Parametric Approach to Surface Screening of a Weak External Electric Field

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We have studied the problem of the penetration of a uniform external electric field at the surface of a metal or degenerate semiconductor within the random-phase approximation. In its most general form, this problem involves the solution of a complex integrodifferential equation. This problem has been studied most recently by Newns using Fourier analysis and numerical inversion of an infinite-dimensional response matrix. We have found that using a parametric representation of the potential, $V(x) = V_0(1-\alpha)^{-1}\ (e^{-\lambda x} - \alpha e^{-2\lambda x})$, in the integral equation led to simple transcendental equations for determining the parameters. The potential which resulted was tested for full self-consistency by using it as a source for a single iteration of the full integral equation. A comparison between the first iteration and results obtained by Newns (for the case $r_s = 2$) showed that they agreed within a few percent.

I. INTRODUCTION

There has been increasing interest during the last few years in studying electron screening at the surface of a metal or a degenerate semiconductor.[1-13] Perhaps the most detailed treatment of electric field penetration into a degenerate electron gas is due to Newns.[14] Newns studied this problem within the random-phase approximation (RPA). By working within a finite slab and using Fourier-analysis techniques, he was able to reduce the problem to the inversion of a large matrix. This he performed numerically to obtain the potential and charge density. The purpose of this paper is to present a rather simple parametric solution to the electric-field-penetration problem within the RPA which approximates the exact solution obtained by Newns within a few percent (for the case of a free-electron metal with $r_s = 2$). In addition, the problem will be formulated in the presence of an external magnetic field perpendicular to the surface of a degenerate electron gas. In such form, it provides the derivation of results which we have used elsewhere with the promise that the derivation would soon be made available.[15]

II. FORMULATION

We consider the problem of a degenerate Fermi gas in the presence of external electric and magnetic fields perpendicular to the surface of the electron gas. We wish to study the electric field penetration within the RPA.

To this end we need to solve Poisson's equation

$$-\frac{d^2V(x)}{dx^2} = \frac{K_0}{\pi}\rho(x), \tag{2.1a}$$

$$\frac{dV(x)}{dx} = F, \tag{2.1b}$$

where $V(x)$ is the electrostatic potential energy as a function of x, the distance into the electron gas measured from the surface, and F is the electric force present at the surface of the Fermi gas. We have expressed energies in units of $\hbar^2/2m$ and charge densities, such as $\rho(x)$, as number densities: This results in a unit of inverse length,

$$K_0 = 8\pi m e^2/\hbar^2\epsilon\ , \tag{2.2}$$

where ϵ is the background dielectric constant (relevant to degenerate semiconductors, where m should then be viewed as the effective mass m^*). $\rho(x)$ is the induced electron charge density, given by

$$\rho(x) = \int R(x, x')V(x')\,dx'. \tag{2.3}$$

$R(x, x')$ is the charge-density response kernel, which, within the RPA and in the presence of a magnetic field H, takes the form

$$R(x, x') = 2\sum_{i,j}\frac{f(\omega(j)) - f(\omega(j))}{\omega(i) - \omega(j) - i\delta} \times \psi_i^*(\vec{\mathbf{r}}')\psi_j(\vec{\mathbf{r}}')\psi_j^*(\vec{\mathbf{r}})\psi_i(\vec{\mathbf{r}}), \tag{2.4}$$

where $f(x)$ is the Fermi-Dirac distribution function, φ_i is the wave function for an electron with energy $\omega(i)$,

$$\psi_i(\vec{\mathbf{r}}) = (L_z)^{-1/2}\, e^{ik_z^i z}\,\varphi_i(y - y_0^i)\ (2/L_x)^{1/2}\sin\nu k_x^i, \tag{2.5}$$

$$\omega(i) = (i + \tfrac{1}{2})E_H + (k_x^i)^2, \quad y_0^i = -2k_z^i/E_H, \tag{2.6}$$

where $\varphi_i(y - y_0^i)$ is the harmonic-oscillator wave function with quantum number i. Note that we have represented the wave functions in the x direction as sine functions, corresponding to the assumption of an infinite potential step at the vacuum–electron-gas interface. E_H is the magnetic energy associated with the Landau levels.

