Accuracy of Transfer Matrix Approaches for Solving the Effective Mass Schrödinger Equation

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(Dated: 16 June 2011, published as IEEE J. Quantum Electron. 45, 1059-1067 (2009))

Abstract—The accuracy of different transfer matrix approaches, widely used to solve the stationary effective mass Schrödinger equation for arbitrary one-dimensional potentials, is investigated analytically and numerically. Both the case of a constant and a position dependent effective mass are considered. Comparisons with a finite difference method are also performed. Based on analytical model potentials as well as self-consistent Schrödinger-Poisson simulations of a heterostructure device, it is shown that a symmetrized transfer matrix approach yields a similar accuracy as the Airy function method at a significantly reduced numerical cost, moreover avoiding the numerical problems associated with Airy functions.

Index Terms—Quantum effect semiconductor devices, Quantum well devices, Quantum theory, Semiconductor heterojunctions, Eigenvalues and eigenfunctions, Numerical analysis, Tunneling, MOS devices

I. INTRODUCTION

TRANSFER matrix methods provide an important tool for investigating bound and scattering states in quantum structures. They are mainly used to solve the one-dimensional Schrödinger or effective mass equation, e.g., to obtain the quantized eigenenergies in quantum well heterostructures and metal-oxide-semiconductor structures or the transmission coefficient of potential barriers [1], [2], [3], [4]. Analytical expressions for the transfer matrices are only available in certain cases, as for constant or linear potential sections and potential steps [4]. An arbitrary potential can then be treated by approximating it for example in terms of piecewise constant or linear segments, for which analytical transfer matrices exist. For constant potential segments, the matrices are based on complex exponentials [1], [2], while the linear potential approximation requires the evaluation of Airy functions [2].

Many applications call for highly accurate methods, e.g., quantum cascade laser structures where layer thickness changes by a few Å already lead to significantly modified wavefunctions, resulting in altered device properties [5], [6]. Also numerical efficiency is crucial, especially in cases where the Schrödinger equation has to be solved repeatedly. Examples are the shooting method where the eigenenergies of bound states are found by energy scans, or Schrödinger-Poisson solvers working in an iterative manner [4]. Besides providing accurate results at moderate computational cost, an algorithm is expected to be numerically robust, and a straightforward implementation is also advantageous.

Besides transfer matrices, also other methods are frequently used, in particular finite difference or finite element schemes [7], [8]. For scattering state calculations, they are complemented by suitable transparent boundary conditions, resulting in the Quantum Transmitting Boundary Method (QTBM) [7], [9]. The transfer matrix method tends to be less numerically stable than the QTBM, since for multiple or extended barriers, numerical instabilities can arise due to an exponential blowup caused by roundoff errors [7]. This issue can however be overcome, for example by using a somewhat modified matrix approach, the scattering matrix method [10]. In this case, the transfer matrices of the individual segments are not used to compute the overall transfer matrix, but rather the scattering matrix of the structure. In addition, transfer matrices have many practical properties, such as their intuitiveness particularly for scattering states, the intrinsic current conservation, and the exact treatment of potential steps, which arise at the interfaces of differing materials. This makes them especially suitable and popular for 1-D heterostructures or metal-oxide-semiconductor structures, providing a simple, accurate and efficient simulation method [4].

As mentioned above, transfer matrices are usually based on a piecewise constant or piecewise linear approximation of an arbitrary potential, giving rise to exponential and Airy function solutions, respectively. The main strength of the Airy function approach is that it provides an exact solution for structures consisting of piecewise linear potentials, and hence only requires few segments for approximating almost linear potentials with sufficient accuracy. On the other hand, Airy functions are much more computationally demanding than exponentials, and also prone to numerical overflow for regions with nearly flat potential [11]. Thus, great care has to be taken to avoid these problems, and to evaluate the Airy functions in an efficient way [12].

It would be desirable to combine the advantages of both methods, namely the accuracy of the piecewise linear approximation and the computational convenience of the exponential
transfer matrix scheme. In this paper, we evaluate the accuracy and efficiency of the different transfer matrix approaches, taking into account both bound and scattering states. In this context, analytical expressions for the corresponding local discretization error are derived. We furthermore evaluate the different approaches numerically on the basis of an analytically solvable model potential, and also draw comparisons to the QTBMs. In particular, we demonstrate that a symmetrized exponential matrix approach is able to provide an accuracy comparable to that of the Airy function method, without having its problems and drawbacks. In our investigation, we will consider both the case of a constant effective mass and the more general case of a position dependent effective mass.

