Screening in modulation-doped quantum wells: Finite-thickness correction

A. B. Henriques
Instituto de Física, Universidade de São Paulo, 05508 São Paulo, Brazil
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The electrostatic potential of a point charge screened by quantum-confined free carriers in a semiconductor heterostructure is calculated analytically, with inclusion of a spatial extension of the screening charge along the growth axis. The resulting expression is tested by computing numerically the binding energy of excitons between $E2$ and $H1$ subbands in a one-side modulation-doped quantum well, giving values in good agreement with experiment. The finite-thickness correction is 2.1 meV for a 150-Å quantum well with a carrier density of 10^{11} cm^{-2}. It is found that the screening effect can be significantly reversed in wide wells with large carrier concentration due to the band-bending effect.

Charge screening is a fundamental issue in the theories of transport and optical properties of semiconductors, and the specifics of the screening effect is related to the dimensionality of the semiconductor system.[1-3] On account of the fact that the Thomas-Fermi screening length for a two-dimensional system is concentration independent, it is predicted that in semiconductor heterostructures and quantum wells (QW's) the screening effect is saturated at high carrier densities. Namely, if the screening carriers are described by a two-dimensional density of states, then a Coulomb center cannot be screened out at any carrier concentration, and a residual and sizable Coulomb interaction will always remain,[4-6] and this preview is supported by experimental data, which show that excitons can be detected in the presence of a high-density quantum-confined electron gas.[7-10] The bleaching of excitons observed at large carrier densities[8-10] is attributed to the phase-space filling[3] (PSF) effect. However, PSF bleaching is only effective for excitons involving filled subband states, and hence excitons between unoccupied subbands are always detected at low temperatures.[7-10] These excitons are described by a binding energy which is reduced from the undoped value on account of screening. Although the screened exciton binding energies have been estimated experimentally,[10] there is some difficulty in comparing the experimental values to the theory, since the latter is usually developed within the strictly two-dimensional limit, or else is not applicable to excitons between excited subbands, since only the electrostatic potential average over the charge distribution in the fundamental subband is available.[1,2,4,6,11] The purpose of this communication is to estimate the correction on the screening effect which follows from the finite thickness of the screening charge along the growth axis when applied to carriers in the excited electronic subbands. To achieve this goal, we consider here the $E2$-$H1$ exciton binding energy in a one-side modulation-doped $Al_xGa_{1-x}As$ quantum well and compare the results with those obtained in the two-dimensional limit and estimate the finite-thickness correction. First, the electrostatic potential of a Coulomb center is calculated in the random-phase approximation (RPA), whereby the spatial extension of the $E1$ screening charge is incorporated via standard variational wave functions. Second, the resulting potential is applied to calculate the $E2$-$H1$ exciton binding energy as a function of well width and carrier density.

Consider a semiconductor heterostructure with electrons occupying states in the fundamental $E1$ subband, and a positive elementary charge at some position z_0 in the growth axis. The electrostatic potential $\varphi(\mathbf{r})$ of the Coulomb center is described by the Poisson equation (in cylindrical coordinates and SI units here)

$$\nabla^2\varphi(\rho,z,z_0)=-(4\pi\kappa/\epsilon)[\rho_{\rm ind}(\rho,z,z_0)+e\delta(\rho)\delta(z-z_0)] , \tag{1}$$

where $\rho_{\rm ind}$ is the screening charge, induced by the positive charge, and ϵ is the dielectric constant, taken to be position independent throughout the structure. Taking advantage of the axial symmetry, it is convenient to Hankel transform[12] φ and $\rho_{\rm ind}$ to obtain

$$\frac{\partial^2\varphi(k,z,z_0)}{\partial z^2}-k^2\varphi(k,z,z_0) = -\frac{4\pi\kappa}{\epsilon}\left[\rho_{\rm ind}(k,z,z_0)+\frac{e}{2\pi}\delta(z-z_0)\right] . \tag{2}$$

