`qwscal` – Quantum Well Scalar Conduction and Valence Subband Software USER'S MANUAL

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1 Purpose of the Software

The program `qwscal` gives the numerical solution 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 subband levels, as well as the spatial dependence of the confined wavefunctions. The solutions are obtained for electrons and for heavy and light holes, although the hole solutions are obtained in the scalar approximation. This means that the hole wavefunction basis states are taken to be spherically symmetric and uncoupled through the hamiltonian. Thus, the valence band solutions are quite similar to the conduction band solutions, differing only as the result of different masses and barrier heights. The associated program `qwkpvb` gives the valence band solution using a more accurate model that does include the appropriate coupling between the valence band basis states. However, `qwkpvb` is much more computationally demanding, taking a longer time than `qwscal` to give a solution. 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. Of course, `qwscal` gives perfectly accurate solutions for the conduction band states, since they are not coupled, as are the valence band states.

For each charge carrier type (electron, heavy hole, light hole), `qwscal` gives the subband levels and wavefunctions for six values of quantum well width, falling within the limits of 25 to 200 Å. The well depth can vary from 0.001 to 1.0 eV, and the carrier effective masses can vary from 0.001 to 1.0 m_0.

2 Design and Operation of the Software

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

$$\left(-\frac{\hbar^2}{2m^*}\frac{d^2}{dx^2} + V(x)\right)\psi(x) = E\psi(x), \tag{1}$$

with

$$V(x) = \begin{cases} V_0, 0 \leq x < a \\ 0, a \leq x \leq a + W \\ V_0, a + W < x \leq b \end{cases},$$

where W and V_0 are the width and depth, respectively, of the quantum well.

The axis x is divided up into a mesh, which for computational purposes, is confined to the interval of total length $b = 300$ Å: $x \in [0, b]$. The effective boundary conditions are $\psi(x) = 0$ for $x < 0$ and for $x > b$. The mesh is subdivided into NMESH=201 nodes with a separation $\Delta x = b/(\texttt{NMESH} - 1) = x_{i+1} - x_i$, for $i = 0, \ldots, \texttt{NMESH} - 1$.

The numerical solution proceeds by converting the differential equation (1) into a finite difference equation:

$$-\frac{\hbar^2}{2m^*}\left[\frac{\psi(x_i + \Delta x) - 2\psi(x_i) + \psi(x_i - \Delta x)}{(\Delta x)^2}\right] + V(x_i)\psi(x_i) = E\psi(x_i), \quad (2)$$

for $i = 1, \ldots, \texttt{NMESH} - 1$,

$$-\frac{\hbar^2}{2m^*}\left[\frac{\psi(x_i + \Delta x) - 2\psi(x_i)}{(\Delta x)^2}\right] + V(x_i)\psi(x_i) = E\psi(x_i), \quad (3)$$

for $i = 0$,

$$-\frac{\hbar^2}{2m^*}\left[\frac{-2\psi(x_i) + \psi(x_i - \Delta x)}{(\Delta x)^2}\right] + V(x_i)\psi(x_i) = E\psi(x_i) \quad (4)$$

for $i = \texttt{NMESH}$. Expressing the wavefunction ψ as an NMESH component vector, whose components are values of ψ at the discrete mesh points x_i, equations 2–4 can be recast as a tridiagonal matrix equation:

$$\begin{aligned} H\Psi &= E\Psi \\ H_{i,j} &= [C_0 - V(x_i)]\delta_{ij} + [-C_0/2](\delta_{i,j-1} + \delta_{i,j+1}) \\ \Psi &= [\psi(x_1), \ldots, \psi(x_{\texttt{NMESH}})], \end{aligned} \quad (5)$$

where $C_0 = \hbar^2/[m^*(\Delta x)^2]$. The program `qwscal` uses a widely available subroutine `TSTURM` to find the eigenvalues, E, and eigenvectors, Ψ, of the hamiltonian, H. Note that the form of the hamiltonian matrix gives rise to the effective boundary conditions $\psi(x) = 0$ for $x < x_1 (= 0)$ and for $x > x_{\texttt{NMESH}} (= b)$.

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.
- Loop over well size.

