The on-top pair-correlation density 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 density \( g(0) \), in both three dimensions and two dimensions. Furthermore, we prove, in general, the ladder theory satisfies the cusp condition for the pair-correlation density \( g(r) \) at zero distance \( r = 0 \).

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I. INTRODUCTION

The pair-correlation density \( g(r) \) 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).\(^{11} \)

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 densities \( g_{\sigma\sigma'}(r) \), with \( g(r) = \frac{1}{2}(g_{uu}(r) + g_{dd}(r)) \).\(^{3, 4, 5, 6, 7, 8, 9} \) In particular, \( g(0) \), the on-top pair-correlation density, which arises totally from \( g_{uu}(0) \) since \( g_{uu}(0) = 0 \), has been well known to play a special role in DFT.\(^{10} \)

The important implication of \( g(0) \) was also realized in many-body theory long ago because the random phase approximation (RPA)\(^{11} \) due to its lack of accurate description of the short-range electron correlations, yields erroneous negative values for \( g(0) \) when the electron densities are not sufficiently high.\(^{12} \)

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).\(^{13, 14, 15, 16} \) In this paper, we attempt to investigate the short-range correlations in terms of 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 following Bethe-Goldstone equation:\(^{23} \)

\[
V_{eff}(\mathbf{p}, \mathbf{p'}; \mathbf{q}) = v(q) + \sum_{k} v(q - k) \times \left( \frac{1 - n(\mathbf{p} + \mathbf{k})}{\epsilon_{\mathbf{p}} + \epsilon_{\mathbf{p'}} - \epsilon_{\mathbf{k}} - \epsilon_{\mathbf{p'} - \mathbf{k}}} \right) V_{eff}(\mathbf{p}, \mathbf{p'}; \mathbf{k}),
\]

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 and \( k_{F} \) is the Fermi momentum, and \( \epsilon_{\mathbf{p}} = \hbar^{2}p^{2}/2m \).

As mentioned above, the RPA gives poor description of the short-range correlations of the electrons, especially for \( g(r) \) as \( r \to 0 \). In fact, the results for \( g_{uu}(r) \) in the RPA violate the following cusp condition: \(^{14, 17, 24, 25, 26, 27} \)

\[
\frac{\partial g_{uu}(r)}{\partial r} \bigg|_{r=0} = \frac{2}{(d-1)a_{B}} g_{uu}(0),
\]

where \( d = 3, 2 \) is the number of spatial dimensions, and \( a_{B} \) is the Bohr radius. It was shown recently\(^{28} \) that the pair-correlation density obtained from the first order perturbation calculation does not satisfy the cusp condition either. In this paper, we prove that \( g_{uu}(r) \) calculated from \( V_{eff}(\mathbf{p}, \mathbf{p'}; \mathbf{q}) \) of Eq.\(^{18} \) satisfies the cusp condition. This indicates the reliability of the LT in the calculations of the pair-correlation density at short range.

The short-range structure of the pair-correlation density is determined by the behavior of the effective potential \( V_{eff}(\mathbf{p}, \mathbf{p'}; \mathbf{q}) \) at large momentum transfer \( q \). In the limiting case, one therefore can approximately replace the momenta of the scattering electrons by zero in Eq.\(^{19} \),

\[
V_{eff}(\mathbf{0}, \mathbf{0}; \mathbf{q}) = v(q) - \sum_{k} v(q - k) \times \frac{1 - n(k)}{2\epsilon_{k}} V_{eff}(\mathbf{0}, \mathbf{0}; \mathbf{k}).
\]

A frequently used approach to solving Eq.\(^{20} \) in the literature is making the following approximation in the Coulomb kernel in the momentum summation: \(^{15, 18, 21, 29, 30} \)

\[
v(q - k) = v(q), \quad q > k
= v(k), \quad k > q.
\]

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, \[13, 20, 30\]

$$g_{\uparrow \downarrow}(0) = \left[ \frac{\sqrt{2\lambda_{3}}/I_{1}(\sqrt{8\lambda_{3}})}{2025 + 3105\lambda_{3} + 1512\lambda_{3}^{2} + 256\lambda_{3}^{3}} \right]^{2}, \tag{5}$$

where $\lambda_{3} = 2\alpha r_{s}/\pi$ with $\alpha = (4/9\pi)^{1/3}$ and $r_{s} = (3/4\pi n)^{1/3}/a_{B}$. A similar result was obtained in 2D,\[13\]

$$g_{\uparrow \downarrow}(0) = \left[ I_{0}(\sqrt{4\lambda_{2}}) \right]^{-2}, \tag{6}$$

where $\lambda_{2} = r_{s}/\sqrt{2}$ with $r_{s} = 1/\sqrt{\pi n a_{B}}$ in 2D. In Eqs. (5) and (6), $I_{n}(x)$ is the $n$th order modified Bessel function.

