On-top pair-correlation function in the homogeneous electron liquid

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The ladder theory, in which the Bethe-Goldstone equation for the effective potential between two scattering particles plays a central role, is well known for its satisfactory description of the short-range correlations in the homogeneous electron liquid. By solving exactly the Bethe-Goldstone equation in the limit of large transfer momentum between two scattering particles, we obtain accurate results for the on-top pair-correlation function $g(0)$, in both three dimensions and two dimensions. Furthermore, we prove, in general, that the ladder theory satisfies the cusp condition for the pair-correlation function $g(r)$ at zero distance $r=0$.

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I. INTRODUCTION

The pair-correlation function $g(r)$ is one of the key concepts in describing the correlation effects, arising from Pauli exclusion principle and Coulomb interaction, in the homogeneous electron liquid (or gas).[1] It also plays a significant role in the constructions of the exchange-correlation energy density functionals in density-functional theory (DFT),[2] since in such constructions the homogeneous electron system is conventionally taken as a reference system. A great deal of theoretical progress has recently been made in giving an accurate evaluation of $g(r)$, or the more specific spin-resolved pair-correlation functions $g_{\sigma\sigma'}(r)$, with $g(r)=\frac{1}{2}[g_{\uparrow\downarrow}(r)+g_{\uparrow\uparrow}(r)]$.[3–9] Huge progress has also been made with the developments in quantum Monte Carlo (QMC) techniques. The QMC results provide rather accurate values for $g(r)$ at intermediate electron-electron distances.[10,11] Unfortunately, present QMC calculations are not capable of providing equivalently accurate evaluation for $g(r)$ at very short ranges and, particularly, the on-top pair-correlation function $g(0)$, which has been well known to play a special role in DFT.[12] In fact, definite discrepancies exist in the present data of $g(0)$, extrapolated from the QMC results for short-range $g(r)$.[4,5,10,13] Future work in QMC calculations aimed at achieving higher accuracy in the short-range $g(r)$ would be desirable. In two dimensions (2D),[11] though a similar problem exists, much better accuracy in $g(0)$ has already been obtained from QMC calculations than in three dimensions (3D).

The important implication of $g(0)$, which arises totally from $g_{\uparrow\downarrow}(0)$ since $g_{\uparrow\uparrow}(0)=0$, was also realized in many-body theory long ago because the random phase approximation (RPA),[14] due to its lack of an accurate description of the short-range electron correlations, yields erroneous negative values for $g(0)$ when the electron densities are not sufficiently high.[15] It is well known that, in many-body theory, the long-range correlations can be rather successfully taken into account in the RPA, while the short-range correlations can be properly described by the ladder theory (LT).[16–19] In this paper, we attempt to investigate the short-range correlations in terms of $g(0)$ in the LT, in both 3D and 2D. In fact, investigations in this direction date back long ago and a great deal of achievement has been made.[16–25]

It is necessary here to give some introduction to the LT. The effective interaction $V_{eff}(\mathbf{p},\mathbf{p}';\mathbf{q})$ in the LT between two scattering electrons with respective momenta $\mathbf{p}$ and $\mathbf{p}'$ satisfies the Bethe-Goldstone equation[26]

$$V_{eff}(\mathbf{p},\mathbf{p}';\mathbf{q}) = v(q) + \sum_{\mathbf{k}} v(\mathbf{q}-\mathbf{k}) \times D(\mathbf{p},\mathbf{p}';\mathbf{k}) V_{eff}(\mathbf{p},\mathbf{p}';\mathbf{k}), \tag{1}$$

where $v(q)$ is the Fourier transform of the Coulomb potential, $n(\mathbf{p})=\theta(k_F-p)$ is the momentum distribution in the noninteracting ground state, k_F is the Fermi momentum, and $\epsilon_p=\hbar^2p^2/2m$. Here $D(\mathbf{p},\mathbf{p}';\mathbf{k})$ is defined as

$$D(\mathbf{p},\mathbf{p}';\mathbf{k}) = \frac{[1-n(\mathbf{p}+\mathbf{k})][1-n(\mathbf{p}'-\mathbf{k})]}{\epsilon_p+\epsilon_{p'}-\epsilon_{\mathbf{p}+\mathbf{k}}-\epsilon_{\mathbf{p}'-\mathbf{k}}}. \tag{2}$$

The momenta $\mathbf{p}$ and $\mathbf{p}'$ of the scattering particles in Eq. (1) are restricted in the Fermi sphere.

As mentioned above, the RPA gives a poor description of the short-range correlations of the electrons, especially for $g(r)$ as $r\to 0$. In fact, the results for $g_{\uparrow\downarrow}(r)$ in the RPA violate the cusp condition[17,20,27–30]

$$\left.\frac{\partial g_{\uparrow\downarrow}(r)}{\partial r}\right|_{r=0} = \frac{2}{(d-1)a_B} g_{\uparrow\downarrow}(0), \tag{3}$$

where $d=3$, 2 is the number of spatial dimensions and a_B is the Bohr radius. It was shown recently that the pair-correlation function obtained from the first-order perturbation calculation does satisfy the cusp condition within first order,[31]

$$\left.\frac{\partial g^{(1)}_{\uparrow\downarrow}(r)}{\partial r}\right|_{r=0} = \frac{1}{a_B} g^{(0)}_{\uparrow\downarrow}(0), \tag{4}$$

in 3D, where $g^{(1)}_{\uparrow\downarrow}(r)$ and $g^{(0)}_{\uparrow\downarrow}(r)$ are the pair-correlation function to the first order and the zeroth order of the electron interaction, respectively, but not the full cusp condition of Eq. (3). In fact, the latter cannot be satisfied in any finite-order perturbation calculations since it results from all multiple-scattering processes as any two electrons coalesce. In this paper, we prove that $g_{\uparrow\downarrow}(r)$ calculated from $V_{eff}(\mathbf{p},\mathbf{p}';\mathbf{q})$ of Eq. (1) satisfies the cusp condition (see also Refs. 20,32). This indicates the reliablity of the LT in the calculations of the pair-correlation function at short range.

