`qwkpvb` – Quantum Well $\mathbf{k} \cdot \mathbf{p}$ Valence Subband Software
USER'S MANUAL

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1 Purpose of the Software

The program `qwkpvb` gives the numerical solution, for holes, to the quantum mechanical problem of a one–dimensional particle in a box, with finite barrier heights. The solution to this type of problem is useful in the design and analysis of semiconductor devices such as quantum well lasers, modulators and detectors.

The software gives the positions of the quantum well valence subband levels, as well as the spatial dependence of the confined hole wavefunctions. The solutions are obtained for heavy holes and for light holes, using the $\mathbf{k} \cdot \mathbf{p}$ method. This means that the hole wavefunction basis states are taken to have a total angular momentum quantum number of $j = 3/2$. The $\mathbf{k} \cdot \mathbf{p}$ coupling between the basis states, in the hamiltonian, gives a more accurate description of the valence subband energy levels and states, than in the uncoupled scalar solutions provided by the complimentary program `qwscal`. The greater modeling accuracy of `qwkpvb` comes at the price of longer computational time. Thus, a reasonable analysis would use `qwscal` to obtain an approximately correct solution for the hole states, possibly as a result of several quick calculations, followed by the use of `qwkpvb` to refine the results with a relatively few, more time–consuming calculations.

The program `qwkpvb` gives the subband levels and wavefunctions for a single quantum well, whose width can vary between 25 to 200 Å, and whose depth can vary from 0.001 to 1.0 eV. The in–plane bandstructure is also calculated along the k_x ($k_y = 0$) and $k_x = k_y$ directions, from $k = 0$, outward.

2 Design and Operation of the Software

The program `qwkpvb` gives the solution to the Schrödinger equation:

$$H\psi(z) = E\psi(z), \tag{1}$$

where H is a 4×4 matrix in the 4–dimensional $j = 3/2$ angular momentum subspace. Explicitly, this hamiltonian is,

$$H = \begin{bmatrix} H_{hh} & b & c & 0 \\ b^\dagger & H_{lh} & 0 & c \\ c^\dagger & 0 & H_{lh} & -b \\ 0 & c^\dagger & -b^\dagger & H_{hh} \end{bmatrix}. \tag{2}$$

The hamiltonian matrix elements are, themselves, operators:

$$H_{hh} = -\frac{\hbar^2}{2m_0}\left[(\gamma_1 + \gamma_2)(k_x^2 + k_y^2) - (\gamma_1 - 2\gamma_2)\frac{\partial^2}{\partial z^2}\right] + V(z) + \delta/2$$

$$
\begin{aligned}
H_{lh} &= -\frac{\hbar^2}{2m_0}\left[(\gamma_1-\gamma_2)(k_x^2+k_y^2)-(\gamma_1+2\gamma_2)\frac{\partial^2}{\partial z^2}\right]+V(z)-\delta/2 \\
b &= -i\frac{\sqrt{3}\hbar^2}{m_0}(-k_y-ik_x)\gamma_3\frac{\partial}{\partial z} \\
c &= \frac{\sqrt{3}\hbar^2}{2m_0}\left[\gamma_2(k_x^2-k_y^2)-2i\gamma_3 k_x k_y\right]. \qquad (3)
\end{aligned}
$$

The parameters here are, m_0, the free electron mass; γ_1, γ_2 and γ_3, the Luttinger valence band parameters; $V(z)$; the potential energy profile of the barriers and the quantum well:

$$
V(z)=\begin{cases} V_0, & 0\le z<a \\ 0, & a\le z\le a+W \\ V_0, & a+W<z\le L \end{cases},
$$

where W and V_0 are the width and depth, respectively, of the quantum well. The width of the first barrier is a and the width of the second barrier is $L-(a+W)$. The parameter δ is the strain energy splitting between the heavy and light holes at $k=0$. This parameter is zero for unstrained material, and is explained in Chapter 3 of "Electronic and Optoelectronic Properties of Semiconductor Structures," by J. Singh, Cambridge University Press ISBN 0-521-82379-X.

