

Chapter 1: General Properties of the Schrödinger Equation

The following set of problems deals with the time-independent *effective-mass Schrödinger equation* (EMSE), which governs the steady-state behavior of an electron in a solid with spatially varying potential profile. The solid may consist of one or more materials (e.g., a heterostructure or superlattice); hence, the effective mass of the electron may vary in space. The EMSE is widely used in studying the electronic and optical properties of solids. The reader should first consult textbooks on EMSE if unfamiliar with the concept [1, 2]. The concept of quantum mechanical wave impedance is introduced to point out the similarity between solutions to the time-independent Schrödinger equation and transmission line theory in classical electrodynamics [3] and microwave theory [4–6].

* Problem 1.1: The effective mass Schrödinger equation for arbitrary spatially varying effective mass $m^*(z)$ and potential $E_c(z)$ profiles

(a) Consider an electron in a solid, which could be a semiconductor or an insulator. We will exclude a metal since the potential inside a metal is usually spatially invariant as a metal cannot sustain an electric field. The potential that an electron sees inside a semiconductor or insulator is the conduction band profile. We will assume that it is time independent and varies only along one direction, which we call the z -direction (see Figure 1.1). The effective mass also varies along that direction.

Show that the stationary solutions of the Schrödinger equation obey the equation

$$\begin{aligned} -\frac{\hbar^2}{2m^*(z)} \left(\frac{d^2}{dx^2} + \frac{d^2}{dy^2} \right) \psi(x, y, z) - \frac{\hbar^2}{2} \frac{d}{dz} \left[\frac{1}{m^*(z)} \frac{d}{dz} \right] \psi(x, y, z) \\ + E_c(z) \psi(x, y, z) = E \psi(x, y, z), \end{aligned} \quad (1.1)$$

where $E_c(z)$ is the conduction band edge and E is the total energy of the electron, which is independent of z because the total energy is a good quantum number in the absence of dissipation. In Equation (1.1),

$$\begin{aligned} E &= E_{\text{kin}}(z) + E_c(z) \quad \text{and} \\ E_{\text{kin}}(z) &= \frac{\hbar^2}{2m_c^*} (k_z^2(z) + k_t^2), \end{aligned} \quad (1.2)$$

where k_z and $k_t = \sqrt{k_x^2 + k_y^2}$ are the longitudinal and transverse components of the electron's wave vector, respectively, while $m_c^* = m^*(0)$ is the effective mass in the

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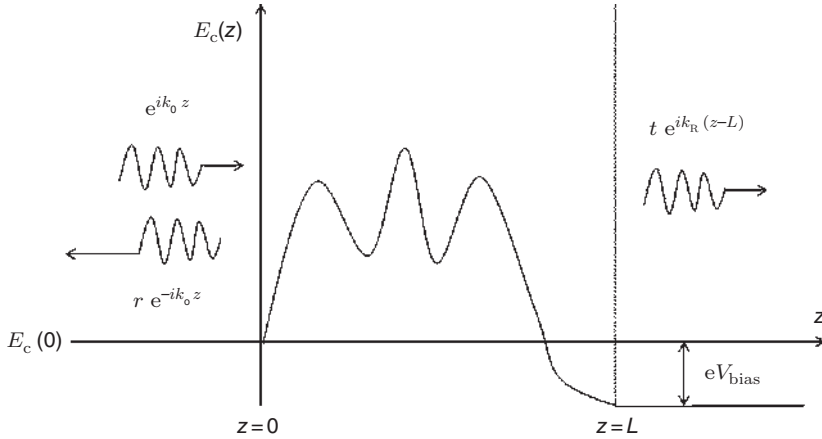


Figure 1.1: Illustration of electron impinging on the left on an arbitrary conduction band energy profile under bias. V_{bias} is the potential difference between the two contacts.

contacts. Since the potential varies only in the z -direction, k_t is spatially invariant, but k_z varies with the z -coordinate.

