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Solving the Schrödinger Equation by the Transfer-Matrix Method

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Abstract. The transfer-matrix method was proposed in the 1940s to solve linear ordinary differential equations. It is broadly studied due to its efficiency and simplicity for solving one-dimensional physical problems. In this work, the method is applied to solve the time-independent Schrödinger equation, in order to improve both the formalism and the computational treatment. Closed-form solutions are derived for quantum wells and periodic potentials of arbitrary profiles. Numerical results are given for symmetric finite-barrier quantum wells and sinusoidal potentials.

Keywords: ordinary differential equation, transfer-matrix method, Schrödinger equation.

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1 Introduction

The transfer-matrix method provides a compact formalism for the study of layered optical systems [7] as well as the one-dimensional (1D) quantum dynamics of a particle in an arbitrary potential [2, 13, 14]. The treatment of the latter case is simpler for potentials whose domain can be divided into a set of intervals such that the general solution of the differential equation is available for each of them. The solution of the differential equation is easier to find for potentials that can be divided into intervals with an available general solution. In such cases, the method produces exact algebraic equations for the energy levels and close-form expressions for the wave functions [19]. Moreover, when an interval consists of N sub-intervals with identical potential profiles, its transfer matrix equals the N-th power of the transfer matrix of a single sub-interval [11].

The 1D time-independent Schrödinger equation for a particle of mass m has the form

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}(x) + V(x)\psi(x) = E\psi(x), \tag{1.1}$$

where x is the position of the particle, E is the particle energy in a quantum stationary state with spatial wave function $\psi(x)$, $V(x)$ is the potential profile, and $\hbar$ is the reduced Planck constant [3]. This second-order linear ordinary differential equation has a fundamental set of two solutions, denoted $\psi_{1,E}(x)$ and $\psi_{2,E}(x)$, for each energy value E.

If the $V(x)$ is a continuous or piece-wise continuous function over an interval I, then $\psi(x)$ is a bounded and continuously differentiable function over I that satisfies

$$\begin{bmatrix} \psi(x) \\ \psi'(x) \end{bmatrix} = W_E(x) \begin{bmatrix} A \\ B \end{bmatrix}, \tag{1.2}$$

for $x \in I$. Here A and B depend on the initial conditions, and

$$W_E(x) = \begin{bmatrix} \psi_{1,E}(x) & \psi_{2,E}(x) \\ \psi'_{1,E}(x) & \psi'_{2,E}(x) \end{bmatrix} \tag{1.3}$$

is the Wronskian matrix. For any initial point x_0 in I, one has

$$\begin{bmatrix} \psi(x) \\ \psi'(x) \end{bmatrix} = T_E(x, x_0) \begin{bmatrix} \psi(x_0) \\ \psi'(x_0) \end{bmatrix}, \tag{1.4}$$

where

$$T_E(x, x_0) = W_E(x) W_E^{-1}(x_0) \tag{1.5}$$

is the matrix that transfers the values of ψ and ψ' from x_0 to x at energy E. It is worth noting that for an arbitrary x_1 in I, the transfer matrix $T_E(x, x_0)$ has the multiplicative property

$$T_E(x, x_0) = T_E(x, x_1)\, T_E(x_1, x_0). \tag{1.6}$$

Since the Wronskian determinant $\det(W_E(x))$ is a constant over the real line [1], we also have

$$\det(T_E(x, x_0)) = 1. \tag{1.7}$$

In this paper, aiming to contribute to modern analytical and numerical applications of the transfer-matrix method, we apply it to solve the Schrödinger equation for arbitrary quantum wells and periodic potentials in one dimension. Quantum wells have great importance in physics and engineering, to model semiconductor electronic devices [13]. Periodic potentials are broadly applied to model electronic states in crystalline structures [9, 12, 17, 6]. Contrasting common approaches [8], we deal with the variable pair $(\psi(x), \psi'(x))$, instead of the constant pair (A, B) [see Equations (1.2) and (1.4)]. This enhances clarity, simplicity and universality: $\psi(x)$ and $\psi'(x)$ have direct physical/geometrical interpretation, the matching conditions between contiguous intervals reduce to continuity conditions, and the transfer matrix is ultimately independent of the chosen fundamental solutions $\psi_{1,E}(x)$ and $\psi_{2,E}(x)$. Furthermore, instead of approximating complex potential profiles by a sequence of piece-wise constant potentials [8], the present formulation assumes that either close-form expressions are available for $\psi_{1,E}(x)$ and $\psi_{2,E}(x)$ or high-accuracy computational procedures can be implemented for their numerical evaluation.