II. TRANSFER MATRIX APPROACH

In a single-band approximation, the wavefunction $\psi$ of an electron with energy $E$ in a one-dimensional quantum structure can be described by the effective mass equation

$$\left[\frac{\hbar^2}{2m^* (z)} \frac{1}{\partial_z} \partial_z + V(z) - E\right] \psi(z) = 0.$$ (1)

Here, the effective mass $m^*$ and the potential $V$ generally depend on the position $z$ in the structure. For applying the transfer matrix scheme, we divide the structure into segments, see Fig. 1 which can vary in length. Potential and effective mass discontinuities can be treated exactly in transfer matrix approaches by applying corresponding matching conditions. To take advantage of this fact and obtain optimum accuracy, the segments should be chosen so that band edge discontinuities, as introduced by heterostructure interfaces, do not lie within a segment, but rather at the border between two segments.

A. Conventional transfer matrices

For the piecewise constant potential approach (Fig. 1(a)), the potential and effective mass in each segment $j$ are approximated by constant values, e.g., $V_j = V(z_j)$, $m^*_j = m^*(z_j)$ for $z_j \leq z < z_{j+1}$ and a jump $V_j \rightarrow V_{j+1}$, $m^*_j \rightarrow m^*_{j+1}$ at the end of the segment. The solution of (1) is for $z_j \leq z < z_{j+1}$ then given by

$$\psi(z) = A_j \exp[i k_j (z - z_j)] + B_j \exp[-i k_j (z - z_j)],$$ (2)

where $k_j = \sqrt{2m^*_j (E - V_j)/\hbar}$ is the wavenumber for $E < V_j$, we obtain $k_j = i \kappa_j = i \sqrt{2m^*_j (V_j - E)/\hbar}$. The matching conditions for the wavefunction at the potential step read

$$\psi(z_0+) = \psi(z_0-) + \left[\partial_z \psi(z_0)\right] m^* (z_0+) = \left[\partial_z \psi(z_0)\right] m^* (z_0-)$$ (3)

where $z_{0+}$ and $z_{0-}$ denote the positions directly to the right and left of the step, here located at $z_0 = z_{j+1}$. The amplitudes $A_{j+1}$ and $B_{j+1}$ are related to $A_j$ and $B_j$ by

$$\begin{pmatrix} A_{j+1} \\ B_{j+1} \end{pmatrix} = T_{j,j+1} \begin{pmatrix} A_j \\ B_j \end{pmatrix},$$ (4)

with the transfer matrix

$$T_{j,j+1} = T_{j-j+1} T_j (\Delta_j) = \begin{pmatrix} \beta_{j+1} e^{i k_j \Delta_j} & \beta_{j+1} e^{-i k_j \Delta_j} \\ \beta_{j+1} e^{i k_j \Delta_j} & \beta_{j+1} e^{-i k_j \Delta_j} \end{pmatrix}.$$ (5)

Equation (5) is the product of the transfer matrix for a flat potential

$$T_j (\Delta_j) = \begin{pmatrix} e^{i k_j \Delta_j} & 0 \\ 0 & e^{-i k_j \Delta_j} \end{pmatrix},$$ (6)

obtained from (2), and the potential step matrix

$$T_j (\Delta_j) = \frac{1}{2\beta_j} \begin{pmatrix} \beta_{j+1} + \beta_j & \beta_{j+1} - \beta_j \\ \beta_{j+1} - \beta_j & \beta_{j+1} + \beta_j \end{pmatrix}$$ (7)

with $\beta_j = k_j/m^*_j$, derived from (3). The relation between the amplitudes at the left and right boundaries of the structure, $A_0, B_0$ and $A_N, B_N$, can be obtained from

$$\begin{pmatrix} A_N \\ B_N \end{pmatrix} = T_{N-1,N} T_{N-2,N-1} \ldots T_{0,1} \begin{pmatrix} A_0 \\ B_0 \end{pmatrix} = \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix} \begin{pmatrix} A_0 \\ B_0 \end{pmatrix}.$$ (8)

where $N$ is the total number of segments. For bound states, this equation must be complemented by suitable boundary conditions. One possibility is to enforce decaying solutions at the boundaries, $A_0 = B_N = 0$, corresponding to $T_{22} = 0$ in (8), which is satisfied only for specific energies $E$, the eigenenergies of the bound states.

