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Changes in nonlinear potential scattering theory in electron gases brought about by reducing dimensionality

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Recent work has shown the essential equivalence of stopping power, force-force correlation function, and phase-shift analysis for nonlinear potential scattering in a three-dimensional electron gas. In the present study, we first demonstrate that the above situation is markedly different when the scattering occurs from a localized potential in a two-dimensional (2D) electron gas. Only to second order in the potential do the three methods referred to above precisely agree. However, all these methods can still be applied in 2D, some fully nonlinear evaluation proving possible. The one-dimensional case is also discussed, albeit more briefly. Scattering from a two-center modeling of the localized potential is also calculated, but now only in the Born approximation, due to the added complication of a noncentral potential. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1947118]

I. INTRODUCTION

Following a vast body of experimental and theoretical studies on three-dimensional metals and alloys,[1,2] attention more recently has focused on two-dimensional systems of itinerant electrons. As an immediate example, on the (111) surfaces of noble metals, e.g., Au, Ag, and Cu, quasiparticles form a two-dimensional electron gas. This has been investigated experimentally by cold scanning tunneling microscopy.[3,4] Turning to physical properties associated with such two-dimensional electron gases (2DEG), the present paper will have as its focus the scattering in such assemblies of the itinerant electrons from localized impurity centers. Then, it is natural enough to proceed with the discussion for spin-compensated impurity systems. However, it is highly relevant to note that both theoretical[5] and experimental[6] studies have appeared recently. In the former, the 2DEG was considered in the presence of a single magnetic impurity (e.g., Co) and the additional scattering phase shift induced by the charge of the Co ion and its specially extended displaced electronic density distribution.[5] Subsequently, scanning tunneling microscopy was employed[6] to measure the phase shift that surface-state electrons suffer when scattering from a single magnetic impurity, which forms a Kondo state.

This is the context then which has motivated the present theoretical study. This follows the earlier discussions,[7,8] of a few aspects of the stopping power of a 2DEG for heavy particles. Two

results utilized there form a valuable starting point for the present study of such a two-dimensional system. First, the transport (tr) cross section is given in the partial wave representation as

$$\sigma_{tr}(k_F) = \frac{4}{k_F} \sum_{m=0}^{\infty} \sin^2[\delta_m(k_F) - \delta_{m+1}(k_F)], \tag{1.1}$$

where k_F denotes the Fermi wave number of the electron gas, related to the Fermi energy E_F by

$$E_F = k_F^2/2. \tag{1.2}$$

In Eq. (1.1), the scattering phase shifts at the Fermi level are denoted by $\delta(k_F)$ for the different partial waves ($m=0,1,\ldots$, etc.). We are interested further in the stopping power $\mathrm{d}E/\mathrm{d}x$ say, at $T=0$, to which the present treatment is restricted, for a heavy ion moving with velocity $\mathbf{v}$. This is related in a direct fashion, as set out in Ref. 7 for slow ions, to the transport cross section σ_{tr} in Eq. (1.1) above

$$\frac{\mathrm{d}E}{\mathrm{d}x} = n_0 v v_F \sigma_{tr}(k_F), \tag{1.3}$$

in which n_0 and v_F are, respectively, the areal density and Fermi velocity of the 2DEG.

The outline of the present investigation is then as follows. In Sec. II below, a force-force correlation function formula, due to Rousseau, Stoddart, and March (RSM),[2,9] in three dimensions, is first adapted to two dimensions. We comment here on the three-dimensional (3D) result. There, the total potential which scatters the electrons is denoted by $V(\mathbf{r})$, and this generates a Dirac density matrix $\gamma(\mathbf{r}_1,\mathbf{r}_2,E)$, which is such that its diagonal element, say $\gamma(\mathbf{r},\mathbf{r},E)$, denotes the integrated local density of electronic states. Correlating the force $-\partial V(\mathbf{r})/\partial \mathbf{r}$ at points $\mathbf{r}_1$ and $\mathbf{r}_2$ via $\partial\gamma(\mathbf{r}_1,\mathbf{r}_2,E)/\partial E$, which is then a generalized density of states, it can readily be shown, when $V(\mathbf{r})$ is assumed to be a central potential $V(r) \equiv V(|\mathbf{r}|)$, to be related to the phase shifts $\delta_l(E)$ for scattering off $V(r)$, via the radial wave functions $R_l(r,E)$ from which the density matrix is constructed. The 3D force-force correlation function formula of RSM is then exactly equivalent to the phase-shift scattering cross section for impurity resistivity of Huang,[10] as shown by one of us.[11] In Sec. II, this 3D situation will be contrasted with that in 2D. Adapting the RSM formula in 3D then leads to the 2D analog set out in Eq. (2.1) below, where account is taken of the Fermi statistics of electrons by considering, as in 3D, that scattering is on the Fermi surface, corresponding to Fermi energy E_F. The 2D phase shift result derived in Eq. (2.15) below for the force-force correlation function is demonstrated here to be distinct from the stopping power in 2D already set out in Eqs. (1.1) and (1.3). This is in contrast to the equivalence of the force-force correlation function and the scattering cross section in 3D which we have discussed above.

Section III is then devoted to studying at some length the Born approximation to this force-force correlation function. In this section, contact is then made with Eqs. (1.1) and (1.3) above. In Sec. IV further illustrations are given by using linear-response formalism for the induced density in 2D. The one-dimensional case of scattering is outlined in Sec. V. Finally, additional and more technical details are summarized in four Appendixes at the end of the paper.

II. FORCE-FORCE CORRELATION FUNCTION IN A TWO-DIMENSIONAL ELECTRON GAS

As indicated above, let us take as starting point a definition of the force-force correlation function in two dimensions as

$$\langle \mathbf{F}\cdot\mathbf{F}\rangle = \int d\mathbf{r}_1 d\mathbf{r}_2 \frac{\partial V(\mathbf{r}_1)}{\partial \mathbf{r}_1}\cdot\frac{\partial V(\mathbf{r}_2)}{\partial \mathbf{r}_2}\left[\frac{\partial \gamma(\mathbf{r}_1,\mathbf{r}_2,E)}{\partial E}\right]^2_{E=E_F}. \tag{2.1}$$

Evidently the two forces $-\partial V(\mathbf{r})/\partial \mathbf{r}$ at two-dimensional position vectors $\mathbf{r}_1$ and $\mathbf{r}_2$ are correlated via the off-diagonal local density of states $N(E,\mathbf{r}_1,\mathbf{r}_2)\equiv \partial\gamma/\partial E$ evaluated at the Fermi level E_F, γ as defined above being the off-diagonal integrated density of states.

