Notes on Quantum Mechanics: Solving the Schrödinger Equation in 1D — Scattering States

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1 Bound and Scatter

At a skate park, a skateboarder rides off the top of one side of a U-shaped ramp that has equal heights on both ends. What is going to happen? In the ideal land of physics, the best that the skateboarded can do is to accelerate to the very bottom of the ramp and then decelerate until they reach the very top of the other end, at which they stop. This is a manifestation of the conservation of energy. The initial, and thus total, energy is the magnitude of the purely gravitational potential energy. At any point in time the total energy of the system cannot exceed that energy.

Now suppose that the ramp is taller on the end that the skateboarder starts from than the other end. What is going to happen now? Now, in the ideal land of physics where the skateboarder magically does not lose any energy in his path, the skateboarder can now ride over the other end with some non-zero velocity and then continue at that velocity if what comes after it is flat.

These two scenarios correspond to what we call *bound* and *scattering* states in Quantum Mechanics. A more fundamental name for *scattering* states would just be *unbound* states. But because unbound states are useful for describing scattering processes because their wavefunctions do not vanish at infinity, we call them *scattering states*. With the intuition from the hypothetical skate park, we can formalize the definitions for bound and scattering states.

$$\begin{cases} E < 0 & \text{Bound States} \\ E > 0 & \text{Scattering States} \end{cases}$$

where E is the total energy of a system. This definition is motivated by the fact that most practical potentials vanish at infinity. If E is smaller than 0 on both sides, then the system is bound, if not, then it is not. It is easy to generalize this definition for potentials that do not go to 0 at infinity (such as the infinite well).

2 Delta Well

The delta potential is defined as follows:

$$V(x) = -\alpha\delta(x) \tag{1}$$

Where $\delta(x)$ is the Dirac Delta Function. The time-independent Schrödinger Equation is then given by:

$$\hat{H}\psi = -\frac{\hbar}{2m}\frac{d^2\psi}{dx^2} - \alpha\delta(x)\psi = E\psi \tag{2}$$

Throughout these notes, we will assume that our wavefunctions are well behaved in the following way:

$$\begin{cases} \psi \text{ is continuous for all x} \\ \frac{d\psi}{dx} \text{ is continous for all x except for where } V(x) \text{ is infinite} \end{cases}$$

We can solve for ψ on both sides of $x = 0$ and avoid dealing with the infinity. On either side of $x = 0$, the potential is zero. Let us first look at the scattering states($E < 0$). In this case, we are essentially faced with the equation $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$. If $E > 0$, then we can write this equation as

$\frac{d^2\psi}{dx^2} = -k^2\psi$, where $k \equiv \frac{\sqrt{2mE}}{\hbar}$. For the left side and right side respectively, the general solutions are sinusoidal:

$$\psi_l = Ae^{ikx} + Be^{-ikx}$$
$$\psi_r = Fe^{ikx} + Ge^{-ikx}$$

By the first boundary condition we obtain that

$$A + B = F + G$$

By the second boundary condition and a quick analysis of the delta potential:

$$F - G = A(1 + 2i\gamma) - B(1 - 2i\gamma)$$

where $\gamma \equiv \frac{m\alpha}{\hbar^2 k}$. To set up the following discussion, let us consider a fixed point on some traveling wave of a fixed shape involving the factor $kx \pm \omega t$. This point's "y-value" must be constant-valued at all times and positions. Therefore $kx \pm \omega t$ is a constant. The plus sign then is associated with a point that has a decreasing x value, and the minus sign is associated with a point that has an increasing x value for obvious reasons.

Under time evolution by the factor $exp(-\frac{iEt}{\hbar})$, the terms associated with B and A represent a wave coming in from the left towards 0 and a wave coming *from* 0 towards the left, respectively. Similarly, the terms associated with G and F represent a wave coming in from the right towards 0 and a wave coming from 0 towards the right respectively. This is a lovely model for scattering processes. We can go ahead and put these wavefunctions in the physical scenario where we send a particle (or particles) from the left towards the potential. This means that $G = 0$ since no particle(s) is coming in from the right. Then, we are left with a system of 2 equations with 3 unknowns. We will express F and B in this underdetermined system in terms of A, which is our "incident" amplitude:

$$B = \frac{i\gamma}{1 - i\gamma}A$$
$$F = \frac{1}{1 - i\gamma}A$$

Recalling that A, B, and F are all amplitudes, their norm squared will give us probabilities of finding the system in any of these three states. We are interested in the probability, or rather the relative probability, of finding the particle reflecting or transmitting through the well:

$$R = \frac{|B|^2}{|A|^2} = \frac{\gamma^2}{1 + \gamma^2} = \frac{1}{1 + (2\hbar^2 E/m\alpha^2)}$$
$$T = \frac{|F|^2}{|A|^2} = \frac{1}{1 + \gamma^2} = \frac{1}{1 + (m\alpha^2/2\hbar^2 E)}$$

