Closed form solution for a double quantum well using Gröbner basis

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Received 12 January 2011
Accepted for publication 13 May 2011
Published 7 June 2011
Online at stacks.iop.org/PhysScr/84/015703

Abstract
Analytical expressions for the spectrum, eigenfunctions and dipole matrix elements of a square double quantum well (DQW) are presented for a general case when the potential in different regions of the DQW has different heights and the effective masses are different. This was achieved by using a Gröbner basis algorithm that allowed us to disentangle the resulting coupled polynomials without explicitly solving the transcendental eigenvalue equation.

PACS numbers: 73.20.P, 73.20.D, 78.66, 03.65.G

1. Introduction
The square double quantum well (DQW) is often used as a toy model to demonstrate the interaction between quantized energy levels brought about by particle tunneling through a potential barrier separating individual wells [1–6]. Recently, the DQW model has attracted considerable attention in semiconductor heterostructure physics, because of its applications in nanoelectronics [7–9]. The tunneling conductance properties of semiconducting DQW devices, as well as drag effects that result from interactions between electrons moving at different velocities in different wells, were discussed recently, for example in the review articles [10, 11].

The presence of transcendental equations that describe the DQW spectrum limits the direct application of analytical methods to tackle the eigenfunction problems. Initially, the problem of finding the eigenfunctions was solved by perturbation theory, assuming that the energy level splitting due to tunneling is small [1]. The most recent analytical approach relies heavily on the symmetry properties of the DQW [6]. Of course, this restriction can be relaxed by resorting to numerical methods [2, 4, 6, 8, 12]. However, in many cases a knowledge of the analytical form of the wave function is highly desirable. For example, in the wave packet dynamics problems, the closed form solution allows one to construct a direct superposition of eigenfunctions in order to make the computational task easy. Here, we demonstrate that one can push the problem further and calculate the relevant eigenfunctions exactly by exploiting a computer-based Gröbner basis algorithm [13]. In sections 2 and 3, the spectrum and eigenfunctions of a general DQW are calculated using the Gröbner basis, and in section 4, the results are applied to find the closed form expression for the optical dipole matrix element of the DQW.

2. Spectrum
The one-dimensional (1D) DQW with flat potentials in each of regions 1–5, as shown in figure 1, is described by the following piecewise function of the coordinate $x$:

$$V(x) = \begin{cases} 
    V_c, & \text{if } x < 0, \\
    0, & \text{if } 0 \leq x \leq a, \\
    V_b, & \text{if } a < x < a+b, \\
    0, & \text{if } a+b \leq x \leq 2a+b, \\
    V_c, & \text{if } x > 2a+b,
\end{cases} \quad (2.1)$$

where $V_c$ is the confining potential (referenced from the bottom of wells) and $V_b$ is the height of the central barrier separating two identical quantum wells. The mirror symmetry of the system ensures that the quantum states of such a DQW have either even or odd parity.

Only bound states will be considered here. These states can be normalized to unity over the entire $x$-axis. The wave
Figure 1. The symmetric DQW with a central barrier of width \( b \) and height \( V_c \). The eigenenergy \( E_n \) is referenced from the bottom of the wells of width \( a \). The electron effective mass in regions 1–5 is assumed to be different.

The function \( \psi(x) \) in regions 1–5 has the following shapes:

\[
\begin{align*}
\psi_1 &= B_1 e^{x_k}, \\
\psi_2 &= A_1 \sin(kx + C_1 \cos kx), \\
\psi_3 &= B_2 e^{x_k(a-x)} + B_3 e^{-x_k(a-x)}, \\
\psi_4 &= A_2 \sin(2a + b - x) + C_2 \cos(k(2a + b - x)), \\
\psi_5 &= B_4 e^{x_k(2a+b-x)},
\end{align*}
\]  