(b) Because the potential does not vary in the x - y plane, the transverse component of the wave function is a plane wave and we can write the wave function in Equation (1.1) as

$$\psi(x, y, z) = \phi(z)e^{i\vec{k}_t \cdot \vec{\rho}}. \quad (1.3)$$

Show that the z -component of the wave function $\phi(z)$ satisfies the following EMSE:

$$\frac{d}{dz} \left[\frac{1}{\gamma(z)} \frac{d}{dz} \right] \phi(z) + \frac{2m_c^*}{\hbar^2} [(E_p + E_t[1 - \gamma^{-1}(z)] - E_c(z))] \phi(z) = 0, \quad (1.4)$$

where $\gamma(z) = \frac{m^*(z)}{m_c^*}$, $E_t = \frac{\hbar^2 k_t^2}{2m_c^*}$, and $E_p = \frac{\hbar^2 k_z^2}{2m_c^*}$.

Solution: Taking into account a spatially varying effective mass along the z -direction, the time-dependent Schrödinger equation describing an electron moving in an arbitrary potential $E_c(z)$ is given by

$$\begin{aligned} & \left[-\frac{\hbar^2}{2m^*(z)} \left(\frac{d^2}{dx^2} + \frac{d^2}{dy^2} \right) - \frac{\hbar^2}{2} \frac{d}{dz} \left(\frac{1}{m^*(z)} \frac{d}{dz} \right) + E_c(z) \right] \Psi(x, y, z, t) \\ & = i\hbar \frac{d\Psi(x, y, z, t)}{dt}. \end{aligned} \quad (1.5)$$

Since all quantities on the left-hand side are time independent by virtue of the fact that the potential is time invariant, we can write the wave function in a product form:

$$\Psi(x, y, z, t) = \psi(x, y, z)\xi(t). \quad (1.6)$$

Substitution of this form in Equation (1.5) immediately yields that $\xi(t) = e^{-iEt/\hbar}$, and $\psi(x, y, z)$ obeys Equation (1.1).

Next, we note that in Equation (1.5) no quantity in the Hamiltonian on the left-hand side (i.e., the terms within the square brackets) depends on more than one coordinate (x , y , or z). Hence, the wave function $\psi(x, y, z)$ can be written as the product of an x -dependent term, a y -dependent term, and a z -dependent term. Furthermore, no quantity depends on the x or y coordinate. Therefore, the x -dependent and y -dependent terms must be plane waves. The z -dependent term will not be a plane wave since both $E_c(z)$ and $m^*(z)$ depend on the z -coordinate. Consequently, we write $\psi(x, y, z)$ as

$$\psi(x, y, z) = e^{ik_x x} e^{ik_y y} \phi(z). \quad (1.7)$$

Plugging this last expression into Equation (1.1) leads to the EMSE for the envelope function $\phi(z)$:

$$\left[-\frac{\hbar^2}{2m^*(z)} (k_x^2 + k_y^2) + \frac{\hbar^2}{2} \frac{d}{dz} \left(\frac{1}{m^*(z)} \frac{d}{dz} \right) \right] \phi(z) = [E - E_c(z)] \phi(z). \quad (1.8)$$

Multiplying both sides of the equation by $\frac{2m_c^*}{\hbar^2}$, we obtain

$$\left[-\frac{2m_c^*}{\hbar^2} \frac{E_t}{\gamma(z)} + \frac{d}{dz} \left(\frac{1}{\gamma(z)} \frac{d}{dz} \right) \right] \phi(z) = \frac{2m_c^*}{\hbar^2} (E - E_c(z)) \phi(z). \quad (1.9)$$

Hence,

$$\frac{d}{dz} \left[\frac{1}{\gamma(z)} \frac{d}{dz} \phi(z) \right] + \frac{2m_c^*}{\hbar^2} \left[E - \frac{E_t}{\gamma(z)} - E_c(z) \right] \phi(z) = 0, \quad (1.10)$$

where $E = E_t + E_p$, $E_p = \frac{\hbar^2 k_z^2}{2m_c^*}$ is the longitudinal kinetic energy (i.e., the kinetic energy associated with the z -component of the motion), and $E_t = \frac{\hbar^2 (k_x^2 + k_y^2)}{2m_c^*}$ is the transverse kinetic energy.

