Applicability of the ladder theory to the three-dimensional homogeneous electron gas

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Emphasizing a proper description of short-range interactions, the ladder theory (LT) is incapable of reliably reproducing any property of the three-dimensional electron gas except for the correlation function at the electron coalescence limit (the on-top density) $g(0)$ and the related large-k tail of the momentum distribution $n(k)$. Because of the violation of the cusp condition, poor accuracy of the predicted $g(r)$ is expected for any nonvanishing r. Although the LT yields components of the correlation energy that satisfy the virial theorem for homogeneous interaction potentials, in the case of the Coulomb potential these components turn out to be infinite. A straightforward analysis shows that any effort at alleviating this problem by introducing a long-range screening is bound to violate the virial condition. A commonly employed approximate version of the LT, which avoids Coulomb singularities, yields incorrect energy components and an unphysical momentum distribution despite producing reasonable values of $g(0)$. Since lessening of the approximation worsens the accuracy of the high-density limit of $g(0)$, this result appears to be due to a fortuitous cancellation of errors.

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I. INTRODUCTION

The recent advances in quantum Monte Carlo (QMC) techniques have brought about a dramatic improvement in the accuracy of energy computations for the three-dimensional homogeneous electron gas (3D HEG).[1] On the other hand, being less amenable to stochastic simulations, other properties of the 3D HEG are usually obtained from approximate treatments of electron correlation. Among those properties, the momentum distribution $n(k)$ and the correlation function $g(r)$ are of particular importance to the development and calibration of density and density matrix functional theories.[2]

Present QMC calculations are capable of yielding reasonably accurate values of $g(r)$ only for the interelectronic distance r that is of the same order of magnitude as the Wigner-Seitz parameter r_s.[3] The currently available estimates of $g(r)$ at shorter distances, afforded by its high-density ($r_s \to 0$) asymptotics,[4] various implementations[3,5] of the Overhauser model,[6] approximations to the ladder theory,[7,8] and hypernetted-chain equations[9] exhibit unacceptable scatter. Even worse situation is encountered for $n(k)$, for which the high-density random phase approximation (RPA) asymptotics is known to be twice the correct value for large magnitudes of k due to the neglect of exchange effects.[10] Attempts at systematically correcting this deficiency[11] yield results in poor agreement with those of other theoretical treatments,[9,12] whereas the published QMC estimates[13] are of doubtful quality. This lack of reliable data hampers the construction of interpolation schemes for $n(k)$ valid over entire ranges of k and r_s.[14]

While the RPA formalism is tailored towards the description of the direct component of long-range electron-electron interactions, the ladder theory (LT) deals primarily with both the direct and exchange parts of short-range correlations, which become important at larger values of r_s.[7] In the case of an exactly solvable one-dimensional fermion system with repulsive δ-function interactions,[15] comparison of the RPA and LT energies with the exact ones reveals a clear superiority of the latter approach.[16] On the other hand, the two published sets of the LT energies of the two-dimensional HEG[17] are mutually inconsistent.

Thus far, the issue of potential merits and drawbacks of the ladder theory applied to the description of the 3D HEG has not been properly addressed, the published calculations[7,8] employing crude approximations and concerning only one property, namely $g(0)$. Prompted by this state of affairs, we have studied the applicability of the LT to the 3D HEG by examining whether the solutions of its equations satisfy such fundamental relations as the cusp condition[18] and the virial theorem.[19] The results of this study are compiled in this paper.