In this paper we have managed to solve exactly Eq. (3) at large momentum transfer for $\lambda$, I. In Eqs. (5) and (6), $I_{n}(x)$ is the $n$th order modified Bessel function.

The paper is organized as follows: In Sect. II, we solve Eq. (3) exactly both in 3D and 2D. In Sect. III, we derive analytically the expressions of Eqs. (7) and (8) for $g_{\uparrow \downarrow}(0)$. We then compare our results with previous ones in the literature in Sect. IV. Sect. V is devoted to conclusions. Some technical points on the solutions for the coefficients of the large momentum expansions of 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. (3) at large momentum transfer $q$ in the effective potential in both 3D and 2D. To this end, we denote $V_{\text{eff}}(0; 0; q)$ as $V_{\text{eff}}(q)$, 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 $k$, Eq. (3) becomes

$$V_{\text{eff}}(q) = \frac{1}{q} - \frac{\lambda_{3}}{2} \int_{1}^{\infty} dk V_{\text{eff}}(k) \frac{1}{qk} \ln \frac{q + k}{|q - k|}, \tag{9}$$

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

$$V_{\text{eff}}(q) = \sum_{n=0}^{\infty} \frac{a_{n}}{q^{2n+2}}, \tag{10}$$

It can be easily confirmed by iteration that no odd power terms in the expansion of $V_{\text{eff}}(q)$ exist in the solution to Eq. (3). The erroneous odd power terms introduced into $V_{\text{eff}}(q)$ in Refs. [13, 20, 30] are purely due to the approximation made in the Coulomb kernel in Eq. (4). We substitute Eq. (10) into Eq. (9), and obtain

$$\sum_{n=0}^{\infty} \frac{a_{n}}{q^{2n+2}} = \frac{1}{q^{2}} - \frac{\lambda_{3}}{2q} \sum_{n=0}^{\infty} a_{n} M_{2n+3}, \tag{11}$$

where

$$M_{2n+3}(q) = \int_{1}^{\infty} dk \frac{1}{k^{2n+3}} \ln \frac{q + k}{|q - k|}, \quad n \geq 0. \tag{12}$$

By carrying through partial integration on the right hand side of Eq. (12), one has,

$$M_{2n+3}(q) = \frac{1}{2n+2} \left[ \ln \frac{q + 1}{q - 1} - 2q \Phi_{n+1}(q) \right], \tag{13}$$

where

$$\Phi_{n+1}(q) = \int_{1}^{\infty} dk \frac{1}{k^{2n+3}} \frac{1}{k^{2} - q^{2}}. \tag{14}$$

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

$$\Phi_{n+1}(q) = - \sum_{m=0}^{n} \frac{1}{q^{2m+2}} \frac{1}{2(n - m) + 1} + \frac{1}{2q^{2n+3}} \ln \frac{q + 1}{q - 1}. \tag{15}$$

Substituting Eq. (15) into Eq. (13) yields,

$$M_{2n+3}(q) = \frac{1}{n + 1} \left[ \sum_{m=0}^{n} \frac{1}{q^{2m+1}} \frac{1}{2(n - m) + 1} + \frac{1}{2} \left( \frac{1}{q^{2n+2}} - 1 \right) \ln \frac{q - 1}{q + 1} \right], \quad n \geq 0. \tag{16}$$