Problem 1.2: The Ben Daniel–Duke boundary condition

Starting with the one-dimensional EMSE derived in the previous problem, show that in addition to the continuity of the wave function required by the postulates of quantum mechanics (see Appendix A), the following quantity must be continuous when taking into account the spatial variation of the effective mass:

$$\frac{1}{m^*(z)} \frac{d\phi(z)}{dz}. \quad (1.11)$$

The continuity of this quantity generalizes the continuity of the first derivative of the wave function typically used in solving quantum mechanical problems. Together with the continuity of the wave function, imposing continuity of this quantity is referred to as the Ben Daniel–Duke boundary conditions [7]. The application of these boundary conditions will be illustrated in several problems throughout the book.

Solution: Our starting point is the time-independent effective one-dimensional Schrödinger equation derived in the previous problem:

$$\frac{d}{dz} \left[\frac{1}{\gamma(z)} \frac{d}{dz} \phi(z) \right] + \frac{2m_c^*}{\hbar^2} \left[E - \frac{E_t}{\gamma(z)} - E_c(z) \right] \phi(z) = 0, \quad (1.12)$$

where $E = E_t + E_p$, $E_p = \frac{\hbar^2 k_z^2}{2m_c^*}$ is the longitudinal kinetic energy, $\gamma(z) = m^*(z)/m_c^*$, where m_c^* is the effective mass in the contacts, and $E_t = \frac{\hbar^2(k_x^2 + k_y^2)}{2m_c^*}$ is the transverse kinetic energy.

Assuming that both $\gamma(z)$ and $E_c(z)$ are either continuous or have finite jumps for all z , we integrate the last Schrödinger equation on both sides from $z_0^- = z_0 - \epsilon$ to $z_0^+ = z_0 + \epsilon$, where ϵ is a small positive quantity. This leads to

$$\frac{1}{\gamma(z)} \frac{d\phi(z)}{dz} \Big|_{z=z_0^-} = \frac{1}{\gamma(z)} \frac{d\phi(z)}{dz} \Big|_{z=z_0^+}. \quad (1.13)$$

As $\epsilon \rightarrow 0$, this last equation shows that the quantity $\frac{1}{m^*(z)} \frac{d\phi(z)}{dz}$ is continuous everywhere [7].

When the effective mass varies in space, the correct boundary condition (involving the spatial derivative of the wave function) to use has been a hotly debated topic. There is some controversy regarding the appropriate form of the Hamiltonian to use in the case of spatially varying effective mass, and the reader is referred to the literature on this topic [8–10].

Preliminary: Linearly independent solutions of the Schrödinger equation

We consider the three-dimensional time-independent Schrödinger equation associated with an electron moving in an arbitrary potential energy profile (such as the conduction band of a semiconductor structure) $E_c(z)$ varying along the z -direction only, as shown in Figure 1.1. If the effective mass of the electron is assumed to be independent of z , the Schrödinger equation for the envelope function component along the z -direction is given by (see Problem 1.1)

$$-\frac{\hbar^2}{2m^*} \ddot{\phi}(z) + E_c(z)\phi(z) = E_p\phi(z), \quad (1.14)$$

where $\ddot{\phi}(z)$ stands for $\frac{d^2}{dz^2}\phi(z)$, the second derivative with respect to z , and E_p is the longitudinal kinetic energy, i.e., the kinetic energy component associated with motion in the z -direction.

The general solution of this second-order differential equation for $\phi(z)$ can be written as a linear combination of two linearly independent solutions [11]. Two solutions $\phi_1(z)$ and $\phi_2(z)$ of a differential equation are linearly independent if the equality $c_1\phi_1(z) + c_2\phi_2(z) = 0$ cannot be satisfied for all z for any choice of (c_1, c_2) except for $c_1 = c_2 = 0$. If non-zero solutions (c_1, c_2) exist, then $\phi_1(z)$ and $\phi_2(z)$ are said to be linearly dependent.