II. THE LADDER THEORY

Consider the three-dimensional homogeneous gas with density ρ consisting of fermions interacting through a potential specified by its Fourier transform $V(\mathbf{p})=V(-\mathbf{p})$ with the large-momentum asymptotics of $\lim_{p\to\infty} p^2\, V(\mathbf{p})=4\pi$. Here and in the following, all the momenta are expressed in units of k_F:

$$k_F=(3\pi^2\rho)^{1/3}, \quad \alpha k_F r_s=1, \quad \alpha=(4/9\pi)^{1/3}, \tag{1}$$

whereas all the potentials are in units of k_F^{-2}. In the ladder theory, the correlation energy density of such a spin-unpolarized gas is given by[7]

$$e_c=-(64\pi^9)^{-1}k_F^3\int_{\Omega(\mathbf{P},\mathbf{p})} d\mathbf{P}\, d\mathbf{p}\int_{\Omega(\mathbf{P},\mathbf{q})} A(\mathbf{P},\mathbf{p},\mathbf{q}) \times[2V(\mathbf{q}-\mathbf{p})-V(\mathbf{q}+\mathbf{p})]\, U(\mathbf{P},\mathbf{p},\mathbf{q})\, d\mathbf{q}, \tag{2}$$

where the effective potential $U(\mathbf{P},\mathbf{p},\mathbf{q})$ solves the Bethe-Goldstone equation

$$U(\mathbf{P},\mathbf{p},\mathbf{q}) = V(\mathbf{q}-\mathbf{p}) - (2\pi)^{-3}k_F^{-1}\int_{\Omega(\mathbf{P},\mathbf{q}')} A(\mathbf{P},\mathbf{p},\mathbf{q}') \times V(\mathbf{q}-\mathbf{q}')\ U(\mathbf{P},\mathbf{p},\mathbf{q}')\ d\mathbf{q}' \tag{3}$$

that ensues from an infinite summation of ladder diagrams. In Eqs. (2) and (3),

$$\Omega(\mathbf{p},\mathbf{q}) \equiv |\mathbf{p}+\mathbf{q}| \geqslant 1 \cap |\mathbf{p}-\mathbf{q}| \geqslant 1,$$
$$\overline{\Omega}(\mathbf{p},\mathbf{q}) \equiv |\mathbf{p}+\mathbf{q}| \leqslant 1 \cap |\mathbf{p}-\mathbf{q}| \leqslant 1 \tag{4}$$

and [note that in fact $A(\mathbf{P},\mathbf{p},\mathbf{q})$ depends only on p and q],

$$A(\mathbf{P},\mathbf{p},\mathbf{q}) = [\varepsilon(\mathbf{P}+\mathbf{q}) + \varepsilon(\mathbf{P}-\mathbf{q}) - \varepsilon(\mathbf{P}+\mathbf{p}) - \varepsilon(\mathbf{P}-\mathbf{p})]^{-1} = (q^2-p^2)^{-1}, \tag{5}$$

where

$$\varepsilon(\mathbf{p}) = (1/2)p^2. \tag{6}$$

Because of its complexity, Eq. (3) cannot be readily solved even with numerical approaches. However, many properties of its solutions can be determined without difficulty.

III. THE CORRELATION FUNCTION AND THE CUSP CONDITION

Functional differentiation of e_c with respect to V yields the correlation contribution $S_c(\mathbf{k})$ to the static structure factor

$$\begin{aligned} S_c(\mathbf{k}) &= 2\rho^{-1}k_F^2\delta e_c/\delta V(\mathbf{k}) \\ &= -(3/4\pi^4)k_F^{-1}\int_{\overline{\Omega}(\mathbf{P},\mathbf{p})} d\mathbf{P}\ d\mathbf{p}\int_{\Omega(\mathbf{P},\mathbf{q})} d\mathbf{q}\ A(\mathbf{P},\mathbf{p},\mathbf{q}) \\ &\quad \times U(\mathbf{P},\mathbf{p},\mathbf{q})\{2[2\delta(\mathbf{q}-\mathbf{p}-\mathbf{k}) - \delta(\mathbf{q}+\mathbf{p}-\mathbf{k})] \\ &\quad - (2\pi)^{-3}k_F^{-1}\int_{\Omega(\mathbf{P},\mathbf{q}')} d\mathbf{q}'\ A(\mathbf{P},\mathbf{p},\mathbf{q}')[2\ U(\mathbf{P},\mathbf{p},\mathbf{q}') \\ &\quad - U(\mathbf{P},-\mathbf{p},\mathbf{q}')]\delta(\mathbf{q}-\mathbf{q}'-\mathbf{k})\}. \end{aligned} \tag{7}$$

