Scattering in one dimension

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I. INTRODUCTION

This writeup accompanies a numerical simulation of particle scattering in one spatial dimension. The simulation can be run on any computer that has Internet access and understands Java. Point your browser to the JAVALAB web page www.pha.jhu.edu/~javalab/ for more information.

The simulation is intended as part of a homework in a senior or graduate-level class in quantum mechanics. It illustrates various aspects of quantum scattering in the simplest physical setting: one spatial dimension. I have deliberately chosen the most basic kind of scatterers—delta potentials—to keep the mathematical sophistication to a minimum and focus on the physics.

To appreciate the physical phenomena illustrated by the program, the user should run simulations in conjunction with theoretical problems suggested in the text. The more difficult problems are marked by an asterisk.

The mathematical formalism of the transfer matrix, well suited for problems of this kind, is described in Sec. II. Interaction of a particle with a single short-range scatterer is discussed in Sec. III. Sec. IV deals with a rudimentary quantum dot formed by two potential barriers. In Sec. V the reader will study propagation of a particle in a one-dimensional crystal formed by a periodic array of delta potentials.

While this writeup is self-contained, the reader may find it helpful to consult additional literature on the use of transfer matrices in quantum mechanics [1, 2]. The formalism is quite popular in other areas of physics, such as statistical mechanics [3] and optics [4].

II. TRANSFER MATRIX

A. Principle of superposition and the transfer matrix

The Schrödinger equation in one spatial dimension,

$$-\frac{\hbar^2}{2m}\psi''(x) + V(x)\psi(x) = E\psi(x), \tag{1}$$

has two linearly independent solutions for a given value of energy E. If we label these solutions $\psi_1(x)$ and $\psi_2(x)$, any other solution of Eq. 1 can be written as their superposition:

$$\psi(x) = c_1\psi_1(x) + c_2\psi_2(x). \tag{2}$$

For a given physical setting, the coefficients c_1 and c_2 are determined by the boundary conditions. For example, if the motion of the particle is restricted to a finite region, we must require that $\psi(-\infty) = 0$ and $\psi(+\infty) = 0$.

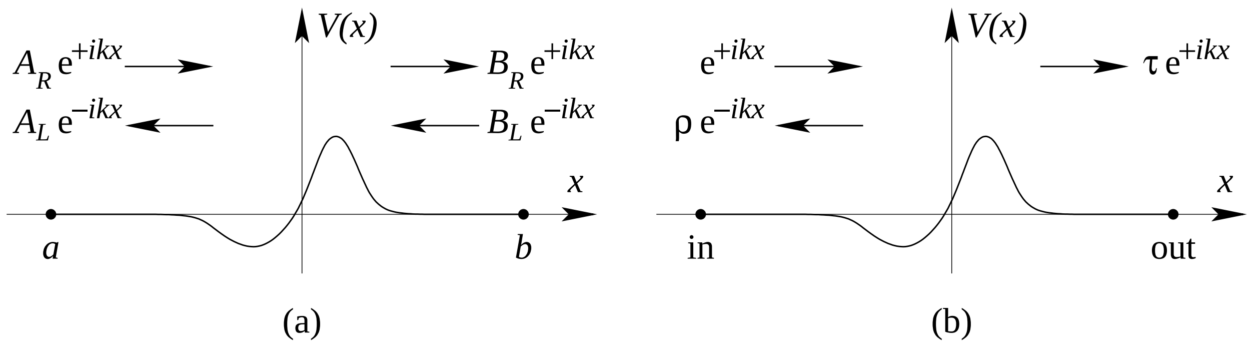

FIG. 1:

