Construction of model dielectric functions for two and three dimensional electron liquids from density functionals

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The Thomas-Fermi (TF) approximation for the static dielectric function of a three-dimensional (3d) electron liquid can be derived by minimizing the TF local-density approximation for the kinetic-energy functional. Here we show that this connection between energy functionals and model dielectric functions is not an artifact, but a general paradigm. Four examples are worked out in detail, by calculating the model dielectric functions that follow, respectively, from (i) exchange corrections to TF theory in 3d, i.e., TF-Dirac theory, (ii) further correlation corrections to TF-Dirac theory in 3d, (iii) TF theory in 2d, and (iv) exchange corrections to TF theory in 2d. Each of these cases has certain interesting features, revealing connections between independent many-body methods, that are discussed in some detail. As a byproduct of these investigations we also find that a common textbook statement about the long-wavelength \((k \to 0)\) limit of the random-phase approximation is not fully correct.

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I. INTRODUCTION

Screening is one of the most important manifestations of many-body effects in metals, semiconductors and plasmas.1,2 In the Thomas-Fermi (TF) approximation,3 static screening in three-dimensional (3-d) electron liquids is described by means of a wave-vector-dependent dielectric function,4–6

\[ \epsilon_{TF}(k) = 1 + \frac{k_{TF}^2}{k^2}, \]  

(1)

where the TF screening wave vector is \(k_{TF} = \sqrt{4k_F^*/\pi a_0}\). Here \(k_F = (3\pi^2n_0)^{1/3}\) and \(a_0 = \hbar^2/mc^2\) denote the Fermi wave vector and the Bohr radius, respectively, and \(n_0\) is the charge density of the unperturbed electron liquid. This model dielectric function is sometimes used in its own right as an approximation for screening in metals, plasmas and doped semiconductors; more frequently, it appears as starting point for, or limiting case of, more sophisticated many-body treatments of screening.4–8 We stress from the outset that our aim in the present work is not the construction of high-precision or material-specific expressions for the dielectric function, but to explore connections between different many-body methods that become visible through the expressions they yield for the dielectric functions.

The Thomas-Fermi approximation to the kinetic energy of a 3-d electron liquid is9,10

\[ T_{TF}[n] = \frac{3\hbar^2(3\pi^2)^{2/3}}{10m} \int d^3r n(r)^{5/3} = C \int d^3r n(r)^{5/3}. \]  

(2)

While both \(\epsilon_{TF}(k)\) and \(T_{TF}[n]\) are widely known and employed concepts, it is worthwhile stressing that the two uses of the label ‘Thomas-Fermi’ are not equivalent: the 3-d TF dielectric function can be obtained from the TF energy functional by one additional approximation, a linearization of the Euler equation resulting from minimizing \(T_{TF}[n]\).7,11 To make our paper self-contained we start, in Sec. II, by briefly recalling this derivation.

The inclusion of many-body effects beyond the TF approximation is in general highly nontrivial, and typically accomplished by either constructing local-field corrections to the random-phase approximation (RPA),7 or by first-principles density-functional calculations of the dielectric functions of realistic materials.12 In Sec. III we show that certain important many-body effects can be incorporated into the TF dielectric function in a much simpler way, by employing the Dirac-Slater local-density approximation (LDA) for the exchange energy.8–10

\[ E_x^{LDA}[n] = -\frac{3e^2}{4} \left( \frac{3}{\pi} \right)^{1/3} \int d^3 r n(r)^{4/3} \]  

(3)

\[ = -D \int d^3 r n(r)^{4/3}. \]  

(4)

Addition of this to the TF energy functional leads to the so-called Thomas-Fermi-Dirac (TFD) approximation.8–10 Further correlation corrections can be described by the local-density approximation9

\[ E_{xc}^{LDA}[n] = E_x^{LDA}[n] + \int d^3 r e_c(n)|_{n \rightarrow n(r)}, \]  

(5)

where \(e_c(n)\) is the per-volume correlation energy of the uniform electron liquid13 underlying common parametrizations of the LDA.9 In Sec. V we derive the dielectric function arising from \(E_{xc}^{LDA}\). Secs. VI and VII extend these calculations to two-dimensional electron liquids, within TF and TFD theory, respectively. As a byproduct of this investigation we also revisit, in Sec. IV,
the long wavelength limit of the three-dimensional dielectric function found in the RPA, which has as nontrivial correction similar to the one found here within TFD theory.

