Image potential of a two-dimensional electron gas

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The image potential of a two-dimensional electron gas (2DEG) in a heterojunction system such as AlGaAs/GaAs is calculated. It is shown that this potential has a substantially different dependence on the electron separation compared to the familiar image potential of a metal. For example, it remains finite as the distance from the surface goes to zero. This happens because of the finite spread of the wave function of two-dimensional electrons in the direction transverse to the surface. Therefore, the image-force lowering of the interface barrier is smaller than it would be near a metallic surface. It is shown that a quite accurate approximation of the image potential is $V_{\rm im}(z_0) = e^2/4\epsilon_2(|z_*| + z_0)$, where e is the electron charge, ϵ_2 is the dielectric constant on the side of the test electron location, z_0 is the electron's distance from the surface, and z_* is the average distance of the 2DEG electrons from the surface.

I. INTRODUCTION

The effect of image-force lowering of the potential barrier at a metal-semiconductor contact is well known.[1] To study the analogous lowering of the heterojunction barrier confining a two-dimensional electron gas (2DEG) (like in a AlGaAs/GaAs system) it is necessary to find the image force produced by the 2DEG. At first glance, it appears that at high electron-sheet concentrations the image force of a 2DEG should be the same as that of a metallic surface. However, as shown below, at small distances from the surface the two effects are quite different. The reason for this is connected with the fact that two-dimensional electrons are on average separated from the surface by a nonvanishing distance z_*. As a result the potential energy of the attraction of the test electron to the induced charge stays finite even when the electron separation from the surface, z_0, goes to zero. Therefore the energy of the test electron, $V_{\rm im}(z_0)$, in the field of the image force can be written in the form

$$V_{\rm im}(z_0) = -\frac{e^2}{4\epsilon_2(|z_*| + |z_0|)} , \qquad (1.1)$$

where ϵ_2 is the dielectric constant on the side of the test electron's location and e is the electron charge.

II. JOINT POTENTIAL OF THE TEST ELECTRON AND THE TWO-DIMENSIONAL GAS

The potential induced by an electron removed from the 2DEG surface by a distance $z_0(z_0 < 0)$, is defined by Poisson's equation

$$\nabla^2 \phi(\mathbf{r},z) + 2S |\zeta(z)|^2 \hat{\phi}(\mathbf{r}) = 0, \quad z > 0 \qquad (2.1a)$$

$$\nabla^2 \phi(\mathbf{r},z) = +(4\pi e/\epsilon_2)\delta(z - z_0)\delta(\mathbf{r}), \quad z < 0 , \qquad (2.1b)$$

where $\mathbf{r}$ is a two-dimensional vector in the plane of the 2DEG, z is the coordinate perpendicular to the plane ($z=0$ corresponds to the heterointerface), ϵ_1 is the dielectric constant on the side of the 2DEG ($z > 0$), $\zeta(z)$ is the

normalized envelope wave function of the lowest subband (we will assume that only this level is occupied),

$$\hat{\phi}(\mathbf{r}) = \int_0^\infty \phi(\mathbf{r},z) |\zeta(z)|^2 dz \qquad (2.2)$$

is the potential, averaged over z,

$$S = (2/R_B)/[1 + \exp(-E_F/T)] \qquad (2.3)$$

is the screening factor of the 2DEG,[2,3] E_F is the Fermi level of the 2DEG relative to the bottom of the first subband, T is the temperature in energy units, R_B is the effective Bohr radius in GaAs ($R_B = \epsilon_1 \hbar^2/m_1 e^2$), and m_1 is the electron effective mass in GaAs.

The second term in the Eq. (2.1a) is the induced charge density in the 2DEG multiplied by $4\pi/\epsilon_1$. It is written in the linear approximation in the potential ϕ. The electron density of the 2DEG is defined by the equation

$$n(\mathbf{r},z) = \frac{m_1 T}{\pi \hbar^2} \ln\{1 + \exp[(E_F - E_1)/T]\} |\zeta(z)|^2 ,$$

