Hole-bound-state calculation for semiconductor quantum wells

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A method for finding bound states in quantum systems described by coupled Schrödinger equations is discussed, and applied to the case of hole-state quantization in semiconductor quantum wells, within the axial approximation.

The conventional one-dimensional Schrödinger equation for a confining potential (quantum well) may be solved numerically for the bound-state energies and wave functions with the following method that has been widely applied due to its simplicity, obtainable accuracy, and low computer-memory requirements. Taking an asymptotically flat confining potential, for example, $\exp(\pm kz)$ type of solutions outside the well, one starts from a point $z=l$, left of the well and, recognizing the fact that a bound-state wave function may include only the decaying-to-left solution $\exp(k_l z), k_l>0$, numerically integrates the Schrödinger equation with initial conditions $\psi'(l)=k_l\psi(l)$ and $\psi(l)=1$, say, with the energy E variable as a parameter. Away from the exact bound-state energies, the calculated wave function at a point $z=$r, right of the well, will be composed of both the decaying-to-right $[\exp(k_r z), k_r<0]$, and the growing-to-right, $\exp(-k_r z)$ solutions, the latter tending to vanish as energy E approaches a bound-state energy, and make the wave function satisfy $\psi'(r)-k_r\psi(r)=0$ (with $k_r<0$). By refining the energy interval where the zero crossing of this expression occurs, bound-state energies may be found with high accuracy, limited essentially by the accuracy of the numerical integration procedure. There are numerous variations of this procedure, designed to fit the particular problem, but it always reduces to a one-dimensional search for energy where the target function undergoes a zero crossing (e.g., Ref. 1).

In cases where a set of basis states is used to describe a quantum system, the corresponding set of coupled Schrödinger equations (in terms of basis-state amplitudes) has to be solved, and it is somewhat less obvious how to apply the present method, since a bound state may be composed of a number of basis states, the relative amplitudes of which are not known in advance at any point.

This type of problem emerges in finding hole-bound states in semiconductor quantum wells, where two (or more) coupled equations have to be solved. As far as we know, the method under discussion has not been applied to this system. A finite-difference-scheme-based method, usable for arbitrary potentials $U(z)$, has been discussed in Ref. 2. Energies and wave functions are found by diagonalization of the matrix emerging from the finite-difference representation of coupled differential equations. Increasing accuracy demands obviously require finer meshes (i.e., larger matrix) and thereby increasing computer-memory requirements and computation time.[2] However, as we discuss below, the present method may be used here with equal efficiency as the conventional, single-component Schrödinger equation, and may provide very high accuracies without the excessive memory requirements typical for the matrix methods.

Within the axial approximation, the heavy- and light-hole Hamiltonian, with z chosen as the quantization axis, reads (e.g., Ref. 2)

$$\begin{bmatrix} P+Q & \tilde{R} \\ \tilde{R}^{+} & P-Q \end{bmatrix} \begin{bmatrix} F_1 \\ F_2 \end{bmatrix} = (E-U) \begin{bmatrix} F_1 \\ F_2 \end{bmatrix}, \tag{1}$$

with

$$\begin{aligned} &P=\gamma_1(k_t^2+k_z^2), \quad Q=\gamma_2(k_t^2-2k_z^2), \quad \tilde{R}=|R|-i|S|, \\ &|R|=(\sqrt{3}/2)(\gamma_2+\gamma_3)k_t^2, \quad |S|=2\sqrt{3}\gamma_3 k_t k_z, \\ &k_t^2=k_x^2+k_y^2, \end{aligned} \tag{2}$$

where the factor $\hbar^2/2m_0$ is absorbed in the Luttinger parameters γ_1, γ_2, and γ_3. In the constant-potential bulk (or the asymptotic barrier regions away from the well, with $U=U_l$ or U_r), Eqs. (1) and (2) may be solved analytically for the $k_z^2(E,k_t^2)$ dependence (given, e.g., in Ref. 3). The two pairs of (generally complex-valued) solutions, k_{z1} and k_{z2} correspond to heavy-hole-like and light-hole-like states. Considering the bound states in a quantum well, none of them should be purely real (otherwise bound states cannot exist at that energy) and should describe an exponentially decaying and exponentially growing state within each pair. The state vector corresponding to a particular k_z is obtained from Eq. (1) as

$$S(k_{zi})=\begin{bmatrix} P-Q-\tilde{R}-E+U \\ P+Q-\tilde{R}^{+}-E+U \end{bmatrix} \equiv \begin{bmatrix} a(k_{zi}) \\ b(k_{zi}) \end{bmatrix} \tag{3}$$

