

where $g_\Lambda(r_{12})$ is given by (2.11) with $j = 2$ and $|\psi_{A+\Lambda}|^2 d\mathbf{r}_\Lambda$ instead of $|\psi_A|^2$. We may therefore write

$$\frac{\delta g_{N\Lambda}(r)}{\delta f(r_{1\Lambda})} \approx \frac{2}{f(r_{1\Lambda})}\{g_{N\Lambda}(r_{1\Lambda})\delta(\mathbf{r}_{1\Lambda}-\mathbf{r}) + \rho g_{N\Lambda}(r_{1\Lambda})g_{N\Lambda}(r)[g(\Lambda)(|\mathbf{r}_{1\Lambda}-\mathbf{r}|)-1]\} \tag{3.2}$$

and

$$\frac{\delta G_{N\Lambda}(r)}{\delta f(r_{1\Lambda})} \approx 2\rho f(r_{1\Lambda})G_{N\Lambda}(r_{1\Lambda})G_{N\Lambda}(r)[f^2_{NN}(|\mathbf{r}_{1\Lambda}-\mathbf{r}|)G(\Lambda)(|\mathbf{r}_{1\Lambda}-\mathbf{r}|)-1] \tag{3.3}$$

The variational principle may now be applied to the energy functional. The variation will be performed by imposing also the integral constraints

$$\rho\int [f^2(r_{1\Lambda})G_{N\Lambda}(r_{1\Lambda})-1]\, d\mathbf{r}_{1\Lambda} = D_1 = \text{finite} \tag{3.4}$$

$$\rho\int [f(r_{1\Lambda})-1]^2 G_{N\Lambda}(r_{1\Lambda})\, d\mathbf{r}_{1\Lambda} = D_2 = \text{finite} \tag{3.5}$$

The first has its origin to the denominator in the distribution function, while the second is a "healing condition."

Owing to the above constraints, two Lagrange multipliers appear in the variational problem. The first Lagrange multiplier (λ_1) is due to (3.4), while the second (λ_2) is due to the healing condition.

The Euler equation of the variational problem is

$$-\frac{\hbar^2}{2\mu_{N\Lambda}}\left\{G_{N\Lambda}(r_{1\Lambda})\frac{d^2f(r_{1\Lambda})}{dr_{1\Lambda}^2}+\left[\frac{2}{r_{1\Lambda}}G_{N\Lambda}(r_{1\Lambda})+\frac{dG_{N\Lambda}(r_{1\Lambda})}{dr_{1\Lambda}}\right]\frac{df(r_{1\Lambda})}{dr_{1\Lambda}}\right\}$$

$$+\left\{\left(-\frac{\hbar^2}{8M_\Lambda}\right)\left[\frac{2}{r_{1\Lambda}}\frac{dG_{N\Lambda}(r_{1\Lambda})}{dr_{1\Lambda}}+\frac{d^2G_{N\Lambda}(r_{1\Lambda})}{dr_{1\Lambda}^2}\right]+V_{N\Lambda}(r_{1\Lambda})G_{N\Lambda}(r_{1\Lambda})\right\}f(r_{1\Lambda})$$

$$+\int d\mathbf{r}\left\{\left(\frac{\hbar^2}{2\mu_{N\Lambda}}-\frac{\hbar^2}{4M_\Lambda}\right)\left[\frac{df(r)}{dr}\right]^2-\frac{\hbar^2}{4M_\Lambda}f(r)\left[\frac{d^2f(r)}{dr^2}+\frac{2}{r}\frac{df(r)}{dr}\right]+V_{N\Lambda}(r)f^2(r)\right\}$$

$$\times\tfrac{1}{2}\frac{\delta G_{N\Lambda}(r)}{\delta f(r_{1\Lambda})}+\lambda_1\left[G_{N\Lambda}(r_{1\Lambda})f(r_{1\Lambda})+\int d\mathbf{r}f^2(r)\tfrac{1}{2}\frac{\delta G_{N\Lambda}(r)}{\delta f(r_{1\Lambda})}\right]$$

$$+\lambda_2\left\{G_{N\Lambda}(r_{1\Lambda})[f(r_{1\Lambda})-1]+\int d\mathbf{r}[f(r)-1]^2\tfrac{1}{2}\frac{\delta G_{N\Lambda}(r)}{\delta f(r_{1\Lambda})}\right\}=0 \qquad (3.6)$$

where the functional derivative $\delta G_{N\Lambda}(r)/\delta f(r_{1\Lambda})$ is given by (3.3).

The study of the asymptotic behavior of this equation at large distances $r_{1\Lambda}$ leads either to $\lambda_1 = 0$ or to a condition similar to that which has been previously obtained [see formula (14) of Grypeos, 1974] but with $G_\Lambda(\mathrm{r}_{12})$ instead of $Z_2^{(0)}(r_{12})$.

The above equation is an integrodifferential equation for the unknown function $f(r_{1\Lambda})$ and may be solved numerically.

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