For the piecewise linear potential approach (Fig. 1(b)), the potential in each segment $j$ is linearly interpolated, $V(z) = V_j + V_{j+1}(z - z_j)$ for $z_j \leq z \leq z_{j+1} + \Delta_j$, with $V_{j+1} = (V_{j+1} - V_j)/\Delta_j$. Equation (1) can then be solved analytically in terms of the Airy functions $Ai$ and $Bi$.

$$\psi(z) = A_j Ai\left( s_j + \frac{z - z_j}{\ell_j} \right) + B_j Bi\left( s_j + \frac{z - z_j}{\ell_j} \right)$$ (9)
for $z_j \leq z \leq z_{j+1}$, with $s_j = (V_j - E)/\varepsilon_j$ and $\ell_j = \varepsilon_j/V_{z,j}$, where
$\varepsilon_j = \sqrt{\hbar^2 V_{z,j}^2/(2m_j^*)}$. We obtain

$$\psi_{j+1} = A_j \psi_j + D_j \ell_j B_j \psi_j,$$
$$\psi'_{j+1} = \ell_j A_j \psi_j + D_j \ell_j B_j \psi_j,$$

and

$$A_j = D_j^{-1} B_j \ell_j, B_j = D_j^{-1} A_j \ell_j,$$

with $D_j = A_j B_j$. Here a prime denotes a derivative with respect to the argument of the Airy
function (for $A'$, $B'$) or the position $z$ (in all other cases).

A position dependent effective mass is treated by assigning
a constant value to each segment $j$, for example $m^*(z_j)$ or preferably $[m^*(z_j) + m^*(z_{j+1})]/2$ (see appendix),
and using the matching conditions (3) at the boundary between
two adjacent segments. A piecewise linear interpolation of $m^*$ as for the potential is not feasible, since then the
solutions of (1) cannot be expressed in terms of Airy functions
anymore. Equations (10), (11) can again be rewritten as a
matrix equation of the form (4), allowing us to treat the
quantum structure using (8) in a similar manner as described
above. Interfaces introducing abrupt potential changes in
the quantum structure must be taken into account explicitly
in the Airy function approach by employing the matching
conditions (3).

B. Symmetrized matrix

In the transfer matrix approach, the amplitudes $A_N$ and $B_N$
at the right boundary of the structure are related to the values
$A_0$ and $B_0$ at the left boundary by repeatedly applying the
transfer matrix. Due to the segmentation of the potential, an
error is introduced in (3) for every propagation step from a
position $z_j$ to $z_{j+1}$, which is typically characterized in terms
of the local discretization error (LDE). The LDE is defined as
the difference between the exact and computed solution at a
position $z_{j+1}$ obtained from a given function value at $z_j$. In
the appendix, the LDE with respect to the amplitudes $A_j$ and
$B_j$ for the transfer matrix (5) is found to be $O(\Delta z^2)$. It can be
improved to $O(\Delta z^3)$ by symmetrizing the matrix, i.e., placing
the potential step in the middle of the segment, see Fig. 1(c).
The resulting transfer matrix then is with $k_j^\pm = (k_j \pm k_{j+1})/2$
given by

$$T_{j,j+1} = T_{j+1} \left(\frac{\Delta j}{2}\right) T_{j-1} T_{j} \left(\frac{\Delta j}{2}\right),$$

where again $k_j = \sqrt{2m_j^* (E - V_j)/\hbar}$, $\beta_j = k_j/m_j^*$.

As in the Airy function approach, interfaces introducing abrupt potential
changes in the quantum structure must be dealt with separately
by applying the matching conditions; here, the corresponding
transfer matrix (7) can be used.

III. Comparison

The improved transfer matrix (12) can be evaluated at a
comparable computational cost as the matrix (5), but exhibits
a superior accuracy. As shown in the appendix, the local
discretization error with respect to the amplitudes $A_j$ and $B_j$
is improved from $O(\Delta z^2)$ to $O(\Delta z^3)$ for arbitrary potentials
and effective masses, i.e., the same order as for the Airy
function approach, which however involves a significantly
higher computational effort.

In the following, we compare the accuracy of the different
methods for an analytically solvable model potential. Here,
polynomial test potentials are not suitable for a general
discussion since their higher order derivatives identically vanish,
which can lead to an increased accuracy in such special cases.
Especially triangular or other piecewise linear potentials are
obviously inadequate since the Airy function approach then
becomes exact. Instead, we choose the exponential ansatz

$$V(z) = V_0 + V_1 \exp(Kz),$$

$$0 \leq z \leq d$$

(see Fig. 2), approaching a linear function for
$K \to 0$. Such a potential cannot be used as a model for the
effective potential profile in the presence of space charges
(13), (14).

