Quantum Mechanics Notes for A. Adams's Lecture Series. Lecture 14: Resonance and the S-Matrix

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Abstract

This paper contains my read-along notes on Lecture Fourteen 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. The fault for any inaccuracies in this paper belongs to the author.

1 Some review

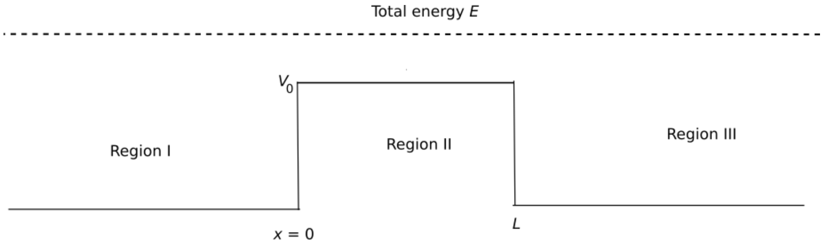

Figure 1. The particle encounters a finite-width rectangular barrier, having total energy greater than the potential step it encounters. Depicted is the well-defined regions of oscillatory behavior.

Since we have scattering from an incoming particle from the left, we set $D = 0$.

Case I: $E > V_0$.

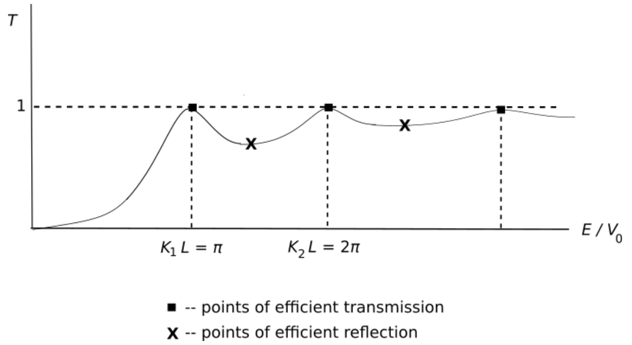

Figure 2. The points where maximal transmissions occur are called *resonances*.

We have resonances (good transmission) at values $k_2L = N\pi$ and $T \to 1$. We have good reflections at values $k_2L = (N + \frac{1}{2})\pi$ and $R \to \dfrac{V_0^2}{(2E - V_0)^2}$.

2 Case of the finite-well barrier

Case I: $E > 0$. This case is similar to the last example, except that from the mathematical point of view we have have replaced V_0 by $-V_0$.

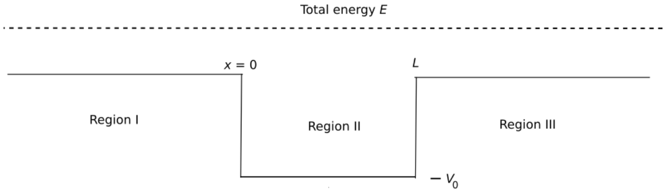

Figure 3. A monocromatic wave comes from the left.

Let

$$g_0^2 = \frac{2mL^2}{\hbar^2} V_0\,, \quad \epsilon = \frac{E}{V_0}\,. \tag{1}$$

This gives us the T value

$$T_{\sqcup} = \frac{1}{1 + \dfrac{1}{4\epsilon(1+\epsilon)} \sin^2(g_0\sqrt{1+\epsilon})}\,. \tag{2}$$

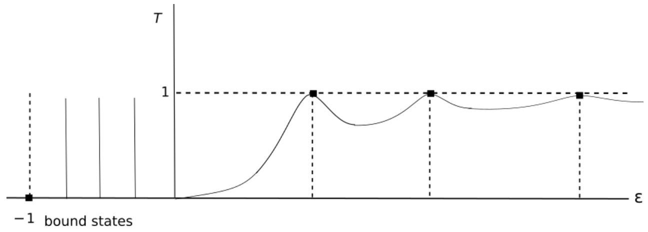

Figure 4. Transmissions with bound states. The lowest ground state is always greater than the bottom of the well.

3 Case of perfect transmission

New situation

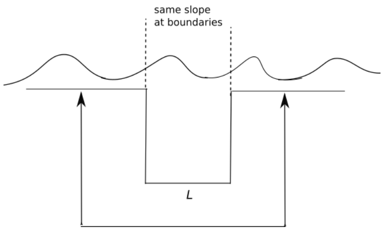

Figure 5. Well Barrier Perfect Transmission. The waveform must have the same amplitude and period on both sides, and a single period inside.

$$T \equiv \frac{|\,R\,|^2}{|\,L\,|^2} = 1\,. \tag{3}$$

So, for the transition amplitude to be one, the waveform must be periodic.