Concept of Wronskian: If ϕ_1 and ϕ_2 are linearly dependent, then $c_1\phi_1(z) + c_2\phi_2(z) = 0$ and $c_1\dot{\phi}_1(z) + c_2\dot{\phi}_2(z) = 0$, where the dot stands for the first derivative with respect to z . Hence, in matrix form, we have

$$\begin{bmatrix} \dot{\phi}_1(z) & \dot{\phi}_2(z) \\ \phi_1(z) & \phi_2(z) \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}. \quad (1.15)$$

This means that the Wronskian $W(z) = \dot{\phi}_1(z)\phi_2(z) - \phi_1(z)\dot{\phi}_2(z)$, which is the determinant of the 2×2 matrix in the last equation, must be identically zero since otherwise only the trivial solution $c_1 = c_2 = 0$ in the last equation would be admissible. Stated differently, for two solutions to be linearly independent, their Wronskian must be non-zero for all z .

Even if $E_c(z)$ has finite discontinuities, it is obvious from Equation (1.14) that $\ddot{\phi}(z)$ exists throughout and, hence, $\phi(z)$ and $\dot{\phi}(z)$ must be continuous.

Since $\phi_1(z), \phi_2(z)$ satisfy the Schrödinger equation in Equation (1.14), it is easy to see that

$$\ddot{\phi}_1(z)\phi_2(z) - \ddot{\phi}_2(z)\phi_1(z) = 0, \quad (1.16)$$

or

$$\frac{d}{dz} [\dot{\phi}_1(z)\phi_2(z) - \dot{\phi}_2(z)\phi_1(z)] = \frac{dW}{dz} = 0. \quad (1.17)$$

Thus, $W(z)$ is a constant independent of z . It is obviously independent of z when it is zero, but it is also independent of z when it is non-zero.

In summary, if the Wronskian $W(z) = 0$, then (ϕ_1, ϕ_2) are linearly dependent, and, if $W(z) \neq 0$, they are linearly independent. If we can find these two linearly independent solutions, their linear combination is the most general solution to the Schrödinger equation. This general solution is

$$\phi(z) = c_1\phi_1(z) + c_2\phi_2(z). \quad (1.18)$$

Typically, two solutions $\phi_1(z)$ and $\phi_2(z)$ of the Schrödinger equation are found such that they obey the boundary conditions

$$\phi_1(0) = 0, \quad \dot{\phi}_1(0) = 1, \quad (1.19)$$

and

$$\phi_2(0) = 1, \quad \dot{\phi}_2(0) = 0. \quad (1.20)$$

These solutions are indeed linearly independent since their Wronskian, which is independent of z , is equal to

$$W(z) = W(0) = \dot{\phi}_1(0)\phi_2(0) - \phi_1(0)\dot{\phi}_2(0) = 1. \quad (1.21)$$

In Chapter 7, we will show that the concept of Wronskian and linearly independent solutions can be used to introduce the concept of a transfer matrix, which is a very powerful approach to solving both bound state and tunneling problems in spatially varying potentials.

**** Problem 1.3: General properties of the one-dimensional time-independent Schrödinger equation**

Suppose two wave functions $\phi_1(z)$ and $\phi_2(z)$ satisfy the following two EMSEs:

$$-\frac{\hbar^2}{2m^*}\ddot{\phi}_1(z) + E_{c1}(z)\phi_1(z) = E_1\phi_1(z), \quad (1.22)$$

and

$$-\frac{\hbar^2}{2m^*}\ddot{\phi}_2(z) + E_{c2}(z)\phi_2(z) = E_2\phi_2(z), \quad (1.23)$$

respectively.

First, multiply Equation (1.22) by $\phi_2(z)$ and Equation (1.23) by $\phi_1(z)$, then subtract one from the other, and finally integrate the difference from z_1 to z_2 . This will yield

$$\begin{aligned} & [\phi_2(z)\phi'_1(z) - \phi_1(z)\phi'_2(z)]_{z_1}^{z_2} \\ &= \frac{2m^*}{\hbar^2} \int_{z_1}^{z_2} [(E_2 - E_{c2}(z)) - (E_1 - E_{c1}(z))] \phi_1(z)\phi_2(z) dz. \end{aligned} \quad (1.24)$$

Starting with the last equation, prove the following statements [11]:

(a) If $E_2 - E_{c2}(z) \geq E_1 - E_{c1}(z)$, there is a node of $\phi_2(z)$ between any two nodes of $\phi_1(z)$.