As emphasized in three dimensions by Rousseau *et al.*,[9] the merit of the corresponding two-dimensional form in Eq. (2.1) is that it is defined for potentials $V(\mathbf{r})$ of lower than circular symmetry. However, it is a valuable starting point in calculating the force-force correlation function $\langle \mathbf{F}\cdot\mathbf{F}\rangle$ in Eq. (2.1) to treat the case of circular symmetry, i.e., $V(\mathbf{r})=V(|\mathbf{r}|)=V(r)$. This is the objective of the present section. For this limiting case of $V(r)$ with circular symmetry, we shall draw also on the treatments by Adhikari[12] and by Tang and Thouless.[13]

Beginning then with the wave function $\psi(r,\theta)$ in polar coordinates defined by $x=r\cos\theta$ and $y=r\sin\theta$, one can write in the asymptotic region, far from the origin of the scattering potential energy $V(r)$, that $\psi(r,\theta)$ consists of a plane wave, propagating say along the x axis, plus a scattered outgoing wave. Both Refs. 12 and 13 adopt the form

$$\psi(r,\theta)_{r\to\infty} \to \exp(ikx) + \sqrt{i/k} f_k(\theta)\frac{\exp(ikr)}{\sqrt{r}}, \tag{2.2}$$

where $f_k(\theta)$ denotes the scattering amplitude. This result (2.2) follows asymptotically from the Schrödinger equation

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial \psi}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2\psi}{\partial\theta^2} + k^2\psi = U\psi, \tag{2.3}$$

where $k^2=2mE/\hbar^2$ and $U(r)=2mV(r)/\hbar^2$. In this case of circular symmetry $V(r)$, one can separate the variables r and θ by writing

$$\psi(r,\theta) = R(r)\Theta(\theta), \tag{2.4}$$

to find

$$\frac{d^2\Theta}{d\theta^2} + m^2\Theta = 0. \tag{2.5}$$

Hence, we have now wave functions of the form following from Eq. (2.4) plus the physically significant solution of Eq. (2.5) as

$$\psi_m(\mathbf{r}_1) = \exp(im\theta_1)R(k_F r_1). \tag{2.6}$$

Returning to the definition (2.1), we can write the energy derivative of the Dirac matrix γ in terms of $\psi_m(\mathbf{r}_1)$ and the energies E_i generated by the one-body Hamiltonian H given by

$$H = -\frac{1}{2}\nabla^2 + V(r), \tag{2.7}$$

as

$$\frac{\partial\gamma}{\partial E} = \sum_i \psi_i^*(\mathbf{r}_1)\psi_i(\mathbf{r}_2)\delta(E-E_i), \tag{2.8}$$

with the complex conjugate satisfying

$$\frac{\partial \gamma^*}{\partial E} = \sum_j \psi_j(\mathbf{r}_1)\psi_j^*(\mathbf{r}_2)\delta(E - E_j). \tag{2.9}$$

Thus, from Eqs. (2.8) and (2.9) it follows that

$$\left|\frac{\partial \gamma}{\partial E}\right|^2_{E=E_F} = \sum_{i,j} \psi_i^*(k_F\mathbf{r}_1)\psi_j(k_F\mathbf{r}_1)\psi_i(k_F\mathbf{r}_2)\psi_j^*(k_F\mathbf{r}_2). \tag{2.10}$$

Replacing i, j by m, m', it follows from Eq. (2.1) for isotropic scattering potentials that

$$\langle \mathbf{F}\cdot\mathbf{F}\rangle = \int r_1 r_2 \frac{\partial V(r_1)}{\partial r_1}\frac{\partial V(r_2)}{\partial r_2}\cos(\theta_2 - \theta_1)\left|\frac{\partial \gamma}{\partial E}\right|^2_{E=E_F} \mathrm{d}r_1\,\mathrm{d}r_2\,\mathrm{d}\theta_1\,\mathrm{d}\theta_2. \tag{2.11}$$

Using the wave functions (2.6), the angular integration in Eq. (2.11) becomes, after some manipulation

$$\begin{aligned}&\frac{1}{2}\sum_{m,m'}\int_0^{2\pi}\int_0^{2\pi}[\exp(i(\theta_2-\theta_1))+\exp(-i(\theta_2-\theta_1))][\exp(i(m-m')\theta_2)\exp(-i(m-m')\theta_1)]\mathrm{d}\theta_1\,\mathrm{d}\theta_2\\ &\quad = 2\pi^2\sum_{m,m'}[\delta(m'=m+1)+\delta(m'=m-1)].\end{aligned} \tag{2.12}$$

Using Eqs. (2.12) and (2.6) in Eq. (2.11), and performing the summation over m' then yields

$$\begin{aligned}\langle \mathbf{F}\cdot\mathbf{F}\rangle = 2\pi^2\sum_m &\int_{r_1} r_1\frac{\partial V(r_1)}{\partial r_1}R_m^*(k_F r_1)[R_{m+1}(k_F r_1)+R_{m-1}(k_F r_1)]\mathrm{d}r_1\int_{r_2} r_2\frac{\partial V(r_2)}{\partial r_2}R_m(k_F r_2)\\ &\times[R_{m+1}^*(k_F r_2)+R_{m-1}^*(k_F r_2)]\mathrm{d}r_2.\end{aligned} \tag{2.13}$$

Using the result of Tang and Thouless[13] that

$$\int r R_{m+1}^*(kr)\frac{\partial V(r)}{\partial r}R_m(kr)\mathrm{d}r = -\frac{k}{\pi}\exp(\delta_m-\delta_{m+1})\sin(\delta_{m+1}-\delta_m) \tag{2.14}$$

then gives

$$\begin{aligned}\langle \mathbf{F}\cdot\mathbf{F}\rangle &= \frac{(2\pi)^2}{2}\left(\frac{k}{\pi}\right)^2\sum_m[\exp(-i(\delta_m-\delta_{m+1}))\sin(\delta_{m+1}-\delta_m)+\exp(i(\delta_{m-1}-\delta_m))\sin(\delta_m-\delta_{m-1})]\\ &\quad\times[\exp(i(\delta_m-\delta_{m+1}))\sin(\delta_{m+1}-\delta_m)+\exp(-i(\delta_{m-1}-\delta_m))\sin(\delta_m-\delta_{m-1})]\\ &= k^2\sum_m[1-\cos(2(\delta_{m+1}-\delta_{m-1}))].\end{aligned} \tag{2.15}$$

The above analysis is analogous to that of Huang[10] in terms of partial waves of orbital angular momentum quantum number l in 3D; there, only the phase shifts δ_l with $k=k_F$ are required, where k_F is the Fermi wave number (independent of l). This two-dimensional result for the force-force correlation function with $V(\mathbf{r})=V(|\mathbf{r}|)$ appears to be new. It must be stressed that this phase-shift result (2.15) for $\langle \mathbf{F}\cdot\mathbf{F}\rangle$ is distinct from the stopping power in Eqs. (1.1) and (1.3).

Though we do not have an analog of Eq. (2.15) for $\langle \mathbf{F}\cdot\mathbf{F}\rangle$ when the isotropy of $V(\mathbf{r})$ is relaxed, it is of immediate interest to treat this more general case in the Born approximation, and this is the essential content of the following section.

