Abstract

abstract-text

1 General Case

1. **Wavefunction solution from Schrodinger's equation**

Before proceeding to derive the prescribed problem set, we can first try to examine a more general case of the system. This may give us more insights in constructing the transfer matrix. We start by modifying the problem set a bit by instead considering the following potential configuration.

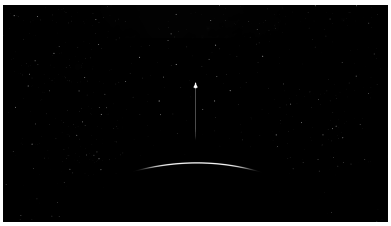

Figure 1: This is a sample figure.

Calculation of the wavefunction is basically finding the solution of a boundary-value problem via Schrodinger's equation along a given interval. The boundary conditions are given by the behavior of two intersecting wavefunctions at a given boundary. The intersection must be continuous (wavefunctions must be equal at the boundary) and smooth (wavefunction derivatives must be equal at the boundary). It should be noted in the special case of a constant potential that the wavefunction can be expressed by an expression parametrized by the potential value and the particles energy. Hence, similar or different parameter values must correspond to similar or different wavefunctions.

The goal of this exercise is to express these conditions ultimately in a matrix form. This is such that a composite matrix can be calculated transforming an incoming wavefunction along any arbitrary sequence of potential steps. The matrix itself possesses properties of the wavefunction at the specified position in space such as transmission and reflection probability amplitude.

2. **Constant potential solution to Schrodinger's equation**

We proceed to derive a general solution to the time-independent Schrodinger equation (TISE) in the region n with constant potential V_n. We denote n as a roman numeral symbol. TISE reads

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi_n(x)}{\mathrm{d}x} + V_n\psi_n(x) = E\psi_n(x) \tag{1}$$

This is simply a constant-coefficient second order ordinary differential equation which is easily recognizable in the form

$$\frac{\mathrm{d}^2\psi_n(x)}{\mathrm{d}x^2} = \frac{2m\left(V_n - E\right)}{\hbar^2}\psi_n(x) \tag{2}$$

which has a solution of form

$$\psi_n(x) = \tau_n \exp\left(ik_n x\right) + \gamma_n \exp\left(-ik_n x\right) \tag{3}$$

where τ_n and γ_n are arbitrary constants of integration and $k_n := \sqrt{(2m(E - V_n))/(\hbar^2)}$. Observe that the wavefunction in a given area n is parametrized by the constants τ_n and γ_n, and potential-dependent k_n. The key to note here is that two neighboring areas n and $n+1$ must have related constants τ_n, τ_{n+1}, γ_n, and γ_{n+1} due to continuity and smoothness conditions. Knowing the relationship between these neighboring constants at a given boundary, we can derive a function that converts a wavefunction from one constant potential to a neighboring constant potential. We proceed to derive this relationship in the next section.

3. **The Hopping Matrix**

From the solution of TISE expressed as in the Eq. (3), continuity requires $\psi_n(x) = \psi_{n+1}(x)$, while smoothness requires $\mathrm{d}\psi_n/\mathrm{d}x = \mathrm{d}\psi_{n+1}/\mathrm{d}x$ That is, in the boundary $x = m$ where m is denoted as a subscript $x_m = m$

$$\tau_n \exp(ik_n x_m) + \gamma_n \exp(-ik_n x_m) = \tau_{n+1} \exp(ik_{n+1} x_m) + \gamma_{n+1} \exp(-ik_{n+1} x_m) \tag{4}$$

$$ik_n \tau_n \exp(ik_n x_m) - ik_n \gamma_n \exp(-ik_n x_m) = ik_{n+1} \tau_{n+1} \exp(ik_{n+1} x_m) - ik_{n+1} \gamma_{n+1} \exp(-ik_{n+1} x_m) \tag{5}$$