(2.2)

where \( k \) is the free-electron wave vector, \( k = \sqrt{2m_0E/h^2} \), in quantum wells of width \( a \). The energy \( E \) is referenced from the bottom of the wells. The wave vectors of evanescent waves in the exponents are \( \chi_b = \sqrt{(2m_b/h^2)(V_b - E)} \) and \( \chi_c = \sqrt{(2m_c/h^2)(V_c - E)} \), where we have introduced different electron masses: namely, \( m_b \) inside the wells, \( m_b \) in the barrier and \( m_c \) in the confining potential. This is typical of semiconductor heterostructures, where the DQW is made of nanometer layers having different forbidden energy gaps. As a result, the electron effective mass depends on the coordinate \( x \). In equations (2.2), there are eight unknown coefficients that must be calculated. Because of symmetry, the number of coefficients, in fact, can be reduced. However, we shall not do this since the Gröbner basis algorithm will take account of symmetry properties of polynomials automatically. The standard BenDaniel–Duke boundary condition \([14]\), which takes into account the mass difference on the right (r) and left (l) sides of the potential step at the coordinates \( X = 0 \), \( X = a \), \( X = a + b \) and \( X = 2a + b \), will be used:

\[
\begin{align*}
\psi_r(X^+) &= \psi_l(X^-), \\
\frac{1}{m_r} \left. \frac{\partial \psi_r}{\partial x} \right|_{X^+} &= \frac{1}{m_l} \left. \frac{\partial \psi_l}{\partial x} \right|_{X^-}.
\end{align*}
\]  

(2.3a,b)

Equations (2.2) and the boundary conditions yield the system of eight linearly dependent equations

\[
\begin{align*}
B_1 - C_1 &= 0, \quad -A_1k/m_0 + B_1 \chi_c/m_c = 0, \quad (2.4a) \\
-A_1k/m_b + B_1 \chi_c/m_c &= 0, \quad C_1k/m_0 = 0, \quad (2.4b) \\
B_1 - B_3 e^{-bX} + A_1 \sin ak + C_1 \cos ak &= 0, \quad (2.4c) \\
B_2 \chi_b - B_2 \chi_b e^{-bX}/m_b + (A_1k \cos ak - C_1k \sin ak)/m_0 &= 0, \quad (2.4d)
\end{align*}
\]

The determinant \( D \) that follows from this system determines the spectrum of discrete energy levels of DQW. The symmetry of the problem ensures the factorization of the determinant

\[
D = m_0^4 m_c^2 m_b^2 e^{-2bV_b} D_4 D_6 = 0,
\]  

(2.5)

where \( D_4 \) and \( D_6 \) refer to symmetric and antisymmetric states, respectively,

\[
\begin{align*}
D_4 &= -km_0 [(\chi_c m_b - \chi_b m_c) + e^{bV_b}(\chi_c m_b + \chi_b m_c)] \cos ak \\
&\quad + [(k^2 m_b m_c + \chi_b \chi_c m_0^2) + e^{bV_b}(k^2 m_b m_c)] \sin ak,
\end{align*}
\]  

(2.6)

\[
D_6 = km_0 [(\chi_c m_b - \chi_b m_c) - e^{bV_b}(\chi_c m_b + \chi_b m_c)] \cos ak \\
&\quad - [(k^2 m_b m_c + \chi_b \chi_c m_0^2) - e^{bV_b}(k^2 m_b m_c)] \sin ak.
\]  

(2.7)

To advance further, the transcendental equations \( D_4(k) = 0 \) and \( D_6(k) = 0 \) that determine, in turn, the spectra of symmetric and antisymmetric discrete energy levels have to be solved explicitly. Unfortunately, these transcendental equations can only be solved by numerical methods. If DQW parameter values are known, then roots of (2.6) and (2.7) define the spectrum of all wave vectors \( k_n \), or equivalently discrete eigenenergies \( E_n = h^2 k_n^2 / 2m_0 \) of the DQW, where \( n \) is the energy level index.

