Approximate Euler–Lagrange Equations for the Ground-State Electron Gas*

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The ground-state wave function for a quantum electron gas is approximated by $\psi=\Phi D$, where D is the ground-state ideal-gas wave function and $\Phi=\exp[-(\frac{1}{2})\Sigma_{i<j}u(r_{ij})]$. Three-body correlation functions in the energy are approximated so that the energy is a functional of only pair-correlation functions. The variational principle is applied by utilizing the functional derivative of the pair-correlation function with respect to $u(r)$. The three- and four-body correlation functions in the functional derivative are approximated in a consistent manner. Use of the Kirkwood superposition approximation for the many-body correlation functions in the functional derivative gives unphysical results. A new approximation to the functional derivative is obtained by using the convolution approximation for the many-body terms. This gives a reasonable result for the asymptotic form of the wave function. The hypernetted-chain functional derivative combined with the convolution approximation for the energy gives the same asymptotic form. When the random-phase approximation to the energy is used with the Gaskell–Broyles–Sahlin–Carley functional derivative, the equation may be solved analytically, giving the same result obtained by Gaskell. The asymptotic form is the same as the two previous methods, namely, $u\sim(e/\hbar)(m/\pi\rho)^{1/2}/r$.

I. INTRODUCTION

We will assume the wave function for the ground-state electron gas is of the form

$$\Psi = D\exp\left(-\frac{1}{2}\sum_{i<j}u(r_{ij})\right), \tag{1.1}$$

where D is the wave function for an ideal gas of spin-$\frac{1}{2}$ fermions and $u(r)$ is a real function to be determined. In the thermodynamic limit, the energy is given by Eq. (2.21) of Ref. 1;

$$E = T + V, \tag{1.2}$$

$$T = E_I + \tfrac{1}{4}\alpha\rho\int g(r)\left(\frac{du(r)}{dr}\right)^2 d\vec{\mathbf{r}} + \tfrac{1}{4}\alpha\rho^2 \times\iint g^{(3)}(r_1, r_2, r_3)\,\nabla_1 u_{12}\cdot\nabla_1 u_{13}\,d\vec{\mathbf{r}}_{12}\,d\vec{\mathbf{r}}_{13}, \tag{1.3}$$

$$V = \tfrac{1}{2}\rho\int G(r)v(r)\,d\vec{\mathbf{r}}, \tag{1.4}$$

where $\alpha=\hbar^2/2m$, E_I is the ideal-gas energy, $v(r)=e^2/r$, $G=g-1$, and the n-body correlation function is defined by

$$g^{(n)}(\vec{\mathbf{r}}_1,\ldots,\vec{\mathbf{r}}_n) = \frac{N!\,\Omega^n}{(N-n)!N^n} \times\frac{\int\cdots\int\Psi^*\Psi\,d\vec{\mathbf{r}}_{n+1}\cdots d\vec{\mathbf{r}}_N}{\int\cdots\int\Psi^*\Psi\,d\vec{\mathbf{r}}_1\cdots d\vec{\mathbf{r}}_N}. \tag{1.5}$$

Several variational calculations[1–6] have been made with the trial wave function in Eq. (1.1). While diverse approximations were employed in the calculations, most authors[1–4] restricted the wave function by using a parametric form for $u(r)$. One purpose of this paper is to explore the result of allowing arbitrary variations of $u(r)$. At the same time, we will be investigating the adequacy of various approximations to the many-body correlation functions.

The Euler–Lagrange equation for the ground-state wave function may be obtained by taking the functional derivative of the energy with respect to $u(r)$. To do this, the functional derivatives of the two- and three-body correlation functions are needed. Lee and Broyles[7] have derived the exact expression,

$$\frac{\delta g(\vec{\mathbf{r}}_{12})}{\delta u(\vec{\mathbf{r}})} = -g(r_{12})\delta(\vec{\mathbf{r}}-\vec{\mathbf{r}}_{12}) - 2\rho g^{(3)}(\vec{\mathbf{r}}_1,\vec{\mathbf{r}}_2,\vec{\mathbf{r}}_1+\vec{\mathbf{r}}) + \tfrac{1}{2}\Omega\rho^2 g(r_{12})g(r) - \tfrac{1}{2}\rho^2\int g^{(4)}(\vec{\mathbf{r}}_1,\vec{\mathbf{r}}_2,\vec{\mathbf{r}}_3,\vec{\mathbf{r}}_3+\vec{\mathbf{r}})\,d\vec{\mathbf{r}}_3. \tag{1.6}$$

The over-all sign is different from that of Lee and Broyles, because their $u(r)$ is defined as the negative of ours.