(b) If $E_{c2}(z) = E_{c1}(z) = E_c(z)$, $E_2 > E_1$, and $\phi_{1,2}(\pm\infty) = \phi'_{1,2}(\pm\infty) = 0$, then ϕ_2 has more nodes than ϕ_1 .

(c) If ϕ_1 and ϕ_2 are solutions of Equations (1.22)–(1.23) with eigenvalues E_1 and E_2 , respectively, and are such that ϕ_1 , ϕ'_1 , ϕ_2 , and ϕ'_2 vanish at either $+\infty$ or $-\infty$, and ϕ_1 and ϕ_2 are linearly independent, then $E_1 \neq E_2$.

Solution:

(a) We prove these assertions indirectly. Let us assume that z_1 and z_2 are the locations of two consecutive nodes of $\phi_1(z)$ and that $\phi_2(z)$ has no node in the interval $[z_1, z_2]$. Since the wave functions can have nodes, both $\phi_1(z)$ and $\phi_2(z)$ must be real (since no solution of the Schrödinger equation that has an imaginary component can vanish anywhere). Furthermore, let us assume (without loss of generality) that $\phi_1(z)$ and $\phi_2(z)$ are both positive within the interval $[z_1, z_2]$ (the proofs for the cases when one is positive and the other negative, or both are negative, are no different from what follows and can be worked out by the reader following the derivation that ensues). Since $\phi_1(z_1) = \phi_1(z_2) = 0$ by assumption, Equation (1.24) leads to

$$\begin{aligned} & \phi_2(z_2)\phi'_1(z_2) - \phi_2(z_1)\phi'_1(z_1) \\ &= \frac{2m^*}{\hbar^2} \int_{z_1}^{z_2} [(E_2 - E_{c2}(z)) - (E_1 - E_{c1}(z))] \phi_1(z)\phi_2(z) dz. \end{aligned} \quad (1.25)$$

Now, since $\phi_1(z)$ vanishes at z_1 and z_2 , and in between these two locations is positive, clearly $\phi_1(z_1 + \epsilon) - \phi_1(z_1) > 0$ and $\phi_1(z_2) - \phi_1(z_2 - \epsilon) < 0$, where ϵ is an infinitesimally small positive quantity. Therefore the spatial derivatives $\phi'_1(z_1)$ and $\phi'_1(z_2)$ are, respectively, positive and negative. Consequently, the left-hand side of the last equation will be negative while the right-hand side is positive, which leads to a mathematical contradiction. Since our original assumption leads to this contradiction, the statement (a) above is proved by *reductio ad absurdum*.

(b) The conditions $\phi_1(\pm\infty) = 0$ and $\phi'_1(\pm\infty)$ imply that the particle is confined to a finite region of the z -axis. The corresponding states are called *bound states*. Letting $E_{c2}(z) = E_{c1}(z)$ in Equation (1.25), we get

$$\phi_2(z_2)\phi'_1(z_2) = \frac{2m^*}{\hbar^2} (E_2 - E_1) \int_{z_1}^{z_2} \phi_1(z)\phi_2(z)dz. \quad (1.26)$$

If $z_1 = -\infty$ and z_2 is the first node of $\phi_1(z)$ from the left, we can, without loss of generality, take $\phi_1(z) > 0$ in the interval $] -\infty, z_2]$. Since $\phi_1(z_2) = 0$ (it is a node) and $\phi_1(z_2 - \epsilon) > 0$ (ϵ is an infinitesimally small positive quantity), obviously the spatial derivate of ϕ_1 at z_2 is negative, i.e., $\phi'_1(z_2) < 0$.

If $\phi_2(z)$ did not have a node in the interval $] -\infty, z_2]$, then its sign will not change within that interval, i.e. the sign will be constant. Since $\phi_{1,2}(\pm\infty) = \phi'_{1,2}(\pm\infty) = 0$ and $\phi_1(z_2) = 0$, we obtain

$$\phi_2(z_2)\phi'_1(z_2) = \frac{2m^*}{\hbar^2} (E_2 - E_1) \int_{-\infty}^{z_2} \phi_1(z)\phi_2(z)dz. \quad (1.27)$$