Consequently

$$\begin{aligned} g(0) &= 1/2 + \rho^{-1}(2\pi)^{-3}k_F^3\int S_c(\mathbf{k})\ d\mathbf{k} \\ &= 1/2 - (9/32\pi^5)k_F^{-1}\int_{\overline{\Omega}(\mathbf{P},\mathbf{p})} d\mathbf{P}\ d\mathbf{p} \\ &\quad \times\int_{\Omega(\mathbf{P},\mathbf{q})} d\mathbf{q}\ A(\mathbf{P},\mathbf{p},\mathbf{q})\ U(\mathbf{P},\mathbf{p},\mathbf{q}) \\ &\quad \times\left[2 - (2\pi)^{-3}k_F^{-1}\int_{\Omega(\mathbf{P},\mathbf{q}')} d\mathbf{q}'\ A(\mathbf{P},\mathbf{p},\mathbf{q}')\ U(\mathbf{P},\mathbf{p},\mathbf{q}')\right] \\ &= (9/4\pi^2)\int_{\overline{\Omega}(\mathbf{P},\mathbf{p})}\left[1 - (2\pi)^{-3}k_F^{-1}\int_{\Omega(\mathbf{P},\mathbf{q})} A(\mathbf{P},\mathbf{p},\mathbf{q})\right. \\ &\quad \left.\times U(\mathbf{P},\mathbf{p},\mathbf{q})\ d\mathbf{q}\right]^2 d\mathbf{P}\ d\mathbf{p}, \end{aligned} \tag{8}$$

as expected.[8] At this point it is convenient to define a different quantity

$$\begin{aligned} \xi(\mathbf{P},\mathbf{p}) &= \lim_{q\to\infty} U(\mathbf{P},\mathbf{p},\mathbf{q})/V(\mathbf{q}-\mathbf{p}) \\ &= 1 - (2\pi)^{-3}k_F^{-1}\lim_{q\to\infty} V(\mathbf{q}-\mathbf{p})^{-1} \\ &\quad \times\int_{\Omega(\mathbf{P},\mathbf{q}')} A(\mathbf{P},\mathbf{p},\mathbf{q}')\ V(\mathbf{q}-\mathbf{q}')\ U(\mathbf{P},\mathbf{p},\mathbf{q}')\ d\mathbf{q}' \\ &= 1 - (2\pi)^{-3}k_F^{-1}\int_{\Omega(\mathbf{P},\mathbf{q}')} A(\mathbf{P},\mathbf{p},\mathbf{q}')\ U(\mathbf{P},\mathbf{p},\mathbf{q}')\ d\mathbf{q}' \end{aligned} \tag{9}$$

that measures the reduction of interaction strength due to short-range screening and allows one to write Eq. (8) in a compact form

$$g(0) = (9/4\pi^2)\int_{\overline{\Omega}(\mathbf{P},\mathbf{p})} \xi(\mathbf{P},\mathbf{p})^2\ d\mathbf{P}\ d\mathbf{p} \geqslant 0. \tag{10}$$