To solve for $V_{eff}(\mathbf{p},\mathbf{p}';\mathbf{q})$ in Eq. (1) and calculate the corresponding pair-correlation function fully numerically is rather difficult. Effort was made in Ref. 20, but with results subject to limitation to a high-density region ($r_s \lesssim 4$) due to slow convergence in the numerical calculation in the lower-density region. Here $r_s=(3/4\pi n)^{1/3}/a_B$ in 3D. [See also Ref. 21, in which, however, $g(r)$ was calculated approximately with $V_{eff}(\mathbf{0},\mathbf{0};\mathbf{q})$ instead.] Therefore, instead of solving $V_{eff}(\mathbf{p},\mathbf{p}';\mathbf{q})$ fully, a common approximation employed to calculate the short-range $g(r)$ is to replace the momenta of scattering electrons $\mathbf{p}$ and $\mathbf{p}'$ in $V_{eff}(\mathbf{p},\mathbf{p}';\mathbf{q})$ by zero. This approximation is generally believed to be reasonable in evaluating $g(r)$ at small r. In fact, the short-range structure of $g_{\uparrow\downarrow}(r)$ is determined by the large-q behavior of the corresponding static structure factor $S_{\uparrow\downarrow}(q)$, the Fourier conjugation of the former. Accordingly, it is determined, in the LT, by that of the effective potential $V_{eff}(\mathbf{p},\mathbf{p}';\mathbf{q})$ at large momentum transfer [see Eq. (40) in Sec. III and Eq. (B2) in Appendix B]. Notice that p, $p' \leqslant k_F$ in Eq. (1). Thus, in the limiting case of calculating $g_{\uparrow\downarrow}(0)$, it should be well justified to replace $\mathbf{p}$ and $\mathbf{p}'$ by zero in $V_{eff}(\mathbf{p},\mathbf{p}';\mathbf{q})$ in Eq. (1),

$$V_{eff}(\mathbf{0},\mathbf{0};\mathbf{q}) = v(q) - \sum_{\mathbf{k}} v(\mathbf{q}-\mathbf{k}) \times \frac{1-n(\mathbf{k})}{2\epsilon_k} V_{eff}(\mathbf{0},\mathbf{0};\mathbf{k}). \tag{5}$$

A frequently used approach to solving Eq. (5) in the literature is making the following approximation in the Coulomb kernel in the momentum summation:[18,21,24,33,34]

$$v(\mathbf{q}-\mathbf{k}) = v(q) \quad (q>k); \quad = v(k) \quad (k>q). \tag{6}$$

With the preceding approximation, an analytical solution for $V_{eff}(\mathbf{0},\mathbf{0};\mathbf{q})$ was obtained which yields the following well-known result for $g_{\uparrow\downarrow}(0)$ in 3D:[18,33,34]

$$g_{\uparrow\downarrow}(0) = [\sqrt{2\lambda_3}/I_1(\sqrt{8\lambda_3})]^2, \tag{7}$$

where $\lambda_3=2\alpha r_s/\pi$ with $\alpha=(4/9\pi)^{1/3}$. A similar result was obtained in 2D,[21]

$$g_{\uparrow\downarrow}(0) = [I_0(\sqrt{4\lambda_2})]^{-2}, \tag{8}$$

where $\lambda_2=r_s/\sqrt{2}$ with $r_s=1/\sqrt{\pi n}a_B$ in 2D. In Eqs. (7) and (8), $I_n(x)$ is the nth-order modified Bessel function.

In this paper we have managed to solve exactly Eq. (5)—i.e., without making the approximation of Eq. (6). Our results for $g_{\uparrow\downarrow}(0)$ are

$$g_{\uparrow\downarrow}(0) = \left[\frac{45(45+24\lambda_3+4\lambda_3^2)}{2025+3105\lambda_3+1512\lambda_3^2+256\lambda_3^3}\right]^2, \tag{9}$$

in 3D, and

$$g_{\uparrow\downarrow}(0) = \left[\frac{15(64+25\lambda_2+3\lambda_2^2)}{960+1335\lambda_2+509\lambda_2^2+64\lambda_2^3}\right]^2, \tag{10}$$

in 2D. Equations (9) and (10) are the main results of this paper.

The paper is organized as follows: In Sec. II, we solve Eq. (5) exactly both in 3D and 2D. In Sec. III, we derive analytically the expressions of Eqs. (9) and (10) for $g_{\uparrow\downarrow}(0)$. We then compare our results with previous ones in the literature in Sec. IV. Section V is devoted to conclusions. Some technical points on the solutions for the effective potentials are given in Appendix A. In Appendix B, we prove the cusp condition in the LT.