The wavefunction is a vector in the 4–dimensional $j=3/2$ angular momentum subspace:

$$
\psi(z)=\begin{bmatrix} \phi_{3/2,3/2}(z) \\ \phi_{3/2,1/2}(z) \\ \phi_{3/2,-1/2}(z) \\ \phi_{3/2,-3/2}(z) \end{bmatrix}. \qquad (4)
$$

This form of the hamiltonian matrix gives the Schrödinger equation for both spin states of both heavy and light holes. These are four coupled partial differential equations.

The axis z is divided up into a mesh, which for computational purposes, is confined to the interval of total length $L=300$ Å: $z\in[0,L]$. The effective boundary conditions are $\psi(z)=0$ for $z<0$ and for $z>L$. The mesh is subdivided into `NMESH`=31 nodes with a separation $\Delta z = L/(\texttt{NMESH}-1) = z_{i+1}-z_i$, for $i=1,\ldots,\texttt{NMESH}-1$.

The numerical solution proceeds by converting the four coupled differential equations (1) into four coupled finite difference equations. First, the 4–element vector wavefunction $\psi(z)$ is converted into Ψ, a $4\cdot\texttt{NMESH}$ element vector, whose elements are the values of $\psi(z)$ at the grid points $z_i, i=1,\ldots,\texttt{NMESH}$:

$$
\begin{aligned}
\Psi &= [\psi(z_1),\ldots,\psi(z_{\texttt{NMESH}})] \\
&= [\phi_{3/2,3/2}(z_1),\phi_{3/2,1/2}(z_1),\phi_{3/2,-1/2}(z_1),\phi_{3/2,-3/2}(z_1),\ldots, \\
&\quad \phi_{3/2,3/2}(z_{\texttt{NMESH}}),\phi_{3/2,1/2}(z_{\texttt{NMESH}}),\phi_{3/2,-1/2}(z_{\texttt{NMESH}}),\phi_{3/2,-3/2}(z_{\texttt{NMESH}})]. \qquad (5)
\end{aligned}
$$

The operation of H on Ψ can be represented as an $\texttt{NMESH} \times \texttt{NMESH}$ operator matrix, whose only non-zero elements are on the diagonal and are the 4×4 hamiltonians that operate on the wavefunction at each grid position,

$$H\Psi = \begin{bmatrix} H & 0 & \cdots & & & & \\ 0 & H & 0 & \cdots & & & \\ & & & \ddots & & & \\ & & & \cdots & 0 & H & 0 \\ & & & & \cdots & 0 & H \end{bmatrix} \begin{bmatrix} \psi(z_1) \\ \psi(z_2) \\ \vdots \\ \psi(z_{\texttt{NMESH}}-1) \\ \psi(z_{\texttt{NMESH}}) \end{bmatrix}. \tag{6}$$

These NMESH equations are then evaluated for $i = 1, \ldots, \texttt{NMESH}$, as,

$$H\psi(z_i) = \begin{bmatrix} H_{hh} & b & c & 0 \\ b^\dagger & H_{lh} & 0 & c \\ c^\dagger & 0 & H_{lh} & -b \\ 0 & c^\dagger & -b^\dagger & H_{hh} \end{bmatrix} \begin{bmatrix} \phi_{3/2,3/2}(z_i) \\ \phi_{3/2,1/2}(z_i) \\ \phi_{3/2,-1/2}(z_i) \\ \phi_{3/2,-3/2}(z_i) \end{bmatrix}. \tag{7}$$

This is a set of four coupled equations, which are:

$$\begin{aligned} H_{hh}\phi_{3/2,3/2}(z_i) + b\phi_{3/2,1/2}(z_i) + c\phi_{3/2,-1/2}(z_i) &= E\phi_{3/2,3/2}(z_i) \\ b^\dagger\phi_{3/2,3/2}(z_i) + H_{lh}\phi_{3/2,1/2}(z_i) + c\phi_{3/2,-3/2}(z_i) &= E\phi_{3/2,1/2}(z_i) \\ c^\dagger\phi_{3/2,3/2}(z_i) + H_{lh}\phi_{3/2,-1/2}(z_i) - b\phi_{3/2,-3/2}(z_i) &= E\phi_{3/2,-1/2}(z_i) \\ c^\dagger\phi_{3/2,1/2}(z_i) - b^\dagger\phi_{3/2,-1/2}(z_i) + H_{hh}\phi_{3/2,-3/2}(z_i) &= E\phi_{3/2,-3/2}(z_i). \end{aligned} \tag{8}$$