Section 2 presents transfer-matrix examples that are applied to deal with either quantum-well bound states in Section 3 or periodic potentials in Section 4. Numerical results and concluding remarks are given in Sections 5 and 6.

2 Transfer-matrix examples

In this section, the transfer matrices for the Schrödinger equation with a constant and a sinusoidal potential are given. The results will be applied to solve two physical problems in Section 5.

2.1 Transfer matrix in a constant potential

Let x and x_0 be in an interval where the potential equals a constant value V, that is, $V(x) = V$. The Schrödinger equation can be written as:

$$\psi''(x) + (K_E)^2\psi(x) = 0, \tag{2.1}$$

where $K_E = \sqrt{2m(E-V)/\hbar^2}$. When $E \neq V$, the Wronskian matrix can be chosen as

$$W_E(x) = \begin{bmatrix} \cos(K_E x) & \frac{1}{K_E}\sin(K_E x) \\ -K_E \sin(K_E x) & \cos(K_E x) \end{bmatrix}, \tag{2.2}$$

the transfer-matrix is given by

$$T_E(x, x_0) = \begin{bmatrix} \cos(K_E(x-x_0)) & \frac{1}{K_E}\sin(K_E(x-x_0)) \\ -K_E \sin(K_E(x-x_0)) & \cos(K_E(x-x_0)) \end{bmatrix}. \tag{2.3}$$

If $E = V$, then $K_E = 0$, the Wronskian matrix can be written as

$$W_E(x) = \begin{bmatrix} 1 & x \\ 0 & 1 \end{bmatrix}, \tag{2.4}$$

and the corresponding transfer matrix is given by

$$T_E(x, x_0) = \begin{bmatrix} 1 & x - x_0 \\ 0 & 1 \end{bmatrix}. \tag{2.5}$$

The transfer matrix is a continuous function of K_E, as the limit of Equation (2.3) when $K_E \to 0$ gives Equation (2.5).

2.2 Transfer-matrix with a sinusoidal potential

For this case, x and x_0 are considered to be in an interval where the potential has a sinusoidal profile that is conveniently written as $V(x) = -A\cos(2\pi x/\lambda)$. The Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}(x) - A\cos(2\pi x/\lambda)\,\psi(x) = E\psi(x), \tag{2.6}$$

can be written as

$$f''(\xi) + [2\epsilon + 2\alpha\cos(2\xi)]f(\xi) = 0, \tag{2.7}$$

where $\xi = \pi x/\lambda$, $f(\xi) = (\lambda/\pi)^{1/2}\,\psi(x)$, $\alpha = A/U$, and $\epsilon = E/U$, with $U = \hbar^2\pi^2/(m\lambda^2)$.

To solve Equation (2.7), it is reduced to the Mathieu equation [1, 4, 6, 5]

$$\frac{d^2f}{d\xi^2}(\xi) + [a - 2q\cos(2\xi)]f(\xi) = 0, \tag{2.8}$$

where $a = 2\epsilon$ and $q = -\alpha$. The fundamental set of solutions can be chosen as

$$f_{1,E}(\xi) = C_{a,q}(\xi) = C_{2\epsilon,-\alpha}(\xi)$$

and

$$f_{2,E}(\xi) = S_{a,q}(\xi) = S_{2\epsilon,-\alpha}(\xi). \tag{2.9}$$

The wave functions read

$$\psi_1(x) = \sqrt{\frac{\pi}{\lambda}}\,C_{2\epsilon,-\alpha}\left(\frac{\pi x}{\lambda}\right)$$