III. FORCE-FORCE CORRELATION FUNCTION IN TWO DIMENSIONS IN THE BORN APPROXIMATION

To calculate $\langle \mathbf{F}\cdot\mathbf{F}\rangle$ in Eq. (2.1) to $\mathcal{O}(V^2)$ for a potential $V(\mathbf{r})$ without circular symmetry, we can make the crucial simplifying approximation that the Dirac density matrix γ in Eq. (2.1) is replaced by its two-dimensional free-electron counterpart $\gamma_0(\mathbf{r}_1,\mathbf{r}_2,E)$. This we obtain following the approach of March and Murray[14,15] in their three-dimensional density matrix perturbation theory, based on the scattering potential $V(r)$ above embedded in an initially uniform free-electron gas. Their main achievement was to start from the canonical, or Bloch density matrix $C(\mathbf{r}_1,\mathbf{r}_2,\beta)$, defined for the one-body Hamiltonian (2.7) having eigenfunctions $\psi_i(\mathbf{r})$ and corresponding eigenvalues ϵ_i as

$$C(\mathbf{r}_1,\mathbf{r}_2,\beta)=\sum_{\text{all}i}\psi_i^*(\mathbf{r}_1)\psi_i(\mathbf{r}_2)\exp(-\beta\epsilon_i):\ \beta=(k_BT)^{-1}. \tag{3.1}$$

The (zero-temperature) Dirac density matrix appearing in Eq. (2.1) is then related to the C matrix in Eq. (3.1) by

$$C(\mathbf{r}_1,\mathbf{r}_2,\beta)=\beta\int_0^\infty \gamma(\mathbf{r}_1,\mathbf{r}_2,E)\exp(-\beta E)\mathrm{d}E. \tag{3.2}$$

A. Free-electron results in two dimensions

It is well known that in D dimensions the free-electron canonical density matrix is given by

$$C_0(\mathbf{r}_1,\mathbf{r}_2,\beta,D)=\frac{1}{(2\pi\beta)^{D/2}}\exp\left(-\frac{|\mathbf{r}_1-\mathbf{r}_2|^2}{2\beta}\right). \tag{3.3}$$

March and Murray were concerned with the three-dimensional case, for which they obtained the Dirac matrix as

$$\gamma_0(\mathbf{r}_1,\mathbf{r}_2,E)_{D=3}=\frac{k_F^3}{2\pi^2}\frac{j_1(k|\mathbf{r}_1-\mathbf{r}_2|)}{k|\mathbf{r}_1-\mathbf{r}_2|}, \tag{3.4}$$

where $j_1(x)$ is the first-order spherical Bessel function $(\sin x - x\cos x)/x^2$, and we have written Eq. (3.4) for single occupied levels.

To obtain the two-dimensional analog, we need the inverse Laplace transform of C_0/β, according to Eq. (3.2), where C_0 is given by Eq. (4.4) with $D=2$. This can be found from Ref. 16 as

$$\gamma_0(\mathbf{r}_1,\mathbf{r}_2,E)=\frac{1}{2\pi}\frac{\sqrt{2E}}{|\mathbf{r}_1-\mathbf{r}_2|}J_1(\sqrt{2E}|\mathbf{r}_1-\mathbf{r}_2|). \tag{3.5}$$

Fortunately, the energy derivative $\partial\gamma/\partial E$ appearing in the force-force formula (2.1) is more compact, and follows after a short calculation using properties of Bessel functions as

$$\frac{\partial\gamma_0(\mathbf{r}_1,\mathbf{r}_2,E)}{\partial E}=\frac{1}{2\pi}J_0(\sqrt{2E}|\mathbf{r}_1-\mathbf{r}_2|). \tag{3.6}$$

An immediate check on the result (3.6) is the density of states $N(E)$ obtained by setting $\mathbf{r}_2=\mathbf{r}_1$ in Eq. (3.6), the result being simply the constant $1/2\pi$ since $J_0(0)=1$. This result (3.6), in conjunction with Eq. (4.7) below, is used in Appendix A to derive the linear response function in two dimensions.

Returning to Eq. (2.1), the force-force correlation function, B denoting the Born approximation, is given, apart from a multiplicative factor, explicitly in terms of the scattering potential $V(\mathbf{r})$ by making use of Eq. (3.6) as