The terms H_{hh}, H_{lh}, b, c, in these equations, are, themselves, operators. When operating on a state $\phi_{j,m_j}(z_i)$, the terms in equation set 8 are:

$$\begin{aligned} H_{hh}\phi_{j,m_j}(z_i) &= \left\{ -\frac{\hbar^2}{2m_0}\left[(\gamma_1+\gamma_2)(k_x^2+k_y^2) - (\gamma_1-2\gamma_2)\frac{\partial^2}{\partial z^2}\right] \right. \\ &\quad \left. +V(z_i) + \delta/2 \right\} \phi_{j,m_j}(z_i) \\ &= \left\{ -\frac{\hbar^2}{2m_0}\left[(\gamma_1+\gamma_2)(k_x^2+k_y^2) - (\gamma_1-2\gamma_2)\frac{-2}{(\Delta z)^2}\right] \right. \\ &\quad \left. +V(z_i) + \delta/2 \right\} \phi_{j,m_j}(z_i) \\ &\quad + \left\{ -\frac{\hbar^2}{2m_0}\left[-(\gamma_1-2\gamma_2)\frac{1}{(\Delta z)^2}\right] \right\} \phi_{j,m_j}(z_{i+1}) \\ &\quad + \left\{ -\frac{\hbar^2}{2m_0}\left[-(\gamma_1-2\gamma_2)\frac{1}{(\Delta z)^2}\right] \right\} \phi_{j,m_j}(z_{i-1}) \\ &= f\phi_{j,m_j}(z_{i+1}) + e_i\phi_{j,m_j}(z_i) + f\phi_{j,m_j}(z_{i-1}) \\ H_{lh}\phi_{j,m_j}(z_i) &= \left\{ -\frac{\hbar^2}{2m_0}\left[(\gamma_1-\gamma_2)(k_x^2+k_y^2) - (\gamma_1+2\gamma_2)\frac{\partial^2}{\partial z^2}\right] \right. \\ &\quad \left. +V(z_i) - \delta/2 \right\} \phi_{j,m_j}(z_i) \end{aligned}$$

$$
\begin{aligned}
&= \left\{ -\frac{\hbar^2}{2m_0}\left[(\gamma_1-\gamma_2)(k_x^2+k_y^2)-(\gamma_1+2\gamma_2)\frac{-2}{(\Delta z)^2}\right]\right. \\
&\quad \left. +V(z_i)-\delta/2\right\}\phi_{j,m_j}(z_i) \\
&\quad +\left\{ -\frac{\hbar^2}{2m_0}\left[-(\gamma_1+2\gamma_2)\frac{1}{(\Delta z)^2}\right]\right\}\phi_{j,m_j}(z_{i+1}) \\
&\quad +\left\{ -\frac{\hbar^2}{2m_0}\left[-(\gamma_1+2\gamma_2)\frac{1}{(\Delta z)^2}\right]\right\}\phi_{j,m_j}(z_{i-1}) \\
&= f^{'}\phi_{j,m_j}(z_{i+1})+e_i^{'}\phi_{j,m_j}(z_i)+f^{'}\phi_{j,m_j}(z_{i-1}) \\
b\phi_{j,m_j}(z_i) &= i\frac{\sqrt{3}\hbar^2}{m_0}(-k_y-ik_x)\gamma_3\frac{\partial}{\partial z}\phi_{j,m_j}(z_i) \\
&= i\frac{\sqrt{3}\hbar^2}{m_0}(-k_y-ik_x)\gamma_3\left(\frac{\phi_{j,m_j}(z_{i+1})-\phi_{j,m_j}(z_{i-1})}{2\Delta z}\right) \\
&= \beta\phi_{j,m_j}(z_{i+1})-\beta\phi_{j,m_j}(z_{i-1}) \\
c\phi_{j,m_j}(z_i) &= -\frac{\sqrt{3}\hbar^2}{2m_0}\left[\gamma_2(k_x^2-k_y^2)-2i\gamma_3k_xk_y\right]\phi_{j,m_j}(z_i). \qquad (9)
\end{aligned}
$$

