Transmission through graded interfaces in the displacement operator method

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Abstract
The transmittivity of a graded heterojunction within the displacement operator framework is studied using the transfer matrix approach. Transmission resonances are observed to be enhanced by large interface widths. The parameter $\gamma$, generator of non-additive translations is observed to orchestrate regimes of enhanced and suppressed transmission.

1. Introduction
In semiconductor materials with non-uniform chemical composition, the effective mass becomes a variable quantity [1–3]. Its dependence on position is engineered according to a grading function that governs the spatial variation of the mole fraction of one of the constituents of the alloy. The grading results in the potential energy function having a similar profile to that of the effective mass [4]. Systems with variable mass have received extensive theoretical attention with regards to enhancing the engineering of electronic optical and transport properties of heterostructures. The methods commonly used in the resolution variable mass systems include: the path integral approach [5], the super symmetric quantum mechanics approach [6] the Darboux Transform method [7], the de Broglie–Bohm approach [8], the factorization approach [9] and the analytic transfer matrix approach [10].

Setting up a proper Hamiltonian with variable mass requires adequate ordering of the effective mass operator and the momentum operator for Hermiticity to be ensured in the kinetic energy operator. There is ambiguity in ordering these operators since this cannot be done in a unique way. This ambiguity is portrayed in the most general variable mass kinetic energy operator proposed by von Roos [11] through 3 parameters termed ‘ordering ambiguity parameters’ which can be set arbitrarily. The non-uniqueness in the definition of a variable mass kinetic energy operator has motivated many authors to attempt consistent theories with variable mass. In the displacement operator approach introduced by Costa et al [12], to arrive at an effective variable mass, one starts from a constant mass system which is assumed to undergo non-additive translations such that the deformed momentum operator describing such displacements gives rise to a position-dependent effective mass. This formalism has been addressed for a system in null and constant potentials [13], double well [14], parabolic [15] and Coulomb-like [16] potentials. Its classical field theory has also been established [17]. Further more, the formalism has been applied successfully in the study of: the influence of interface potential on the effective mass in Ge nanostructures [18], Quantum confinement in Si and Ge quantum wells [19], the role of quantum confinement in luminescence efficiency of group IV nanostructures [20]. Yet its effective application to compositionally graded interfaces has not been addressed.

In this work, in a bid to assess the transmittivity of a heterointerface whose grading produces an effective mass profile that conforms to the displacement operator-derived effective mass function introduced in section 2, we have in section 3 presented the model and in section 4, applied the transfer matrix approach. Sensitivity of the transmission to system energy, interface width and the space deformation parameter have been discussed alongside features such as the need to readjust the definition of transmission probability in terms of probability currents within the variable mass scenario. Concluding remarks are presented in section 5.
2. Position-dependent mass Schrödinger equation

The generalized form for the position-dependent effective mass Schrödinger equation was proposed by von Roos \([11]\) as follows:

\[
\frac{1}{4}(m^0 p^0 \nabla^2 + m^0 p^0 \nabla^0) \psi(x) + [V(x) - E] \psi(x) = 0,
\]

where \(p = -i\hbar \partial_x\), and the ordering ambiguity parameters \(a, b,\) and \(c\) in the kinetic energy operator can be chosen arbitrarily but are constrained by the relation \(a + b + c = -1\). By setting the parameters as: \(a = c = -\frac{1}{4}\) and \(b = -\frac{1}{2}\), equation (1) reads

\[
-\frac{\hbar^2}{2} \left[ \frac{1}{m^{1/4}} \frac{d}{dx} \frac{1}{m^{1/4}} \frac{d}{dx} \right] \psi(x) + [V(x) - E] \psi(x) = 0.
\]

Performing the substitution \(\psi(x) = m^{1/4} \psi(x)\), equation (2) takes the following non-Hermitian form:

\[
-\frac{\hbar^2}{2} \left[ \frac{1}{m^{1/4}} \frac{d}{dx} \frac{1}{m^{1/4}} \frac{d}{dx} \right] \psi(x) + [V(x) - E] \psi(x) = 0.
\]

The systems equations (4) and (2), related through the transformation equation (3), will have the same set of eigenvalues and will differ only at the level of their eigenstates.

