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LETTER TO THE EDITOR

The effect of the image potential on the binding energy of hydrogenic impurities in semiconductor quantum wells

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Abstract. We report the results of a variational calculation of the binding energy of shallow donors in quantum wells along with the effects of the image potential.

In the past few years a great deal of interest has been shown in the properties of hydrogenic impurities in semiconductor microstructures. This interest is due to the fact that studies of shallow impurity states yield considerable information about the properties of the host semiconductor microstructure. The energy levels associated with such shallow states are found near the sub-band edges. The Coulomb binding energy has been the focus of most of the theoretical work. The discontinuities of both the conduction- and valence-band edges at the heterointerfaces build potential wells for electrons and holes in those layers which have been filled by the smaller-gap semiconductor. The motion of carriers in the direction perpendicular to the layer plane is confined, while the motion in the layer plane is free. This leads to the quantization of the carrier energy. The first calculation of the shallow-donor binding energy in a single quantum well was performed by Bastard (1981) assuming an infinitely deep potential well. Mailhiot *et al* (1982) and Green and Bajaj (1983) have presented results for the binding energies of the ground and several excited states as a function of the thickness of the quantum well. The complex structure of the valence band in the case of shallow acceptors was taken into account by Masselink *et al* (1983). Brum *et al* (1985) and Wenming Liu and Min Cai (1989) have reported theoretical results on the electric field dependence of the impurity binding energy in quantum well structures. The effect of spatially dependent screening was studied by Csavinszky and Elabsy (1985), Oliveira and Falicov (1986), Brum *et al* (1984) and Oliveira (1988). Experimentally, the first observation of impurity-related features in optical spectra was researched by Miller *et al* (1982). Recently various experimental measurements of the properties of hydrogenic impurities have been reported by Shanabrook (1987).

In this paper we show a variational calculation within the effective-mass approximation of the binding energy of shallow donors in quantum wells along with the effects of the image potential. The image effects arise due to the different polarizabilities of the different semiconductors forming the semiconductor microstructure.

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In the framework of the effective-mass approximation, the Hamiltonian of a hydrogenic donor in the quantum well is given by

$$H = -\frac{\hbar^2}{2m_e}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2}{\partial \varphi^2}\right] - \frac{\hbar^2}{2m_e}\frac{\partial^2}{\partial z_e^2} + V_e(z_e) + V^c(r; z_e, z_D) \tag{1}$$

where m_e is the effective mass of the conduction electron around the impurity. The position of this electron is designated by $\boldsymbol{x}_e$ and the donor position by $\boldsymbol{x}_D$, and (r, φ) are the relative coordinates in the x–y plane. $V_e(z_e)$ is the confining potential for the electron in the conduction band and $V^c(r; z_e, z_D)$ is the electron–donor interaction potential in the quantum well. The quantum well considered here is realized as a double heterostructure (DHS) consisting of a smaller-gap semiconductor ($\nu = 1$) for $a > z > 0$ (for instance GaAs) which is symmetrically embedded between a wider-gap semiconductor ($\nu = 2$) for $z > a$ and $0 > z$ (for instance $Ga_{1-x}Al_xAs$).

The trial wavefunction used in the variational calculation of the binding energy is

$$\psi(\boldsymbol{x}_e, \boldsymbol{x}_D) = \sum_K \varphi_K^e(z_e) g_K(\boldsymbol{x}_e, \boldsymbol{x}_D). \tag{2}$$

Here we assume that the Hamiltonian H is dominated by V_e. Hence we use the assumption of the strong-confinement limit. For simplicity we use $g_K(\boldsymbol{x}_e, \boldsymbol{x}_D) = g(r, \varphi)$. Separability in r, φ and z_e of $\psi(\boldsymbol{x}_e, \boldsymbol{x}_D)$ has been shown to give accurate results for GaAs–$Ga_{1-x}Al_xAs$ quantum wells with thicknesses in the range from about 3 to 30 nm (Brum and Bastard 1985). The function $\varphi_K^e(z_e)$ is the envelope wavefunction of electrons defined by the single-particle equation

$$\left(-\frac{\hbar^2}{2m_e}\frac{d^2}{dz_e^2} + V_e(z_e)\right)\varphi_K^e(z_e) = \mathscr{E}_K^e \varphi_K^e(z_e). \tag{3}$$