and

$$\psi_2(x) = \sqrt{\frac{\pi}{\lambda}}\,S_{2\epsilon,-\alpha}\left(\frac{\pi x}{\lambda}\right), \tag{2.10}$$

and the Wronskian matrix becomes

$$W_E(x) = \frac{\pi^2}{\lambda^2}\begin{bmatrix} C_{2\epsilon,-\alpha}(\frac{\pi x}{\lambda}) & S_{2\epsilon,-\alpha}(\frac{\pi x}{\lambda}) \\ C'_{2\epsilon,-\alpha}(\frac{\pi x}{\lambda}) & S'_{2\epsilon,-\alpha}(\frac{\pi x}{\lambda}) \end{bmatrix}. \tag{2.11}$$

Therefore, the transfer matrix form x_0 to x is given by

$$T_E(x,x_0) = \begin{bmatrix} C_{2\epsilon,-\alpha}(\xi) & S_{2\epsilon,-\alpha}(\xi) \\ C'_{2\epsilon,-\alpha}(\xi) & S'_{2\epsilon,-\alpha}(\xi) \end{bmatrix} \begin{bmatrix} C_{2\epsilon,-\alpha}(\xi_0) & S_{2\epsilon,-\alpha}(\xi_0) \\ C'_{2\epsilon,-\alpha}(\xi_0) & S'_{2\epsilon,-\alpha}(\xi_0) \end{bmatrix}^{-1}, \tag{2.12}$$

where $\xi = \pi x/\lambda$ and $\xi_0 = \pi x_0/\lambda$.

3 Bound states of an arbitrary quantum well

We consider a quantum well of width a with arbitrary profile $V_w(x)$ over the interval $-a/2 < x < a/2$, cladded between semi-infinite leftward and rightward barriers of heights V_l and V_r, respectively. This is given by the potential

$$V(x) = \begin{cases} V_l, & \text{if } x \le -a/2 \\ V_w(x), & \text{if } -a/2 < x < a/2 \\ V_r, & \text{if } x \ge a/2. \end{cases} \tag{3.1}$$

The discrete energy levels satisfy $\min(V_w(x)) \le E \le \min(V_l, V_r)$.

For $x < -a/2$, the bound wave functions have the form

$$\psi(x) = \psi(-a/2)e^{\kappa_E^{(l)}(x+a/2)} \tag{3.2}$$

where $\kappa_E^{(l)} = \sqrt{2m(V_l - E)/\hbar^2}$. This implies

$$\begin{bmatrix} \psi(-a/2) \\ \psi'(-a/2) \end{bmatrix} = \psi(-a/2) \begin{bmatrix} 1 \\ \kappa_E^{(l)} \end{bmatrix}. \tag{3.3}$$

Similarly, for $x > a/2$ we obtain

$$\psi(x) = \psi(a/2)e^{-\kappa_E^{(r)}(x-a/2)} \tag{3.4}$$

and

$$\begin{bmatrix} \psi(a/2) \\ \psi'(a/2) \end{bmatrix} = \psi(a/2) \begin{bmatrix} 1 \\ -\kappa_E^{(r)} \end{bmatrix}, \tag{3.5}$$

with $\kappa_E^{(r)} = \sqrt{2m(V_r - E)/\hbar^2}$.

Considering the region $-a/2 \leq x \leq a/2$, we find

$$\begin{bmatrix} \psi(a/2) \\ \psi'(a/2) \end{bmatrix} = M_E \begin{bmatrix} \psi(-a/2) \\ \psi'(-a/2) \end{bmatrix}, \tag{3.6}$$

where $M_E = T_E(a/2, -a/2)$. Then, putting (3.3) and (3.5) into (3.6), we get

$$\psi(a/2) \begin{bmatrix} 1 \\ -\kappa_E^{(r)} \end{bmatrix} = M_E \, \psi(-a/2) \begin{bmatrix} 1 \\ \kappa_E^{(l)} \end{bmatrix}, \tag{3.7}$$