If the effective mass is chosen in the form

\[
m(x) = \frac{m_0}{(1 + \gamma x)^2} \quad \text{in} \quad 0 \leq x \leq L,
\]

where \(0 \leq x \leq L\) is the interfacial region between two dissimilar semiconductors where the effective mass is variable. We note that \(m(x)\) as in equation (4) remains finite within the domain if the parameter \(\gamma\) satisfies the constraint

\[
\gamma \geq 0.
\]

Using equations (3), (4) can be rewritten as

\[
\left[ \frac{\hbar^2}{2m_0} (1 + \gamma x) \frac{d}{dx} \frac{1}{1 + \gamma x} \frac{d}{dx} - V(x) + E \right] \psi(x) = 0.
\]

From where identifying the deformed momentum operator

\[
p_\gamma = -i\hbar \left( 1 + \frac{\gamma}{x} \frac{d}{dx} \right),
\]

it becomes clear that equation (8) is exactly the same as the displacement operator-derived Schrödinger equation \([12]\) which was arrived at, starting with an infinitesimal translation operator of the form

\[
T_\gamma (dx) = 1 + \frac{dx}{\hbar} p_\gamma.
\]

The commutation relation

\[
-i\hbar \left[ \frac{1}{m^{1/4}} \frac{d}{dx} \frac{1}{m^{1/4}} \right] x = -i\hbar (1 + \gamma x) = [p_\gamma, x],
\]

implies that the original system equation (2) and the transformed system equation (4) in addition to being isospectral, have the same form for the uncertainty product which reads

\[
\Delta x \Delta p_\gamma \geq \frac{\hbar}{2} (1 + \gamma (x)).
\]

3. Application to compositionally graded interfaces

Consider a ternary alloy such as Al\(_x\)Ga\(_{1-x}\)As in which the mole fraction \(\delta\) of Al is varied at the interface according to the grading function.
The grading profile in equation \((12)\) is experimentally realizable. In practice, tailoring the grading profile makes it possible to fabricate quantum wells of desired shapes \([4, 21]\).

The effective mass for the entire structure, with profile shown in figure 1 is given in the three ensuing regions by

\[
M(x) = \begin{cases} 
  m_0 & \text{in } x < 0 \\
  \frac{m_0}{(1 + \gamma x)^2} & \text{in } 0 \leq x \leq L, \\
  m_L & \text{in } x > L
\end{cases}
\]

and the potential energy function reads

\[
U(x) = \begin{cases} 
  V_0 & \text{in } x < 0 \\
  \frac{V_0}{(1 + \gamma x)^2} & \text{in } 0 \leq x \leq L, \\
  V_L & \text{in } x > L
\end{cases}
\]

where

\[
V_L = \frac{V_0}{(1 + \gamma L)^2} = V_0 \delta(L) = V_0 \delta_L,
\]

\[
m_L = \frac{m_0}{(1 + \gamma L)^2} = m_0 \delta(L) = m_0 \delta_L.
\]

By defining the effective mass discontinuity as \(\delta_L = \frac{m_0}{m_L}\), it can be seen that the parameter \(\gamma\) is given by

\[
\gamma = \frac{1}{L} (\delta_L^{1/2} - 1),
\]

and is completely determined by the material parameters (the effective mass mismatch \(\delta_L\) and the interface width \(L\)). Since \(m_0 > m_L\), it follows from equation \((16)\) that \(\gamma\) satisfies the constraint equation \((6)\).

With the graded interface of width \(L\) located at \(0 \leq x \leq L\), it is apparent that \(\gamma x \geq 0\). This guarantees that the momentum operator equation \((2)\) and the fundamental commutator equation \((5)\) will not vanish anywhere within the interface. This also shows that the domain of \(\delta\) is \(0 \leq \delta \leq 1\), which is to be expected for any grading function.

