Binding energies of hydrogenic impurities in finite-quantum-well structures with effective-mass mismatch: Simple and accurate variational treatments

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Simple two- and three-dimensional (2D and 3D) effective-mass approximations are applied to the calculation of the energy levels due to hydrogenic impurities in finite-quantum-well structures. For two materials with identical effective masses the 2D and 3D treatments both give results of accuracy comparable to that of more sophisticated numerical calculations. In the case of effective-mass mismatch, however, only the 2D treatment can satisfy the correct boundary conditions, which leads to the introduction of an equivalent parallel effective mass. The method is shown to be accurate and can be extended to the determination of all levels derived from different subbands.

I. INTRODUCTION

Recent advances in crystal-growth techniques have allowed numerous experimental[1–3] and theoretical[4–12] studies of one-dimensional periodic structures such as superlattices (SL's) and quantum wells (QW's). Calculations of the shallow hydrogenic impurity levels have been performed,[4–8] and they give evidence of the finite potential-barrier influence[5–7] which first appeared in Ref. 12. Here, we establish the first very simple model that can accurately treat a mismatch in effective masses.

We first treat the case of a SL made of two materials having the same effective masses, using the three- (3D) and two-dimensional (2D) (more adapted to the 2D feature of QW's) effective-mass approximations (EMA). The donor center position varies from the center to the edge of the well. We also give a simple analytical formula that describes the asymptotic behavior of very narrow or large QW's.

In Sec. III we apply the above-mentioned models to more realistic cases (where the two materials present different electronic effective masses m_1^* and m_2^*). We point out that only the 2D EMA model can treat this problem in order to satisfy the required boundary conditions. This model imposes to consider an equivalent effective mass derived from the SL band structure (we give its expression as a function of m_1^*, m_2^*, L, and V_0—the latter two denoting well width and depth, respectively). We show that for moderately narrow wells the influence of the effective-mass mismatch cannot be neglected (for $m_1^*=0.067$ and $m_2^*=0.1$, the relative change in binding energy is $+30\%$ with respect to the case $m_1^*=m_2^*=0.067$). Our single-parameter variational approach gives results comparable with those obtained by much more sophisticated calculations.[5] We also give the analytical asymptotical behavior for weak or large L.

II. SUPERLATTICES MADE OF TWO MATERIALS WITH THE SAME EFFECTIVE MASS

Here, we will neglect tunneling effects between the equivalent wells of the SL and thus study a finite quantum well where $V(z)=V_0$ if $|z|>L/2$, and $V=0$ otherwise. Let us first rapidly recall the simple model first proposed by Bastard[4] for infinite quantum wells. For shallow levels belonging to a single band of the host materials, the single-impurity problem can be described by the Hamiltonian

$$H=\frac{p^2}{2m}+V(z)-\frac{e^2}{\kappa[\rho^2+(z-z_i)^2]^{1/2}}\ , \tag{1}$$

where ρ is the distance from the impurity in the plane parallel to the layers, z_i is the impurity's position in the perpendicular direction, and κ is the relative dielectric constant of the medium (assumed to be identical in both layers).

The energy levels are obtained by a variational treatment, with the trial wave function

$$\psi=N\exp\left[-\frac{1}{\lambda}[\rho^2+(z-z_i)^2]^{1/2}\right]\psi_0(z)\ , \tag{2}$$

where $\psi_0(z)$ is the z-dependent eigenfunction of the Hamiltonian corresponding to the system without any impurity. Here, we apply this treatment to the case of finite wells. Figures 1(a) and 2 show the variations of binding energy with L, the well width, for different well depths, for an on-center and on-edge impurity, respectively. The results for a central impurity are equivalent to those recently obtained by Chaudhuri.[7]

In a previous work[8,9] we derived a 2D EMA for infinite quantum wells. Let us briefly recall this formalism,