Finally, substituting Eq. (16) into Eq. (11), and comparing the same power orders of $1/q$, one obtains the following equations for $a_{n}$:

$$a_{0} = 1 - \lambda_{3} \sum_{n=0}^{\infty} \frac{a_{n}}{2n + 1}, \tag{17}$$

and

$$a_{n} = - \frac{\lambda_{3}}{2n + 1} \sum_{l=0}^{\infty} \frac{a_{l}}{2(l - n) + 1}, \quad n \geq 1. \tag{18}$$
Equations 17 and 18 for \( a_n \) can be solved exactly in principle. In fact, by making the truncation of \( a_n = 0 \) for \( n \geq 3 \), a nearly exact solution can be obtained as

\[
a_0 = \frac{45(45 + 24 \lambda_3 + 4 \lambda_3^2)}{D_3},
\]

\[
a_1 = \frac{15 \lambda_3 (45 + 8 \lambda_3)}{D_3},
\]

and

\[
a_2 = \frac{45 \lambda_3 (3 + 4 \lambda_3)}{D_3},
\]

where

\[
D_3 = 2025 + 3105 \lambda_3 + 1512 \lambda_3^2 + 256 \lambda_3^3.
\]

In Appendix A, we show that the preceding solution for \( a_0 \), which is directly related to \( g_{eff}(0) \), as shown in the next section, is very close to the exact numerical solution to Eqs. 17 and 18. 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. 10, and hence a truncation solution like the preceding one is almost exact.

**B. 2D**

In 2D, we make use of the following expression,

\[
\frac{2\pi}{|q-k|} = \int dr e^{i(q-k)\cdot r} \frac{1}{r},
\]

and rewrite Eq. 20 as follows:

\[
V_{eff}(q) = \frac{1}{q} - \frac{\lambda_2}{(2\pi)^2} \int dk \theta(k-1) \frac{1}{k^2} V_{eff}(k)
\]

\[
\times \int dr e^{i(q-k)\cdot r} \frac{1}{r},
\]

Carrying out the angular integrations of \( k \) and \( r \), we have

\[
V_{eff}(q) = \frac{1}{q} - \lambda_2 \int_0^\infty dr \int_1^\infty dk \frac{1}{k} V_{eff}(k)
\]

\[
\times J_0(qr) J_0(kr),
\]

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

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

No even power terms exist in the solution to Eq. 25. Again, the erroneous even power terms 15 appear in \( V_{eff}(q) \) due to the approximation made in Eq. 14.

We substitute Eq. 26 into Eq. 25, and obtain

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

where

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

Carrying out the integration over \( k \) in Eq. 28, one obtains,

\[
N_{2n}(q) = \sum_{m=1}^n (-2)^{m-1} \frac{(n-1)!}{(n-m)!}
\]

\[
\times \int_0^\infty dx J_0(x/q) J_m(x)/x, n \geq 1.
\]

The integral on the right hand side of Eq. 29 can be expressed in terms of the hypergeometric function as follows, 31

\[
\int_0^\infty dx J_0(x/q) J_m(x)/x = \frac{\Gamma(\frac{1}{2})}{2^m \Gamma(1) \Gamma(m + \frac{1}{2})}
\]

\[
\times F\left(\frac{1}{2} - m + \frac{1}{2}; 1; \frac{1}{q^2}\right), n \geq 1.
\]

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

\[
N_{2n}(q) = \sum_{m=1}^n (-2)^{m-1} \frac{(n-1)!}{(n-m)!} (2m-1)!!
\]

\[
\times \frac{\Gamma(\frac{1}{2})}{2^m \Gamma(1) \Gamma(m + \frac{1}{2})}
\]

\[
\times F\left(\frac{1}{2} - m + \frac{1}{2}; 1; \frac{1}{q^2}\right), n \geq 1.
\]

Substituting Eq. 31 into Eq. 27, and comparing the same power orders of \( 1/q \), one finally gets

\[
c_0 = 1 - \lambda_2 \sum_{n=0}^\infty \frac{c_n}{2n+1},
\]

and

\[
c_n = \lambda_2 (-1)^n \sum_{m=0}^{n-1} \frac{(2m)!}{(2m+1)!!} \sum_{l=0}^\infty \frac{1}{l} \sum_{m=0}^l \frac{(-2)^m}{(l-m)!(2m+1)!!},
\]

for \( n \geq 1 \).