(the form we prefer for calculating state vectors, since it never leads to an identity-zero vector for any value of E and k_t). Certainly, at exact bound-state energies only the outward decaying states exist in bulk regions surrounding

the well [denote their **k** vectors as $+k_{1,2l}$ on the left and $+k_{1,2r}$ on the right, the $(-)$ sign being reserved for the outward-growing states].

Inside the well region, the system of coupled differential equations, obtained by substituting $k_z \rightarrow -id/dz$ in Eq. (1),

$$\begin{aligned}(\gamma_1-2\gamma_2)\frac{d^2F_1}{dz^2} &= [(\gamma_1+\gamma_2)k_t^2+U(z)-E]F_1 \\ &\quad +(\sqrt{3}/2)(\gamma_2+\gamma_3)k_t^2F_2 \\ &\quad -2\sqrt{3}\gamma_3 k_t\frac{dF_2}{dz}\ , \\ (\gamma_1+2\gamma_2)\frac{d^2F_2}{dz^2} &= [(\gamma_1-\gamma_2)k_t^2+U(z)-E]F_2 \\ &\quad +(\sqrt{3}/2)(\gamma_2+\gamma_3)k_t^2F_1 \\ &\quad +2\sqrt{3}\gamma_3 k_t\frac{dF_1}{dz}\ ,\end{aligned} \tag{4}$$

has to be solved (γ's are assumed here to be positionally independent). To apply the present method, we first calculate the two state vectors left from the well, corresponding to the outward-decaying solutions (k_{1l} and k_{2l}), i.e.,

$$S(k_{1,2l})=[a(k_{1,2l}),\ b(k_{1,2l})]^T\ .$$

Now, integrate the system (4) with pure k_{1l} input state, i.e., with initial conditions $F_1(l)=a(k_{1l})$, $F_2(l)=b(k_{1l})$ and, hence,

$$F_1'(l)=k_{1l}a(k_{1l}),\quad F_2'(l)=k_{1l}b(k_{1l})\ .$$

The calculated solution at $z=r$ (denoted as the state vector $S^{(1)}$) includes both the outward-decaying and outward-growing solutions. It should be decomposed in terms of state vectors of the right barrier

$$S^{(1)}= C_1^{(1)}S(k_{1r})+C_2^{(1)}S(k_{2r})+\bar{C}_1^{(1)}S(-k_{1r}) +\bar{C}_2^{(1)}S(-k_{2r})\ , \tag{5}$$

where the upper index (1) denotes that this solution stems from the pure k_{1l} input state on the left. Using the fact that the derivative of a bulk state vector is simply its amplitude times the corresponding k, the decomposition (5) is given as the solution of the linear inhomogeneous system of equations

$$\begin{bmatrix} a(k_{1r}) & a(-k_{1r}) & a(k_{2r}) & a(-k_{2r}) \\ b(k_{1r}) & b(-k_{1r}) & b(k_{2r}) & b(-k_{2r}) \\ k_{1r}a(k_{1r}) & -k_{1r}a(-k_{1r}) & k_{2r}a(k_{2r}) & -k_{2r}a(-k_{2r}) \\ k_{1r}b(k_{1r}) & -k_{1r}b(-k_{1r}) & k_{2r}b(k_{2r}) & -k_{2r}b(-k_{2r}) \end{bmatrix} \begin{bmatrix} C_1^{(1)} \\ \bar{C}_1^{(1)} \\ C_2^{(1)} \\ \bar{C}_2^{(1)} \end{bmatrix} = \begin{bmatrix} F_1(r) \\ F_2(r) \\ F_1'(r) \\ F_2'(r) \end{bmatrix} \tag{6}$$

