Correlation energy of a two-dimensional electron gas from static and dynamic exchange-correlation kernels

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We calculate the correlation energy of a two-dimensional homogeneous electron gas using several available approximations for the exchange-correlation kernel $f_{xc}(q, \omega)$ entering the linear dielectric response of the system. As in the previous work of Lein et al. [Phys. Rev. B 67, 13431 (2000)] on the three-dimensional electron gas, we give attention to the relative roles of the wave number and frequency dependence of the kernel and analyze the correlation energy in terms of contributions from the $(q, i\omega)$ plane. We find that consistency of the kernel with the electron-pair distribution function is important and in this case the nonlocality of the kernel in time is of minor importance, as far as the correlation energy is concerned. We also show that, and explain why, the popular Adiabatic Local Density Approximation performs much better in the two-dimensional case than in the three-dimensional one.

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I. INTRODUCTION

Fluids of electronic carriers with essentially two-dimensional (2D) dynamics in semiconductor structures present a rich phenomenology, in which dynamical correlations take increasing importance as the electron density is lowered. Many of the electron-electron interaction effects can be understood with the help of the homogeneous electron gas (EG) model. A central role in the theory of short-range correlations in the EG is played by the wave number and frequency dependent exchange-correlation kernels or equivalently by the local field factors entering the linear response properties of the model. These provide key inputs for some applications of density functional theory and for studies of quasi-particle properties such as the effective mass and the effective Landé g-factor. These properties are known from experiment for carriers in semiconductor structures over a wide range of carrier density. A great deal of accurate information has come from quantum Monte Carlo (QMC) studies, but theoretical understanding continues to draw interest.

The exchange-correlation kernel $f_{xc}(q, \omega)$ entering the dielectric response of the EG determines its correlation energy through the fluctuation-dissipation theorem relating the imaginary part of the inverse dielectric function to van Hove’s dynamic structure factor $S(q, \omega)$. Starting from $S(q, \omega)$ an integration over frequency is needed to obtain the electron-pair structure factor $S(q)$, which in Fourier transform describes the shape of the instantaneous exchange-correlation (Pauli-Coulomb) hole surrounding an average electron located at the origin. From $S(q)$ the ground-state energy $E_g$ can be calculated by means of further integrations over wave number and over coupling strength (see for instance Ref. 4) and the correlation energy $\varepsilon_c$ is defined, as usual, as the difference between $E_g$ and its Hartree-Fock value.

For the 3D EG Lein et al. have analyzed in detail this procedure for calculating the correlation energy, with particular attention to the roles of the wave number and frequency dependence of $f_{xc}(q, \omega)$. While the wave number dependence of the kernel is physically related to the spatial shape of the exchange-correlation hole, as already remarked, its frequency dependence reflects the inertia of the hole as the electron at the origin moves through the EG. When the frequency dependence of $f_{xc}(q, \omega)$ is omitted and its wave number dependence is approximated by its leading long-wavelength term, one is accounting for short-range exchange and correlation effects in the EG only through the compressibility sum rule (see for instance Ref. 3). This approximation provides the basis for the so-called Adiabatic Local Density Approximation (ALDA), which has often been used in dealing with time-dependent phenomena in inhomogeneous electronic systems in the low-frequency regime.

In the present work we extend the analysis of Lein et al. to the 2D EG by examining how several known forms of $f_{xc}(q, \omega)$ perform in regard to the calculation of its correlation energy over a range of values for the coupling strength. The standard of comparison is the parametrized form reported for the correlation energy by Rapisarda and Senatore from their Diffusion QMC results. The paper is organized as follows. In Sec. II we report the detailed expressions relating $\varepsilon_c$ to $f_{xc}(q, \omega)$ and in Sec. III we list the various forms of $f_{xc}(q, \omega)$ that we have considered. Section IV presents our main numerical results and discusses them with special emphasis on the usefulness of the ALDA in 2D as compared with 3D. Finally, in an Appendix we briefly comment on the scaling properties of the exchange-correlation kernel for inhomogeneous electron fluids of arbitrary dimensionality.
II. CORRELATION ENERGY FROM EXCHANGE-CORRELATION KERNELS