These equations can be applied for all $i = 1, \ldots,$ NMESH, provided that it is understood that $\phi_{j,m_j}(z_0) = \phi_{j,m_j}(z_{\text{NMESH}}+1) = 0$. The symbols introduced to compress the notation are:

$$
\begin{aligned}
e_i &= -\frac{\hbar^2}{2m_0}\left[(\gamma_1+\gamma_2)(k_x^2+k_y^2)-(\gamma_1-2\gamma_2)\frac{-2}{(\Delta z)^2}\right]+V(z_i)+\delta/2 \\
e_i^{'} &= -\frac{\hbar^2}{2m_0}\left[(\gamma_1-\gamma_2)(k_x^2+k_y^2)-(\gamma_1+2\gamma_2)\frac{-2}{(\Delta z)^2}\right]+V(z_i)-\delta/2 \\
f &= -\frac{\hbar^2}{2m_0}\left[-(\gamma_1-2\gamma_2)\frac{1}{(\Delta z)^2}\right] \\
f^{'} &= -\frac{\hbar^2}{2m_0}\left[-(\gamma_1+2\gamma_2)\frac{1}{(\Delta z)^2}\right] \\
\beta &= i\frac{\sqrt{3}\hbar^2}{m_0}(-k_y-ik_x)\gamma_3\left(\frac{1}{2\Delta z}\right). \qquad (10)
\end{aligned}
$$

The hamiltonian that operates on the vector Ψ is a $4\cdot$NMESH $\times\, 4\cdot$NMESH matrix. The elements of this matrix are calculated by the routine `kpham`. In the program, NMESH $= 31$. The hamiltonian matrix can be considered to be the sum of four matrices, one for each of the operators H_{hh}, H_{lh}, b, c. In what follows, to display the layout of the hamiltonian matrix, a smaller value of NMESH $= 3$ will be used. Using the compressed notation for the operators in equation 10, these four matrices are as follows.

The matrix of the operator H_{hh} is laid out in the following way.

z_1				z_2				z_3			
$3/2$	$1/2$	$-1/2$	$-3/2$	$3/2$	$1/2$	$-1/2$	$-3/2$	$3/2$	$1/2$	$-1/2$	$-3/2$
e_1				f							
			e_1				f				
f				e_2				f			
			f				e_2				f
				f				e_3			
							f				e_3

The matrix of the operator H_{lh} is laid out in the following way.

z_1				z_2				z_3			
$3/2$	$1/2$	$-1/2$	$-3/2$	$3/2$	$1/2$	$-1/2$	$-3/2$	$3/2$	$1/2$	$-1/2$	$-3/2$
	$e_1^{'}$				$f^{'}$						
		$e_1^{'}$				$f^{'}$					
	$f^{'}$				$e_2^{'}$				$f^{'}$		
		$f^{'}$				$e_2^{'}$				$f^{'}$	
					$f^{'}$				$e_3^{'}$		
						$f^{'}$				$e_3^{'}$	

The matrix of the operator b is laid out in the following way.

z_1				z_2				z_3			
$3/2$	$1/2$	$-1/2$	$-3/2$	$3/2$	$1/2$	$-1/2$	$-3/2$	$3/2$	$1/2$	$-1/2$	$-3/2$
					β						
				β^*							
							$-\beta$				
						$-\beta^*$					
	$-\beta$								β		
$-\beta^*$								β^*			
			β								$-\beta$
		β^*								$-\beta^*$	
					$-\beta$						
				$-\beta^*$							
							β				
						β^*					

The matrix of the operator c is laid out in the following way.

z_1				z_2				z_3			
$3/2$	$1/2$	$-1/2$	$-3/2$	$3/2$	$1/2$	$-1/2$	$-3/2$	$3/2$	$1/2$	$-1/2$	$-3/2$
		c									
			c								
c^*											
	c^*										
						c					
							c				
				c^*							
					c^*						
										c	
											c
								c^*			
									c^*		

The sum of these four matrices is the following total hamiltonian matrix.