A. Position independent effective mass

For now, we assume a constant effective mass $m^*$. Then, the
analytical solutions of the form

$$\psi = c_1 J_\mu(a) + c_2 Y_\mu(a),$$

exist for the potential (13), with constants $c_1$ and $c_2$. Here, $J_\mu$ and $Y_\mu$ are Bessel functions of the first and second kind, and
the parameters are given by

$$\mu = 2\sqrt{2m^* (V_0 - E)},$$
$$a(z) = 2\sqrt{-2m^* V_1}/\exp\left(\frac{1}{2}Kz\right).$$

For our simulations, the different transfer matrix approaches
discussed in Section (11) are used to compute an overall matrix
based on (6), from which the required quantities can be extracted.
First, we investigate the barrier structure shown in
Fig. 2(a), which can be characterized in terms of a transmission

![Fig. 2. Exponential model potential with $d = 10$ nm and $K = -1/d$, used for evaluating the accuracy of various methods. (a) Barrier. (b) Quantum well.](image-url)
The symmetrized transfer matrix approach and the Airy function method exhibit a superior accuracy especially for small $K$, corresponding to a weak curvature of the potential. While the error of the unsymmetrized matrix approach and the QTBM show only a weak dependence on $K$, the Airy function method becomes exact for $K \to 0$, where the potential becomes piecewise linear. Interestingly, also the symmetrized transfer matrix approach has a vanishing error $\varepsilon_T$ for a specific value of $K$, at $Kd \approx 0.167$.

Now we apply the different numerical methods to the bound states of the potential well shown in Fig. 2(b), Again assuming a constant effective mass of $m^* = 0.067 m_e$, evaluation of (14) yields two bound states with eigenenergies $E_1 = -0.1343$ eV and $E_2 = -0.067$ eV.
and $E_2 = -0.0129 \text{eV}$, respectively. In the following, we compare the accuracy of the numerically found eigenenergies $E_{\text{num}}$, as obtained by the unsymmetrized and the symmetrized transfer matrix approach and the Airy function method, corresponding to the expressions (5), (12), and (10), respectively. Here, we again divide the structure into $N$ segments of equal length $\Delta = d/N \propto N^{-1}$. Fig. 5 shows the relative error $\varepsilon_E(N) = |1 - E_{\text{num}}(N)/E|$ for the first and the second bound state as a function of $N$. As for the transmission coefficient in Fig. 5, the error scales with $N^{-1} \propto \Delta$ for the unsymmetrized matrix approach and with $N^{-2} \propto \Delta^2$ for the other methods. Again, the symmetrized matrix approach and the Airy function method exhibit a comparable value of $\varepsilon_E(N)$, being far superior to the unsymmetrized matrix approach.

B. Position dependent effective mass

Now we compare the accuracy of the different methods for a position dependent effective mass $m^*(z)$. Here, we choose the same exponential ansatz for the potential as above, see (13) and Fig. 2. For an effective mass of the form $m^* = m_0^* \exp(-Kz)$, again an analytical solution exists:

$$\psi = c_1 J_{\mu}(a) \exp(-Kz/2) + c_2 Y_{\mu}(a) \exp(-Kz/2),$$

with

$$\mu = -\sqrt{1 + 8m_0^*V_1/K^2\hbar^2},$$

$$a(z) = 2\sqrt{-2m_0^* (V_0 - E)}/K \exp\left(-\frac{1}{2}Kz\right).$$

The transfer matrix definitions (5), (12) are also valid for position dependent effective masses. In the Airy function approach (10), a position dependent effective mass can be accounted for by assuming a constant value within each segment, as discussed at the end of Section 1A. Here, we assign the averaged mass $(m_j^* + m_{j+1}^*)/2$ rather than $m_j^*$ to each segment, since then the third order LDE, found for the amplitudes $A$ and $B$ in the case of position independent masses, is also preserved for the position dependent case, see the appendix.

Fig. 6 corresponds to Fig. 3 but now for a position dependent effective potential with $m^* = 0.2m_e \exp(-Kz)$ for $0 \leq z \leq d$ and $m^* = 0.067m_e$ otherwise. The exact transmission coefficient for an electron with energy $E = 0$, as obtained by evaluating (16), is now $T = 5.376 \times 10^{-10}$. From Fig. 6, we can see that also here the error scales with $N^{-1} \propto \Delta$ for the unsymmetrized matrix approach and with $N^{-2} \propto \Delta^2$ for the other methods, compare Fig. 3. Again, the symmetrized matrix approach and the Airy function method are the most accurate, with the symmetrized matrix approach being numerically much more efficient.

For the sake of completeness, Fig. 7 is shown as the counterpart of Fig. 4 but now taking into account a position dependent effective mass as above. Again, the symmetrized matrix approach and the Airy function method have a superior accuracy especially for small values of $K$, corresponding to a weak curvature of the potential.