II. EXACT SOLUTION TO THE BETHE-GOLDSTONE INTEGRAL EQUATION AT LARGE TRANSFER MOMENTUM

In this section, we present our solution to Eq. (5) at large momentum transfer $\mathbf{q}$ in the effective potential in both 3D and 2D. To this end, we denote $V_{eff}(\mathbf{0},\mathbf{0};\mathbf{q})$ as $V_{eff}(q)$ and reduce the momenta with unit k_F and potentials with $v(k_F)$, respectively. We present our solution for the 3D case in subsection A and the 2D case in subsection B, separately.

A. 3D

After carrying out the angular integrations in the summation of the momentum $\mathbf{k}$, Eq. (5) becomes

$$V_{eff}(q) = \frac{1}{q^2} - \frac{\lambda_3}{2}\int_1^\infty dk V_{eff}(k)\frac{1}{qk}\ln\left|\frac{q+k}{q-k}\right|. \tag{11}$$

We expand $V_{eff}(q)$ in powers of $1/q$,

$$V_{eff}(q) = \sum_{n=0}^{\infty} \frac{a_n}{q^{2n+2}}. \tag{12}$$

It can be easily confirmed by iteration that no odd power terms in the expansion of $V_{eff}(q)$ exist in the solution to Eq. (11). The erroneous odd-power terms introduced into $V_{eff}(q)$ in Refs. 18,33,34 are purely due to the approximation made in the Coulomb kernel in Eq. (6). We substitute Eq. (12) into Eq. (11) and obtain

$$\sum_{n=0}^{\infty} \frac{a_n}{q^{2n+2}} = \frac{1}{q^2} - \frac{\lambda_3}{2q}\sum_{n=0}^{\infty} a_n M_{2n+3}, \tag{13}$$

where

$$M_{2n+3}(q) = \int_1^\infty dk \frac{1}{k^{2n+3}}\ln\left|\frac{q+k}{q-k}\right|, \quad n \geqslant 0. \tag{14}$$

By carrying through partial integration on the right-hand side of Eq. (14), one has

$$M_{2n+3}(q) = \frac{1}{2n+2}\left[\ln\frac{q+1}{q-1} - 2q\Phi_{n+1}(q)\right], \tag{15}$$

where

$$\Phi_{n+1}(q) = \int_1^\infty dk \frac{1}{k^{2n+2}}\frac{1}{k^2-q^2}. \tag{16}$$

$\Phi_{n+1}(q)$ defined in the preceding equation can be evaluated to be

$$\Phi_{n+1}(q) = -\sum_{m=0}^{n} \frac{1}{q^{2m+2}} \frac{1}{2(n-m)+1} + \frac{1}{2q^{2n+3}} \ln\frac{q+1}{q-1}. \tag{17}$$

Substituting Eq. (17) into Eq. (15) yields

$$M_{2n+3}(q) = \frac{1}{n+1}\left[\sum_{m=0}^{n} \frac{1}{q^{2m+1}} \frac{1}{2(n-m)+1} + \frac{1}{2}\left(\frac{1}{q^{2n+2}} - 1\right)\ln\frac{q-1}{q+1}\right], \quad n \geqslant 0. \tag{18}$$

Finally, substituting Eq. (18) into Eq. (13) and comparing the same power orders of $1/q$, one obtains the following equations for a_n:

$$a_0 = 1 - \lambda_3 \sum_{n=0}^{\infty} \frac{a_n}{2n+1} \tag{19}$$

and

$$a_n = -\frac{\lambda_3}{2n+1} \sum_{l=0}^{\infty} \frac{a_l}{2(l-n)+1}, \quad n \geqslant 1. \tag{20}$$

Equations (19) and (20) for a_n can be solved exactly in principle. In fact, by making the truncation of $a_n=0$ for $n \geqslant 3$, a nearly exact solution can be obtained as

$$a_0 = \frac{45(45 + 24\lambda_3 + 4\lambda_3^2)}{D_3}, \tag{21}$$

$$a_1 = \frac{15\lambda_3(45 + 8\lambda_3)}{D_3}, \tag{22}$$

and

$$a_2 = \frac{45\lambda_3(3 + 4\lambda_3)}{D_3}, \tag{23}$$

where

$$D_3 = 2025 + 3105\lambda_3 + 1512\lambda_3^2 + 256\lambda_3^3. \tag{24}$$

In Appendix A, we show that the preceding solution for a_0, which is directly related to $g_{\uparrow\downarrow}(0)$, as shown in the next section, is very close to the exact numerical solution to Eqs. (19) and (20). In fact, the large-momentum behavior of $V_{eff}(q)$ is dominated by the leading terms in the large-q expansion of $V_{eff}(q)$ in Eq. (12), and hence a truncation solution like the preceding one is almost exact.

B. 2D

In 2D, we make use of the expression

$$\frac{2\pi}{|\mathbf{q}-\mathbf{k}|} = \int d\mathbf{r} e^{i(\mathbf{q}-\mathbf{k})\cdot\mathbf{r}} \frac{1}{r} \tag{25}$$

and rewrite Eq. (5) as follows:

$$V_{eff}(q) = \frac{1}{q} - \frac{\lambda_2}{(2\pi)^2} \int d\mathbf{k}\, \theta(k-1) \frac{1}{k^2} V_{eff}(k) \times \int d\mathbf{r} e^{i(\mathbf{q}-\mathbf{k})\cdot\mathbf{r}} \frac{1}{r}. \tag{26}$$

Carrying out the angular integrations of **k** and **r**, we have

$$V_{eff}(q) = \frac{1}{q} - \lambda_2 \int_0^{\infty} dr \int_1^{\infty} dk \frac{1}{k} V_{eff}(k) \times J_0(qr) J_0(kr), \tag{27}$$

where $J_n(x)$ is the nth-order Bessel function. We expand $V_{eff}(q)$ in the powers of $1/q$ as follows:

$$V_{eff}(q) = \sum_{n=0}^{\infty} \frac{c_n}{q^{2n+1}}. \tag{28}$$

No even-power terms exist in the solution to Eq. (27). Again, the erroneous even-power terms[21] appear in $V_{eff}(q)$ due to the approximation made in Eq. (6).