These expressions can be compactified when converting them into a matrix form. Defining a vector $\vec{\psi}_n(x)$ as

$$\vec{\psi}_n(x) = \begin{bmatrix} \tau_n \exp(ik_n x) \\ \gamma_n \exp(-ik_n x) \end{bmatrix} \tag{6}$$

The conditions Eqs. (4) and (5) can be converted into a 2-dimensional linear system expressed compactly as

$$\begin{bmatrix} 1 & 1 \\ ik_n & -ik_n \end{bmatrix} \vec{\psi}_n(x_m) = \begin{bmatrix} 1 & 1 \\ ik_{n+1} & -ik_{n+1} \end{bmatrix} \vec{\psi}_{n+1}(x_m) \tag{7}$$

Hence, we can define a matrix $M(U_n, U_{n+1})$ such that

$$\vec{\psi_n}(x_m) = M(U_n, U_{n+1}) \vec{\psi_{n+1}} \tag{8}$$

We can find M by simply inverting the matrix

$$invert \tag{9}$$

where we can define

$$M_s(U_n, U_{n+1}) = \begin{bmatrix} 1 & 1 \\ ik_{n+1} & -ik_{n+1} \end{bmatrix} \tag{10}$$

4. **The Running Matrix**

We have derived a matrix that can transform a wavefunction from a potential to another given only the potential difference. However, note that this can only be used at the boundaries between each potential. We still need to traverse the constant potential itself. Similarly, we can also derive a matrix as follows. Doing this allows us to remain in a region n and use the same wavefunction. Consider the two non-boundary points $x_{m1} = m_1$ and $x_{m2} = m_2$ in the region n. Then,

$$\vec{\psi}_n(x_{m1}) = \begin{bmatrix} \tau_n \exp(ik_n x_{m1}) \\ \gamma_n \exp(-ik_n x_{m1}) \end{bmatrix} \qquad \vec{\psi}_n(x_{m2}) = \begin{bmatrix} \tau_n \exp(ik_n x_{m2}) \\ \gamma_n \exp(-ik_n x_{m2}) \end{bmatrix} \tag{11}$$

To transform $\vec{\psi}_n(x_{m1})$ into $\vec{\psi}_n(x_{m2})$, a trivial transformation can be used.

$$\begin{bmatrix} \tau_n \exp(ik_n x_{m1}) \\ \gamma_n \exp(-ik_n x_{m1}) \end{bmatrix} = \begin{bmatrix} \exp(ik_n(x_{m2} - x_{m1})) & 0 \\ 0 & \exp(-ik_n(x_{m2} - x_{m1})) \end{bmatrix} \begin{bmatrix} \tau_n \exp(ik_n x_{m2}) \\ \gamma_n \exp(-ik_n x_{m2}) \end{bmatrix} \tag{12}$$

But $x_{m2} - x_{m1}$ is simply the length of the region n we denote as L_n. Hence,

$$\vec{\psi}_n(x_{m2}) = \begin{bmatrix} \exp(ik_n L_n) & 0 \\ 0 & \exp(-ik_n L_n) \end{bmatrix} \vec{\psi}_n(x_{m1}) \tag{13}$$

where we can define

$$M_r(L_n, U_n) = \begin{bmatrix} \exp(ik_n L_n) & 0 \\ 0 & \exp(-ik_n L_n) \end{bmatrix} \tag{14}$$

This is the running matrix we denote as $M_r(L_n, U_n)$ which is dependent on the length L_n of the region of constant potential U_n.