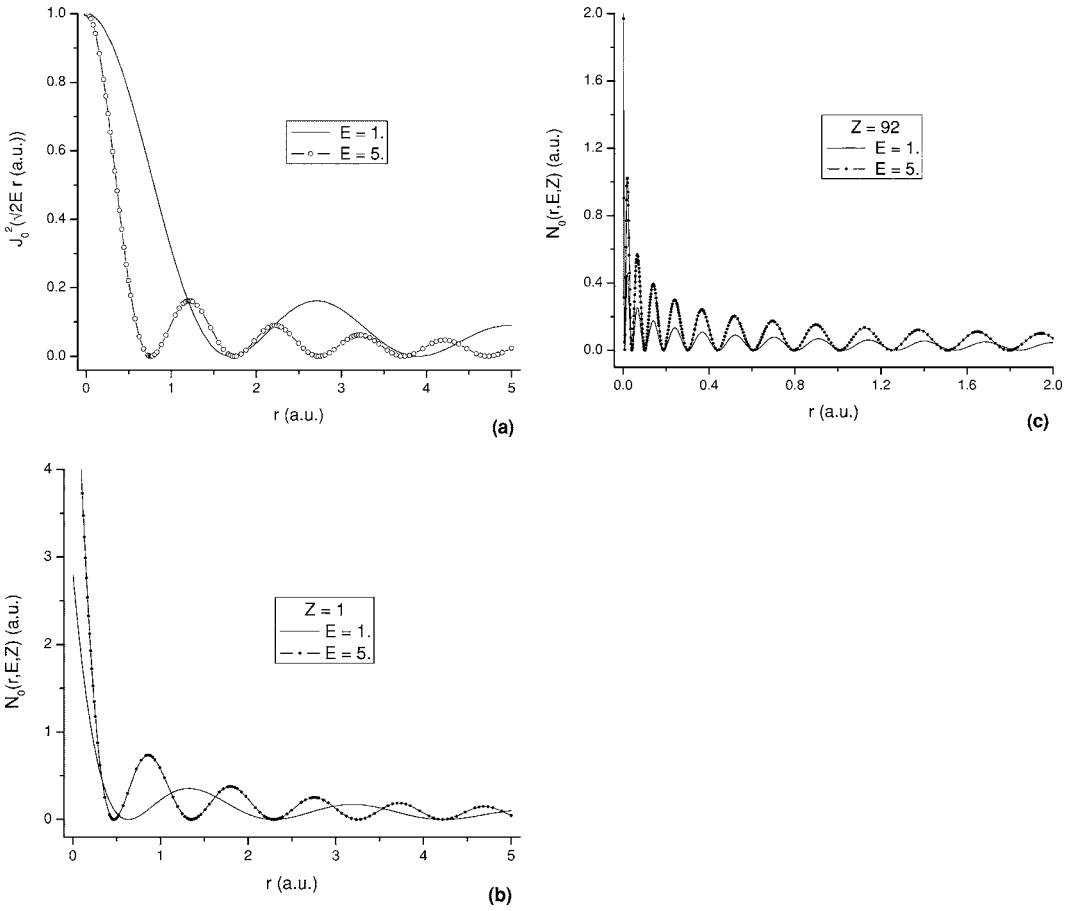

FIG. 1. (a) Plot of $J_0^2(\sqrt{2E}r)$ appearing in force-force correlation function set out in Eq. (3.7), versus r, for two values of E [compare also Eq. (D4)]. Other curves shown are (b) and (c) the s-state ($m=0$) component of the local density of states $N_0(r,E,Z)$ generated by a bare Coulomb potential ($-Z/r$) embedded in a two-dimensional electron gas, for $Z=1$ and 92 and the same two values of energy E as in the plot of J_0^2. Apart from an unimportant normalization factor, J_0^2 is the limit of $N_0(r,E,Z)$ as Z tends to zero.

$$\langle \mathbf{F}\cdot\mathbf{F}\rangle_B \propto \int d\mathbf{r}_1\, d\mathbf{r}_2 \frac{\partial V(\mathbf{r}_1)}{\partial \mathbf{r}_1}\cdot\frac{\partial V(\mathbf{r}_2)}{\partial \mathbf{r}_2} J_0^2(\sqrt{2E}|\mathbf{r}_1-\mathbf{r}_2|). \tag{3.7}$$

Some examples relating to Eq. (3.7) are set out in Appendixes C and D below. By way of illustration, we show in Fig. 1 a plot of $J_0^2(\sqrt{2E}r)$ versus r for two values of E. For comparison, we show the local density of states $N_0(r,E,Z)$ for the bare Coulomb potential energy $-Ze^2/r$ given in Eq. (C3), which reduces to $J_0^2(\sqrt{2E}r)$ when $Z=0$, apart from an unimportant normalization factor.

B. Scattering from a model two-center potential in two dimensions and in Born approximation

Dimers of impurities on nonmagnetic substrates provide a very active research field in scanning tunneling spectroscopy at the atomic scale.[17] This activity motivates the present subsection on the role of reduced dimensionality in associated scattering processes.

Consider the case of two equivalent scattering centers in a 2D electron gas. Let $\mathbf{R}$ be the vector joining the centers, $\mathbf{n}_0$ a unit vector in the direction of incidence, $\mathbf{n}_1$ a unit vector in the direction of scattering, and $\mathbf{k}$ the scattering wave vector of electrons. Due to the Fermi statistics $\mathbf{k}=\mathbf{k}_F$ is, in fact, the practically important value. As a first approximation we regard the two centers as scattering independently but coherently. Therefore, the result obtained will be generally

valid (even for strong scattering by the single center) if $kR \gg 1$. Following closely the standard[18,19] derivation in the 3D case, one obtains for the 2D differential cross section the following expression, in this so-called independent-atom approximation:

$$d\sigma(k,\theta)d\theta = 2|f_k(\theta)|^2(1+\cos[k(\mathbf{n}_0-\mathbf{n}_1)\cdot\mathbf{R}])d\theta, \tag{3.8}$$

where $\cos\theta = \mathbf{n}_0\cdot\mathbf{n}_1$. The function $f_k(\theta)$ is given in Eq. (2.2).

Practically, due to the random orientations of dimers (diclusters), the averaged cross section $d\sigma_{av}(k,\theta)$ is required. Therefore, we average over all orientations of the vector $\mathbf{R}$ in 2D by using Eqs. (3.715.18) of Ref. 20 and obtain

$$d\sigma_{av}(k,\theta)d\theta = 2|f_k(\theta)|^2[1+J_0(qR)]d\theta, \tag{3.9}$$

in which $q=2k\sin(\theta/2)$, the momentum transfer. In the first-order Born approximation the scattering amplitude $f_k^B(\theta)$ is related simply to the Fourier transform of the single-atom screened potential $V(q)$. Thus, in this case we have

$$|f_k^B(\theta)|^2 = \frac{1}{2\pi k}|V(q)|^2. \tag{3.10}$$

For the $kR \gg 1$ condition, Eq. (3.9) is applicable also for stronger scattering using partial-wave expansion.[12,13] In the so-called leading ($m=0$) phase-shift approximation, one gets the usual expression

$$|f_k(\theta)|^2 = \frac{2}{\pi k}\sin^2(\delta_0(k)). \tag{3.11}$$

If the unitary limit, as prescribed by the 2D Friedel sum rule,[8] is a valid approximation, one may use $\delta_0=\pi/2$ in Eqs. (3.11) and (3.9).

Various angular integrals of $d\sigma_{av}(k,\theta)$ need, in the leading phase-shift method, only a simple averaging of the $J_0[2k\sin(\theta/2)R]$ factor. Applying the standard expansion

$$J_0(qR) = \sum_{m=-\infty}^{\infty} J_m^2(kR)\exp(im\theta), \tag{3.12}$$

in Eq. (3.9), the total (t) cross section becomes

$$\sigma_{av}^t(k) = \frac{8}{k}\sin^2(\delta_0(k))(1+[J_0(kR)]^2), \tag{3.13}$$

for this case. This quantity may prove useful in estimating the dephasing time due to elastic scattering of surface-state electrons by dimer impurities.

Other angle-weighted cross sections (transport, diffusion) require more detailed, but feasible, calculations for the important 2D case.

IV. LINEAR RESPONSE FUNCTION GIVING THE DISPLACED FERMION DENSITY AROUND A "PERTURBING POTENTIAL" $V(\mathbf{r})$ IN A TWO-DIMENSIONAL UNIFORM ELECTRON GAS

Though our main purpose has been to evaluate the force-force correlation function defined in Eq. (2.1) to all orders in the scattering potential $V(|\mathbf{r}|)$ in Eq. (2.13), and to illustrate this by presenting numerical results at the Born level, it seemed of interest, in view of the usefulness of the March-Murray result[14,15] for the density $\rho(\mathbf{r})$ in three dimensions, namely

$$\rho_{3d}(\mathbf{r}) - \rho_0 = \text{const.} \times \int d\mathbf{r}' V(\mathbf{r}') \frac{j_1(2k_F|\mathbf{r}-\mathbf{r}'|)}{|\mathbf{r}-\mathbf{r}'|^2}, \tag{4.1}$$

where $\rho_0 = k_F^3/6\pi^2$, and the constant is given in Eq. (A2), to obtain the corresponding two-dimensional result. This then is the purpose of the present section. We shall take as starting point the work of Stoddart, March, and Stott,[21] who write Eq. (4.1) more generally as

$$\Delta\rho(\mathbf{r}) = \int d\mathbf{r}' V(\mathbf{r}') F(|\mathbf{r}-\mathbf{r}'|, E), \tag{4.2}$$

where

$$\frac{\partial F}{\partial E} = 2\,\mathrm{Re}\left[G(\mathbf{r},\mathbf{r}',E) \frac{\partial \gamma(\mathbf{r},\mathbf{r}',E)}{\partial E} \right]. \tag{4.3}$$