We substitute Eq. (28) into Eq. (27) and obtain

$$\sum_{n=0}^{\infty} \frac{c_n}{q^{2n+1}} = \frac{1}{q} - \frac{\lambda_2}{q} \sum_{n=1}^{\infty} c_{n-1} N_{2n}(q), \tag{29}$$

where

$$N_{2n}(q) = \int_0^{\infty} dx J_0(x) \int_1^{\infty} dk \frac{1}{k^{2n}} J_0(kx/q). \tag{30}$$

Carrying out the integration over k in Eq. (30), one obtains

$$N_{2n}(q) = \sum_{m=1}^{n} (-2)^{m-1} \frac{(n-1)!}{(n-m)!} \times \int_0^{\infty} dx J_0(x/q) J_m(x)/x^m, \quad n \geqslant 1. \tag{31}$$

The integral on the right-hand side of Eq. (31) can be expressed in terms of the hypergeometric function as follows:[35]

$$\int_0^{\infty} dx J_0(x/q) J_m(x)/x^m = \frac{\Gamma\left(\frac{1}{2}\right)}{2^m \Gamma(1) \Gamma\left(m+\frac{1}{2}\right)} \times F\left(\frac{1}{2}, -m+\frac{1}{2}; 1; \frac{1}{q^2}\right), \quad n \geqslant 1, \tag{32}$$

where $\Gamma(\alpha)$ is the gamma function. Therefore, one has

$$N_{2n}(q) = \sum_{m=1}^{n} (-2)^{m-1} \frac{(n-1)!}{(n-m)!\,(2m-1)!!} \times F\left(\frac{1}{2}, -m+\frac{1}{2}; 1; \frac{1}{q^2}\right), \quad n \geqslant 1. \tag{33}$$

Substituting Eq. (33) into Eq. (29) and comparing the same power orders of $1/q$, one finally gets

$$c_0 = 1 - \lambda_2 \sum_{n=0}^{\infty} \frac{c_n}{2n+1} \quad (34)$$

and

$$c_n = \lambda_2 (-)^{n-1} \frac{(2n)!}{2^{3n} n!^3} \sum_{l=0}^{\infty} c_l l\,! \sum_{m=0}^{l} (-2)^m \times \frac{(2m+1)(2m-1)\cdots(2m-2n+3)}{(l-m)\,!\,(2m+1)\,!\,!}, \quad (35)$$

for $n \geqslant 1$.

Similarly to the 3D case, Eqs. (34) and (35) can be solved exactly in principle. In fact, a nearly exact solution can be obtained as follows by the truncation of $c_n=0$ for $n \geqslant 3$:

$$c_0 = \frac{15(64 + 25\lambda_2 + 3\lambda_2^2)}{D_2}, \quad (36)$$

$$c_1 = \frac{30\lambda_2(8+\lambda_2)}{D_2}, \quad (37)$$

and

$$c_2 = \frac{45\lambda_2(1+\lambda_2)}{D_2}, \quad (38)$$

where

$$D_2 = 960 + 1335\lambda_2 + 509\lambda_2^2 + 64\lambda_2^3. \quad (39)$$

III. RESULTS FOR $g_{\uparrow\downarrow}(r)$ AT SMALL r

The spin-antiparallel pair-correlation function in the LT can be shown to be[18,21]

$$g_{\uparrow\downarrow}(r) = \frac{4}{n^2} \sum_{\mathbf{p},\mathbf{p}'}{}' \left| 1 + \sum_{\mathbf{q}} D(\mathbf{p},\mathbf{p}';\mathbf{q}) \times V_{eff}(\mathbf{p},\mathbf{p}';\mathbf{q}) e^{i\mathbf{q}\cdot\mathbf{r}} \right|^2, \quad (40)$$

where the prime on the summations over $\mathbf{p}$ and $\mathbf{p}'$ means the restrictions $0 \leqslant p$ and $p' \leqslant k_F$. Below we present the results for the 3D and 2D cases in subsections A and B, respectively. We will reduce r with unit $1/k_F$.

A. 3D

Using the approximate solution $V_{eff}(q)$ for $V_{eff}(\mathbf{p},\mathbf{p}';\mathbf{q})$, one obtains[20]

$$g_{\uparrow\downarrow}(r) = \left[1 - \lambda_3 \int_1^{\infty} dq V_{eff}(q) j_0(qr) \right]^2. \quad (41)$$

Trivially,

$$g_{\uparrow\downarrow}(0) = \left[1 - \lambda_3 \int_1^{\infty} dq V_{eff}(q) \right]^2. \quad (42)$$

With the expression of Eq. (12), one has

$$g_{\uparrow\downarrow}(0) = a_0^2. \quad (43)$$

Equation (19) has been made use of in obtaining the preceding result. The expression for a_0 is given in Eq. (21), with which we obtain the final result of Eq. (9). Furthermore, it is straightforward to show, from Eq. (41), that, at small r,

$$g_{\uparrow\downarrow}(r) = g_{\uparrow\downarrow}(0) + \frac{\pi}{2}\lambda_3 g_{\uparrow\downarrow}(0) r. \quad (44)$$

