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Generalized Slater-Jastrow trial function: Application to the electron gas at high density

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The function $u(i,j)=u(|\mathbf{r}_i-\mathbf{r}_j|)$, in terms of which variational trial functions of the Slater-Jastrow type are expressed, is generalized to include dependence on the electron momenta as well as on the electron-pair separations. The resulting Euler equations are used to evaluate the ground-state coulomb correlation energy giving $\epsilon_c=0.0622\log(r_s)-0.1441$ Ry, where r_s is the ratio of the radius of a sphere, containing, on average one electron, to the Bohr radius. This correlation energy is 0.050 Ry lower than the corresponding result $\epsilon_c=0.0622\log(r_s)-0.094$ Ry found by Gell-Mann and Brueckner. Also evaluated are the corresponding correlation corrections to the Hartree-Fock (HF) exchange potential energy and to the average exchange charge density as a function of distance. The correction to the HF exchange potential energy is shown to cancel the divergence of the HF exchange energy at the Fermi energy so that the electron effective mass remains finite.

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I. INTRODUCTION

Since the early work of Gaskell[1] the Slater-Jastrow (SJ) trial function has been widely employed in the study of the electron gas.[2–8] This trial function is usually written as

$$\Psi_{\mathrm{SJ}}=\Psi_{\mathrm{HF}}\exp\left[\sum_{i_1\neq i_2=1}^{N}u(i_1,i_2)\right], \tag{1}$$

where $\Psi_{\mathrm{HF}}=|\{[U(j;i)]\}|$ is the Hartree-Fock (HF) determinant and $\{[U(j;i)]\}$ is an $N\times N$ matrix of plane waves

$$U(j;i)=\frac{1}{\sqrt{V}}\exp[\imath k_F\boldsymbol{\beta}(j)\cdot\mathbf{r}_i]\sigma(j) \tag{2}$$

with columns $j=1,2,\ldots,N$ specifying electron momenta $\hbar k_F\boldsymbol{\beta}(j)$ and spin $\sigma(j)$, where $k_F=(3\pi^2N/V)^{1/3}=(3\pi^2n_o)^{1/3}$ is the Fermi momentum and rows $i=1,2,\ldots,N$ specifying electron-coordinate dependence. We shall consider the unpolarized gas where half of the N spins are parallel to a chosen z axis and half antiparallel.

In the present work we will be interested in the high-density regime where r_s, a parameter whose smallness measures the density of the gas, is less than or on the order of unity. In particular, r_s is defined as the ratio of the radius of a sphere containing on average one electron to the Bohr radius so that $r_s=(3/4\pi n_o)^{1/3}/(\hbar^2/me^2)$.

Of the authors referenced above only Talman[6] provides an algebraic relation for the coulomb-correlation energy per electron at high densities. This takes the form[9]

$$\epsilon_T=0.0570\log(r_s)-0.094\ \text{Ry}.$$

We may compare this with the well-known evaluation of the coulomb-correlation energy by Gell-Mann and Brueckner (GB), who employed the random-phase approximation of Rayleigh-Schrödinger perturbation theory to obtain[10]

$$\epsilon_{\mathrm{GB}}=0.0622\log(r_s)-0.094\ \text{Ry}.$$

The Rayleigh-Ritz principle tells us that ϵ_T represents an upper limit for the correlation energy so that, for $r_s<1$, these two estimates are not in conflict since $\epsilon_{\mathrm{GB}}<\epsilon_T$.

There is, however, no *a priori* line of reasoning which guarantees that the GB estimate for the correlation energy is actually correct. Where the ground-state energy of a system has a perturbation series in the appropriate coupling constant then one may expect the diagrammatic methods of quantum-field theory to provide precisely correct results in each order. No such guarantee exists in the case of the electron gas where a perturbation series in the parameter r_s does not exist.[11] Both the HF equations and first-order Rayleigh-Schrödinger perturbation theory are however known to give correctly the first two terms in the expression for the system energy per electron, the HF kinetic and exchange energies, but the question as to the correct form of the correlation energy at high density remains open.

In this work we introduce pair functions which are generalizations of the two electron functions $u(i_1,i_2)$ in Eq. (1). These functions, which depend on the momenta as well as the positions of pairs of electrons, are employed, within the variational framework of the derivation[12] of the original HF equations, to evaluate the correlation energy. The correlation energy thus obtained is found to lie 0.050 Ry *below* ϵ_{GB} so that there is reason to expect that the present estimation of the correlation energy is superior to both the results of Talman and of Gell-Mann and Brueckner.

Just as the GB result, even when extended through the $r_s\log(r_s)$ term,[13,14] cannot be applied successfully at metallic densities, as it predicts a positive and therefore nonphysical result for $r_s\gtrsim 2.5$, neither can the present result. There are a variety of methods which do give the correlation energy in the range $1<r_s<10$ and the results from eight of these have recently been summarized by Unezawa and Tsuneyuki.[15] At $r_s=1$, where formulas valid at high density and at metallic densities may be expected to overlap, our present variational result shows closest agreement with the transcorrelated (TC) method[15,16] where both methods give $\epsilon\approx-0.144$ Ry with slope ≈ 0.06 Ry per unit change in r_s.[17]

The key to successfully generalizing the HF equations to embrace pair functions lies in the choice of the variational trial functions and associated normalization conditions. Since the HF one-electron functions depend on both momentum and spin as well as on position, it is natural to introduce pair functions with an arbitrary dependence on momenta and spin as well as position. This is in contrast to the SJ trial function where the pair functions are dependent on position only. That the correlation energy may be lowered by introducing additional momentum dependence in the trial function is supported by the results of calculations for the correlation energy which include backflow[8] where the single electron functions $U(j;i)$ (plane waves for the electron gas) are modified by the multiplicative factor $\exp[\imath \mathbf{k}\cdot\Sigma_{m\neq i}\eta(|\mathbf{r}_i-\mathbf{r}_m|)(\mathbf{r}_i-\mathbf{r}_m)]$ with η determined so as to minimize the system energy.

II. GENERALIZED SJ TRIAL FUNCTION

In manipulating the SJ trial function with a view toward generalization, we shall find it convenient to introduce antisymmetrizing operators A^j and A_i such that

$$A^j[U(1;1)U(2;2)\cdots U(N;N)] = \sum_{(j_1,j_2,\ldots,j_N)=P(1,2,\ldots,N)} (-1)^P \times U(j_1;1)U(j_2;2)\cdots U(j_N;N), \tag{3}$$

where P is the number of nearest-neighbor interchanges necessary to produce the sequence of integers $\{j_1,j_2,\ldots,j_N\}$ starting from the sequence $\{1,2,\ldots,N\}$ and where $P\{1,2,\ldots,N\}$ is one of the $N!$ permutations of the integers $\{1,2,\ldots,N\}$. A similar relation holds for A_i, i.e.,

$$A_i[U(1;1)U(2;2)\cdots U(N;N)] = \sum_{(i_1,i_2,\ldots,i_N)=P(1,2,\ldots,N)} (-1)^P \times U(1;i_1)U(2;i_2)\cdots U(N;i_N), \tag{4}$$

where now P equals the number of nearest-neighbor interchanges necessary to produce the sequence of integers $\{i_1,i_2,\ldots,i_N\}$ starting from the sequence $\{1,2,\ldots,N\}$. It will be seen that $\Psi_{\mathrm{HF}}=A^j[\Pi_{j=1}^N U(j;j)]=A_i[\Pi_{i=1}^N U(i;i)]$.

Now consider the general term in the expansion of the exponent in Eq. (1). This is

$$T_n=\Psi_{\mathrm{HF}}\frac{1}{n!}\sum_{i_1\neq i_2=1}^{N}\sum_{i_3\neq i_4=1}^{N}\cdots\sum_{i_{2n-1}\neq i_{2n}=1}^{N} u(i_1,i_2) \times u(i_3,i_4)\cdots u(i_{2n-1},i_{2n}) \rightarrow \Psi_{\mathrm{HF}}\frac{1}{n!}\sum_{i_1,i_2,\ldots,i_{2n}=1}^{N}{}' u(i_1,i_2)u(i_3,i_4)\cdots u(i_{2n-1},i_{2n}), \tag{5}$$

where the prime superscript indicates that terms for which one or more pairs of the indices $\{i_1,i_2,\ldots,i_{2n}\}$ become equal are to be omitted from the summation. The final replacement here constitutes a nearly exact equality for $n^2 \ll N$. Sinanoglu[18] has discussed the analogous approximation for atoms and molecules in terms of the negligibility of linked clusters relative to "simultaneous" unlinked clusters.

It might at first appear that we need no terms nonlinear in the pair functions here since we wish to limit ourselves to the consideration of Euler Equations which are no worse that linear in the pair functions. This however is not the case. The presence of terms nonlinear in the pair functions contributes in an essential way to the normalization of the trial function and thus to the Euler Equations and to the correlation energy. For terms with $n \lesssim N$ the replacement in Eq. (5) does indeed change the nature of the trial function; this in a way which renders it more convenient in what follows while substantially modifying only the highly nonlinear portion of the SJ trial function which, historically, has played no role in applications to the electron gas.

We can write T_n in Eq. (5) in terms of a sum over $1\leq i_1 < i_2 < \cdots < i_{2n} \leq N$ as

$$T_n=\Psi_{\mathrm{HF}}\frac{1}{n!}\sum_{1\leq i_1<i_2<\cdots<i_{2n}\leq N} \times \sum_{\{i'_1,i'_2,\ldots,i'_{2n}\}=P\{i_1,i_2,\ldots,i_{2n}\}} u(i'_1,i'_2)\cdots u(i'_{2n-1},i'_{2n}). \tag{6}$$

Positioning Ψ_{HF} now to the *right* of the sum over $1\leq i_1 < i_2 < \cdots i_{2n} \leq N$ in Eq. (6) allows us to repeatedly expand[19] the HF determinant as a sum over columns of products of minors $M=A^j[U(j_1;i_1)\cdots U(j_{2n};i_{2n})]$ with their algebraic compliments, or cofactors, $D(j_1,\ldots,j_{2n};i_1,\ldots,i_{2n})$, where the minors M are formed from elements (i.e., plane waves) in rows $i_1 < i_2 < \cdots i_{2n}$, chosen to agree, for each such expansion, with the (changing) values of the summation indices $\{i\}$ on the right in Eq. (6), and from all possible sets of columns $1\leq j_1 < j_2 < \cdots j_{2n} \leq N$. Specifically we write

$$T_n=\frac{1}{n!}\sum_{1\leq i_1<i_2<\cdots i_{2n}\leq N} \times \sum_{1\leq j_1<j_2<\cdots j_{2n}\leq N} A^j[U(j_1;i_1)\cdots U(j_{2n};i_{2n})] \times D(j_1,\ldots,j_{2n};i_1,\ldots,i_{2n}) \times \sum_{(i'_1,\ldots,i'_{2n})=P(i_1,i_2,\ldots,i_{2n})} u(i'_1,i'_2)\cdots u(i'_{2n-1},i'_{2n}), \tag{7}$$

where $D(j_1,\ldots,j_{2n};i_1,\ldots,i_{2n})=(-1)^{i_1+i_2+\cdots i_{2n}+j_1+j_2+\cdots j_{2n}} \times M'(j_1,\ldots,j_{2n};i_1,\ldots,i_{2n})$ and where, in turn, M' is the $N-2n$ by $N-2n$ minor of Ψ_{HF} obtained by deleting the rows and columns conserved in M.