Thus, to obtain the two-dimensional counterpart of Eq. (4.1), we shall write, for the uniform gas, that

$$\frac{\partial F_0(\mathbf{r},\mathbf{r}',E)}{\partial E} = 2 \frac{\partial \gamma_0(\mathbf{r},\mathbf{r}',E)}{\partial E}\,\mathrm{Re}[G_0(\mathbf{r},\mathbf{r}',E)]. \tag{4.4}$$

Here, G_0 is the free-particle Green function in two dimensions. This is related to the canonical density matrix $C_0(\mathbf{r},\mathbf{r}',\beta)$ discussed above by

$$\mathcal{L} C_0(\mathbf{r},\mathbf{r}',\beta) = G_0(\mathbf{r},\mathbf{r}',-E). \tag{4.5}$$

With C_0 again given by Eq. (3.3) with $D=2$, the Laplace transform $\mathcal{L}$ above can be obtained as

$$\mathcal{L} C_0(\mathbf{r},\mathbf{r}',\beta) = \frac{K_0(\sqrt{2E}|\mathbf{r}-\mathbf{r}'|)}{\pi} \tag{4.6}$$

where $K_0(x)$ is the modified Bessel function.[16] Using Eqs. (4.5) and (4.6), we thus find

$$G_0(\mathbf{r},\mathbf{r}',E) = \frac{K_0(i\sqrt{2E}|\mathbf{r}-\mathbf{r}'|)}{\pi}. \tag{4.7}$$

Since $\partial\gamma_0/\partial E$ is known in terms of J_0 from Eq. (3.6), we have $\partial F_0/\partial E$ by appealing to Eq. (4.4). We note that Zhang[22] has obtained a more compact form in **k**-space, although he then invokes the Meijer function in the **r**-space representation we focus on in the present study. The above theory is extended somewhat in Appendix A.

V. ONE-DIMENSIONAL SCATTERING

Having contrasted nonlinear scattering in 2D and 3D electron gases from a localized potential, we turn, albeit briefly, to consider what further changes are introduced by dimensionality reduction to the case of 1D. We follow March and Murray,[14,15] who dealt completely with 3D plane wave perturbation theory, by starting from the integral equation derived from the well-known Bloch equation[23] for the canonical density matrix $C(x,x_0,\beta)$, where

$$C(x,x_0,\beta) = \sum_{\text{all}\,i} \psi_i(x)\psi_i^*(x_0)\exp(-\beta\epsilon_i). \tag{5.1}$$

In Eq. (5.1), $\psi_i(x)$ and the corresponding eigenvalues ϵ_i satisfy

$$H\psi_i = \epsilon_i \psi_i, \tag{5.2}$$

where the one-dimensional Hamiltonian is simply

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x). \tag{5.3}$$

Evidently, completeness yields from Eq. (5.1) at $\beta=0$

$$C(x,x_0,0) = \delta(x-x_0), \tag{5.4}$$

and this is built in the integral form of the Bloch equation, namely

$$C(x,x_0,\beta) = C_0(x,x_0,\beta) - \int_0^\beta d\beta_1 \int dx_1 C_0(x,x_1,\beta-\beta_1)V(x_1)C(x_1,x_0,\beta_1). \tag{5.5}$$

In Eq. (5.5), C_0 is the free-particle density matrix[23]

$$C_0(x,x_0,\beta) = \frac{1}{\sqrt{2\pi\beta}}\exp\left(-\frac{(x-x_0)^2}{2\beta}\right). \tag{5.6}$$

The β_1 integration can be removed by a Laplace transform on β ($\rightarrow E$) to yield ($C\rightarrow\tilde{C}$)

$$\tilde{C}(x,x_0,E) = \tilde{C}_0(x,x_0,E) - \int \mathrm{d}x_1\, \tilde{C}_0(x,x_1,E)V(x_1)\tilde{C}(x_1,x_0,E). \tag{5.7}$$

The Laplace transform of Eq. (5.6) is readily obtained as[24]

$$\tilde{C}_0(x,x_0,E) \equiv \mathcal{L}C_0(x,x_0,\beta) = \frac{1}{\sqrt{2E}}\exp(-\sqrt{2E}|x-x_0|). \tag{5.8}$$

If in Eq. (5.7) we then work to first order in the "perturbing" potential $V(x)$, we find

$$\tilde{C}(x,x_0,E) = \frac{1}{\sqrt{2E}}\exp(-\sqrt{2E}|x-x_0|) - \frac{1}{2E}\int \mathrm{d}x_1\, V(x_1)\exp(-\sqrt{2E}\{|x-x_1|+|x_1-x_0|\}). \tag{5.9}$$

Inverting the Laplace transform ($E\rightarrow\beta$) in Eq. (5.9) readily yields

$$C(x,x_0,\beta) = \frac{1}{\sqrt{2\pi\beta}}\exp\left(-\frac{(x-x_0)^2}{2\beta}\right) - \frac{1}{2}\int \mathrm{d}x_1\, V(x_1)\mathrm{erfc}\left(\sqrt{\frac{2}{\beta}}\frac{\{|x-x_1|+|x_1-x_0|\}}{2}\right). \tag{5.10}$$

The Dirac density matrix $\gamma(x,x_0,E)$ then follows as the inverse Laplace transform of $C(x,x_0,\beta)/\beta$, and is given by

$$\gamma(x,x_0,E) = \frac{\sin(\sqrt{2E}|x-x_0|)}{\pi|x-x_0|} - \int \mathrm{d}x_1\, V(x_1)\left[\frac{1}{2} - \frac{\mathrm{Si}(\sqrt{2E}\{|x-x_1|+|x_1-x_0|\})}{\pi}\right], \tag{5.11}$$

which is the 1D analog of the first-order 3D result of March and Murray.[14,15]