IV. EXAMPLE: Schrödinger-Poisson solver

In the following, we apply the transfer matrices discussed above to a real-world example, namely finding the wavefunctions and eigenenergies of the quantum cascade laser (QCL) structure described in [15]. The goal is to evaluate and compare the performance of the different approaches for a practical problem, and to discuss the inclusion of additional important effects. Specifically, we here also account for energy-band nonparabolicity, and complement the Schrödinger equation by the Poisson equation to take into account space charge effects. In practice, extensive parameter scans have to be performed for QCL design optimization. Thus, the simulation of QCLs calls for especially efficient methods, the more so as the self-consistent solution of the Schrödinger-Poisson system results in a further increase of the numerical effort.

In simulations, the QCL structure is defined by an infinitely repeated elementary sequence of multiple wells and barriers (called a period). For such a structure under bias, it is sufficient to compute the eigenenergies and corresponding wave functions for a single energy interval given by the bias.
matrix result for and Airy function matrix approach at single period are shown for the unsymmetrized, symmetrized the obtained energy levels and wave functions squared of a various temperatures, considering the seven lowest levels (i.e., with lowest energies leading to an additional potential $-e\Delta$), difference scheme on a is achieved. For the Poisson equation (18), we employ a finite Poisson equations are iteratively solved until self-consistency neutrality condition within one period. The Schrödinger and adopted, such as applying Fermi-Dirac statistics [3], [17] parameter range. Thus, for solving the Schrödinger-Poisson transport simulations [6], this is prohibitive for design opti-structure. The chemical potential do not depend on the choice of the elementary period in the structure. Especially, this ensures that the simulation results to correctly reflect the invariance properties of the biased band edge $E_n^*$ is the lattice temperature, and $m^*$ is the effective mass, here taken to be the value of the well material. In [19], we use the energy of a state relative to the conducton band edge $E_n = E_n - \int V |\psi_n|^2 \, dz$ rather than $E_n$ itself to correctly reflect the invariance properties of the biased structure. Especially, this ensures that the simulation results do not depend on the choice of the elementary period in the structure. The chemical potential $\mu$ is found from the charge neutrality condition within one period. The Schrödinger and Poisson equations are iteratively solved until self-consistency is achieved. For the Poisson equation (13), we employ a finite difference scheme on a 1 Å-grid, where we use [5] and [9] to appropriately interpolate the eigenfunctions obtained from the Schrödinger solver.

Simulations of the QCL in [15] have been performed at various temperatures, considering the seven lowest levels (i.e., with lowest energies $E_n$) within each period. In Fig. [8], the obtained energy levels and wave functions squared of a single period are shown for the unsymmetrized, symmetrized and Airy function matrix approach at $T = 300$ K, using a segment length of $\Delta = 2$ nm. Also the symmetrized transfer matrix result for $\Delta = 0.1$ nm is plotted for reference. The

\begin{equation}
\begin{aligned}
-\partial_z [e(z) \partial_z \varphi(z)] &= e \left[ N(z) - \sum_n n_{2D,n} |\psi_n(z)|^2 \right], \\
&= e \left[ \int |\psi_n(z)|^2 \, dz \right]
\end{aligned}
\end{equation}

leading to an additional potential $-e\Delta$ in (1). Here, $\epsilon(z)$ is the permittivity, $e$ is the elementary charge, $N(z)$ is the doping concentration, and $n_{2D,n}$ is the electron sheet density of level $n$ with wave function $\psi_n(z)$. While for an operating QCL, $n_{2D,n}$ can only be exactly determined by detailed carrier transport simulations [6], this is prohibitive for design optimizations of experimental QCL structures over an extended parameter range. Thus, for solving the Schrödinger-Poisson system, simpler and much faster approaches are commonly adopted, such as applying Fermi-Dirac statistics [3], [17].

\begin{equation}
n_{2D,n} = \frac{m^*}{\pi \hbar^2} k_B T \ln \left( 1 + \exp \left( \frac{\mu - E_n}{k_B T} \right) \right),
\end{equation}

where $\mu$ is the chemical potential, $k_B$ is the Boltzmann constant, $T$ is the lattice temperature, and $m^*$ is the effective mass.

\section{V. Conclusion}

In conclusion, we have compared the accuracy of different transfer matrix approaches, as used for solving the effective mass Schrödinger equation with an arbitrary one-dimensional potential and a constant or position dependent effective mass. In particular, the local discretization error has been derived for the Airy function approach resulting from a piecewise linear approximation of the potential, and for unsymmetrized and symmetrized transfer matrices based on a piecewise constant potential approximation. Furthermore, numerical simulations have been performed to evaluate the numerical accuracy of the different approaches for scattering and bound states, employing exponential test potentials. Comparisons to the finite difference method, specifically the QTBM, have also been carried out. Additionally, self-consistent Schrödinger-Poisson device simulations are presented.