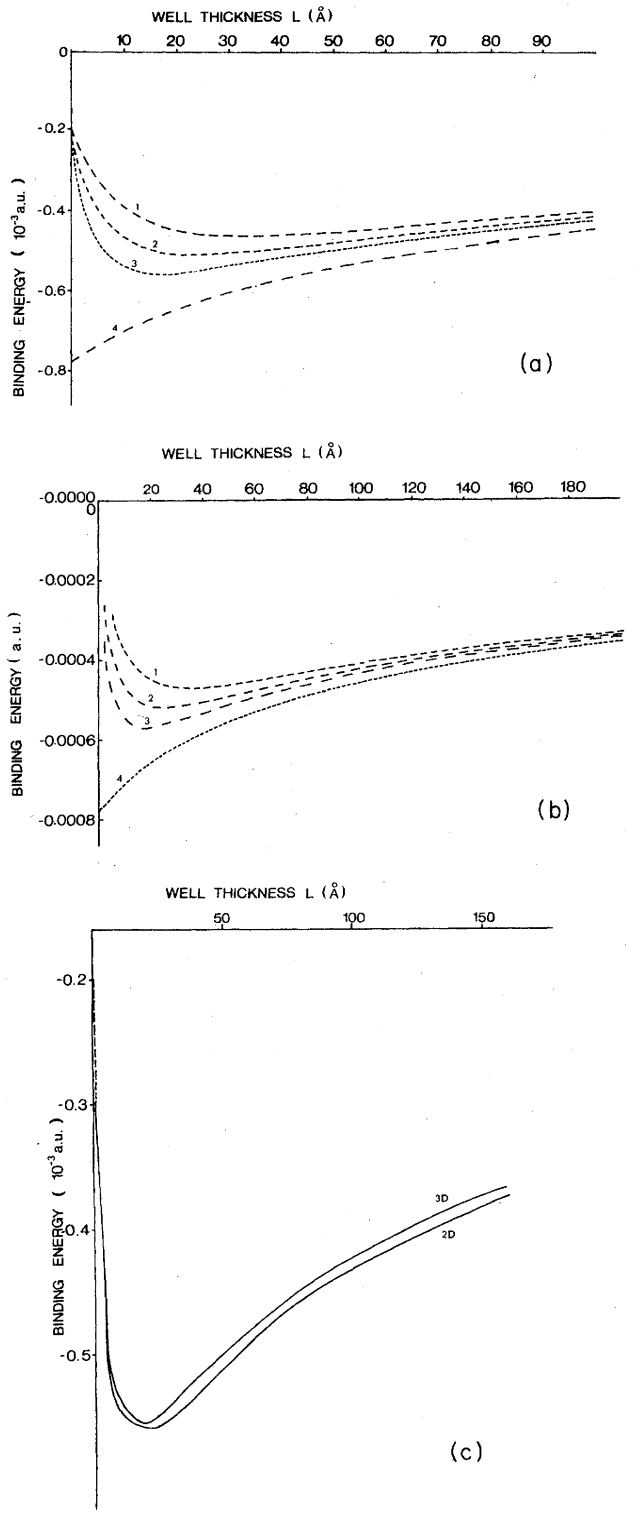

FIG. 1. Energy of the donor ground state with respect to the first conduction subband, as a function of the slab thickness, for different barrier potentials. Impurity at the center of the well; $\kappa=13.1$, $m^*=0.067$. 1 a.u. = 27.2 eV. (a) 3D EMA, $V_0=106$ meV (curve 1), 265 meV (curve 2), 424 meV (curve 3), and infinite (curve 4). (b) 2D EMA, $V_0=212$ meV (curve 1), 424 meV (curve 2), 848 meV (curve 3), and infinite (curve 4). (c) Comparison between the 3D and the 2D EMA and asymptotic behavior (dashed line) for very small L and $V_0=424$ meV.