In scattering problems the boundary conditions are different. If the scattering potential has a finite extent or vanishes quickly as $x \to \infty$ [Fig. 1(a)], the motion of the particle is asymptotically free; the wavefunction consists of the right-mover e^{+ikx} and left-mover e^{-ikx}:

$$\begin{aligned} \psi(x) &\sim A_R\,\mathrm{e}^{+ikx} + A_L\,\mathrm{e}^{-ikx} \text{ as } x \to -\infty, \\ \psi(x) &\sim B_R\,\mathrm{e}^{+ikx} + B_L\,\mathrm{e}^{-ikx} \text{ as } x \to +\infty. \end{aligned} \tag{3}$$

For a particle incident from the left, one specifies the amplitude of the incoming wave at one end (e.g. $A_R = 1$) and requires that there be no incoming wave at the other end: $B_L = 0$ [Fig. 1(b)]. We will be interested in computing the amplitudes of the reflected wave $A_L = \rho$ and that of the transmitted wave $B_R = \tau$.

The principle of superposition (2) guarantees that there is a linear relation between the wave amplitudes on both sides of the scatterer:

$$\begin{pmatrix} B_R\mathrm{e}^{+ikb} \\ B_L\mathrm{e}^{-ikb} \end{pmatrix} = \begin{pmatrix} T_{RR} & T_{RL} \\ T_{LR} & T_{LL} \end{pmatrix} \begin{pmatrix} A_R\mathrm{e}^{+ika} \\ A_L\mathrm{e}^{-ika} \end{pmatrix}. \tag{4}$$

The coefficients T_{ij} form the *transfer matrix.* They are fully determined by the scattering potential $V(x)$ and are independent of the boundary conditions.

Be aware that the transfer matrix depends on the choice of basis vectors. For example, instead of specifying the amplitudes of the right and left-moving waves, as in Eq. 3, we could write a linear relation between the values of the wavefunction and its derivative at two different points:

$$\begin{pmatrix} \psi(b) \\ \psi'(b) \end{pmatrix} = \begin{pmatrix} T_{00} & T_{01} \\ T_{10} & T_{11} \end{pmatrix} \begin{pmatrix} \psi(a) \\ \psi'(a) \end{pmatrix}. \tag{5}$$

Here the indices 0 and 1 signify the "zeroth" and first derivatives of ψ.

Transfer matrices are convenient mathematical objects. Suppose we know how the wavefunctions "propagate" from point a to point b and also from b to c:

$$\begin{pmatrix} \psi(b) \\ \psi'(b) \end{pmatrix} = T(b,a) \begin{pmatrix} \psi(a) \\ \psi'(a) \end{pmatrix}, \qquad \begin{pmatrix} \psi(c) \\ \psi'(c) \end{pmatrix} = T(c,b) \begin{pmatrix} \psi(b) \\ \psi'(b) \end{pmatrix}.$$

Propagation from a to c is then described by the product of the transfer matrices:

$$\begin{pmatrix} \psi(c) \\ \psi'(c) \end{pmatrix} = T(c,a) \begin{pmatrix} \psi(a) \\ \psi'(a) \end{pmatrix}, \text{ where } T(c,a) = T(c,b)\,T(b,a). \tag{6}$$

The multiplicative property (6) is rather useful. We can connect simple scatterers as building blocks to create an intricate potential landscape and determine its transfer matrix by simple multiplication.

Transfer matrices contain all physical information about scattering. As shown in Appendix A, the amplitude of the transmitted wave is $\tau = k_{\mathrm{in}}/(k_{\mathrm{out}}T_{LL})$, where k_{in} and k_{out} are the wavenumbers of the incoming and outgoing waves. In all our calculations $k_{\mathrm{out}} = k_{\mathrm{in}}$, so that the transmission amplitude τ and transmission probability t are as follows:

$$\tau = 1/T_{LL}, \quad t = 1/|T_{LL}|^2. \tag{7}$$

(Caution! These formulas work for $k_{\mathrm{out}} = k_{\mathrm{in}}$ only!)