therefore at zero temperature, in contrast to the three-dimensional case, the induced charge $e\delta n(r,z)$ is proportional to the change in the electron energy δE_1 in the potential $\phi(r,z)$. At finite temperature the ratio of the second-order term in δE_1 to the first is $\beta = \delta E_1/2T\{1 + \exp[(E_F - E_1)/T]\}$. In the case of degeneracy ($\Delta E = E_F - E_1 > 0$) this ratio has a maximum, relative to the parameter $\Delta E/T$, at 1.27 and $\beta = \beta_{\rm max} = 0.14\Delta E_1/\Delta E$. In GaAs the value of ΔE is equal to $\pi \hbar^2 n_s/m_1 = 8$ meV at the surface concentration of the 2DEG $n_s = 2 \times 10^{11}$ cm^{-2}. The value ΔE_1 can be estimated using the image potential $\Delta E_1 = V_{\rm im}(z_0)$ [see Eq. (1.1)]. If we take $z_* = 25$ Å then for GaAs $\Delta E_1 = 10$ meV. This estimation shows that $\beta_{\rm max}$ is of the order 0.14 at the temperature $T = 8/1.27$ meV (73 K). With increasing surface concentration the parameter β decreases due to the increase of the Fermi energy. Hence, the linear approximation of the induced charge that is used in the Eq. (2.1a) is valid for all temperatures and concentrations in the practical range.

The Eq. (2.1) is subject to the boundary conditions:

$$\phi(r,z)=0 \quad \text{when } r\rightarrow\infty \text{ and } z\rightarrow\pm\infty . \tag{2.4}$$

Performing the Fourier transformation

$$\phi(\mathbf{q},z)=\int \phi(\mathbf{r},z)\exp(-i\mathbf{q}\cdot\mathbf{r})d^2\mathbf{r} , \tag{2.5}$$

we obtain

$$d^2\phi(\mathbf{q},z)/dz^2-q^2\phi(\mathbf{q},z)=-2S\,|\,\zeta(z)\,|^2\widehat{\phi}(\mathbf{q}), \quad z>0 \tag{2.6a}$$

$$d^2\phi(\mathbf{q},z)/dz^2-q^2\phi(\mathbf{q},z)=(4\pi e/\epsilon_2)\delta(z-z_0), \quad z<0 , \tag{2.6b}$$

where

$$\widehat{\phi}(\mathbf{q})=\int \phi(\mathbf{q},z)\,|\,\zeta(z)\,|^2 dz=\int \widehat{\phi}(\mathbf{r})\exp(-i\mathbf{q}\cdot\mathbf{r})d^2\mathbf{r} \tag{2.7}$$

and the boundary condition becomes $\phi(\mathbf{q},z)\rightarrow0$ for $z\rightarrow\pm\infty$.

The solution of Eq. (2.6) is given by

$$\phi(\mathbf{q},z)=A_1\exp(-qz)+\widehat{\phi}(\mathbf{q})F(z), \quad z>0 \tag{2.8a}$$

$$\phi(\mathbf{q},z)=A_2\exp(qz)-(2\pi e/q\epsilon_2)\exp(-q\,|\,z-z_0\,|\,), \quad z<0 , \tag{2.8b}$$

where

$$F(z)=-\frac{S}{q}\int_0^\infty |\,\zeta(z')\,|^2\exp(-q\,|\,z-z'\,|\,)dz', \quad z>0 . \tag{2.9}$$

Here, we used a different particular solution of Eq. (2.6a) from that chosen in Ref. 4.

The coefficients A_1 and A_2 are determined from the continuity of the electric field and the potential at the interface. They are given by

$$A_1=\frac{1}{(1+\lambda)}\left[\widehat{\phi}(\mathbf{q})\left[\frac{F'(0)}{q}-\lambda F(0)\right]\right.$$
$$\left.-\frac{4\pi e\lambda}{q\epsilon_2}\exp(-q\,|\,z_0\,|\,)\right] , \tag{2.10}$$

$$A_2=\frac{1}{(1+\lambda)}\left[\widehat{\phi}(\mathbf{q})\left[\frac{F'(0)}{q}+F(0)\right]\right.$$
$$\left.+\frac{2\pi e(1-\lambda)}{q\epsilon_2}\exp(-q\,|\,z_0\,|\,)\right] ,$$

where $\lambda=\epsilon_2/\epsilon_1$, and the prime indicates the derivative of the function $F(z)$ with respect to z.