  - Loop over carrier type: electron, HH, LH
    * Set the barrier and well positions.
    * Set the potential profile.
    * Set the initial eigenvalue search range.
    * Calculate the hamiltonian matrix elements.
    * Initialize other input to the eigen-solver.
    * Solve for the eigenvalues and eigenvectors.
    * Possibly reduce upper limit of eigenvalue search range.
    * Output selected eigenvalues and eigenvectors.
    * Update calculation progress chart.
  - Do next carrier type.
- Do next well size.
- Finish calculation progress chart.
- Finish and close the information output file.
- Output lowest level wavefunctions, for each well size.
- Close the solution output files.

The program requires one single input file, `qwscal.inp`. This contains values of the three carrier effective masses, the two bandedge discontinuities and the six well widths. And example of this file is:

```
qwscal input parameters
 0.067    m^*_e; electron effective mass, in units of m0
 0.45     m^*_hh; heavy hole "       "         "      "
 0.09     m^*_lh; light hole "       "         "      "
 0.3      dE_c; conduction band discontinuity, in units of eV
 0.13     dE_v; valence      "       "         "      "     "
 130.0    w1; quantum well width #1; in units of angstroms
 140.0    w2; quantum well width #2; "         "      "
 150.0    w3; quantum well width #3; "         "      "
 160.0    w4; quantum well width #4; "         "      "
 170.0    w5; quantum well width #5; "         "      "
 180.0    w6; quantum well width #6; "         "      "
```

The first word of the first line must be "`qwscal`". This is used by the program to confirm the identity of the input file. The format of the masses and bandedge discontinuities must be `f6.3`. The format of the well widths 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 ten output files:

- one file of general information: `qwinfo.dat`;

- three files containing up to 10 subband levels for all six well widths: `qwsbel.dat` (electrons), `qwsbhh.dat` (heavy holes), `qwsblh.dat` (light holes);
- three files containing up to 10 wavefunctions for the last (and generally largest) well width listed in `qwscal.inp`: `qwwwel.dat` (electrons), `qwwwhh.dat` (heavy holes), `qwwwlh.dat` (light holes);
- three files containing the lowest level wavefunctions for each of the six well widths: `qww1el.dat` (electrons), `qww1hh.dat` (heavy holes), `qww1lh.dat` (light holes).

The limitation of up to 10 solutions in six of the files arises from the fact that the number of solutions found depends on the values of effective mass and well depth, and therefore varies from one parameter set to another. If a given set of parameters results in ten or less solutions, all of these are output in the files `qwsbel.dat`, `qwsbhh.dat`, `qwsblh.dat`, `qwwwel.dat`, `qwwwhh.dat`, `qwwwlh.dat`. On the other hand, if more than ten solutions are found, then only the lowest ten solutions are output. This achieves a practical limit on the size of the output files and satisfies most pedagogical purposes. To find the total number of states bound in the quantum well, these numbers are given for each of the charge carrier types in the file `qwinfo.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 `qwscal.inp`, above, `qwscal` generates the following `qwinfo.dat`.

```
GENERAL CALCULATION INFORMATION FROM PROGRAM qwscal.


            Eff. Mass (m0)     Barrier Ht. (eV)
            ------------------------------------
Electron       .067                 .300
Heavy Hole     .450                 .130
Light Hole     .090                 .130


Well #     Well Width W (A)
---------------------------
   1           130.0
   2           140.0
   3           150.0
   4           160.0
   5           170.0
   6           180.0


Calculation Mesh
----------------
Pitch dx =   1.50 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


Solutions
---------
Well #   EL #s   EL #b   HH #s   HH #b   LH #s   LH #b
-------------------------------------------------------
   1       5       3       8       6       3       3
   2       5       4       8       6       3       3
   3       5       4       8       6       4       3
   4       5       4       9       7       4       3
   5       5       4       9       7       4       3
   6       5       5       9       8       4       3


Energy level and wavefunction files
-----------------------------------
Subband energies, up to 10, for each W:
   electrons:   qwsbel.dat
   heavy holes: qwsbhh.dat
   light holes: qwsblh.dat

Wavefunctions, up to 10, at largest W:
   electrons:   qwwwel.dat
   heavy holes: qwwwhh.dat
   light holes: qwwwlh.dat

Lowest state wavefunctions, for each W:
   electrons:   qww1el.dat
   heavy holes: qww1hh.dat
   light holes: qww1lh.dat
```

First, the effective masses (in units of free electron mass) and barrier heights (in units of eV) are given for each charge carrier type.

Next, the six values of well width are given (in units of Å).

