Abstract

It is possible to fabricate mesoscopic structures where at least one of the dimensions is of the order of de Broglie wavelength for cold electrons. By using semiconductors, composed of more than one material combined with a metal slip-gate, two-dimensional quantum tubes may be built. We present a method for predicting the transmission of low-temperature electrons in such a tube. This problem is mathematically related to the transmission of acoustic or electromagnetic waves in a two-dimensional duct. The tube is asymptotically straight with a constant cross-section. Propagation properties for complicated tubes can be synthesised from corresponding results for more simple tubes by the so-called Building Block Method. Conformal mapping techniques are then applied to transform the simple tube with curvature and varying cross-section to a straight, constant cross-section, tube with variable refractive index. Stable formulations for the scattering operators in terms of ordinary differential equations are formulated by wave splitting using an invariant imbedding technique. The mathematical framework is also generalised to handle tubes with edges, which are of large technical interest. The numerical method consists of using a standard MATLAB ordinary differential equation solver for the truncated reflection and transmission matrices in a Fourier sine basis. It is proved that the numerical scheme converges with increasing truncation.

1 Introduction

In the search for faster computers critical parts are becoming smaller. Today, it is possible to build mesoscopic structures where some dimensions are of the order of the de Broglie wavelength for cold electrons. Often the electron motion is confined to two dimensions. Consequently, it may be necessary, at least for some computer parts, to include quantum effects in the design process.

A large number of studies, devoted to such quantum effects, have been carried out in recent years and a review is given by Londegan et al [1]. Many
investigations aim at understanding the physical properties of a particular quantum tube rather than developing reliable mathematical and numerical methods that can be used in a more general context. The research has given valuable knowledge on the physical behaviour but also reports on the limitations of the methods used. For instance, Lin & Jaffe [2] report that a straightforward matching at the boundary of a circular bend does not converge, demonstrating the numerical problems with such a method. An illposedness is present in quantum tube scattering and some type of regularisation is therefore required to avoid large errors. Often, the tubes have sharp corners to facilitate manufacturing but also to enhance quantum effects. The presence of corners with attached singularities requires special treatment.

Scattering of electrons in quantum tubes, see figure 1, is theorywise related to the scattering of acoustic and electromagnetic waves in ducts. Nilsson [3] treats a general method for the acoustic transmission in curved ducts with varying cross-sections. Wellposedness, i.e. stability, is achieved in an asymptotic sense. The mathematical framework guarantees consistent results and allows for sharp corners and a proof for numerical convergence is given. We set out to present a quantum version of the results of Nilsson [3]. In this way the problems reported on convergence [2] and on inconsistent mathematical results would be resolved.

The paper is organised as follows. An introduction to scattering in quantum tubes is given in section 2 and a mathematical model is formulated in section 3. The Building block Method which is a systematic method to analyse complicated tubes in terms of results for simple tubes is also briefly described. Then in section 4 the scattering problem for the curved tube with varying cross-section and constant potential is reformulated to a scattering problem for a straight tube with a varying refractive index. The solution to this problem is presented in section 5 and a discussion on numerical methods are also given.
2 Tubes in quantum heterostructures

A schematic view of a quantum heterostructure is shown in figure 2 following Wu et al. Electrons are emitted from the n-type doped AlGaAs layer, migrate into the GaAs layer and stay close to the boundary to the AlGaAs layer. In this way a very narrow layer of electrons which are free to move in a plane is formed. Nearly all the electrons in this two-dimensional gas are in the same quantum state. By applying a negative potential on the metal electrodes on the top of the heterostructure in figure 1, the electrons are banished from the region below the electrodes. For relatively low voltages, the effective potential in the tube for one electron is close to the square-well potential. As a consequence the electrons in the two-dimensional gas are further restricted to a tube that in form is a mirror picture of the gap between the two electrodes. This quantum tube links the electrons between the two two-dimensional gases on both sides of the strip formed by the electrodes.

![Diagram of heterostructure and split-gate structure.](image)

Figure 2: Schematic picture of heterostructure and split-gate structure.