Of course, one obvious difference between 2D and 3D scattering and the 1D case to be discussed further below is that in the 1D system there are only two discrete directions for scattering: forward and backward along a line. Below, we restrict our discussion to symmetric localized potentials $V(x)$ satisfying

$$V(x) = V(-x). \tag{5.12}$$

The 1D analog of the customary Lippmann-Schwinger equation takes the form

$$\psi_k(x) = \phi_k(x) + \int_{-\infty}^{\infty} G_0(x,x')V(x')\psi_k(x')\mathrm{d}x', \tag{5.13}$$

where $\phi_k(x)$ is the free-particle wave function $\exp(ikx)$. The one-dimensional Green function $G_0(x,x')$ is given by

$$G_0(x,x') = -\frac{i}{2k}\exp(ik|x-x'|), \tag{5.14}$$

which is readily verified to be the Laplace transform ($\mathcal{L}$) of the canonical density matrix (3.3) with respect to β for the case $D=1$, since

$$\mathcal{L}C = G_0(x,x'):E = k^2. \tag{5.15}$$

Using Eq. (5.14) in (5.13), the following asymptotic form of $\psi_k(x)$ results:

$$\psi_k(x) \to \exp(ikx) + \frac{i}{k}f_k(\epsilon)\exp(ikx), \tag{5.16}$$

where $f_k(\epsilon)$ is the analog of the scattering amplitude in higher dimensions. However, as discussed above, there are but two scattering directions in 1D, corresponding to $\epsilon = \pm 1$. This is to be contrasted with the continuum of scattering angles in both 2D and 3D. The differential cross sections in these two directions in the 1D case are given by

$$\sigma_\epsilon = \frac{1}{k^2}|f_k(\epsilon)|^2, \tag{5.17}$$

while the total cross section σ takes the form

$$\sigma = \frac{1}{k^2}[|f_k(+1)|^2 + |f_k(-1)|^2]. \tag{5.18}$$

To press the analogy with higher dimensions, we have now just two partial waves. For potentials satisfying Eq. (5.12), these two partial waves are distinct, with even and odd parity. It is to be noted that the cross section σ, in principle an observable, has units of length L squared in 3D, L in 2D, and is dimensionless according to Eq. (5.18) in 1D.

Analogs of the optical theorem and the unitarity relation again exist, paralleling here the 2D and 3D scattering, but we shall not go into further detail. It is worth adding, in concluding this brief discussion of 1D scattering, that the above can be usefully illustrated for a potential $V(x)$ which is the Dirac delta function (see the discussion in 3D in Ref. 25), but we shall not go into further detail since the 3D example was treated fully for a similar, completely localized, scattering center.

VI. DISCUSSION AND FUTURE DIRECTIONS

Our principal aim has been to demonstrate the effect of dimensionality reduction on the 3D results given earlier[25] for nonlinear scattering by a localized potential. For the 2D case, which is the main focus of the present study, it is striking that the stopping power problem summarized in Eqs. (1.1) and (1.3) turns out, beyond the Born approximation, to be distinct from the force-force correlation function $\langle \mathbf{F}\cdot\mathbf{F}\rangle$ defined in Eq. (2.1) in 2D. These are essentially identical to all orders in the localized scattering potential V in 3D. It is possible in 2D that there are "frictional effects" in surfaces, the theory of which has been discussed by d'Agliano and co-workers,[26] which may mirror $\langle \mathbf{F}\cdot\mathbf{F}\rangle$, but it remains to be proved that this latter correlation function is indeed an observable in 2D, whereas it is established that this is the case, though not distinct from stopping power or transport cross section, in 3D. Here, we believe for the first time, $\langle \mathbf{F}\cdot\mathbf{F}\rangle$ in Eq. (2.1) has been

calculated analytically in terms of phase shifts at the Fermi level, and is given for 2D in Eq. (2.13). This is evidently closely related to, but nevertheless distinct from, Eq. (1.1) in terms of the same input information, for the transport cross section.

Further directions of interest for the future, which were already touched on in the Introduction, are scattering in essentially two dimensions from a single magnetic impurity. Here, the spin-dependent theoretical approach of Stoddart and March[27] may well find application, and the two-dimensional version should prove of considerable interest for the future.

APPENDIX A: r-SPACE LINEAR RESPONSE FUNCTION $F(|\mathbf{r}-\mathbf{r}'|,E)$ IN TWO DIMENSIONS

The object of this appendix is to give the two-dimensional form of the result of March and Murray[14]

$$\Delta\rho(\mathbf{r},E)=\int F_{3d}(|\mathbf{r}-\mathbf{r}'|,E)V(\mathbf{r}')\mathrm{d}\mathbf{r}', \tag{A1}$$

for the displaced charge below energy E created by a perturbing potential $V(\mathbf{r})$ inserted into an initially uniform electron gas. The result of Ref. 14 was explicitly [compare Eq. (4.1)]

$$F_{3d}(R,E)=-\frac{mE}{\pi^3\hbar^2}\frac{j_1(2\sqrt{2E}R)}{R^2}. \tag{A2}$$

Below, we derive an analogous form to Eq. (A2) in two dimensions. As shown by Stoddart, March, and Stott,[21] for the uniform Fermi gas as the unperturbed system, $\partial F(R,E)/\partial E$ is given by Eq. (4.3) of the main text, where the free-electron 2D Green function has been given in Eq. (4.7) in terms of the Bessel function K_0. Likewise, $\partial\gamma/\partial E$ is known in 2D in terms of J_0 from Eq. (3.6), and inserting these results into Eq. (4.3) and forming the energy derivative yields, after using the identity

$$\mathrm{Re}[K_0(ikR)]=-Y_0(kR)/2\pi, \tag{A3}$$

the result

$$F(R,E)=-\frac{1}{2\pi}\int^E J_0(\sqrt{2E}R)Y_0(\sqrt{2E}R)\mathrm{d}E. \tag{A4}$$

Performing the integration, one finds

$$F(R,E)=-\frac{E}{2\pi}[J_0(\sqrt{2E}R)Y_0(\sqrt{2E}R)+J_1(\sqrt{2E}R)Y_1(\sqrt{2E}R)]+f(R). \tag{A5}$$

But, the energy-independent function $f(R)$ must be zero since $\Delta\rho(R,E=0)=0$, and thus, for the displaced charge at the origin $\Delta\rho(0,E)$, one obtains

$$\Delta\rho(0,E)=-ZE\int_0^\infty [J_0(\sqrt{2E}r)Y_0(\sqrt{2E}r)+J_1(\sqrt{2E}r)Y_1(\sqrt{2E}r)]\mathrm{d}r, \tag{A6}$$

for the case of the bare Coulomb potential, by way of illustration. From Ref. 20, we have

$$\int_0^\infty J_\nu(ax)Y_\nu(ax)\mathrm{d}x=-\frac{1}{2a},\quad [\nu>-1/2,a>0], \tag{A7}$$

and hence

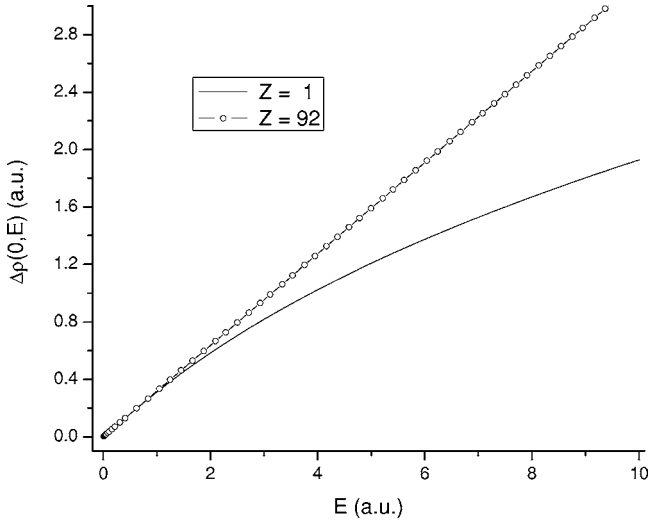

FIG. 2. Displaced charge $\Delta\rho(0,E)$ at nucleus, resulting from a bare Coulomb potential $(-Z/r)$ embedded in a two-dimensional electron gas, for $Z=1$ and 92, versus energy E, as given in Eq. (A9).