The symmetrized transfer matrix approach and the Airy function method exhibit a comparable accuracy, being superior to the other methods investigated. However, the symmetrized matrix approach achieves this at a significantly reduced numerical cost, moreover avoiding the numerical problems associated with Airy functions. All in all, the symmetrized transfer matrix approach is shown to combine the numerical efficiency
and straightforwardness of its unsymmetrized counterpart with the superior accuracy of the Airy function method.

**APPENDIX A**

**LOCAL DISCRETIZATION ERROR**

In the following, we derive the local discretization error (LDE) for the different types of transfer matrices. In this context, we investigate the piecewise constant potential approximation based on matrix (5) and its symmetrized version (12), as well as the piecewise linear potential scheme (10). As mentioned in Section II, the segments are chosen so that band edge discontinuities in the structure coincide with the borders between two segments, enabling an exact treatment in terms of the matching conditions (3). Thus, for our error analysis we imply that the potential and effective mass vary smoothly within each segment, i.e., have a sufficient degree of differentiability. Otherwise, no further assumptions about the potential shape and effective mass are made. The local discretization error for \( \psi \) at \( z = z_{j+1} \) is

\[
\tau_{j+1}^\psi = \psi_{j+1} - \psi(z_{j+1}),
\]

where \( \psi_{j+1} \) is the approximate wavefunction value at \( z_{j+1} \) obtained by the transfer matrix approach from a given value \( \psi(z_j) = \psi_j \) at \( z_j \), while \( \psi(z_{j+1}) \) is the exact solution. For evaluating the LDE, it is helpful to express \( \psi(z_{j+1}) \) in terms of a Taylor series,

\[
\psi(z_{j+1}) = \psi_j + \psi_j' \Delta_j + \frac{1}{2} \psi_j'' \Delta_j^2 + \frac{1}{6} \psi_j''' \Delta_j^3 + \frac{1}{24} \psi_j^{(4)} \Delta_j^4 + O(\Delta_j^5).
\]

(21)

Analogously, we can define an LDE for the derivative \( \psi' \),

\[
\tau_{j+1}^{\psi'} = \psi_{j+1}' - \psi'(z_{j+1}),
\]

(22)

and express \( \psi'(z_{j+1}) \) as

\[
\psi'(z_{j+1}) = \psi_j' + \psi_j'' \Delta_j + \frac{1}{2} \psi_j''' \Delta_j^2 + \frac{1}{6} \psi_j^{(4)} \Delta_j^3 + O(\Delta_j^4).
\]

(23)

**A. Piecewise constant potential approximation**

Using (22), we can relate \( A_j \) and \( B_j \) to the wavefunction at position \( z_j \),

\[
A_j = \frac{1}{2} \left( \psi_j - \frac{1}{k_j} \psi_j' \right),
\]

\[
B_j = \frac{1}{2} \left( \psi_j + \frac{1}{k_j} \psi_j' \right),
\]

(24)

and express the LDEs for the amplitudes \( A \) and \( B \) in terms of \( \tau_{j+1}^\psi \) and \( \tau_{j+1}^{\psi'} \).

\[
\tau_{j+1}^A = A_{j+1} - A(z_{j+1}) = \frac{1}{2} \left( \tau_{j+1}^\psi - \frac{1}{k_{j+1}} \tau_{j+1}^{\psi'} \right),
\]

\[
\tau_{j+1}^B = B_{j+1} - B(z_{j+1}) = \frac{1}{2} \left( \tau_{j+1}^\psi + \frac{1}{k_{j+1}} \tau_{j+1}^{\psi'} \right).
\]

(25)

For the unsymmetrized transfer matrix, we obtain from (3) with the expressions (4) and (5)

\[
\psi_{j+1} = A_{j+1} + B_{j+1} = \exp(ik_j \Delta_j) A_j + \exp(-ik_j \Delta_j) B_j,
\]

\[
\psi_{j+1}' = ik_{j+1} (A_j + B_j - 1).
\]

(26)

For calculating the LDE, we insert the expressions (26) and (21) into (20), where we express \( A_j \) and \( B_j \) by (24) and use (1) to rewrite the derivatives \( \psi_j^{(n)} \) in (21) as

\[
\psi_j^{(n)} = -\frac{k_j^2}{m_j^*} \psi_j + \frac{m_j^{*''}}{m_j^*} \psi_j',
\]

\[
\psi_j^{(3)} = -\frac{(m_j k_j^2)^2}{m_j^*} \psi_j + k_j^2 \psi_j' + \frac{m_j^{*'''}}{m_j^*} \psi_j'',
\]