At the large-k limit

$$\begin{aligned} S(\mathbf{k}) - 1 = S_c(\mathbf{k}) &= -(3/4\pi^4)k_F^{-1}\int_{\overline{\Omega}(\mathbf{P},\mathbf{p})} d\mathbf{P}\ d\mathbf{p} \\ &\quad \times\left\{2[2\ A(\mathbf{P},\mathbf{p},\mathbf{k}+\mathbf{p})\ U(\mathbf{P},\mathbf{p},\mathbf{k}+\mathbf{p})\right. \\ &\quad - A(\mathbf{P},\mathbf{p},\mathbf{k}-\mathbf{p})\ U(\mathbf{P},\mathbf{p},\mathbf{k}-\mathbf{p})] - (2\pi)^{-3}k_F^{-1} \\ &\quad \times\int_{\Omega(\mathbf{P},\mathbf{q})} A(\mathbf{P},\mathbf{p},\mathbf{q})\ U(\mathbf{P},\mathbf{p},\mathbf{q})\ A(\mathbf{P},\mathbf{p},\mathbf{q}-\mathbf{k}) \\ &\quad \left.\times[2\ U(\mathbf{P},\mathbf{p},\mathbf{q}-\mathbf{k}) - U(\mathbf{P},-\mathbf{p},\mathbf{q}-\mathbf{k})]d\mathbf{q}\right\} \end{aligned} \tag{11}$$

as it is always possible to find a combination of vectors that simultaneously satisfy the conditions imposed by the delta functions and the integration domains. Combining Eqs. (5), (9), and (11) with the assumed asymptotics of $V(\mathbf{k})$ yields

$$\lim_{k\to\infty} k^4[1 - S(\mathbf{k})] = (3/\pi^3)k_F^{-1}\int_{\overline{\Omega}(\mathbf{P},\mathbf{p})} [1+\xi(\mathbf{P},\mathbf{p})]\xi(\mathbf{P},\mathbf{p})\ d\mathbf{P}\ d\mathbf{p}, \tag{12}$$

from which it follows that:[18]

$$\begin{aligned} g'(0) \equiv dg(r)/dr|_{r=0} &= (3\pi/8)\,k_F\lim_{k\to\infty} k^4[1 - S(\mathbf{k})] \\ &= (9/8\pi^2)\int_{\overline{\Omega}(\mathbf{P},\mathbf{p})} [1+\xi(\mathbf{P},\mathbf{p})]\ \xi(\mathbf{P},\mathbf{p})\ d\mathbf{P}\ d\mathbf{p} \\ &= g(0) + (9/8\pi^2)\int_{\overline{\Omega}(\mathbf{P},\mathbf{p})} [1-\xi(\mathbf{P},\mathbf{p})]\ \xi(\mathbf{P},\mathbf{p})\ d\mathbf{P}\ d\mathbf{p} \\ &\geqslant g(0), \end{aligned} \tag{13}$$

the equality being attained only when $\xi(\mathbf{P},\mathbf{p}) \equiv 1$. Thus, the ladder theory violates the cusp condition[18] for $g(r)$, approaching it only asymptotically at the $r_s \to 0$ limit.

IV. THE MOMENTUM DISTRIBUTION AND ITS ASYMPTOTICS

The correlation contribution $n_c(\mathbf{k})$ to the momentum distribution is also available through functional differentiation

$$\begin{aligned} n_c(\mathbf{k}) &= (1/2)\ \delta e_c/\delta\varepsilon(\mathbf{k}) \\ &= (128\pi^9)^{-1}k_F \int_{\Omega(\mathbf{P},\mathbf{p})} d\mathbf{P}\ d\mathbf{p} \int_{\Omega(\mathbf{P},\mathbf{q})} d\mathbf{q}\ U(\mathbf{P},\mathbf{p},\mathbf{q}) \\ &\quad \times [2\ U(\mathbf{P},\mathbf{p},\mathbf{q}) - U(\mathbf{P},-\mathbf{p},\mathbf{q})][A(\mathbf{P},\mathbf{p},\mathbf{k}-\mathbf{P})^2 \\ &\quad \times \delta(\mathbf{q}-\mathbf{k}+\mathbf{P}) + A(\mathbf{P},\mathbf{p},\mathbf{P}-\mathbf{k})^2\ \delta(\mathbf{q}+\mathbf{k}-\mathbf{P}) \\ &\quad - A(\mathbf{P},\mathbf{k}-\mathbf{P},\mathbf{q})^2\ \delta(\mathbf{p}-\mathbf{k}+\mathbf{P}) \\ &\quad - A(\mathbf{P},\mathbf{P}-\mathbf{k},\mathbf{q})^2\ \delta(\mathbf{p}+\mathbf{k}-\mathbf{P})]. \end{aligned} \tag{14}$$