3 Mathematical model

Consider a two-dimensional tube with interior $\Omega'$ according to figure 1. The boundary $\Gamma'$ consists of two continuous curves, $\Gamma'_+$ and $\Gamma'_-$, which are piecewise $C^2$. The upper boundary $\Gamma'_+$ can be continuously deformed to $\Gamma'_-$ within $\Omega'$. Outside a bounded region the duct is straight with constant widths $a$ and $b$, respectively. These terminating ducts are called the left and the right termi-
nating duct or L and R for short. We use stationary scattering theory for one electron in an effective potential, with time dependence \( \exp(-iEt/\hbar) \), assuming that the wave function \( \psi \) satisfies the time-independent Schrödinger equation
\[
\triangle \psi + k^2 \psi = 0 \quad \text{in } \Omega',
\]
where \( k^2 = 2m^*E/\hbar \) and \( m^* \) is the effective mass. Usually \( k^2 \) is called energy. The effective potential is assumed to be a square well meaning that \( \psi_{\Gamma'} = 0 \).

In a tube with constant cross-section the harmonic wavefunction \( \psi \) can be uniquely decomposed in leftgoing and rightgoing parts by \( \psi = \psi^+ + \psi^- \). Super indices "\( + \)" and "\( - \)" indicate rightgoing or plus and leftgoing or minus waves respectively. Let \( \psi^+_{in} \) and \( \psi^-_{in} \) be known incoming waves in the terminating ducts. \( \psi^+_\text{in} \) is present in the left and \( \psi^-\text{in} \) in the right one. Let us write
\[
\begin{align*}
\psi &= \psi^+_\text{in} + R^+ \psi^+_\text{in} + T^- \psi^-\text{in} \quad \text{in L} \\
\psi &= \psi^-\text{in} + R^- \psi^-\text{in} + T^+ \psi^+_\text{in} \quad \text{in R},
\end{align*}
\]
where for example the last two terms in (1a) are minus waves and the equation defines the left reflection mapping \( R^- \) that maps the incoming wave to an outgoing one in L. The scattering problem consists of finding the mappings \( R^+, T^-, R^- \) and \( T^+ \) as functions of energy for a given duct. In summary we have
\[
\begin{align*}
\triangle \psi + k^2 \psi &= 0 \quad \text{in } \Omega' \\
\psi_{\Gamma'} &= 0 \\
\psi^+ &= \psi^+_\text{in} \quad \text{in L} \\
\psi^- &= \psi^-\text{in} \quad \text{in R},
\end{align*}
\]

There is always a solution to (2), and except for a discrete number of eigenenergies \( k^2 = k^2_i, i = 1, 2, 3, ..., \) the solution is unique. When \( k^2 = k^2_i \), an eigenenergy, there exists a solution without incoming but with outgoing waves.

The use of the Building Block Method or transfer matrix formalism is very efficient for the solution of scattering problems. In this method a tube with a complicated geometry is divided into two parts usually where the tube is straight. These two parts are converted to the type shown in figure 1 by extending the terminating tubes to infinity. A sub tube for the tube shown in figure 1 originates from the left part and is depicted in figure 3. The Building Block Method gives a procedure for calculating the mappings \( R^+, T^-, R^- \) and \( T^+ \) for the entire tube in terms of the corresponding scattering properties for the sub tubes. This procedure can be repeated to get several sub tubes. Rather than using a general numerical package for conformal mappings we have for the calculations in this paper employed the Schwarz-Christoffel mapping for a duct with corners and rounding the corners using the methods of Henrici. Required analytic integrations are performed in MATHEMATICA.

We recall the standard duct theory in a form that illustrates the illposed-
Figure 3: Sub-tube with interior $\Omega'$ and upper boundary $\Gamma'_+$ and lower boundary $\Gamma'_-. b/a = 0.6.$

ness of the problem and we have

$$\psi = \psi^+ + \psi^- = \sum_{n=1}^{\infty} A_n^+ e^{i\alpha_n x} \varphi_n(y) + \sum_{n=1}^{\infty} A_n^- e^{-i\alpha_n x} \varphi_n(y), \quad (3)$$

with $\varphi_n(y) = \sin(n\pi y/a)$ and $\alpha_n = \sqrt{k^2 - n^2\pi^2/a^2}$, $\text{Im} \alpha_n \geq 0$. It is convenient to define the operator $B_0$ by

$$\begin{cases} B_0 f = \sum_{n=1}^{\infty} \alpha_n f_n \varphi_n, \\ f(y) = \sum_{n=1}^{\infty} \alpha_n f_n \varphi_n(y) \end{cases} \quad (4)$$