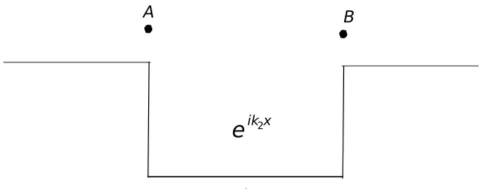

Figure 6. Well-Barrier question: What's the probability that an incoming wave from the left, that reaches point A, will arrive at point B?

$$\begin{aligned} t_{\sqcup} &= t_{\llcorner} e^{ik_2L} t_{\lrcorner} + t e^{ik_2L} r e^{ik_2L} r e^{ik_2L} t + \cdots \\ &= t e^{ik_2L} t \left(\frac{1}{1 - |\,r\,|^2 e^{2ik_2L}} \right) \\ &= e^{ik_2L} \,|\,t\,|^2 \frac{1}{1 - |\,r\,|^2 e^{2ik_2L}}\,, \end{aligned} \tag{4}$$

where the first step involved a geometric series. This result has accounted for all the possible means of contributing to the transmission, being with and without reflections.

Therefore,

$$t_{\sqcup} = \frac{1}{e^{ik_2} - \dfrac{2i}{T_{\lrcorner}} \sin(k_2L)}\,. \tag{5}$$

Next, we extract the magnitude.

$$|\,t_{\sqcup}\,|^2 = \frac{1}{1 + \dfrac{1}{4\epsilon(\epsilon+1)} \sin^2\left(g_0\sqrt{\epsilon+1}\right)} = T\,. \tag{6}$$

4 Realistic modeling of a particle

Now we complicate matters by moving on to the case of a realistic model of a particle moving to the right.

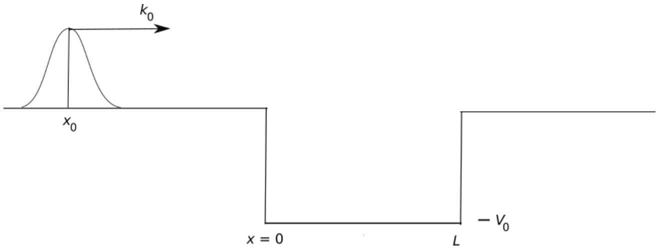

Figure 7. Well-Barrier with a gaussian approaching from the left.

We begin with the wavepacket for a free particle:

$$\psi(x,0) = N e^{-\dfrac{(x-x_0)^2}{2a^2}} e^{ik_0 x} \,. \tag{7}$$

In preparation of time-evolving this gaussian, first we expand in energy eigenstates:

$$\psi(x,0) = \int dk \frac{e^{ikx}}{\sqrt{2\pi}} f(k) \,, \tag{8}$$

where

$$f(k) = \widetilde{\psi}(x,0) \tag{9}$$

is the Fourier transform,

$$f(k) = \widetilde{N} e^{-\dfrac{a^2(k-k_0)^2}{2}} e^{-ikx_0} \tag{10}$$

As these are energy eigenstates, under time evolution they are merely multiplied by a phase:

$$\psi(x,t) = \int dk \frac{e^{ikx}}{\sqrt{2\pi}} f(k) e^{i(kx-\omega t)} \,, \tag{11}$$

where $\dfrac{\hbar^2 k^2}{2m} = \hbar\omega$.

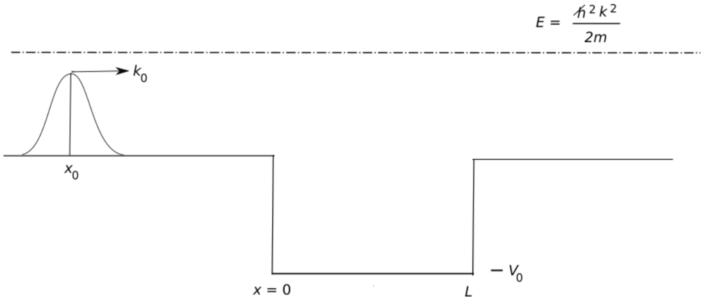

Figure 8. Well-Barrier with initial wavenumber k_0.