Note that $R + T = 1$ as we would expect; the particle either reflects or transmits. It does not disappear. T increases and R decreases as E increases, as we might expect. What is strange is that although the potential takes a *downhill* direction, *the particle can still reflect back.* How strange is that! Imagine if you drove a car off a cliff but you just get reflected back by ... thin air? — how strange that would be but also how many lives that would save! This is a truly determinedly different behavior from what we are used to in our everyday lives.

If $V(x) = \alpha\delta(x)$ as opposed to $V(x) = -\alpha\delta(x)$, the reflection and transmission coefficients are unchanged, as one can quickly verify. This is even more mind-boggling. You are just as likely to pass through a potential barrier (technically termed *tunneling through a potential barrier*) as to cross a potential well. This would easily be total nonsense to anyone who has not studied quantum mechanics.

3 Finite Square Well

A Finite Square Well can be given by the following potential:

$$V(x) = \begin{cases} -V_o & |x| \leq a \\ 0 & |x| > a \end{cases}$$

We will now examine the scattering states allowed by the Finite Square Well potential. Assuming that $E > 0$, the solutions to the left and the right of the potential step are the same as that derived for the Dirac Well Potential:

$$\psi_l = Ae^{ikx} + Be^{-ikx}$$
$$\psi_r = Fe^{ikx} + Ge^{-ikx}$$

In between, the solution also takes a similar form, with the wave number being $l \equiv \frac{\sqrt{2m(E+V_o)}}{\hbar}$:

$$\psi_m = \alpha e^{ilx} + \beta e^{-ilx} \equiv C\sin(lx) + D\cos(lx)$$

Imposing the same set of boundary conditions on the wavefunctions and their derivatives at $x = a$ and $x = -a$ and assuming that $G = 0$ (scattering from the left), we find that

$$B = i\frac{\sin(2la)}{2kl}(l^2 - k^2)F$$
$$F = \frac{e^{-2ika}}{\cos(2la) - i\frac{k^2+l^2}{2kl}\sin(2la)}A$$

The transmission coefficient $T = \frac{|F|^2}{|A|^2}$ is given by:

$$T = \frac{1}{1 + \frac{V_o^2}{4E(E+V_o)}\sin^2\left(\frac{2a}{\hbar}\sqrt{2m(E+V_o)}\right)}$$

The term involving sine squared has a curious character: it equals zero when $\frac{2a}{\hbar}\sqrt{2m(E_n + V_o)} = n\pi$ for an integer n — or in other words, we get perfect transmission when $E_n + V_o = \frac{n^2\pi^2\hbar^2}{2m(2a)^2}$. These allowed energies resemble the form of that of an *infinite* square well with a width of $2a$! This remarkable phenomenon is called the **Ramsauer-Townsend Effect**. Here is an intuitive explanation for it: the allowed wavefunctions inside an inifte square well has the property that it is perfectly "periodic" in the sense that the behavior of the wavefunction entering the well is captured by the wavefunction leaving the well due to the boundary conditions being that $\psi = 0$ as well as the uniform sinusoidal nature of the wavefunctions. Therefore, whatever enters the well *must* be matched by what leaves the well, and thus we get perfect transmission of the wavefunction.

4 Dispersion of the Gaussian

Scattering states are not normalizable, as we have saw in the last two scenarios. Therefore, we turn our attention to building wave packets that can actually help us model scattering processes. In particular, we focus our attention on the **Gaussian** wave packet — as one can show, it is the wave packet with the minimum uncertainty *when initialized.* This is the case because, as we will show, the wave packet disperses and eventually flattens out.