5. **The Transfer Matrix**

To transfer from one general point to another, one simply needs to "run" through the length L_n of a constant potential U_n using M_r and "hop" from potential U_n across U_{n+1} using M_h. That is, to find the composite transfer matrix, we perform these runs and hops by repeatedly multiplying the vector $\vec{\psi}_n$. Of course, one needs to keep in mind that the potential U_n is conveniently stored in k_n. We can compose the first events: entering the first potential entrance and traversing the first potential.

$$\vec{\psi_2}(x) = M_r(L_1, U_1)M_h(U_0, U_1)\vec{\psi_0}(x) \tag{15}$$

This converts the wavefunction of incoming wave (region 0) into the wavefunction in the (region 2)

We can compose the matrices as

$$M_r(L_1, U_1)M_h(U_0, U_1) = \prod_{n_0=0}^{n_f=2} M_r(L_{n+1}, U_{n+1})M_h(U_n, U_{n+1}) \tag{16}$$

Hence, if we define a general transfer matrix as

$$M_t(n_0, n_f) := \prod_{n_0}^{n_f} M_r(L_{n+1}, U_{n+1})M_h(U_n, U_{n+1}) \tag{17}$$

we can first calculate the transfer matrix of a given potential configuration and parametrize it with respect to physical parameters (E,m). Again, this matrix allows us to enter one potential and exit through another. That is

$$\vec{\psi}_{n_0}(x) = M_t(n_0, n_f)\vec{\psi}_{n_f}(x) \tag{18}$$

M_t encodes properties of the potential (its configuration shape as dictated by steepness and width of each individual well) and properties of the particle (mass and energy).

2 Answers to Problem Set 5

1. **Wavefunction solution from Schrodinger's equation**

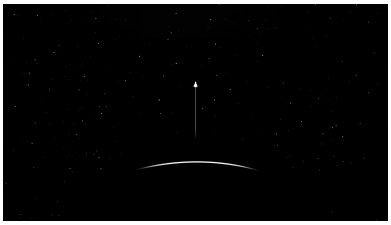

Figure 2: This is a sample figure.

Show that :

- in region II, for $E < V_0$, $\psi = C\ \exp\ (-\beta x) + D\ \exp\ (\beta x)$ where $\beta = \sqrt{2m(V_0 - E)/\hbar^2}$
- in region III, for $E < V_0$, $\psi = F\ \exp\ (ikx) + G\ \exp\ (-ikx)$ where $k = \sqrt{2mE/\hbar^2}$

2. **Incoming wave boundary condition**

Show that the boundary conditions at $x = 0$ is

$$\begin{aligned} A + B &= C + D \\ ik(A - B) &= \beta(D - E) \end{aligned}$$

or

$$\begin{bmatrix} 1 & 1 \\ ik & -ik \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ \beta & -\beta \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix}$$

3. **Outgoing wave boundary condition**

Show that the boundary conditions at $x = a$ is

$$\begin{aligned} D\ \exp\ (\beta a) + C\ \exp(-\beta a) &= F\ \exp\ (ika) + G\ \exp(-ika) \\ \beta(D\ \exp\ (\beta a) - C\ \exp(-\beta a)) &= ik(F\ \exp\ (ika) + G\ \exp(-ika)) \end{aligned}$$

or

$$\begin{bmatrix} \exp\ (\beta a) & \exp\ (-\beta a) \\ \beta\ \exp\ (\beta a) & -\beta\ \exp\ (-\beta a) \end{bmatrix} \begin{bmatrix} D \\ C \end{bmatrix} = \begin{bmatrix} \exp\ (ika) & \exp\ (-ika) \\ ik\ \exp\ (ika) & -ik\ \exp\ (-ika) \end{bmatrix} \begin{bmatrix} F \\ G \end{bmatrix}$$

4. **Constant potential matrix**

Find the constant potential transition matrix M_0 where

$$M_0 \begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} C \\ D \end{bmatrix}$$

,

5. **Potential step matrix**

Find the potential step transition matrix M_s where

$$M_s \begin{bmatrix} D \\ C \end{bmatrix} = \begin{bmatrix} F \\ G \end{bmatrix}$$

6. **The transfer matrix**

Find the potential step transition matrix M_s where

$$M_s \begin{bmatrix} D \\ C \end{bmatrix} = \begin{bmatrix} F \\ G \end{bmatrix}$$