For the numerical calculations we are interested in the simplest model potential in which the quantum well has infinite barriers. Within this simple square-well potential the envelope wavefunction is given by

$$\varphi_K^e(z_e) = \sqrt{\frac{2}{a}}\sin\left(\frac{\pi(K+1)}{a} z_e\right) \tag{4}$$

and the sub-band energies by

$$\mathscr{E}_K^e = (\hbar^2\pi^2/2m_e a)(K+1)^2 \qquad K = 0, 1, 2, 3, \ldots. \tag{5}$$

Using equations (2), (3) and (4) in the Schrödinger equation of the hydrogenic donor one obtains

$$\left\{-\frac{\hbar^2}{2m_e}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2}{\partial \varphi^2}\right] + V_K^c(r; z_D)\right\} g(r, \varphi) = \mathscr{E}^K g(r, \varphi). \tag{6}$$

Here the matrix element of the electron–donor interaction is given by

$$V_K^c(r; z_D) = \int dz_e\, (\varphi_K^e(z_e))^2 V^c(r; z_e, z_D). \tag{7}$$

We minimize the expectation value $E^K(\lambda) = \langle g|H|g\rangle/\langle g|g\rangle$ using equation (3) and obtain, by this variational procedure, the binding energy $E_B^K = -\mathrm{Min}\, E^K \omega$ which is the rigorous upper bound for the true binding energy.

For $g(r, \varphi)$ we use the 1s-like function

$$g_{1s}(r) = N\,e^{-(\lambda/a_0^*)r} \tag{8}$$

with λ the variational parameter and N a normalization constant. $a_0^* = 4\pi\varepsilon_0\varepsilon_{s1}\hbar^2/m_e e^2$ is the effective bulk Bohr radius of the electron ($a_0^* = 10.29$ nm for GaAs) with ε_{s1} the static dielectric constant of material 1.

With respect to the bulk case, the electron–donor interaction is modified by image effects arising from the different polarization of the different semiconductors in the layered system. To calculate the electron–donor interaction potential we solve first Poisson's equation together with the boundary conditions of the electrostatics and in a second step we calculate the electrostatic energy for an electron–donor pair at the positions $\boldsymbol{x}_e$ and $\boldsymbol{x}_D$. This interaction potential is given by

$$V^c(r; z_e, z_D) = \frac{1}{2\pi}\int_0^\infty dq_\parallel\, q_\parallel [J_0(q_\parallel r)(V^{DIR}(q_\parallel; z_e, z_D) + V^{SIM}(q_\parallel; z_e, z_D)) + V^{SIM}(q_\parallel; z_e) + V^{SIM}(q_\parallel; z_D)] \tag{9}$$

with $q_\parallel = |\boldsymbol{q}_\parallel|$ being the absolute value of the wavevector $\boldsymbol{q}_\parallel$ in the x–y plane and $J_0(q_\parallel r)$ the Bessel function of the first kind. The matrix elements $V_K^c(r; z_D)$ of the interaction potential (9) are calculated according to equation (7). We write the matrix elements in the form

$$V_K^c(q_\parallel; z_D) = -(e^2/2\varepsilon_0\varepsilon_{s1}q_\parallel) f_K(q_\parallel; z_D) \tag{10}$$

with the form factor

$$f_K(q_\parallel; z_D) = \int dz_e\,(\varphi_K^e(z_e))^2 f(q_\parallel; z_e, z_D). \tag{11}$$