II. TF DIELECTRIC FUNCTION IN THREE-DIMENSIONAL ELECTRON LIQUIDS

This derivation, although elementary, will be presented in some detail, because it serves as a model for the more complicated cases treated afterwards. The 3-d TF total-energy functional is

\[ E_{TF}[n] = T_{TF}[n] + \frac{e^2}{2} \int d^3r \int d^3r' \frac{n(r)n(r')}{|r - r'|} + \int d^3r n(r)v_{ext}(r), \]  

(6)

where the second term on the right-hand-side (rhs) is the electrostatic (Hartree) energy of the charge distribution \( n(r) \) with itself, and the third term describes the potential energy of this charge distribution in the external potential \( v_{ext}(r) \), composed of a smeared-out background of positive charge with constant density \( n_{bg} \) and potential \( v_{bg} \) and an additional test charge \( n_{test}(r) \) with potential \( v_{test}(r) \). It is the screening of this test charge, which is normally taken to be a point charge, that the theory aims to describe. Equilibrium is characterized by the condition \( \delta(E_{TF}[n] - \mu N)/\delta n(r) = 0 \), where the total particle number \( N = \int d^3r n(r) \) and the chemical potential \( \mu \) at zero temperature is the Fermi energy \( \epsilon_F \). This minimization leads to the Euler equation

\[ \frac{5}{3} Cn(r)^{2/3} + v_{ext}(r) + v_H(r) - \mu = 0, \]  

(7)

where the Hartree potential is \( v_H = \delta E_H[n]/\delta n = e^2 \int d^3r' n(r')/|r - r'| \). Solving Eq. (7) for \( n(r) \) we find

\[ n(r) = \left( \frac{3}{5C} \right)^{3/2} (\mu - v_s(r))^{3/2}, \]  

(8)

where we have introduced the effective, or screened, potential \( v_s \), which is \( v_H + v_{ext} \). If this potential is weak, i.e., \( v_s/\mu \ll 1 \), Eq. (8) can be linearized to give

\[ n(r) = \left( \frac{3\mu}{5C} \right)^{3/2} \left( 1 - \frac{3}{2} \frac{v_s(r)}{\mu} \right). \]  

(9)

By introducing the charge density of the unperturbed system, \( n_0 = k_F^2/3\pi^2 \) (where \( h^2k_F^2/2m = \mu \)), and the corresponding 3-d density of states, \( g_0 = mk_F/h^2\pi^2 \), we can write this as

\[ n(r) = n_0 - g_0 v_s(r) =: n_0 + n_{ind}. \]

The screened potential becomes

\[ v_s(r) = v_{ext}(r) + e^2 \int d^3r' \frac{n_0(r') + n_{ind}(r')}{|r - r'|}. \]  

(10)

Stability of the unperturbed electron liquid (with \( v_{ext} = 0 \)) requires \( n_0 = -n_{bg} \), so that the background-contribution to \( v_{ext} \) is cancelled precisely by the first term arising from the integral. Hence,

\[ v_s(r) = v_{ext}(r) + e^2 \int d^3r' \frac{n_{ind}(r')}{|r - r'|}. \]  

(11)

Upon Fourier transformation this becomes

\[ v_s(k) = v_{ext}(k) + e^2 F[n_{ind}(r)][F(1/r)], \]  

(12)

where \( F \) stands for the 3-d Fourier transform operator. In the second term we have used the convolution theorem to decompose the Fourier transform of the Hartree potential into a product of two Fourier transforms. By substituting \( n_{ind} = -g_0 v_s \) in this equation, using \( F[1/r] = 4\pi/k^2 \), and solving for \( v_s \), we obtain

\[ v_s(k) = \frac{v_{ext}(k)}{1 + e^2 g_0 F[1/r]} = \frac{v_{test}(k)}{1 + \frac{4\pi e^2}{a_0\mu k^2}} = \frac{v_{test}(k)}{\epsilon_{TF}(k)}, \]  