We find that $B_0^2 = \partial_x^2 + k^2$ and $\partial_x \psi^\pm = \pm iB_0 \psi^\pm$. The initial value problem,

$$\begin{cases} \partial_x \psi^+(x) = iB_0 \psi^+(x), \\ \psi^+(0) = \psi_0, \end{cases} \quad (5)$$

is illposed for $x < 0$, but not for $x > 0$. If an attenuated plus wave is marched to the left an exponential growth is found. To avoid the illposedness, $\psi$ is decomposed and the plus waves are calculated by marching to the right and minus waves in the opposite direction.

4 Reformulated scattering problem

To be able to use powerful spectral methods it is advantageous to transform the tube to a flat boundary. It is enough, according to the Building Block Method, to consider the scattering in the sub tubes and we restrict ourselves to the first part as shown in figure 3. One way of transforming the tube is to use a conformal mapping $w(\zeta)$ transforming the interior $\Omega'$ of the tube with variable cross-section in the $\zeta = x + iy$ plane (figure 3) to the interior $\Omega$ of a straight
tube with constant cross-section in the $w = u + iv$ plane. The straight tube is described by $-\infty < u < \infty$, $0 < v < a$.

Introducing $\phi(u, v) = \psi(x, y)$ we get

$$\begin{align*}
\partial^2_u \phi + B^2(u) \phi &= 0 \text{ in } \Omega \\
\phi(u, 0) &= \phi(u, a) = 0, u \in \mathbb{R},
\end{align*}$$

with $B^2(u) = \partial_u^2 + k^2 \mu(u, v)$ and $\mu = |d\zeta/dw|^2$. $\mu(u, v)^{-1}$ can be denoted as a refractive index for the straight tube. In figure 4, $\mu$ related to the simple tube in figure 3 is depicted. The factor $\mu(u, v)$ is asymptotically constant at both ends of the tube or more precisely $\mu(u, v) = \mu_\pm + O(e^{\mp |cu|}), u \to \pm \infty$ with $\mu_- = 1$ and $\mu_+ = (b/a)^2$.

We use a first order description and rewrite (6a) as

$$\begin{align*}
\partial_u \left( \begin{array}{c} \phi \\ \partial_u \phi \end{array} \right) &= \left( \begin{array}{cc} 0 & 1 \\ -B^2 & 0 \end{array} \right) \left( \begin{array}{c} \phi \\ \partial_u \phi \end{array} \right).
\end{align*}$$

To avoid illposedness the decomposition $\phi = \phi^+ + \phi^-$ is introduced which must be identical to the corresponding decomposition (\ref{eq:decomposition}) in regions where $\mu$.

Figure 4: $\mu(u, v)$ in the straight duct. Parameters as in figure 3. $\mu^{-1}$ is the refractive index.
is a constant. The new state variables \((\phi^+, \phi^-)\) are introduced via the linear relation

\[
\begin{pmatrix}
\phi \\
\partial_u \phi
\end{pmatrix} = \begin{pmatrix}
1 & 1 \\
iC & -iC
\end{pmatrix}
\begin{pmatrix}
\phi^+ \\
\phi^-
\end{pmatrix}.
\] (8)

Solving (8) for \(\phi^+\) and \(\phi^-\) and taking the \(u\)-derivative and using a similar notation as Fishman [10], we find that

\[
\partial_u \begin{pmatrix}
\phi^+ \\
\phi^-
\end{pmatrix} = \begin{pmatrix}
\alpha & \beta \\
\gamma & \delta
\end{pmatrix}
\begin{pmatrix}
\phi^+ \\
\phi^-
\end{pmatrix},
\] (9)

where

\[
\begin{align*}
\alpha &= \frac{1}{2}[(\partial_u C^{-1})C + iC^{-1}B^2 + iC] \\
\beta &= \frac{1}{2} - (\partial_u C^{-1})C + iC^{-1}B^2 - iC] \\
\gamma &= \frac{1}{2} - (\partial_u C^{-1})C - iC^{-1}B^2 + iC] \\
\delta &= \frac{1}{2} [(\partial_u C^{-1})C - iC^{-1}B^2 - iC]
\end{align*}
\] (10)