Similarly to the 3D case, Eqs. 32 and 33 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 \( n \geq 3 \):

\[
c_0 = \frac{15(64 + 25 \lambda_2 + 3 \lambda_3^2)}{D_2},
\]

\[
c_1 = \frac{30 \lambda_2 (8 + \lambda_2)}{D_2},
\]

and

\[
c_2 = \frac{45 \lambda_2 (1 + \lambda_2)}{D_2},
\]

where

\[
D_2 = 960 + 1335 \lambda_2 + 509 \lambda_2^2 + 64 \lambda_3.
\]
III. RESULTS FOR $g_{\uparrow\downarrow}(r)$ AT SMALL $r$

The spin-antiparallel pair-correlation density in the LT can be shown to be \cite{15,18}

$$g_{\uparrow\downarrow}(r) = \frac{4}{n^2} \sum_{p,p'} |1 + \sum_{q} D(p,p';q) \times V_{eff}(p,p';q)e^{iqr}|^2$$ \hspace{1cm} (38)

where the prime on the summations over $p, p'$ means the restrictions $0 \leq p, p' \leq k_F$, and $D(p,p';q)$ is defined as,

$$D(p,p';q) = \frac{(1-n(p+q))(1-n(p'-q))}{\epsilon_p + \epsilon_{p'} - \epsilon_{p+q} - \epsilon_{p'-q}}$$ \hspace{1cm} (39)

Below we present the results for the 3D and 2D cases in subsection A and B, respectively. We will reduce $r$ with unit $1/k_F$.

A. 3D

Using the approximate solution $V_{eff}(q)$ for $V_{eff}(p,p';q)$, one obtains \cite{17}

$$g_{\uparrow\downarrow}(r) = \left[ 1 - \lambda_3 \int_{1}^{\infty} dq V_{eff}(q)j_0(qr) \right]^2.$$ \hspace{1cm} (40)

Trivially,

$$g_{\uparrow\downarrow}(0) = \left[ 1 - \lambda_3 \int_{1}^{\infty} dq V_{eff}(q) \right]^2.$$ \hspace{1cm} (41)

With the expression of Eq. (10), one has

$$g_{\uparrow\downarrow}(0) = a_0^2.$$ \hspace{1cm} (42)

Equation (17) has been made use of in obtaining the preceding result. The expression for $a_0$ is given in Eq. (19), with which we obtain the final result of Eq. (7). Furthermore, it is straightforward to show, from Eq. (10), that at small $r$,

$$g_{\uparrow\downarrow}(r) = g_{\uparrow\downarrow}(0) + \frac{\pi}{2} 3\gamma g_{\uparrow\downarrow}(0)r.$$ \hspace{1cm} (43)

B. 2D

In 2D, one has,

$$g_{\uparrow\downarrow}(r) = \left[ 1 - \lambda_2 \int_{1}^{\infty} dq \frac{1}{q} V_{eff}(q)J_0(qr) \right]^2.$$ \hspace{1cm} (44)

Similar derivation to that in the 3D case leads to

$$g_{\uparrow\downarrow}(0) = \epsilon_0^2,$$ \hspace{1cm} (45)

or, by the use of Eq. (34), the final result of Eq. (8). Furthermore, from Eq. (44), one can obtain

$$g_{\uparrow\downarrow}(r) = g_{\uparrow\downarrow}(0) + 2\lambda_2 g_{\uparrow\downarrow}(0)r.$$ \hspace{1cm} (46)

IV. COMPARISONS AND DISCUSSIONS

First of all, at limiting high density, we have, from Eq. (7),

$$g_{\uparrow\downarrow}(0) = 1 - 2\lambda_3 = 1 - 0.663r_s,$$ \hspace{1cm} (47)

in 3D. Equation (47) is the same as the corresponding Yasuhara’s result \cite{20}. We note that, the first order perturbation calculation, \cite{10,21,25,32} which is believed to approach to the exact result at high density limit, yields a result of $1 - 0.7317r_s$. We plot $g(0) \times r_s$ calculated from Eq. (7) in Fig. 1, in comparison with that calculated from Eq. (47) \cite{15,20,23,30}. Notice that the discrepancy between Eq. (7) and Eq. (47), which appears not minor, arises purely from the approximation of Eq. (4) made in obtaining Eq. (5) in Yasuhara’s theory. In effect, Lowy and Brown \cite{16} had thrown doubt on the validity of the approximation of Eq. (4) made in Yasuhara’s theory. We hence justify their doubt, at least for the limiting short range correlations. The result based on Overhauser’s proposal (Eq. (26) in Ref. [33]) is also shown in Fig. 1. The comparison hence indicates that the coincidence between Overhauser’s result (and the corresponding numerical result of Gori-Giorgi and Perdew \cite{3}) and Yasuhara’s is accidental.

