# Quantum Mechanics Notes for A. Adams's Lecture Series. Lecture 12: The Dirac Well and Scattering off the Finite Step

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**Abstract**

This paper contains my notes on Lecture Twelve of Allan Adams's 2013 presentation on Quantum Mechanics for his MIT Video Lecture Series (8.04). These notes are meant to aid the reader in following Prof. Adams's presentation, without having to take copious notes. However, I don't intend to publish notes on all the lectures.

## 1 The Free Particle

We imagine a particle of mass $m$ moving to the right at speed $v$. Of course, a free particle is not subject to external forces. Now, we need to come up with a quantum mechanical description of the particle and its motion. We will express its wave function as a superposition of waves in an energy eigenstate:

$$\phi_E = Ae^{i(kx-\omega t)} + Be^{i(kx+\omega t)} \,, \tag{1}$$

which is a solution to the time-dependent Schrödinger Equation, where $E = \hbar^2 k^2/2m$.

$e^{i(kx-\omega t)}$ is a right-moving wave, and

$e^{i(kx+\omega t)}$ is a left-moving wave.

However, $\phi_E$ as given above is not normalizable, so we need to do something else. The standard thing to do here is to construct a wavepacket which is normalizable! Let

$$\phi_k = \frac{1}{\sqrt{2\pi}} e^{ikx} \,, \tag{2}$$

such that

$$\langle\, \phi_k \mid \phi_{k'} \,\rangle = \delta(k-k') \,, \tag{3}$$

which is the next-best-thing to being able to normalize a plane wave. Anyway, it is not possible to place a particle in an energy eigenstate for a free particle. What we can do is to build a wavepacket out of these solutions.

So, we investigate the wavepacket. Consider a free particle in a minimum uncertainty $\psi$, that being a gaussian:

$$\psi(x,0) = \frac{1}{\sqrt{a\sqrt{\pi}}} e^{-x^2/2a^2} \,, \tag{4}$$

So, what is $\psi(x,t)$?

I) One method is to use the time-dependent Schrödinger equation.

II) Another method is to expand $\psi$ into energy eigenstates, each of which we know how it evolves in time.

According to the Spectral Theorem for any observable, the corresponding operator has a basis of eigenfunctions

$$\psi(x,0) = \sum_n c_n \phi_n(x)\,. \tag{5}$$

Thus,

$$\psi(x,t) = \sum_n c_n \phi_n(x) e^{-iE_n t/\hbar}\,, \tag{6}$$

where

$$\hat{E}\phi_n = E_n \phi_n\,. \tag{7}$$

But,

$$\psi(x,0) = \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}} (e^{ikx})\widetilde{\psi}(k) = \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}}\, e^{ikx}\, \frac{\sqrt{a}}{\pi^{1/4}}\, e^{-k^2a^2/2}\,, \tag{8}$$

where wee have use the Fourier transform. Next, we time-evolve this to get

$$\psi(x,t) = \frac{\sqrt{a}}{\pi^{1/4}} \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}}\, e^{i(kx-\omega_k t)}\, e^{-x^2a^2/2}\,, \tag{9}$$

where $\omega_k = \dfrac{\hbar k^2}{2m}$. Hence,

$$\psi(x,t) = \sqrt{\frac{a}{\sqrt{\pi}}} \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}} e^{i(kx - \frac{\hbar k^2}{2m}t)}\, e^{-k^2a^2/2} = \sqrt{\frac{a}{\sqrt{\pi}}} \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}} e^{ikx} e^{-\frac{k^2}{2}(a^2 + i\frac{\hbar k}{m}t)}\,,$$

which yields

$$\psi(x,t) = \sqrt{\frac{a}{\sqrt{\pi}}} \frac{1}{\sqrt{a^2 + i\frac{\hbar}{m}t}}\, e^{-\frac{x^2}{2\left(a^2+i\frac{\hbar}{m}t\right)}}\,. \tag{10}$$

Therefore, the probability goes as

$$P(x,t) = \frac{1}{\sqrt{\pi}} \frac{1}{\sqrt{a^2 + \left(\frac{\hbar}{2ma}\right)^2 t^2}}\, e^{-\dfrac{x^2}{2\left(a^2 + \left(\frac{\hbar}{2ma}\right)^2 t^2\right)}}\,. \tag{11}$$

where $\dfrac{1}{\sqrt{a^2 + \left(\frac{\hbar}{2ma}\right) t^2}}$ is the amplitude, which is getting smaller in time.