Under `Calculation Mesh` are given the value of Δx (`dx`) and the position of the barriers. In the above example, the first barrier extends from $x = 0$ Å to $x = 50$ Å; for the first well width $W = 130$ Å, the well extend from $x = 50$ Å to $x = 180$ Å and the second barrier extends from $x = 180$ Å to $x = 300$ Å; for the last well width $W = 180$ Å, the well extend from $x = 50$ Å to $x = 230$ Å and the second barrier extends from $x = 230$ Å to $x = 300$ Å.

Under `Solutions`, for each well width and each charge carrier type, the total number of solutions found (`#s`) and the number of solutions bound in the quantum well (`#b`), are shown. In the above example, for the first well, a total of five electron solutions were found by `TSTURM`, the lowest three of which were bound in the quantum well. For the second, through fifth wells, four of the five found solutions were bound in the quantum well. In the sixth well, all five solutions were bound in the quantum well. The columns headed `HH` pertain to the heavy hole and the ones headed `LH` pertain to the light hole. The reason that the total number of solutions found (`#s`) may exceed the number bound in the quantum well (`#b`), is that the effective boundary conditions, discussed above, of $\psi(x) = 0$ for $x < 0$ and for $x > b$, are equivalent to imposing barriers

of infinite height to the left of the first barrier and to the right of the second barrier. The additionally found solutions, that are not bound in the quantum well, are therefore modeling artifacts, arising as states boundin the artificial infinite quantum well imposed at the calculation boundaries. These additional solutions, therefore, do not represent realistic states in the semiconductor system and should be disregarded. In fact, since there are `NMESH`=201 grid points used in the calculation, `TSTURM` can, in principle, find 201 solutions. All, except the lowest ones, bound in the quantum well, are calculational artifacts.

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

2.2 Contents of `qwsb??.dat`

Up to 10 found subband energy levels, are given in these three files. The file `qwsbel.dat` contains data for electrons, `qwsbhh.dat` contains data for heavy holes, `qwsblh.dat` contains data for light holes. The energy levels are given for each of the six wel widths, one well width per line. The first column of each file is the well width, in units of Å. From the second column, on, are the subband energy levels, in ascending order, from lowest to highest value found. Using the parameters shown in `qwscal.inp`, above, the contents of `qwsbel.dat` are:

```
130.0     .2237E-01     .8813E-01     .1918E+00     .3100E+00     .3474E+00
140.0     .1968E-01     .7777E-01     .1705E+00     .2851E+00     .3455E+00
150.0     .1775E-01     .7026E-01     .1548E+00     .2628E+00     .3448E+00
160.0     .1583E-01     .6277E-01     .1388E+00     .2384E+00     .3367E+00
170.0     .1420E-01     .5641E-01     .1251E+00     .2165E+00     .3177E+00
180.0     .1300E-01     .5168E-01     .1149E+00     .1998E+00     .2981E+00
```

Although each row (well width) of the file gives five energy levels, not all are solutions bound in the quantum well. Referring to the contents of `qwscal.inp`, the electron barrier height is 0.3 eV. For the first well width, $W = 130$ Å, only the first three energy levels are below 0.3 eV. The remaining two solutions lie above the barrier and are not present in the real semiconductor system, as discussed above. For well widths in the range of $W = 140$ Å to 170 Å, four levels are found to lie within the quantum well, while all five levels are bound in the last well, of width $W = 180$ Å.

The contents of the other two files `qwsbhh.dat` and `qwsblh.dat`, yield to a similar interpretation, for heavy and light holes, respecitively.

2.3 Contents of `qwww??.dat`

Up to 10 found wavefunctions are given, as functions of position across the calculation grid, in these files. Due to the great amount of data involved, only the wavefunctions pertaining to the last of the six well widths, given in `qwscal.inp`,