(13)

in agreement with the definitions following Eq. (1). For the screening of a point charge with \( v_{test}(k) = 4\pi e^2/k^2 \) this becomes

\[ v_s(k) = \frac{4\pi e^2}{k^2 + \epsilon_{TF}^2}. \]  

(14)

Minimization of the TF kinetic-energy functional followed by a minimization of the resulting Euler equation thus reproduces the TF dielectric function

\[ \epsilon_{TF}(k) = 1 + \frac{4\pi e^2}{a_0\mu k^2}. \]  

(15)

In the following sections we explore whether this connection between energy functionals and model dielectric functions remains valid in more complex situations, characterized by additional exchange and correlation terms in the functional, and in two dimensions.

III. TFD DIELECTRIC FUNCTION IN THREE-DIMENSIONAL ELECTRON LIQUIDS

The fact that dielectric functions can be derived from energy functionals opens up the possibility to incorporate additional physics into a model dielectric function by using a more complete energy functional. To illustrate this we now deduce an expression that incorporates exchange effects into the TF dielectric function. Starting point is the 3-d TFD energy functional

\[ E_{TFD}[n] = E_{TF}[n] + E^{LDA}_x[n], \]  

(16)

where the functionals on the rhs are defined in Eq. (6) and (4), respectively. The Euler equation corresponding to this functional is

\[ \frac{5}{3} C n(r)^{2/3} + v_{ext}(r) + v_H(r) - \frac{4}{3} D n(r)^{1/3} - \mu = 0. \]  

(17)
In accordance with common practice in density-functional theory, we regard the exchange term on the rhs as a contribution to the effective potential, now defined as

\[ v_s = v_{\text{ext}} + v_H + v_x = v_{\text{ext}} + v_H - (4D/3)n_0^{1/3}. \]  

(18)

The induced density change is defined in terms of this potential as before, via \( n(r) = n_0 - g_0v_s(r) =: n_0 + n_{\text{ind}}(r) \), and the counterpart to Eq. (12) becomes

\[ v_s(k) = v_{\text{test}}(k) + e^2F[n_{\text{ind}}(r)]F \left[ \frac{1}{r} \right] - \frac{4D}{3}F[n_0^{1/3}]. \]  

(19)

To evaluate this expression in closed form we linearize again, assuming consistently that \( n_{\text{ind}} \ll n_0 \), i.e., the self-consistent modification of the density distribution due to the test charge is small compared to the density of the original unperturbed system. This allows us to write \( n_0^{1/3} \approx n_0^{1/3}(1 + n_{\text{ind}}/3n_0) \), and the preceding equation becomes

\[ v_s(k) = v_{\text{test}}(k) + e^2F[n_{\text{ind}}(r)]F \left[ \frac{1}{r} \right] - \frac{4D}{3}F[n_0^{1/3}] - \frac{4D}{3}g_0n_0^{2/3}F[n_{\text{ind}}]. \]  

(20)

The last term can be handled as before, by using \( n_{\text{ind}} = -g_0v_{\text{sc}} \). Since \( n_0 \) is spatially constant, the Fourier transform of the second-to-last term contributes only at \( k = 0 \). Solving the preceding equation for \( v_s \) we find

\[ v_s(k) = v_{\text{test}}(k) - 4DF[n_0^{1/3}]/3 \frac{k_F}{\pi a_0 k_F} \frac{\pi}{\pi a_0 k_F} - \frac{1}{\pi a_0 k_F} \frac{1}{\pi a_0 k_F} \frac{1}{\pi a_0 k_F}, \]  

(21)

where we have substituted the explicit expressions for \( g_0, n_0 \) and \( D \) in terms of universal functions and the Fermi wave vector. To identify the dielectric function \( \epsilon \) we consider again the screening of a point charge, with \( v_{\text{test}} = 4\pi e^2/k^2 \). After a little algebra we find

\[ \epsilon_{\text{TFD}}(k) = 1 + \frac{4k_F}{\pi a_0 k_F^2} \frac{1}{\pi a_0 k_F} = \epsilon_{\text{TF}}(k) - \frac{\alpha r_s}{\pi}, \]  

(22)

where in the last step we have introduced the usual electron gas parameters \( r_s = 1/\alpha a_0 k_F \) and \( \alpha = (4/9\pi)^{1/3} \). Eq. (22) illustrates how exchange-corrections modify the TF dielectric function, and also illustrates how by starting from suitable energy functionals additional physics can be built into models for the dielectric function.