Next in Eq. (7) we position the determinant $A^j[U(j_1;i_1)\cdots U(j_{2n};i_{2n})]$ to the right of the sum over permutations $P\{i_1,\ldots,i_{2n}\}$ and note that, for each such permutation, we can write

$$A^j[U(j_1;i_1)\cdots U(j_{2n};i_{2n})]=(-1)^P A^j[U(j_1;i'_1)\cdots U(j_{2n};i'_{2n})], \tag{8}$$

where P is the number of nearest-neighbor interchanges necessary to carry the sequence of integers $\{i_1,i_2,\ldots,i_{2n}\}$ into the sequence $\{i'_1,i'_2,\ldots,i'_{2n}\}$. Thus Eq. (7) becomes

$$T_n = \frac{1}{n!} \sum_{\substack{1 \le j_1 < j_2 < \cdots < j_{2n} \le N \\ 1 \le i_1 < i_2 < \cdots < i_{2n} \le N}} A^j \Bigg[\sum_{\{i'_1, \ldots, i'_{2n}\} = P\{i_1, i_2, \ldots, i_{2n}\}} (-1)^P \times U(j_1; i'_1) U(j_2; i'_2) u(i'_1, i'_2) \times \cdots \times U(j_{2n-1}; i'_{2n-1}) U(j_{2n}; i'_{2n}) u(i'_{2n-1}, i'_{2n}) \Bigg] \times D(j_1, \ldots, j_{2n}; i_1, \ldots, i_{2n}), \tag{9}$$

where the square-bracketed quantity will be recognized as the determinant $A_i[U(j_1;i_1)U(j_2;i_2)u(i_1,i_2)\cdots U(j_{2n-1};i_{2n-1}) \times U(j_{2n};i_{2n})u(i_{2n-1},i_{2n})]$.

Thus we have finally

$$T_n = \frac{1}{n!} \sum_{\substack{1 \le j_1 < j_2 < \cdots < j_{2n} \le N \\ 1 \le i_1 < i_2 < \cdots < i_{2n} \le N}} A^j A_i \Bigg[\prod_{k=1}^{2n-1} U(j_k; i_k) U(j_{k+1}; i_{k+1}) \times u(i_k, i_{k+1}) \Bigg] D(j_1, \ldots, j_{2n}; i_1, \ldots, i_{2n}). \tag{10}$$

This form of the Slater-Jastrow trial function lends itself to the generalization

$$U(j_1;i_1)U(j_2;i_2)u(i_1,i_2) \to U(j_1;i_1)U(j_2;i_2)\tilde{f}(j_1,j_2;i_1,i_2) \equiv f(j_1,j_2;i_1,i_2) \tag{11}$$

so that now, instead of a single function u, one has $N(N-1)/2$ pair functions f, one for each pair j_1, j_2; $1 \le j_1 < j_2 \le N$. In terms of the continuum momenta $\hbar k_F \boldsymbol{\beta}_1$, $\hbar k_F \boldsymbol{\beta}_2$; $0 \le \beta_1$, $\beta_2 \le 1$, u (now $\tilde{f}$) will depend on $|\mathbf{r}|$, β_1, β_2, $\mathbf{r} \cdot \boldsymbol{\beta}_1$, $\mathbf{r} \cdot \boldsymbol{\beta}_2$, and $\boldsymbol{\beta}_1 \cdot \boldsymbol{\beta}_2$ where $\mathbf{r} \equiv \mathbf{r}_1 - \mathbf{r}_2$. Thus we have the more general trial function

$$\Psi = \sum_{n=0}^{[N/2]} \frac{1}{n!} \sum_{\substack{1 \le j_1 < j_2 < \cdots < j_{2n} \le N \\ 1 \le i_1 < i_2 < \cdots < i_{2n} \le N}} A_i^j \Bigg[\prod_{k=1}^{2n-1} f(j_k, j_{k+1}; i_k, i_{k+1}) \Bigg] \times D(j_1, \ldots, j_{2n}; i_1, \ldots, i_{2n}), \tag{12}$$

where, by convention, we take the $n=0$ term to be just Ψ_{HF}.

A desirable characteristic of the trial function Eq. (12) becomes apparent upon evaluation of the density matrices

$$\rho^{(m)}(\mathbf{r}'_1, \mathbf{r}'_2, \ldots, \mathbf{r}'_m; \mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_m) = \int d\mathbf{r}_{m+1} d\mathbf{r}_{m+2} \ldots d\mathbf{r}_N \Psi^*(\mathbf{r}'_1, \mathbf{r}'_2, \ldots, \mathbf{r}'_m, \mathbf{r}_{m+1}, \mathbf{r}_{m+2}, \ldots, \mathbf{r}_N) \times \Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_m, \mathbf{r}_{m+1}, \mathbf{r}_{m+2}, \ldots, \mathbf{r}_N),$$

for $m=1,2,3$. Neglecting terms cubic in the pair functions, it can be shown[20] that

$$\rho^{(3)}(\mathbf{r}'_1, \mathbf{r}'_2, \mathbf{r}'_3; \mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = -2\rho^{(1)}(\mathbf{r}'_1; \mathbf{r}_1)\rho^{(1)}(\mathbf{r}'_2; \mathbf{r}_2)\rho^{(1)}(\mathbf{r}'_3; \mathbf{r}_3) + \rho^{(2)}(\mathbf{r}'_1, \mathbf{r}'_2; \mathbf{r}_1, \mathbf{r}_2)\rho^{(1)}(\mathbf{r}'_3; \mathbf{r}_3) + \rho^{(2)} \times (\mathbf{r}'_1, \mathbf{r}'_3; \mathbf{r}_1, \mathbf{r}_3)\rho^{(1)}(\mathbf{r}'_2; \mathbf{r}_2) + \rho^{(2)} \times (\mathbf{r}'_2, \mathbf{r}'_3; \mathbf{r}_2, \mathbf{r}_3)\rho^{(1)}(\mathbf{r}'_1; \mathbf{r}_1),$$

which is the quantum analog of the Mayer cluster expansion[21] when three particle interactions are neglected.

The generalized Slater-Jastrow trial function Eq. (12) has been previously employed to examine coulomb correlations in Be and LiH by Sinanoglu[18] and to the electron gas by Szasz,[22,23] who considered only the $n=0$ and $n=1$ terms, and by Porter,[20] who treated the more general case. [In what follows we shall quote extensively from this latter paper which we shall refer to as I. Equation numbers referenced from this paper are denoted by Eq.(I.eqno).]

Both Porter[20] and Szasz[23] arrived at the conclusion that the one-electron functions and the pair functions are orthogonal in the sense that

$$\int d\mathbf{r}_1 U^*(j'_1;1) f(j_1,j_2;1,2) = 0; \quad j'_1, j_1 \ne j_2 = 1,2, \ldots, N, \tag{13}$$

Szasz, by an *a priori* examination of the trial wave function and Porter by explicit inclusion of all integrals of the form Eq. (13) throughout; whereupon Eq. (13) follows from an inspection of the two electron Euler Equation. In the interest of a simplified notation we shall, in the present work, impose these orthogonality relations from the outset when reporting results from I.

To examine the effect of the nonlinear terms in the pair functions Eq. (12), suppose first that these terms are absent, as in the work of Szasz. Then, if we require that contributions to the system energy from the $n=0$ and $n=1$ terms in Eq. (12) be of order unity (rather that say $1/N$) with respect to one another, the pair functions must be normalized such that $[f(j_1,j_2;1,2), f(j_1,j_2;1,2)]$ is of order unity with respect to N. [Szasz[23] uses $\int |f(j_1,j_2;1,2)|^2 d\mathbf{r}_1 d\mathbf{r}_2 = 1$; $j_1, j_2 = 1, \ldots, N$ where the one-electron functions are required to be orthonormal $[U(j_1;1), U(j_2;1)] = \delta(j_1,j_2)$.] By contrast the presence of the large number of nonlinear terms in Eq. (12) requires [see Eq.(I.7)] the orthogonality relations

$$[U(j'_1;1), U(j_1;1)] + \sum_{j_2=1}^{N} [1 + \lambda(j_2)]^{-1} \times [A^j f(j'_1, j_2; 1,2), A_i^j f(j_1, j_2; 1,2)] = [1 + \lambda(j_1)]\delta(j'_1, j_1); \quad j_1, j'_2 = 1,2, \ldots, N \tag{14}$$

if the pair function contribution is to be of order unity with respect to that of the one-electron functions. Here the normalization constants $\lambda(j)$ are of order unity with respect to N and are determined by Eqs. (2) and (14).

III. CALCULATION OF THE ENERGY INTEGRAL

The one- and two-electron Euler equations result, respectively, from variations with respect to $U^*(j_1;1)$ and $f^*(j_1,j_2;1,2)$ of the system energy integral

$$E=\left[\Psi,\left(-\frac{\hbar^2}{2m}\sum_i \partial^2/\partial\mathbf{r}^2+\sum_{i<j}e^2/|\mathbf{r}_i-\mathbf{r}_j|\right)\Psi\right]/(\Psi,\Psi). \tag{15}$$

Note that no assumptions are made relative to the parametric form of the pair functions, only the parameterization of the many-body wave function in terms of the pair functions is specified as in Eq. (12). Below we shall refer to the one-electron Euler equation as the "generalized HF" equation and to the two-electron Euler equation as the "pair" equation.

The calculation of the energy integral proceeds in two steps: first a calculation of the numerator in Eq. (15) in which only the first two terms $n=0,1$ in Eq. (12) are considered and second the modification of these results to include the quotients remaining after cancellations of the contributions made by the nonlinear terms in Eq. (12) to the numerator and denominator of Eq. (15). To illustrate, consider the contribution to the kinetic energy arising from terms linear in the pair functions in Ψ and Ψ^* to the numerator of Eq. (15). This can be written[24]

$$\sum_{j_1\neq j_2=1}^{N}\left[f(j_1,j_2;1,2),\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial\mathbf{r}_1^2}+\frac{\partial^2}{\partial\mathbf{r}_2^2}\right)A_i^jf(j_1,j_2;1,2)\right],$$

where we have used the orthogonality conditions Eq. (13). If we now include contributions of the nonlinear terms in Eq. (12) to numerator and denominator in Eq. (15) this expression is found[24] to be modified to the form

$$\sum_{j_1\neq j_2=1}^{N}[1+\lambda(j_1)]^{-1}[1+\lambda(j_2)]^{-1}$$
$$\times\left[f(j_1,j_2;1,2),\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial\mathbf{r}_1^2}+\frac{\partial^2}{\partial\mathbf{r}_2^2}\right)A_i^jf(j_1,j_2;1,2)\right], \tag{16}$$

where the $\lambda(j)$, to second order in the pair functions, are given in view of Eqs. (2) and (14), by $\lambda(j_1)=\Sigma_{j_2}[A^jf(j_1,j_2;1,2),A_i^jf(j_1,j_2;1,2)]$. In general, the effect of the nonlinear terms in Eq. (12) is to insert a multiplicative factor $[1+\lambda(j)]^{-1}$ under each appearance of a sum over particle identity j.