To obtain an equation for $\widehat{\phi}(\mathbf{q})$, we multiply Eq. (2.8a) by $|\,\zeta(z)\,|^2$ and integrate it with respect to z from $z=0$ to $z=\infty$. We find

$$\widehat{\phi}(\mathbf{q})$$
$$=-\frac{4\pi e\lambda}{q\epsilon_2}\frac{\chi(q)\exp(-q\,|\,z_0\,|\,)}{[1-\widetilde{F}(q)](1+\lambda)+[\lambda F'(0)-F(0)/q]\chi(q)} , \tag{2.11}$$

where

$$\widetilde{F}(q)=\int_0^\infty F(z)\,|\,\zeta(z)\,|^2 dz , \tag{2.12}$$

$$\chi(q)=\int_0^\infty |\,\zeta(z)\,|^2\exp(-qz) . \tag{2.13}$$

III. ELECTRON POTENTIAL ENERGY

As yet, we have calculated the potential $\phi(\mathbf{r},z)$ which is the sum of the electron potential $\phi_0(\mathbf{r},z)$ and the potential of the charges induced by it in the two-dimensional gas. Only half of the latter is the image potential which is of interest to us.

According to Eq. (2.5) the potential of the system electron plus 2DEG is equal to

$$\phi(\mathbf{r},z)=\frac{1}{(2\pi)^2}\int \phi(\mathbf{q},z)\exp(i\mathbf{q}\cdot\mathbf{r})d^2\mathbf{q} . \tag{3.1}$$

The self-electron potential can be written in the form

$$\phi_0(\mathbf{r},z)=-\frac{e}{\epsilon_2[r^2+(z-z_0)^2]^{1/2}}$$
$$=-\frac{e}{\epsilon_2}\int_0^\infty J_0(qr)\exp(-q\,|\,z-z_0\,|\,)dq , \tag{3.2}$$

where $J_0(x)$ is a Bessel function of zeroth order. Thus, the potential energy $V_0(z_0)$ of an electron separated by a distance $|\,z_0\,|$ from the heterointerface can be found as the limit

$$V(z_0)=\lim_{\substack{z\rightarrow z_0 \\ r\rightarrow0}}\tfrac{1}{2}[-e\phi(r,z)+e\phi_0(r,z)] . \tag{3.3}$$

Using the representation for the Bessel function

$$J_0(x)=(1/2\pi)\int_{-\pi}^\pi \exp[ix\cos(\alpha)]d\alpha \tag{3.4}$$

and Eqs. (3.1) and (3.2) we can rewrite Eq. (3.3) in the form

$$V(z_0)=-\lim_{\substack{z\rightarrow z_0 \\ r\rightarrow0}}\int_0^\infty \frac{1}{2}\left[\frac{e}{2\pi}q\phi(q,z)+(e^2/\epsilon_2)\exp(-q\,|\,z-z_0\,|\,)\right]J_0(qr)dq , \tag{3.5}$$

where we took advantage of the fact that the function $\phi(q,z)$ depends only on the absolute value of $\mathbf{q}$.

Because $z_0<0$ in Eq. (3.5) we must use Eq. (2.8b) and the result we obtain is of the form

$$V(z_0)=-\lim_{\substack{z\rightarrow z_0 \\ r\rightarrow0}}\frac{e}{4\pi}\int_0^\infty qA_2J_0(qr)\exp(qz)dz . \tag{3.6}$$

Substituting A_2 into Eq. (3.6), we obtain

$$V(z_0) = \frac{-1}{(1+\lambda)} \left[\frac{e^2(1-\lambda)}{2\epsilon_2|z_0|} + \frac{e}{2\pi} \int_0^\infty q\hat{\phi}(q) \left[\frac{F'(0)}{q} + F(0) \right] \exp(-q|z_0|)dq \right] . \tag{3.7}$$

The first term in Eq. (3.7) is trivial. It is connected with the surface charge polarization induced at the heterointerface. If the external electron is located in a medium which has a larger dielectric constant than the medium in which the 2DEG gas is located ($\lambda > 1$) then the induced charge is negative. In the AlGaAs/GaAs system $\lambda < 1$ and therefore this effect increases the attractive force of the 2DEG. The influence of the polarization effect on the electron-electron interaction and the subband levels was studied in Ref. 5. The second term in Eq. (3.7) describes the effect of the 2DEG.

To proceed with the calculation we must choose a particular envelope wave function for the lowest subband of the 2DEG. As was shown in Ref. 6, the best analytical wave function (which gives for the energy of the first subband a value that is different from the exact numerical value by less than 2%) is given by

$$\zeta(z) = \frac{\alpha^{[(2\nu+1)/2]}}{\Gamma^{1/2}(2\nu+1)} z^\nu \exp(-\alpha z/2) , \tag{3.8}$$

where the parameters α and ν are defined by

$$\alpha = 2[2\pi(4\nu^2-1)N^*(\nu)/R_B]^{1/3} , \tag{3.9}$$

$$N^*(\nu) = N_{\text{depl}} + n_s(39+5\nu)/2^7 , \tag{3.10}$$

$$\nu = \frac{1}{4} - \delta + \left[\delta^2 + \frac{5\delta}{2} + \frac{11}{48} \right]^{1/2} , \tag{3.11}$$

$$\delta = (64N_{\text{depl}} + 39n_s/2)/15n_s .$$

n_s is the surface concentration of the 2DEG and N_{depl} is the surface concentration of the ionized impurity centers in the depletion region on the side of the 2DEG.

