

Problem 1. (15 points) Mathematical Preliminaries: Facts about Unitary Operators

- (a) **(3 points)** Suppose ϕ_u is an eigenfunction of U with eigenvalue u , ie

$$U\phi_u = u\phi_u$$

We thus have that

$$(U\phi_u|U\phi_u) = (u\phi_u|u\phi_u) = |u|^2(\phi_u|\phi_u)$$

On the other hand, since U is unitary, $U^\dagger U = 1$, we have

$$(U\phi_u|U\phi_u) = (\phi_u|U^\dagger U\phi_u) = (\phi_u|1\phi_u) = (\phi_u|\phi_u)$$

This tells us that,

$$|u|^2(\phi_u|\phi_u) = (\phi_u|\phi_u)$$

Thus, unless $\phi_u = 0$, we must have that

$$|u|^2 = 1$$

ie, all eigenvalues u of a Unitary operator must be pure phases, $u = e^{i\theta}$

- (b) **(2 points)** The condition for U to be Hermitian is that $U^\dagger = U$. The condition for U to be Unitary is that $U^\dagger U = 1$. Thus the condition for an operator to be both Unitary and Hermitian is that $UU = 1$ – ie, the only Unitary operators which are also Hermitian are those which square to one.

Note that can be easily seen from the eigenvalues: Hermitian implies the eigenvalues are all real; Unitary implies the eigenvalues are all pure phases; the only numbers which are both real and pure phases are ± 1 ; thus the eigenvalues of a Unitary Hermitian operator are all ± 1 and square to one.

So: can a Unitary operator be Hermitian? Yes, but only if it squares to one. Is a generic Unitary operator Hermitian? No!

- (c) **(4 points)** Suppose M is Hermitian, $M^\dagger = M$. We'd like to see that $U = e^{iM}$ is Unitary, ie that $U^\dagger U = 1$. By definition of the exponential of an operator,

$$U = e^{iM} = \sum_{n=0}^{\infty} \frac{(iM)^n}{n!}$$

Since M is Hermitian, iM is anti-Hermitian, ie $(iM)^\dagger = -iM$, so

$$U^\dagger = \sum_{n=0}^{\infty} \frac{(-iM^\dagger)^n}{n!} = e^{-iM} \tag{1}$$

Thus,

$$U^\dagger U = e^{-iM} e^{iM} = 1$$

- (d) **(1 points)** We want to see that the product of two Unitary operators is also Unitary. Suppose A and B are Unitary, $A^\dagger A = 1$ and $B^\dagger B = 1$, and let $W = AB$. Then

$$W^\dagger = (AB)^\dagger = B^\dagger A^\dagger \quad \Rightarrow \quad W^\dagger W = (B^\dagger A^\dagger)AB = B^\dagger(A^\dagger A)B = B^\dagger B = 1$$

So $W = AB$ is Unitary.

- (e) **(1 points)** The length of a vector v is defined as $|v| = \sqrt{\langle v|v \rangle}$ (in Dirac notation). Let's make the notation $|u\rangle = U|v\rangle$. The length of u is:

$$|u| = \sqrt{\langle u|u \rangle} = \sqrt{\langle v| \underbrace{U^\dagger U}_I |u \rangle} = \sqrt{\langle v|v \rangle} = |v|. \quad (2)$$

So Unitary operators preserve the length of vectors.

- (f) **(4 points)** Since \hat{p} is a Hermitian operator, also

$$-\frac{L}{\hbar}\hat{p}, \quad (3)$$

being the multiplication of \hat{p} by a real number, is Hermitian. Indeed, from Problem set 6 we know that

$$\left(-\frac{L}{\hbar}\hat{p}\right)^\dagger = \hat{p}^\dagger \left(-\frac{L}{\hbar}\right)^\dagger = \hat{p} \left(-\frac{L}{\hbar}\right) = -\frac{L}{\hbar}\hat{p}. \quad (4)$$

Likewise, since \hat{x} is a Hermitian operator, also

$$\frac{q}{\hbar}\hat{x}, \quad (5)$$

is Hermitian. Thus, from part (c), we know that

$$\hat{T}_L = e^{i\left(-\frac{L}{\hbar}\hat{p}\right)} \quad \hat{B}_q = e^{i\left(\frac{q}{\hbar}\hat{x}\right)}, \quad (6)$$

are Unitary operators.