(27)

with \( k_j = \sqrt{2 m_j^* (E - V_j) / h} \). A Taylor expansion then yields

\[
\tau_{j+1}^\psi = \cos(k_j \Delta_j) \psi_j + \sin(k_j \Delta_j) k_j^{-1} \psi_j'
\]

\[
- \psi_j - \psi_j'' \Delta_j - \frac{1}{2} \psi_j''' \Delta_j^2 + \frac{1}{6} \psi_j^{(4)} \Delta_j^3 + O(\Delta_j^4)
\]

\[
= -\frac{1}{2} m_j^{*''} \psi_j' \psi_j + \frac{1}{6} \left( \frac{m_j k_j^2 \psi_j'}{m_j^*} - \frac{m_j^{*''} \psi_j'}{m_j^*} \right) \Delta_j^3
\]

\[
+ O(\Delta_j^4).
\]

(28)

Analogously, by inserting the expressions (26) and (23) into (22) we obtain

\[
\tau_{j+1}^{\psi'} = \frac{m_j^{*++1}}{m_j^*} \left( \psi_j' \cos(k_j \Delta_j) - k_j \sin(k_j \Delta_j) \psi_j \right)
\]

\[
- \psi_j - \psi_j'' \Delta_j - \frac{1}{2} \psi_j''' \Delta_j^2 + O(\Delta_j^3)
\]

\[
= \left( \frac{m_j^{*+1}}{m_j^*} - 1 - m_j^{*''} \Delta_j \right) \psi_j' + \frac{m_j^*}{m_j^*} - m_j^{*+1} k_j^2 \psi_j \Delta_j
\]

\[
+ \frac{1}{2} \left( \frac{m_j k_j^2 \psi_j'}{m_j^*} - \frac{m_j^{*''} \psi_j'}{m_j^*} \right) \psi_j' \Delta_j^2
\]

\[
+ O(\Delta_j^4)
\]

\[
= \left( \frac{(m_j k_j^2)^2}{2 m_j^*} - \frac{m_j^{*''}}{m_j^*} k_j^2 \right) \psi_j \Delta_j^2 + O(\Delta_j^3),
\]

(29)

where we use \( m_j^{*+1} = m_j^* + m_j^{*''} \Delta_j + \frac{1}{2} m_j^{*'''} \Delta_j^2 + O(\Delta_j^3) \) to obtain the last line of (29). Thus, \( \tau_{j+1}^\psi \) is \( O(\Delta_j^2) \) (\( O(\Delta_j^4) \) for a constant effective mass), and \( \tau_{j+1}^{\psi'} \) is \( O(\Delta_j^3) \). With (29), we see that both \( \tau_{j+1}^A \) and \( \tau_{j+1}^B \) are \( O(\Delta_j^2) \).

In a similar manner, we obtain for the symmetrized matrix (12) \( \tau_{j+1}^A = O(\Delta_j^2) \) and \( \tau_{j+1}^B = O(\Delta_j^3) \). More precisely, the calculation yields for a constant \( m^* \)

\[
\tau_{j+1}^A = \frac{1}{24} (k_j^2)^2 \psi_j \Delta_j^2 + O(\Delta_j^3),
\]

\[
\tau_{j+1}^{\psi'} = -\frac{1}{12} (k_j^2)^2 \psi_j \Delta_j^3 - \frac{1}{24} (k_j^2)^2 \psi_j \Delta_j^3 + O(\Delta_j^3),
\]

(30)

(and a somewhat more complicated expression for a position dependent effective mass). This means that \( \tau_{j+1}^A \) and \( \tau_{j+1}^B \) are now \( O(\Delta_j^3) \).
B. Piecewise linear potential approximation

For computing the LDEs (20) and (22) of the Airy function approach, we proceed in a manner similar as above. Equations (10) and (11) give the relation between values \( \psi_j, \psi'_j \) at \( z_j \) and the numerical result \( \psi_{j+1}, \psi'_{j+1} \) obtained at \( z_{j+1} \) from the Airy function approach:

\[
\psi_{j+1} = \frac{1}{D_j} \left[ \text{Ai}(s_j + \frac{\Delta_j}{\ell_j}) \text{Bi}'(s_j) - \text{Ai}'(s_j) \text{Bi}(s_j + \frac{\Delta_j}{\ell_j}) \right] \psi_j
+ \frac{\ell_j}{D_j} \left[ \text{Ai}(s_j) \text{Bi}(s_j + \frac{\Delta_j}{\ell_j}) - \text{Ai}(s_j + \frac{\Delta_j}{\ell_j}) \text{Bi}(s_j) \right] \psi'_j
= \left( 1 + \frac{s_j}{2 \ell_j} \Delta_j^2 + \frac{1}{6 \ell_j^3} + \frac{s_j^2}{24 \ell_j^5} \Delta_j^4 \right) \psi_j
+ \left( \Delta_j + \frac{s_j}{6 \ell_j^2} \Delta_j^3 + \frac{1}{12 \ell_j^3} \right) \psi'_j + O(\Delta_j^5),
\]