Using their method, one may also derive the exact functional derivative of $g^{(n)}$:

$$\frac{\delta g^{(n)}(\vec{\mathbf{r}}_1,\ldots,\vec{\mathbf{r}}_n)}{\delta u(r)} = -g^{(n)}(\vec{\mathbf{r}}_1,\ldots,\vec{\mathbf{r}}_n)\sum_{1\le i<j\le n}\delta(\vec{\mathbf{r}}_{ij}-\vec{\mathbf{r}}) - \rho\sum_{i=1}^{n}g^{(n+1)}(\vec{\mathbf{r}}_1,\ldots,\vec{\mathbf{r}}_n,\vec{\mathbf{r}}_i+\vec{\mathbf{r}}) - \tfrac{1}{2}\rho^2\left(\int_\Omega g^{(n+2)}(\vec{\mathbf{r}}_1,\ldots,\vec{\mathbf{r}}_{n+1},\vec{\mathbf{r}}_{n+1}+\vec{\mathbf{r}})\,d\vec{\mathbf{r}}_{n+1} - \Omega g^{(2)}(r)g^{(n)}(\vec{\mathbf{r}}_1,\ldots,\vec{\mathbf{r}}_n)\right). \tag{1.7}$$

Since the latter functional derivative is so complicated, even for $n=3$, we will only consider the alternative of directly approximating $g^{(3)}$ in the energy so that it is a functional only of pair-correlation functions; then, only Eq. (1.6) is needed to obtain the Euler–Lagrange equation. Thus, approximations are needed for $g^{(3)}$ and $g^{(4)}$. It will, generally, be impractical to solve the equations which will be obtained; however, it will be possible to obtain some information about the wave function from these equations. In particular, we shall assume that for very large particle separations

$$u(r)\sim a/r \tag{1.8}$$

and shall obtain the value of the constant from the Euler–Lagrange equation. It will be necessary to assume that $G(r)=g(r)-1$ is short ranged, i.e., it falls off at least as fast as r^{-4} for large r; but, it will not be necessary to assume any particular asymptotic form for $G(r)$. We will also obtain the slope of u at the origin under the assumption that for small r

$$u(r)\to(\text{const})+br. \tag{1.9}$$

The Kirkwood superposition approximation[8] (KSA) will be used in Sec. II. In Sec. III, the convolution approximation[9–11] (CA) to $g^{(3)}$ and $g^{(4)}$ will be used to get the functional derivative and the asymptotic form. In addition, an approach employing the random-phase approximation[12] (RPA) and the Gaskell–Broyles–Sahlin–Carley (GBSC) formula[6,13] will be presented in Sec. IV. In this case, an analytic expression for the Fourier transform of $u(r)$ will be obtained. In Sec. V, the hypernetted-chain (HNC) functional derivative is combined with the CA to the energy.

Before any approximations are made, two relations will be obtained, which are satisfied by the exact functional derivative. These will be useful in testing and understanding the approximations which will be considered in later sections. The change in potential energy V due to an arbitrary variation $\delta u(\vec{r})$ away from any function $u_1(r)$ is

$$\delta V=\int\left(\frac{\delta V}{\delta u(\vec{r})}\right)_{u_1}\delta u(\vec{r})\,d\vec{r}. \tag{1.10}$$

If we consider a variation which is the same for all $\vec{r}$, $\delta u(\vec{r})=\epsilon$, then V is unchanged. Hence

$$\int\left(\frac{\delta V}{\delta u(r)}\right)_{u_1}d\vec{r}=0. \tag{1.11}$$

Similarly, from Eq. (1.5), $g(r)$ is unchanged under such a variation:

$$\int\left(\frac{\delta g(\vec{r}_{12})}{\delta u(\vec{r})}\right)_{u_1}d\vec{r}=0. \tag{1.12}$$

Note that the functional derivative given by Eq. (1.6) satisfies this relation.