If we desire a pair equation linear in the pair functions we need to retain terms only through those quadratic in the pair functions in the energy integral. Thus the only necessary appearances of the factor $[1+\lambda(j)]^{-1}$ are in connection with the HF kinetic- and potential-energy (PE) terms in the energy integral where they contribute to the logarithmic and constant terms in the correlation energy.

IV. EULER EQUATIONS AND THEIR SOLUTION

As in the usual derivation of the HF equations,[12] we associate with the conditions Eq. (14) a matrix of N^2 Lagrange multipliers. It is shown in I that this matrix may be diagonalized to give N real constants $\epsilon(j)$ which are just the generalized HF exchange energies for the electron gas. The lengthy energy integral needed to evaluate Eq. (15) is given explicitly in Eq.(I.15), where terms proportional to the orthogonality integral on the left in Eq. (13) are explicitly retained. (Although integrals of the form Eq. (13) vanish, their *variations* with respect to the one and two electron functions do not.) The Euler equations obtained from Eq. (15) are given in I as Eqs.(I.25) and (I.26). The latter two relations are reproduced here in a more succinct notation in Appendix A in Eqs. (A1) and (A2).

In the following it is convenient to introduce a slightly different notation for the pair functions. Since the trial function Ψ introduces pair functions exclusively in the combination $A_i^jf(j_1,j_2;1,2)$ we lose no generality in requiring $f(j_1,j_2;1,2)=f(j_2,j_1;2,1)$ so that we can write

$$A_i^jf(j_1,j_2;1,2)=2f(j_1,j_2;1,2)-2f(j_2,j_1;1,2)$$
$$\equiv F(j_1,j_2;1,2)-F(j_2,j_1;1,2). \tag{17}$$

With the single electron functions given as in Eq. (2), it is shown in Appendix A that spatial Fourier analysis of the pair equation leads to the following expression for the pair functions to first order in r_s:

$$F(j_1,j_2;1,2)=\frac{\alpha r_s}{2\pi^2}U(j_1;1)U(j_2;2)$$
$$\times\int d\mathbf{q}\,\exp[\imath k_F\mathbf{q}\cdot(\mathbf{r}_1-\mathbf{r}_2)]\Theta(|\mathbf{q}+\boldsymbol{\beta}_1|-1)$$
$$\times\Theta(|\mathbf{q}-\boldsymbol{\beta}_2|-1)\frac{q[\ell(q;z_1)+\ell(q;-z_2)]}{q+z_1-z_2}, \tag{18}$$

where $F(j_1,j_2;1,2)=2f(j_1,j_2;1,2)$ and $z_i=\boldsymbol{\beta}_i\cdot\mathbf{q}/q;\ i=1,2$, and where $\ell(q;z_1)$ satisfies

$$\ell(q;z_1)=-\frac{1}{q^2}\left[q^2+\frac{2\alpha r_s}{\pi}K(q;z_1)\right]^{-1}\left[\frac{1}{2}+\frac{2\alpha r_s}{\pi}\right.$$
$$\left.\times\frac{1}{2\pi}\int_{\beta_2<1}d\boldsymbol{\beta}_2\frac{q\Theta(|\mathbf{q}+\boldsymbol{\beta}_2|-1)\ell(q;z_2)}{q+z_1+z_2}\right]. \tag{19}$$

Here Θ is the unit step function, which vanishes for negative values of its argument, and

$$K(q;z_1)=\frac{1}{2\pi}\int_{\beta_2<1}d\boldsymbol{\beta}_2\frac{\Theta(|\mathbf{q}+\boldsymbol{\beta}_2|-1)}{q^2+q(z_1+z_2)}. \tag{20}$$

Finally we have defined $\alpha=(4/9\pi)^{1/3}$. We have also replaced summations over the indices j_k by integrations over the corresponding β_k; $k=1,2$; each with a sum over the corresponding spin.

In Eq. (18) we have neglected contributions of order (r_s^2) as these do not contribute to the logarithmic or constant terms in the correlation energy with which we are concerned here. Note that Eq. (18) is consistent with the symmetry property $F(j_1,j_2;1,2)=F(j_2,j_1;2,1)$ and with the orthogonality property Eq. (13).

The function F is small everywhere except near the Fermi surface where β_1 and β_2 are $\lesssim 1$. This is consistent with the backflow correction studied by Kwon, Ceperley, and Martin[8] which is largest for $k\lesssim k_F$.

V. CORRELATION ENERGY

The correlation energy per electron $\epsilon_c = E/N - \epsilon_{\mathrm{HF}}$ is obtained from the expression for the system energy E [Eq. (I.15)] through terms quadratic in the pair functions and the HF energy, $\epsilon_{\mathrm{HF}} = 3/(5\alpha^2 r_s^2) - 27\alpha^2/(8r_s)$ Ry, as one over N times the sum of three terms: (1) a kinetic-energy term [this term was incorrectly[24] omitted from Eq. (I.15)]

$$\frac{1}{2}\sum_{j_1 \neq j_2 = 1}^{N} \left\{ F(j_1,j_2;1,2), -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial \mathbf{r}_1^2} + \frac{\partial^2}{\partial \mathbf{r}_2^2}\right) \times [F(j_1,j_2;1,2) - F(j_2,j_1;1,2)] \right\},$$

(2) a potential-energy contribution

$$\sum_{j_1 \neq j_2 = 1}^{N} Re\left\{ U(j_1;1)U(j_2;2), \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} \times [F(j_1,j_2;1,2) - F(j_2,j_1;1,2)] \right\}$$

and (3) a contribution from the normalization constants λ of the form

$$-\sum_{j_1=1}^{N} \lambda(j_1)\left[U(j_1;1), -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial \mathbf{r}_1^2} U(j_1;1) \right],$$

where, up to terms bilinear in the pair functions

$$\lambda(j_1) = \sum_{j_2=1}^{N} [F(j_1,j_2;1,2), F(j_1,j_2;1,2) - F(j_2,j_1;1,2)]. \tag{21}$$

Here we have included exchange corrections to each of the three terms. Such exchange terms were neglected in I but are necessary here to correctly calculate the constant term of ϵ_c.

Using Eq. (18) we find, because of the partial cancellation of terms (1) and (3), and expressing the result in Ry

$$\epsilon_c = [\epsilon_{direct}] + [\epsilon_{exch}] = \frac{3}{\pi^2}\frac{1}{(2\pi)^3}\int_{\beta_1,\beta_2<1} d\mathbf{q}\, d\boldsymbol{\beta}_1 d\boldsymbol{\beta}_2 \frac{q\Theta(|\mathbf{q} + \boldsymbol{\beta}_1| - 1)\Theta(|\mathbf{q} + \boldsymbol{\beta}_2| - 1)}{q + z_1 + z_2} \times \left(\left[q^2[\ell(q;z_1) + \ell(q,z_2)]^2 + \frac{2}{q^2}[\ell(q;z_1) + \ell(q;z_2)] \right] + \left[\frac{1}{2q^2}|\mathbf{q} + \boldsymbol{\beta}_1 + \boldsymbol{\beta}_2|^2 \right] \right). \tag{22}$$

The exchange term, which gives rise to the second square-bracketed term on the right here, includes an additional factor of one half since, for this term, the spins $\sigma(j_1)$ and $\sigma(j_2)$ must agree. Because exchange contributions do not diverge with $r_s \to 0$, limiting values for the functions $\ell(q;z)$, as $r_s \to 0$, from Eq. (19), namely, $\ell(q;z) \to_{r_s \to 0} -1/(2q^4)$, have been invoked. The nine-dimensional integral for ϵ_{exch} in Eq. (22) is identical with the second-order exchange energy encountered in the analysys via Rayleigh-Schrödinger perturbation theory[25] and has been evaluated by Onsager[26] as $\epsilon_{exch} = 0.0484$ Ry.

To evaluate ϵ_{direct} it is convenient to isolate the portion of $\ell(q;z_1)$ which leads to the logarithmically divergent contribution to the correlation energy by introducing in Eq. (19) the new dependent variable

$$\ell 1\left(\frac{q}{\sqrt{2\alpha r_s/\pi}};z_1\right) = \frac{2\alpha r_s}{\pi}\left\{ q^2 \ell(q;z_1) + \frac{1}{2}\left[q^2 + \frac{2\alpha r_s}{\pi}K(q;z_1) \right]^{-1} \right\}. \tag{23}$$

Then, dropping terms of order (r_s) with respect to unity, it is straightforward to show that $\ell 1$ satisfies

$$\ell 1(p;z_1) = \frac{1}{p^2 + k(z_1)}\int_0^1 dz_2 \frac{z_2}{z_1 + z_2} \times \left\{ \frac{1}{2[p^2 + k(z_2)]} - \ell 1(p;z_2) \right\}, \tag{24}$$

where we have defined $p = q/\sqrt{2\alpha r_s/\pi}$ and where

$$k(z) \equiv 1 - z\log[(1+z)/z].$$

Equation (24) is solved numerically in Appendix B.

The integrations over the vectors $\boldsymbol{\beta}$ in Eqs. (19), (20), and (22) are facilitated by adopting cylindrical coordinates (ρ, ϕ, z) with symmetry axis z along $\mathbf{q}$. Then, if $\tilde{F}$ is an arbitrary function of z, we can write

$$(2\pi)^{-1}\int_{\beta<1} d\boldsymbol{\beta}\Theta(|\mathbf{q}+\boldsymbol{\beta}|-1)\widetilde{F}(z) = \begin{cases} q\int_0^{1-q/2} dz_1 z_1 \widetilde{F}(z-q/2) & \\ +\dfrac{1}{2}\int_{1-q}^{1} dz(1-z^2)\widetilde{F}(z); & 0<q<2 \\ \dfrac{1}{2}\int_{-1}^{1} dz(1-z^2)\widetilde{F}(z); & q>2. \end{cases} .$$

Returning to Eq. (22) we find

$$\epsilon_{direct} = \frac{3}{2\pi^2}\Bigg\{ -\int_0^2 \frac{dq}{q^3}\left[\int_{1-q}^{1} dz_1(1-z_1^2)\int_{1-q}^{1} dz_2(1-z_2^2) + 2q\int_{1-q}^{1} dz_1(1-z_1^2)\int_{-q/2}^{1-q} dz_2(2z_2+q)\right]\frac{1}{q+z_1+z_2}$$
$$-\int_2^{\infty}\frac{dq}{q^3}\int_{-1}^{1} dz_1(1-z_1^2)\int_{-1}^{1} dz_2(1-z_2^2)\frac{1}{q+z_1+z_2} + 4\int_0^2 dq q^5\int_0^{1-q/2} dz_1' z_1'\int_0^{1-q/2} dz_2'\frac{z_2'}{z_1'+z_2'}$$
$$\times\left\{q^2[\ell(q;z_1'-q/2)+\ell(q,z_2'-q/2)]^2 + \frac{2}{q^2}[\ell(q;z_1'-q/2)+\ell(q;z_2'-q/2)]\right\}\Bigg\}. \tag{25}$$

Since the initial two integrals over q in Eq. (25) do not diverge as $r_s \to 0$, we have replaced the factor $\{q^2[\ell(q;z_1)+\ell(q;z_2)]^2+(2/q^2)[\ell(q;z_1)+\ell(q;z_2)]\}$ in each of the corresponding integrands by its limiting value $-1/q^6$ as $r_s \to 0$. In the final integral over $0 \le q \le 2$ in Eq. (25), which diverges logarithmically as $r_s \to 0$, we have defined $z_i' = z_i + q/2;\ i=1,2$. In the following we drop these primes, using $z_i' \to z_i;\ \ i=1,2$.