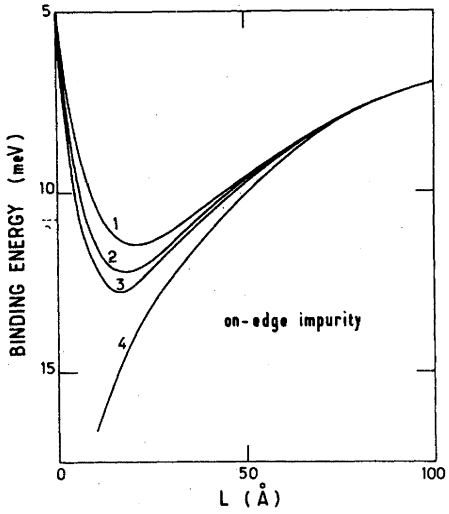

FIG. 2. 3D EMA binding energy for the donor ground state as a function of the GaAs layer thickness for an impurity on edge; $m^*=0.067$, $\kappa=13.1$, $V_0=212$ meV (curve 1), 318 meV (curve 2), 424 meV (curve 3), and infinite (curve 4).

which we extend here to the case of a finite QW.

In the absence of impurity, the energy dispersion curves can be grouped into two-dimensional subbands, due to quantification in the z direction. We can thus write the impurity states derived from a 2D subband as

$$|\psi\rangle=\sum_{\vec{k}_{||}} a_{\vec{k}_{||}} |\psi_{\vec{k}_{||}}\rangle , \tag{3}$$

where $|\psi_{\vec{k}_{||}}\rangle$ are the Bloch states of parallel wave vector $\vec{k}_{||}$ relative to this subband. We can then derive the 2D effective-mass equation,

$$\left[\epsilon(\vec{k}^{\,0}_{||})-E-\frac{\hbar^2}{2m^*_{||}}\Delta_{||}+U(r_{||})\right]F(\vec{r}_{||})=0 . \tag{4}$$

$\epsilon(\vec{k}^{\,0}_{||})$ is the bottom of the subband considered, and $m^*_{||}$ is obtained from the band structure in the absence of impurity by

$$\frac{2}{m^*_{||}}=\frac{2}{\hbar^2}\frac{\partial^2\epsilon}{\partial k^2_{||}}\bigg|_{k^0_{||}} . \tag{5}$$

$U(\vec{r}_{||})$, the effective impurity potential, is an average of $V(\vec{r}_{||},z)$ over z, defined as

$$U(\vec{r}_{||})=\int_{-\infty}^{+\infty} C(z)V(\vec{r}_{||},z)dz , \tag{6}$$

$$C(z)=\int |\psi_{\vec{k}^{\,0}_{||}}(\vec{r}_{||},z)|^2 d^2r_{||} . \tag{7}$$

With a trial function $F(\vec{r}_{||})=Ne^{-\alpha r_{||}}$, the lowest impurity-state binding energy below the lowest subband is obtained by minimization of the variational energy $E(\alpha)$,

$$E(\alpha)=\epsilon(k^0_{||})+E_B(\alpha) , \tag{8}$$

$$E_B(\alpha)=\frac{h^2\alpha^2}{2m^*_{||}}-\frac{8\alpha^2e^2}{\kappa}\int_0^\infty f^2(z)F(z)dz , \tag{9}$$

where $F(z)$ is given by

$$F(z)=\frac{z\pi}{2}[H_1(2\alpha z)-N_1(2\alpha z)]-z\ , \tag{10}$$

where H_1 and N_1 are Struve and Neuman functions of the order 1, and $f(z)$ is the subband eigenstate at $k_{||}^0$. In Fig. 1(b) we have reported, for different well depths, the variations of binding energy with the well width. Figure 1(c) allows the comparison between 2D and 3D EMA. The 2D EMA is slightly better over the usual range of L values. It becomes poorer for large L when the impurity eigenstate is close to the bulk one. This is also the case for very small L. In both limits we can obtain a very simple analytical approximation by using a trial function $\exp(-\alpha r)$ (which is exact for $L=0$ and $L=\infty$). Then, the impurity energy level is equal to

$$E(\alpha)=\frac{\hbar^2\alpha^2}{2m^*}-\frac{e^2\alpha}{\kappa}+V_0e^{-\alpha L}\left[1+\frac{\alpha L}{2}\right]. \tag{11}$$

In Fig. 1(c) the results given by this expression are identical to those of the 3D calculation for thin layers with $L<10$ Å. In the large-L limit it becomes valid for quite thick layers (more than 1000 Å). For moderately narrow layers, the 2D EMA is slightly superior to the 3D EMA. The interest in the 2D EMA will become obvious in the case of an effective-mass mismatch (inside and outside the well).