II. KIRKWOOD SUPERPOSITION APPROXIMATION

The KSA[8] for $g^{(n)}$ is given by

$$g^{(n)}(\vec{r}_1,\ldots,\vec{r}_n)=\sum_{i<j\le n}g(r_{ij}). \tag{2.1}$$

Applying this approximation, with $n=3$, to Eq. (1.3) gives[1]

$$E=E_I+\tfrac{1}{2}\rho\int G(r)v(r)\,d\vec{r}+\tfrac{1}{4}\alpha\rho\int g(r)\left(\frac{du(r)}{dr}\right)^2 d\vec{r}$$
$$+\tfrac{1}{4}\alpha\rho^2\iint G_{23}g_{12}g_{13}\nabla_1u_{12}\cdot\nabla_1u_{13}\,d\vec{r}_{12}\,d\vec{r}_{13}. \tag{2.2}$$

Using the KSA for $g^{(3)}$, $g^{(4)}$, and $g^{(5)}$, one can obtain an approximation to the functional derivative[7]

$$\frac{\delta g(\vec{r}_{12})}{\delta u(\vec{r})}=-g(r)\delta(\vec{r}-\vec{r}_{12})-2\rho g(r)g(r_{12})G(\vec{r}-\vec{r}_{12}). \tag{2.3}$$

Becker[5] took the functional derivative of the energy, given by Eq. (2.2), and utilized Eq. (2.3) to obtain an integrodifferential equation for u. He then obtained the asymptotic form of u. Unfortunately, his treatment contains several errors; the most serious of these involves a sign error in obtaining his Eq. (41) from Eq. (37). When the correct sign is used, the final result for the asymptotic form of $u(r)$ is

$$u(r)\sim\pm i(e/\hbar)(m/\pi\rho)^{1/2}/r. \tag{2.4}$$

This imaginary result is unacceptable. The implication is that the KSA has made the Euler–Lagrange equation inconsistent.

Let us now examine this calculation in more detail. The KSA to the Euler–Lagrange equation for u may be written

$$-\frac{2}{\alpha}g(r)v(r)-\frac{4}{\alpha}\rho g(r)\int v(t)g(t)G(\vec{r}-\vec{t})\,d\vec{t}-2\nabla\cdot\{g(r)[\nabla u(r)+\vec{J}(r)]\}-g(r)\nabla u(r)\cdot[\nabla u(r)+2\vec{J}(r)]$$
$$-2\rho g(r)\int g(t)G(\vec{r}-\vec{t})\nabla u(t)\cdot[\nabla u(t)+2\vec{J}(t)]\,d\vec{t}-\rho g(r)\left(\tilde{X}^2(1+2\rho\tilde{G})+2\rho\tilde{G}(k)\int\frac{\tilde{X}^2(\vec{k}-\vec{l})\tilde{G}(l)\,d\vec{l}}{(2\pi)^3}\right)^F=0, \tag{2.5}$$

where

$$\tilde{X}(k)=\frac{d}{dk}\left(\frac{g}{r}\frac{du}{dr}\right)^F, \tag{2.6}$$

$$\vec{J}(r)=\nabla_r[\rho\tilde{X}(k)\tilde{G}(k)/k]^F, \tag{2.7}$$

and the tilde and the superscript F denote the

Fourier transform

$$\tilde{G}(k)=\int G(r)e^{-i\vec{k}\cdot\vec{r}}d\vec{r}\,. \tag{2.8}$$

If we assume that $G(r)$ is short ranged and that $u(r)\sim a/r$, then at large r the leading terms are of order r^{-1}. The large-r form is determined by the small-k contributions from the Fourier transforms. To get the small-k behavior of $\tilde{X}$ we replace g by unity in Eq. (2.6) and use a Fourier-transform identity to obtain

$$\tilde{X}(k)\to k\tilde{u}(k)\to 4\pi a/k \quad \text{as } k\to 0\,. \tag{2.9}$$