If the confinement of the $E1$ electron along the growth axis is less than $\approx 2a_B$, where a_B is the bulk exciton Bohr radius calculated with the transverse exciton mass, then to a good approximation[13,4] the positive charge will not modify the electronic wave-function component in z, and in the random-phase approximation the induced charge will be given by[1,4,2]

$$\rho_{\rm ind}(k,z,z_0)=-\frac{\epsilon}{2\pi\kappa}sf(k/2k_F)\chi_{E1}^2(z)\langle\varphi(k,z_0)\rangle , \tag{3}$$

where the $E1$ subband is assumed parabolic, described by an effective mass m^*, $s=2\kappa e^2m^*/\epsilon\hbar^2$ is a screening constant,

$$\langle\varphi(k,z_0)\rangle=\int\chi_{E1}^2(z)\varphi(k,z,z_0)dz ,$$

and at $T=0$ K

$$f(k/2k_F)=\begin{cases}1, & k<2k_F\\ 1-[1-(2k_F/k)^2]^{1/2}, & k\geq 2k_F\end{cases},$$

where k_F is the Fermi wave vector. The factor $f(k/2k_F)$ accounts for the finiteness of the Fermi surface and ensures the absence of screening when the subband is empty (that is, when $k_F=0$). Equation (3) is identical to the semiclassical Thomas-Fermi approximation if the factor $f(k/2k_F)$ is substituted by unity.[1] Under condition (3) we obtain the general solution to Eq. (2):

$$\varphi(k,z,z_0)=\frac{\kappa e}{\epsilon k}\left[e^{-k|z-z_0|}-\frac{sf(k/2k_F)P(k,z_0)P(k,z)}{k+sf(k/2k_F)\langle P(k)\rangle}\right], \tag{4}$$

where $P(k,z)=\int e^{-k|z-z'|}\chi_{E1}^2(z')dz'$, and the average is taken as before.

In order to incorporate the finite thickness of the screening charge into our model, the particle density $\chi_{E1}^2(z)$ can be approximated by standard variational wave functions. For low carrier densities, when the band bending is small, a good approximation is

$$\chi_{E1}(z)=\begin{cases}(2/L)^{1/2}\cos\pi z/L, & |z|\leq L\\ 0, & |z|>L,\end{cases}$$

where parameter L is adjusted to obtain the best agreement with the Hartree wave function. For this wave function we obtain

$$P(k,z)=\begin{cases}1, & k=0\\ \frac{2\beta}{kL}\operatorname{senh}(kL/2)e^{-k|z|}, & k\neq 0,\ |z|\leq L/2\\ \frac{2\beta}{kL}[1+2(kL/2\pi)^2\cos^2\pi z/L-e^{-kL/2}\cosh(kz)], & k\neq 0,\ |z|>L/2\end{cases}$$

and

$$\langle P(k)\rangle=\begin{cases}1, & k=0\\ (3-\beta)/kL-2(\beta/kL)^2(1-e^{-kL}), & k\neq 0,\end{cases}$$

where $\beta=[1+(kL/2\pi)^2]^{-1}$. For higher carrier densities, when the band bending is significant, the modified Fang-Howard wave function can be used (Ref. 2, pp. 166 and 186):

$$\chi_{E1}(z)=\begin{cases}Nz_b\exp(k_bz/2), & z\leq 0\\ N(z+z_b)\exp(-bz/2), & z>0,\end{cases}$$

where $z_b=2/(b+k_bm_w/m_b)$, $N=(b^3/2)^{1/2}[1+bz_b+\frac{1}{2}b^2z_b^2(1+b/k_b)]^{-1/2}$, $k_b=2(2m_bV_b)^{1/2}/\hbar$, m_w and m_b are the electron effective mass in the well and in the barrier, respectively, and $V_b=1.247\times 0.65x$ eV is the conduction-band discontinuity at the $Al_xGa_{1-x}As/GaAs$ interface. In order to obtain the best agreement with the Hartree wave function, parameters b and x were adjusted. For the modified Fang-Howard wave function the result is