Interestingly, the resulting additive exchange correction to the TF dielectric function, \( -\alpha r_s/\pi \), turns out to be the same already known to appear as the multiplicative Hartree-Fock correction to the sound velocity \( \epsilon \), compressibility \( \kappa \) and spin susceptibility \( \chi \) of the 3-d electron gas:1,2

\[ \epsilon_{\text{TFD}}(k) - \epsilon_{\text{TF}}(k) = 1 - \frac{k^2}{\kappa_0^2} = 1 - \frac{k^2}{\kappa_0^2} = 1 - \frac{\chi_0}{\chi} = -\frac{\alpha r_s}{\pi}. \]  

(23)

The behaviour of \( \epsilon_{\text{TFD}}(k) \) for two different densities is illustrated in Fig. 1. Exchange is seen to reduce screening (i.e., to lead to a dielectric function closer to \( \epsilon = 1 \) for all \( k \)). This behaviour is easily understood because exchange tends to keep particles apart, thereby making screening less effective. The limits of validity of Eq. (22) are similar to that of ordinary TF theory, restricting the use of (22) to high and slowly varying densities (small \( r_s \) and \( k \to 0 \)).

IV. LONG WAVELENGTH LIMIT OF THE RANDOM-PHASE APPROXIMATION

In the random-phase approximation the static dielectric function is given by1,2,4–7

\[ \epsilon_{\text{RPA}}(k) = 1 + \frac{k^2 F}{2k^2} \left[ 1 + \frac{1}{2\pi} (1 - x^2) \ln \left| \frac{1 + x}{1 - x} \right| \right], \]  

(24)

where \( x = k/2k_F \). In textbooks1,2,5,6,11,14 it is usually argued that in the limit \( x \to 0 \) the term in square brackets tends to 1, because, to linear order in \( x \), \( \ln \left| \frac{1 + x}{1 - x} \right| \to 2x \), so that the RPA dielectric function for long wavelength density oscillations becomes \( \epsilon_{\text{RPA}}(k \to 0) = \epsilon_{\text{TF}}(k) \) and thus recovers the TF result. (See, e.g., Eq. (5.65) of Ref. 1, p. 105 of Ref. 11, p. 140 of Ref. 6, Eq. (5.35) of Ref. 2, or Eq. (28.9) of Ref. 14.)

This statement, however, is not fully correct. More precisely, it is not consistent in orders of \( k \). To the order in \( k \) to which TF theory provides an approximation to \( \epsilon(k) \), i.e., constant plus \( 1/k^2 \), it is not enough to expand the logarithm in Eq. (24) to linear order in \( x \). Instead, the expansion must be carried to cubic order, which after

FIG. 1: Three-dimensional Thomas-Fermi (dashed curves) and Thomas-Fermi-Dirac (continuous curves) dielectric function vs. wave vector \( k/k_F \), for \( r_s = 6 \) (upper curves) and \( r_s = 3 \) (lower curves). For comparison purposes we also include the \( k \to 0 \) limit of the static RPA dielectric function (dotted curves), as given in Eq. (26). For the density dependence of the TF and TFD dielectric functions see Fig. 3.
multiplication by the prefactor $\frac{1}{3}(1-x^2)$ also contributes a constant term to $\epsilon^{RPA}(k)$. The RPA dielectric function thus has the $k \to 0$ expansion

$$\epsilon_{RPA}(k \to 0) = \frac{4k_F}{\alpha_0 r_s} k^{-2} + \left(1 - \frac{1}{3} \frac{\alpha r_s}{\pi}\right) k^0 + O(k^2)$$

$$= \epsilon_{TF}(k) - \frac{1}{3} \frac{\alpha r_s}{\pi} + O(k^2).$$

In the extreme $k \to 0$ limit all constants can be neglected compared to $1/k^2$, and RPA and TF theory do indeed predict the same divergence. However, already at the level of constant corrections to this limit, RPA and TF differ, and the TF dielectric function in the form $1 + \frac{k^2_{TF}/k^2}$ is never obtained as a long wavelength limit from the RPA (except in the extreme case $r_s = 0$).