We consider a fluid of electrons moving in a plane and interacting by the $e^2/r$ law. The correlation energy (per electron) can be written in terms of the difference between the potential energy of the fluid and the exchange energy, integrated over the coupling-strength parameter $\lambda$

$$\varepsilon_c = \frac{1}{2} \int_0^{\pi} d\lambda \int \frac{d^2q}{(2\pi)^2} v_{q}^{\lambda} [S_{\lambda}(q) - S_{HF}(q)].$$

(1)

Here $v_{q}^{\lambda} = 2\pi \lambda/q$ is the 2D Fourier transform of the Coulomb potential with strength $\lambda$, $S_{\lambda}(q)$ is the structure factor of an EG with interactions $v_{q}^{\lambda}$ and $S_{HF}(q)$ is the Hartree-Fock structure factor,

$$S_{HF}(q) = \begin{cases} \frac{2}{\pi} \left[ \arcsin(q) + \sqrt{1 - q^2} \right] & \text{for } q < 1 \\ \frac{1}{1 - q^2} & \text{for } q > 1 \end{cases}$$

(2)

where $q = q/(2k_F)$ with $k_F = (2\pi n)^{1/2}$ being the Fermi wave number determined by the 2D electron density $n$. The fluctuation-dissipation theorem relates the structure factor to the density-density response function $\chi_{\rho\rho}(q, iu)$ calculated on the imaginary frequency axis,

$$S_{\lambda}(q) = -\frac{\hbar}{\pi n} \int_0^{\infty} du \chi_{\rho\rho}(q, iu).$$

(3)

The response function can in turn be expressed through the frequency-dependent exchange-correlation kernel $f_{xc}(q, \omega)$ on the imaginary frequency axis,

$$\chi_{\rho\rho}(q, iu) = \frac{\chi_0(q, iu)}{1 - [v_{q}^{\lambda} + f_{xc}(q, iu)]\chi_0(q, iu)}$$

(4)

where

$$\chi_0(q, iu) = -m_{\pi}^{1/2} \left[ 1 - \frac{1}{\sqrt{2\lambda}} \sqrt{f(\bar{q}, \bar{u}) + \sqrt{f^2(\bar{q}, \bar{u}) + 4\bar{q}^2\bar{u}^2}} \right]$$

(5)

is the density-density response function of the 2D ideal Fermi gas. Here, $\bar{u} = mu/\hbar k_F q$ and $f(\bar{q}, \bar{u}) = q^2 - \bar{u}^2 - 1$.

From Eqs. (3) and (4) it is possible to rewrite Eq. (1) in the form

$$\varepsilon_c = -\frac{\hbar}{4\pi^2\pi n} \int_0^{\infty} dq d\lambda \int_0^{\pi} d\lambda v_{q}^{\lambda} \frac{[\chi_0(q, iu)]^2 [v_{q}^{\lambda} + f_{xc}(q, iu)]}{1 - [v_{q}^{\lambda} + f_{xc}(q, iu)]\chi_0(q, iu)}.$$
III. APPROXIMATE KERNELS FOR THE HOMOGENEOUS ELECTRON GAS

We have tested five main forms of the kernel $f_{xc}(q, iu)$. In three of these (designated by the acronyms ALDA, DPGT, and STLS) the frequency dependence of the kernel is omitted. A dynamical kernel has been used in the approximations designated by QSTLS and AKA. Some details are as follows.

(i) ALDA: for the homogeneous electron gas the adiabatic local density approximation omits both the wave number and the frequency dependence of the kernel. It amounts to taking into account the compressibility sum rule by setting

$$f_{xc}^{ALDA}(q, iu) = \frac{1}{n^2 \kappa_0} \left( 1 - \frac{\kappa_0}{\kappa} \right)$$

where $\kappa$ is the compressibility of the EG and $\kappa_0$ that of the ideal Fermi gas, given in 2D by $\kappa_0 = \pi r_s^4/2$ in units of $a_B^2$/Ryd. The ratio $\kappa_0/\kappa$ is related to the correlation energy (in Ryd units) by

$$\frac{\kappa_0}{\kappa} = 1 - \frac{\sqrt{2}}{\pi} r_s + \frac{r_s^4}{8} \left[ \frac{d^2 \epsilon_c}{dr_s^2} - \frac{1}{r_s} \frac{d \epsilon_c}{dr_s} \right].$$

We evaluate this input from the parametrized form of $\epsilon_c(r_s)$ of Rapisarda and Senatoro.  