Using the wave function (3.8), we obtain for $F(0)$, $F'(0)$, $X(q)$, and $\tilde{F}(q)$ the following expressions:

$$F(0) = \frac{-S\alpha^{(2\nu+1)}}{q(q+\alpha)^{(2\nu+1)}}, \quad F'(0) = qF(0) ,$$

$$X(q) = \left[\frac{\alpha}{\alpha+q} \right]^{(2\nu+1)} , \tag{3.12}$$

$$\tilde{F}(q) = -\frac{8S\Gamma(2\nu+3/2)}{\pi^{1/2}q\Gamma(2\nu+2)} \left[\frac{\alpha}{\alpha+q} \right]^3$$

$$\times F(2\nu+1, -2\nu; 2\nu+2; (\alpha-q)/2\alpha) , \tag{3.13}$$

where $F(\alpha,\beta,\gamma,z)$ is the hypergeometric function. Then Eq. (3.7) becomes

$$V(z_0) = \frac{-e^2(1-\lambda)}{4\epsilon_2(1+\lambda)|z_0|}$$
$$+ \frac{eS\alpha^{(2\nu+1)}}{2\pi(1+\lambda)} \int_0^\infty \frac{\hat{\phi}(q)\exp(-q|z_0|)}{(q+\alpha)^{(2\nu+1)}}dq , \tag{3.14}$$

where

$$\hat{\phi}(q) = -\frac{4\pi e\lambda}{\epsilon_2}$$

$$\times \frac{[\alpha/(\alpha+q)]^{(2\nu+1)}\exp(-q|z_0|)}{(1+\lambda)q[1-F(q)] - S(\lambda-1)(\alpha/\alpha+q)^{(4\nu+2)}} . \tag{3.15}$$

From Eq. (3.14) we see that in the formal limit $S\to 0$, i.e., when the screening length tends to infinity the effect of the image force disappears.

In another limit corresponding to two-dimensional electrons located at the surface (i.e., to the case of the extreme localization of the wave function (3.8): ($\alpha\to\infty$), Eq. (3.14) takes the form
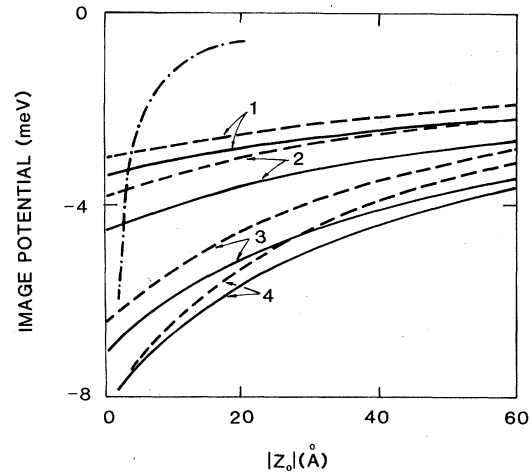

FIG. 1. Image potential as a function of the distance $|z_0|$ from the surface. Solid curves have been calculated by using Eq. (3.14) without the polarization potential V_{pol}. The dashed curves have been calculated by using Eq. (1.1). The dotted curve is the polarization image potential V_{pol}. The curves 1, 2, 3, and 4 are calculated for $n_s = 5\times10^{11}$, 10^{12}, 5×10^{12}, and 10^{13} cm^{-2}.