Interestingly, the additional term $-\alpha r_s/3\pi$ needed to make the $k \to 0$ expansion of the static RPA consistent in orders of $k$ is, up to a factor $1/3$ the same additional term we found above as an exchange correction to the TF dielectric function.

V. CORRELATION CORRECTIONS TO THE THOMAS-FERMI DIELECTRIC FUNCTION

Further many-body effects can be included by adding the local-density approximation for correlation, Eq. (5) to the TFD energy functional. We introduce the derivatives

$$v_{xc}[n](r) = \frac{\delta E_{xc}[n]}{\delta n(r)}$$

and

$$f_{xc}[n](r,r') = \frac{\delta^2 E_{xc}[n]}{\delta n(r)\delta n(r')}.$$  

and note that in the LDA, Eq. (5), the exchange-correlation kernel $f_{xc}$ is

$$f_{xc}^{LDA}[n](r,r') = \frac{\partial^2 e_{xc}(n)}{\partial n^2} |_{n-n(r)} \delta(r-r')$$

$$= :f_{xc}^{LDA}[n] \delta(r-r'),$$

where the second equality defines the functional $f_{xc}^{LDA}[n]$. The Fourier transform of $f_{xc}^{LDA}[n]$ is simply related to that of the static local-field factor $G(k)$ via

$$f_{xc}^{LDA}[n](k) = -\epsilon^2 F \left[\frac{1}{|r|}\right] G(k),$$

where $-\epsilon^2 F[1/|r|]$ is the Fourier transform of the Coulomb interaction.

By going through the same steps as before we find for the dielectric function corresponding to correlation-corrected TFD theory

$$\epsilon_{TFDC}(k) = 1 + \frac{4k_F}{\alpha_0 \pi k^2} + g_0 f_{xc}^{LDA}[n_0]$$

$$= \epsilon_{TF}(k) + g_0 f_{xc}^{LDA}[n_0].$$

Interestingly, the inclusion of correlation, already on the linearized LDA level, has introduced the exchange-correlation kernel $f_{xc}$ in the corrected TF dielectric function, and thus lead to a dependence on local-field corrections that would ordinarily only be expected in sophisticated beyond-RPA dielectric functions.\cite{1,2,7} The wave-vector dependence of the local-field correction, however, is lost in the linearization.

VI. TF DIELECTRIC FUNCTION IN TWO-DIMENSIONAL ELECTRON LIQUIDS

Next, we extend the above analysis to two dimensions, where our starting point is the 2-d local-density approximation to the kinetic-energy functional,

$$T_{TF,2}[n] = \frac{\pi k^2}{2m} \int d^2 r n(r)^2. \quad (34)$$

(Here and below 2-d energy functionals and dielectric functions are distinguished from their 3-d counterparts by a subscript 2. For all other quantities no confusion can arise, and to avoid cluttering the formulas we use the same symbol for them in 2-d as in 3-d.) By following exactly the same steps as before we find the Euler equation

$$\frac{\pi k^2}{m} n(r) + v_{ext}(r) + v_{H}(r) - \mu = 0. \quad (35)$$

Unlike Eq. (8) in 3-d, this density-potential relation is already linear, and no further approximation is needed to
write it in the form \( n(r) = n_0 + n_{\text{ind}}(r) \). The 2-d Fermi wave vector is related to the 2-d density via \( n_0 = \frac{k_F^2}{2\pi} \), and in terms of the 2-d density of states \( g_0 = m/\pi^2 \)

one immediately identifies \( n_{\text{ind}} = -g_0 v_s \). All remaining steps are the same as in 3-d, and from the 2-d Fourier transform \( \mathcal{F}[1/r] = 2\pi/k \) one readily obtains

\[
\frac{v_{\text{test}}(k)}{1 + e^2 g_0 \mathcal{F}[1/r]} = \frac{v_s(k)}{1 + \frac{1}{g_0}} = \frac{v_{\text{test}}(k)}{\epsilon_{TF,2}(k)}. \tag{36}
\]