5 Continuing, using the Heaviside Step Function

The Heaviside Step Function $\theta(x)$ is defiined on the real numbers, and has the values

$$\theta(x) = \begin{cases} 0 & \text{for} \quad x < 0 \,, \\ \frac{1}{2} & \text{for} \quad x = 0 \,, \\ 1 & \text{for} \quad x > 0 \,. \end{cases} \tag{12}$$

We can use this function to 'turn on' a function after a particular value. But for the sake of integration the value of $\theta(0)$ can be ignored.

Now, the energy eigenstates

$$\phi_k = \frac{1}{2\pi} \left[e^{ikx}\theta(-x) + re^{-ikx}\theta(-x) + te^{ikx}\theta(x) \right] , \tag{13}$$

where r is the amplitude of reflection and t is the amplitude of transmission. Next, we decompose the wavefunctions in terms of actual eigenstates.

$$\begin{aligned}\psi(x,0) &= \int \frac{dk}{\sqrt{2\pi}} \widetilde{f}(k)\phi(k) \quad (\text{where} \quad \phi(k) = \phi_k) \\ &= \int \frac{dk}{\sqrt{2\pi}} \left[\widetilde{f}(k)e^{i(kx)}\theta(-x) + \widetilde{f}re^{-i(kx)}\theta(-x) + \widetilde{f}te^{i(kx)}\theta(x)\right] . \end{aligned} \tag{14}$$

Hence,

$$\psi(x,t) = \int \frac{dk}{\sqrt{2\pi}} \left[\widetilde{f}(k)e^{i(kx-\omega t)}\theta(-x) + \widetilde{f}re^{-i(kx+\omega t)}\theta(-x) + \widetilde{f}te^{i(kx-\omega t)}\theta(x)\right] . \tag{15}$$

The terms above that contain the factor $e^{i(kx-\omega t)}$ have central peaks that move to the right; whereas, the terms above that contain the factor $e^{-i(kx+\omega t)}$ have central peaks that move to the left.

Let's look at (15) when $t = 0$:

$$\psi(x,0) = \int dk\widetilde{f}(k)e^{ikx}\theta(-x) = G(x_0, k_0, t=0)\theta(-x)\,, \tag{16}$$

where G is the "gaussian." Now, put in the time dependence:

$$\psi(x,t) = \int dk\widetilde{f}(k)e^{i(kx-\omega t)}\theta(-x) = G(x_0, k_0, t)\theta(-x)\,. \tag{17}$$

We interpret $\widetilde{f}(k)$ as the envelope of a plane-wave packet moving to the right, and localized in space and in momentum k_0.

6 The Method of Stationary Phase

The location of the peak of the wavepacket satisfies

$$\frac{d}{dk}(kx - \omega(k)t)\Big|_{k_0} = 0\,. \tag{18}$$

This becomes

$$\left(x - \frac{d\omega}{dk}t\right)\Big|_{k_0} = 0\,, \tag{19}$$

where $d\omega/dk = \hbar k/m$. Therefore,

$$x(t) = \frac{\hbar k}{m}t = v_0 t\,, \tag{20}$$

where v_0 is the classical velocity.

7 The Big Question

What happens when the wavepacket hits the barrier? Regarding $\psi(x,t)$ in (15), in positive time t the term $\widetilde{f}(k)e^{i(kx-\omega t)}\theta(-x)$ is zero. However, the reflection term $\widetilde{f}(k)re^{-i(kx-\omega t)}\theta(-x)$, because it moves to the left, turns on for $x < 0$.

But for $x > 0$, $\widetilde{f}(k)te^{i(kx-\omega t)}\theta(x)$ turns on and $\theta(x) = 1$. So, let's focus on this term.

$$\int \frac{dk}{\sqrt{2\pi}} \widetilde{f}te^{i(kx-\omega t)}\,. \tag{21}$$

Now, t is the transmission probability with a phase. Let's make this explicit

$$t = \sqrt{T} e^{-\varphi(k)} \,, \tag{22}$$

So, what can we find out about this phase?

$$\int \frac{dk}{\sqrt{2\pi}} f \sqrt{T} e^{i(kx-\omega t-\varphi)} \,. \tag{23}$$