(31)

\[
\psi'_{j+1} = \frac{1}{D_j \ell_j} \left[ \text{Ai}'(s_j + \frac{\Delta_j}{\ell_j}) \text{Bi}(s_j) \right] \psi_j
- \text{Bi}'(s_j + \frac{\Delta_j}{\ell_j}) \text{Ai}(s_j) \psi_j
+ \frac{1}{D_j} \left[ \text{Ai}(s_j) \text{Bi}'(s_j + \frac{\Delta_j}{\ell_j}) - \text{Ai}'(s_j + \frac{\Delta_j}{\ell_j}) \text{Bi}(s_j) \right] \psi'_j
= \left( \frac{s_j}{2 \ell_j} \Delta_j^2 + \frac{1}{6 \ell_j^3} + \frac{s_j^2}{3 \ell_j^3} \Delta_j^3 \right) \psi_j
+ \left( 1 + \frac{s_j}{2 \ell_j^2} \Delta_j^2 + \frac{1}{3 \ell_j^3} \Delta_j^3 \right) \psi'_j + O(\Delta_j^5),
\]

(32)

with \( D_j = \text{Ai}(s_j) \text{Bi}(s_j) - \text{Ai}'(s_j) \text{Bi}(s_j) \). The exact results \( \psi(z_{j+1}) \) and \( \psi'(z_{j+1}) \) are again expressed by the Taylor series expansions (21) and (23), respectively, where we rewrite the derivatives \( \psi^{(n)}_j \) in terms of \( \psi_j \) and \( \psi'_j \). For a constant effective mass, we have

\[
\psi'_j = \ell_j^{-2} s_j \psi_j,
\]

\[
\psi^{(3)}_j = \ell_j^{-2} s_j \psi'_j + \ell_j^{-3} \frac{V'_j}{V_{z,j}} \psi_j,
\]

\[
\psi^{(4)}_j = \ell_j^{-4} s_j^2 \psi_j + 2 \ell_j^{-3} \frac{V'_j}{V_{z,j}} \psi'_j + \ell_j^{-3} \frac{V''_j}{V_{z,j}} \psi_j,
\]

with \( V_{z,j} = (V'_{j+1} - V_j) / \Delta_j \), and obtain with the expressions (20), (21) and (31)

\[
\tau^\psi_{j+1} = \psi_{j+1} - \psi(z_{j+1}) = - \frac{1}{24} (k_j')^\nu \psi_j \Delta_j^4 + O(\Delta_j^5),
\]

(34)

and with (22), (23) and (32)

\[
\tau^{\psi'}_{j+1} = \psi'_{j+1} - \psi'(z_{j+1}) = - \frac{1}{12} (k_j')^\nu \psi_j \Delta_j^3 + O(\Delta_j^4),
\]

(35)

where \( k_j = \sqrt{2m_j^* (E - V_j) / \hbar} \). Using (11), we can express the LDEs for the amplitudes \( A \) and \( B \) in terms of \( \tau^\psi_{j+1} \) and \( \tau^{\psi'}_{j+1} \), and obtain \( \tau^\psi_{j+1} = O(\Delta_j^3), \tau^{\psi'}_{j+1} = O(\Delta_j^3) \).

As described in Section 1.5.A, a position dependent effective mass can in the Airy function approach be treated by assuming a constant value within each segment \( j \), e.g., \( m_j^* = m^* (z_j) \), and applying the matching conditions (5) at the section boundaries (2). The result for \( \psi'_{j+1} \) in (32) has thus to be multiplied by \( m^*_j / m^*_k \) before inserting it into (22). While \( \tau^{\psi'}_{j+1} \) is still \( O(\Delta_j^3) \), \( \tau^{\psi'}_{j+1} \) drops to \( O(\Delta_j^2) \), now yielding \( \tau^{\psi'}_{j+1} = O(\Delta_j^3), \tau^{\psi} = O(\Delta_j^3) \). The error analysis also shows that \( \tau^{\psi'}_{j+1} \) and thus \( \tau^{\psi} \) can be improved to \( O(\Delta_j^3) \) by assigning an averaged mass \( (m_j^* + m_{j+1}^*) / 2 \) rather than \( m_j^* \) to each segment, and applying the matching conditions correspondingly.

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