(ii) DPGT: an analytical expression for the static kernel $f_{xc}(q, 0)$ as a function of $r_s$ in the range $0 \leq r_s \leq 10$ has been obtained by Davoudi et al. by fitting the available Diffusion Monte Carlo data for the local field factor in the 2D EG. Their expression embodies the compressibility sum rule as well as the asymptotic high-$q$ behavior of the static kernel. By setting

$$f_{xc}^{DPGT}(q, iu) = f_{xc}^{QMC}(q, 0)$$

we are evidently omitting the frequency dependence of the kernel but taking into account its "exact" dependence on wave number at low frequency.

(iii) STLS: the Singwi-Tosi-Land-Sjölander approximation omits the frequency dependence of the kernel by relating it self-consistently to the structure factor $S(q)$ through

$$f_{xc}^{STLS}(q, iu) = \frac{1}{n} \int \frac{d^2 \mathbf{k}}{(2\pi)^2} \frac{\mathbf{q} \cdot \mathbf{k}}{q^2} v_k \left[ S(|\mathbf{q} - \mathbf{k}|) - 1 \right].$$

This expression was justified by an analysis of kinetic equations in the presence of a time-dependent weak external potential and has been used rather widely in the literature.

(iv) QSTLS: a frequency dependence of the local field factor in an STLS-type self-consistent theory has been included by later authors. We adopt in particular the expression

$$f_{xc}^{QSTLS}(q, iu) = \frac{1}{n} \int \frac{d^2 \mathbf{k}}{(2\pi)^2} \frac{\chi_0(q, \mathbf{k}; iu)}{\chi_0(q, iu)} v_k \left[ S(|\mathbf{q} - \mathbf{k}|) - 1 \right]$$

where the function $\chi_0(q, \mathbf{k}; iu)$ is given by

$$\chi_0(q, \mathbf{k}; iu) = -\frac{m}{\pi \hbar^2} c (1 - r).$$

Here $c = \mathbf{q} \cdot \mathbf{k}/q^2$ and

$$r^2 = -\frac{y^2 + z^2 - c^2}{2c^2} + \left[ (y^2 + z^2 - c^2)^2 + 4y^2 z^2 \right]^{1/2}$$

with $y = 2k_F/q$ and $z = 2mu/\hbar q^2$.

(v) AKA: Atwal et al. have recently proposed an analytic expression for the dynamical local field factor which is based on many-body perturbation theory and on known sum rules, in the same spirit as in the work of Richardson and Ashcroft on the 3D EG. With the notations of Ref. 16,

$$f_{xc}^{AKA}(q, iu) = -v_q \left[ G_s(q, iu) + G_n(q, iu) \right]$$

where

$$G_s(q, iu) = \frac{a_s(u)q + b_n(u)q^3}{1 + c_s(u)q + d_n(u)q^3}$$

and

$$G_n(q, iu) = \frac{a_n(u)q + b_n(u)q^3}{1 + c_n(u)q + d_n(u)q^3}.$$
and
\[ G_n(q, iu) = \frac{a_n(u)q + b_n(u)q^7}{1 + c_n(u)q + d_n(u)q^6}. \]  
(18)

Here \( a_{s,n}(u) \), \( b_{s,n}(u) \), \( c_{s,n}(u) \) and \( d_{s,n}(u) \) are functions of frequency and depend on two input parameters, which are the contact value \( g(0) \) of the pair distribution function and the correlation energy. In our calculations we have replaced Eqs. (41) and (52) of Ref. 14 for \( d_{s,n}(u) \), which contain typographical errors, by the following expressions communicated to us by Dr. G. S. Atwal:

\[ d_s(\omega) = \frac{\zeta_s \lambda_0^0}{6(\zeta_s \lambda_0^0 - 1 + g(0))(1 + \omega^4)} + \frac{\lambda_s^\infty \omega}{[1 - g(0)](1 + \omega^4)}, \]  
(19)

\[ d_n(\omega) = \frac{\zeta_n \lambda_n^0}{(5\zeta_n \lambda_n^0 + 2\lambda_n^\infty)(1 + \omega^4)} + \frac{\gamma_n \omega^2}{[5\gamma_n \omega(1 + 0.38\omega)^2](1 + 0.38\omega)^4(1 + \omega^4)}. \]  
(20)

For expressions of the other functions and of the various parameters the reader is referred to the original paper.

