Transfer Matrices Applied to Quantum Dot Systems

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Christopher Brown

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Abstract

Quantum dots in semiconductor systems can be used to increase electron excitation in crystals by introducing intermediate bands betwen the main valence and conduction bands. Using the method of transfer matrices, we investigate how an electron interacts with a spherically symmetric potential well boundary. This result then can be generalized by creating a periodic lattice of similar potential wells.

1 Introduction

In recent years there has been a large push in the photovoltaic community to explore and incorporate quantum dots in p-n junction systems [12]. Normal p-n junction systems are formed by growing a semiconductor doped with p-material (materials that donate holes to the bulk system, or in other words accept electrons) on top of a semiconductor doped with n-material (materials that donate electrons to the bulk system). This sets up an electron donation gradient, resulting in electron/hole diffusion force

and a net electric field across the depletion zone [2]. A simple p-n junction will broaden

the valence and conduction bands within the semiconductor device by adding levels for

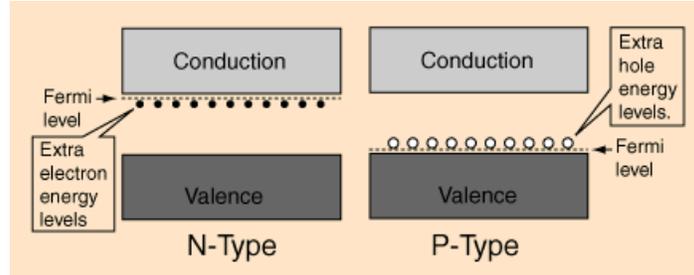holes and electrons. This can be seen in Figure 1 [5].

Figure 1: This figure shows the broadening of the valence and conduction bands due to extra states donated by the doped semiconductors. The extra hole states are donated by the p-doped semiconductor region, while the extra electrons are donated by the n-doped semiconductor region.[7]

Quantum dots (QD) are small nearly one dimensional structures within crystals

that alter the properties of the bulk crystal [8]. These QD structures can be made

by doping the semiconductor with a separate material, or by deforming the already

present semiconductor lattice to create tiny quantum wells [10] . QDs are incredibly

advantageous to use in semiconductor systems since they are quite tunable. Properties

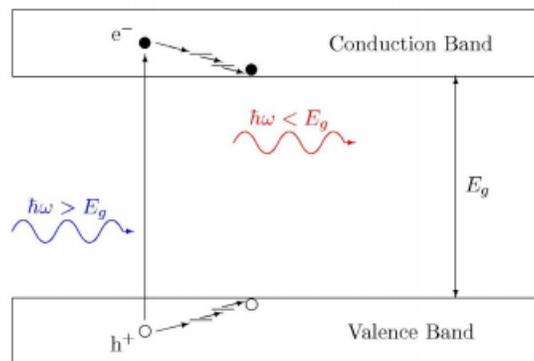of the dots highly depend on their size, and obviously upon their chemical make up.

Figure 2: This figure shows how a significantly energetic photon can excite an electron from the valence band into the conduction band. If the photon does not have the energy equivalent to the band gap energy, the electron will not excite into the conduction band.[2]

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The addition of QD systems in a semiconductor can also create intermediate bands between the main valence and conduction bands [11]. When a significantly energized photon is absorbed by a valence electron, it can jump the band gap. This is shown in Figure 2. But if the photon does not have energy equivalent or greater than that of the band gap, the electron will not be displaced out of the valence band. It is therefore beneficial to have intermediate bands between the valence band and conduction band so that less energetic photons can excite electrons out of the valence band, eventually ending up into the main conduction band [2]. Figure 3 shows how one can arrange intermediate bands much like ladder rungs up to the conduction band.
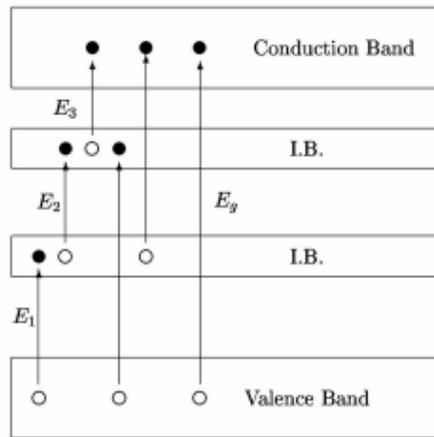

Figure 3: This figure shows how intermediate bands can be formed to facilitate excitation of electrons out of the valence band [2].