The contributions to the form factor $f(q_\parallel; z_e, z_D)$ are (Wendler *et al* 1990)

$$f^{DIR}(q_\parallel; z_e, z_D) = e^{-q_\parallel|z_e - z_D|} \tag{12}$$

$$f^{MIM}(q_\parallel; z_e, z_D) = \varepsilon_{s12}\frac{e^{-q_\parallel(a-z_e)} + \varepsilon_{s12}\,e^{-q_\parallel(a+z_e)}}{e^{q_\parallel a} - \varepsilon_{s12}^2\,e^{-q_\parallel a}}\,e^{q_\parallel z_D} + \varepsilon_{s12}\frac{e^{q_\parallel(a-z_e)} + \varepsilon_{s12}^2\,e^{-q_\parallel(a-z_e)}}{e^{q_\parallel a} - \varepsilon_{s12}^2\,e^{-q_\parallel a}}\,e^{-q_\parallel z_D} \tag{13}$$

$$f^{SIM}(q_\parallel; z_e) = \frac{\varepsilon_{s12}}{2(e^{q_\parallel a} - \varepsilon_{s12}^2\,e^{-q_\parallel a})}(e^{-q_\parallel(a-2z_e)} + e^{q_\parallel(a-2z_e)} + 2\varepsilon_{s12}\,e^{-q_\parallel a}) \tag{14}$$

$$f^{SIM}(q_\parallel; z_D) = \frac{\varepsilon_{s12}}{2(e^{q_\parallel a} - \varepsilon_{s12}^2\,e^{-q_\parallel a})}(e^{-q_\parallel(a-2z_D)} + e^{q_\parallel(a-2z_D)} + 2\varepsilon_{s12}\,e^{-q_\parallel a}) \tag{15}$$

with

$$\varepsilon_{s12} = (\varepsilon_{s1} - \varepsilon_{s2})/(\varepsilon_{s1} + \varepsilon_{s2}). \tag{16}$$

The potentials include two parts: the direct Coulomb part (equation (12)) and the image parts (equations (13)–(15)). The image contribution for the interaction potential consists of the mutual image potential among two charged particles and their image charges; and the self-image potentials of two particles due to their image charges.

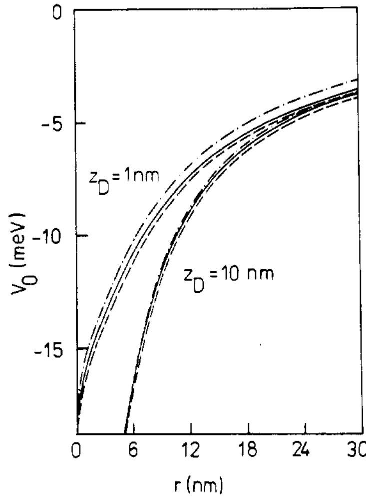

Figure 1. Electron–donor interaction potential for a GaAs–$Ga_{1-x}Al_xAs$ DHS without any image contribution (full curve); without the self-image contribution (broken curve); and with all image contributions (chain curve) for a = 20 nm and r = 1 nm.

We note that the self-image potentials are neglected in the work of Keldysh (1979). According to their physical origin, the self-image potentials do not depend on the difference r between the electron and the donor in the x–y plane.

For large thicknesses of the quantum well ($a \to \infty$) both image contributions vanish as in the case $\varepsilon_{s2} \to \varepsilon_{s1}$. But for large distances r the direct and the mutual-image parts go to zero. The form factor $f_K(q_\parallel; z_D)$ for $K = 0$ is given by

$$f_0^{\mathrm{DIR}}(q_\parallel; z_D) = \frac{1}{q_\parallel a}(2 - \mathrm{e}^{-q_\parallel(a-z_D)} - \mathrm{e}^{-q_\parallel z_D}) + \frac{(q_\parallel a)}{(q_\parallel a)^2 + (2\pi)^2}(\mathrm{e}^{-q_\parallel z_D} + \mathrm{e}^{-q_\parallel(a-z_D)}) - \frac{2q_\parallel a}{(q_\parallel a)^2 + (2\pi)^2}\cos\left(\frac{2\pi}{a}z_D\right) \tag{17}$$