Figure 1. Plot of the effective mass, potential and the first three eigenstates of a system at a heterojunction graded according to the displacement operator formalism. Parameter values used are: \(m_0 = 0.146\), \(V_L = 0.5\), \(\hbar = 1\), \(L = 20\). With this choice of the interface width, only the ground satisfies \(E < V\).
Effecting the variable change
\[ u = \int_{0}^{x} \frac{dx}{(1 + \gamma x)}; \quad (1 + \gamma x) = e^{\omega}; \quad (1 + \gamma x) \frac{d}{du} = \frac{d}{dx}, \] (17)
the potential energy function becomes
\[ U(u) = \begin{cases} V_0 & \text{in } u \leq 0 \\ V_0 e^{-\gamma u} & \text{in } 0 < u < \frac{1}{\gamma} \ln (1 + \gamma u) \\ V_1 & \text{in } u \geq \frac{1}{\gamma} \ln (1 + \gamma u) \end{cases}. \] (18)

Since we are interested in transmission through the structure, it is necessary to solve the Schrödinger equation in each region and match the solutions across the boundaries. At the graded interface, the similarity transformation equation (17) reduces the time-independent Schrödinger equation to the constant mass problem
\[ \frac{\hbar^2}{2m_0} \frac{d^2}{du^2} \psi(u) + [V_0 e^{-\gamma u} - E] \psi(u) = 0. \] (19)

With the substitutions
\[ z = \frac{\sqrt{2m_0 V_0}}{E} e^{-\gamma u}; \quad n = \frac{\sqrt{-2m_0 E}}{E}, \] (20)
equation (14) can be rewritten as
\[ z^2 \frac{d^2}{dz^2} \psi(z) + z \frac{d}{dz} \psi(z) - [z^2 + n^2] \psi(z) = 0, \] (21)
whose solution in the limit \( L \to \infty \) is obtained in terms of the modified Bessel functions \( I_n/K_n \) of the first/second kinds respectively, i.e.
\[ \psi_n(z) = C I_n(z) + D K_n(z), \] (22)
and the spectral values are
\[ E_n = \frac{-\hbar^2 \gamma^2 n^2}{2m_0}. \] (23)

Using equations (3) and (17) the solution to the original problem is obtained as
\[ \phi_n(x) = Cm(x)^{1/4} I_n \left[ \frac{2m_0 V_0}{\hbar \gamma} (1 + \gamma x)^{-1} \right] + Dm(x)^{1/4} K_n \left[ \frac{\sqrt{2m_0 V_0}}{\hbar \gamma} (1 + \gamma x)^{-1} \right]. \] (24)

For finite \( L \), an exact analytic solution is not possible, however, an estimate of the bound states can be obtained numerically. The first three eigenstates are shown on figure 1 while the first ten eigenvalues obtained through the finite element method \([22]\) are given on table 1.

### 4. Evaluation of transmission probability

To evaluate the transmission probability, we will use the transfer matrix method. Approximation of the grading profile and consequently the potential and effective mass is customarily done by slicing the graded region in to \( n \) rectangular barriers \([23]\) with \( n + 1 \) interfaces located at \( x_0, x_1, ... x_n \), where \( x_0 = 0 \) and \( x_n = L \). We will take the effective mass and potential in each piece as the classical average in that region such that
\[ m_i = \frac{1}{x_{i+1} - x_i} \int_{x_i}^{x_{i+1}} m_0 \frac{dx}{(1 + \gamma x)^2} = \frac{m_0}{(x_{i+1} + 1)(x_i + 1)}, \]
\[ V_i = \frac{1}{x_{i+1} - x_i} \int_{x_i}^{x_{i+1}} V_0 \frac{dx}{(1 + \gamma x)^2} = \frac{V_0}{(x_{i+1} + 1)(x_i + 1)}, \] (25)
where \( i = 0, 1, 2, ... n - 1 \). The wave vector in each piece will be
\[ k_i = \sqrt{2m_i(E_n - V_i)}/\hbar^2, \] (26)
and the solution to Schrödinger equation in each piece will be
\[ \phi = C_i e^{ik_i x} + D_i e^{-ik_i x}. \] (27)
In the limit of a single barrier, the solution