For screening of a point charge (36) becomes

\[
v_s(k) = \frac{2\pi e^2}{k + k_{TF}}, \tag{37}
\]

where in 2-d \( k_{TF} = 2/a_0 \). The resulting density-independent expression

\[
\epsilon_{TF,2}(k) = 1 + \frac{2}{a_0} \frac{1}{k} \tag{38}
\]

for the 2-d TF dielectric function is well known, e.g., in the context of 2-d electron liquids in semiconductor heterostructures.\(^{15,18}\)

Interestingly, the 2-d TF dielectric function follows rigorously from the 2-d TF kinetic energy functional, without an additional linearization. Hence, in this sense, (36) is a stronger result than its 3-d counterpart (13).\(^{16}\) However, this stronger result is an artifact of two-dimensionality, arising because the 2-d kinetic energy is quadratic in \( n(r) \), and its density-derivative linear.

On the other hand, the fact that \( \epsilon_{TF,2}(k) \) is obtained from \( T_{TF,2}[n] \) in the same way \( \epsilon_{TF}(k) \) is obtained from \( T_{TF}[n] \) shows that the relation between energy functionals and dielectric functions in itself is not an artifact of three-dimensionality.\(^{17}\)

\section{VII. TFD DIELECTRIC FUNCTION IN TWO-DIMENSIONAL ELECTRON LIQUIDS}

Finally, we work out the form of the exchange corrections to the two-dimensional Thomas-Fermi dielectric function. The per-particle exchange energy of a uniform two-dimensional electron liquid is \(-8\sqrt{2}/(3\pi r_s) R_y\),\(^{19,20}\) where \( r_s = 1/(a_0\sqrt{\pi}) \) and \( R_y = e^2/2a_0 \). The local-density approximation for \( E_{x,2}[n] \) is thus

\[
E_{x,2}^{\text{LDA}}[n] = -\frac{4}{3} \sqrt{\frac{2}{\pi}} e^2 \int d^2r \, n^{3/2}. \tag{39}
\]

The 2-d TFD Euler equation can be cast in the same form as before, \( n(r) = n_0 + n_{\text{ind}}(r) \), where in 2-d \( n_0 = k_F^2/2\pi \) and \( n_{\text{ind}} = -g_0 v_s \), with \( v_s = v_{\text{ext}} + v_H + v_z \) and \( v_z = -2e^2 \sqrt{2n}/\pi r_s \). The Hartree potential arising from the unperturbed density \( n_0 \) and the potential energy in the positive background (contained in \( v_{\text{ext}} \)) cancel again, and by means of the convolution theorem the Fourier-transformed screened potential becomes

\[
v_s(k) = v_{\text{ext}}(k) + e^2 \mathcal{F}_2[n_{\text{ind}}(r)] \mathcal{F}_2 \left[ \frac{1}{r} \right] - 2e^2 \sqrt{\frac{\pi}{r}} \mathcal{F}_2[\sqrt{n}]. \tag{40}
\]

The Fourier transforms in the second term on the rhs are easily evaluated by using \( n_{\text{ind}} = -g_0 v_s(k) \) and \( \mathcal{F}_2[1/r] = 2\pi/k \). To evaluate the Fourier transforms in the third term we linearize in terms of \( n_{\text{ind}}/n_0 \), as before, and obtain

\[
\mathcal{F}_2[\sqrt{n_0 + n_{\text{ind}}}] \approx \mathcal{F}_2[\sqrt{n_0}] - \frac{1}{2\sqrt{n_0}} \mathcal{F}_2[n_{\text{ind}}]. \tag{41}
\]

Hence, for the 2-d screening of a point charge with \( v_{\text{test}}(r) = e^2/r \), we obtain

\[
v_s(k) = \frac{2\pi e^2}{k} \left( 1 + \frac{1}{a_0} \frac{1}{k} - \frac{\sqrt{2}}{\pi r_s} \right), \tag{42}
\]

where we have used \( r_s = \sqrt{2}/a_0 k_F \) for the 2-d density parameter \( r_s \), and, as before, \( k \delta(k) \equiv 0 \). As in the 3-d case, the derivation from a kinetic-energy functional allows us to build exchange effects in a simple way into the TF dielectric function.