Separating ϵ_{direct} in Eq. (25) into a potential-energy contribution, which depends linearly on ℓ, and a kinetic-energy contribution, which is quadratic in ℓ, and expressing the functions ℓ in terms of $\ell 1$ as in Eq. (23) gives

$$\epsilon_{direct\ \ PE} = -0.38630 + \frac{12}{\pi^2}\int_0^2 dq\int_0^{1-q/2} dz_1 z_1\int_0^{1-q/2} dz_2\frac{z_2}{z_1+z_2}\frac{1}{2}\frac{d}{dq}\{-\log[q^2+2\alpha r_s k(z_1)/\pi]\}$$
$$+\frac{24}{\pi^2}\int_0^{2/\sqrt{2\alpha r_s/\pi}} dp p\int_0^{1-1/2p\sqrt{2\alpha r_s/\pi}} dz_1 z_1 \ell 1(p;z_1)\int_0^{1-1/2p\sqrt{2\alpha r_s/\pi}} dz_2\frac{z_2}{z_1+z_2} \tag{26}$$

and

$$\epsilon_{direct\ \ KE} = 0.19315 + \frac{12}{\pi^2}\int_0^2 dq\int_0^{1-q/2} dz_1 z_1\int_0^{1-q/2} dz_2\frac{z_2}{z_1+z_2}$$
$$\times\frac{1}{8}\frac{d}{dq}\left\{\log[q^2+2\alpha r_s k(z_1)/\pi] + \frac{2\alpha r_s k(z_1)/\pi}{q^2+2\alpha r_s k(z_1)/\pi} + \frac{k(z_1)\log[q^2+2\alpha r_s k(z_1)/\pi] - k(z_2)\log[q^2+2\alpha r_s k(z_2)/\pi]}{k(z_1)-k(z_2)}\right\}$$
$$+\frac{12}{\pi^2}\int_0^{2/\sqrt{2\alpha r_s/\pi}} dp p^3\int_0^{1-1/2p\sqrt{2\alpha r_s \pi}} dz_1 z_1 \ell 1(p;z_1)\int_0^{1-1/2p\sqrt{2\alpha r_s/\pi}} dz_2\frac{z_2}{z_1+z_2}$$
$$\times\left[\ell 1(p;z_1)+\ell 1(p;z_2) - \frac{1}{p^2+k(z_1)} - \frac{1}{p^2+k(z_2)}\right]. \tag{27}$$

Since factors of q^2 scale as r_s under the integrals in Eqs. (26) and (27), we have again replaced in these relations $K(q;z-q/2)$ [$=k(z)+$ terms of order (q^2)] by simply $k(z)$. The initial integral over q in both Eqs. (26) and (27) has been cast in a form suitable for integration by parts on q, while, in the remaining integrals over $\ell 1$, the variable of integration $p=q/\sqrt{2\alpha r_s/\pi}$ has been introduced. Note that upper limits $2/\sqrt{2\alpha r_s/\pi}$ and $1-\frac{1}{2}p\sqrt{2\alpha r_s/\pi}$ appearing in Eqs. (26) and (27) may be replaced, respectively, by infinity and unity if we omit terms of higher order in r_s.

Using the Leibniz integral rule[19] to rewrite the derivatives with respect to q to the *left* of the z_1 and z_2 integrations in Eqs. (26) and (27) and putting $r_s=0$ everywhere except where an infinity would result gives, respectively,

$$\epsilon_{direct\ \mathrm{PE}} = -0.38630 + \frac{6}{\pi^2}\int_0^1 dz_1 z_1 \int_0^1 dz_2 \frac{z_2}{z_1+z_2}\log(2\alpha r_s k(z_1)/\pi) + \frac{12}{\pi^2}\int_0^2 dq \log q \frac{d}{dq}\left(\int_0^{1-q/2} dz_1 z_1 \int_0^{1-q/2} dz_2 \frac{z_2}{z_1+z_2}\right)$$
$$+ \frac{24}{\pi^2}\int_0^\infty dpp \int_0^i dz_1 z_1 \ell 1(p;z_1)\int_0^1 dz_2 \frac{z_2}{z_1+z_2}, \tag{28}$$

and

$$\epsilon_{direct\ KE} = 0.19315 - \frac{3}{2\pi^2}\int_0^1 dz_1 z_1 \int_0^1 dz_2 \frac{z_2}{z_1+z_2}\left\{\log[2\alpha r_s k(z_1)/\pi] + 1 + \frac{k(z_1)\log[2\alpha r_s k(z_1)/\pi] - k(z_2)\log[2\alpha r_s k(z_2)/\pi]}{k(z_1)-k(z_2)}\right\}$$
$$- \frac{6}{\pi^2}\int_0^2 dq \log q \frac{d}{dq}\left(\int_0^{1-q/2} dz_1 z_1 \int_0^{1-q/2} dz_2 \frac{z_2}{z_1+z_2}\right) + \frac{12}{\pi^2}\int_0^\infty dpp^3 \int_0^1 dz_1 z_1 \ell 1(p;z_1)\int_0^1 dz_2 \frac{z_2}{z_1+z_2}$$
$$\times\left[\ell 1(p;z_1) + \ell 1(p;z_2) - \frac{1}{p^2+k(z_1)} - \frac{1}{p^2+k(z_2)}\right]. \tag{29}$$

A more cumbersome alternative to the above procedure for extracting the logarithmic term from ϵ_c consists of writing the q integrations in Eqs. (26) and (27) as sums of integrals over $0 < q < q_c$ and $q_c < q < 2$, where $r_s \ll q_c \ll 1$ and then showing that dependence on q_c vanishes from the final result.[27,28]

Substituting Eqs. (B1) and (B9) in Eqs. (28) and (29) and performing the integrations numerically gives finally

$$\epsilon_{direct\ \mathrm{PE}} = 0.1244 \log r_s - 0.2607 \tag{30}$$

and

$$\epsilon_{direct\ KE} = -0.0622 \log r_s + 0.0682 \tag{31}$$

so that

$$\epsilon_c = \epsilon_{direct\ \mathrm{PE}} + \epsilon_{direct\ KE} + \epsilon_{exch} = 0.0622 \log r_s - 0.1441. \tag{32}$$

[This last result may also be obtained by term by term integration of the Neumann series expansion of Eq. (24).] Equation (32) gives an upper limit for the correlation energy at high density which, for $r_s \gtrsim 10^{-3}$, is approximately 10% *less* than the variational estimate obtained by Talman,[6] from a Slater-Jastrow trial function and about 0.05 Ry less, for all r_s, than the result of Gell-Mann and Brueckner.[10]

VI. VIRIAL THEOREM

In addition to the Rayleigh-Ritz principle, the variational method has the advantage that it allows contributions to the correlation energy, arising from alterations in the kinetic and potential energies as the interaction is turned on, to be separately calculated and thus to allow a test of the virial theorem. For the electron-gas correlation energy $\epsilon_c = \epsilon_{KE} + \epsilon_{\mathrm{PE}}$ with N, the total number of electrons, fixed, the virial theorem gives[29]

$$2\epsilon_{KE} + \epsilon_{\mathrm{PE}} = -r_s \frac{d}{dr_s}\epsilon_{\mathrm{PE}}. \tag{33}$$

Note that, with N fixed, the correlation contribution to the kinetic energy is independent[29] of r_s so that the usual term $-r_s d\epsilon_{KE}/dr_s$ does not appear on the right in Eq. (33). In this connection observe that ϵ_{KE} arises from cancellations between the two nominally infinite terms (1) and (3) above. The latter of these, which is proportional to $\lambda(j_1)$, arises from the normalization contribution to the energy integral. Due to the presence of the Lagrange multipliers introduced in I, such contributions are not subject to variation with respect to the pair functions and thus, in particular, are not subject to variation with respect to r_s.

Splitting ϵ_{exch} into kinetic- and potential-energy contributions, $\epsilon_{exch} = \epsilon_{exch\ KE} + \epsilon_{exch\ \mathrm{PE}}$, we find, using Eqs. (30) and (31),

$$\epsilon_{KE} = \epsilon_{direct\ KE} + \epsilon_{exch\ KE}$$
$$= -0.0622 \log(r_s) + 0.0682 - 0.0484,$$

and

$$\epsilon_{\mathrm{PE}} = \epsilon_{direct\ \mathrm{PE}} + \epsilon_{exch\ \mathrm{PE}} = 0.1244 \log(r_s) - 0.2607 + 0.0968.$$

These kinetic- and potential-energy contributions to the correlation energy satisfy the relation Eq. (33) *exactly* to the accuracy already implicit in Eqs. (30) and (31).

VII. CORRELATION CORRECTION TO THE HF EXCHANGE PE

Here we wish to determine $\epsilon_c(j_1)$, the correlation correction to the HF exchange potential energy.[12] We have $\epsilon(j_1) = \epsilon_{\mathrm{HF}}(j_1) + \epsilon_c(j_1)$ with

$$\epsilon_{\mathrm{HF}}(j_1) = V \sum_{spin(j_1)} \left(U^*(j_1;1)\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial \mathbf{r}_1^2}\right)U(j_1;1) - \sum_{j_2=1}^{N} \int d\mathbf{r}_2 \times U^*(j_1;1)U^*(j_2;2)\frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|}U(j_2;1)U(j_1;2)\right),$$

or, in terms of the rydberg energy unit

$$\epsilon_{\mathrm{HF}}(\beta_1) = \frac{\beta_1^2}{\alpha^2 r_s^2} - \frac{9\alpha^2}{2r_s}\left(1 + \frac{1-\beta_1^2}{2\beta_1}\log\frac{1+\beta_1}{1-\beta_1}\right); \quad 0 < \beta_1 < 1.$$

From the generalized HF equation, Eq. (A1), we have

$$\epsilon_c(j_1) = V \sum_{spin(j_1)} \sum_{j_2=1}^{N} \int d\mathbf{r}_2 U^*(j_1;1)U^*(j_2;2)\frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} \times [F(j_1,j_2;1,2) - F(j_2,j_1;1,2)] \tag{34}$$

so that, using Eq. (18), and expressing the result in rydbergs, we have

$$\epsilon_c(\beta_1) = \frac{1}{\pi^4}\int d\mathbf{q}\int_{\beta_2 \le 1} d\boldsymbol{\beta}_2 \frac{q\Theta(|\mathbf{q}+\boldsymbol{\beta}_1| - 1)\Theta(|\mathbf{q}+\boldsymbol{\beta}_2| - 1)}{q + z_1 + z_2} \times [\ell(q;z_1) + \ell(q;z_2)]\left(\frac{2}{q^2} - \frac{1}{|\mathbf{q}+\boldsymbol{\beta}_1+\boldsymbol{\beta}_2|^2}\right), \tag{35}$$

where again $z_i = \boldsymbol{\beta}_i \cdot \mathbf{q}/q;\ i = 1,2$.