2   Theory

We begin by considering a three dimensional spherical potential well contained in another medium. This serves to simulate the quantum dot in our semiconductor. The sphere has radius a and is assumed to have a potential of zero. We also assume a three dimensional wave incident on our barrier. Because of spherical symmetry, we can reduce our problem down to only the radial component, as we assume our wavefunction can

be separated into independent variables. We look for a solution to the radial portion of the spherical Schrödinger equation,

$$[\frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2}]\psi(r) = 0 \tag{1}$$

These solutions are linear combinations of the spherical Bessel functions, j_l and n_l, but neither describe a traveling wave. For this situation we need a function in the vein of $e^{\pm ikr}$ that we used in the one dimensional problem [1]. We can look to the spherical Hankel functions, also known as Bessel functions of the third to do this job,

$$h_l^{(1)}(z) \equiv j_l(z) + in_l(z) \qquad\qquad h_l^{(2)}(z) \equiv j_l(z) - in_l(z) \tag{2}$$

If we assume, like we always do, that $\psi(r)$ is made up of linearly independent solutions, as such,

$$\psi(r) = A\phi(r) + B\chi(r) \tag{3}$$

then we can represent outgoing and incoming waves by these independent solutions, where

$$\phi(r) = h_l^{(1)}(kr) \qquad\qquad \chi(r) = h_l^{(2)}(kr) \tag{4}$$

Now we look at the spherical barrier. We must not only equate the wavefunction describing the inner part of the sphere with the wavefunction describing the outer part of the sphere at $r = a$, but we must also equate the first derivative of each wavefunction (inside and out) at the surface of the sphere.

$$\psi_{in}(a) = \psi_{out}(a) \qquad\qquad \psi'_{in}(a) = \psi'_{out}(a) \qquad (5)$$

We can construct these equalities in a convenient matrix form,

$$\begin{pmatrix} \phi_{in} & \chi_{in} \\ \phi'_{in} & \chi'_{in} \end{pmatrix} \begin{pmatrix} A_{in} \\ B_{in} \end{pmatrix} = \begin{pmatrix} \phi_{out} & \chi_{out} \\ \phi'_{out} & \chi'_{out} \end{pmatrix} \begin{pmatrix} A_{out} \\ B_{out} \end{pmatrix} \qquad (6)$$

Let us now relabel our matrices, for convenience, as such:

$$\mathbf{M}_i(a) = \begin{pmatrix} \phi_i & \chi_i \\ \phi'_i & \chi'_i \end{pmatrix} \qquad\qquad \mathbf{\Psi}_i = \begin{pmatrix} A_i \\ B_i \end{pmatrix} \qquad (7)$$

This allows us to rewrite equation (6) as

$$\mathbf{M}_{in}(a)\mathbf{\Psi}_{in} = \mathbf{M}_{out}(a)\mathbf{\Psi}_{out} \qquad (8)$$

By rearranging our matrices, we can solve for the outer coefficients, A_{out} and B_{out},

$$\mathbf{\Psi}_{out} = \mathbf{M}_{out}^{-1}(a)\mathbf{M}_{in}(a)\mathbf{\Psi}_{in} \qquad (9)$$

Now we have our transfer matrix $\mathbf{M}_{out}^{-1}(a)\mathbf{M}_{in}(a)$ which we can multiply and expand as such:

$$\mathbf{\Gamma} = \mathbf{M}_{out}^{-1}(a)\mathbf{M}_{in}(a) = \frac{1}{\phi_{out}\chi'_{out} - \phi'_{out}\chi_{out}} \begin{pmatrix} \phi_{in}\chi'_{out} - \phi'_{in}\chi_{out} & \chi_{in}\chi'_{out} - \chi'_{in}\chi_{out} \\ \phi_{out}\phi'_{in} - \phi'_{out}\phi_{in} & \phi_{out}\chi'_{in} - \phi'_{out}\chi_{in} \end{pmatrix} \qquad (10)$$

We can analytically express each term in our transfer matrix by taking the appropriate

derivatives, noting that

$$\frac{\partial}{\partial z}(h_l^{(1)}(z)) = \frac{1}{2}(h_{l-1}^{(1)}(z) - \frac{h_l^{(1)}(z) + zh_{l+1}^{(1)}(z)}{z}) \tag{11}$$

and likewise for $h_l^{(2)}$, and that with each derivative, a $\frac{1}{m^*}$ drops out, where m^* is the effective electron mass. Our transfer matrix, Γ, then can be expanded as

$$\Gamma = \frac{ia^2 k_{out}}{2m^*(2l+1)} \begin{pmatrix} n_{11} & n_{12} \\ n_{21} & n_{22} \end{pmatrix} \tag{12}$$