Once again, by stationary phase,

$$\frac{d}{dk}(kx - \omega(k)t - \varphi)\bigg|_{k_0} = 0 \,, \tag{24}$$

yields $x - v_0 t - \frac{d\varphi}{dk}\Big|_{k_0} = 0$. But $\frac{d\varphi}{dk} = \frac{d\omega}{dk}\frac{d\varphi}{d\omega} = v_0 \hbar \frac{d\varphi}{dE}$. This implies that

$$x_{\text{peak}} = v_0\Big(t + \hbar \frac{d\varphi}{dE}\Big) \,, \tag{25}$$

where, again, x is the position of the wavepacket peak. However, the term $\hbar \frac{d\varphi}{dE}$ constitutes a shift. Interpretation: Classically, the particle speeds up over the potential well, and slows down when it leaves it. For a very deep well, the particle traverses the gap nearly instantaneously.

At $x > L$, $x = v_0\big(t + \frac{L}{v_0}\big)$, where L/v_0 is the lost time traversing the gap.

$$\Delta t_{\text{CL}} = \frac{L}{v_0} = \hbar \frac{d\varphi}{dE}\bigg|_{k_0} \,. \tag{26}$$

For amplitude C/A (see the last lecture)

$$\varphi = k_2 L - \arctan\left(\frac{k_1^2 + k_2^2}{2k_1k_2}\tan(k_2L)\right) \,, \tag{27}$$

where the RH term should simplify near resonance.

$$k_2 L = N\pi \Longrightarrow \hbar \frac{d\varphi}{dE}\bigg|_{k_0} = \frac{L}{2v_0}\left(1 + \frac{E}{V_0}\right) \approx \frac{L}{2v_0} \,. \tag{28}$$

Thus the QM result B is halved compared to the classical result.

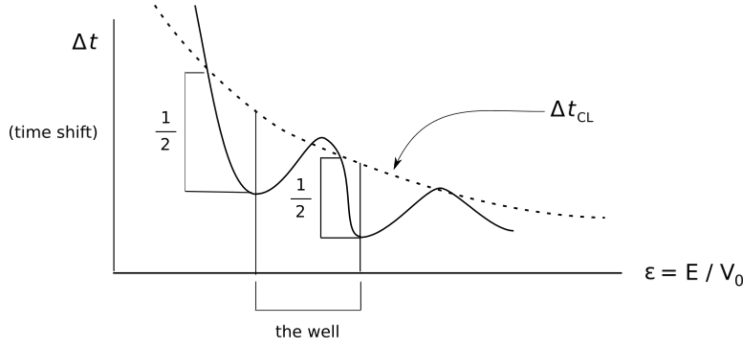

Figure 9. The QM particle moves slower across the well.

8 The S-Matrix

Let $V(x)$ be an unknown potential as in Fig. 10. The resonances contain the information to solve for E and V.

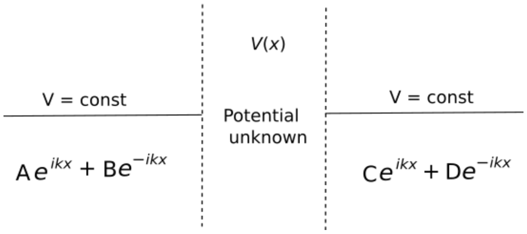

Figure 10. The Unknown Potential with solutions, $E > V_0$.

Let's ramp-up to a more general situation. Suppose we extend into the gap incoming from the left (A) and from the right (D). We can attempt a matrix formulation which provides us a linear relationship

$$\begin{pmatrix} B \\ C \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \begin{pmatrix} A \\ D \end{pmatrix} , \tag{29}$$

which will conserve probability. Knowing the values of $S_{ij}(E)$ solves the scattering problem.

So, what properties must S satisfy?

1) Stuff doesn't disappear, thus,

$$|\,A\,|^2 + |\,D\,|^2 = |\,B\,|^2 + |\,C\,|^2 , \tag{30}$$

which can be given the matrix representation

$$\begin{aligned} \begin{pmatrix} A^* & D^* \end{pmatrix} \begin{pmatrix} A \\ D \end{pmatrix} &= \begin{pmatrix} B^* & C^* \end{pmatrix} \begin{pmatrix} B \\ C \end{pmatrix} \\ &= \begin{pmatrix} A^* & D^* \end{pmatrix} S^\dagger S \begin{pmatrix} A \\ D \end{pmatrix} , \end{aligned} \tag{31}$$