In a special case when the DQW heterostructure is fabricated from two types of nanolayers (labeled \( b \) and \( 0 \), we have that \( V_c = V_b \) and \( m_c = m_0 \). Then \( \chi_c = \chi_b \), and the determinants (2.6) and (2.7) simplify to

\[
D_{h=2} = -2k \chi_b m_0 m_b e^{-bV_b} \cos ak \\
&\pm \left[ (k^2 m_b^2 + \chi_b^2 m_0^2) + e^{bV_b}(k^2 m_b^2 - \chi_b^2 m_0^2) \right] \sin ak = 0,
\]  

(2.8)

where the plus/minus signs correspond to symmetric/antisymmetric states. When \( m_1 = m_0 \), further simplification is possible:

\[
\begin{align*}
D_{h=2} &= 2 \cos ak + (\xi - \xi^{-1}) \sin ak \\
&\pm (\xi + \xi^{-1}) \sin ak e^{bV_b} = 0,
\end{align*}
\]  

(2.9)

where now \( k = \sqrt{2m_0E/h} \), \( \chi = \sqrt{2m_0(V - E)/h} \) and \( \xi = \chi / k = \sqrt{(V - E)/E} \). Here the plus/minus sign corresponds to the antisymmetric/symmetric state relative to the center of the DQW structure, respectively. Expression (2.9) can be found in [7, 12], where the energy in the presented formulae is counted from the top of the wells. When the barrier width \( b \to \infty \), equation (2.9) goes back to the well-known formula for an isolated quantum well.
When the particle energy $E$ is larger than the height $V_0$ of the barrier but smaller than the confining potential, $V_0 < E < V_c$, the particle remains localized. The only difference is that in the regions 2–4 the wave function now oscillates, i.e. the eigenfunctions $\psi(x)$ here are described by trigonometric functions alone. It is easy to see that the above solution at $E < V_0$ remains valid if we account for hyperbolic function properties $\sinh(i\chi_2) = i\sin\chi_2$, $\cosh(i\chi_2) = \cos\chi_2$ and note that in this case $\chi_b$ can be replaced by $i\chi_b = \sqrt{(2m_0/h^2)(E - V_0)}$.

3. Eigenfunctions

The coefficients in the wave function (2.2) depend on $k_n$. Since the spectrum $k_n$ (or $E_n = h^2k_n^2/2m_0$) is determined by roots of the transcendental equations (2.6) and (2.7), one is obliged to solve these equations by using numerical methods. Nonetheless, as we shall see, the eigenfunctions can be explicitly calculated with the help of the Gröbner basis algorithm [13, 15] without any reference to the roots at all. Roughly speaking, a Gröbner basis for a system of polynomial equations is a different system of simpler polynomials having the same roots as do the original ones. Calculation of the Gröbner basis to some extent resembles reducing a square matrix to a triangular matrix. For further calculations, it is convenient to introduce the following half-angle variables:

$$x = \tan(bk/2), \quad y = \tan(ak/2),$$

and express sine and cosine functions in (2.4a)–(2.4f) and (2.6) (or (2.7) in the case of antisymmetric eigenfunctions) through the polynomial variables $x$ and $y$:

$$\sin ak = \frac{2x}{1 + x^2}, \quad \cos ak = \frac{1 - x^2}{1 + x^2},$$

$$\sin bk = \frac{2y}{1 + y^2}, \quad \cos bk = \frac{1 - y^2}{1 + y^2}.$$  

Calculating the Gröbner basis for coefficients $A$, $B$ and $C$ and requesting that new variables $x$ and $y$ be eliminated, the program Mathematica generates a basis that consists of 146 polynomials. However, it should be stressed that the program can find the Gröbner basis only if the spectrum equation, either (2.6) or (2.7), is appended to the original polynomial system (2.4a)–(2.4f). The following simplest polynomials were selected for symmetric states:

$$A_1 = A_2 = C_2 = \frac{\chi_km_0}{km_c},$$

$$B_1 = B_4 = C_1 = C_2,$$

$$B_2 = B_3 = \frac{\pm C_2m_0e^{b\nu}m_0 \sqrt{k^2m_0^2 + \chi_b^2m_0^2}}{m_c[k^2m_0^2(1 + e^{b\nu})^2 + \chi_b^2m_0^2(-1 + e^{b\nu})^2]^{1/2}},$$