In Fig. 2, we plot $g(0) \times r_s$ in 2D calculated from Eq. (8), together with that from Eq. (47), \cite{15}. Once again, we emphasize that the discrepancy is totally due to the approximation of Eq. (4) made in obtaining Eq. (8). However, at limiting high density, both equations yield
the following same result:

\[ g_{\uparrow\downarrow}(0) = 1 - 2\lambda_2. \]  

(48)

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 [33] for the strong-coupling limit.

\[ \tilde{D}_3 = 2480625 + 4158000\lambda_3^3 + 2437200\lambda_3^2 + 634880\lambda_3^1 + 65536\lambda_3^0. \]  

(A5)

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 proved that, the ladder theory satisfies the cusp condition for the pair-correlation density 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 density.

The main results obtained in this paper are, in effect, Eq. (9) and Eq. (8) given in the Introduction, in three dimensions and two dimensions respectively, for the on-top pair-correlation density in the homogeneous electron liquid. These results have been derived by solving Eq. (3), 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 is determined by the large transfer momentum behavior of the effective potential. The major theoretical progress made in this paper is that we have removed the approximation of Eq. (4) frequently made in the literature for the Coulomb kernel in solving Eq. (3). Our solution to Eq. (3) is thus exact.

\[ a_0 = \frac{175(14175 + 9585\lambda_3^3 + 2520\lambda_3^2 + 256\lambda_3^1)}{D_3}, \] 

(A1)

\[ a_1 = \frac{105\lambda_3(7875 + 2480\lambda_3 + 256\lambda_3^2)}{D_3}, \] 

(A2)

\[ a_2 = \frac{105\lambda_3(1575 + 2280\lambda_3 + 256\lambda_3^2)}{D_3}, \] 

(A3)

\[ a_3 = \frac{175\lambda_3(405 + 576\lambda_3 + 256\lambda_3^2)}{D_3}, \] 

(A4)

where

\[ D_3 = 2480625 + 4158000\lambda_3 + 2437200\lambda_3^2 + 634880\lambda_3^3 + 65536\lambda_3^4. \]  

(A5)

APPENDIX A: ON THE SOLUTIONS TO EQS. (17) AND (18), AND EQS. (32) AND (33).

A nearly exact solution for \( a_0 \) to Eqs. (17) and (18) has been given in Eq. (19) in Sect. III by the truncation of \( a_n = 0 \) for \( n \geq 3 \). Below we give the solution for \( a_n \) by the truncation of \( a_n = 0 \) for \( n \geq 4 \).

\[ a_0 = \frac{175(14175 + 9585\lambda_3^3 + 2520\lambda_3^2 + 256\lambda_3^1)}{D_3}, \] 

(A1)

\[ a_1 = \frac{105\lambda_3(7875 + 2480\lambda_3 + 256\lambda_3^2)}{D_3}, \] 

(A2)

\[ a_2 = \frac{105\lambda_3(1575 + 2280\lambda_3 + 256\lambda_3^2)}{D_3}, \] 

(A3)

\[ a_3 = \frac{175\lambda_3(405 + 576\lambda_3 + 256\lambda_3^2)}{D_3}, \] 

(A4)

\[ D_3 = 2480625 + 4158000\lambda_3 + 2437200\lambda_3^2 + 634880\lambda_3^3 + 65536\lambda_3^4. \]  

(A5)
In Fig. 3, we plot the results for $a_0$ calculated from Eqs. [19] and [A1], together with the corresponding exact numerical solution to Eqs. [17], and [18]. There is basically no difference among them. We present the expressions of Eqs. (17), and (18) and (A1), together with the corresponding exact numerical solution to Eqs. (19) above for possible future reference.

Similar expressions for the 2D case are given below.

$$c_0 = \frac{35(12288 + 6000\lambda_2^2 + 1121\lambda_2^4 + 80\lambda_2^3)}{D_2}, \quad (A6)$$

$$c_1 = \frac{1680\lambda_2(64 + 14\lambda_2 + \lambda_2^3)}{D_2}, \quad (A7)$$

$$c_2 = \frac{105\lambda_2(192 + 207\lambda_2 + 16\lambda_2^3)}{D_2}, \quad (A8)$$

and

$$c_3 = \frac{350\lambda_2(24 + 25\lambda_2 + 8\lambda_2^3)}{D_2}, \quad (A9)$$

where

$$D_2 = 430080 + 640080\lambda_2 + 290307\lambda_2^2 + 55472\lambda_2^3 + 4096\lambda_2^4.$$  (A10)

The corresponding illustration is given in Fig. 4.