Interestingly, our final expression

\[
\epsilon_{TFD,2}(k) = 1 + \frac{2}{a_0} \frac{1}{k} - \frac{\sqrt{2}}{\pi} r_s = \epsilon_{TF,2}(k) - \frac{\sqrt{2}}{\pi} r_s \tag{43}
\]

has acquired a density dependence, through \( r_s(n) = 1/(a_0\sqrt{\pi}) \). Inclusion of exchange thus removes the unphysical density-independence of \( \epsilon_{TF,2}(k) \) obtained in the 2-d TF approximation (36). The behaviour of the 2-d TF and TFD dielectric functions as a function of wave vector and density is illustrated in Figs. 2 and 3. Correlation corrections could be included in two dimensions in the same way as in three dimensions. In the interest of brevity we refrain from showing the straightforward extension of the above expressions to this case.

On the other hand, we stress that in 2-d we obtain the same chain of equalities as in 3-d, relating the additive correction to the dielectric function with multiplicative renormalization of the sound velocity, compressibility and spin susceptibility of the 2-d electron gas:\(^{21,22}\)

\[
\epsilon_{TFD,2}(k) - \epsilon_{TF,2}(k) = 1 - \frac{s^2}{s_0^2} = 1 - \frac{k_s^2}{k_0^2} = 1 - \frac{\chi_0}{\chi} = -\frac{\sqrt{2} r_s}{\pi} \tag{44}
\]

Eq. (23) thus carries over to 2-d, with a modified density dependence.

\section{VIII. SUMMARY AND ASSESSMENT}

While the 2d and 3d TF dielectric functions \( \epsilon_{TF}(k) \) and \( \epsilon_{TF,2}(k) \), given in Eqs. (15) and (38), are well known
features that were not obvious from the 3-d TF case, but are revealed by deriving model dielectric constants from density functionals.

Specifically in the 3-d TFD case, we found that the exchange contribution to the TF dielectric function yields a term of the same form as the long-wavelength expansion of the RPA, if that expansion is carried out consistently in orders of \( k \). The standard way of identifying \( \epsilon_{TF}(k) \) as the \( k \rightarrow 0 \) limit of the static RPA is not consistent in orders of \( k \). Further correlation terms lead, already on the linearized LDA level, to a simple dependence of the dielectric function on local-field factors.

Unlike the connection between the TF dielectric function and the Yukawa potential in real space, that between the TF dielectric function and energy functionals carries over to two-dimensions, where \( \epsilon_{TFD}(k) \) turns out to be a more robust expression than \( \epsilon_{TF}(k) \) in 3-d, because it can be derived from the 2-d TF kinetic-energy functional without any linearization. Upon including exchange (TFD), a density dependence reappears in the 2-d dielectric function, which is lost in the usual 2-d TF dielectric function. In both 2d and 3d, the additive exchange contribution to the dielectric function turns out to be the same as the multiplicative exchange renormalization factor of other observables, such as the spin susceptibility.

The existence of a connection between a class of energy functionals and a set of model dielectric functions opens the question whether more detailed models for \( \epsilon(k) \) can be obtained from the more complex energy functionals in use in modern density-functional theory. Models for frequency-dependent dielectric functions may be accessible via time-dependent density-functional theory.23

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16. This is not immediately obvious from the alternative
derivation of $\varepsilon_{TF,2}$ via the usual textbook arguments regarding screening of slowly varying potentials.

To illustrate that this transfer from 3-d to 2-d is by no means trivial, we remind the reader of the alternative derivation of 3-d TF screening from a short-range Yukawa potential in real space, $v_Y(r) = e^{2e^{-k_{TF}r}}/r$. Here screening is described by the exponential decay of the potential away from the origin, where the point charge to be screened is placed. The 3-d Fourier transform of this short-range potential is

$$\mathcal{F}[v_Y(r)] = \frac{4\pi}{k^2} \frac{1}{1 + \frac{k_T^2}{k^2}},$$

which identical to (14). However, this identification does not carry over to 2-d: The 2-d Fourier transform of the Yukawa potential is

$$\mathcal{F}[v_Y(r)] = \frac{2\pi e^2}{\sqrt{k^2 + k_{TF}^2}},$$

which is not identical to (37). Hence, the relation Yukawa-potential—TF dielectric function is peculiar to 3-d systems, while the one between energy functionals and the dielectric function carries over to 2-d.