z_1				z_2				z_3			
3/2	1/2	−1/2	−3/2	3/2	1/2	−1/2	−3/2	3/2	1/2	−1/2	−3/2
e_1		c		f	β						
	$e_1^{'}$		c	β^*	$f^{'}$						
c^*		$e_1^{'}$				$f^{'}$	$-\beta$				
	c^*		e_1			$-\beta^*$	f				
f	$-\beta$			e_2		c		f	β		
$-\beta^*$	$f^{'}$				$e_2^{'}$		c	β^*	$f^{'}$		
		$f^{'}$	β	c^*		$e_2^{'}$				$f^{'}$	$-\beta$
		β^*	f		c^*		e_2			$-\beta^*$	f
				f	$-\beta$			e_3		c	
				$-\beta^*$	$f^{'}$				$e_3^{'}$		c
						$f^{'}$	β	c^*		$e_3^{'}$	
						β^*	f		c^*		e_3

This is the form of the hamiltonian matrix for this example `NMESH` = 3. For the actually used `NMESH` = 31, the extension of this layout is straightforward resulting in a 124×124 matrix. The program `qwkpvb` calls a subroutine `kpham` to calculate all of the elements of the hamiltonian matrix. Note that the form of the hamiltonian matrix gives rise to the effective boundary conditions $\psi(z) = 0$ for $z < z_1$ and for $z > z_{\texttt{NMESH}}$.

The program operates as follows.

- Input the parameters.
- Set the mesh pitch.
- Open the general information output file.
- Open the solution output files.
- Start calculation progress chart.
- Set the barrier and well positions.
- Set the potential profile.
- Loop over in-plane wavevectors k_y and k_x.
  - Calculate $\mathbf{k} \cdot \mathbf{p}$ hamiltonian matrix elements.
  - Solve for the eigenvalues and eigenvectors.
  - Output selected eigenvalues and eigenvectors.
  - Update calculation progress chart.

- Do next in-plane wavevector.
- Finish calculation progress chart.
- Finish and close the information output file.
- Close the energy output file.

The program requires one single input file, `qwkpvb.inp`. This contains values of the three Luttinger valence bandstructure parameters, the strain energy splitting, the bandedge discontinuity and the quantum well width. An example of this file is:

```
qwkpvb input parameters
 6.85     Gamma_1: Luttinger valence band parameter
 2.1      Gamma_2:     "           "            "
 2.9      Gamma_3:     "           "            "
 0.0      Delta: Strain energy, in units of eV
 0.1      dE_v; Valence band discontinuity, in units of eV
 130.0    w0; Quantum well width, in units of angstroms
```

The first word of the first line must be "`qwkpvb`". This is used by the program to confirm the identity of the input file. The format of the Luttinger parameters, the strain energy splitting and the bandedge discontinuity must be `f6.3`. The format of the well width must be `f6.1`. The text following the numerical values is not used by the program, and is shown only for the user's benefit.

The program generates 14 output files:

- one file of general information: `qwinfo.dat`;
- one file, `qwkpen.dat`, containing the quantum well subbandstructure for both the heavy and light holes, consisting of the lowest 12 eigenvalues;
- twelve files, `qwkpwf01.dat`—`qwkpwf12.dat`, containing the spatial dependence of each of the 12 lowest level wavefunctions for $k_x = k_y = 0$, corresponding to the $\mathbf{k}_{\|} = 0$ energy values in `qwkpen.dat`.

The specific contents of each of the output files are as follows.

2.1 Contents of `qwinfo.dat`

For the input parameter values shown in the example of `qwkpvb.inp`, above, `qwkpvb` generates the following `qwinfo.dat`.

```
GENERAL CALCULATION INFORMATION FROM PROGRAM qwkpvb.


Bandstructure Parameters
------------------------
Gamma_1     6.850
Gamma_2     2.100
Gamma_3     2.900
Delta (eV)  0.000



Well Parameters
---------------
Well width =  130.0 A
Well depth =  0.100 eV


Calculation Mesh
----------------
Pitch dz =   10.0 A
Barrier 1 - Well interface at X = 50.0 A
Well - Barrier 2 interface at X = 50.0 + W  A
Total calculation mesh from 0 to  300.0 A


Energy level and wavefunction files
-----------------------------------
Subband energies, top 12:
   qwkpen.dat

Wavefunctions, top 12, at Kx=Ky=0:
    #     file
     1    qwkpwf01.dat
     2    qwkpwf02.dat
     3    qwkpwf03.dat
     4    qwkpwf04.dat
     5    qwkpwf05.dat
     6    qwkpwf06.dat
     7    qwkpwf07.dat
     8    qwkpwf08.dat
     9    qwkpwf09.dat
    10    qwkpwf10.dat
    11    qwkpwf11.dat
    12    qwkpwf12.dat
```

First, the Luttinger valence band parameters and the strain energy splitting (in units of eV) are given, followed by the quantum well parameters of width (in units of Å) and depth (in units of eV).