where $C_2$ was replaced by $C_{2s}$ to identify the state symmetry. The sign of coefficients $B_2$ and $B_3$ has to ensure derivative continuity at points $a$ and $a + b$. It is a straightforward matter to verify that the solution (3.3) indeed satisfies the initial equations (2.4a)–(2.4f). In (3.3) all amplitudes are expressed through a single coefficient $C_{2s}$, which in turn can be found from the normalization condition of the total wave function $\psi(x)$. Integration over the $x$-axis yields the normalization constant in the form

$$C_{2s} = km_c(G_1 + C_{2s})^{-1/2},$$

where

$$G_1 = \chi_b^{-1}\left[\chi^2 - (m_c + m_0a\chi_e)\right],$$

$$G_2 = \frac{m_0(k^2m_0^2 + \chi_b^2m_0^2)(b\chi_bk^2m_0 + (k^2m_0^2 + \chi_b^2m_0^2)m_0\sinh b\chi_b)}{\chi_b(k^2m_0^2 - \chi_b^2m_0^2 + (k^2m_0^2 + \chi_b^2m_0^2)cosh b\chi_b)}.$$  

If all masses are assumed to be equal ($m_0 = m_b = m_e = 1$), the normalization constant simplifies to

$$C_{2s} = \sqrt{\chi_b} \left[\left(1 + \frac{\chi_c^2}{k^2}\right) \left(\frac{a\chi_b + \chi_c^2}{\chi_b}\right)^2 \frac{b\chi_bk^2 + (k^2 + \chi_c^2)cosh b\chi_b}{k^2 - \chi_b^2 + (k^2 + \chi_c^2)cosh b\chi_b}\right]^{-1/2}.$$  

Quite a similar calculation for the antisymmetric (C2 → C2s) states yields

$$B_1 = B_4 = -C_1 = C_2s, \quad -A_1 = A_2 = C_2 \frac{\chi_km_0}{km_c},$$

$$B_2 = B_3 = \frac{\pm C_2m_0e^{b\nu}(k^2m_0^2 + \chi_b^2m_0^2)^{1/2}}{m_c[k^2m_0^2(1 + e^{b\nu})^2 + \chi_b^2m_0^2(1 + e^{b\nu})^2]^{1/2}},$$

where the choice of sign again follows from the derivative continuity condition. The normalization constant in this case is

$$C_{2s} = km_c(H_1 + H_2)^{-1/2},$$

where

$$H_1 = \chi_b^{-1}\left[k^2m_0^2(1 + a\chi_e) + m_0\chi_c^2(m_c + m_0a\chi_e)\right],$$

$$H_2 = \frac{m_0(k^2m_0^2 + \chi_b^2m_0^2)(b\chi_bk^2m_0 + (k^2m_0^2 + \chi_b^2m_0^2)m_0\sinh b\chi_b)}{\chi_b(k^2m_0^2 - \chi_b^2m_0^2 + (k^2m_0^2 + \chi_b^2m_0^2)cosh b\chi_b)}.$$  

When all masses become equal, the normalization constant $C_{2s}$ reduces to

$$C_{2s} = \sqrt{\chi_b} \left[\left(1 + \frac{\chi_c^2}{k^2}\right) \left(\frac{a\chi_b + \chi_c^2}{\chi_b}\right)^2 \frac{b\chi_bk^2 + (k^2 + \chi_c^2)cosh b\chi_b}{k^2 - \chi_b^2 + (k^2 + \chi_c^2)cosh b\chi_b}\right]^{-1/2}.$$  

As far as a more general nonsymmetric DQW problem is concerned, the calculations of the Gröbner basis indicate that, in contrast to solutions (3.3) and (3.8), at least one of the coefficients $A$, $B$ or $C$ includes the trigonometric functions. In this case, the determinant $D$ does not factorize to symmetric and asymmetric parts either.
4. The dipole matrix element

The knowledge of eigenfunctions allows one to proceed with analytical calculations. As an example, we shall find a closed form expression for dipole matrix elements between even \( \psi_s(k_m, x) \) and odd \( \psi_a(k_m, x) \) discrete states:

\[
d_{ns,ma} = \int_{-\infty}^{\infty} \psi_s^*(k_s, x) \left( x - a - \frac{b}{2} \right) \psi_a(k_m, x) \, dx
\]

\[
= 2d_1 + 2d_2 + d_3.
\]