Inspection of the integration domains in Eq. (14) readily produces

$$\begin{aligned} n_c(\mathbf{k}) &= -(8\pi^6)^{-1}k_F^{-2} \int_{\Omega(\mathbf{P},\mathbf{q})\cap|2\mathbf{P}-\mathbf{k}|\leqslant 1} A(\mathbf{P},\mathbf{k}-\mathbf{P},\mathbf{q})^2 \\ &\quad \times U(\mathbf{P},\mathbf{k}-\mathbf{P},\mathbf{q})[2\ U(\mathbf{P},\mathbf{k}-\mathbf{P},\mathbf{q}) \\ &\quad - U(\mathbf{P},\mathbf{P}-\mathbf{k},\mathbf{q})]d\mathbf{P}\ d\mathbf{q} \quad \text{for } k \leqslant 1 \end{aligned} \tag{15}$$

and

$$\begin{aligned} n_c(\mathbf{k}) &= (8\pi^6)^{-1}k_F^{-2} \int_{\Omega(\mathbf{P},\mathbf{p})\cap|2\mathbf{P}-\mathbf{k}|\geqslant 1} A(\mathbf{P},\mathbf{p},\mathbf{k}-\mathbf{P})^2 \\ &\quad \times U(\mathbf{P},\mathbf{p},\mathbf{k}-\mathbf{P})[2U(\mathbf{P},\mathbf{p},\mathbf{k}-\mathbf{P}) \\ &\quad - U(\mathbf{P},-\mathbf{p},\mathbf{k}-\mathbf{P})]\ d\mathbf{P}\ d\mathbf{p} \quad \text{for } k \geqslant 1. \end{aligned} \tag{16}$$

Combining Eqs. (5), (9), (10), and (16) with the assumed asymptotics of $V(\mathbf{k})$ yields

$$\begin{aligned} \lim_{\mathbf{k}\to\infty} k^8\ n_c(\mathbf{k}) &= (2/\pi^4)k_F^{-2} \int_{\Omega(\mathbf{P},\mathbf{p})} \xi(\mathbf{P},\mathbf{p})^2\ d\mathbf{P}\ d\mathbf{p} \\ &= (8/9\pi^2)k_F^{-2}\ g(0) \end{aligned} \tag{17}$$

as expected.[20]

V. THE CHEMICAL POTENTIAL, THE VIRIAL THEOREM, AND THE KINETIC ENERGY

The correlation contribution μ_c to the chemical potential reads

$$\begin{aligned} \mu_c &= \partial e_c/\partial\rho = (k_F/3\rho)\ \partial e_c/\partial k_F \\ &= (3\rho)^{-1}\Bigg\{ 4e_c + (64\pi^9)^{-1}k_F^3 \int_{\Omega(\mathbf{P},\mathbf{p})} d\mathbf{P}\ d\mathbf{p} \int_{\Omega(\mathbf{P},\mathbf{q})} A(\mathbf{P},\mathbf{p},\mathbf{q}) \\ &\quad \times [2U(\mathbf{P},\mathbf{p},\mathbf{q}) - U(\mathbf{P},-\mathbf{p},\mathbf{q})]\ U(\mathbf{P},\mathbf{p},\mathbf{q})\ d\mathbf{q} \Bigg\}. \end{aligned} \tag{18}$$