To generalize the concept of transmission operators we make them \(u\)-dependent, using a similar notation as Fishman [10]

\[
\begin{pmatrix}
\phi^+(u_2) \\
\phi^-(u_1)
\end{pmatrix} = \begin{pmatrix}
T^+(u_2, u_1) & R^-(u_1, u_2) \\
R^+(u_2, u_1) & T^-(u_1, u_2)
\end{pmatrix}
\begin{pmatrix}
\phi^+(u_1) \\
\phi^-(u_2)
\end{pmatrix},
\] (11)

assuming that \(u_1 \leq u_2\) and suppressing the explicit \(u\)-dependence. It is assumed for (11) that the scattering problem has a unique solution or that homogenous solutions are removed. A homogenous solution is usually called a bound state.

Next we find a differential equation for the scattering operators \(T^+(u_2, u_1)\), \(R^-(u_1, u_2)\), \(R^+(u_2, u_1)\) and \(T^-(u_1, u_2)\) in (11) using the invariant imbedding technique [10], [11]. It is required that the incoming wave from the right, \(\phi^-(u_2)\), is vanishing. Then put \(u_1 = u\), find \(\partial_u \phi^-(u)\) from (11), use (11) once more to obtain

\[
\partial_u R^+(u_2, u) = \gamma + \delta R^+(u_2, u) - R^+(u_2, u)\alpha - R^+(u_2, u)\beta R^+(u_2, u),
\] (12)

In a similar manner we get

\[
\partial_u T^+(u_2, u) = -T^+(u_2, u)\alpha - T^+(u_2, u)\beta R^+(u_2, u).
\] (13)

The stability properties of (12) and (13) are of central importance. In the flat regions where \(B = B_+\) or \(B_-\) we have \(C = B\) and \(\partial_u C^{-1} = 0\) implying that \(\beta = \gamma = 0\) and \(\alpha = -\delta = iB\). Similarly (12) and (13) reduce to \(\partial_u X^+ = -iBX^+, X^+ = R^+\) or \(T^+\), equations which are well-posed for marching to the left. The initial values to accompany (12) and (13) are \(R^+(u_2, u_2) = 0\) and \(T^+(u_2, u_2) = I\), where \(I\) is the identity operator.

We choose \(C = B_- + f(u)(B_+ - B_-)\) that is independent of \(v\). Here \(f\) is increasing and smooth with \(\lim_{u \to -\infty} f(u) = 0\), and \(\lim_{u \to \infty} f(u) = 1\).
5 Solution of the scattering problem

For the numerical solution of the scattering operator we expand $\phi$ in a Fourier sine series and $\mu$ in a Fourier cosine series:

$$
\phi(u, v) = \sum_{n=1}^{\infty} \phi_n(u) \phi_n(v),
$$

$$
\mu(u, v) = \sum_{n=0}^{\infty} \mu_n(u) \xi_n(v),
$$

where $\xi_n(v) = \cos(n\pi/a)$. Using the notation $\phi = (\phi_0, \phi_1, \ldots)^T$ we find that

$$
\frac{d^2 \phi(u)}{du^2} + B^2(u) \phi(u) = 0.
$$

The matrix elements of $B^2(u)$ are given by

$$
B^2(u)_{nm} = \frac{k^2}{2} [\mu_{m+n}(u) - \mu_{m-n}(u) - \mu_m + \mu_{-m}(u)] - \frac{n^2 \pi^2}{a^2} \delta_{nm}, \quad n, m = 0, 1, 2, \ldots,
$$

and it is understood in (16) that $\mu_l(u) = 0$ for negative $l$.