In determining the input for this form of the kernel we have again used the form of Rapisarda and Senatore for \( \varepsilon_c(r_s) \) and followed Atwal et al. in taking the values of \( g(0) \) from an interpolation formula proposed by Polini et al. We have also checked simple variants of this scheme, taking \( g(0) \) from calculations in the ladder approximation or dropping the frequency dependence of \( f_{x\text{c,\ AKA}}(q, iu) \).

IV. NUMERICAL RESULTS AND DISCUSSION

We turn to a presentation of our numerical results, which are collected in Figures 1-4. In Figure 1 (top panel) we show the difference between the correlation energy calculated by means of Eqs. (7) and (8) and the "exact" correlation energy \( \varepsilon_{x\text{c,AMC}}(r_s) \) from the parametrization of Ref. 15, for electron densities in the range 0.5 \( \leq r_s \leq 10 \). In 2D this range extends into the intermediate-to-strong coupling regime. In the bottom panel of Figure 1 we report the calculated correlation energies in the weak-coupling regime 0 \( \leq r_s \leq 0.8 \), to show that none of the theories that we have examined satisfies the exactly known limiting expression for \( r_s \to 0 \),

\[ \varepsilon_c(r_s) \to -0.385 - \frac{2\sqrt{2}}{3\pi}(10 - 3\pi)r_s \ln r_s + o(r_s). \]  
(21)

This panel also reports the correlation energy given by the Random Phase Approximation (RPA), which corresponds to setting the exchange-correlation kernel to zero and evidently is badly in error even at low \( r_s \).

Turning to the results shown in the top panel of Figure 1, a pleasant surprise in 2D is that ALDA does not overestimate badly the correlation energy as was shown by Lein et al. to be the case in 3D. In fact, in the range 2 \( \leq r_s \leq 10 \) the ALDA results are seen to be quite close to the DPGT results, in which the full nonlocality of the static kernel in space has been included. The reason for this can be inferred from the work of Davoudi et al., who showed that in 2D satisfying the compressibility sum rule reproduces quite accurately the \( q \)-dependence of the static kernel almost up to \( q \approx 2k_F \). Following Lein et al. we have also examined frequency-dependent forms of the long-wavelength kernel and in particular that proposed by Qian and Vignale. We have found that this overestimates the correlation energy by as much as \( \approx 0.1 \) Ryd at \( r_s = 3 \). It appears, therefore, that nonlocality of the kernel in space should be included if its nonlocality in time is accounted for in the calculation of the correlation energy.

This is, of course, what is being done in the AKA calculation. The average deviation of its results in the top panel of Figure 1 is approximately 0.02 Ryd, which is somewhat better than in ALDA or in DPGT. Taking \( g(0) \) in the AKA kernel from the ladder-diagram calculation raises this deviation to about 0.03 Ryd and, most importantly, dropping the frequency dependence of the AKA kernel brings it to about 0.04 Ryd. The summary conclusion of all these calculations is, therefore, that as far as the correlation energy in 2D is concerned one does already fairly well by taking a constant exchange-correlation kernel adjusted to the compressibility sum rule and that nonlocality of the kernel in both space and time needs including in order to obtain some improvement in the results.

Figure 1 in its top panel further shows that STLS gives a very good estimate of the correlation energy, with a deviation of about 0.004 Ryd on average. In this case inclusion of the frequency dependence of the kernel by means of the QSTLS recipe has only a minor effect, bringing the average deviation down to about 0.0035. Consistency of the exchange-correlation kernel with the electron-pair structure thus appears to be important, as far as the calculation of the correlation energy is concerned. This fact may give a useful suggestion for further improvement of the more
sophisticated kernels that have been proposed in the more recent work. We may also remark that Dobson et al.\(^\text{24}\) have recently extended the STLS scheme to inhomogeneous electronic systems and shown that it gives good results for the correlation energy of jellium slabs of finite thickness, lying within 3% of the Diffusion Monte Carlo results of Acioli and Ceperley.\(^\text{25}\)