The sum over all but one of the transverse quantum numbers is easily performed in (2.4), and one finds

$$R(x, x') = \frac{1}{\pi^2}E_H L_y L_z \sum_n \int_0^\infty\int dk'\,dk\,\frac{f(\omega_k^n) - f(\omega_{k'}^n)}{\omega_k^n - \omega_{k'}^n - i\delta}$$

$$\times \sin kx \sin k'x \sin kx' \sin k'x', \qquad (2.7)$$

where

$$\omega_k^n = E_H(n+\tfrac{1}{2}) + k^2 . \qquad (2.8)$$

Combining (2.7), (2.3), and (2.1), one sees that the solution of Poisson's equation actually involves solving a complex integrodifferential equation:

$$-\frac{d^2V(x)}{dx^2} = \frac{K_0}{\pi}\int_\infty^\infty R(x,x')V(x')\,dx' . \qquad (2.9)$$

To obtain an approximate solution to (2.9), we assume that we can represent $V(x')$ near the surface, in the region where it is largest, by a simple parametric form: The form we have found most convenient is a sum of exponentials:

$$V_{\exp}(x) = -[V_0/(1-\alpha)](e^{-\lambda x} - \alpha e^{-2\lambda x}). \qquad (2.10)$$

This three-parameter representation for $V(x)$ is inserted into the right-hand side of (2.9), converting it into a differential equation. This equation can be integrated straight away and the first iteration of the integrodifferential equation obtained in terms of known functions. The parameters are now determined in a self-consistent fashion by requiring that the value of the parametrized potential and the first interation agree both with respect to their value and their first derivative at the origin. These two conditions, coupled with the requirement that the electric field at the surface is fixed by the boundary condition (2.1b), constitute three equations for determining the parameters α, λ, and V_0. If the first iteration and the parametrized form of the potential agree rather well over the region where the potential is large, as we will see that they do, we will have obtained an approximate solution to the integrodifferential equation. Since the procedure outlined above is a hybrid between an iterative and self-consistent solution, we will adopt the iterative form of the potential as our solution to (2.9).

III. EXPONENTIAL RESPONSE

For the procedure adopted above to work, we need an expression for the induced charge density produced by an exponential potential of the form

$$V_0 e^{-\alpha x} . \qquad (3.1)$$

Inserting (3.1) into (2.3) and (2.7) and doing the x' integration, we find

$$\rho(x) = \frac{E_H V_0}{2\pi^2}\int_0^\infty dk \int_0^\infty dk' \,\frac{f(\omega_k^n) - f(\omega_{k'}^n)}{\omega_k^n - \omega_{k'}^n} \sin kx \sin k'x \times\left(\frac{\alpha}{\alpha^2+(k-k')^2} - \frac{\alpha}{\alpha^2+(k+k')^2}\right) . \qquad (3.2)$$

Specializing to zero temperature,

$$\rho(x) = \frac{E_H V_0}{\pi^2}\int_0^{k_n} dk \int_{k_n}^\infty dk' \,\frac{1}{k^2-k'^2} \sin kx \sin k'x \times\left(\frac{\alpha}{\alpha^2+(k-k')^2} - \frac{\alpha}{\alpha^2+(k+k')^2}\right) , \qquad (3.3)$$

where

$$k_n = [E_F - E_H(n+\tfrac{1}{2})]^{1/2} \qquad (3.4)$$

and E_F is the Fermi energy.