$$\Delta\rho(0,E) = \frac{ZE}{\sqrt{2E}} = Z\sqrt{\frac{E}{2}}, \quad E \neq 0. \tag{A8}$$

In fact, for $V=-Z/r$, this result (A8) has the fully nonlinear generalization

$$\Delta\rho(0,E) = \frac{E}{\pi}\tanh\left(\frac{Z\pi}{\sqrt{2E}}\right), \tag{A9}$$

which is equivalent to Eq. (A8) to first order in Z. Equation (A9) is plotted as a function of energy E for $Z=1$ and $Z=92$ in Fig. 2. The following appendix adds some further nonlinear results associated still with the unscreened Coulomb potential.

APPENDIX B: SOME FURTHER PROPERTIES GENERATED BY THE BARE COULOMB POTENTIAL IN TWO DIMENSIONS

The real-space Schrödinger equation in plane polar coordinates (r,θ) reads

$$\left[-\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) - \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2} + V(\mathbf{r})\right]\psi(\mathbf{r}) = E\psi(\mathbf{r}), \tag{B1}$$

where, writing

$$\psi(\mathbf{r}) = R(r)\Theta(\theta), \tag{B2}$$

we have

$$\Theta(\theta) = \frac{1}{\sqrt{2\pi}}\exp(im\theta). \tag{B3}$$

The corresponding radial equation, with $E=-k_0^2$, say, is

$$\frac{d^2R}{dr^2} + \frac{1}{r}\frac{dR}{dr} + \left[\frac{2}{r} - k_0^2 - \frac{m^2}{r^2}\right]R = 0. \tag{B4}$$

The normalized wave functions are then

$$\psi_{nm}(\mathbf{r}) = \sqrt{\frac{k_0^3(n-|m|)!}{\pi(n+|m|)!}}(2k_0r)^{|m|}\exp(-k_0r)L_{n-|m|}^{2|m|}(2k_0r)\exp(im\theta), \tag{B5}$$

where L as usual denotes the associated Laguerre polynomial.

In three dimensions, Heilmann and Lieb[28] (HL) calculated the total density of the entire spectrum of bound states of the hydrogen atom. Below, we note one property for the two-dimensional case that is much simpler than for the three-dimensional case, namely the density $\rho_\infty(r)$ at $r=0$. Using the definition in two dimensions that

$$\rho_\infty(r) = \sum_{n=0}^{\infty}\sum_{m\leqslant n}\psi^*(\mathbf{r})\psi(\mathbf{r}), \tag{B6}$$

one has from Eq. (B5) the result

$$\rho_\infty(r) = \sum_{n=0}^{\infty}\sum_{m\leqslant n}\frac{k_0^3(n-|m|)!}{\pi(n+|m|)!}(2k_0r)^{2|m|}\exp(-2k_0r)[L_{n-|m|}^{2|m|}(2k_0r)]^2. \tag{B7}$$

At $r=0$, the above summation simplifies (because only $m=0$ terms contribute) to

$$\rho_\infty(0) = \sum_{n=0}^{\infty}\frac{k_0^3}{\pi}, \tag{B8}$$

where the bound-state energy levels are given by

$$E = -k_0^2 = -\frac{1}{(n+1/2)^2}. \tag{B9}$$

Using the summation in Ref. 16, namely

$$(1-2^{-n})\zeta(n) = \sum_{k=0}^{\infty}(2k+1)^{-n}, \tag{B10}$$

with $n=3$ yields the closed result

$$\rho_\infty(0) = \frac{7}{\pi}\zeta(3), \tag{B11}$$

where ζ denotes the Riemann zeta function. This result can be further generalized to N closed shells as

$$\rho_N(0) = \frac{7}{\pi}\zeta(3) + \frac{\Psi(2,N+3/2)}{2\pi}, \tag{B12}$$

and Fig. 3 shows a plot of this equation as a function of N. The value $\rho_\infty(0)$ is solely due to the spherically symmetric wave functions corresponding to $m=0$ (s states) and hence $\rho_\infty(0)=\rho_{\infty s}(0)$.

Kato's theorem, discussed by one of us in Ref. 29, has then the generalization to D dimensions for nuclear charge Ze given by

$$\left.\frac{\partial\rho(r)}{\partial r}\right|_{r=0} = -\frac{4Z}{(D-1)}\rho_s(r)\Big|_{r=0}, \tag{B13}$$

and means that, for $Z=1$ and $D=2$

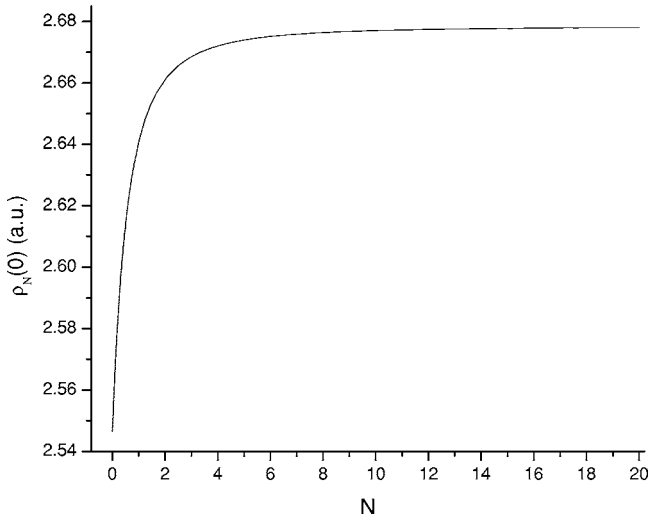

FIG. 3. Plot of electron density $\rho_N(0)$ at the nucleus given by Eq. (B12) for a two-dimensional hydrogen-like atom, versus the number of closed shells N.

$$\left.\frac{\partial\rho(r)}{\partial r}\right|_{r=0} = -\frac{28}{\pi}\zeta(3). \tag{B14}$$

This implies, in particular, that after differentiating $\rho_\infty(r)$ in Eq. (B7) with respect to r, the summation over m can be performed and the result then relates to the s-like ($m=0$) density according to Eq. (B13).