B. 2D

In 2D, one has

$$g_{\uparrow\downarrow}(r) = \left[1 - \lambda_2 \int_1^{\infty} dq \frac{1}{q} V_{eff}(q) J_0(qr) \right]^2. \quad (45)$$

A similar derivation to that in the 3D case leads to

$$g_{\uparrow\downarrow}(0) = c_0^2 \quad (46)$$

or, by the use of Eq. (36), the final result of Eq. (10). Furthermore, from Eq. (45), one can obtain

$$g_{\uparrow\downarrow}(r) = g_{\uparrow\downarrow}(0) + 2\lambda_2 g_{\uparrow\downarrow}(0) r, \quad (47)$$

Evidently, the cusp condition of Eq. (3) is satified in both Eqs. (44) and (47). In fact, in Appendix B we shall show that Eq. (3) is satisfied, in general, in the full ladder theory.

IV. COMPARISONS AND DISCUSSIONS

First of all, at limiting high density, we have, from Eq. (9),

$$g_{\uparrow\downarrow}(0) = 1 - 2\lambda_3 = 1 - 0.663 r_s, \quad (48)$$

in 3D. Equation (48) is the same as the corresponding Yasuhara's result.[33] We note that, the first-order perturbation calculation,[12,27,31,36] which is believed to approach the exact result at the high-density limit, yields a result of $1 - 0.7317 r_s$. We plot $g(0) \times r_s$ calculated from Eq. (9) in Fig. 1, in comparison with that calculated from Eq. (7).[18,33,34] Notice that the discrepancy between Eqs. (7) and (9), which appears not minor, arises purely from the approximation of Eq. (6) made in obtaining Eq. (7) in Yasuhara's theory. In effect, Lowy and Brown[19] had thrown doubt on the validity of the approximation of Eq. (6). We hence justify their doubt, at least for the limiting short-range correlations. The result calculated from two-electron wave functions (geminals), obtained from the Schrödinger equation with a two-body scattering potential in Ref. 37 is also shown in Fig. 1 (see also later developments in the geminal approach in Refs. 5,8,38).

It might be useful to mention that the Bethe-Goldstone equation is essentially the two-body Schrödinger equation with the effects of the Fermi-gas background taken into account explicitly. Thus, in methodology, an approach to the pair-correlation function based on the Bethe-Goldstone equation is closely related to the geminal approach. In both, it is assumed that the contribution from two-body interaction dominates the short-range correlations. This should be essentially exact for the limiting case of $g(0)$. Hence, to achieve a

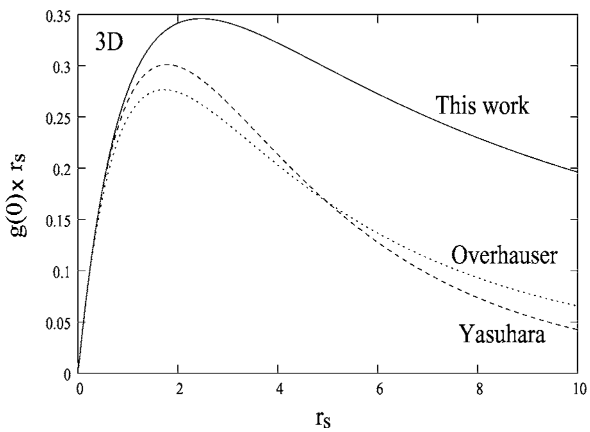

FIG. 1. On-top pair-correlation function multiplied by r_s in 3D. The result of this work [Eq. (9)] is compared with Eq. (7) (Yasuhara's formula in Refs. 18,33,34) and the Overhauser formula [Eq. (26) in Ref. 37].

better understanding of the results for $g(0)$, further investigation into the relation between the LT and the geminal method might be helpful.

In Fig. 2, we plot $g(0)\times r_s$ in 2D calculated from Eq. (10), together with that from Eq. (8).[21] Once again, we emphasize that the discrepancy is totally due to the approximation of Eq. (6) made in obtaining Eq. (8). However, at limiting high density, both equations yield the following same result:

$$g_{\uparrow\downarrow}(0) = 1 - 2\lambda_2. \tag{49}$$

For a comparison, we have also shown in Fig. 2 the result of Eq. (17) in Ref. 7, which was proposed by Polini *et al.* based on an interpolation between the first-order (second-order in terms of the correlation energy) calculation for the weak-coupling limit and Overhauser-type calculation[37] for the strong-coupling limit.

V. CONCLUSIONS

The proper approach to the short-range electron correlations in many-body theory is the ladder theory, in which the effective potential between two scattering particles satisfies the Bethe-Goldstone equation of Eq. (1). In this paper, we have shown in detail that the ladder theory satisfies the cusp condition for the pair-correlation function in the homogeneous electron liquid. This enhances our belief in the capability of the ladder theory in describing the short-range correlations, especially in calculating the pair-correlation function.