III. ONE DELTA POTENTIAL

A. Physics

One of the simplest scatterers in one dimension is the zero-range potential

$$V(x) = \frac{\hbar^2\kappa}{2m}\,\delta(x). \tag{8}$$

Note the choice of units. The strength of the potential is characterized by the coupling constant κ having the dimension of the inverse length. The coupling constant will be compared to the particle wavenumber k, which has the same units. Keep in mind that momentum of the particle is not conserved thanks to the scattering. Therefore, think of k as a measure of *energy*, $E = \hbar^2k^2/2m$.

For a fixed wavenumber k, we have two quantities with the dimension of the inverse length: k and κ. The physical properties of the model will depend on the only dimensionless parameter, their ratio. It is therefore reasonable to expect that the probability of scattering is small for $\kappa/k \ll 1$ and approaches unity for $\kappa/k \gg 1$.

B. Mathematics

For starters, let us compute the transfer matrix of the delta potential (8) in the basis of the wavefunction and its derivative (5). By integrating the Schrödinger equation

$$-\psi''(x) + \kappa\delta(x)\psi(x) = k^2\psi(x)$$

over the infinitesimal interval $x \in (-0; +0)$ we obtain

$$\psi'(+0) - \psi'(-0) = \kappa\psi(0).$$

The first derivative has a step discontinuity at $x = 0$, while $\psi(x)$ itself is continuous. Thus

$$\begin{pmatrix} \psi(+0) \\ \psi'(+0) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ \kappa & 1 \end{pmatrix} \begin{pmatrix} \psi(-0) \\ \psi'(-0) \end{pmatrix}. \tag{9}$$

C. Problems

1. Show that a chunk of free space of length a has the transfer matrix

$$T_{\text{free}}(a) = \begin{pmatrix} \mathrm{e}^{+ika} & 0 \\ 0 & \mathrm{e}^{-ika} \end{pmatrix} \tag{10}$$

in the basis of right and left-movers (4).

2. Show that the transfer matrix of the delta potential (8) in the plane-wave basis (3) is

$$T_{\delta}(\kappa) = \begin{pmatrix} 1 - \mathrm{i}\kappa/2k & -\mathrm{i}\kappa/2k \\ \mathrm{i}\kappa/2k & 1 + \mathrm{i}\kappa/2k \end{pmatrix}. \tag{11}$$

3. Compute the transmission and reflection amplitudes for the delta potential (8). Compare the exact result to the first Born approximation:

$$\rho_{\text{Born}} = -\frac{m}{2\pi\hbar^2}\int_{-\infty}^{\infty} V(x)\,\mathrm{e}^{2\mathrm{i}kx}\,dx. \tag{12}$$

IV. TWO DELTA POTENTIALS: A QUANTUM DOT

A. Physics

Let us put together a rudimentary quantum dot by erecting two delta potentials of strength κ a distance a apart. A particle can be injected into the dot from the outside, bounce between the walls and leak out again. Now that we have three inverse lengths in the problem (k, κ and $1/a$), we will observe a less monotone behavior.

Investigate the behavior of the transmission amplitude $\tau(k)$ with the aid of the simulator for several values of the barrier height κ and dot size a. In favorable conditions you will observe a series of narrow maxima in transmission. At the peaks of these "resonances" the particle experiences *perfect* transmission $|\tau|^2 = 1$.

B. Mathematics

The transfer matrix of the dot can be computed as a product of the transfer matrices of its three constituents: the left barrier, the inside of the dot and the right barrier,

$$T_{\text{dot}} = T_{\delta}(\kappa)\; T_{\text{free}}(a)\; T_{\delta}(\kappa). \tag{13}$$

C. Problems

4. Explain the physical origin of these transmission resonances. Determine approximately their locations.

5*. Estimate the width of a *narrow* resonance.