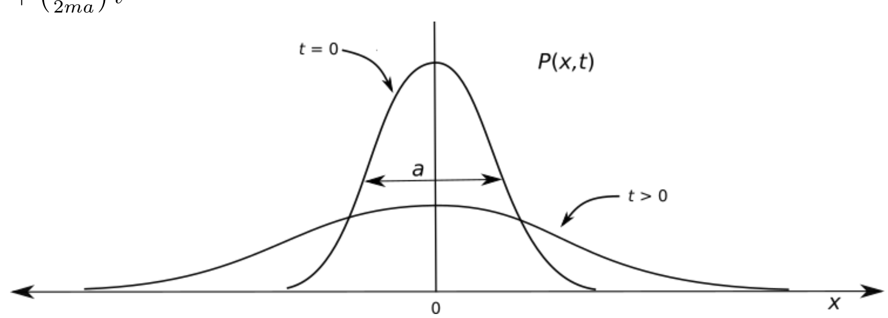


Figure 1. The probability function on $x$ and $t$. The packet width as a function of $t$ is $\sqrt{a^2 + \left(\frac{\hbar}{2ma}\right)^2 t^2}$.

And the width of the wavepacket is given by $\left(a^2 + \left(\frac{\hbar}{2ma}\right)^2 t^2\right)$ of the exponential, which is getting wider in time. This wave spreads with velocity $v = \hbar/2ma$, where $a$ is the packet width at $t = 0$.

Question 1: How do we build a wavefunction such that its width goes to a minimum at some time later than $t = 0$?

Question 2: How do we make the particle move?

Phase Velocity:

$$v_p = \frac{\omega}{k} = \frac{\hbar k}{2m} = \frac{v_c}{2}\,, \tag{12}$$

where $v_c$ is the classical velocity. However, the group velocity of a wavpacket $v_g$ is given by

$$v_g = \frac{\partial\omega}{\partial k} = \frac{\hbar k}{m} = v_c\,, \tag{13}$$

where $\omega = \hbar k^2/2m$. Hence,

$$v_p = \tfrac{1}{2} v_c\,. \tag{14}$$

## 2 The drop-off potential

We begin by examining a particle moving from the left in a constant potential and then it suddenly encountering a (sharp) potential drop off as seen in Fig. 2.

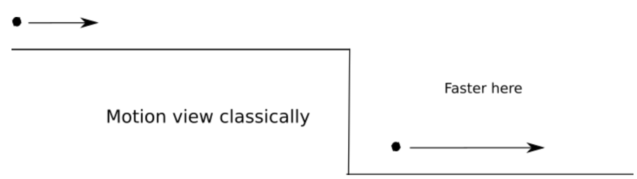


Figure 2. Classically, the particle will speed up after encountering the drop-off potential.

Now, we see what happens to a wavepacket in the same situation.

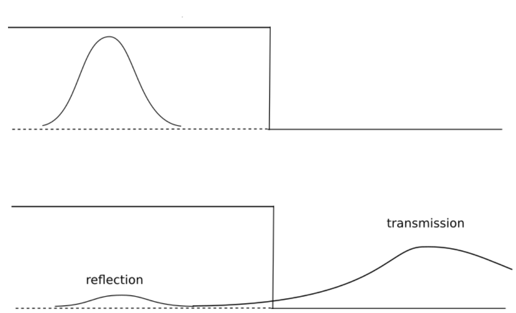


Figure 3. On top, the wavepacket approaches from the left. On bottom, we see that the particle will probably be found on the other side of the potential drop-off, but there is some chance for a reflection of the wavepacket. In this situation, the particle energy was greater than the potential height.