(4.1)

Here the subscripts \( s \) and \( a \) refer to, respectively, even and odd symmetry states and \( d_i \) is the contribution of the \( i \)th region indicated in figure 1. For a general case, the expressions for dipole components \( d_{ns,ma} \) are rather complicated. For simplicity, below we present the expressions for the case when masses in all regions are equal, \( m_c = m_h = m_o \) and the central and confining barrier heights coincide, \( \chi_c = \chi_h = \chi \). Since the energy of symmetric and antisymmetric states differ, the wave vectors \( k \) and \( \chi \) are supplied by indices \( s \) and \( a \). Thus, the dipole expressions have two kinds of wave vectors, \( k_s \) and \( k_a \), and evanescent modes \( \chi_s \) and \( \chi_a \).

In the first and fifth regions, the contribution to the dipole is

\[
d_1 = d_5 = d_{1N}/d_{1D},
\]

where

\[
d_{1N} = \left[ 2 (2a + b)(\chi_s + \chi_a) \right] r_s r_a,
\]

\[
r_s = \sqrt{\chi_a \left[ (k_s^2 - \chi_s^2) + (k_s^2 + \chi_s^2) \cosh b \chi_s \right]},
\]

\[
r_a = \sqrt{\chi_a \left[ -(k_s^2 - \chi_s^2) + (k_s^2 + \chi_s^2) \cosh b \chi_s \right]},
\]

and

\[
d_{1D} = 2(k_s + \chi_s)^2 \sqrt{(k_s^2 + \chi_s^2)(k_s^2 + \chi_a^2)} \delta_s \delta_a,
\]

\[
\delta_s = \left[ -(k_s^2 + 1 + a \chi_s) + k_s^2 [1 + (a + b) \chi_a] \right.
\]

\[
+ (k_s^2 + \chi_s^2) \left. [1 + (a + b) \chi_a] \cosh b \chi_s + \sinh b \chi_a \right]^{1/2},
\]

\[
\delta_a = \left[ (k_s^2 + 1 + a \chi_s) - k_s^2 [1 + (a + b) \chi_a] \right.
\]

\[
+ (k_s^2 + \chi_s^2) \left. [1 + (a + b) \chi_a] \cosh b \chi_s + \sinh b \chi_a \right]^{1/2}.
\]

In the second region, it is

\[
d_2 = d_{2N}/d_{2D},
\]

where

\[
d_{2N} = -4r_s r_a \left[ (k_s - k_a)^2 (p_1 - p_3) - (k_s + k_a)^2 (p_2 - p_4) \right],
\]

\[
p_1 = \left[ b(k_s + k_a)(k_s + k_a + x_h) + 2k_s k_a - 2\chi_h \chi_s \right] \cos \left( k_s - k_a \right),
\]

\[
p_2 = \left[ b(k_s - k_a)(k_s + k_a - x_h) - 2k_s k_a - 2\chi_h \chi_s \right] \cos \left( k_s + k_a \right),
\]

\[
p_3 = \left[ b(k_s + k_a)(k_s + k_a - x_h) - 2k_s k_a - 2\chi_h \chi_s \right] \sin \left( k_s + k_a \right),
\]

\[
p_4 = \left[ b(k_s - k_a)(k_s + k_a + x_h) + 2k_s k_a - 2\chi_h \chi_s \right] \sin \left( k_s - k_a \right),
\]

\[
\text{Figure 2. The energies of the GaAs/Ga}_{0.8}\text{Al}_{0.2}\text{As DQW as a function of the central barrier width at } a = 6 \text{ nm.}
\]

\[
d_{2D} = \frac{(k_s^2 - k_a^2)^2}{(\chi_h + \chi_a)^2} d_{1D}.
\]

One can see that trigonometric functions, which will give the oscillations of matrix elements versus the well width, appear only here.