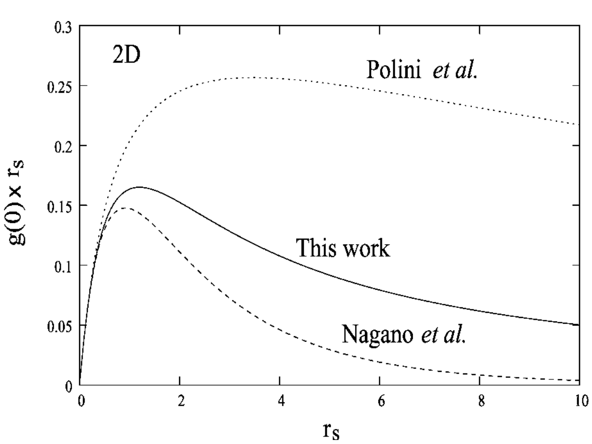

FIG. 2. On-top pair-correlation function multiplied by r_s in 2D. The result of this work [Eq. (10)] is compared with Eq. (8) (formula of Nagano *et al.* in Ref. 21) and the formula of Polini *et al.* [Eq. (17) in Ref. 7].

The main results obtained in this paper are, in effect, Eqs. (9) and (10) given in the Introduction, in three dimensions and two dimensions, respectively, for the on-top pair-correlation function in the homogeneous electron liquid. These results have been derived by solving Eq. (5), in which the two scattering particles in the Bethe-Goldstone equation are approximately taken to be static. This approximation should be reasonable since the limiting short-range structure of the pair-correlation function is dominated by the large-transfer-momentum behavior of the effective potential in the ladder theory. The major theoretical progress made in this paper is that we have removed the approximation of Eq. (6) frequently made in the literature for the Coulomb kernel in solving Eq. (5). Our solution to Eq. (5) is thus exact.

A final remark might be necessary. Though our solution to Eq. (5) for the effective potential $V_{eff}(\mathbf{0},\mathbf{0};\mathbf{q})$ between two scattering particles is exact, the latter is approximate to $V_{eff}(\mathbf{p},\mathbf{p}';\mathbf{q})$ in the ladder theory. Furthermore, the fact that the ladder theory (without the approximation of $p=p'=0$) can properly describe the short-range correlations does not necessarily imply that it is capable of yielding exact $g(0)$. Therefore, the results in Eqs. (9) and (10) by no means can be regarded as "exact."

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APPENDIX A: THE SOLUTIONS TO EQS. (19) and (20) AND EQS. (34) and (35)

A nearly exact solution for a_0 to Eqs. (19) and (20) has been given in Eq. (21) in Sec. III by the truncation of $a_n=0$ for $n\geqslant 3$. Below we give the solution for a_n by the truncation of $a_n=0$ for $n\geqslant 4$:

$$a_0 = \frac{175(14175 + 9585\lambda_3 + 2520\lambda_3^2 + 256\lambda_3^3)}{\tilde{D}_3}, \tag{A1}$$

$$a_1 = \frac{105\lambda_3(7875 + 2480\lambda_3 + 256\lambda_3^2)}{\tilde{D}_3}, \tag{A2}$$

$$a_2 = \frac{105\lambda_3(1575 + 2280\lambda_3 + 256\lambda_3^2)}{\tilde{D}_3}, \tag{A3}$$

and

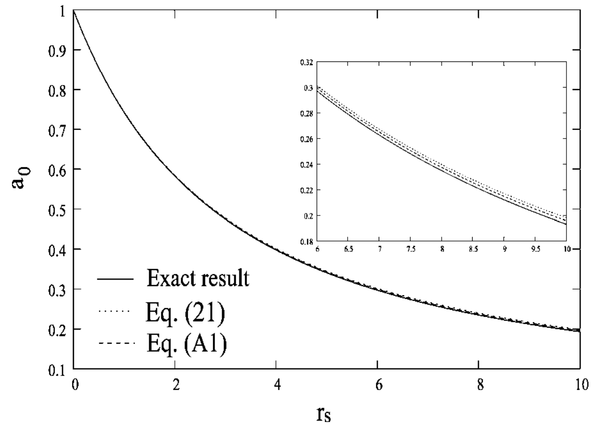

FIG. 3. a_0 calculated from Eqs. (21) and (A1), together with the exact numerical result. The inset shows the large-r_s region.

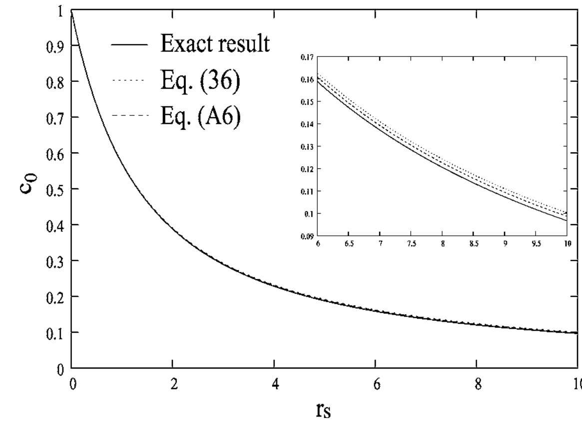

FIG. 4. c_0 calculated from Eqs. (36) and (A6), together with exact numerical result. The inset shows the large-r_s region.

$$a_3 = \frac{175\lambda_3(405 + 576\lambda_3 + 256\lambda_3^2)}{\tilde{D}_3}, \tag{A4}$$

where

$$\tilde{D}_3 = 2480625 + 4158000\lambda_3 + 2437200\lambda_3^2 + 634880\lambda_3^3 + 65536\lambda_3^4. \tag{A5}$$

In Fig. 3, we plot the results for a_0 calculated from Eqs. (21) and (A1), together with the corresponding exact numerical solution to Eqs. (19) and (20). There is basically no difference among them. We present the expressions of Eqs. (A1)–(A4) above for possible future reference.