$$f_0^{\mathrm{MIM}}(q_\parallel; z_D) = \frac{\varepsilon_{s12}}{1 - \varepsilon_{s12}^2\,\mathrm{e}^{-2q_\parallel a}}\left[\left(\mathrm{e}^{-q_\parallel(a-z_D)} + \varepsilon_{s12}\,\mathrm{e}^{-q_\parallel(a+z_D)} + \mathrm{e}^{-q_\parallel z_D} + \varepsilon_{s12}\,\mathrm{e}^{-q_\parallel(2a-z_D)}\right)\left(\frac{1}{q_\parallel a}(1 - \mathrm{e}^{-q_\parallel a}) + \frac{q_\parallel a\,(\mathrm{e}^{-q_\parallel a} - 1)}{(q_\parallel a)^2 + (2\pi)^2}\right)\right] \tag{18}$$

$$f_0^{\mathrm{SIM}}(q_\parallel; z_D) = \frac{\varepsilon_{s12}}{(1 - \varepsilon_{s12}^2\,\mathrm{e}^{-2q_\parallel a})2}\left[(1 - \mathrm{e}^{-2q_\parallel a})\left(\frac{1}{q_\parallel a} - \frac{q_\parallel a}{(q_\parallel a)^2 + \pi^2}\right) + \mathrm{e}^{-2q_\parallel(a-z_D)} + \mathrm{e}^{-2q_\parallel z_D} + 4\varepsilon_{s12}\,\mathrm{e}^{-2q_\parallel a}\right]. \tag{19}$$

In figure 1 the potential V_0^c is plotted against r for a GaAs–$Ga_{0.75}Al_{0.25}As$ quantum well with 20 nm thickness ($\varepsilon_{s1} = 12.87$ and $\varepsilon_{s2} = 12.21$) for two different positions z_D of the donor. It is seen that the attraction of the electron is stronger for a position of the donor in the centre of the quantum well ($z_D = 10$ nm) than if the donor is in the near vicinity of the heterointerface ($z_D = 1$ nm or equivalently, because of the symmetry, $z_D = 19$ nm). Further, it is to be seen that the effects of the image parts are more pronounced if the donor is in the near vicinity of the heterointerfaces. This is apparent because in this case more field lines are localized in the medium $\nu = 2$.

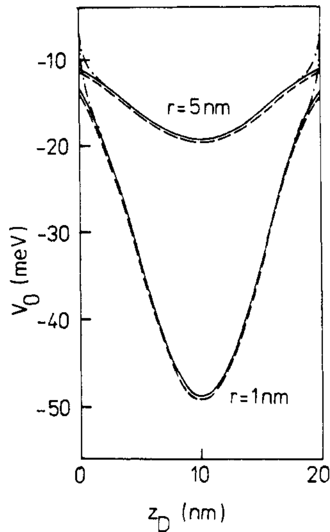

Figure 2. Electron–donor interaction potential for a $GaAs–Ga_{1-x}Al_xAs$ DHS without any image contribution (full curve); without the self-image contribution (broken curve); and with all image contributions (chain curve) for two different distances r between the electron and the donor in the $x–y$ plane.

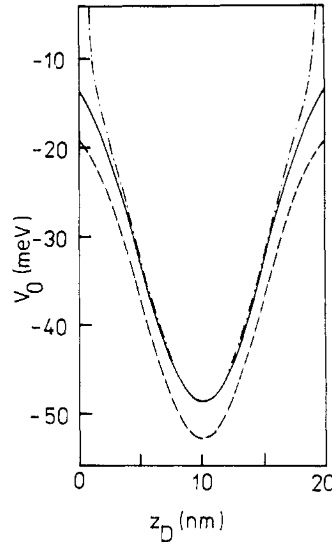

Figure 3. Electron–donor interaction potential for a DHS with $\varepsilon_{s1}/\varepsilon_{s2} = 1.81$ without any image contribution (full curve); without the self-image contribution (broken curve); and with all image contributions (chain curve) for $a = 20$ nm and $r = 1$ nm.