The next step in processing (3.3) is to rewrite

$$\sin kx \sin k'x \to \tfrac{1}{2}[\cos(k-k')x - \cos(k+k')x]$$

and to notice that the integrand is a separable function of the variables $\omega' = k + k'$ and $\omega = k - k'$. Making this change of variables, it becomes a straightforward although somewhat tedious task to show that

$$\rho(x) = \frac{E_H V_0}{\pi^2 16\alpha}\int_\infty^\infty \frac{d\omega}{\omega}\cos x\omega \left(\ln\frac{(2k_n+\omega)^2+\alpha^2}{(2k_n-\omega)^2+\alpha^2} - \frac{\omega^2}{\alpha^2+\omega^2} \times \ln\frac{(2k_n+\omega)^2}{(2k_n-\omega)^2}\right) . \qquad (3.5)$$

Examination of the integrand reveals that it is well behaved at $\omega = 0$, has integrable singularities at $\pm 2k_n$, and vanishes more rapidly at infinity than ω^{-2}. A more convenient form for $\rho(x)$ can be obtained by means of contour integration,

$$\rho(x) = \frac{E_H V_0}{16\alpha\pi^2}\,\mathrm{Re}\int_c \frac{dz}{z}\, e^{izx}\left(\ln\frac{(2k_n+z)^2+\alpha^2}{(2k_n-z)^2+\alpha^2} - \frac{z^2}{z^2+\alpha^2} \times \ln\frac{(2k_n+z)^2+\epsilon_0^2}{(2k_n-z)^2+\epsilon_0^2}\right) , \qquad (3.6)$$

where $z = \omega + i\omega_1$, and we have closed the contour in the upper-half of the complex z plane. ϵ_0 is an infinitesimal introduced to remove the branch cut of the logarithm from the real axis. If we shrink the contour c, we find that we pick up three contributions to the integral—one from the pole at $z = i\alpha$, another from the logarithmic branch cut from $z = -2k_n + i\alpha$ to $2k_n - i\alpha$, and the third from the logarithmic branch cut from $-2k_n + i\epsilon$ to $2k_n + i\epsilon$. Combining these contributions one finds

$$\rho(x) = \frac{E_H V_0}{2\pi^2}\sum_n \left(\frac{1-e^{-\alpha x}}{\alpha}\int_0^{2k_n} \frac{t\sin xt}{t^2+\alpha^2}\,dt - e^{-\alpha x} \times \int_0^{2k_n}\frac{1-\cos xt}{t^2+\alpha^2}\,dt\right). \qquad (3.7)$$

The charge density can be divided into two parts. The first is short range, decaying exponentially, while the second part is long range and oscillatory. This long-range part is just the Friedel oscillations set up by the surface potential. For small x, $\rho(x)$ behaves as x^2, which we expect since that is also the behavior of the charge density near the surface within our model. Note that the Friedel term is necessary to ensure this behavior. In the limit $\alpha \to 0$, corresponding to a slowly varying potential,

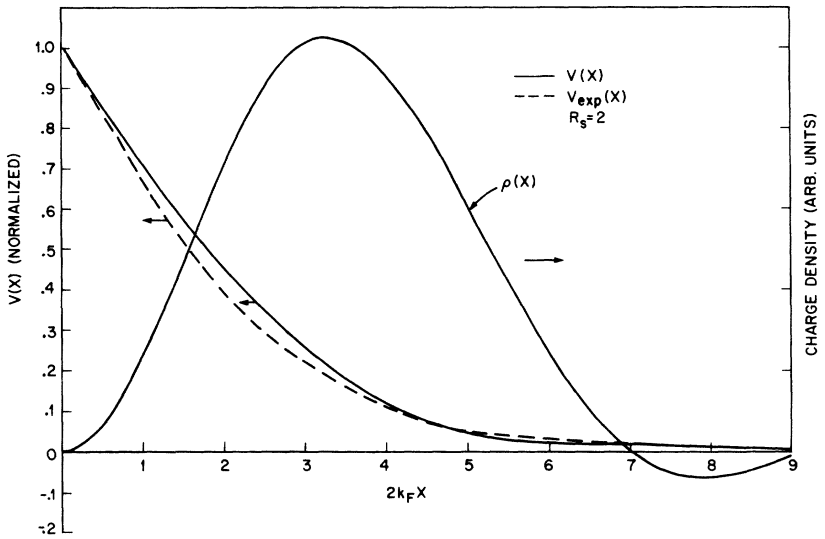

FIG. 1. Self-consistent parametric potential and its first iteration compared for $r_s=2$. The charge density $\rho(x)$ induced by the parametric potential is also plotted.

$$\rho(x) \to \frac{e^2 E_H V_0}{2\pi^2} \sum_n \frac{\sin^2 k_n x}{k_n} , \tag{3.8}$$

which is just proportional to the position-dependent density of states.