Hence, the virial theorem[19]

$$3\ \rho\ \mu_c = 4\ e_c + t_c \tag{19}$$

demands that the correlation component t_c of the kinetic energy density equals

$$\begin{aligned} t_c &= (64\pi^9)^{-1}k_F^3 \int_{\Omega(\mathbf{P},\mathbf{p})} d\mathbf{P}\ d\mathbf{p} \int_{\Omega(\mathbf{P},\mathbf{q})} A(\mathbf{P},\mathbf{p},\mathbf{q}) \\ &\quad \times [2\ U(\mathbf{P},\mathbf{p},\mathbf{q}) - U(\mathbf{P},-\mathbf{p},\mathbf{q})]U(\mathbf{P},\mathbf{p},\mathbf{q})d\mathbf{q}. \end{aligned} \tag{20}$$

On the other hand

$$\begin{aligned} t_c &= (4\pi^3)^{-1}k_F^5 \int \varepsilon(\mathbf{k})n_c(\mathbf{k})d\mathbf{k} \\ &= (32\pi^9)^{-1}k_F^3 \int_{\Omega(\mathbf{P},\mathbf{p})} d\mathbf{P}\ d\mathbf{p} \int_{\Omega(\mathbf{P},\mathbf{q})} [\varepsilon(\mathbf{P}+\mathbf{q}) - \varepsilon(\mathbf{P}+\mathbf{p})] \\ &\quad \times A(\mathbf{P},\mathbf{p},\mathbf{q})^2 U(\mathbf{P},\mathbf{p},\mathbf{q})[2U(\mathbf{P},\mathbf{p},\mathbf{q}) - U(\mathbf{P},-\mathbf{p},\mathbf{q})]d\mathbf{q}, \end{aligned} \tag{21}$$

which, by virtue of Eq. (5), affords Eq. (20) after a trivial manipulation. Thus, despite its nonvariational character, the ladder theory is consistent with the virial theorem.

VI. THE CASE OF THE COULOMBIC POTENTIAL AND APPROXIMATE SOLUTIONS

In the particular case of the Coulombic potential

$$V(\mathbf{q}) = 4\pi|\mathbf{q}|^{-2}, \tag{22}$$

the integral

$$I(0) = \int_{\Omega(\mathbf{P},\mathbf{p})} d\mathbf{P}\ d\mathbf{p} \int_{\Omega(\mathbf{P},\mathbf{q})} A(\mathbf{P},\mathbf{p},\mathbf{q})\ V(\mathbf{q}-\mathbf{p})^2 d\mathbf{q} \tag{23}$$

diverges due to the well-known singularity at $\mathbf{q}=\mathbf{p}$.[21] Consequently, although the Bethe-Goldstone Eq. (3) can be iterated for small values of r_s (large values of k_F), e_c does not possess a power expansion in terms of r_s. Still, one may inquire whether the summation of ladder diagrams leads to a finite e_c (as it does in the case of ring diagrams[21]). In order to answer this question, one isolates the singularity by writing

$$U(\mathbf{P},\mathbf{p},\mathbf{q}) = V(\mathbf{q}-\mathbf{p}) + W(\mathbf{P},\mathbf{p},\mathbf{q}) \tag{24}$$

and substituting $W(\mathbf{P},\mathbf{p},\mathbf{q})$ into Eq. (3), which yields

$$W(\mathbf{P},\mathbf{p},\mathbf{p}) \approx -(2\pi)^{-3}\ k_F^{-1}[I_1(\mathbf{P},\mathbf{p}) + W(\mathbf{P},\mathbf{p},\mathbf{p})I_2(\mathbf{P},\mathbf{p})]. \tag{25}$$