## 3 Other potentials

For the case of a particle encoutnering a step function potential extending off to infinity to the right, and with particle energy less than the potential height, the wavepacket will extend into the classically forbidden area for a little ways, for a lilttle time, anmd then bnasically reflect back to the left. This is referred to as 'penetration into the barrier.'

Next case, the particle encounters a finite-width barrier.

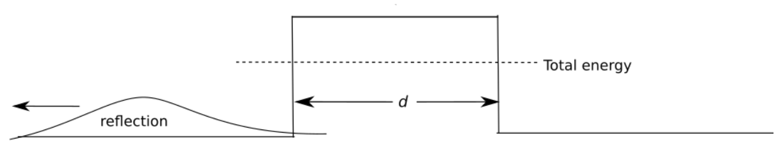


Figure 4. The particle encounters a finite-width barrier, having total energy less than the potential step it encounters. Depicted is the near total reflection off the barrier.

Thus we see that the behavior of the wavepacket in the finite width case is roughly the same as in the infinite-width situation. However, if we take the width $d$ of the finite-width barrier to vanishingly small, then the wavepacket tends to cross the barrier almost as if it isn't even there. It's as if the wider the finite-width barrier is, the greater the pushback on the incoming wavepacket.

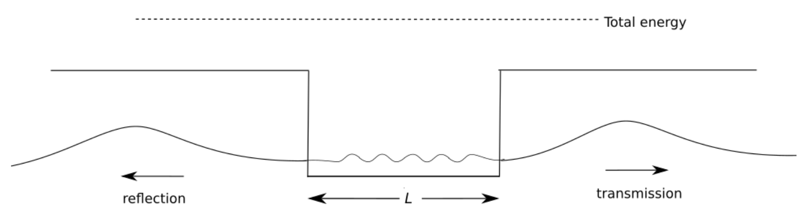


Figure 5. The particle encounters a potential, having total energy greater than the height of the potential well. We expect both transmission and reflection. The ratio of transmission to reflection will depend on length $L$.

## 4 Building Solutions

1. Find the energy eigenstates for the case of the step potential when the incoming energy is less than the potential height.

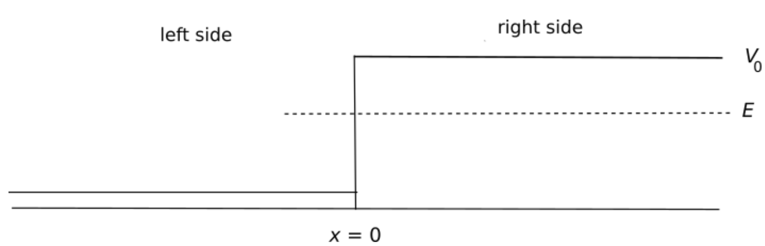


Figure 6. A free particle encounters a step potential.

$$\phi_E = \begin{cases} Ae^{ikx} + Be^{-ikx} & \text{left side}, \quad \frac{\hbar^2 k^2}{2m} = E\,, \\ Ce^{\alpha x} + De^{-\alpha x} & \text{right side}, \quad \frac{\hbar^2 \alpha^2}{2m} = V_0 - E\,. \end{cases} \tag{15}$$

But the term with $e^{\alpha x}$ will blowup; therefore, we must set $C = 0$ to stop that. At $x = 0$, we need $\phi, \phi'$ to be continuous functions. Thus,

$$\phi: \quad A + B = D\,, \tag{16}$$

$$\phi': \quad ik(A - B) = -\alpha D\,. \tag{17}$$

where

$$D = \frac{2k}{K + i\alpha}\,, \qquad B = \frac{k - i\alpha}{k + i\alpha} \tag{18}$$

What is the condition on the energy? None, because energy states are continuous.