Let us assume that the constant sign of $\phi_2(z)$ in the interval is positive. Then, since $\phi'_1(z_2) < 0$, the left-hand side of the last equation becomes negative while the right-hand side remains positive, leading to an absurdity. The reader can verify that the same absurdity would have arisen if we had assumed that the constant sign of $\phi_2(z)$ in the interval was negative, instead of positive. Therefore, the assumption that $\phi_2(z)$ has a constant sign in the interval $] -\infty, z_2]$ is invalid. As a consequence, the wave function $\phi_2(z)$ must have at least one node to the left of the first node of $\phi_1(z)$. According to part (a), there must be at least one node of $\phi_2(z)$ between any two nodes of $\phi_1(z)$. In a similar fashion, it can be shown that there is at least one node of $\phi_2(z)$ to the right of the last node of $\phi_1(z)$. Thus, $\phi_2(z)$ has at least one more node than $\phi_1(z)$, and part (b) is proved.

(c) Suppose $E_1 = E_2$. Then, since $\phi_1(z)$ and $\phi_2(z)$ are solutions of the same EMSE with the same energy $E_1 = E_2$, we can define a Wronskian W . Furthermore, since $\phi_1(z)$ and ϕ_2 are linearly independent, their Wronskian, $W(z) = \phi'_1(z)\phi_2(z) - \phi_1(z)\phi'_2(z)$, is a constant *different* from zero. But W is independent of the z -coordinate and, because either $W(+\infty)$ or $W(-\infty)$ vanishes, W must be exactly zero. Once again, we have a contradiction, which tells us that our original assumption must have been incorrect and therefore $E_1 \neq E_2$. Two (or more) linearly independent states having the same energy eigenvalues are said to be *degenerate*. This last property shows that *bound states of a particle in a one-dimensional potential are always non-degenerate*.

*** Problem 1.4: Bound states of a particle moving in a one-dimensional potential of even parity**

Show that the bound state solutions of the one-dimensional Schrödinger equation in a one-dimensional potential of even parity have either odd or even parity.

Solution: If the one-dimensional potential energy profile has even parity, then it is symmetric about $z = 0$, i.e., $E_c(z) = E_c(-z)$. In that case, if $\phi(z)$ is solution of the one-dimensional EMSE in Equation (1.14), then clearly so is $\phi(-z)$.

Any wave function $\phi(z)$ can be written as a sum of a symmetric part $\phi_+(z)$ and an antisymmetric part $\phi_-(-z)$:

$$\phi(z) = \frac{1}{2}[\phi(z) + \phi(-z)] + \frac{1}{2}[\phi(z) - \phi(-z)] = \phi_+(z) + \phi_-(-z). \quad (1.28)$$

For an even $E_c(z)$, since both $\phi(z)$ and $\phi(-z)$ are solutions of Equation (1.14), so must be $\phi_+(z)$ and $\phi_-(z)$ since they are linear combinations of $\phi(z)$ and $\phi(-z)$.

From the results of Problem 1.3, the bound states of a general one-dimensional $E_c(z)$ are non-degenerate. Hence, the bound states of a particle moving in an even $E_c(z)$ must have a definite parity, i.e., must be either odd (antisymmetric) or even (symmetric).

*** Problem 1.5: Quantum measurement**

The “particle in a one-dimensional box” problem is one of the simplest problems in quantum mechanics. It refers to an electron confined within a one-dimensional box with infinite barriers. The eigenstates (or allowed wave functions) of the electron are given by (see Problem 3.5):

$$\phi_n(z) = \sqrt{\frac{2}{W}} \sin\left(\frac{n\pi z}{W}\right), \quad (1.29)$$

where n is an integer ($n = 1, 2, 3, \dots$) and W is the width of the box. Each value of n defines an eigenstate.

The corresponding energy eigenvalues are given by

$$E_n = n^2 \frac{\hbar^2 \pi^2}{2m^* W^2}, \quad (1.30)$$

and they are all distinct or non-degenerate, in keeping with what was proved in Problem 1.2.

For an electron injected into a quantum box of width W at time $t = 0$ in the state

$$\phi(0) = A \left[i\sqrt{2} \sin\left(\frac{3\pi z}{W}\right) - \sin\left(\frac{7\pi z}{W}\right) + 2 \sin\left(\frac{9\pi z}{W}\right) \right] e^{i(k_x x + k_y y)}, \quad (1.31)$$

where the plane of the quantum well is the (x, y) plane:

(a) Find the value of A .