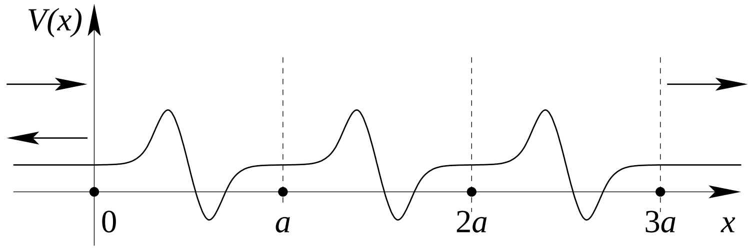

FIG. 2:

V. PERIODIC ARRAY OF DELTA POTENTIALS: A CRYSTAL

A. Physics

Consider now scattering from a periodic array of potential barriers. When the number of barriers L is finite, the situation is qualitatively similar to the case $L = 2$ (the quantum dot): the transmission probability $|\tau|^2$ oscillates as a function of k. By introducing yet another dimensionless parameter (L) we have made the problem more complicated. Can we ever disentangle this mess?

We can get rid of the extra variable by taking the limit $L \to \infty$. Doing so has a double benefit of simplifying the algebra and bringing about qualitatively new physics. Energy of a particle moving in a periodic potential has allowed bands separated by gaps. A particle whose energy lies in a forbidden gap cannot propagate in the crystal.

We can investigate the structure of energy bands and gaps by performing scattering experiments on a finite array of L identical unit cells. A long enough crystal is nontransparent for a particle whose energy lies in a gap.

Use the simulator to map out the band structure of k for some values of potential strength κ and period a. It helps to vary L at fixed κ and a in order to make sure that the "crystal" indeed becomes less transparent as L grows.

B. Mathematics

For a periodic crystal containing L unit cells, the transfer matrix can be written as $T = T_0^L$, where T_0 is the transfer matrix for a single unit cell (Fig. 2). Let us inject particles on the left ($x = 0$) and observe them on the right ($x = La$) by measuring the transmission amplitude τ. As discussed at the end of Sec. II,

$$\frac{1}{\tau} = T_{LL} = \begin{pmatrix} 0 & 1 \end{pmatrix} T \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 & 1 \end{pmatrix} T_0^L \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

The explicit form of the transmission coefficient for large but finite L is too cumbersome to be dealt with directly. We need a trick to simplify the matter.

The general strategy in such cases is to identify the largest eigenvalue of the unit-cell transfer matrix T_0. It will dominate the observable quantities in the limit $L \to \infty$.

Being a 2×2 matrix, T_0 has two eigenvalues:

$$T_0 \begin{pmatrix} \alpha_1 \\ \beta_1 \end{pmatrix} = \lambda_1 \begin{pmatrix} \alpha_1 \\ \beta_1 \end{pmatrix}, \quad T_0 \begin{pmatrix} \alpha_2 \\ \beta_2 \end{pmatrix} = \lambda_2 \begin{pmatrix} \alpha_2 \\ \beta_2 \end{pmatrix}.$$

For convenience, let us normalize the eigenvectors in such a way that

$$\begin{pmatrix} \alpha_1 \\ \beta_1 \end{pmatrix} + \begin{pmatrix} \alpha_2 \\ \beta_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

After simple algebra,

$$1/\tau = \beta_1 \lambda_1^L + \beta_2 \lambda_2^L. \tag{14}$$

Consider now $1/\tau$ as a function of L. If one eigenvalue exceeds the other in absolute terms, say $|\lambda_1| > |\lambda_2|$, we can neglect the contribution of the smaller eigenvalue and write

$$\tau \sim \beta_1^{-1} \lambda_1^{-L} \text{ as } L \to \infty. \tag{15}$$

What can we say about the eigenvalues of a transfer matrix in general? Periodicity of the potential guarantees that the particle momentum at $x = 0$ and $x = a$ is the same. Therefore, $\det T_0 = 1$ (see Appendix A). Because the determinant of a matrix equals the product of its eigenvalues, we find that $\lambda_1 \lambda_2 = 1$. Two cases are then possible.