Similar expressions for the 2D case are given below:

$$c_0 = \frac{35(12288 + 6000\lambda_2 + 1121\lambda_2^2 + 80\lambda_2^3)}{\tilde{D}_2}, \tag{A6}$$

$$c_1 = \frac{1680\lambda_2(64 + 14\lambda_2 + \lambda_2^2)}{\tilde{D}_2}, \tag{A7}$$

$$c_2 = \frac{105\lambda_2(192 + 207\lambda_2 + 16\lambda_2^2)}{\tilde{D}_2}, \tag{A8}$$

and

$$c_3 = \frac{350\lambda_2(24 + 25\lambda_2 + 8\lambda_2^2)}{\tilde{D}_2}, \tag{A9}$$

where

$$\tilde{D}_2 = 430080 + 640080\lambda_2 + 290307\lambda_2^2 + 55472\lambda_2^3 + 4096\lambda_2^4. \tag{A10}$$

The corresponding illustration is given in Fig. 4.

To more clearly show that the present analytical solutions to $V_{eff}(q)$ are nearly exact, we have numerically solved Eq. (5) in both 3D and 2D. In Fig. 5, the exact numerical solution, in 3D, is compared with that of Eq. (12) with the truncation made in Sec. II A and a_0, a_1, and a_2 given in Eqs. (21)–(23). They turn out to be rather close. We have also included the result of Eq. (12) with the truncation made in this appendix and a_0, a_1, a_2, and a_3 given in Eqs. (A1)–(A4). A similar illustration for the 2D case is presented in Fig. 6.

APPENDIX B: CUSP CONDITION IN THE LADDER THEORY

Due to the singularity of the Coulomb potential between electrons, the many-body Schrödinger wave function has a cusp when any two electrons coalesce.[39–41] This fact leads to the cusp condition of Eq. (3) (Ref. 17, 20, and 27–30) for the pair-correlation function (also known as Kimball relation in the literature of many-electron theory). It was claimed in Ref. 20 that the cusp condition is valid in the LT. However, recently it was claimed[32] that Eq. (3) is not satisfied in the LT. In this appendix, we give a rigorous proof for Eq. (3) in the LT. The proof will be formulated in 3D.

We start with the definition of the spin-antiparallel static structure factor as follows:

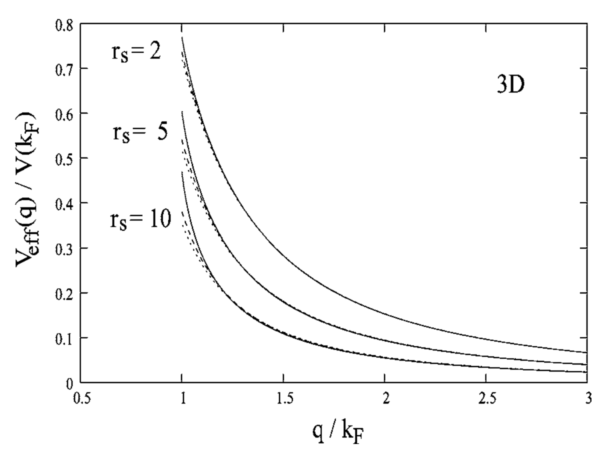

FIG. 5. $V_{eff}(q)$ [in units of $V(k_F)$] as a function of q/k_F for $r_s = 2, 5, 10$ in 3D. The solid lines, exact numerical solution to Eq. (5); dotted lines, Eq. (12) with a_0, a_1, a_2 given in Eqs. (21)–(23), and $a_n = 0$ for $n \geqslant 3$; dashed lines, Eq. (12) with a_0, a_1, a_2, a_3 given in Eqs. (A1)–(A4), and $a_n = 0$ for $n \geqslant 4$.

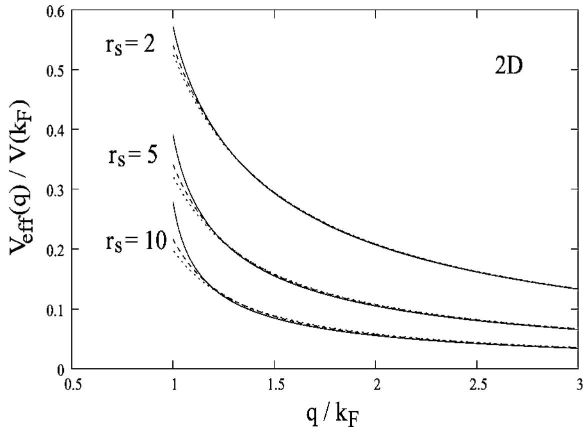

FIG. 6. $V_{eff}(q)$ [in units of $V(k_F)$] as a function of q/k_F for r_s =2, 5, 10 in 2D. The solid lines, exact numerical solution to Eq. (5); dotted lines, Eq. (28) with c_0, c_1, c_2 given in Eqs. (36)–(38), and c_n=0 for $n \geq 3$; dashed lines, Eq. (28) with c_0, c_1, c_2, c_3 given in Eqs. (A6)–(A9), and c_n=0 for $n \geq 4$.