Under `Calculation Mesh` are given the value of Δz (`dz`) and the position of the barriers. In the above example, the first barrier extends from $z = 0$ Å to $z = 50$ Å; the well extends from $z = 50$ Å to $z = 180$ Å; the second barrier extends from $z = 180$ Å to $z = 300$ Å.

Under `Energy level and wavefunction files`, the filenames of each of the other 13 output files are given. These will now be discussed.

2.2 Contents of `qwkpen.dat`

This 14–column file contains the valence subband structure for the lowest 12 subband, as functions of the in–plane wavevector (k_x, k_y). Column by column, the contents are as follows.

Col. #	Quantity
1	k_x (Å^{-1})
2	k_y "
3	E_{1a} (eV)
4	E_{1b} "
5	E_{2a} "
6	E_{2b} "
7	E_{3a} "
8	E_{3b} "
9	E_{4a} "
10	E_{4b} "
11	E_{5a} "
12	E_{5b} "
13	E_{6a} "
14	E_{6b} "

The energy pairs E_{ia} and E_{ib} are the same, because of two-fold spin degeneracy in the symmetric quantum well. The first 10 lines of `qwkpen.dat` give the bandstructure as $\mathbf{k}_\parallel$ varies from $k_x = k_y = 0$, along the [100] direction, to $k_x = 0.027$ Å^{-1}, $k_y = 0$. Then, the remaining nine lines of the file give the bandstructure as $\mathbf{k}_\parallel$ varies from $k_x = k_y = 0.003$ Å^{-1}, along the [110] direction, to $k_x = k_y = 0.027$ Å^{-1}. Depending on the quantum well depth, all of the given subbandstructure may not correspond to states that are bound in the quantum well. This is because the effective boundary conditions, discussed above, of $\psi(z) = 0$ for $z < 0$ and for $z > z_{\texttt{NMESH}}$, are equivalent to imposing barriers of infinite height to the left of the first barrier and to the right of the second barrier. This gives rise to further quantized solutions, lying above the barriers, which are modeling artifacts. These are states bound in the artificial infinite quantum well imposed at the calculation boundaries. These solutions, above the tops of the barriers, do not represent realistic states in the semiconductor system and should be disregarded. In fact, since there are `NMESH`=31 grid points used in the calculation, the software can, in principle, find 31 solutions at each value of wavevector. All, except those below the barrier edge, are calculational artifacts.

2.3 Contents of `qwkpwf??.dat`

Each of the 12 files, `qwkpwf01.dat`—`qwkpwf12.dat` has 11 columns, giving a $\mathbf{k}_{\|} = 0$ wavefunction as a function of position across the calculation grid. Column by column, the contents are as follows.

Col. #	Quantity
1	z (Å)
2	V (eV)
3	$\|\psi\|^2$
4	$\mathrm{Re}(\phi_{3/2,3/2}(z))$
5	$\mathrm{Im}(\phi_{3/2,3/2}(z))$
6	$\mathrm{Re}(\phi_{3/2,1/2}(z))$
7	$\mathrm{Im}(\phi_{3/2,1/2}(z))$
8	$\mathrm{Re}(\phi_{3/2,-1/2}(z))$
9	$\mathrm{Im}(\phi_{3/2,-1/2}(z))$
10	$\mathrm{Re}(\phi_{3/2,-3/2}(z))$
11	$\mathrm{Im}(\phi_{3/2,-3/2}(z))$

Each of the wavefunction files corresponds to one of the subbands, given in `qwkpen.dat`, at $\mathbf{k}_{\|} = 0$, as listed below.