- $|\lambda_1| > 1 > |\lambda_2|$. By keeping the largest eigenvalue only, we find that the transmission coefficient vanishes exponentially with L (see Eq. 15). The wavenumber k lies in an energy gap.
- $|\lambda_1| = |\lambda_2| = 1$. In this case we must keep both eigenvalues when evaluating $1/\tau$. The dependence on L is oscillatory, rather than exponential. The particle has a good chance of getting through the crystal even if L is large. The wavenumber k belongs to one of the allowed energy bands.

In our simulations, the unit cell includes a delta potential of strength κ and a chunk of free space of length a. Depending on where you choose the origin of the unit cell, its transfer matrix will be one of these expressions:

$$T_0 = \begin{cases} T_\delta(\kappa)\, T_{\text{free}}(a), \\ T_{\text{free}}(a)\, T_\delta(\kappa), \\ T_\delta(\kappa/2)\, T_{\text{free}}(a)\, T_\delta(\kappa/2), \\ T_{\text{free}}(a/2)\, T_\delta(\kappa)\, T_{\text{free}}(a/2), \\ \ldots \end{cases} \tag{16}$$

C. Problems

6. Compute the eigenvalues of the unit-cell transfer matrix (16). Derive a condition that determines the allowed bands and forbidden gaps of k. Solve it (numerically) for the same values of κ and a that you used in your simulations. Does your theory agree with experiment?

7*. For a particle in a gap, the transmission coefficient decays exponentially with L: $t = |\tau|^2 \sim C\mathrm{e}^{-L/\xi}$. Determine the localization length ξ.

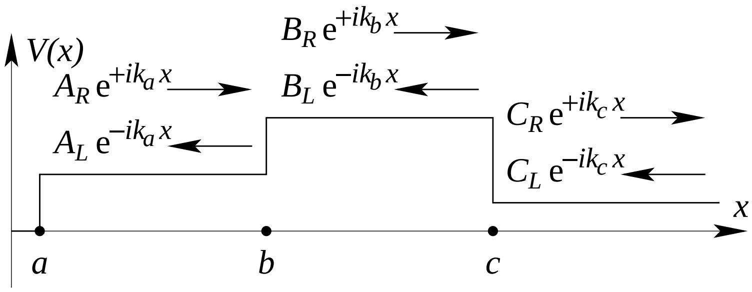

FIG. 3:

[1] E. Merzbacher, *Quantum Mechanics,* Wiley, New York (1998).

[2] J.S. Walker and J. Gathright, Am. J. Phys. **62,** 408 (1994).

[3] N. Goldenfeld, *Lectures on phase transitions and the renormalization group,* Addison-Wesley, Reading (1992).

[4] A.E. Siegman, *Lasers,* Oxford University Press, Oxford (1986).

APPENDIX A: GENERAL PROPERTIES OF THE TRANSFER MATRIX

1. Determinant of the transfer matrix

Complete determination of the transfer matrix amounts to solving the Schrödinger equation (1). Therefore finding the transfer matrix of an arbitrary scattering potential is not a simple exercise. Nevertheless, some properties of the transfer matrix are universal. Notice, in particular, that $\det T = 1$ in Eqs. 9, 11, and 10.

More generally, the determinant of a transfer matrix between points $x = x_0$ and $x = x_1$ is given by the ratio of the local wavenumbers:

$$\det T(x_1, x_0) = \frac{k_0}{k_1}, \quad \text{where } \frac{\hbar^2 k_i^2}{2m} \equiv E - V(x_i). \tag{A1}$$

Proof. This result is easy to derive for a "Manhattan skyline" potential, consisting of finite segments $V(x) = \text{const}$ (Fig. 3).