In this section we examine $\epsilon_c(j_1)$ in the limit $r_s \to 0$, with $\beta_1 < 1$. Following this, in the subsection on effective mass, we consider the limit of the derivative $d\epsilon_c(\beta_1)/d\beta_1$ as $\beta_1 \to 1$, with r_s remaining finite.

For simplicity we consider here, for the first of these cases, just the r_s-dependent contribution to $\epsilon_c(\beta_1)$. It is this contribution which is responsible for the logarithmically divergent portion of $\epsilon_{direct\ \mathrm{PE}}$ in Eq. (30). Choosing cylindrical coordinates with z axis along $\mathbf{q}$ for the $\boldsymbol{\beta}_2$ integration and spherical coordinates (q,θ,ϕ) with z axis along $\boldsymbol{\beta}_1$ for the $\mathbf{q}$ integration, and retaining only terms which depend on r_s as $r_s \to 0$, we find

$$\begin{aligned}\epsilon_{\mathrm{c}}(\beta_1) \underset{r_s \approx 0}{\longrightarrow} &- \frac{4}{\pi^2}\int_{1-\beta_1}^{1+\beta_1} dq \int_{(1-\beta_1^2-q^2)/2q\beta_1}^{1} d(\cos\,\theta)\int_0^{1-q/2} \frac{dz_2 z_2}{\frac{q}{2} + \beta_1 \cos\,\theta + z_2} \\ &\times\left[\frac{1}{q^2 + (2\alpha r_s/\pi)K(q;\beta_1 \cos\,\theta)} + \frac{1}{q^2 + (2\alpha r_s/\pi)K\left(q;z_2 - \frac{q}{2}\right)}\right] \\ = &- \frac{4}{(1-b)\pi^2}\int_b^{2-b} dq \int_{b(2-b)/2q}^{1-b+q/2} dz_1' \int_0^{1-q/2} \frac{dz_2 z_2}{z_1' + z_2} \\ &\times\left[\frac{1}{q^2 + (2\alpha r_s/\pi)K\left(q;z_1' - \frac{q}{2}\right)} + \frac{1}{q^2 + (2\alpha r_s/\pi)K\left(q;z_2 - \frac{q}{2}\right)}\right],\end{aligned} \tag{36}$$

where, to obtain the final equality we have defined $z_1' = \beta_1 \cos\,\theta + q/2$ and $b = 1 - \beta_1$.

Next, to examine the behavior of $\epsilon_c(\beta_1)$ for small r_s it is convenient to express $\epsilon_c(\beta_1) = \epsilon_c(1-b)$ in the form

$$\epsilon_c(1-b) = \frac{d}{db}\int_0^b db' \epsilon_c(1-b')$$

so that, dropping the prime from the dummy variable z_1' in Eq. (36)

$$\begin{aligned}\epsilon_c(1-b) \underset{r_s \approx 0}{\longrightarrow} &- \frac{4}{\pi^2}\frac{d}{db}\int_0^b dq \int_0^q \frac{db'}{1-b'}\int_{b'(2-b')/2q}^{1-b'+q/2} dz_1 \\ &\times \int_0^{1-q/2} \frac{dz_2 z_2}{z_1 + z_2}\left[\frac{1}{q^2 + (2\alpha r_s/\pi)k(z_1)} + \frac{1}{q^2 + (2\alpha r_s/\pi)k(z_2)}\right].\end{aligned} \tag{37}$$

To obtain Eq. (37) we have interchanged the order of integration with respect to b' and q in Eq. (36) according to

$$\int_0^b db' \int_{b'}^{2-b'} dq \to \int_0^b dq \int_0^q db' + \int_b^{2-b} dq \int_0^b db' + \int_{2-b}^{2} dq \int_0^{2-q} db' \tag{38}$$

and have observed that only the first integral on the right in the prescription Eq. (38) need be retained as large contributions to the square-bracketed factor in Eq. (36) occur only for $q \approx 0$. In Eq. (37) we have also made use of the observation that $K(q, z - q/2) = k(z)$ plus negligibly small terms of order (q^2).

Setting in Eq. (37), both b' and q to zero in comparison to unity and replacing the variable of integration b' by $x = b'/q$ gives

$$\epsilon_c(1-b) = -\frac{4}{\pi^2}\frac{d}{db}\int_0^b dq \int_0^1 q dx \int_x^1 dz_1 \int_0^1 \frac{dz_2}{z_1+z_2} \times \left[\frac{1}{q^2+(2\alpha r_s/\pi)k(z_1)} + \frac{1}{q^2+(2\alpha r_s/\pi)k(z_2)}\right]. \tag{39}$$

Again interchanging the order of integration

$$\int_0^1 dx \int_x^1 dz_1 \to \int_0^1 dz_1 \int_0^{z_1} dx$$

and carrying out the x integration, which gives just a factor of z_1, we find

$$\begin{aligned}\epsilon_c(1-b) &= -\frac{4}{\pi^2}\frac{d}{db}\int_0^b dqq \int_0^1 dz_1 \int_0^1 \frac{dz_2 z_1 z_2}{z_1+z_2} \times \left[\frac{1}{q^2+(2\alpha r_s/\pi)k(z_1)} + \frac{1}{q^2+(2\alpha r_s/\pi)k(z_2)}\right] \\ &= -\frac{8b}{\pi^2}\int_0^1 \frac{dz_1 z_1 k(z_1)}{b^2+(2\alpha r_s/\pi)k(z_1)}.\end{aligned} \tag{40}$$

Thus

$$\epsilon_c(\beta_1) = -\frac{8}{\pi^2(1-\beta_1)}\int_0^1 \frac{dz_1 z_1 k(z_1)}{1+\mu k(z_1)}, \tag{41}$$

where $\mu \equiv 2\alpha r_s/[\pi(1-\beta_1)^2]$. Because $k(z)$ is a slowly varying function, order three and higher Gauss-Legendre integration can be used to produce accurate approximations to the integral here.

Using Eq. (41) it is straightforward to verify that

$$\epsilon_{direct\ \ \mathrm{PE}} = \frac{3}{8\pi}\int_{\beta_1<1} d\boldsymbol{\beta}_1 \epsilon_c(\beta_1) \underset{r_s\to 0}{\to} 0.1244 \log(r_s)$$

in agreement with Eq. (30).

VIII. ELECTRON EFFECTIVE MASS AT THE FERMI ENERGY

It is known[25] that the effective mass of electrons in jellium

$$\frac{m_{eff}}{m} = 1 + \frac{m}{k_F^2}\frac{d}{\beta_1 d\beta_1}[\epsilon_{\mathrm{HF}}(\beta_1) + \epsilon_c(\beta_1)]$$

remains finite as $\beta_1 \to 1$. This implies that the logarithmic divergence of $d[\epsilon_{\mathrm{HF}}(\beta_1)]/d\beta_1 \to (-2/\pi\alpha r_s)\log(1-\beta_1)$ as $\beta_1 \to 1$ is canceled by a similar divergence of $d\epsilon_c(\beta_1)/d\beta_1$ as $\beta_1 \to 1$. Here we use Eq. (35) to investigate this question.

Once again, the exchange term in Eq. (35) may be neglected as it leads to contributions to the rate of change in ϵ_c with respect to β_1 which do not diverge as $\beta_1 \to 0$. Choosing coordinate axes as above gives a relation similar to that on the immediate right in Eq. (36) except that the contribution of the functions $\ell 1$ in Eq. (23) is now considered, as these latter functions contribute in the limit $\beta_1 \to 1$, with r_s finite.

We have then

$$\begin{aligned}\epsilon_c(\beta_1) \underset{\beta_1\to 1}{\to} \epsilon_{c\ \ direct}(\beta_1) = -\frac{4}{\pi^2}\int_{1-\beta_1}^{1+\beta_1} dq \int_{(1-\beta_1^2-q^2)/2q\beta_1}^{1} d[\cos(\theta)] \int_0^{1-q/2} \frac{dz_2 z_2}{q/2+\beta_1\cos(\theta)+z_2} \Bigg\{ \frac{1}{q^2+(2\alpha r_s/\pi)K[q;\beta_1\cos(\theta)]} \\ -\frac{\pi}{\alpha r_s}\ell 1\left[\frac{q}{\sqrt{2\alpha r_s/\pi}};\beta_1\cos(\theta)\right] + \frac{1}{q^2+(2\alpha r_s/\pi)K(q;z_2)} - \frac{\pi}{\alpha r_s}\ell 1\left[\frac{q}{\sqrt{2\alpha r_s/\pi)}};z_2\right]\Bigg\}\end{aligned} \tag{42}$$

There are several contributions to $d\epsilon_c(\beta_1)/d\beta_1$ but only one of these diverges at $\beta_1 = 1$, this being the contribution arising from the variation in the lower limit of the integration over $\cos(\theta)$. Considering just this contribution, we have

$$\begin{aligned}\frac{d\epsilon_c(\beta_1)}{d\beta_1} \underset{\beta_1\to 1}{\to} \frac{4}{\pi^2}\int_{1-\beta_1}^{1+\beta_1} dq\left(-\frac{1}{2q}\right)\left(\frac{1-q^2}{\beta_1^2}+1\right)\int_0^{1-q/2} \frac{z_2 dz_2}{(1-\beta_1^2)/2q+z_2} \Bigg\{ \frac{1}{q^2+(2\alpha r_s/\pi)K[q;(1-\beta_1^2)/2q-q/2]} \\ -\frac{\pi}{\alpha r_s}\ell 1\left[\frac{q}{\sqrt{(2\alpha r_s/\pi}};\frac{1-\beta_1^2}{2q}-\frac{q}{2}\right] + \frac{1}{q^2+(2\alpha r_s/\pi)K(q;z_2)} - \frac{\pi}{\alpha r_s}\ell 1\left[\frac{q}{\sqrt{(2\alpha r_s/\pi)}};z_2\right]\Bigg\}\end{aligned} \tag{43}$$

Here we are interested in contributions arising from values of q such that $1-\beta_1 < q \ll q_c$, where we may take $q_c \ll r_s$, as these dominate the expression Eq. (43) as $\beta_1 \to 1$. Accordingly, Eq. (43) gives

$$\frac{d\epsilon_c(\beta_1)}{d\beta_1}\underset{\beta_1\to 1}{\to} -\frac{2}{\pi\alpha r_s}\int_{1-\beta_1}^{q_c}\frac{dq}{q}\int_0^1 dz_2\left\{\frac{1}{k[(1-\beta_1)/q]} - 2\ell 1\left(0;\frac{1-\beta_1}{q}\right)+\frac{1}{k(z_2)}-2\ell 1(0;z_2)\right\} \tag{44}$$

Introducing the new variable of integration $z=q_c(1-\beta_1)/q$ in the nontrivial q integrations here, and performing the trivial q integrations, gives

$$\frac{d\epsilon_c(\beta_1)}{d\beta_1}\underset{\beta_1\to 1}{\to} -\frac{2}{\pi\alpha r_s}\left\{\int_{1-\beta_1}^{q_c}\frac{dz}{z}\left[\frac{1}{k(z/q_c)}-2\ell 1(0;z/q_c)\right] + [-\log(1-\beta_1)]\int_0^1 dz_2\left[\frac{1}{k(z_2)}-2\ell 1(0;z_2)\right]\right\} \tag{45}$$

Since $q_c \gg 1-\beta_1$ and since the dominant contributions to the first integrand here arise where $z \gtrsim 1-\beta_1$, we may replace this integrand by $1/k(0^+)-2\ell 1(0;0)=1-2\ell 1(0;0)$. Equation (45) then gives

$$\frac{d\epsilon_c(\beta_1)}{d\beta_1}\underset{\beta_1\to 1}{\to} = \frac{2\log(1-\beta_1)}{\pi\alpha r_s}\left\{1-2\ell 1(0;0) + \int_0^1 dz_2\left[\frac{1}{k(z_2)}-2\ell 1(0;z_2)\right]\right\}. \tag{46}$$

Numerical integration in the second integral here gives 1.00003 while $1-2\ell 1(0;0)$ evaluates numerically to 0.001. However putting $p=0$ and $z_1\to 0$ in the integral equation Eq. (24) gives the more exact result

$$\int_0^1 dz_2\left[\frac{1}{k(z_2)}-2\ell 1(0;z_2)\right] = 2\ell 1(0;0).$$

Thus we have cancellation of the divergence of $d\epsilon(\beta_1)/d\beta_1$ as $\beta_1\to 1$ so that the effective electron mass remains finite at the Fermi energy.