(b) Find the wave function at time t .

(c) What is the expectation value of the electron's energy?

Solution: (a) Normalization of the wave function requires $A^2 \frac{W}{2} (2 + 1 + 4) = 1$, hence $A = \sqrt{\frac{2}{7W}}$.

(b) The wave function at time t is

$$\begin{aligned} \phi(t) = \sqrt{\frac{2}{7W}} & \left[i\sqrt{2} \sin\left(\frac{3\pi z}{W}\right) e^{\frac{iE_3 t}{\hbar}} - \sin\left(\frac{7\pi z}{W}\right) e^{\frac{iE_7 t}{\hbar}} \right. \\ & \left. + 2 \sin\left(\frac{9\pi z}{W}\right) e^{\frac{iE_9 t}{\hbar}} \right] e^{i(k_x x + k_y y)}, \end{aligned} \quad (1.32)$$

where E_n is given by Equation (1.30).

(c) The expectation value of the energy is independent of time and given by

$$\begin{aligned} \langle E \rangle &= \frac{2E_3 + E_7 + 4E_9}{7} \\ &= \frac{\hbar^2}{14m^*} [2 \times 3^2 + 7^2 + 4 \times 9^2] \left(\frac{\pi}{W}\right)^2 \\ &= \frac{391\hbar^2}{14m^*} \left(\frac{\pi}{W}\right)^2. \end{aligned} \quad (1.33)$$

** Problem 1.6: Concept of quantum mechanical wave impedance

Starting with Problem 1.1, show that the Schrödinger equation for a particle moving in a general potential energy profile $E_c(z)$ (assuming constant effective mass)

$$\frac{d^2}{dz^2} \phi(z) + \beta^2 \phi(z) = 0, \quad (1.34)$$

where

$$\beta^2 = \frac{2m^*}{\hbar^2} \left[E - E_c(z) - \frac{\hbar}{2m^*} (k_x^2 + k_y^2) \right] \quad (1.35)$$

and (k_x, k_y) are the components of the transverse momentum, can be rewritten as two first-order differential equations

$$\frac{dv(z)}{dz} = -Zu(z) \quad (1.36)$$

and

$$\frac{du(z)}{dz} = -Yv(z) \quad (1.37)$$

if we introduce the two variables

$$u = \phi(z) \quad (1.38)$$

and

$$v = -\frac{2\hbar}{m^*i} \frac{d\phi}{dz}. \quad (1.39)$$

What are the expressions for Z and Y ?

This is equivalent to defining a quantum mechanical wave impedance $Z(z)$ as follows [12]:

$$Z(z) = \frac{v(z)}{u(z)} = \left(\frac{2\hbar}{im^*} \right) \frac{\frac{d\phi(z)}{dz}}{\phi(z)}. \quad (1.40)$$

Solution: Based on the definitions in Equations (1.38) and (1.39), we get

$$\frac{du}{dz} = \frac{d\phi}{dz} = -\frac{m^*}{2i\hbar}v \quad (1.41)$$

and

$$\frac{dv}{dz} = -\frac{2i\hbar}{m^*} \frac{d^2\phi}{dz^2} = \left(\frac{2i\hbar\beta^2}{m^*} \right) u, \quad (1.42)$$

which can be recast as

$$\frac{dv}{dz} = -Zu \quad (1.43)$$

and

$$\frac{du}{dz} = -Yv \quad (1.44)$$

by introducing the quantities

$$Y = \frac{m^*}{2i\hbar} \quad (1.45)$$

and

$$Z = -\frac{2i\hbar\beta^2}{m^*}. \quad (1.46)$$

Equations (1.43) and (1.44) look similar to the transmission line equations in electromagnetic field theory [3–5] if we use the transformations

$$V(z) \rightarrow -\frac{2i\hbar}{m^*} \frac{d\phi}{dz} \quad (1.47)$$

and

$$I(z) \rightarrow \phi(z). \quad (1.48)$$

The Schrödinger Equation (1.34) is therefore equivalent to two first-order coupled differential equations:

$$\frac{dv(z)}{dz} = -ZI(z), \quad (1.49)$$

$$\frac{dI(z)}{dz} = -YV(z). \quad (1.50)$$

This is equivalent to defining a quantum mechanical wave impedance $Z_{\text{QM}}(z)$ as follows [12]:

$$Z_{\text{QM}}(z) = \frac{2\hbar}{im^*} \frac{(d\phi(z)/dz)}{\phi(z)}. \quad (1.51)$$