$$P(k,z)=N^2e^{k_bz}\left[\frac{z_b^2}{2k_b}(1-2k_bz)+\frac{c(b+k_b)}{(b+k_b)^3}\right],\quad z<0,\ k=k_b,$$

$$P(k,z)=N^2\left[\left[\frac{z_b^2}{k_b-k}+\frac{c(b+k)}{(b+k)^3}\right]e^{kz}-\frac{2kz_b^2}{(k_b-k)(k_b+k)}e^{k_bz}\right],\quad z<0,\ k\neq k_b,$$

$$P(k,z)=N^2e^{-bz}\left[\frac{z_b^2}{k_b+b}+\frac{4b^3z^3+6b^2z^2(2bz_b+1)+3(2bz+1)(2b^2z_b^2+2bz_b+1)}{12b^3}\right],\quad z\geq 0,\ k=b,$$

$$P(k,z)=N^2\left[\left[\frac{z_b^2}{k_b+k}+\frac{c(b-k)}{(b-k)^3}\right]e^{-kz}-\frac{2[a_2(z_b+z)^2+a_1(z_b+z)+a_0]}{(b-k)^3}e^{-bz}\right],\quad z\geq 0,\ k\neq b,$$

and

$$\langle P(k)\rangle=N^4\left[\frac{z_b^4}{k_b(k_b+k)}+\frac{2z_b^2c(b+k)}{(b+k)^3(k_b+k)}+\frac{z_b^4}{b(b+k)}+\frac{2(2b+k)z_b^3}{b^2(b+k)^2}+\frac{(8b^2+9bk+3k^2)(2b^2z_b^2+2bz_b+1)}{2b^5(b+k)^3}\right],$$

where $a_0=2k(3b^2+k^2)/(b+k)^3$, $a_1=4bk(b-k)/(b+k)^2$, $a_2=k(b-k)^2/(b+k)$, and $c(x)=x^2z_b^2+2xz_b+2$.

Given the screened electrostatic potential $\varphi(k,z,z_0)$, we can compute the binding energy of an exciton between excited subbands (say, subbands $E2$ and $H1$) by finding the fundamental eigenvalue E of the equation[14,15]

$$\left[\frac{-\hbar^2}{2\mu\rho}\frac{\partial}{\partial\rho}\left[\rho\frac{\partial}{\partial\rho}\right]+V(\rho)-E\right]\phi(\rho)=0, \tag{5}$$

where

$$V(\rho) = -e \int k\, dk\, J_0(k\rho)\varphi(k,z,z_0)\chi_{E2}^2(z)\chi_{H1}^2(z_0)dz\, dz_0 \tag{6}$$

and μ is the in-plane exciton reduced mass.

Now the calculation procedure can be described. Wave functions $\chi_{E1}(z)$, $\chi_{E2}(z)$, and $\chi_{H1}(z)$ were obtained in the Hartree approximation as described in Ref. 15. Limiting ourselves to the Hartree approximation means that the exchange-correlation correction to the subband particle densities[1] has not been included in our model, however, for n-type quantum wells in the electric quantum limit this correction is small and will not significantly alter the Hartree result (Ref. 2, p. 165). Wave function $\chi_{E1}(z)$ was then approximated by a best-fit analytical expression to give the electrostatic potential (4), and $\chi_{E2}(z)$ and $\chi_{H1}(z)$ were used to calculate integral (6) by Gaussian quadratures,[16] and finally the $E2$-$H1$ exciton binding energy was calculated by a numerical solution[15] to (5). In the calculations, we consider a one-side modulation doped GaAs-$Al_xGa_{1-x}As$ QW with $Al_{0.3}Ga_{0.7}As$ barriers, the dielectric constant was taken to be 12.6, the electron mass $(0.07+0.08x)m_0$, the in-plane $H1$ hole mass $0.25m_0$,[17,15] and the $H1$ mass along the z direction $(0.38+0.1x)m_0$, where $x=0$ in the well and $x=0.3$ in the barriers. The conduction-band offset was taken to be $0.65\,\Delta E_G$, where $\Delta E_G = 1.247x$ eV.