i.e.,

$$M_E \begin{bmatrix} 1 \\ \kappa_E^{(l)} \end{bmatrix} = \lambda_E \begin{bmatrix} 1 \\ -\kappa_E^{(r)} \end{bmatrix}, \tag{3.8}$$

with $\lambda_E = \psi(a/2)/\psi(-a/2)$. This means that the two-dimensional vector in the left-hand side should be perpendicular to the vector $(\kappa_E^{(r)}, 1)$, i.e.,

$$\begin{bmatrix} \kappa_E^{(r)} & 1 \end{bmatrix} M_E \begin{bmatrix} 1 \\ \kappa_E^{(l)} \end{bmatrix} = 0. \tag{3.9}$$

This equation leads to the discrete energy levels of the particle in the quantum well of arbitrary profile $V_w(x)$ for $-a/2 < x < a/2$. The quantum-well transfer matrix M_E depends on such a profile.

For each energy level, the ratio $\psi(a/2)/\psi(-a/2)$ is given by Equation (3.8) as

$$\lambda_E = \begin{bmatrix} 1 & 0 \end{bmatrix} M_E \begin{bmatrix} 1 \\ \kappa_E^{(l)} \end{bmatrix}. \tag{3.10}$$

4 Energy bands in an arbitrary periodic potential

For a periodic potential of period λ, i.e., satisfying $V(x + \lambda) = V(x)$, a complete set of solutions fulfills the Bloch condition [13]

$$\psi_{k,E}(x + \lambda) = e^{ik\lambda} \psi_{k,E}(x),$$

where k is the crystalline wave vector. The derivative of the wave function obeys the same condition, namely

$$\psi'_{k,E}(x + \lambda) = e^{ik\lambda} \psi'_{k,E}(x). \tag{4.1}$$

For an arbitrary point x_0, we have

$$\begin{bmatrix} \psi_{k,E}(x_0+\lambda) \\ \psi'_{k,E}(x_0+\lambda) \end{bmatrix} = M_E \begin{bmatrix} \psi_{k,E}(x_0) \\ \psi'_{k,E}(x_0) \end{bmatrix} = e^{ik\,\lambda} \begin{bmatrix} \psi_{k,E}(x_0) \\ \psi'_{k,E}(x_0) \end{bmatrix}. \tag{4.2}$$

where $M_E = T_E(x_0+\lambda, x_0)$ is the transfer matrix of a unit cell. This means that $e^{ik\,\lambda}$ is an eigenvalue of M_E, i.e.,

$$\det\left(M_E - Ie^{ik\,\lambda}\right) = 0, \tag{4.3}$$

where I is the identity matrix. Considering Equation (1.7), the latter equation is equivalent to

$$S_E = \cos(k\lambda), \tag{4.4}$$

where S_E is the semi-trace of M_E.

On the one hand, the energy levels where $|S_E| \leq 1$ are allowed, leading to the so-called energy bands [9]. The dependence of E on k for each energy band is implicitly given by Equation (4.4). On the other hand, the energy levels where $|S_E| > 1$ are forbidden. They form gaps in the energy spectrum [9].

5 Numerical Results

Here, the equations in Sections 2, 3 and 4, are applied to solve the time-independent Schrödinger equation for a symmetric finite-barrier quantum well and a periodical sinusoidal potential. The numerical calculations and the graphical work have been implemented in Wolfram Mathematica [5].

5.1 Energy levels in a symmetric finite quantum well

The potential of the usual symmetric finite-barrier quantum well is given by Equation (3.1), with $V_w(x) = 0$ and $V_l = V_r = V_b$, where V_b is the barrier height. Then, Equation (3.9) becomes

$$\begin{bmatrix} \kappa_E & 1 \end{bmatrix} M_E \begin{bmatrix} 1 \\ \kappa_E \end{bmatrix} = 0, \tag{5.1}$$

where $\kappa_E = \sqrt{2m(V_b - E)/\hbar^2}$. Moreover, according to Equation (2.3), the quantum-well transfer matrix is given by

$$M_E = T_E(a/2, -a/2) = \begin{bmatrix} \cos(K_E\, a) & \frac{1}{K_E}\sin(K_E\, a) \\ -K_E \sin(K_E\, a) & \cos(K_E\, a) \end{bmatrix}, \tag{5.2}$$

with $K_E = \sqrt{2mE/\hbar^2}$.