$$\phi = C e^{ik_0 x} + D e^{-ik_0 x},$$

for which imposing the respect of boundary conditions yields the spectrum

$$E_n = \frac{\hbar^2 \pi^2 n^2}{2mL^2} + V_0,$$

has to be matched to the plane wave solutions

$$Ae^{ik_0 x} + Be^{-ik_0 x}, \quad x < 0,$$

and

$$Ge^{ik_x x} + Fe^{-ik_x x}, \quad x > L,$$

where $k_0 = \sqrt{2m_0 (E - V_0) / \hbar^2}$ and $k_L = \sqrt{2m_L (E - V_L) / \hbar^2}$. This results in the following linear system:

$$\begin{pmatrix}
1 & 1 & -1 & -1 & 0 & 0 \\
-i k_0 & -ik_0 & -ik_L & i k_L & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & e^{ik_L} & e^{-ik_L} & -e^{ik_L} & -e^{-ik_L} \\
0 & 0 & i k_L e^{ik_L} & -i k_L e^{-ik_L} & i k_L e^{ik_L} & -i k_L e^{-ik_L}
\end{pmatrix}
\begin{pmatrix}
A \\
B \\
C_L \\
D_L \\
G \\
F
\end{pmatrix}
= \begin{pmatrix}
0 \\
0 \\
0 \\
0 \\
0 \\
0
\end{pmatrix}.$$

Assuming no incoming waves from $x > L$, $F$ can be set to zero. The currents are

$$J_{x<0} = \frac{\hbar}{m_0} \left| \psi' \right| \frac{d}{dx} \psi' = \frac{\hbar k_0}{m_0} (|A|^2 - |B|^2) = J_{in} - J_{ref},$$

$$J_{x>L} = \frac{\hbar k_L}{m_L} |G|^2 = J_{tr}.$$

To determine the transmission probability, we consider that the transmitted current is proportional to the difference between the incident and reflected currents. i.e.

$$\mathcal{J} = (J_{in} - J_{ref}) \propto J_{tr},$$

$$= \alpha J_{tr}.$$

The transmission probability is

$$T = \alpha \frac{J_{tr}}{J_{in}} = \alpha \delta^{3/2} \left| \frac{E - V_L}{E - V_0} \right|^2 \left| \frac{G}{A} \right|^2.$$

From equation (35), choosing the dimensionless constant $\alpha$ such that

$$\alpha \delta^{3/2} = 1,$$

it follows that equation (34) can be rewritten as

$$\mathcal{J} = \delta^{-3/2} J_{tr},$$

which is equivalent to the current in equation (9) of [24].

| $n$ | $E$ |
|-----|-----|
| 1   | 0.43000 |
| 2   | 0.71145 |
| 3   | 1.13486 |
| 4   | 1.72597 |
| 5   | 2.48683 |
| 6   | 3.41817 |
| 7   | 4.52123 |
| 8   | 5.79804 |
| 9   | 7.25161 |
| 10  | 8.86614 |

Table 1. Bound state energy levels at the graded interface, at an interface width of $L = 20$. 

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Equation (35) shows that only $A$ and $G$ are necessary to determine the transmission probability. Solving equation (32) for $A$ and $G$ yields

$$T = \frac{4k_0^2 k_1^2}{k_1^2 (k_0 + k_L)^2 - (k_0^2 - k_1^2)(k_1^2 - k_L^2) \sin^2(2k_iL)}.$$  

(38)

In the situation where properties of the end regions are the same ($k_0 = k_L$), equation (38) reduces to the transmission probability of the square barrier or the square well given by

$$T = \left(1 + \frac{V_i^2}{4E(E - V_0)} \sin^2(2k_iL)\right)^{-1}.$$  

(39)