where the elements of the matrix are

$$n_{11} = k_{out}h_l^{(1)}(ak_{in})[lh_{l-1}^{(2)}(ak_{out})-(l+1)h_{l+1}^{(2)}(ak_{out})]-k_{in}h_l^{(2)}(ak_{out})[lh_{l-1}^{(1)}(ak_{in})-(l+1)h_{l+1}^{(1)}(ak_{in})]$$
$$\tag{13a}$$

$$n_{12} = k_{out}h_l^{(2)}(ak_{in})[lh_{l-1}^{(2)}(ak_{out})-(l+1)h_{l+1}^{(2)}(ak_{out})]-k_{in}h_l^{(2)}(ak_{out})[lh_{l-1}^{(2)}(ak_{in})-(l+1)h_{l+1}^{(2)}(ak_{in})]$$
$$\tag{13b}$$

$$n_{21} = -k_{out}h_l^{(1)}(ak_{in})[lh_{l-1}^{(1)}(ak_{out})-(l+1)h_{l+1}^{(1)}(ak_{out})]+k_{in}h_l^{(1)}(ak_{out})[lh_{l-1}^{(1)}(ak_{in})-(l+1)h_{l+1}^{(1)}(ak_{in})]$$
$$\tag{13c}$$

$$n_{22} = -k_{out}h_l^{(2)}(ak_{in})[lh_{l-1}^{(1)}(ak_{out})-(l+1)h_{l+1}^{(1)}(ak_{out})]+k_{in}h_l^{(1)}(ak_{out})[lh_{l-1}^{(2)}(ak_{in})-(l+1)h_{l+1}^{(2)}(ak_{in})]$$
$$\tag{13d}$$

While this looks extremely messy, we must keep in mind that we're looking for ground-state energy values [9]. This sets $l = 0$, which causes half of our terms in equations (13a-d) to disappear. The resulting matrix is much more manageable. Before we go through the trouble of rewritting this transfer matrix, let us touch on how we will go about finding our transmission probability. If we have a transfer matrix of a system, we can obtain the transmission amplitude, t, by setting our transmission and reflection

coefficients, A_{in}, B_{in}, etc. as such

$$\begin{pmatrix} 1 \\ r \end{pmatrix} = \Gamma \begin{pmatrix} t \\ 0 \end{pmatrix} \tag{14}$$

By doing so, we have assumed that there is only a traveling wave coming from within the sphere. There is no wave traveling from outside hitting the barrier from the other direction. Thus our inner-to-outer wave can only transmit, or reflect. This then allows us to find our transfer probability, T, by

$$T = \frac{1}{|t|^2} \tag{15}$$

where

$$t = \Gamma_{11} = n_{11} \tag{16}$$

From this probability we can begin to look at transmission energy states. This formulation will provide peaks at singular energy values. If we were to generalize this mechanism though, we could simulate a periodic lattice of these quantum dot-like well regions. Each well we add, we split the transmission peaks accordingly. Thus, if we add n wells, we'll split the energy spectrum n times, resulting in a band structure rather than a peak spectrum.

Generalizing our formulation of the transfer matrix is fairly easy due to our existing notation. If we had n boundaries (it is important to note that we must account for every boundary encountered, not just each region or well), then we would have n transfer matrices describing each boundary interaction. To obtain the resulting energy band spectrum, we can express the n interactions as

$$\begin{pmatrix} 1 \\ r \end{pmatrix} = \Gamma_1 \Gamma_2 \Gamma_3 ... \Gamma_n \begin{pmatrix} t \\ 0 \end{pmatrix} \tag{17}$$

where the indices 1,2,3,...,n, are the order of the boundaries the incoming wave encounters. In this notation it becomes quite easy to deal with multiple barriers. Doing so should make modeling the band structure of a semiconductor crystal doped with quantum dot-like wells fairly straight forward.

3 Future Work

The next step in our model is to tune the intrinsic values such that intermediate bands appear in our semiconductor system. Beyond that we would also like to introduce excitons into the model. Excitons, electrons excited from the valence band into the conduction band, also leave behind a hole in the valence band. These two particles (it is convenient to approximate the hole as a particle) are then bound by the Coulomb force. We can, in a way, treat this electron-hole system as a quasi-particle in our crystal [6]. By including this into our model, we could begin to effectively predict photocurrents from QD doped photovoltaics.

4 Conclusion

Quantum dots can be formed through many different methods, and through control over their size and composition can have many different properties. We begin a formulation of the energy states that can transmit out of the quantum dots in our system. By approximating the dots as spherically symmetric potentials and the electrons as incoming waves. Once an appropriate transfer matrix is constructed, we can generalize the system as a periodic lattice of quantum wells. This splits the transmission energy peaks into a energy band spectrum. Further work can be done to generalize and tune this model. Using this technique could help predict the structure and composition of better photovoltaic cells.

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