The next step is to calculate the potential which results from substituting (3.7) into (2.1). It is straightforward to do the required x integration within the integral sign. We find for the induced potential

$$V(x) = \frac{K_0 V_0 E_H}{\alpha} \sum_n \int_0^{2k_n} \frac{1}{\alpha^2+t^2} \left[\frac{\sin xt}{t} + e^{-\alpha x}\left(\frac{1}{\alpha} - \frac{(t^3-3t\alpha^2)\sin xt + (\alpha^3-3t^2\alpha)\cos tx}{(t^2+\alpha^2)^2}\right)\right] dt \tag{3.9a}$$

$$\equiv V_0 G(x,\alpha). \tag{3.9b}$$

IV. SELF-CONSISTENT EQUATIONS

We are now able to determine the self-consistent parameters V_0, α, and λ which enter the parametric potential (2.9). For the purpose of this paper we will specialize to zero magnetic field. The application of this work to finite magnetic field has been made by the authors[15] in the context of strong electric fields where it is necessary to include the contribution of bound states to the screening of the electric field. The three conditions to be required of V_{exp} are

$$F = \frac{dV_{exp}(0)}{dx} , \tag{4.1a}$$

$$F = \frac{dV(0)}{dx} , \tag{4.1b}$$

$$V_{exp}(0) = V(0) , \tag{4.1c}$$

where $V(x)$ is the potential energy that results if V_{exp} is substituted into the right-hand side of (2.9). Using (2.10), condition (4.1a) reduces to

$$F = \lambda V_0 [(1-2\alpha)/(1-\alpha)] . \tag{4.2}$$

To obtain expressions for (4.1b) and (4.1c) we need the zero-magnetic-field limit of (3.9b). It is a trivial task to show that this is obtained by replacing

$$E_H \textstyle\sum_n \int_0^{2k_n} \cdots dt \to \int_0^{2k_F} [k_F^2 - (\frac{1}{2}t)^2] \cdots dt, \tag{4.3}$$

so that (3.9) becomes

$$V(x) = \frac{K_0 V_0}{\pi\alpha} \int_0^{2k_F} \frac{k_F^2 - (\frac{1}{2}t)^2}{\alpha^2+t^2} \left[\frac{\sin xt}{t} + e^{-\alpha x}\left(\frac{1}{\alpha} - \frac{(t^3-3t\alpha^2)\sin xt + (\alpha^3-3t^2\alpha)\cos xt}{(t^2+\alpha^2)^2}\right)\right] dt . \tag{4.4}$$

Evaluating (4.4) and its derivative at $x=0$, one finds for (4.1b) and (4.1c)

$$F = \frac{K_0 V_0}{2\pi}\left[b\left(\frac{\lambda}{2k_F}\right) - \alpha b\left(\frac{\lambda}{k_F}\right)\right] \Big/ (1-\alpha) , \tag{4.5}$$

where

$$b(x) = 1/x - \tan^{-1}(1/x) , \tag{4.6}$$

and

TABLE I. Parameters λ and α as well as $[V_0(dV/dx)^{-1}]_{x=0}$ plotted vs r_s for a free-electron gas and comparison made to Newns's results for $[V_0(dV/dx)^{-1}]_{x=0}$.

r_s	$\frac{\lambda}{k_F}$	α	$\left(V_0/\frac{dV}{dx}\right)\Big\|_{x=0}^{\text{ours}}$	$\left(V_0/\frac{dV}{dx}\right)\Big\|_{x=0}^{\text{Newns}}$
2	1.25	0.355	0.98	0.95
4	1.70	0.387	1.75	1.67