For the tube in the physical $\zeta-$plane we require that locally both the potential and the kinetic part of the energy are finite, that is both

$$
\int_X |\psi|^2 \, dxdy < \infty
$$

and

$$
\int_X |\nabla \psi|^2 \, dxdy < \infty
$$

for all finite regions $X$ inside the tube. We say that $\psi$ belongs to the Sobolev space $H^1_{\text{loc}}$ meaning that $\psi$ and its first derivatives are locally square integrable. Transformed to the straight duct the local finite energy requirement means

$$
\int_U |\phi|^2 \, dudv < \infty
$$

and

$$
\int_U |\nabla \phi|^2 \, dudv < \infty
$$

for all finite regions $U$ inside the tube. For a smooth boundary $\phi$ is more regular, and also the second derivatives of $\phi$ are square integrable, that is $\phi \in H^2_{\text{loc}}$. It follows from the theory of Grisvard [12] that also the second derivatives of $\phi$ are square integrable, which means that $\phi \in H^2_{\text{loc}}$. According to a graph theorem [13] $\phi \in H^2_{\text{loc}}$ implies that $\phi(u, \cdot) \in H^{3/2}(0, a)$, meaning that up to $3/2$ derivatives are square integrable. To interpret this regularity with fractional derivatives we define, following Taylor [13], the function space

$$
D_s = \left\{ f \in L^2(0, a) : \sum_{n=0}^{\infty} |f_n|^2 \left(1 + n^2\right)^s < \infty \right\}, \quad s \geq 0,
$$

with $f = \sum_{n=1}^{\infty} f_n \varphi_n$ and $f_n = (f, \varphi_n)/(\varphi_n, \varphi_n)$. $D_s$ is a Hilbert space with the norm

$$
||f||^2_{D_s} = (f, f) = \sum_{n=1}^{\infty} |f_n|^2 \left(1 + n^2\right)^s.
$$

Taylor [13] shows that $D_0 = L^2(0, a)$, $D_1 = H^1_0(0, a)$, $D_2 = H^2(0, a) \cap H^1_0(0, a)$ and that $\partial_s D_s = D_{s-1}$, $s \geq 1$. In this terminology we have that for a smooth boundary $\phi(u, \cdot) \in D_{3/2}$. 

8
The operator $\partial^2_v$ is self-adjoint on $D_{3/2}$. Thus, we may define $B_{\pm}$ by

$$B_{\pm} f = \sum_{n=1}^{\infty} \sqrt{k^2\mu_{\pm} - n^2\pi^2/a^2} f_n \varphi_n,$$

assuming that the branch $\text{Im} > 0$ of the square root is taken. It is clear that $T^+, R^-, R^+$ and $T^-$ are mappings $D_{3/2} \rightarrow D_{3/2}$ and $B_{\pm}: D_s \rightarrow D_{s-1}, s \geq 1$.

For tubes with edges in the $\zeta$-duct things are a little more complicated. With no restriction on the sharpness of the edges we cannot improve that $\phi \in H^1_{\text{loc}}$, implying $\phi(u, \cdot) \in D_{1/2}$. Then, as an intermediate step in our calculations $B_{\pm}\phi$ should be in the space $D_{-1/2}$. Such a derivative must of course be interpreted as a distribution. However, the end result, i.e. scattered wave function belongs to $D_{1/2}$. To generalise we define by duality for positive $s$

$$D_{-s} = \left\{ g : \int_0^a f(v) g(v) dv < \infty \text{ for all } f \in D_s \right\}.$$

Multiplication by $\sqrt{\mu}$ is an operator $D_{1/2} \rightarrow D_{-1/2}$ and if $s \geq 1/2$ we have the following mapping properties: $B_{\pm}: D_s \rightarrow D_{s-1}, \partial_v: D_s \rightarrow D_{s-1},$ and $T^+, R^-, R^+$ and $T^-$ are mappings $D_s \rightarrow D_s$.

The equations (12-13) can only in very special cases be solved in a closed form. Therefore some type of numerical scheme is used. Generally a numerical method cannot give uniform convergence for the entire space $D_s$. In a practical application it is usually sufficient to know the effect of the scattering matrices on the lowest eigenfunctions, the first $N_0$ say. A practical method is therefore to truncate the matrix representation of (12) - (13) to $N >> N_0$ and solve the finite-dimensional ordinary differential equation with a standard numerical routine. Nilsson [3] proves that such a procedure converges when $N \rightarrow \infty$.

Presently, numerical results are not available for the quantum tube scattering. However, Nilsson [3] presents results for the acoustic case where the Neumann rather than the Dirichlet boundary condition applies. He reports that for the lowest order reflection coefficient $N = 1$, i.e. a scalar solution, is accurate up to $ka = 1.5$, $N = 2$ gives a good and $N = 5$ gives a perfect description up to $ka = 6$. Energy conservation holds for all $N$.

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