The third (barrier) region contribution to the dipole is

\[
d_3 = d_{3N}/d_{3D},
\]

where

\[
d_{3N} = -4e^{(1/2)(b \chi_s + \chi_a)} k_s k_a r_s r_a \left[ v_1 \cosh \frac{b \chi_s}{2} + v_2 \sinh \frac{b \chi_s}{2} \right],
\]

\[
v_1 = -b \chi_s (\chi_s^2 + \chi_a^2) \cosh \frac{b \chi_s}{2} + 4 \chi_s \chi_a \sinh \frac{b \chi_s}{2},
\]

\[
v_2 = -2(\chi_s^2 + \chi_a^2) \cosh \frac{b \chi_s}{2} + 4b \chi_s (\chi_s^2 - \chi_a^2) \sinh \frac{b \chi_s}{2},
\]

and

\[
d_{3D} = \frac{1}{2} (\chi_s - \chi_a)^2 s_s s_a d_{1D},
\]

\[
s_s = \sqrt{ \left[ (1 + e^{b \chi_s})^2 k_s^2 + (1 - e^{b \chi_s})^2 \chi_s^2 \right] / (k_s^2 + \chi_s^2) },
\]

\[
s_a = \sqrt{ \left[ (1 - e^{b \chi_s})^2 k_s^2 + (1 + e^{b \chi_s})^2 \chi_s^2 \right] / (k_s^2 + \chi_s^2) }.
\]

Figure 2 shows the dependences of the first two energy levels \( E_{1s} \) and \( E_{2a} \) as a function of the inner barrier width. The following parameter values that are typical of GaAs/Ga_{0.8}Al_{0.2}As DQW heterostructures were used: \( a = 6 \) nm, \( b = (1-15) \) nm, \( V_c = V_b = 0.1671 \) eV, \( m_0 = 0.067m_e \) and \( m_c = m_h = 0.0836m_e \), where \( m_e \) is the electron mass in vacuum. The increase in the energy difference between levels with a decrease in \( b \) is assigned to the tunnel coupling of levels.

Figure 3(a) demonstrates the size of optical dipole matrix elements between pairs of adjacent levels, \( d_{1s,2a} \) and \( d_{2a,3s} \), as a function of the barrier width. Figure 3(b) shows the contribution of individual regions to the dipole \( d_{1s,2a} \).

It is clear that the general trend and magnitude of dipole elements in figure 3(a) can be understood if one assumes that only quantum wells contribute to the total dipole. In this approximation, the functions \( \psi_1 = \psi_3 = \psi_5 = 0 \), while...
Figure 3. (a) Dipole matrix elements $d_{1s,2a}$ and $d_{2a,3s}$ as a function of barrier width $b$. (b) The contributions of individual regions to the dipole matrix $d_{1s,2a}$.

$\psi_2$ and $\psi_4$ can be approximated by half-period sine functions. Then $d_{1s,2a}$ reduces to

$$d_{1s,2a} \approx \frac{2}{a} \int_0^a \sin \frac{\pi x}{a} \left( x - a - \frac{b}{2} \right) \left( - \sin \frac{\pi x}{a} \right) \, dx$$

$$= \frac{a + b}{2}. \tag{4.11}$$

The formula shows that the dipole size increases linearly with the barrier width $b$ as long as $b$ remains much smaller than the excitation light wavelength. For $2a - 3s$ optical transitions, one of the sines should be replaced by $\sin(2\pi x/a)$. Then, a similar calculation yields $d_{2s,3s} \approx 16a/9\pi^2$, which is independent of the barrier width. The deviations from the obtained expressions, in figure 3(a), come from the evanescent mode contribution in the barrier and confining potential regions.

In conclusion, the presented example shows that the application of a Gröbner basis algorithm in some cases allows one to find closed form expressions for the total wave function and therefore to calculate the dipole matrix elements exactly without directly solving the transcendental equations that determine the spectrum of the DQW. Of course, the described method can be applied to other quantum systems for which eigenvalue equations cannot be explicitly solved exactly.

Acknowledgment

This work was supported by EU grant number VP2-1.4-ŪM-03-K-01-019, ‘Science for Business and Society’.

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