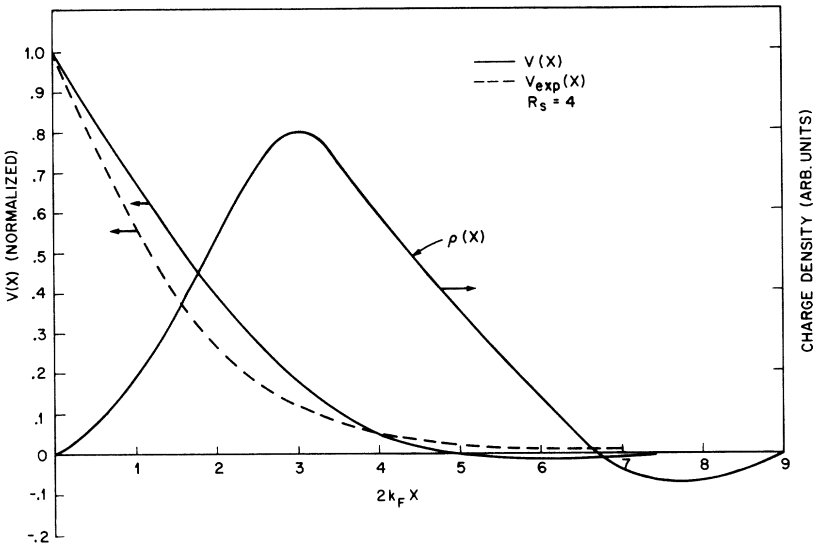

FIG. 2. Self-consistent parametric potential and its first iteration compared for r_s=4. The charge density $\rho(x)$ induced by the parametric potential is also plotted.

$$1 = \frac{K_0}{8\pi k_F}\left[a\left(\frac{\lambda}{2k_F}\right) - \alpha\, a\left(\frac{\lambda}{k_F}\right)\right] \Big/ (1-\alpha), \tag{4.7}$$

where

$$a(x) = \frac{1}{x^2(1+x^2)} + \frac{1}{x^3}\left(\frac{\pi}{2} - \tan^{-1}\frac{1}{x}\right). \tag{4.8}$$

Equations (4.2), (4.5), and (4.7) constitute the set which determines α, λ, and V_0. We can eliminate α and V_0 to obtain a single transcendental equation for $y = \lambda/2k_F$:

$$[\eta a(y) - 1]/[\eta a(2y) - 1] = [y - 2\eta b(y)]/[2y - 2\eta b(2y)], \tag{4.9}$$

where

$$\eta = K_0/8\pi k_F. \tag{4.10}$$

V. RESULTS AND DISCUSSIONS

The solution of (4.5) is trivially obtained by graphical methods. It admits two roots, one of which has $\alpha < 1$, the other $\alpha > 1$. We have studied systematically only the former. Once α, λ, and V_0 have been determined for a given k_F and K_0, we calculated $V(x)$ and $\rho(x)$ from (4.4) and the zero-field limit of (3.7).

In order to make contact with the work of Newns and assess the accuracy of the method, we have calculated $V(x)$ and $\rho(x)$ for a free-electron gas in which $r_s = 2$ and $r_s = 4$. In Table I we have listed for a given r_s the values of λ, α, and $V(0)(dV/dx)^{-1}$ and we obtained and compared it with the Newns value. The agreement is quite satisfactory. Before proceeding further with the comparison, we would like to turn to an examination of the internal consistency of our solution. It is clear that our procedure is most accurate at small values of r_s. In Figs. 1 and