IX. CORRELATION CORRECTION TO THE EXCHANGE CHARGE DENSITY

The probability density at a distance r from one electron and averaged over all electrons is given by $\rho(r)=\rho_{\mathrm{HF}}(r)+\rho_c(r)$, where[12]

$$\rho_{\mathrm{HF}}(r) = \frac{V}{N}\sum_{j_1\neq j_2=1}^{N} U^*(j_1;1)U^*(j_2;2)U(j_2;1)U(j_1;2) = \frac{n_o}{2}\left[3\frac{\sin k_F r - k_F r\cos k_F r}{(k_F r)^3}\right]^2 \tag{47}$$

and

$$\rho_c(r) = -\frac{V}{N}\sum_{j_1\neq j_2=1}^{N} U^*(j_1;1)U^*(j_2;2)[F(j_1,j_2;1,2) - F(j_2,j_1;1,2)]. \tag{48}$$

This function is closely related to both the diagonal terms of the second-order density matrix, Eq.(I.27) and, in view of Eq. (11), to the Slater-Jastrow pair function $u(r)$. The calculation of $\rho_c(r)$ is much simplified by considering only the leading term in r_s and by expanding in powers of $1/(k_F r)$. With $F(j_1,j_2;1,2)$ from Eq. (18), the direct contribution to $\rho_c(r)$ becomes

$$\rho_{c\ direct}(r) = n_o\left(\frac{3}{4\pi}\right)^2\frac{\alpha r_s}{2\pi^2}\int d\mathbf{q}\int_{\beta_1,\beta_2<1} d\boldsymbol{\beta}_1 d\boldsymbol{\beta}_2 \times\frac{q\Theta(|\mathbf{q}+\boldsymbol{\beta}_1|-1)\Theta(|\mathbf{q}+\boldsymbol{\beta}_2|-1)}{q+z_1+z_2}\left(\frac{1}{q^4}\right), \tag{49}$$

where we have taken the limit as $r_s\to 0$ in the integrand and have considered that $\ell 1(p;z)\sim p^{-4}$ for large p. Here again we define $z_i=\mathbf{q}\cdot\boldsymbol{\beta}_i/q$, for $i=1,2$.

Introducing cylindrical coordinates for the $\boldsymbol{\beta}_1$ and $\boldsymbol{\beta}_2$ integrations and spherical coordinates, with z axis along $\mathbf{r}$, for the $\mathbf{q}$ integration, we find

$$\rho_{c\ direct}(r) = \frac{9}{2\pi}\frac{n_o\alpha r_s}{k_F r}\left[\int_0^2 dq\,\sin(k_F r q)f(q) + \int_2^\infty dq\,\sin(k_F r q)f1(q)\right], \tag{50}$$

where we have also performed the integrations over the angles θ and ϕ specifying $\mathbf{q}/q$. Here

$$f(q) \equiv \int_0^{1-q/2} dz_1 z_1\int_0^{1-q/2} dz_2\frac{z_2}{z_1+z_2} + \frac{1}{q}\int_0^{1-q/2} dz_1 z_1\int_{1-q}^{1} dz_2\frac{(1-z_2)^2}{q/2+z_1+z_2} + \frac{1}{4q^2}\int_{1-q}^{1} dz_1(1-z_1^2)\int_{1-q}^{1} dz_2\frac{(1-z_2)^2}{q+z_1+z_2} \tag{51}$$

and

$$f1(q) \equiv \frac{1}{4q^2}\int_{-1}^{1} dz_1(1-z_1^2)\int_{-1}^{1} dz_2\frac{(1-z_2^2)}{q+z_1+z_2}. \tag{52}$$

Since the integrands in Eq. (50) (as well as their first derivatives) become equal at $q=2$, $\rho_{c\ direct}(r)$ has no $\cos(2k_F r)$ dependence at lowest order in $1/(k_F r)$. Integrating in Eq. (50) by parts gives

$$\rho_{c\ direct}(r) = \frac{9}{2\pi}\frac{n_o\alpha r_s}{k_F r}\left[-\frac{\cos(k_F r q)}{k_F r}f(q)\Big|_0^2 + \int_0^2 dq f'(q)\frac{\cos(k_F r q)}{k_F r} - \frac{\cos(k_F r q)}{k_F r}f1(q)\Big|_2^\infty + \int_2^\infty dq f1'(q)\frac{\cos(k_F r q)}{k_F r}\right] \tag{53}$$

and continuing with such integrations gives

$$\rho_{c\ direct}(r) = \frac{9\alpha r_s}{2\pi k_F r}\left\{\frac{f(0^+)}{k_F r} - \frac{f''(0^+)}{(k_F r)^3} + \frac{\cos(2k_F r)}{(k_F r)^3}\right.$$
$$\left.\times[f''(2^-) - f1''(2^+)] + \cdots\right\}$$
$$= \frac{3}{\pi} n_o \alpha r_s\left[\frac{1-\log(2)}{(k_F r)^2} + \frac{1-\cos(2k_F r)}{8(k_F r)^4}\right.$$
$$\left. + O(k_F r)^{-6}\right]. \tag{54}$$

Substituting from Eq. (18), the exchange term in Eq. (48) becomes

$$\rho_{c\ exch}(r) = -n_o\left(\frac{3}{4\pi}\right)^2\frac{\alpha r_s}{2\pi^2}\int_{\beta_1,\beta_2<1} d\boldsymbol{\beta}_1 d\boldsymbol{\beta}_2$$
$$\times\exp[\imath k_F\mathbf{r}\cdot(\boldsymbol{\beta}_1+\boldsymbol{\beta}_2)]\int d\mathbf{q}\,\exp(\imath k_F\mathbf{q}\cdot\mathbf{r})$$
$$\times\frac{q\Theta(|\mathbf{q}+\boldsymbol{\beta}_1|-1)\Theta(|\mathbf{q}+\boldsymbol{\beta}_2|-1)}{q+z_1+z_2}\left(\frac{1}{2q^4}\right), \tag{55}$$

where again $z_i=\mathbf{q}\cdot\boldsymbol{\beta}_i/q$; $i=1,2$. Here $\rho_{c\ exch}(r)$ falls off with increasing $k_F r$ much more rapidly than does $\rho_{c\ direct}(r)$ and hence is negligible. This is because each of the $\boldsymbol{\beta}$ integrations in Eq. (55) produces an additional factor $(k_F r)^{-5/2}$ relative to the direct term. It is evident that $\rho_{c\ direct}(r)$ in Eq. (54) dominates the HF exchange probability density for $k_F r \gtrsim 1/\sqrt{r_s}$.

For $r\to 0$, $\rho_c(r)$ vanishes for parallel spins due to the exchange term. For antiparallel spins, inspection of Eq. (50), where $\sin(k_F rq)/(k_F rq) < 1$ for all $q>0$, shows that $\rho_{c\ direct}(r)$ has a maximum. Thus, to the extent that the wave function Eq. (12) can be approximated by a Slater-Jastrow trial function, that is, by Eq. (1) with $u(r)=-\rho_c(r)/n_o$, Ψ attains a minimum as any pair of electrons approach one another, regardless of spin.

APPENDIX A: EULER-LAGRANGE EQUATIONS

In the following we refer to the one-electron Euler equation as the generalized HF equation because of its obvious similarity the HF equation(s). The generalized HF equation with the electron-gas Hamiltonian is

$$\left[\epsilon(j_1) + \frac{\hbar^2}{2m}\frac{\partial^2}{\partial\mathbf{r}_1^2}\right]U(j_1;1)$$
$$= \sum_{j_2=1}^{N}[1-\lambda(j_2)]\int_V d\mathbf{r}_2 U^*(j_2;2)\frac{e^2}{|\mathbf{r}_1-\mathbf{r}_2|}U(j_1;1)U(j_2;2)$$
$$+ \sum_{j_2=1}^{N}\int_V d\mathbf{r}_2 U^*(j_2;2)\frac{e^2}{|\mathbf{r}_1-\mathbf{r}_2|}[-U(j_2;1)U(j_1;2)$$
$$+ F(j_1,j_2;1,2) - F(j_2,j_1;1,2)], \tag{A1}$$

where we have neglected terms quadratic in the pair functions with the single exception of the product of the nominally infinite Hartree term with the normalization constants $\lambda(j)$. The Hartree term is canceled by contributions to the system energy from the background of compensating positive charge in which the electrons move.[11]

The pair equation can be expressed succinctly in terms of the projection operators $\widetilde{P}(\mathbf{r}_i)$, where $\widetilde{P}(\mathbf{r}_i)$ projects from its operand that portion orthogonal to each of the $\{U(j;i)\}$; $j=1,2,\ldots,N$, $i=1,2$. For example, for $i=1$

$$\widetilde{P}(\mathbf{r}_1) = 1 - \sum_{j_1'=1}^{N} U(j_1';1)\int_V d\mathbf{r}_1' U^*(j_1';1')\widetilde{\bigcirc}(\mathbf{r}_1\to\mathbf{r}_1'), \tag{A2}$$

where, in turn, $\widetilde{\bigcirc}(\mathbf{r}_1\to\mathbf{r}_1')$ acts to replace coordinates $\mathbf{r}_1$ by $\mathbf{r}_1'$. Neglecting terms quadratic in the pair functions, the pair equation Eq.(I.26) is

$$\left[\epsilon(j_1) + \epsilon(j_2) + \frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial\mathbf{r}_1^2} + \frac{\partial^2}{\partial\mathbf{r}_2^2}\right)\right]A_i^j f(j_1,j_2;1,2)$$
$$= \widetilde{P}(\mathbf{r}_1)\widetilde{P}(\mathbf{r}_2)\frac{e^2}{|\mathbf{r}_1-\mathbf{r}_2|}A^j[U(j_1;1)U(j_2;2) + A_i f(j_1,j_2;1,2)] + \widetilde{P}(\mathbf{r}_1)\sum_{j_3=1}^{N}\int_V d\mathbf{r}_3 U^*(j_3;3)\frac{e^2}{|\mathbf{r}_1-\mathbf{r}_3|}$$
$$\times A^j[U(j_1;1)A_i f(j_2,j_3;2,3)] + \widetilde{P}(\mathbf{r}_2)\sum_{j_3=1}^{N}\int_V d\mathbf{r}_3 U^*(j_3;3)\frac{e^2}{|\mathbf{r}_2-\mathbf{r}_3|}A^j[U(j_2;2)A_i f(j_1,j_3;1,3)]$$
$$+ \sum_{j_3=1}^{N}\int_V d\mathbf{r}_3 U^*(j_3;3)\left(\frac{e^2}{|\mathbf{r}_1-\mathbf{r}_3|} + \frac{e^2}{|\mathbf{r}_2-\mathbf{r}_3|}\right)A^j[U(j_3;3)A_i f(j_1,j_2;1,2)]. \tag{A3}$$