Plugging (5.2) into (5.1) we get the transcendental equation

$$\cos(K_E\, a) + \frac{1}{2}\sin(K_E\, a)\left(\frac{\kappa_E}{K_E} - \frac{K_E}{\kappa_E}\right) = 0, \tag{5.3}$$

which leads to the energy levels. This can be solved for both $\cos(K_E\, a)$ and $\sin(K_E\, a)$ as

$$\begin{bmatrix} \cos(K_E\, a) \\ \sin(K_E\, a) \end{bmatrix} = \pm\frac{1}{\sqrt{1+g_E^2}} \begin{bmatrix} g_E \\ 1 \end{bmatrix}, \tag{5.4}$$

with

$$g_E = \frac{1}{2}\left(\frac{K_E}{\kappa_E} - \frac{\kappa_E}{K_E}\right). \tag{5.5}$$

According to Equation (3.10), this leads to

$$\lambda_E = \cos(K_E\, a) + \frac{\kappa_E}{K_E}\sin(K_E\, a) = \pm 1 \tag{5.6}$$

Hence, the wave function satisfies $\psi(-x) = \lambda_E\, \psi(x)$. The case $\lambda_E = 1$ ($\lambda_E = -1$) corresponds to even (odd) wave functions.

To compare with the literature, we calculate

$$\cot(K_E a/2) = \frac{\cos(K_E a/2)}{\sin(K_E a/2)} = \frac{1+\cos(K_E a)}{\sin(K_E a)} = g_E + \lambda_E\sqrt{1+g_E^2}. \tag{5.7}$$

As expected [10, 13], even states satisfy

$$\cot(K_E a/2) = g_E + \sqrt{1+g_E^2} = \frac{K_E}{\kappa_E}, \tag{5.8}$$

whereas odd states fulfill

$$\cot(K_E a/2) = g_E - \sqrt{1+g_E^2} = -\frac{\kappa_E}{K_E}. \tag{5.9}$$

Conveniently, the numerical results are given in appropriate units: $\epsilon = E/U$ and $\alpha = V_b/U$, with $U = \hbar^2/(2ma^2)$. Thus, the dimensionless energy levels are given by the roots of

$$p(\epsilon) = \cos(\sqrt{\epsilon}) + \frac{1}{2}\sin(\sqrt{\epsilon})\left(\sqrt{\frac{\alpha-\epsilon}{\epsilon}} - \sqrt{\frac{\epsilon}{\alpha-\epsilon}}\right). \tag{5.10}$$

Moreover, the energies of the even ($\lambda_E = 1$) and odd ($\lambda_E = -1$) states are given by the roots of

$$q_{\lambda_E}(\epsilon) = \cos(\sqrt{\epsilon}) + \sqrt{\frac{\alpha-\epsilon}{\epsilon}}\,\sin(\sqrt{\epsilon}) - \lambda_E. \tag{5.11}$$

A graphical analysis of Equation (5.10) can be performed from Figure 5.1. The points where the curve intersects the ϵ axis correspond to the bound states of the particle in the quantum well.

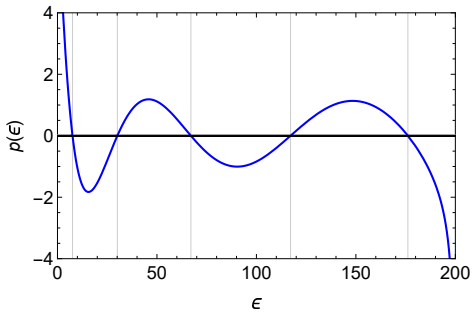

Figure 5.1: Graph of $p(\epsilon)$ given by Equation (5.10) for $\alpha = 200$.