Both

$$I_1(\mathbf{P},\mathbf{p}) = \int_{\Omega(\mathbf{P},\mathbf{q})} A(\mathbf{P},\mathbf{p},\mathbf{q})\ V(\mathbf{q}-\mathbf{p})^2\ d\mathbf{q} \tag{26}$$

and

$$I_2(\mathbf{P},\mathbf{p}) = \int_{\Omega(\mathbf{P},\mathbf{q})} A(\mathbf{P},\mathbf{p},\mathbf{q})\ V(\mathbf{q}-\mathbf{p})\ d\mathbf{q}, \tag{27}$$

which can be readily computed, diverge for $\mathbf{q}=\mathbf{p}$. Next, one examines the finiteness of the integral [compare Eqs. (2), (3), and (25)]:

$$\begin{aligned} I(k_F) &= \int_{\bar{\Omega}(\mathbf{P},\mathbf{p})} d\mathbf{P}\ d\mathbf{p} \int_{\Omega(\mathbf{P},\mathbf{q})} A(\mathbf{P},\mathbf{p},\mathbf{q})\ V(\mathbf{q}-\mathbf{p}) U(\mathbf{P},\mathbf{p},\mathbf{q})\ d\mathbf{q} \\ &= -(2\pi)^3 k_F \int_{\bar{\Omega}(\mathbf{P},\mathbf{p})} W(\mathbf{P},\mathbf{p},\mathbf{p}) d\mathbf{P}\ d\mathbf{p} \\ &\approx \int_{\bar{\Omega}(\mathbf{P},\mathbf{p})} I_1(\mathbf{P},\mathbf{p})[1+(2\pi)^{-3}k_F^{-1}\ I_2(\mathbf{P},\mathbf{p})]^{-1} d\mathbf{P}\ d\mathbf{p}. \end{aligned} \tag{28}$$

Numerical experiments with varying quadrature grids indicate that $I(k_F)$ is infinite. Therefore, unlike the RPA approach, the ladder theory does not yield a finite correlation energy.

Consider the high-density limit of $g(0)$ obtained by substituting $V(\mathbf{q}-\mathbf{p})$ for $U(\mathbf{P},\mathbf{p},\mathbf{q})$ in Eq. (8) and retaining only the term linear in k_F^{-1}:

$$\begin{aligned} g(0) &= (9/4\pi^2) \int_{\bar{\Omega}(\mathbf{P},\mathbf{p})} [1-2(2\pi)^{-3}k_F^{-1} I_2(\mathbf{P},\mathbf{p})]\ d\mathbf{P}\ d\mathbf{p} + \ldots \\ &= (1/2) - (9/16\pi^5) k_F^{-1} \int_{\bar{\Omega}(\mathbf{P},\mathbf{p})} I_2(\mathbf{P},\mathbf{p}) d\mathbf{P}\ d\mathbf{p} + \ldots \\ &= (1/2) - (5\pi)^{-1}(\pi^2 + 6\ \ln 2 - 3) k_F^{-1} + \ \ldots\ . \end{aligned} \tag{29}$$

This limit turns out to be identical with the leading term in the exact asymptotics[4]—an expected result taking into account that the lowest-order ring and ladder diagrams coincide. On the other hand, inspection of Eqs. (15) and (16) shows that $n_c(\mathbf{k})$ diverges at $k=1$.

In principle, the divergences in e_c, t_c, μ_c, and $n_c(\mathbf{k})$ could be remedied by incorporating a long-range screening in the Coulombic $V(\mathbf{q})$, i.e., altering it in such a way that it remains finite at $q\to 0$. However, the dependence of the resulting $V(\mathbf{q})$ on k_F required by a proper description of such screening would give rise to violation of the virial theorem [compare Eq. (18)].[22]