The quantity $Z_{\text{QM}}(z)$ does not have the unit of ohms (it has the unit of velocity), but is a useful concept to solve some bound state and tunneling problems, as illustrated in Chapter 7.

Suggested problems

- Consider a particle with the one-dimensional wave function

$$\phi(z) = N (a^2 + z^2)^{-1/2} e^{\frac{ip_0 z}{\hbar}}, \quad (1.52)$$

where a , p_0 , and N are real constants.

- (1) Find the normalization constant N .
- (2) Determine the probability of finding the particle in the interval $-(a/\sqrt{5}) \leq z \leq (a/\sqrt{5})$.
- (3) What is the expectation value of the momentum?

- Consider a particle in a box defined by the potential profile:

$$V(z) = 0 \text{ if } |z| \leq W \text{ and } V(z) = \infty \text{ if } |z| \geq W.$$

At time $t = 0$ the wave function $\phi_0(z)$ is an even function of z .

- (1) What are the possible values resulting from a measurement of the kinetic energy?
- (2) How soon after $t = 0$ will the particle return to its initial state if left undisturbed? (If the particle is left undisturbed, it periodically visits the initial state. This is known as Poincaré recurrence).

12 Problem Solving in Quantum Mechanics

- Consider a particle described by the one-dimensional harmonic oscillator Hamiltonian (see Appendix B)

$$H = \frac{p^2}{2m^*} + \frac{1}{2}m^*\omega^2 z^2. \quad (1.53)$$

At time $t = 0$, the particle is described by the following wave function:

$$\phi(z) = N(1 + 3\alpha^2 z^2)e^{-\frac{1}{2}\alpha^2 z^2}, \quad (1.54)$$

where $\alpha = m^*\omega/\hbar^{1/2}$ and N is the normalization constant.

- (1) Find the value of N .
 - (2) What are the possible outcomes of the measurement of the total energy of the particle and with what probabilities?
 - (3) Write down the analytical expression of the wave function of the particle at time t .
- When the mass of a particle varies with position, the mass and momentum operators do not commute. The kinetic operator must be modified. Von Ross proposed the following kinetic operator [10]:

$$T(z) = \frac{1}{4}(m^\alpha p m^\beta p m^\gamma + m^\gamma p m^\beta p m^\alpha), \quad (1.55)$$

with $\alpha + \beta + \gamma = -1$.

In this case, show that the Schrödinger equation becomes

$$\begin{aligned} \frac{d^2}{dz^2}\phi(z) - \frac{m'(z)}{m(z)}\frac{d}{dz}\phi(z) \\ + \left[\frac{1}{2} \left(r m'' - s \frac{m'^2}{m^2} \right) + \frac{2m(z)}{\hbar^2}(E - E_c(z)) \right] \phi(z) = 0, \end{aligned} \quad (1.56)$$

where $r = \alpha + \gamma$, $s = \alpha(\gamma + 2) - \gamma(\alpha + 2)$. Furthermore, $m' = \frac{dm}{dz}$ and $m'' = \frac{d^2m}{dz^2}$.

- Starting with the results of the previous problem, show that the first derivative of $\phi(z)$ can be eliminated by making the transformation $\phi(z) = \sqrt{m(z)}\psi(z)$. Show that the resulting effective Schrödinger equation for $\psi(z)$ is given by

$$\begin{aligned} \frac{d^2}{dz^2}\phi(z) + \left[(1+r) \left\{ \frac{m'(z)}{2m(z)} \right. \right. \\ \left. \left. - \left(\frac{3}{4} + \frac{s}{2} \right) \frac{m'^2}{m^2} + m(E - E_c(z)) \right\} \right] \psi(z) = 0. \end{aligned} \quad (1.57)$$

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