are output to these files. Each row of each file corresponds to a single position, x, within the calculation grid. There are `NMESH`=201 rows in each file. The first column of each file gives the position, in units of Å, ranging from 0 to 300 Å. The second column give the potential energy profile, in units of eV. From the third column, on, are the wavefunctions, which directly correspond, one for one, with the subband levels in the corresponding `qwsb??.dat` file. The given wavefunctions correspond to the energy values in the last line (last well width) of the corresponding `qwsb??.dat`. Using the parameters, shown above, for `qwscal.inp`, some of the contents of `qwwwel.dat` are:

```
   .0     .300     .1503E-03    -.3557E-03     .7123E-03    -.1445E-02     .3026E-02
  1.5     .300     .3024E-03    -.7149E-03     .1430E-02    -.2895E-02     .6051E-02
  3.0     .300     .4579E-03    -.1081E-02     .2158E-02    -.4357E-02     .9078E-02
   .
   .

148.5     .000     .1188E+00     .3456E-01    -.1071E+00    -.6246E-01     .8397E-01
150.0     .000     .1183E+00     .3970E-01    -.1035E+00    -.7083E-01     .7630E-01
151.5     .000     .1178E+00     .4475E-01    -.9940E-01    -.7864E-01     .6772E-01
   .
   .

297.0     .300     .9272E-04     .2448E-03     .5984E-03     .1687E-02     .6291E-02
298.5     .300     .6124E-04     .1619E-03     .3965E-03     .1121E-02     .4194E-02
300.0     .300     .3045E-04     .8054E-04     .1975E-03     .5595E-03     .2097E-02
```

Column 3 contains the ground state wavefunction. Columns 4 through 7, of this example, contain the remaining four quantum well bound wavefunctions, in the order of ascending energy.

The contents of the other two files, `qwwwhh.dat` and `qwwwlh.dat`, yeild to a similar interpretation, for heavy and light holes, respectively.

2.4 Contents of `qww1??.dat`

The ground state wavefunctions for each of the six quantum well widths, are given as functions of position across the calculation grid, in these files. Each row of each file corresponds to a single position, x, within the calculation grid. From the second column to the seventh column, are the wavefunctions, corresponding to the first through sixth quantum well widths. The given wavefunctions correspond to the energy values in the first column of the corresponding `qwsb??.dat` file. Using the parameters, shown above, for `qwscal.inp`, some of the contents of `qww1el.dat` are:

```
   .0     .2352E-03     .2112E-03     .1938E-03     .1764E-03     .1615E-03     .1503E-03
  1.5     .4730E-03     .4248E-03     .3898E-03     .3548E-03     .3248E-03     .3024E-03
  3.0     .7159E-03     .6430E-03     .5901E-03     .5371E-03     .4918E-03     .4579E-03
   .
   .

148.5     .1064E+00     .1138E+00     .1175E+00     .1195E+00     .1196E+00     .1188E+00
150.0     .1038E+00     .1119E+00     .1160E+00     .1184E+00     .1189E+00     .1183E+00
151.5     .1011E+00     .1098E+00     .1144E+00     .1173E+00     .1182E+00     .1178E+00
   .
```

.

```
297.0     .4692E-05     .8593E-05     .1464E-04     .2764E-04     .5281E-04     .9272E-04
298.5     .3099E-05     .5676E-05     .9672E-05     .1826E-04     .3488E-04     .6124E-04
300.0     .1541E-05     .2823E-05     .4809E-05     .9077E-05     .1734E-04     .3045E-04
```

Column 2 contains the wavefunction for the first well width ($W = 130$ Å). Columns 3 through 7, contain the wavefunctions for the second through sixth well widths (140 Å — 180 Å). The contents of the other two files, `qww1hh.dat` and `qww1lh.dat`, yield to a similar interpretation, for heavy and light holes, respectively.

3 Examples

3.1 Compilation

```
% f77 -o qwscal.exe qwscal.f (or) % f90 -o qwscal.exe qwscal.f
(or)
% f90 -o qwscal.exe qwscal.f (or) % f90 -o qwscal.exe qwscal.f
qwscal.f:
 MAIN qwscal:
        tsturm:
        epslon:
        pythag:
%
```

3.2 Running

```
% qwscal.exe
```

```
                Calculation Progress
 Start |-------------------------------------| Finish
       |=====================================|
                  Calculation Done
```

```
% ls -1 qw*.dat
qwinfo.dat
qwsbel.dat
```

```
qwsbhh.dat
qwsblh.dat
qww1el.dat
qww1hh.dat
qww1lh.dat
qwwwel.dat
qwwwhh.dat
qwwwlh.dat
%
```

3.3 Variation of input parameters

Parameters in the input file `qwscal.inp` can be varied within the following ranges. Effective masses can vary from 0.001 to 1.0 m_0. Bandedge discontinuities can vary from 0.001 to 1.0 eV. Quantum well widths can vary from 25 to 200 Å. Generally, the quantum well widths are ordered in `qwscal.inp` from smallest to largest, although this is not necessary.