III. SUPERLATTICES WITH AN EFFECTIVE-MASS MISMATCH

In this case, Eq. (9), derived from the 2D EMA, remains valid as long as one uses $m_{||}^*$ and $f(z)$ derived from the new system without impurity. This means that we have to describe the new subband structure. If the levels we study are not too far from the conduction-band bottom, we can approximate the system Hamiltonian inside the QW by

$$H_1=\frac{p^2}{2m_1^*} \tag{12}$$

and the one outside the QW by

$$H_2=\frac{p^2}{2m_2^*}+V_0\ , \tag{13}$$

where m_1 and m_2 are the bulk effective masses of GaAs ($0.067m_0$) and $Ga_{1-x}Al_xAs$ [$0.1m_0$ for $x=0.4$ (Ref. 6)], respectively. The perfect-system wave function can still be factorized under the form $f(z)\exp(i\vec{k}_{||}\cdot\vec{r}_{||})$. The problem thus reduces to a Schrödinger equation for $f(z)$ whose even solutions are of the form

$$\begin{aligned} &f(z)=C\cos(kz) \ \text{ if } |z|<L/2\ , \\ &f(z)=C'\exp(-\lambda z) \ \text{ if } z>L/2\ , \\ &f(-z)=f(z)\ , \end{aligned} \tag{14}$$

with

$$k^2=\frac{2m_1^*}{\hbar^2}E-\vec{k}_{||}^{\,2}\ ,\quad \lambda^2=\frac{2m_2^*}{\hbar^2}(V_0-E)+\vec{k}_{||}^{\,2}\ , \tag{15}$$

where the values of k and λ can be obtained by writing the continuity equations at $z=L/2$. Here we have to write the continuity of the wave function f and of the current density, i.e., of the quantity $(1/m^*)(df/dz)$.[13] Once k and λ are known through

$$\frac{k}{m_1^*}\tan\left[k\frac{L}{2}\right]=\frac{\lambda}{m_2^*}\ , \tag{16}$$

it is a simple matter to evaluate

$$\left.\frac{\partial^2E}{\partial k_{||}^2}\right|_{k_{||}^0}$$

via (15) and (16). Then, using (5), we obtain the equivalent effective mass $m_{||}^*$, given by

$$\frac{1}{m_{||}^*}=\frac{1}{m_1^*}\left[1+\frac{m_1^*}{m_2^*}\left[\frac{m_1^*}{m_2^*}-1\right]\cos^2(k_0L/2)\frac{1}{1+(m_1^*/m_2^*-1)\cos^2(k_0L/2)+(k_0L/2)\tan(k_0L/2)}\right], \tag{17}$$

with k_0 being given from (15) and (16) with $k_{||}=0$.

The behavior of $m_{||}^*$ as a function of the layer thickness is represented in Fig. 3. We can now apply Eq. (9) and obtain the binding energies given in Fig. 4. We must notice that our 2D approach has allowed the reduction of a system of two materials with different effective masses to a much simpler one corresponding to one material with one single equivalent effective mass.

It is important to note that a 3D approach, with a trial function as given in Eq. (2), could not satisfy the current-continuity condition and thus is not adapted to the treatment of effective-mass mismatch. Thus we have derived a very simple method, suited to the treatment of impurities in quantum-well structures with effective-mass mismatch and adapted to the determination not only of the ground state but also of all excited states (note that $m_{||}^*$ will depend on the subband). The accuracy of this 2D EMA treatment can be judged by consideration of Fig. 5,