where $S^\dagger$ is the adjoint of S. Anyway, this forces the conclusion that

$$S^\dagger S = I , \tag{32}$$

where I is the unit 2×2 matrix. This, in turn, implies that S is unitary, and that the eigenvalues of S are phases:

$$s_1 = e^{i\varphi_1} , \quad s_2 = e^{i\varphi_2} . \tag{33}$$

Certain mathematical constraints on S (derived on the problem set) require that

$$|\,S_{11}\,| = |\,S_{22}\,| , \quad |\,S_{12}\,| = |\,S_{21}\,| , \tag{34}$$

and

$$|\,S_{12}\,|^2 + |\,S_{21}\,|^2 = 1 , \quad S_{11} S_{12}^* + S_{21} S_{22}^* = 0 . \tag{35}$$

Special case: All input is from the left.

$$D = 0 , \quad A = 1 . \tag{36}$$

Then,

$$\frac{B}{A} = S_{11}\,, \quad \frac{C}{A} = S_{21}\,. \tag{37}$$

But

$$r_{\leftarrow} = \frac{B}{A}\,, \quad t_{\rightarrow} = \frac{C}{A}\,. \tag{38}$$

and

$$|\,S_{11}\,| = |\,S_{22}\,| \Longrightarrow (|\,r_{\leftarrow}\,| = |\,r_{\rightarrow}\,|) \;\&\; (|\,t_{\leftarrow}\,| = |\,t_{\rightarrow}\,|)\,, \tag{39}$$

and lastly,

$$|\,S_{12}\,|^2 + |\,S_{11}\,|^2 = 1 \quad \Longrightarrow \quad T + R = 1\,. \tag{40}$$

Suppose we try a time reversal, $t \to -t$. Assuming time-reversal invariance (as in electrostatics), then ψ is a solution if and only if ψ^* is also a solution.

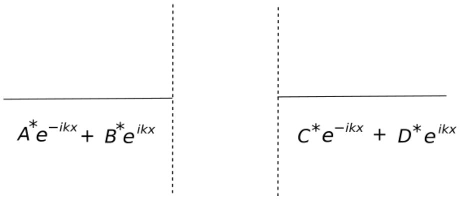

Figure 11. In time reversal, we conjugate ψ. $E > V_0$.

The outgoing solution, then, is

$$\begin{pmatrix} A^* \\ D^* \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \begin{pmatrix} B^* \\ C^* \end{pmatrix}\,, \tag{41}$$

From this, we have that

$$S^* S = I\,, \quad \text{and} \quad S^T = S \quad \Longrightarrow \quad S_{21} = S_{12} \quad \text{(i.e., same phases)}\,. \tag{42}$$

The values of the S-matrix can be determined by experimental measurment. This is enough to determine the bound-state energies of a system.

$$\begin{pmatrix} B \\ C \end{pmatrix} = S_E \begin{pmatrix} A \\ D \end{pmatrix}\,, \tag{43}$$

at a given energy $E > V_0$.

But, what if $E < 0$ (?) for a bound state? In this case, we set $k \to i\alpha$.

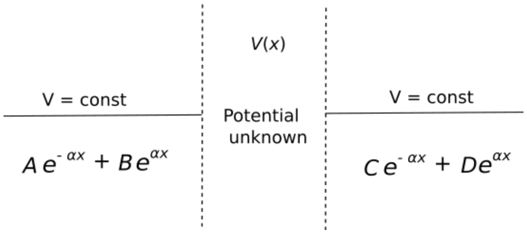

Figure 12. Unknown potential with bounds states.

What about the normalization requirement? We take $A = 0$, for otherwise for $x \to -\infty$, the A-term blows-up. Similarly, $D = 0$. All this implies

$$\begin{pmatrix} A \\ D \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} , \tag{44}$$

which implies that for

$$\begin{pmatrix} B \\ C \end{pmatrix} \neq \begin{pmatrix} 0 \\ 0 \end{pmatrix} , \tag{45}$$

S must have a pole: $S \sim 1/0$. Look at

$$S_{21} = t_{\sqcup} = \frac{2k_1 k_2 e^{ik_2 L}}{2k_1 k_2 \cos(k_2 L) - i(k_1^2 + k_2^2)\sin(k_2 L)} , \tag{46}$$

which implies that the following relation gives the bound states for the square well.

$$\frac{2k_2}{2} \tan\left(\frac{2k_2}{2}\right) = \frac{k_1 L}{2} . \tag{47}$$