We turn now to Figures 2-4, in which following again Lein et al.\(^\text{8}\) we provide an analysis of the correlation energy at \(r_s = 1\) into contributions from correlations between density fluctuations of different wave vectors and different imaginary frequencies. Equations (7) and (8) naturally define a wave-vector analysis \(\varepsilon_c(q)\) if we write

\[
\varepsilon_c = \int_0^\infty \varepsilon_c(q) d(q/k_F)
\]

and an imaginary-frequency analysis \(\varepsilon_c(u)\) if we write

\[
\varepsilon_c = \int_0^\infty \varepsilon_c(u) d(2mu/\hbar k_F^2).
\]

Gori-Giorgi et al.\(^\text{26}\) have obtained an "exact" wave-vector analysis through the Fourier transform of the coupling-averaged correlation-hole density and built an analytic model for it by combining exactly known limiting behaviors with Diffusion Monte Carlo data, as in the work of Perdew and Wang on the 3D EG.

Figure 2 compares the results for \(\varepsilon_c(q)\) given by the theories of present interest with the QMC ones that have kindly been communicated to us by Dr. P. Gori-Giorgi.\(^\text{26}\) While all theories perform similarly well in this test, it is pleasant to notice the reasonably good behavior shown by the ALDA. Finally, the imaginary-frequency analysis of the various theories is reported in Figures 3 and 4, in the low-\(u\) and large-\(u\) regimes respectively. As in the 3D case,\(^\text{8}\) in all theories \(\varepsilon_c(u)\) starts with a finite negative value at \(u = 0\) and vanishes at large \(u\). In ALDA \(\varepsilon_c(u)\) becomes positive at \(u \approx 7\hbar k_F^2/(2m)\) and ultimately vanishes from above.

To conclude our work, in Appendix A we briefly comment on how the coupling-constant dependence of the frequency-dependent exchange-correlation kernel in an inhomogeneous electronic system of arbitrary dimensionality may be found from the knowledge of its density dependence at full coupling strength.

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**APPENDIX A: SCALING OF THE INHOMOGENEOUS EXCHANGE-CORRELATION KERNEL**

From time-dependent density functional theory and dynamical scaling Lein et al.\(^\text{8}\) have derived a coordinate-scaling relation in dimensionality \(D=3\) for the coupling-constant dependence of the exchange-correlation kernel \(f_{xc}[n](r, r'; \omega)\) of an inhomogeneous many-electron system.

It is easy to generalize their proof to an inhomogeneous system in arbitrary space dimensionality \(D\): namely, it is possible to prove that

\[
f_{xc}[n](r, r'; \omega) = \lambda^2 f_{xc}[n'](\lambda r, \lambda r'; \omega/\lambda^2)
\]

where \(n'(r, t) = \lambda^{-D} n(r/\lambda, t/\lambda^2)\). In fact, the dimensionality of the system enters the proof only insofar as integrations of the time-dependent density \(n(r, t)\) over space are involved.

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FIG. 1: Top panel: deviation of approximate correlation energy from the QMC correlation energy of Rapisarda and Senatore (in units of Ryd) as a function of $r_s$ for $0.5 \leq r_s \leq 10$ (the AKA results are omitted for $r_s \geq 8$ where they do not seem to vary smoothly). Bottom panel: approximate and QMC correlation energy (in units of Ryd) as a function of $r_s$ for $0 \leq r_s \leq 0.8$ (the QMC results also embody the limiting form in Eq. (21)).
FIG. 2: Wave-vector analysis of the correlation energy per electron (in units of Ryd) at \( r_s = 1 \) as a function of \( q/k_F \).

FIG. 3: Imaginary-frequency analysis of the correlation energy per electron (in units of Ryd) at \( r_s = 1 \) as a function of \( 2m u/(\hbar k_F^2) \) in the low-\( u \) regime. In the inset an enlargement of the results from ALDA, QSTLS and DPGT is shown.
FIG. 4: Imaginary-frequency analysis of the correlation energy per electron (in units of Ryd) at $r_s = 1$ as a function of $2mu/(\hbar k_F^2)$ in the large-$u$ regime.