We start out with an arbitrary Gaussian wave packet at $t = 0$:

$$\psi(x, 0) = Ae^{-\frac{x^2}{2a^2}}$$

where A is a normalization constant. We then take the Fourier Transform of this wave packet:

$$\psi(x, 0) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{ikx}Be^{-\frac{k^2a^2}{2}}\,dk$$

where B is some constant irrelevent to what we are getting at right now. In the step above, I used the fact that the Fourier Transform of a Gaussian with width a is another Gaussian but with width $\frac{1}{a}$. This step is essentially building a localized position-space wavefunction by summing up infinitely many (position-wise unlocalized) momentum-space eigenfunctions. We can then attach the standard factor for time evolution:

$$\psi(x, t) == \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{i(kx-\omega(k)t)}Be^{-\frac{k^2a^2}{2}}\,dk$$

where $\omega(k)$ is the angular frequency by which a plane wave with wave number k evolves. This integral evaluates to:

$$\psi(x,t) = N(t)\exp\left(-\frac{x^2}{2(a^2 + i\frac{\hbar}{m}t)}\right)$$

where $N(t)$ is another normalization factor inversely proportional to $\frac{t}{a}$. This equation tells us two things:

1. The Gaussian Packet gets wider as time passes.
2. The Gaussian Packet gets shorter as time passes, and the rate of such shortening is dependent on the initial width only.

These two facts combine together to give us a dispersive Gaussian packet that "spreads out" overtime. The more localized the wave packet is at the beginning, the faster it will spread out.

5 The S-Matrix

The S-Matrix is a neat and general way to summarize information about a scattering process. Let there be a potential that goes to zero at infinities, as in many physical cases, but has some arbitrary behavior (which can be a delta well or a finite well...) in a contiguous region. We can call this a *localized potential*. We can send a wave packet in from the left and then measure what comes out the right side of the localized potential without worrying about potential messy behavior in between. As in the previous sections, our left signal is going to be in the form $\psi_l = Ae^{ikx} + Be^{-ikx}$ and our right signal is going to be in the form $\psi_r = Fe^{ikx} + Ge^{-ikx}$. We are able to impose four different boundary conditions on this physical system, two for each of the left and right interfaces. With this knowledge, it is possible to relate the left and right as follows:

$$\begin{pmatrix} B \\ F \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \begin{pmatrix} A \\ G \end{pmatrix}$$

A more semantically sensible way to write it would be this:

$$\begin{pmatrix} B \\ F \end{pmatrix} = \begin{pmatrix} r_l & t_r \\ t_l & r_r \end{pmatrix} \begin{pmatrix} A \\ G \end{pmatrix}$$

where $|r|^2 = R$ and $|t|^2 = T$. For instance, the equation $B = r_l A + t_r G$ can be loosely interpreted as "*the amplitude of the wave that moves away from the left interface towards $-\infty$ is made up of the reflected amplitude of the wave that moves from $-\infty$ towards the left interface as well as the transmitted amplitude from the wave that moves from ∞ towards the right interface*". When we are dealing with a scattering process from the left, we can set $G = 0$.

The scattering matrix for the Dirac Well, for instance, would look like

$$\begin{pmatrix} \sqrt{\frac{1}{1+(2\hbar^2E/m\alpha^2)}} & \sqrt{\frac{1}{1+(m\alpha^2/2\hbar^2E)}} \\ \sqrt{\frac{1}{1+(m\alpha^2/2\hbar^2E)}} & \sqrt{\frac{1}{1+(2\hbar^2E/m\alpha^2)}} \end{pmatrix}$$

by symmetry. This 2×2 matrix can be generalized to an arbitrary operator $\hat{S}(E)$ such that $\phi_{in} = \hat{S}(E)\phi_{out}$. Note that an **S-Matrix has to be unitary** based on the physical constraints on wavefunctions, on which they act. Specifically, the idea is that the probability current has to be continuous across the potential. Otherwise that would mean a particle has a non-zero chance of magically stopping or disappearing into thin air for some reason; probability current from left into potential has to be equal to the probability current from potential to right. In an equation:

$$|A|^2 - |B|^2 = |F|^2 - |G|^2$$

or

$$|B|^2 + |F|^2 = |A|^2 + |G|^2$$

Then by the definition of S we have

$$|F|^2 + |B|^2 = \begin{pmatrix} B^* & F^* \end{pmatrix} \begin{pmatrix} B \\ F \end{pmatrix} = \begin{pmatrix} A^* & G^* \end{pmatrix} S^\dagger S \begin{pmatrix} A \\ G \end{pmatrix} = |A|^2 + |G|^2 \tag{3}$$

which implies that S has to be unitary. Based on this observation, we can then conclude that $|r_l|^2 + |t_l|^2 = 1$ and $|r_r|^2 + |t_r|^2 = 1$. Furthermore, we can conclude that $r_l^* t_r + t_l^* r_r = 0$ and that $t_r^* r_l + r_r^* t_l = 0$. This further implies that the columns of the an S-Matrix are orthogonal unit vectors. This fact is a reflection of the constraint that the net probability flow across the potential has to be zero.