Also, since the pair-correlation function is normalized so that $\tilde{G}(0)=-1/\rho$, we find that for large r:

$$\vec{J}(r)\sim-\nabla u\,. \tag{2.10}$$

It can then be shown that for large r only the first, second, and last terms of Eq. (2.5) contribute to order r^{-1}; the other terms fall off at least as fast as r^{-4}. Furthermore, the integral in the last term is finite at $k=0$ and does not contribute to this order. Hence, for large r, Eq. (2.5) reduces to

$$-\frac{2e^2}{\alpha r}+\frac{4e^2}{\alpha r}+\rho\left[\left(\frac{4\pi a}{k}\right)^2\right]^F=0 \tag{2.11}$$

or

$$\frac{2e^2}{\alpha r}+\frac{4\pi a^2\rho}{r}\sim 0\,. \tag{2.12}$$

Solving this for a gives the imaginary result stated in Eq. (2.4).

To understand why this approximation does not work, we integrate the KSA to the functional derivative given by Eq. (2.3) to obtain,

$$\int\left(\frac{\delta g(\vec{r})}{\delta u(\vec{t})}\right)_{\mathrm{KSA}}d\vec{t}=g(r)\left(1-2\rho\int G(t)G(\vec{r}-\vec{t})\,d\vec{t}\right)\neq 0\,. \tag{2.13}$$

Thus, Eq. (1.12) is not satisfied by the KSA functional derivative.

The first two terms in Eq. (2.5) are the variation of the potential energy. As stated in Eq. (2.12), the sum of these terms is asymptotic to $2e^2/\alpha r$. Since the sum multiplied by r^2 is finite everywhere, the integral condition in Eq. (1.11) cannot be satisfied, because the integral does not converge at large r. Hence, it appears that the unacceptable error was in the use of the KSA to calculate the functional derivative, rather than in approximating the three-body term in the energy by the KSA. While this result indicates that there is a serious problem in using the KSA functional derivative on the electron gas, it does not necessarily indicate that its application to helium is incorrect.[7] Because the interatomic potential is short ranged, errors in the functional derivative at large r may not be fatal.

The slope of $u(r)$ at the origin can be obtained rather easily. For very small r, the first term and that part of the third term containing $\nabla^2 u$ dominate Eq. (2.5). This gives

$$-\frac{2}{\alpha}g(r)\frac{e^2}{r}-\frac{4g(r)}{r}\frac{du(r)}{dr}\to 0\,. \tag{2.14}$$

Hence,

$$u'(0)=-me^2/\hbar^2=-1/a_0\,, \tag{2.15}$$

where a_0 is the Bohr radius. Note that this result depends only on the local term in the functional derivative, i.e., that part which contains the δ function. On the other hand, the approximation to the functional derivative involves only the nonlocal part.

III. CONVOLUTION APPROXIMATION

The CA to $g^{(3)}$ was introduced by Jackson and Feenberg.[9] It was later[10] extended to $g^{(4)}$. Wu and Chien[11] then stated and proved the approximation to $g^{(n)}$ for arbitrary n. The CA was derived with the requirements that the correlation functions be symmetric in all of the coordinates and that the sequential relations be satisfied:

$$\rho\int g^{(n+1)}(\vec{r}_1,\ldots,\vec{r}_{n+1})\,d\vec{r}_{n+1}=(N-n)g^{(n)}(\vec{r}_1,\ldots,\vec{r}_n)\,. \tag{3.1}$$

Even though the KSA does not satisfy the sequential relations, in the derivation of the KSA to the functional derivative it was assumed that

$$g^{(5)}_{\mathrm{KSA}}/g^{(4)}_{\mathrm{KSA}}=g^{(5)}/g^{(4)}\,, \tag{3.2}$$

and then the sequential relation was used with $n=4$ in deriving Eq. (2.3). Hence, the CA may give better results than the KSA. The CA for $g^{(3)}$ is[9]

$$g^{(3)}(\vec{r}_1,\vec{r}_2,\vec{r}_3)=g_{12}g_{13}g_{23}-G_{12}G_{13}G_{23}+\rho\int G_{14}G_{24}G_{34}\,d\vec{r}_4\,. \tag{3.3}$$