Wavefunction File	Corresp. Subband
`qwkpwf01.dat`	E_{1a}
`qwkpwf02.dat`	E_{1b}
`qwkpwf03.dat`	E_{2a}
`qwkpwf04.dat`	E_{2b}
`qwkpwf05.dat`	E_{3a}
`qwkpwf06.dat`	E_{3b}
`qwkpwf07.dat`	E_{4a}
`qwkpwf08.dat`	E_{4b}
`qwkpwf09.dat`	E_{5a}
`qwkpwf10.dat`	E_{5b}
`qwkpwf11.dat`	E_{6a}
`qwkpwf12.dat`	E_{6b}

Only if the corresponding subband, at $\mathbf{k}_{\|} = 0$, lies below the edge of the barrier, does a wavefunction correspond to a physically real state; otherwise, it is a calculational artifact, as discussed above.

3 Examples

3.1 Compilation

```
% f77 -o qwkpvb.exe qwkpvb.f
or
% f90 -o qwkpvb.exe qwkpvb.f
qwkpvb.f:
 MAIN qwkpvb:
        kpham:
        htridi:
        htribk:
        imtql2:
%
```

3.2 Running

```
% qwkpvb.exe



 Calculation Progress
   1/ 19 of the way done.
   2/ 19 of the way done.
   3/ 19 of the way done.
   4/ 19 of the way done.
   5/ 19 of the way done.
   6/ 19 of the way done.
   7/ 19 of the way done.
   8/ 19 of the way done.
   9/ 19 of the way done.
  10/ 19 of the way done.
  11/ 19 of the way done.
  12/ 19 of the way done.
  13/ 19 of the way done.
  14/ 19 of the way done.
  15/ 19 of the way done.
  16/ 19 of the way done.
  17/ 19 of the way done.
  18/ 19 of the way done.
  19/ 19 of the way done.
 Calculation Done
```

```
% ls -1 qw*.dat
qwinfo.dat
qwkpen.dat
qwkpwf01.dat
qwkpwf02.dat
qwkpwf03.dat
qwkpwf04.dat
qwkpwf05.dat
qwkpwf06.dat
qwkpwf07.dat
qwkpwf08.dat
qwkpwf09.dat
qwkpwf10.dat
qwkpwf11.dat
qwkpwf12.dat
%
```

3.3 Variation of input parameters

Parameters in the input file `qwkpvb.inp` can be varied within the following ranges. Luttinger valence band parameters can vary from 0 to 10. The strain energy splitting can vary from -0.5 to 0.5 eV. The bandedge discontinuity can vary from 0.001 to 1.0 eV. The quantum well width can vary from 25 to 200 Å.

4 Trouble Shooting

For any problems not covered below, refer to the source code of `qwkpvb.f`. It has extensive and detailed documentation.

4.1 Interpretation of source level error messages

```
Error:  incorrect input file.
Check contents of file "qwkpvb.inp".
Program halting.
```

The value of the identification string read from the parameter input file is not the expected value of "`qwkpvb`". This may indicate that the contents of `qwkpvb.inp` are generally bad. Fix: carefully compare the contents of your

copy of `qwkpvb.inp` with those of the original distribution file, and correct any differences other than possible numerical differences in the parameters. Ensure that the same number of parameters exist and that they pertain to the same physical quantities.

```
Error:  input value of Gamma_1 out of valid range.
Input value = GAMMA
Valid range = [GAMIN,GAMAX]
Program halting.
```

The value of Luttinger parameter γ_1, read from the input parameter file `qwkpvb.inp` is outside of the valid range of `[GAMIN,GAMAX] = [0,10]`. Fix: make sure that γ_1, second line of `qwkpvb.inp` is within the above range and that it is in the format of `f6.3` .

```
Error:  input value of Gamma_2 out of valid range.
Input value = GAMMA
Valid range = [GAMIN,GAMAX]
Program halting.
```

The value of Luttinger parameter γ_2, read from the input parameter file `qwkpvb.inp` is outside of the valid range of `[GAMIN,GAMAX] = [0,10]`. Fix: make sure that γ_2, third line of `qwkpvb.inp` is within the above range and that it is in the format of `f6.3`.

```
Error:  input value of Gamma_3 out of valid range.
Input value = GAMMA
Valid range = [GAMIN,GAMAX]
Program halting.
```

The value of Luttinger parameter γ_3, read from the input parameter file `qwkpvb.inp` is outside of the valid range of `[GAMIN,GAMAX] = [0,10]`. Fix: make sure that γ_3, fourth line of `qwkpvb.inp` is within the above range and that it is in the format of `f6.3`.

```
Error:  input value of Delta out of valid range.
Input value = DELTA
Valid range = [-DELMAX,DELMAX]
Program halting.
```

The value of the strain energy splitting, δ, read from the input parameter file `qwkpvb.inp` is outside of the valid range of `[-DELMAX,DELMAX] = [-0.5,0.5]`.