Figure 5.2 displays the energy levels of a finite quantum well with different values of the dimensionless parameter α. For $\alpha = 150$, only two energy levels appear, for $\alpha = 200$, three energy levels appear, and for $\alpha = 250$, four energy levels appear. Therefore, the higher the value of α, the more energy levels are found.

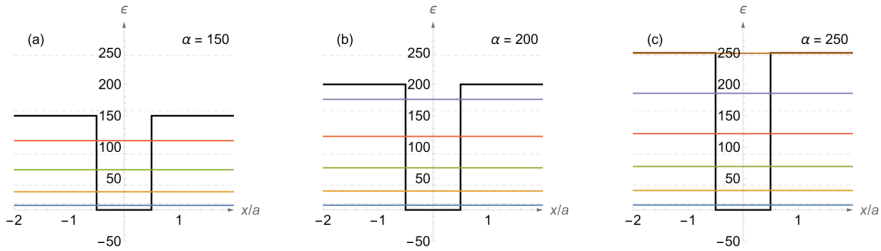

Figure 5.2: Energy levels of a particle in a finite quantum well for three values of the dimensionless parameter: (a) $\alpha = 150$, (b) $\alpha = 200$, and (c) $\alpha = 250$.

5.2 Energy bands of the sinusoidal potential

Now we consider the sinusoidal potential $V(x) = -A\cos(2\pi x/\lambda)$ whose transfer matrix was calculated in Subsection 2.2. The energy bands of the particle are given by Equation (4.4), where S_E can be taken as the semi-trace of the transfer matrix M_E from 0 to λ. According to Equation (2.12), and considering that $S_{2\epsilon,-\alpha}(0) = C'_{2\epsilon,-\alpha}(0) = 0$, we have

$$\begin{aligned} M_E &= T_E(\lambda, 0) \\ &= \begin{bmatrix} C_{2\epsilon,-\alpha}(\pi) & S_{2\epsilon,-\alpha}(\pi) \\ C'_{2\epsilon,-\alpha}(\pi) & S'_{2\epsilon,-\alpha}(\pi) \end{bmatrix} \begin{bmatrix} C_{2\epsilon,-\alpha}(0) & S_{2\epsilon,-\alpha}(0) \\ C'_{2\epsilon,-\alpha}(0) & S'_{2\epsilon,-\alpha}(0) \end{bmatrix}^{-1} \\ &= \begin{bmatrix} \dfrac{C_{2\epsilon,-\alpha}(\pi)}{C_{2\epsilon,-\alpha}(0)} & \dfrac{S_{2\epsilon,-\alpha}(\pi)}{S'_{2\epsilon,-\alpha}(0)} \\ \dfrac{C'_{2\epsilon,-\alpha}(\pi)}{C_{2\epsilon,-\alpha}(0)} & \dfrac{S'_{2\epsilon,-\alpha}(\pi)}{S'_{2\epsilon,-\alpha}(0)} \end{bmatrix}. \end{aligned} \tag{5.12}$$

Hence, we obtain

$$S_E = \frac{1}{2}\,\mathrm{Tr}(M_E) = \frac{1}{2}\left(\frac{C_{2\epsilon,-\alpha}(\pi)}{C_{2\epsilon,-\alpha}(0)} + \frac{S'_{2\epsilon,-\alpha}(\pi)}{S'_{2\epsilon,-\alpha}(0)}\right), \tag{5.13}$$

in good agreement with the literature [1, 18].