This approximation has the disadvantage of the resulting $g^{(3)}$ not necessarily being non-negative, while the KSA to $g^{(3)}$ is always non-negative. Inserting Eq. (3.3) into Eq. (1.3) gives

$$E=E_I+\tfrac{1}{2}\rho\int G(r)v(r)\,d\vec{r}+\tfrac{1}{4}\alpha\rho\int g(r)\left(\frac{du(r)}{dr}\right)^2 d\vec{r}+\tfrac{1}{4}\alpha\rho^2\iint G_{23}(1+G_{12}+G_{13})\nabla_1 u_{12}\cdot\nabla_1 u_{13}\,d\vec{r}_{12}\,d\vec{r}_{13}+\tfrac{1}{4}\alpha\rho^3\iint G_{14}G_{24}G_{34}\nabla_1 u_{12}\cdot\nabla_1 u_{13}\,d\vec{r}_{12}\,d\vec{r}_{13}\,d\vec{r}_4\,. \tag{3.4}$$

This expression may be rearranged to give a more compact expression,

$$E=E_I+\tfrac{1}{2}\alpha\rho\int\tilde{G}\tilde{v}\,d\vec{k}/(2\pi)^3+\tfrac{1}{4}\alpha\rho\int k^2\tilde{u}^2S\,d\vec{k}/(2\pi)^3+\tfrac{1}{4}\alpha\rho\int G\nabla T\cdot\nabla T\,d\vec{r}\,, \tag{3.5}$$

where T is defined by

$$\tilde{T} = S\tilde{u} \tag{3.6}$$

and S is the structure factor,

$$S = 1 + \rho\tilde{G} . \tag{3.7}$$

The Euler–Lagrange equation can now be obtained by setting the variation of the energy, with respect to $u(\vec{1})$, to zero:

$$\int\left(\frac{2}{\alpha}\tilde{v}(k) + \rho k^2\tilde{u}^2 + \int \nabla T\cdot\nabla T e^{-i\vec{k}\cdot\vec{r}}d\vec{r}\right)\frac{\delta\tilde{G}(\vec{k})}{\delta u(\vec{1})}\frac{d\vec{k}}{(2\pi)^3} + \frac{2l^2\tilde{u}(l)S(l)}{(2\pi)^3} - 2\int\frac{\delta T(\vec{r})}{\delta u(\vec{1})}\nabla\cdot(G\nabla T)d\vec{r} = 0 . \tag{3.8}$$

From the definition of T in Eq. (3.6), we find

$$\frac{\delta T(\vec{r})}{\delta\tilde{u}(\vec{1})} = \frac{S(l)\,e^{i\vec{1}\cdot\vec{r}}}{(2\pi)^3} + \rho\int\tilde{u}(k)\frac{\delta\tilde{G}(\vec{k})}{\delta\tilde{u}(\vec{1})}\frac{e^{i\vec{k}\cdot\vec{r}}d\vec{k}}{(2\pi)^3} . \tag{3.9}$$

Inserting this result in the previous equation gives

$$2l^2\tilde{u}(l)S(l) - 2S(l)[\nabla\cdot(G\nabla T)]^F + \int\tilde{P}(k)\frac{\delta\tilde{G}(\vec{k})}{\delta\tilde{u}(\vec{1})}d\vec{k} = 0 , \tag{3.10}$$

where $\tilde{P}$ has been defined as

$$\tilde{P}(k) = (2/\alpha)\tilde{v}(k) + \rho k^2\tilde{u}^2(k) + [\nabla T\cdot\nabla T]^F - 2\rho\tilde{u}(k)[\nabla\cdot(G\nabla T)]^F . \tag{3.11}$$

We now need the CA to the functional derivative of G, in order to evaluate the last term of Eq. (3.10). The exact expression for the functional derivative of g, Eq. (1.6), contains both $g^{(3)}$ and $g^{(4)}$. The CA expression for $g^{(4)}$ contains 58 terms.[11] When it is applied to the four-body term in Eq. (1.6), the result is