The profile of the potential energy and effective mass are more accurately taken into consideration if the number of barriers is large. Therefore the result equation (38) becomes more accurate for large $n$. To perform the computation for $n > 1$, it is more convenient to rewrite equation (32) in terms of a product of two types of $2 \times 2$ matrices. The first type

$$d_{i-1,i} = \frac{1}{k_{i-1}} \left( \begin{array}{cc} k_{i-1} + k_i & k_{i-1} - k_i \\ k_{i-1} - k_i & k_{i-1} + k_i \end{array} \right)$$  

(40)

characterizes the discontinuity at each interface while the second

$$p_i(x_i) = \left( \begin{array}{cc} e^{ik_i x_i} & 0 \\ 0 & e^{-ik_i x_i} \end{array} \right)$$  

(41)

characterizes propagation in each region. A composition of their product is the transfer matrix given by

$$\text{Tr} = \prod_{i=1}^{n-1} p_i(x_i) d_{i-1,i} p_i^{-1}(x_i)$$  

(42)

and the transmission probability is

$$T = \left| \frac{1}{\text{Tr}_{11}} \right|^2.$$  

(43)

Figure 2 shows the transmission probability for three different numbers of barriers. At $n = 1$, numerical evaluation of equation (42) coincides with formula equation (38) and is represented by the solid curve. As the number of slices is increased, the initial resonance peaks shift away from $T = 1$ line and the curve progressively settles to a final shape which becomes indistinguishable beyond $n = 20$. 
Figures 3 and 4 show the transmission probability for three values of the interface width. It is noticed that as $L$ tends to zero, no resonance peaks are observed and the probability curve takes the shape obtained for an abrupt heterojunction (curve with large dashing). As $L$ is increased, the resonance peaks start to show up and they increase in number with increasing $L$.

Figure 5 shows the dependence of the transmission coefficient on $\gamma$, the parameter responsible for non-additive translations. When the system’s energy is just slightly greater than the barrier height, transmission is greatly suppressed as $\gamma$ increases (solid curve). When $E \gg V$, the interface becomes transparent (dashed line). The smaller $E$ is as compared to $V$, the more reflection is favored. An example is illustrated by the dotted line. This line has a small positive gradient showing that increasing $\gamma$ enhances transmission in this regime.
5. Conclusion

We have shown that the displacement operator method can be used to describe compositionally graded heterostructures in a very neat way when the grading function is in an inverse power law form. In this circumstance, the parameter $\gamma$ which characterizes the non-additive translations of a quantum mechanical particle is a function of the effective mass mismatch $L$ and the interface width $L$. Apparently, the varying mass affects the conservation of current such that $L^{1/2}$ appears as the proportionality constant between currents in the incident and the target regions. It was necessary to introduce the dimensionless constant $\alpha$ in equation (34) to ensure current conservation similar to the redefinition of charge and current conservation in $\mathcal{PT}$-symmetric systems with position-dependent effective mass [25]. One notes too that it is $\delta$, the grading function that distinguishes the BenDaniel–Duke boundary conditions [26] for variable mass systems from the usual boundary conditions for constant mass systems ($\delta = 1$). In the present context, it is apparent that the grading function is a position-dependent effective mass mismatch function.

The advantage of grading is apparent in the appearance of transmission resonances when $L$ is increased from zero. At small $L$, it is observed that the transmission probability curve resembles that of a single abrupt heterointerface (large dashing curve in figure 3). This unique shape of the transmittivity profile at $L \to 0$ is the reason why different kinetic energy operators at this limit become indistinguishable [27]. A remarkable feature here though is that for $E > V$, the initial resonant peaks occur below the $T = 1$ level.

The parameter $\gamma$ responsible for non-additive translations and consequently for the variable mass, suppresses transmission when the system’s energy is about the same as the barrier height and enhances tunneling when the system is not endowed with sufficient energy to go over the barrier. If one considers the source of the non-additive translations to be scattering with impurity atoms, then this model produces results in line with the fact that an engineered disposition of impurity atoms in a crystal leads to high carrier mobility and superconductivity [28].

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