Since $A_i^j f(j_1,j_2;1,2)=F(j_1,j_2;1,2)-F(j_2,j_1;1,2)$, it is clear that the pair equation Eq. (A3) consists of the difference of two relations, one giving $F(j_1,j_2;1,2)$ in terms of $F(j_1,j_2;1,2)$ and $F(j_2,j_1;1,2)$ and a second relation which duplicates the first, with the exception only that the roles of j_1 and j_2 are reversed. Consequently, we retain the physical content of Eq. (A3) by considering only the first of these relations

$$\begin{aligned}&\left[\epsilon(j_1)+\epsilon(j_2)+\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial\mathbf{r}_1^2}+\frac{\partial^2}{\partial\mathbf{r}_1^2}\right)\right]F(j_1,j_2;1,2)\\
&\quad=\tilde{P}(\mathbf{r}_1)\tilde{P}(\mathbf{r}_2)\frac{e^2}{|\mathbf{r}_1-\mathbf{r}_2|}[U(j_1;1)U(j_2;2)+F(j_1,j_2;1,2)]\\
&\qquad+\tilde{P}(\mathbf{r}_1)\sum_{j_3=1}^{N}\int_V d\mathbf{r}_3U^*(j_3;3)\frac{e^2}{|\mathbf{r}_1-\mathbf{r}_3|}[U(j_1;1)F(j_2,j_3;2,3)-U(j_1;1)F(j_3,j_2;2,3)+U(j_3;2)F(j_1,j_2;2,3)]\\
&\qquad+\tilde{P}(\mathbf{r}_2)\sum_{j_3=1}^{N}\int_V d\mathbf{r}_3U^*(j_3;3)\frac{e^2}{|\mathbf{r}_2-\mathbf{r}_3|}[U(j_2;2)F(j_1,j_3;1,3)-U(j_2;2)F(j_3,j_1;1,3)+U(j_3;2)F(j_2,j_1;1,3)]\\
&\qquad+\sum_{j_3=1}^{N}\int_V d\mathbf{r}_3U^*(j_3;3)\left(\frac{e^2}{|\mathbf{r}_1-\mathbf{r}_3|}+\frac{e^2}{|\mathbf{r}_2-\mathbf{r}_3|}\right)[U(j_3;3)F(j_1,j_2;1,2)+U(j_1;3)F(j_2,j_3;1,2)+U(j_2;3)F(j_3,j_1;1,2)].\end{aligned}\tag{A4}$$

The initial terms in each of the four square-bracketed factors on the right in Eq. (A4) determine the pair functions to first order in r_s. The remaining exchange terms make contributions to F which are bilinear in r_s and which do not contribute to the logarithmic or constant terms of the correlation energy. We drop these terms in what follows.

The initial term in the final square-bracketed factor of Eq. (A4) is nominally infinite, and, together with the initial term on the right in Eq. (A1), is canceled when terms associated with the positive charged background are included in the Hamiltonian. To explain this cancellation in more detail we note that the effect of the background of positive charge is to cancel the Hartree term

$$\sum_{j_1\neq j_2}\left[U(j_1;1)U(j_2;2),\frac{e^2}{|\mathbf{r}_1-\mathbf{r}_2|}U(j_1;1)U(j_2;2)\right]$$

from the system energy E. In the energy expression for E, Eq.(I.15), the HF Hartree term appears as the sum of two terms

$$\begin{aligned}&\frac{1}{2}\sum_{j_1\neq j_2}[1+\lambda(j_1)]^{-1}[1+\lambda(j_2)]^{-1}\\
&\quad\times\left[U(j_1;1)U(j_2;2),\frac{e^2}{|\mathbf{r}_1-\mathbf{r}_2|}U(j_1;1)U(j_2;2)\right]\quad\text{and}\\
&\frac{1}{2}\sum_{j_1\neq j_2,j_3}\left[F(j_1,j_2;1,2)U(j_3;3),\left(\frac{e^2}{|\mathbf{r}_1-\mathbf{r}_3|}\right.\right.\\
&\quad\left.\left.+\frac{e^2}{|\mathbf{r}_2-\mathbf{r}_3|}\right)U(j_3;3)F(j_1,j_2;1,2)\right].\end{aligned}$$

Because of the introduction of Lagrange multipliers in I, variations in the normalization integral (Ψ,Ψ) of Eq. (15) are not calculated. Thus, since the factor $[1+\lambda(j_1)]^{-1}[1+\lambda(j_2)]^{-1}\approx[1-\lambda(j_1)-\lambda(j_2)]$ above arises from this normalization integral, [see Eq. (I.A15)], only the latter of these two separately infinite terms contributes to Eq. (A3). It is this contribution which gives the direct part of the final term in Eq. (A4). Thus this final term, as well as the Hartree term in Eq. (A1), modified now by the factor $[1+\lambda(j_3)]^{-1}\approx[1-\lambda(j_3)]$, is canceled, up to terms quadratic in the pair functions, by the self-energy of the positively charged background.

Next, since $U^*(j_1;1)U^*(j_2;2)F(j_1,j_2;1,2)$ contributes to the diagonal part of the second-order density matrix given in I, this product must depend only on the difference $(\mathbf{r}_1-\mathbf{r}_2)$. Thus we may express the pair functions in terms of their Fourier transforms $f[\mathbf{q};\boldsymbol{\beta}(j_1),\boldsymbol{\beta}(j_2)]$ as

$$\begin{aligned}F(j_1,j_2;1,2)&=V^2U(j_1;1)U(j_2;2)\frac{k_F^3}{(2\pi)^3}\int d\mathbf{q}\\
&\quad\times\exp[\imath k_F\mathbf{q}\cdot(\mathbf{r}_1-\mathbf{r}_2)]f[\mathbf{q};\boldsymbol{\beta}(j_1),\boldsymbol{\beta}(j_2)];\\
&\quad j_1\neq j_2=1,2,\ldots,N\end{aligned}\tag{A5}$$

In these equations, as well as in what follows, the momenta are measured in units of the Fermi momentum k_F.

Multiplying on right and left in Eq. (A4) by $U^*(j_1;1)U^*(j_2;2)$ and taking the Fourier transform with respect to $\mathbf{r}_1-\mathbf{r}_2$ gives, putting

$$\frac{1}{N}\sum_{j_3}\rightarrow\sum_{spin(j_3)}\frac{3}{8\pi}\int_{\beta(j_3)<1}d\boldsymbol{\beta}(j_3)\tag{A6}$$

and with $\epsilon(j)\approx\beta^2(j)/\alpha^2r_s^2$ from Eq. (A1)

$$\begin{aligned}&[q^2+\mathbf{q}\cdot(\boldsymbol{\beta}_1-\boldsymbol{\beta}_2)]f(\mathbf{q};\boldsymbol{\beta}_1,\boldsymbol{\beta}_2)+\frac{\alpha r_s}{\pi^2q^2}\int_{\beta_3<1}d\boldsymbol{\beta}_3[\Theta(|\mathbf{q}+\boldsymbol{\beta}_1|\\
&\quad-1)f(\mathbf{q};\boldsymbol{\beta}_3,\boldsymbol{\beta}_2)+\Theta(|\mathbf{q}-\boldsymbol{\beta}_2|-1)f(\mathbf{q};\boldsymbol{\beta}_1,\boldsymbol{\beta}_3)]\\
&\quad=-\frac{4\alpha r_sn_o}{3\pi N^2q^2}\Theta(|\mathbf{q}+\boldsymbol{\beta}_1|-1)\Theta(|\mathbf{q}-\boldsymbol{\beta}_2|-1)\end{aligned}\tag{A7}$$

Here we have defined $\alpha=(4/9\pi)^{1/3}$ and have written $\boldsymbol{\beta}_i$ for $\boldsymbol{\beta}(j_i)$; $i=1,2,3$. Also Θ is the unit step function which vanishes for negative values of its argument. Sums over spins $\sigma(j)$ give an additional factor of 2.

It can be verified by direct substitution that a solution of Eq. (A7) can be written in the form

$$f(\mathbf{q};\boldsymbol{\beta}_1,\boldsymbol{\beta}_2) = \frac{4\alpha r_s n_o}{3\pi N^2}\Theta(|\mathbf{q}+\boldsymbol{\beta}_1|-1)\Theta(|\mathbf{q}-\boldsymbol{\beta}_2|-1) \times \frac{q[\ell(q;z_1)+\ell(q;-z_2)]}{q+z_1-z_2}, \tag{A8}$$

where $z_i = \boldsymbol{\beta}_i\cdot\mathbf{q}/q$; $i=1,2$; $0\leq z_1$, $z_2\leq 1$ and where $\ell(q;z_1)$ satisfies Eq. (19). Substitution of Eq. (A8) in Eq. (A5) gives Eq. (18).