$$\begin{aligned}\rho\int g^{(4)}(\vec{r}_1,\vec{r}_2,\vec{r}_3,\vec{r}_3+\vec{r})d\vec{r}_3 &= \rho\Omega g_{12}g(r) - 4g_{12}g(r) \\ &+ 2\rho[1+G(r)+G_{12}]F(\vec{r}_{12}-\vec{r}) \\ &+ 4\rho\int G_{13}G_{23}[G(\vec{r}_{13}-\vec{r})+\rho F(\vec{r}_{13}-\vec{r})]d\vec{r}_3 \\ &+ 4\rho^2\int\int G_{14}G_{23}G_{34}H(\vec{r}_{34}-\vec{r})d\vec{r}_3 d\vec{r}_4 ,\end{aligned} \tag{3.12}$$

where we have defined

$$\tilde{F} = \tilde{G}^2 \quad\text{and}\quad H(r) = G(r) + \tfrac{1}{2}\rho F(r) . \tag{3.13}$$

Inserting this result and the CA for $g^{(3)}$ into Eq. (1.6) gives the CA to the function derivative:

$$\begin{aligned}\frac{\delta g(\vec{r}_{12})}{\delta u(\vec{r})} &= -g_{12}\delta(\vec{r}-\vec{r}_{12}) - 2\rho[1+G(r)+G_{12}]H(\vec{r}_{12}-\vec{r}) \\ &- 4\rho^2\int G_{13}G_{23}H(\vec{r}_{13}-\vec{r})d\vec{r}_3 \\ &- 2\rho^3\int\int G_{14}G_{23}G_{34}H(\vec{r}_{34}-\vec{r})d\vec{r}_3 d\vec{r}_4 .\end{aligned} \tag{3.14}$$

With some tedious but straightforward algebra, one may demonstrate that this functional derivative satisfies Eq. (1.12). A more compact result may be obtained for the double Fourier transform of the functional derivative:

$$\frac{\delta\tilde{G}(\vec{k})}{\delta\tilde{u}(\vec{1})} = -S^2(k)\delta(\vec{k}-\vec{1}) + \tilde{G}(\vec{k}-\vec{1})S^2(l)/(2\pi)^3 . \tag{3.15}$$

Substituting this result into Eq. (3.10) gives the CA to the Euler–Lagrange equation

$$2l^2\tilde{u}(l)S(l) - S^2(l)\tilde{P}(l) - 2S(l)[\nabla\cdot(G\nabla T)]^F - S^2(l)\int S^2(k)\tilde{P}(k)\tilde{G}(\vec{k}-\vec{1})d\vec{k}/(2\pi)^3 = 0 . \tag{3.16}$$

We will now examine Eq. (3.16) at small l. From our assumption about the large-r behavior of u,

$$\tilde{u}(l) \to 4\pi a/l^2 \qquad \text{as } l\to 0 , \tag{3.17}$$

and, therefore,[4]

$$S(l) \to l^2/4\pi\rho a . \tag{3.18}$$

The divergence theorem can be used to show that $[\nabla\cdot(G\nabla T)]^F$ is zero at $l=0$. Then, the first two terms of Eq. (3.11) dominate $\tilde{P}$ at small l,

$$\tilde{P}(l) \to \frac{8\pi e^2/\alpha + 16\pi^2a^2\rho}{l^2} . \tag{3.19}$$

Hence, the integral in the last term of Eq. (3.16) is finite at $l=0$, because the integrand is finite everywhere and $\tilde{G}(\vec{k}-\vec{1})$ makes it short ranged in k. Retaining only those terms of order l^2 in Eq. (3.16), we obtain contributions from the first two terms,

$$\frac{2l^2}{\rho} - \frac{e^2l^2}{2\pi\alpha\rho^2a^2} - \frac{l^2}{\rho} \to 0 . \tag{3.20}$$

Hence, solving for a, we get

$$a = (e/\hbar)(m/\pi\rho)^{1/2} , \tag{3.21}$$

in agreement with Gaskell[6] and the result from the effective-potential method of Dunn and Broyles.[14]

The variation of the potential energy enters Eq. (3.16) through the first term in $\tilde{P}(l)$. At small l, the leading term is

$$-(2/\alpha)S^2(l)\tilde{v}(l) \to 0(l^2) . \tag{3.22}$$

Therefore, the condition of Eq. (1.11) is satisfied,

$$\int\left(\frac{\delta V}{\delta u(r)}\right)_{CA}d\vec{r} = \left(\frac{\delta V}{\delta\tilde{u}(l)}\right)_{l=0} = 0 . \tag{3.23}$$

Thus, both conditions on the functional derivative, derived in Sec. I, are satisfied by the CA.