**APPENDIX B: CUSP CONDITION IN THE LADDER THEORY**

Due to the singularity of the Coulomb potential between electrons, the many-body Schrödinger wavefunction has a cusp when any two electrons coalesce. [34, 35]

This fact leads to the cusp condition of Eq. [24] for the pair-correlation density (also known as Kimball relation in the literature of many-electron theory). Recently it was claimed that Eq. [24] is not satisfied in the LT. [37] In this appendix, we give a rigorous proof for Eq. [24] in the LT. The proof will be formulated in 3D.

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

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

where $\hat{n}_\sigma(q)$ 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. (18) as [14, 15]:

$$S_{\uparrow\downarrow}(q) = \frac{1}{n} \sum_{p,p'} \left[ 2D(p,p';q)V_{\text{eff}}(p,p';q) + \sum_k D(p,p';k)V_{\text{eff}}(p,p';k) \times D(p,p';k - q)V_{\text{eff}}(p,p';k - q) \right]. \quad (B2)$$

Next we examine the large momentum structure of $S_{\uparrow\downarrow}(q)$. For $p, p' \leq k_F$ and $q \rightarrow \infty$, one has, from Eqs. (14) and (39):

$$D(p,p';q) \ V_{\text{eff}}(p,p';q) = \frac{1}{2\epsilon_q} v(q)$$

$$\times \left[ 1 + \sum_k \sum_{p,p'} D(p,p';k)V_{\text{eff}}(p,p';k) \right]. \quad (B3)$$

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

$$\sum_k D(p,p';k)V_{\text{eff}}(p,p';k)$$

$$\times D(p,p';q - k)V_{\text{eff}}(p,p';q - k)$$

$$= \frac{1}{\epsilon_q} v(q) \left[ 1 + \sum_k \sum_{p,p'} D(p,p';k)V_{\text{eff}}(p,p';k) \right]$$

$$\times \sum_{k'} D(p,p';k')V_{\text{eff}}(p,p';k'). \quad (B4)$$

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

$$\lim_{q \rightarrow \infty} \sum_k f(k)g(q - k) = 2\{q\} \sum_k f(k), \quad (B5)$$

if $\lim_{q \rightarrow \infty} f(q) \sim O(1/q^4)$. It seems that a mistake occurs in Ref. [37] 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. [37].
Substituting Eqs. (B3) and (B4) into Eq. (B2), one has

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

(B6)

On the other hand, from Eq. (38), we have

\[ g_{\uparrow\downarrow}(0) = \frac{4}{3\pi} \sum_{\mathbf{p}, \mathbf{p}'} \left( 1 + \sum_{\mathbf{q}} D(\mathbf{p}, \mathbf{p}'; \mathbf{q}) \times V_{\text{eff}}(\mathbf{p}, \mathbf{p}'; \mathbf{q}) \right)^2. \]  

(B7)

Comparing Eq. (B6) and Eq. (B7) yields

\[ S_{\uparrow\downarrow}(q) = \frac{2\pi^2 nm}{q^4} g_{\uparrow\downarrow}(0). \]  

(B8)

Combining the preceding result with the following well-known relation \(^{24}\),

\[ \lim_{q \to \infty} q^4 S_{\uparrow\downarrow}(q) = -2\pi n \frac{\partial g_{\uparrow\downarrow}(r)}{\partial r} \bigg|_{r=0}, \]  

(B9)

one proves the cusp condition of Eq. (2) in the LT.

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

\[ S_{\uparrow\downarrow}(q) = -\frac{\pi e^2 n m}{q^2} g_{\uparrow\downarrow}(0), \]  

(B10)

in the LT. Combining the above result with the following relation \(^{33}\)

\[ \lim_{q \to \infty} q^3 S_{\uparrow\downarrow}(q) = -\frac{1}{2} \pi n \frac{\partial g_{\uparrow\downarrow}(r)}{\partial r} \bigg|_{r=0}, \]  

(B11)

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

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