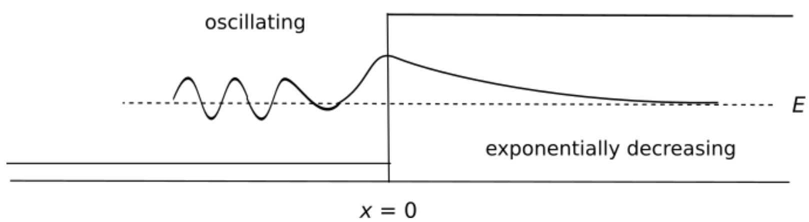


Figure 7. A free particle encounters a step potential.

Next, we convert to time dependence.

$$\phi_E = \begin{cases} Ae^{i(kx-\omega t)} + Be^{-i(kx+\omega t)} & \text{left side}, \quad \frac{\hbar^2 k^2}{2m} = E\,, \\ Ce^{\alpha x} + De^{-\alpha x} & \text{right side}, \quad \frac{\hbar^2 \alpha^2}{2m} = V_0 - E\,, \end{cases} \tag{19}$$

where $e^{i(kx-\omega t)}$ is right-moving and $e^{-i(kx+\omega t)}$ is left-moving.

Next we calculate $|\,B\,|^2$:

$$|\,B\,|^2 = BB^* = \frac{k - i\alpha}{k + i\alpha}\,\frac{k + i\alpha}{k - i\alpha} = 1\,. \tag{20}$$

We can invent parameters $\rho$ and $\mu$ to characterize $B$ in polar form, beginning with

$$k + i\alpha = \rho e^{i\mu}\,, \tag{21}$$

$$k - i\alpha = \rho e^{-i\mu}\,. \tag{22}$$

Hence,

$$B = \frac{k - i\alpha}{k + i\alpha} = \frac{\rho e^{-i\mu}}{\rho e^{i\mu}} = e^{-2i\mu}\,. \tag{23}$$

Thus, $B$ is pure phase. And the left-moving term on the LHS has the same magnitude as the right-moving term, which implies a standing wave. The effectof this is that the barrier acts as a mirror, reflecting the incoming wave by adding a phase to it. Redefining that phase, we get

$$B = e^{i\phi}\,, \tag{24}$$

where $\phi$ is called the *scattering phase shift*. To get arbitrarily good reflections, make $V_0$ large, which then makes $\alpha$ large and $k$ is small, and so $B \to -1$.

## 5 The Conservation Equation

$$\rho = |\,\psi\,|^2 \,, \quad J^x = \frac{\hbar}{2mi}(\psi^* \partial_x \psi - \psi \partial_x \psi^*) \tag{25}$$

(where $J^x$ is the current in the $x$ direction), satisfying

$$\frac{\partial \rho(x,t)}{\partial t} = -\frac{\partial}{\partial x} J^x \,. \tag{26}$$

Notation:

$$\psi = \begin{cases} \psi_I + \psi_R & \text{Left}\,, \\ \psi_T & \text{Right}\,, \end{cases} \tag{27}$$

where $\psi_I$ is $\psi$ incident and $\psi_R$ is $\psi$ reflected. Next, we keep track of how much stuff is going to the left compared to how much is going to the right. We need the probability current: Let $J_I$ be the incident current

$$J_I = \frac{\hbar k}{m} |\,A\,|^2 \,. \tag{28}$$

Then plug $\psi_I$ into $J$:

$$J_R = -\frac{\hbar k}{m} |\,B\,|^2 \,, \tag{29}$$

$$J_T = 0 \,. \tag{30}$$

The transmission probability goes as

$$T \equiv \left|\, \frac{J_T}{J_I} \,\right| \,, \tag{31}$$

which in this case is zero. And $R = 1 - T$.