Tedious but straightforward manipulation of Eq. (3.16) for large l reveals that the leading terms are of order l^{-2}. Setting the sum of the coefficients of these terms equal to zero gives the same result as obtained in Sec. II for $u'(0)$.

IV. RPA AND GBSC RELATION

Variational calculations[1,6] have been performed, using the GBSC relation, to obtain $g(r)$ and the RPA for the energy. Both of these approximations are expected to be good only for high densities. However, this section has been included because, within these approximations, the Euler–Lagrange equation may be solved analytically. The RPA[12] for the energy may be written[1]

$$E = E_I + \tfrac{1}{2}\rho \int \tilde{G}\tilde{v}\, d\vec{k}/(2\pi)^3 + \tfrac{1}{4}\alpha\rho \int k^2 \tilde{u}^2 S\, d\vec{k}/(2\pi)^3 . \tag{4.1}$$

Note that this is the same as the CA expression, except that the last term of Eq. (3.5) is missing.

The GBSC relation[6,13] is

$$S = 1 + \rho\tilde{G} = S_I/(1 + \rho\tilde{u}S_I), \tag{4.2}$$

where S_I is the structure factor for an ideal Fermi gas. Then it follows from Eq. (4.2) that

$$\frac{\delta\tilde{G}(k)}{\delta\tilde{u}(l)} = -S^2(k)\delta(\vec{k} - \vec{l}), \tag{4.3}$$

which is the same as the first term in the CA expression given by Eq. (3.15). Setting the variation of the energy with respect to $\tilde{u}(l)$ equal to zero then gives

$$-\tfrac{1}{2}\rho S^2\tilde{v} + \tfrac{1}{2}\alpha\rho l^2 S\tilde{u} - \tfrac{1}{4}\alpha\rho^2 l^2 S^2\tilde{u}^2 = 0 . \tag{4.4}$$

This algebraic equation may be solved using Eq. (4.2) to give

$$\tilde{u} = \frac{2\tilde{v}S_I}{\epsilon + (\epsilon^2 + 2\rho\epsilon\tilde{v}S_I^2)^{1/2}}, \tag{4.5}$$

where $\epsilon = \alpha l^2$. This is the same result obtained by Gaskell.[6] This is to be expected, since the approximations appear to be equivalent, but the derivation is much simpler here.

Note that the asymptotic form is the same as that found using the CA in Sec. III. Also, $u'(0)$ is easily shown to be the same as that obtained in Secs. II and III. Furthermore, both conditions on the functional derivative, Eqs. (1.11) and (1.12), are satisfied.

V. HYPERNETTED-CHAIN AND CONVOLUTION APPROXIMATIONS

In this section, we will obtain some properties of $u(r)$ which are directly applicable to a recent variational calculation,[4] which used the CA for the energy, Eq. (3.5), and the HNC integral equation to obtain $g(r)$. Here, the HNC functional derivative will be applied to the CA energy expression. The HNC approximation is[15]

$$g(r) = e^{N(r) - u(r)}, \tag{5.1}$$

where

$$\tilde{N} = \rho\tilde{G}^2/S. \tag{5.2}$$

The Euler–Lagrange equation obtained from Eq. (3.5) is given by Eq. (3.10). It may be written

$$\tilde{Q}(k) = -2k^2\tilde{u}(k)S(k) + 2S(k)[\nabla\cdot(G\nabla T)]^F, \tag{5.3}$$

where we have introduced

$$\tilde{Q}(k) = \int \tilde{P}(l)\frac{\delta\tilde{G}(\vec{l})}{\delta\tilde{u}(\vec{k})}\, d\vec{l}, \tag{5.4}$$

with T and $\tilde{P}$ defined in Eqs. (3.6) and (3.11). Utilizing the symmetry of the functional derivative, we may write

$$\tilde{Q}(k) = \int \tilde{P}(l)\frac{\delta\tilde{G}(\vec{k})}{\delta\tilde{u}(\vec{l})}\, d\vec{l} . \tag{5.5}$$