In figures 2 and 3 we present the calculated potentials against the donor position z_D in the quantum well. As expected, we find that the absolute value of the potential decreases if the donor is placed outside the centre of the quantum well. This is more pronounced for smaller distances r between the electron and donor. It is to be seen from figure 2 that for small distances r the influence of the image effects increases more if the donor is localized near the heterointerface than if it is at larger distances. We can conclude that for the system $GaAs–Ga_{0.75}Al_{0.25}As$ ($\varepsilon_{s1}/\varepsilon_{s2} = 1.05$) the influence of the image effects is very small in magnitude.

In figure 3 we have plotted the potential against the donor position z_D for a system with $\varepsilon_{s1}/\varepsilon_{s2} = 1.81$ (for instance Si–CaF_2: $\varepsilon_{s1} = 12.0$ and $\varepsilon_{s2} = 6.63$). It is to be seen that in this case the image contribution cannot be neglected. Further, the mutual and the self-image parts are of the same order.

In the figures 4 and 5 we have plotted the binding energy of the hydrogenic donor against the donor positon z_D within the quantum well. For GaAs the effective Rydberg constant is $\text{Ryd}^* = \hbar^2/2m_e a_0^{*2} = 5.43$ meV. From consideration of figure 4 it is seen that the binding energies with all image contributions and without them are nearly the same. Hence the two image parts, the mutual and the self-image part, have equal magnitudes but different signs. Therefore, the inclusion of the self-image term is important and cannot be neglected as done by Keldysh (1979). This is also true for the case of $\varepsilon_{s1}/\varepsilon_{s2} = 1.81$ (figure 5). Here the differences are more pronounced as in the case $\varepsilon_{s1}/\varepsilon_{s2} = 1.05$. Hence these contributions become important, especially if the donor is at a position near the heterointerface.

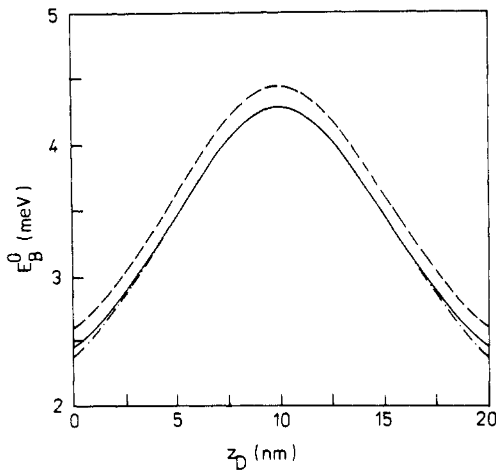

Figure 4. Binding energy of a donor within a GaAs–$Ga_{1-x}Al_xAs$ DHS without any image contribution (full curve); without the self-image contribution (broken curve); and with all image contributions (chain curve) for $a = 20$ nm.

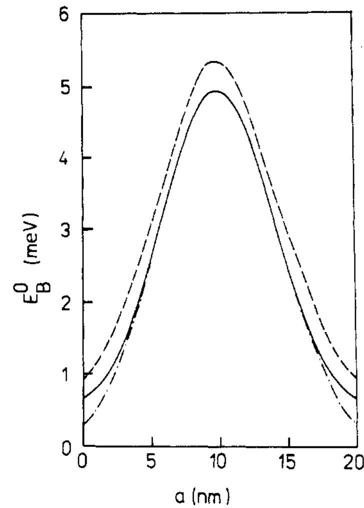

Figure 5. Binding energy of a donor within a DHS with $\varepsilon_{s1}/\varepsilon_{s2} = 1.81$ (we use for simplicity the same electron mass as in figure 4) without any image contribution (full curve); without the self-image contribution (broken curve); and with all image contributions (chain curve) for $a = 20$ nm.

In conclusion we note that the image potential effects on the hydrogenic donor binding energy are weak, especially for the system GaAs–$Ga_{1-x}Al_xAs$ and for donor positions in the centre of the quantum well. But our calculations show that the inclusion of only the mutual image potential can give wrong results, especially for systems with larger differences in the background dielectric constants.

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