APPENDIX C: DIFFERENTIAL EQUATION SATISFIED BY THE DIAGONAL LOCAL DENSITY OF STATES $N(r,E)$ FOR THE $m=0$ COMPONENT

Denoting the $m=0$ component of the local density of states by $N_0(r,E,Z)$, we have the differential equation, with primes denoting derivatives with respect to r, as

$$\frac{r^2}{2E}N_0''' + \frac{3r}{2E}N_0'' + \left[4r\left(r+\frac{1}{E}\right)+\frac{1}{2E}\right]N_0' + \left[4\left(r+\frac{1}{2E}\right)+\frac{1}{2E}\left(4+\frac{1}{r}\right)\right]N_0 = 0. \tag{C1}$$

Dropping the "potential energy" term $1/r$, one can readily verify that Eq. (C1) is satisfied by the free-electron result

$$N_0(r,E,Z=0) = \text{const.} \times [J_0(\sqrt{2E}r)]^2. \tag{C2}$$

The physical solution (with $V(r)=-Z/r$ now the 2D Coulomb potential) of Eq. (C1) is

$$N_0(r,E,Z) = \text{const.} \times \frac{\mathcal{M}(-iZ/k,0,i2kr)^2}{r}, \tag{C3}$$

where $\mathcal{M}$ denotes the Whittaker function (see also Fig. 1 of the main text).

APPENDIX D: COULOMB LOCAL DENSITY OF STATES AND FREE-ELECTRON LIMIT

In the main text we proved that

$$\frac{\partial\gamma_0}{\partial E} = \frac{1}{2\pi}J_0(\sqrt{2E}|\mathbf{r}-\mathbf{r}'|), \tag{D1}$$

which we now expand in terms of angular functions $\exp(im\phi)$, where $\cos(\phi)=\mathbf{r}\cdot\mathbf{r}'/rr'$, to write

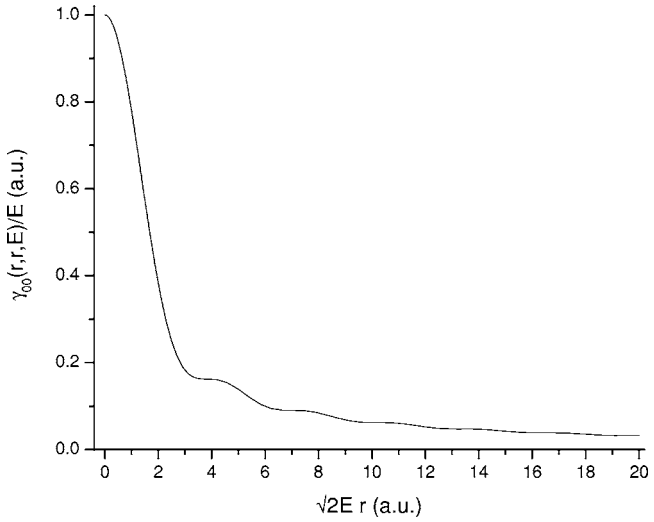

FIG. 4. s-state ($m=0$) electron density $\gamma_{00}(r,r,E)$ for a two-dimensional free electron gas, as given by Eq. (D6). Actual plot is $\gamma_{00}(r,r,E)/E$ versus $\sqrt{2E}r$.

$$\frac{\partial\gamma_0}{\partial E}=\sum_{m=-\infty}^{\infty}\frac{\partial\gamma_{0m}(r,r')}{\partial E}\exp(im\phi). \tag{D2}$$

Then, it follows directly from Eqs. (D1) and (D2) above that

$$\frac{\partial\gamma_{00}(r,r')}{\partial E}=\frac{1}{2\pi}\int_0^{2\pi}J_0(\sqrt{2E}|\mathbf{r}-\mathbf{r}'|)d\phi. \tag{D3}$$

From Ref. 20, Eq. 6.684.1, we have that the integral on the right-hand side of Eq. (D3) is a product of Bessel functions of order zero, and hence we obtain explicitly

$$\frac{\partial\gamma_{00}(r,r')}{\partial E}=J_0(\sqrt{2E}r)J_0(\sqrt{2E}r'). \tag{D4}$$

Performing the energy integration, and using the physical boundary condition that $\partial\gamma_{00}/\partial E\to 0$ as $E\to 0$, we find the $m=0$ component of the Dirac density matrix for the free-electron gas in 2D as

$$\gamma_{00}(r,r',E)=\frac{\sqrt{2E}}{(r'^2-r^2)}[r'J_0(\sqrt{2E}r)J_1(\sqrt{2E}r')-rJ_0(\sqrt{2E}r')J_1(\sqrt{2E}r)]. \tag{D5}$$

Taking the limit of Eq. (D5) as $r'\to r$ yields

$$\gamma_{00}(r,r,E)=E[J_0^2(\sqrt{2E}r)+J_1^2(\sqrt{2E}r)]. \tag{D6}$$

This result (D6) is plotted in Fig. 4 as a function of r for two different values of the energy E.

1. Coulomb analogue

For the continuous spectrum of the hydrogen-like atom with $V(r)=-Z/r$ in two dimensions, the radial wave function corresponding to $m=0$ is

$$R_0(kr) = C_{k0} \exp(-ikr)\,{}_1F_1(iZ/k + 1/2, 1, i2kr), \tag{D7}$$

where ${}_1F_1$ denotes the confluent hypergeometric function, and hence, apart from a multiplying factor which can depend on energy and Z, we can write the analog of Eq. (D4) in the limit $r \to r'$ as

$$\left.\frac{\partial \gamma_{m=0}(r,r',Z)}{\partial E}\right|_{r'=r} = \left|{}_1F_1(iZ/k + 1/2, 1, i2kr)\right|^2 : k = \sqrt{2E}. \tag{D8}$$

Allowing $Z \to 0$ in Eq. (D8), we can make use of the identity (Ref. 20, Eq. 9.215.3)

$${}_1F_1(b + 1/2, 2p + 1, i2z) = \Gamma(p+1)\left(\frac{Z}{2}\right)^{-p} \exp(iz) J_p(z), \tag{D9}$$

for the case $p=0$ to verify that, apart from a factor already referred to, Eq. (D8) correctly leads back to the free-electron result (D4) in the limit $Z \to 0$ and $r'=r$.

The force-force correlation function formula can then be written explicitly as a quadrature involving $(\partial V(r_1)/\partial \mathbf{r}_1)\cdot(\partial V(r_2)/\partial \mathbf{r}_2)$ multiplied by $(\partial \gamma_{m=0}/\partial E)^2 = R_0(kr_1)R_0(kr_2)$, the analog if the higher terms for $m \neq 0$ in Eq. (D2) are assumed small for the Coulomb case. However, the detail proliferates and we shall therefore not give it.

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