$$S_{\uparrow\downarrow}(q) = \frac{1}{N}\langle \hat{n}_\uparrow(-\mathbf{q})\hat{n}_\downarrow(\mathbf{q})\rangle - \frac{N}{2}\delta_{\mathbf{q},0}, \tag{B1}$$

where $\hat{n}_\sigma(\mathbf{q})$ is the spin-resolved density operator and N is the particle number. It has been shown that the spin-antiparallel static structure factor in the LT can be expressed in terms of the effective potential of Eq. (1) as[17,21]

$$S_{\uparrow\downarrow}(q) = \frac{1}{n}\sum_{\mathbf{p},\mathbf{p}'}{}' \Big[2D(\mathbf{p},\mathbf{p}';\mathbf{q})V_{eff}(\mathbf{p},\mathbf{p}';\mathbf{q}) + \sum_{\mathbf{k}} D(\mathbf{p},\mathbf{p}';\mathbf{k})V_{eff}(\mathbf{p},\mathbf{p}';\mathbf{k}) \times D(\mathbf{p},\mathbf{p}';\mathbf{k}-\mathbf{q})V_{eff}(\mathbf{p},\mathbf{p}';\mathbf{k}-\mathbf{q})\Big]. \tag{B2}$$

Next we examine the large-momentum structure of $S_{\uparrow\downarrow}(q)$. For p, $p' \leq k_F$ and $q \to \infty$, one has, from Eqs. (1),

$$D(\mathbf{p},\mathbf{p}';\mathbf{q})V_{eff}(\mathbf{p},\mathbf{p}';\mathbf{q}) = -\frac{1}{2\epsilon_q}v(q) \times \left[1 + \sum_{\mathbf{k}} D(\mathbf{p},\mathbf{p}';\mathbf{k})V_{eff}(\mathbf{p},\mathbf{p}';\mathbf{k})\right], \tag{B3}$$

which evidently goes to zero in the order of $O(1/q^4)$. Therefore,

$$\sum_{\mathbf{k}} D(\mathbf{p},\mathbf{p}';\mathbf{k})V_{eff}(\mathbf{p},\mathbf{p}';\mathbf{k}) \times D(\mathbf{p},\mathbf{p}';\mathbf{q}-\mathbf{k})V_{eff}(\mathbf{p},\mathbf{p}';\mathbf{q}-\mathbf{k}) = -\frac{1}{\epsilon_q}v(q)\left[1 + \sum_{\mathbf{k}} D(\mathbf{p},\mathbf{p}';\mathbf{k})V_{eff}(\mathbf{p},\mathbf{p}';\mathbf{k})\right] \times \sum_{\mathbf{k}'} D(\mathbf{p},\mathbf{p}';\mathbf{k}')V_{eff}(\mathbf{p},\mathbf{p}';\mathbf{k}'). \tag{B4}$$

In obtaining Eq. (B4), we have used the relation

$$\lim_{q\to\infty}\sum_{\mathbf{k}} f(\mathbf{k})f(\mathbf{q}-\mathbf{k}) = 2f(\mathbf{q})\sum_{\mathbf{k}} f(\mathbf{k}) \tag{B5}$$

if $\lim_{q\to\infty} f(\mathbf{q}) \sim O(1/q^4)$. It seems that a mistake occurs in Ref. 32 due to a possible miss of the factor 2 on the right-hand side of the preceding equation, as it was employed to derive Eq. (12) from Eq. (11) in Ref. 32.

Substituting Eqs. (B3) and (B4) into Eq. (B2), one has

$$S_{\uparrow\downarrow}(q) = -\frac{1}{n}\frac{v(q)}{\epsilon_q}\sum_{\mathbf{p},\mathbf{p}'}{}'\left[1 + \sum_{\mathbf{k}} D(\mathbf{p},\mathbf{p}';\mathbf{k}) \times V_{eff}(\mathbf{p},\mathbf{p}';\mathbf{k})\right]^2. \tag{B6}$$

On the other hand, from Eq. (40), we have

$$g_{\uparrow\downarrow}(0) = \frac{4}{n^2}\sum_{\mathbf{p},\mathbf{p}'}{}'\left[1 + \sum_{\mathbf{q}} D(\mathbf{p},\mathbf{p}';\mathbf{q}) \times V_{eff}(\mathbf{p},\mathbf{p}';\mathbf{q})\right]^2. \tag{B7}$$

Comparing Eqs. (B6) and (B7) yields

$$S_{\uparrow\downarrow}(q) = -\frac{2\pi e^2 nm}{q^4} g_{\uparrow\downarrow}(0). \tag{B8}$$

Equation (B8) was also given in Ref. 20. Combining the preceding result with the well-known relation[27]

$$\lim_{q\to\infty} q^4 S_{\uparrow\downarrow}(q) = -2\pi n \left.\frac{\partial g_{\uparrow\downarrow}(r)}{\partial r}\right|_{r=0}, \tag{B9}$$

one proves the cusp condition of Eq. (3) in the LT.

The above proof can be straightforwardly extended to the 2D case. In fact, in 2D, it can be similarly shown

$$S_{\uparrow\downarrow}(q) = -\frac{\pi e^2 nm}{q^3} g_{\uparrow\downarrow}(0), \tag{B10}$$

in the LT. Combining the above result with the relation[42]

$$\lim_{q\to\infty} q^3 S_{\uparrow\downarrow}(q) = -\frac{1}{2}\pi n \left.\frac{\partial g_{\uparrow\downarrow}(r)}{\partial r}\right|_{r=0}, \tag{B11}$$

leads to Eq. (3) for the 2D case.

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