Figure 1 shows the exciton binding energy as a function of carrier density obtained in the Thomas Fermi approximation, in the two-dimensional limit [that is, by taking $\chi_{E1}^2 = \delta(z)$ at the inverted interface] and finally the result of (4). For larger carrier densities than shown, the $E2$ subband starts to be populated, and the PSF mechanism of exciton bleaching would have to be included. It can be seen from Fig. 1 that the finite thickness of the screening charge enhances the screening effect, and this is expected since the larger the well, the closer we are to the bulk situation, where we know that the binding energy vanishes at large carrier concentration. The finite-thickness correction is quite substantial at any significant doping level [for instance, 2.1 meV (2.3 meV) at a carrier density of 10^{11} cm^{-2} for $L_z = 150$ Å ($L_z = 200$ Å)]. Moreover we can see that for a one-side modulation-doped QW, there is a critical carrier density (around 10^{11} cm^{-2}), above which the screening strength undergoes a turning point. The latter effect is a consequence of the spatial separation of the $E1$ electron and the $E2$-$H1$ exciton due to the band bending [as can be seen from (3), the screening charge density decreases when the $H1$ hole moves away from the $E1$ electron]. This effect should be more pronounced in wider wells, where the spatial separation is stronger. In Fig. 1(b) the $E2$-$H1$ binding energy for a 200-Å well, which can be considered as an upper limit for the reliability of the approximations used here, is shown. For the largest carrier density allowed by the electric quantum limit, the $E2$-$H1$ binding energy obtained is around 2.0 meV (3.5 meV in the two-dimensional limit), which compares to the experimental value of 1.6±0.2 meV for a QW of the same parameters.[10]

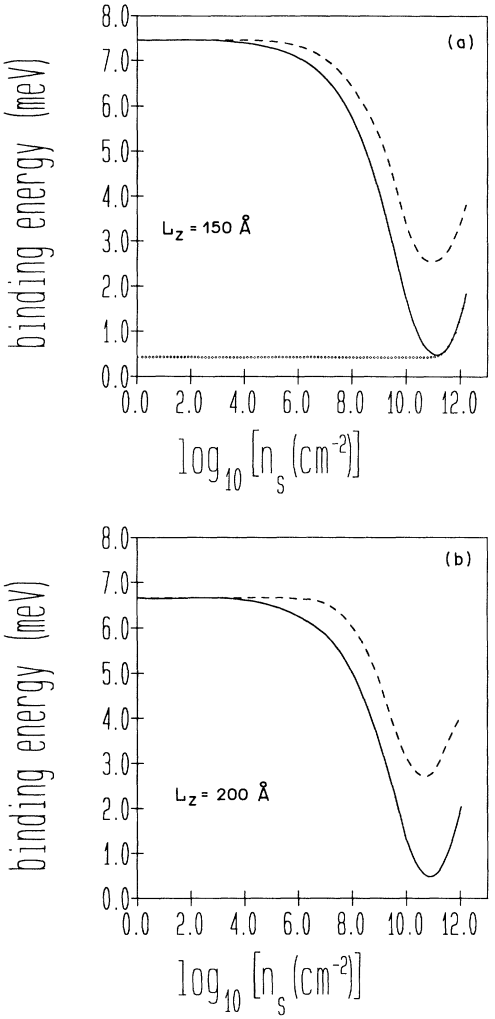

FIG. 1. Binding energy for $E2$-$H1$ excitons in a one-side modulation-doped QW (a) $L_z = 150$ Å, (b) $L_z = 200$ Å. Dotted line is the Thomas-Fermi result; dashed line is the RPA result in the two-dimensional limit; solid line is the RPA result with account of finite thickness of the screening charge.

In conclusion, we have shown that the finite-thickness correction on the screening effect is significant, and this correction was calculated for the $E2$-$H1$ exciton binding energy for a one-side modulation-doped QW. On increasing the carrier density in the $E1$ subband, the screening effect can be significantly reversed due to band bending and spatial separation of the screening charge and the exciton.

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