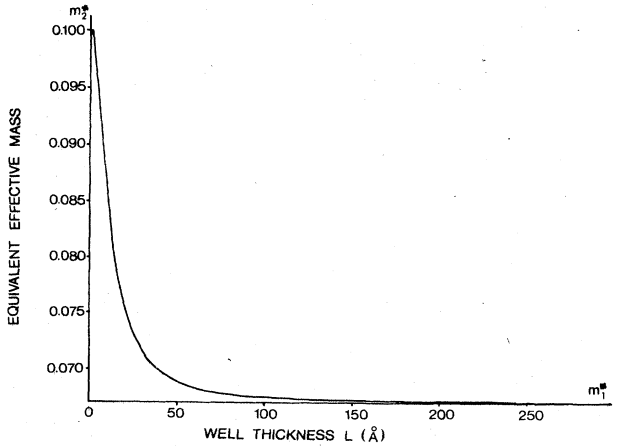

FIG. 3. Variations of the equivalent parallel effective mass with the well width ($m_1^*=0.067$ inside the well and $m_2^*=0.1$ outside the well) ($V_0=424$ meV, $\kappa=13.1$).

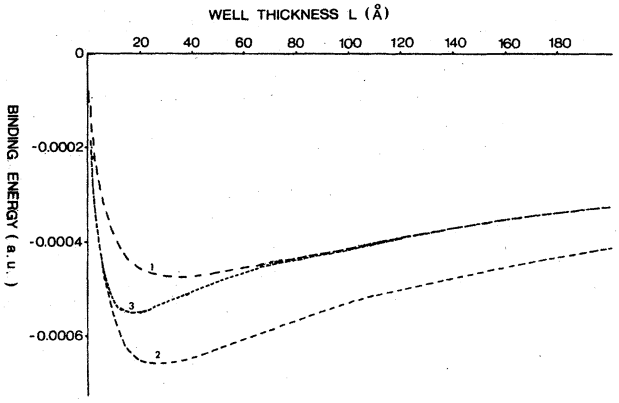

FIG. 4. Influence of the effective-mass mismatch: binding energy of the donor ground state for $m_1^*=m_2^*=0.1$ (curve 2), $m_1^*=m_2^*=0.067$ (curve 1), and $m_1^*=0.067$ and $m_2^*=0.1$ (curve 3); $V_0=0.220$ meV, $\kappa=13.1$. Impurity at the center of the well.

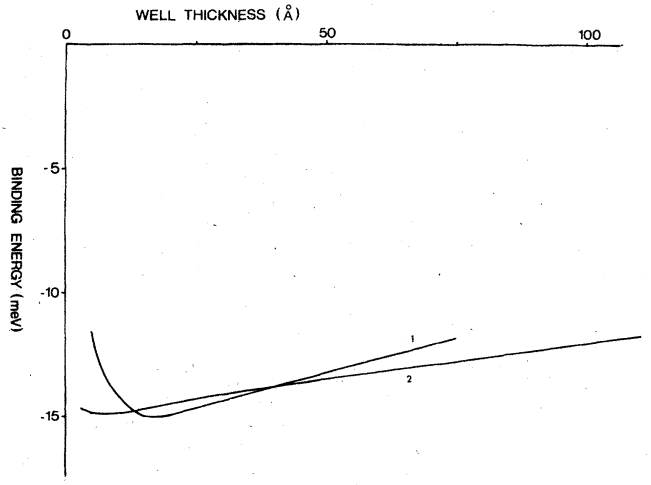

FIG. 5. Comparison between our results (curve 1) and more sophisticated calculations (Ref. 5) (curve 2) ($m_1=0.067$, $m_2=0.1$, $\kappa=13.1$, and $V_0=424$ meV) for the donor ground-state impurity at the center of the well.

where our result is compared to a much more sophisticated calculation[5] (for the binding energy of a ground state with an on-center impurity). In the range of moderately narrow (10—50 Å) superlattices we obtain a larger binding energy, showing that our variational function is quite adapted to the problem.

IV. CONCLUSION

We have presented different models that are quite simple and can accurately predict the ground-state binding energy of hydrogenic impurities in finite-quantum-well structures. Both 3D and 2D effective-mass approximations are comparable for materials with identical effective mass. In case of effective-mass mismatch only the 2D treatment can be made to satisfy the correct boundary condition, i.e., the current continuity. The binding energies are found to be comparable to those of much more sophisticated numerical treatments. Finally, an interesting aspect of the 2D model is that it can also be applied to the prediction of all excited states derived from any of the subbands.

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