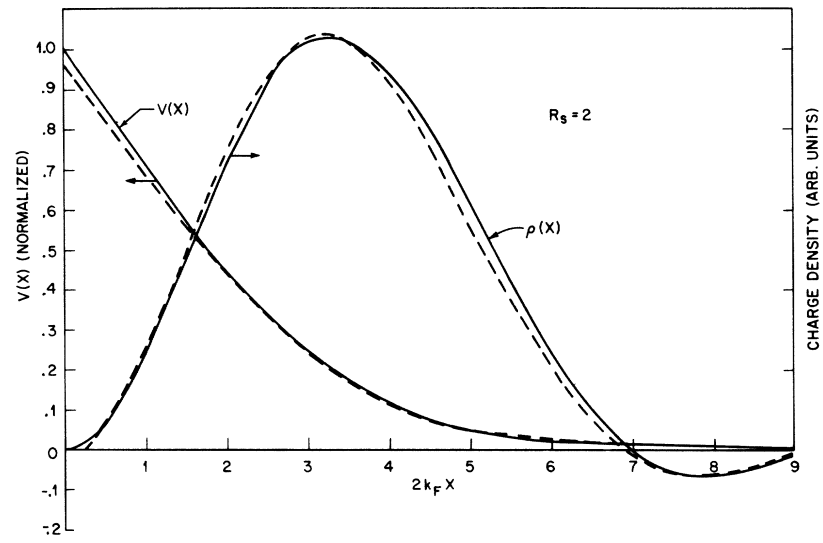

FIG. 3. Iteration potential and charge density calculated in this paper (solid line) compared with those obtained by Newns for r_s=2.

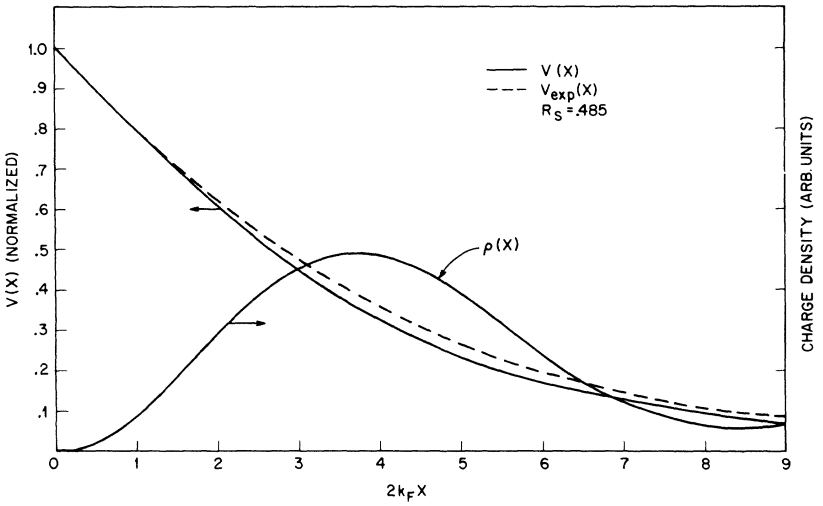

FIG. 4. Self-consistent potential and its iteration compared and the charge density plotted for $r_s = 0.485$, corresponding to the parameters relevant to InAs with $m^* = 0.02$, $\epsilon = 15$, and $k_F = 0.01$ Å^{-1}.

2 we have plotted both $V_{exp}(x)$ and $V(x)$ for $r_s = 2$ and 4, respectively. For the case $r_s = 2$, $V(x)$ and $V_{exp}(x)$ agree very well as to their general shape and magnitude, and for $r_s = 4$, the agreement is satisfactory. In Fig. 3 we have compared $V(x)$ and $\rho(x)$ with those values obtained by Newns. We believe this agreement to be excellent.

The two cases just considered correspond to electron gases at metallic densities. While the modifications of the screening at the surface compared with the Thomas-Fermi result are sizable for these cases, the modifications being greatest for large r_s, it is also true that the RPA is strictly valid only for $r_s < 1$. We have found, however, that the case of narrow-band degenerate semiconductors is an excellent example of a system where the effective r_s is much less than 1 and at the same time the deviations from bulk screening are still substantial. For example, the r_s value of InAs with an effective mass of 0.02 and a dielectric constant of 15 is 0.485 when the doping is 2×10^{16}, corresponding to a Fermi energy of 20 meV (see Fig. 4). For this example, the bulk Thomas-Fermi screening distance is approximately 200 Å, while we calculate that the comparable distance as measured by

$$V(x=0)\Big/\frac{dV}{dx}\ (x=0)$$

is 257 Å. Note also that for this case, V_{exp} and $V(x)$ are in extremely close agreement, and we expect therefore that our results for the logarithmic potential should be rather good.

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