4 Trouble Shooting

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

4.1 Interpretation of source level error messages

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

The value of the identification string read from the parameter input file is not the expected value of "`qwscal`". This may indicate that the contents of `qwscal.inp` are generally bad. Fix: carefully compare the contents of your copy of `qwscal.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 electron m^* out of valid range.
Input value = AM
```

```
Valid range = [AMMIN,AMMAX]
Program halting.
```

The value of electron effective mass, AM, read from the input parameter file qwscal.inp is outside of the valid range of [AMMIN,AMMAX] = [0.001,1.0]. Fix: make sure that the electron effective mass, second line of qwscal.inp is within the above range and that it is in the format of f6.3.

```
Error:  input value of heavy hole m^* out of valid range.
Input value = AM
Valid range = [AMMIN,AMMAX]
Program halting.
```

The value of heavy hole effective mass, AM, read from the input parameter file qwscal.inp is outside of the valid range of [AMMIN,AMMAX] = [0.001,1.0]. Fix: make sure that the heavy hole effective mass, second line of qwscal.inp is within the above range and that it is in the format of f6.3.

```
Error:  input value of light hole m^* out of valid range.
Input value = AM
Valid range = [AMMIN,AMMAX]
Program halting.
```

The value of light hole effective mass, AM, read from the input parameter file qwscal.inp is outside of the valid range of [AMMIN,AMMAX] = [0.001,1.0]. Fix: make sure that the light hole effective mass, second line of qwscal.inp is within the above range and that it is in the format of f6.3.

```
Error:  input value of CB discontinuity out of valid range.
Input value = V0
Valid range = [V0MIN,V0MAX]
Program halting.
```

The value of conduction band discontinuity, V0, read from the input parameter file qwscal.inp is outside of the valid range of [V0MIN,V0MAX] = [0.001,1.0]. Fix: make sure that the CB discontinuity, fifth line of qwscal.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 = [V0MIN,V0MAX]
Program halting.
```

The value of valence band discontinuity, V0, read from the input parameter file qwscal.inp is outside of the valid range of [V0MIN,V0MAX] = [0.001,1.0]. Fix: make sure that the VB discontinuity, fifth line of qwscal.inp is within the above range and that it is in the format of f6.3.

```
Error:  input value of well width #I out of valid range.
Input value = W0
Valid range = [W0MIN,W0MAX]
Program halting.
```

The value of quantum well width #I, W0, read from the input parameter file qwscal.inp is outside of the valid range of [W0MIN,W0MAX] = [100.0,200.0]. Fix: make sure that the I-th, well width, I+6-th line of qwscal.inp is within the above range and that it is in the format of f6.1.

```
Error: M subbands found in interval [LB,UB].
This exceeds initial estimate of MM subbands.
Program halting.
```

More subbands (M) were found in the specified energy interval [LB,UB], than the initial stated estimate of MM subbands. The eigen-solver TSTURM reserves only MM elements to return the found eigenvalues and therefore does not have enough storage to return the complete solution. Fix: increase the value of MM input to TSTURM, to be at least as large as M. This requires alteration of the program source code.

```
Error: convergence failure for wavefunction #X.
Program halting.
```

The routine TSTURM has failed to compute the X-th eigenvector within five iterations. Quick fix: decrease the interval [LB,UB] so that less than X eigensolutions are found. Better fix: study the source code of TSTURM and figure out why the convergence is failing in this case. This requires alteration of the program source code.

```
Error: unclassified non-normal return from TSTURM;  IERR = X
Program halting.
```

The value of the error flag IERR does not correspond to a classified error, nor to a normal, no-error condition. The returned value of IERR is X. This requires examination of the source code.

4.2 Trouble associated with the input file

Erroneous behavior of the program may result from the use of an input file `qwscal.inp` whose contents do not conform to rather strict formatting specifications. The first six characters of the first line of the file `qwscal.inp` must be "`qwscal`". The rest of this line is arbitrary. The effective masses and band edge discontinuities 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 six quantum well widths must appear in the first six columns of the seventh through twelfth lines of the input file. These values must have their decimal point in the fifth column, being in the FORTRAN format of `f6.1`. The text on lines 2 through 12, 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 `qwscal` are discussed here.

One limitation of the model concerns the discrete nature of the calculation grid. The mesh pitch Δx 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 Δx. Thus, wells which are only a few Δx 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 `qwscal`.