We now require the HNC approximation to Q. This can be accomplished by applying the same method as used in Sec. II of Ref. 16 to obtain an integral equation for $\tilde{Q}(k)$. Equation (5.5), here, corresponds to Eq. (2.9) of Ref. 16 and P corresponds to $-V^*$ in Ref. 16. The integral equation for $\tilde{Q}$ is then given by Eq. (2.11) of Ref. 16,

$$\tilde{Q} = -S^2(gP)^F + S^2\{G[(S^2 - 1)\tilde{Q}/S^2]^F\}^F . \tag{5.6}$$

Equation (5.6) must now be solved using the expression for $\tilde{Q}$ in Eq. (5.3). First examine the small-k limit. The first term of Eq. (5.3) dominates at small k. Using the small-k limits of $\tilde{u}$ and S given in Eqs. (3.17) and (3.18), we find

$$\tilde{Q}(k) \to -2k^2/\rho . \tag{5.7}$$

Since the last term in Eq. (5.6) does not contribute to this order and g may be replaced by unity, Eq. (5.6) reduces to

$$-2k^2/\rho \to -k^4\tilde{P}(k)/16\pi^2\rho^2 a^2 . \tag{5.8}$$

We may now use Eq. (3.19) for the small-k form of $\tilde{P}$ and solve for a. We obtain

$$a = (e/\hbar)(m/\pi\rho)^{1/2}, \tag{5.9}$$

in agreement with previous results.

To examine the small-r, large-k limit, replace S by 1 in Eq. (5.3). Also, replace $T(r)$ by $u(r)$ and retain only the $\nabla^2 u$ from the last term. This gives

$$Q(r) \to \frac{4g(r)}{r}\frac{du}{dr} . \tag{5.10}$$

Equation (5.6) reduces to

$$Q(r) \to -g(r)P(r), \tag{5.11}$$

but

$$P(r) \to 2v(r)/\alpha . \tag{5.12}$$

Hence, we find

$$\frac{2}{r}\frac{du}{dr} \to -\frac{e^2}{\alpha r} \tag{5.13}$$

or

$$u'(0) = -1/a_0 \tag{5.14}$$

as before.

VI. CONCLUSIONS

The KSA to the functional derivative has been shown to be unsatisfactory for the electron gas. This is illustrated by the appearance of a long-range term in the variation of the potential energy, which should not be present. However, no evidence has been found to indicate that the KSA to the three-body term in the energy is poor. Indeed, numerical calculations indicate that the KSA and CA energies are in good agreement in the metallic density region.[4] The combination of the RPA and the GBSC relation gives an acceptable asymptotic form; however, these two approximations are generally limited to high densities. The CA gives the same large- and small-r results as the GBSC-RPA. Because of the additional terms present in the CA formulas, the CA may be valid at lower densities than the GBSC-RPA. This has been confirmed by a parametric variational calculation in the metallic density region of the electron gas.[4]

All four methods give identical values for $u'(0)$, except for the GBSC-RPA; this is because the local term in the functional derivative is not approximated. The GBSC-RPA does approximate this term by replacing $g(r)\delta(\vec{r}-\vec{r}\,')$ by $\delta(\vec{r}-\vec{r}\,')$. However, the energy is approximated by replacing $g(r)$ in the second term in Eq. (1.3) by unity. These two errors cancel to give $u'(0)=-1/a_0$.

The CA, GBSC-RPA, and HNC-CA methods give the same asymptotic form for $u(r)$. Hence, we feel that it would be advantageous if parametric variational calculations were to incorporate these limits in the parametric form chosen for $u(r)$. This economy would then allow additional parameters to determine the other features of $u(r)$ more accurately.

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Focusing of Photon Echoes

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It is shown that the radius of curvature R'' of the photon echo is related to the radius of curvature R of the first pulse and R' of the second pulse by $1/R''=2/R'-1/R$ and yields a focusing effect for the photon echo.

I. INTRODUCTION

The anomalous response of an atom or molecule to a sequence of two saturating pulses of visible or infrared radiation has led to the unusual effect which is known as the photon echo.[1,2] After the initial observation of this effect,[2] subsequent efforts were directed toward a study[3] and an explana-