APPENDIX B: NUMERICAL SOLUTION OF EQ. (24)

Our approach here is to first obtain a symmetric kernel through a change of dependent variable in Eq. (24) and then to approximate this kernel as a sum of products of the Chebyshev polynomials. Inserting the change of dependent variable

$$n(p;z_1) \equiv \sqrt[4]{1-(2z_1-1)^2}\sqrt{z_1[p^2+k(z_1)]}\times \ell 1(p;z_1) \tag{B1}$$

into Eq. (24) shows that n satisfies the integral equation

$$n(p;z_1) = \int_0^1 dz_2 \frac{G(p;z_1,z_2)-H(p;z_1,z_2)n(p;z_2)}{\sqrt{1-(2z_2-1)^2}}, \tag{B2}$$

where

$$G(p;z_1,z_2) \equiv \frac{z_2\sqrt{z_1}\sqrt[4]{1-(2z_1-1)^2}\sqrt{1-(2z_2-1)^2}}{2(z_1+z_2)\sqrt{[p^2+k(z_1)][p^2+k(z_2)]}}$$

and where $H(p;z_1,z_2)=H(p;z_2,z_1)$ is given by

$$H(p;z_1,z_2) \equiv \frac{\sqrt{z_1z_2}\sqrt[4]{[1-(2z_1-1)^2][1-(2z_2-1)^2]}}{(z_1+z_2)\sqrt{[p^2+k(z_1)][p^2+k(z_2)]}}.$$

The solution of Eq. (B2) is facilitated by approximating the kernel H, as well as the function G, by a sum of products of the first $\tilde{N}$ Chebyshev polynomials[30]

$$T_j(z) = \cos[j\arccos(z)];\quad j=0,1,\ldots,\tilde{N}-1$$

as

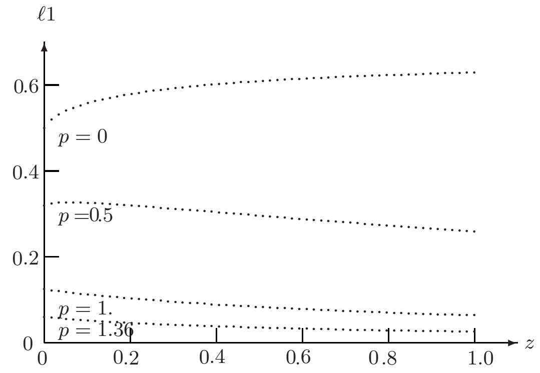

FIG. 1. $\ell 1(p;z)$ vs z for $p=0,0.5,1,1.36$.

$$G(p;z_1,z_2) \approx \sum_{j,k=1}^{\tilde{N}} g_{j,k}T_{j-1}(2z_1-1)T_{k-1}(2z_2-1) \tag{B3}$$

and

$$H(p;z_1,z_2) \approx \sum_{j,k=1}^{\tilde{N}} h_{j,k}T_{j-1}(2z_1-1)T_{k-1}(2z_2-1), \tag{B4}$$

where

$$g_{j,k} = \frac{4}{\tilde{N}^2}\left(1-\frac{\delta_{j,1}}{2}\right)\left(1-\frac{\delta_{k,1}}{2}\right) \times \sum_{n,m=1}^{\tilde{N}} G\left(p;\frac{X_{2,n}+1}{2},\frac{X_{2,m}+1}{2}\right)X_{j,n}X_{k,m}$$

with an exactly similar expression for $h_{j,k}$ in terms of $H(p;z_1,z_2)$. Here, in turn

$$X_{i,j} \equiv \cos\left[\pi\frac{(i-1)(j-1/2)}{\tilde{N}}\right].$$

In view of the orthogonality and normalization relations satisfied by the Chebyshev polynomials

$$\int_0^1 dz\frac{T_{i-1}(2z-1)T_{j-1}(2z-1)}{\sqrt{1-(2z-1)^2}} = \frac{\pi}{4}\delta_{i,j}(1+\delta_{i,1});$$

$$i,j=1,2,\ldots,\tilde{N} \tag{B5}$$

substituting Eqs. (B3) and (B4) into Eq. (B2) gives

$$n(p;z_1) = \sum_{j=1}^{\tilde{N}}\left(\frac{\pi}{2}g_{j,1}-\sum_{k=1}^{\tilde{N}}h_{j,k}\zeta_k\right)T_{j-1}(2z_1-1). \tag{B6}$$

In Eq. (B6) we have defined

$$\zeta_i = \int_0^1 dz_1 T_{i-1}(2z_1-1)\frac{n(p;z_1)}{\sqrt{1-(2z_1-1)^2}}.$$

Multiplying through in Eq. (B6) by

$$\left(1-\frac{\delta_{i,1}}{2}\right)\frac{T_{i-1}(2z_1-1)}{\sqrt{1-(2z_1-1)^2}}$$

for each $i=1,2,\ldots,\tilde{N}$ and integrating over $0\leq z_1\leq 1$ gives, in view of Eq. (B5)

$$\left(1-\frac{\delta_{i,1}}{2}\right)\zeta_i = \frac{\pi^2}{8}g_{i,1}-\frac{\pi}{4}\sum_{j=1}^{\tilde{N}}h_{i,j}\zeta_j;\quad i=1,2,\ldots,\tilde{N}. \tag{B7}$$

Rearranging, we may write

$$M\boldsymbol{\zeta} = \mathbf{c}, \tag{B8}$$

where $M\equiv[(m_{i,j})]$ is the symmetric, positive definite $\tilde{N}\times\tilde{N}$ matrix with elements

$$m_{i,j} = \frac{\pi}{4} h_{i,j} + \delta_{i,j}\left(1 - \frac{\delta_{i,1}}{2}\right)$$

and where $\mathbf{c}$ and $\boldsymbol{\zeta}$ are column vectors

$$\mathbf{c} = \frac{\pi^2}{8}[g_{1,1}, g_{2,1}, \ldots, g_{\tilde{N},1}]^T$$

and

$$\boldsymbol{\zeta} = [\zeta_1, \zeta_2, \ldots, \zeta_{\tilde{N}}]^T.$$

Solving Eq. (B8) for $\boldsymbol{\zeta} = M^{-1}\mathbf{c}$ and substituting in Eq. (B6) gives finally

$$n(p;z_1) = \sum_{j=1}^{\tilde{N}} \left[\frac{\pi}{2} g_{j,1} - \sum_{k=1}^{\tilde{N}} h_{j,k}(M^{-1}\mathbf{c})_k \right] T_{j-1}(2z_1 - 1), \tag{B9}$$

whence $\ell 1$ follows from Eq. (B1).

In the present work we have used $\tilde{N} = 30$, as larger $\tilde{N}$ give little added accuracy. Additional accuracy was, however, obtained by replacing $\ell 1(p;z)$ by its equivalent on the right in Eq. (24), thus reducing the concentration of error near $z = 0$, and then by putting $\ell 1_{\text{best}}(p;z) = \ell 1(p;z) + \delta(p;z)$, where $\delta(p;z)$ satisfies an integral equation of the form Eq. (24) except now with an inhomogeneous term on the order of 10^3 times smaller than that found in Eq. (24). The method of solution above was then reapplied to $\delta(p;z)$. This diminished the quotient of the difference in right- and left-hand members of Eq. (24), when evaluated with $\ell 1(p;z) = \ell 1_{\text{best}}(p;z)$, to $\ell 1_{\text{best}}(p;z)$ itself to less than 10^{-4} for all $p \geq 0$ and $0.02 \leq z \leq 1$ and 10^{-3} for all p and $0 \leq z < 0.02$.

Solutions were obtained over a 60×60 grid of $(p;z)$ values. Equally spaced z values, $z_i = (i-1)/59$ were used with the exception of z_1 which was taken to be 0.00035 to avoid numeric instability. Cubic extrapolation from results at $z = z_1, z_2, z_3$, and z_4 was then used, for each value of p considered, to estimate the result at $z = 0$. For p, 31 equally spaced values on $[0,1]$ plus 29 values between 1 and 30, as determined from the reciprocals of those values chosen on (0,1), were used. Cubic spline interpolation from these 3600 values completed the solution for $p \leq 10$. For p greater than 10, $\ell 1(p;z)$ falls off almost exactly as p^{-4}; and, $\ell 1(p;z)$ attains values no larger than 10^{-4}, times those typically realized for $0 < p < 1$. Since the cubic spline interpolations, otherwise employed, produce small nonphysical oscillations in the unexamined intervals $10 < p < 15$ and $15 < p < 30$; we replaced $\ell 1(p;z)$; by $\ell 1(10;z) \times (10/p)^4$; for; $p > 10$.

Figure 1, which is based on data generated by MATHCAD,[31] shows plots of $\ell 1(p;z)$ for values 0., 0.5, 1, and 1.36 of the parameter p.

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[1] T. Gaskell, Proc. Phys. Soc. Lond. **77**, 1182 (1961).

[2] M. S. Becker, A. A. Broyles, and T. Dunn, Phys. Rev. **175**, 224 (1968).

[3] D. K. Lee and F. H. Ree, Phys. Rev. A **6**, 1218 (1972).

[4] M. A. Pokrant and F. A. Stevens, Jr., Phys. Rev. A **7**, 1630 (1973).

[5] F. A. Stevens, Jr. and M. A. Pokrant, Phys. Rev. A **8**, 990 (1973).

[6] J. D. Talman, Phys. Rev. A **10**, 1333 (1974).

[7] D. Ceperley, Phys. Rev. B **18**, 3126 (1978).

[8] Y. Kwon, D. M. Ceperley, and R. M. Martin, Phys. Rev. B **58**, 6800 (1998).

[9] Talman's result reads $\epsilon_T = 0.0570 \log r_s - 0.1324$ Ry $+ \epsilon_{exch}$ where the exchange contribution is estimated by Talman to be 0.040 Ry at densities of physical interest ($r_s \approx 5$). Here we have used $\epsilon_{exch} = 0.0484$ Ry, the second-order exchange energy from Rayleigh-Schroedinger perturbation theory since this value is known to be accurate for small r_s.

[10] M. Gell-Mann and K. A. Brueckner, Phys. Rev. **106**, 364 (1957).

[11] A. L. Fetter and J. D. Walecka, *Quantum Theory of Many-Particle Systems* (McGraw-Hill, New York, 1971), pp. 21–22 and 94–95.

[12] J. C. Slater, *Quantum Theory of Atomic Structure*, Vol. 2 (McGraw-Hill, New York, 1960), p. 1–30 and Appendix 22.

[13] D. F. DuBois, Ann. Phys. (N.Y.) **7**, 174 (1959), Appendix C.

[14] W. J. Carr, Jr. and A. A. Maradudin, Phys. Rev. **133**, A371 (1964).

[15] N. Umezawa and S. Tsuneyuki, J. Chem. Phys. **119**, 10015 (2003).

[16] Naoto Umezawa and Shinji Tsuneyuki, Phys. Rev. B **69**, 165102 (2004).

[17] The slope was obtained by fitting a quadratic to TC data points at $r_s = 1$, 2, and 3.

[18] O. Sinanoglu, J. Chem. Phys. **36**, 706 (1962).

[19] G. A. Korn and K. T. M. Korn, *Handbook for Scientists and Engineers*, 2nd ed. (Courier Dover, Mineola, NY, 2000).

[20] J. C. Porter, Phys. Rev. **140**, A732 (1965).

[21] J. E. Mayer and M. G. Mayer, *Statistical Mechanics of Fluids* (Wiley and Sons, New York, 1940).

[22] L. Szasz, Phys. Rev. **126**, 169 (1962).

[23] L. Szasz, Phys. Rev. **132**, 936 (1963), see Eq.(3.4).

[24] J. C. Porter, Ph.D. thesis, Purdue University (1965), eqs.5.21 and C.13.

[25] G. D. Mahan, *Many-Particle Physics*, 2nd ed. (Plenum, New York, 1990), pp. 399–384.

[26] L. Onsager, L. Mittag, and M. J. Stephen, Ann. Phys. **473**, 71 (1966).

[27] K. Sawada, Phys. Rev. **106**, 372 (1957).

[28] K. Sawada, K. A. Brueckner, N. Fukuda, and R. Brout, Phys. Rev. **108**, 507 (1957).

[29] P. N. Argyres, Phys. Rev. **154**, 410 (1967).

[30] W. H. Press, B. P. Flannery, S. A. Teukolsky, and W. T. Vetterling, *Numerical Recipes* (University of Cambridge, Melbourne, Australia, 1986), pp. 80–94.

[31] MATHCAD14, Mathsoft Engineering Inc., 101 Main St., Cambridge, MA, 02142–1521 (2008).