The singularity at $\mathbf{q}=\mathbf{p}$ is also avoided (although in a spurious way) in an approximation, employed in all the LT calculations on the 3D HEG performed to date,[7,8] that consistently replaces $U(\mathbf{P},\mathbf{p},\mathbf{q})$ with $\bar{U}(\mathbf{q})=U(\mathbf{0},\mathbf{0},\mathbf{q})$ in Eqs. (3) and (9) by inserting the factor $(2\pi^2/9)\delta(\mathbf{P})\delta(\mathbf{p})$ in front of $d\mathbf{P}\ d\mathbf{p}$ in Eqs. (2), (10), (13), (14), and (21). The resulting approximate equations read

$$e_c = -(18\pi^5)^{-1} k_F^3 \int_1^\infty q^{-2}\ \bar{U}(q)\ dq, \tag{30}$$

$$\bar{U}(q) = 4\pi\ q^{-2} - (\pi k_F q)^{-1} \int_1^\infty q'^{-1} \ln\left|\frac{q+q'}{q-q'}\right|\ \bar{U}(q')\ dq', \tag{31}$$

$$\bar{\xi} \equiv \xi(\mathbf{0},\mathbf{0}) = (4\pi)^{-1} \lim_{q\to\infty} q^2 \bar{U}(q), \tag{32}$$

$$g(0) = (1/2)\bar{\xi}^2, \tag{33}$$

$$g'(0) = (1/4)(1+\bar{\xi})\bar{\xi}, \tag{34}$$

$$\begin{aligned} n_c(k) &= (36\pi^4)^{-1} k_F^{-2}\ \eta(k-1)\ \bar{U}(k)^2 k^{-4} \\ &\quad - (9\pi^3)^{-1} k_F^{-2} \int_1^\infty \bar{U}(q)^2\ q^{-2}\ dq\ \delta(\mathbf{k}), \end{aligned} \tag{35}$$

and

$$t_c = (72\pi^6)^{-1} k_F^3 \int_1^\infty \bar{U}(q)^2\ dq, \tag{36}$$

where $\eta(x)$ is the Heaviside step function. Thus, although the values of $g(0)$ afforded by this approximation appear to be reasonable,[8] with the high-density asymptotics

$$g(0) = (1/2) - (2/\pi) k_F^{-1} + \ldots \tag{37}$$

suffering from a 10% (0.6366 vs 0.7021) error in the term proportional to k_F^{-1}, the correlation contributions e_c and t_c possess the $r_s\to 0$ limits of

$$e_c = -t_c = -(2/27\pi^4)\ k_F^3 + \ \ldots\ = -(2/9\pi^2)\rho + \ \ldots\ , \tag{38}$$

that are predictably devoid of the logarithmic terms. Even worse, the approximate effect of electron correlation on the momentum distribution is spuriously limited to $k=0$ and $k\geqslant 1$.

A lesser approximation that involves setting $\mathbf{P}=\mathbf{0}$ (rather than $\mathbf{P}=\mathbf{p}=\mathbf{0}$ as above), brings back the singularities and *worsens* the high-density asymptotics of $g(0)$. Finally, it should also be noted that a crude approximation to $V(\mathbf{q})$, which allows for an explicit solution of Eq. (31) in terms of Bessel functions,[7] results in a serious underestimation of $g(0)$ (by as much as a factor of 2 at $r_s\approx 5$)[8] and thus should be avoided.

VII. CONCLUSIONS

Emphasizing a proper description of short-range interactions, the LT is incapable of reliably reproducing any property of the three-dimensional electron gas except for the correlation function at the electron coalescence limit (the on-top density) $g(0)$ and the related large-k tail of the momentum distribution $n(k)$. However, because of the violation of the cusp condition, poor accuracy of the predicted $g(r)$ is expected for any nonvanishing r. Despite its nonvariational character, the LT yields components of the correlation energy

that satisfy the virial theorem for homogeneous interaction potentials. However, in the case of the Coulomb potential all the energy components turn out to be infinite. A straightforward analysis shows that any effort at alleviating this problem by introducing a long-range screening is bound to violate the virial condition.

An approximate version of the LT, which avoids Coulomb singularities, yields incorrect energy components and an unphysical momentum distribution despite producing reasonable values of $g(0)$. Since lessening of the approximation worsens the accuracy of the high-density limit of $g(0)$, this result appears to be due to a fortuitous cancellation of errors.

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