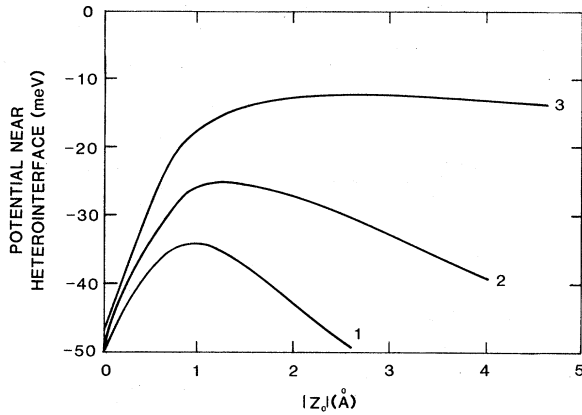FIG. 2. Shape of the potential barrier near a heterointerface: curve 1, $n_s = 10^{12}$ cm^{-2}; curve 2, $n_s = 5 \times 10^{12}$ cm^{-2}; curve 3, $n_s = 10^{13}$ cm^{-2}.
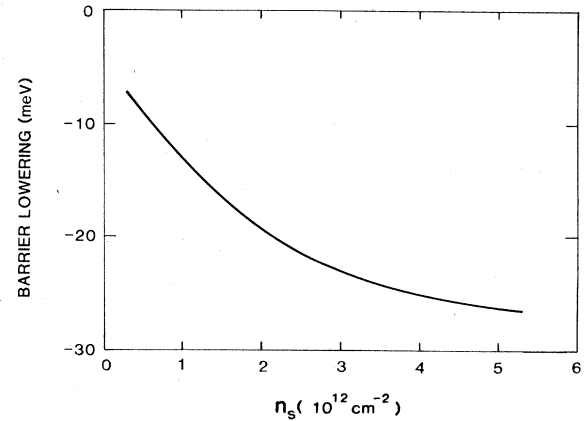

FIG. 3. Heterojunction barrier lowering as a function of the electron sheet concentration.

$$V(z_0) = -\frac{e^2(1-\lambda)}{4\epsilon_2(1+\lambda)|z_0|} - \frac{2e^2 S}{\epsilon_1(1+\lambda)} \int_0^\infty [q(1+\lambda)+2S]^{-1} \exp(-2q\,|z_0|)dq$$

$$= -\frac{e^2}{2(1+\lambda)} \left[\frac{1-\lambda}{2|z_0|} - \frac{\gamma}{\epsilon_1} \exp(\gamma\,|z_0|)Ei(-\gamma\,|z_0|) \right], \tag{3.16}$$

where $\gamma = 4S/(1+\lambda)$, and

$$Ei(-y) = -\int_y^\infty [\exp(-t)/t]dt$$

is the integral exponent function.[7] When the product $S\,|z_0|$ goes to infinity, then $V(z_0) \to e^2/(4\epsilon_2\,|z_0|\,)$, i.e., the image potential energy has the same form as it has near a metallic surface. The parameter $S\,|z_0|$ cannot be increased by increasing the 2DEG surface concentration because the screening length practically does not depend on concentration. Therefore, this inequality is fulfilled only at large distances from the surface.

To analyze effects of the 2DEG image force in real situations we have to integrate Eq. (3.14) numerically, using the expression (3.15) for $\hat{\phi}(q)$. It is useful to consider separately the polarization part of the full image potential and the proper image potential of two-dimensional electrons. We will denote them as V_{pol} and V_{im}, respectively.

Figure 1 shows the dependence of V_{im} on the distance $|z_0|$ for several values of the 2DEG concentration. The dotted line shows the dependence of the polarization potential. The parameters we used are $m_1 = .067m_0$, $\epsilon_1 = 12.85$, $\epsilon_2 = 11.93$ ($x = 0.37$ in Al$_x$Ga$_{1-x}$As), and we have assumed that $N_{depl} \ll n_s$. We see that in the limit $z_0 \to 0$, V_{im} tends to a constant value unlike the metallic image potential that approaches infinity. We can also see

that the value of V_{pol} becomes smaller than V_{im} within the distance of several angstroms. The dashed curves in Fig. 1 were plotted by using Eq. (1.1) and appropriate concentrations. The value z_* was taken equal to $(2\nu+1)/\alpha$.[6] A comparison of these curves with the solid line shows that the nonvanishing separation of the 2DEG from the surface is the main factor that influences the image potential of the 2DEG. The Eq. (1.1) is a good approximation of the detailed calculation. As can be seen, the difference with exact solution is of the order of 10%. In Fig. 2 we have plotted the full image potential plus the potential $-z_0 E(0)$ of the electric field $E(0)$ that is equal, near the heterointerface, to $4\pi e n_s/\epsilon_2$. This gives the barrier shape near a heterointerface. The lowering of the barrier is of the order of 20 meV when $n_s = 10^{12}$ cm^{-2}. The dependence of the barrier lowering on the concentration n_s is plotted in Fig. 3.

ACKNOWLEDGMENTS

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