Fix: make sure that δ, fifth line of `qwkpvb.inp` is within the above range and that it is in the format of `f6.3`.

```
Error:  input value of VB discontinuity out of valid range.
Input value = V0
Valid range = [VOMIN,VOMAX]
Program halting.
```

The value of valence band discontinuity, V_0, read from the input parameter file `qwkpvb.inp` is outside of the valid range of `[VOMIN,VOMAX] = [0.001,1.0]`. Fix: make sure that the VB discontinuity, sixth line of `qwkpvb.inp` is within the above range and that it is in the format of `f6.3`.

```
Error:  input value of well width out of valid range.
Input value = W0
Valid range = [WOMIN,WOMAX]
Program halting.
```

The value of quantum well width, W, read from the input parameter file `qwkpvb.inp` is outside of the valid range of `[WOMIN,WOMAX] = [25.0,200.0]`. Fix: make sure that the well width, seventh line of `qwkpvb.inp` is within the above range and that it is in the format of `f6.1`.

```
Error: on return from IMTQL2.
Eigenvalue #J has not been determined after 30 iterations.
Program halting.
```

Fix: learn operation of the subroutine `IMTQL2` to debug this problem.

4.2 Trouble associated with the input file

Erroneous behavior of the program may result from the use of an input file `qwkpvb.inp` whose contents do not conform to rather strict formatting specifications. The first six characters of the first line of the file `qwkpvb.inp` must be "`qwkpvb`". The rest of this line is arbitrary. The Luttinger valence band parameters, the strain energy splitting and the valence band discontinuity must appear in the first six columns of the second through sixth lines of the input file. These values must have their decimal point in the third column, being in the FORTRAN format of `f6.3`. The quantum well width must appear in the first six columns of the seventh input line. It must have its decimal point in the fifth column, being in the FORTRAN format of `f6.1`. The text on lines 2 through 7, following the numerical data, is arbitrary.

4.3 Trouble associated with overwriting previously existing files

All output files are newly created with each run. If any of the ten output files remains from a previous run, the program will crash at the point that it tries to create the file. The solution is to either remove the files from the previous run, or the more them or otherwise change their names. This is so as to avoid inadvertently overwriting data from other computations.

4.4 Trouble associated with exceeding realistic model capabilities

Although any model can be incorrectly applied in a virtually limitless number of ways, only some of the more likely problems using `qwkpvb` are discussed here.

One limitation of the model concerns the discrete nature of the calculation grid. The mesh pitch Δz determines the finest scale that can be spatially resolved. This can give rise to a degree of roughness in the spatial variation of the wavefunction. Also, the transition between barrier and well is not abrupt, but is indistinguishable from a linear variation in potential energy over the distance Δz. Thus, wells which are only a few Δz wide may not be accurately modeled as being abruptly edged square wells.

Another limitation concerns the finite extent of the calculation grid. Used properly, the wavefunction is very nearly zero well before reaching either end of the grid. Given an adequately thick pair of barriers, low-level solutions generally will satisfy this requirement. However, as the energy increases, the wavefunction penetrates the barriers to an increasing extent and beyond some energy value, will not be sufficiently small as the ends of the calculation grid are approached. In this case, the effective boundary conditions, which force the wavefunction to be zero outside of the calculation grid, will be significant. The nature of the wavefunction will be primarily determined by the artificial effective infinite potential barriers beyond the calculation grid. For increasing energy, solutions will have a diminishing dependence on the quantum well. As discussed earlier, these solutions are not physically correct and are merely artifacts of the model. The physically correct solutions are a continuum of states above the barrier together with a series of resonance levels that play a role in the scattering of continuum states by the potential of the quantum well. However, these are not correctly calculated by `qwkpvb`.