The blue curves in Figure 5.3 display the behavior of S_E given by Equation (4.4), for three values of the parameter α. The yellow ranges are

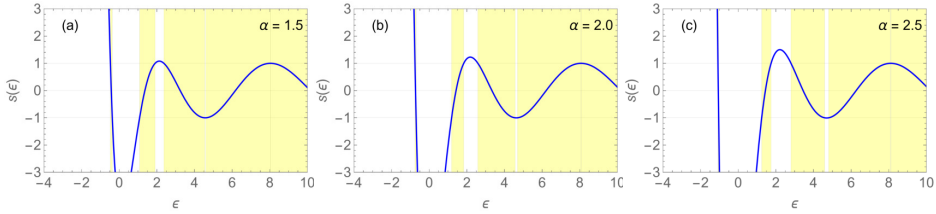

Figure 5.3: Energy bands (yellow ranges) and gaps (white ranges) for a particle in a sinusoidal potential for different values of the dimensionless parameter: (a) $\alpha = 1.5$, (b) $\alpha = 2.0$ and (c) $\alpha = 2.5$. The curve is for the semi-trace S_E.

the energy bands, whereas the white ranges between them are the energy gaps. We observe that the energy bands narrow and the energy gaps widen as the parameter α increases.

Figure 5.4 displays the dispersion relation (energy versus wave vector) for the lowest five energy bands in Figure 5.4. These are continuous and periodic functions of period $2\pi/\lambda$. Their derivatives on the wave vector are also continuous almost everywhere. In general, kinks may appear at vanishing energy gaps. It is noteworthy that the sinusoidal potential allows for arbitrarily small energy gaps, but none of them is null [16].

6 Conclusions

The transfer-matrix method has been applied to solve the Schrödinger equation in one-dimension to find the allowed energy levels of a particle in a quantum well, and in a periodic potential, with arbitrary profiles. This should simplify calculations for complex profiles, even in the case where the transfer matrix needs to be found by approximate numerical methods. Analytical and numerical results were given for symmetric finite-barrier quantum wells and sinusoidal periodic potentials. They were found in agreement with the literature [10, 13].

For the finite quantum well, a graphical analysis of the energy spectrum

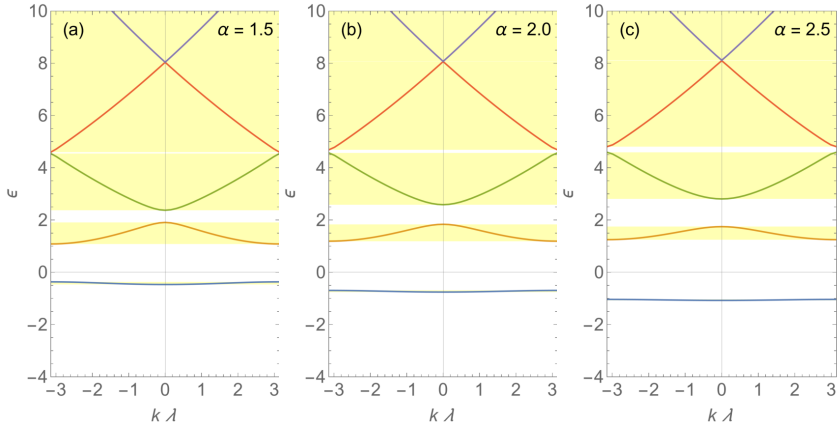

Figure 5.4: As of Figure 5.3, but including the dependence of the energy ϵ on the crystalline wave vector k. The lowest five energy bands are displayed in different colors. Part of the fifth one is above the displayed energy range.

was performed for different values of a dimensionless parameter α that is proportional to the product of the particle mass, the well depth and the square of the well width. The higher the value of α, the more energy levels were observed.

For the sinusoidal potential, the method led to a band structure that is typical for particles in crystalline solids, with analytical expressions in agreement with the literature [1, 18]. Numerical calculations were given for different values of a dimensionless parameter α that is proportional to the product of the particle mass, the potential amplitude and the squared potential period. As α increases, the bands become narrower while the energy gaps become wider.

Our formulation can be applied to solve the Schrödinger equation for a variety of potential profiles in a clear, simple, universal and accurate way. Beyond these benefits for students, physicists, engineers and the like, the formulation should be useful to develop/benchmark trending alternate methods, such as those using neural networks/machine learning techniques [15].

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