The transfer matrix for the step at $x = b$ can be obtained as follows. Continuity of the wavefunction and its first derivative at $x = b$,

$$\begin{aligned}\psi(b) &= A_R\,\mathrm{e}^{+\mathrm{i}k_a b} + A_L\,\mathrm{e}^{-\mathrm{i}k_a b} = B_R\,\mathrm{e}^{+\mathrm{i}k_b b} + B_L\,\mathrm{e}^{-\mathrm{i}k_b b},\\ \psi'(b) &= \mathrm{i}k_a\left(A_R\,\mathrm{e}^{+\mathrm{i}k_a b} - A_L\,\mathrm{e}^{-\mathrm{i}k_a b}\right) = \mathrm{i}k_a\left(B_R\,\mathrm{e}^{+\mathrm{i}k_b b} - B_L\,\mathrm{e}^{-\mathrm{i}k_b b}\right),\end{aligned}$$

can be rewritten in the matrix form

$$\begin{pmatrix} B_R\,\mathrm{e}^{+\mathrm{i}k_b b} \\ B_L\,\mathrm{e}^{-\mathrm{i}k_b b}\end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 + k_a/k_b & 1 - k_a/k_b \\ 1 - k_a/k_b & 1 + k_a/k_b\end{pmatrix}\begin{pmatrix} A_R\,\mathrm{e}^{+\mathrm{i}k_a b} \\ A_L\,\mathrm{e}^{-\mathrm{i}k_a b}\end{pmatrix}.$$

This immediately yields the transfer matrix (and its determinant) for a step:

$$T_{\text{step}}(b) = \frac{1}{2}\begin{pmatrix} 1 + k_a/k_b & 1 - k_a/k_b \\ 1 - k_a/k_b & 1 + k_a/k_b\end{pmatrix}, \qquad \det T_{\text{step}}(b) = \frac{k_a}{k_b}.$$

Add free space on the left (from a to b):

$$\det T(b,a) = \det\left[T_{\text{step}}(b)\, T_{\text{free}}(b,a)\right] = \det T_{\text{step}}(b)\ \det T_{\text{free}}(b,a) = \frac{k_a}{k_b} \times 1 = \frac{k_a}{k_b}.$$

Put two plateaus together:

$$\det T(c,a) = \det\left[T(c,b)\, T(b,a)\right] = \det T(c,b)\ \det T(b,a) = \frac{k_b}{k_c}\,\frac{k_a}{k_b} = \frac{k_a}{k_c},$$

independent of the intermediate momentum k_b. Generalization to n steps is obvious. Finally, any smooth potential can be approximated by a Manhattan skyline with an infinite number of steps yielding the desired result (A1). Q.E.D.

2. Amplitude of the transmitted wave

The transfer matrix can be used to compute complex amplitudes of transmission and reflection. For the situation depicted in Fig. 1(b), the reflected wave has the amplitude $A_L = \rho$, while the transmitted wave has the amplitude $B_R = \tau$. Both τ and ρ can be expressed in terms of the transfer matrix. Substitute them into Eq. 4:

$$\begin{pmatrix} \tau \\ 0 \end{pmatrix} = T \begin{pmatrix} 1 \\ \rho \end{pmatrix}, \text{ or } \begin{pmatrix} 1 \\ \rho \end{pmatrix} = T^{-1} \begin{pmatrix} \tau \\ 0 \end{pmatrix}.$$

Thus we see that the transmission amplitude τ is given by the RR element of the inverse matrix T^{-1}:

$$\frac{1}{\tau} = \left(T^{-1}\right)_{RR} = \frac{T_{LL}}{\det T}.$$

Substitution of an earlier results (A1) yields

$$\tau = \frac{k_{\text{in}}}{k_{\text{out}} T_{LL}}. \tag{A2}$$

3. Probability of transmission

To determine the probability of transmission, compare the *fluxes* of incoming and outgoing particles. The fluxes are products of the probability densities and particle velocities $v = \hbar k/m$. Therefore the transmission probability is

$$t = \frac{|B_R|^2 k_{\text{out}}}{|A_R|^2 k_{\text{in}}} = \frac{|\tau|^2 k_{\text{out}}}{k_{\text{in}}} = \frac{k_{\text{in}}}{|T_{LL}|^2\, k_{\text{out}}}. \tag{A3}$$