with only the amplitudes of outward-growing states, $\bar{C}_1^{(1)}$ and $\bar{C}_2^{(1)}$ actually being of interest. The whole procedure is then repeated with initial conditions for integrating (4) corresponding to pure k_{2l} input state, i.e., $F_1(l)=a(k_{2l})$, $F_2(l)=b(k_{2l})$, $F_1'(l)=k_{2l}a(k_{2l})$, and $F_2'(l)=k_{2l}b(k_{2l})$, and the coefficients $\bar{C}_1^{(2)}$ and $\bar{C}_2^{(2)}$ finally calculated.

A particular linear combination of k_{1l} and k_{2l} input states on the left [with amplitudes $\psi(k_{1l})$ and $\psi(k_{2l})$, respectively] that makes the outward-growing states right of the well disappear, is a quantum-well eigenstate. Writing this in the transfer-matrix form

$$\begin{bmatrix} \psi(-k_{1r}) \\ \psi(-k_{2r}) \end{bmatrix} = \begin{bmatrix} \bar{C}_1^{(1)} & \bar{C}_1^{(2)} \\ \bar{C}_2^{(1)} & \bar{C}_2^{(2)} \end{bmatrix} \begin{bmatrix} \psi(k_{1l}) \\ \psi(k_{2l}) \end{bmatrix}\ , \tag{7}$$

it is obviously the zero crossing (as energy varies) of the determinant of the matrix (7) that determines hole-bound-state energies. The accuracy of finding bound states is determined by the accuracy of the numerical integration of the system (4), and may be easily controlled. With a given known bound-state energy, the correspond-

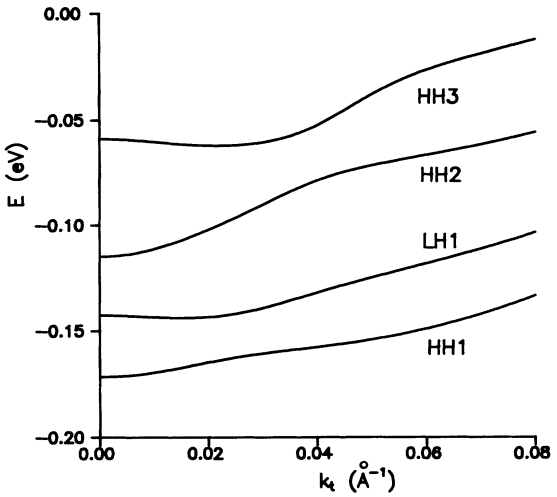

FIG. 1. The dispersion of the lowest four hole-bound states in truncated parabolic confining potential, $U(z)=-U_0[1-(2z/r-1)^2]$ for $0<z<r$, and $U(z)=0$ otherwise, with $U_0=0.2$ eV and $r=100$ Å. Numerical integration should be performed only between $z=0$ and $z=r$, since the potential is flat outside this segment. The Luttinger parameters are taken as $\gamma_1=6.85$, $\gamma_2=2.10$, and $\gamma_3=2.90$ (corresponding to GaAs), as in Ref. 4.

ing wave function is found by integrating (4) with the initial conditions at $z=l$, including both k_{1l} and k_{2l} states, with relative weights given by $\bar{C}_2^{(2)}-\bar{C}_1^{(2)}$ and $\bar{C}_2^{(1)}-\bar{C}_1^{(1)}$, respectively [i.e., by the null-space vector of the matrix (7) that becomes singular at bound-state energies].

A sample calculation of heavy- and light-hole bound-state dispersion, within the axial approximation, is given in Fig. 1.

This method may be straightforwardly generalized to more complex systems, e.g., for heavy and light holes, without the axial approximation, or with the split-off band included as well, etc. The only difference is that all (or most of) the steps discussed above would have to be performed numerically.

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