Finally, note that, acting with \hat{T}_L on any function $f(x)$, and keeping into account Equation (1),

$$\hat{T}_{-L}f(x) = f(x+L) = e^{i\frac{L}{\hbar}\hat{p}}f(x) = \left(e^{-i\left(\frac{L}{\hbar}\hat{p}\right)}\right)^\dagger = T_L^\dagger f(x). \quad (7)$$

In the same way, acting with \hat{B}_q on $f(x)$,

$$\hat{B}_{-q}f(x) = e^{i\frac{-qx}{\hbar}}f(x) = e^{-i\left(\frac{q}{\hbar}\hat{x}\right)}f(x) = \left(e^{-i\left(\frac{q}{\hbar}\hat{x}\right)}\right)^\dagger f(x) = \hat{B}_q^\dagger f(x). \quad (8)$$

Since Equations (7) and (8) hold for any function $f(x)$, we conclude that the first and the last members are equal at the operator level, and thus

$$\hat{T}_{-L} = \hat{T}_L^\dagger, \quad \hat{B}_{-q} = \hat{B}_q^\dagger. \quad (9)$$

Problem 2. (20 points) Quantum Evolution is Unitary

- (a) **(3 points)** The square modulus of the wavefunction $|\psi(x, t)|^2$ is the probability density of finding the particle at position x at time t . Since we want our particle to exist somewhere, we require the total probability to be equal to unity, i.e. $\int |\psi(x, t)|^2 dx = 1$. Time evolution must preserve the total probability, so the time-evolution operator must preserve the norm of the wavefunction – i.e., \hat{U}_t must be Unitary.
- (b) **(5 points)** Given a wavefunction $\psi(x, 0)$ at time $t = 0$, and using the definition¹ of the evolution operator \hat{U}_t , we can deduce the wavefunction at time t_1 by acting with the evolution operator as,

$$\psi(x, t_1) = \hat{U}_{t_1} \psi(x, 0). \quad (10)$$

We can then deduce the wavefunction at a subsequent time $t_1 + t_2$ by acting again with the evolution operator as,

$$\psi(x, t_1 + t_2) = \hat{U}_{t_2} \psi(x, t_1) = \hat{U}_{t_2} \hat{U}_{t_1} \psi(x, 0). \quad (11)$$

On the other hand, we can also determine the wavefunction at time $t_1 + t_2$ directly with a single application of the evolution operator,

$$\psi(x, t_1 + t_2) = \hat{U}_{t_1+t_2} \psi(x, 0). \quad (12)$$

But physically, the wavefunction at time $t_1 + t_2$ is completely determined by the wavefunction at time $t = 0$ – the evolution of the wavefunction is deterministic. Our two expressions for $\psi(x, t_1 + t_2)$ thus must agree. Since this logic applies regardless of the initial wavefunction, it must be true that, as operators,

$$\hat{U}_{t_2} \hat{U}_{t_1} = \hat{U}_{t_1+t_2}. \quad (13)$$

- (c) **(4 points)** Consider the state $\psi(x, t)$, which is the evolution of the state $\psi(x, 0)$ at time $t = 0$. Thus we can write

$$\psi(x, t) = \hat{U}_t \psi(x, 0). \quad (14)$$

Using the Schrödinger equation, we obtain

$$\left(\partial_t \hat{U}_t \right) \psi(x, 0) = \partial_t \left(\hat{U}_t \psi(x, 0) \right) = -\frac{i}{\hbar} \hat{E} \hat{U}_t \psi(x, 0), \quad (15)$$

¹Note that we are assuming that the system is time-translationally invariant, i.e. that if $\psi(x, t) = \hat{U}_t \psi(x, 0)$, then $\psi(x, t + t_o) = \hat{U}_t \psi(x, t_o)$, i.e. that *how the wavefunction evolves does not depend on time*. This is equivalent to assuming that the energy operator, \hat{E} , is time-independent. In general, we may relax this assumption by allowing the evolution operator to depend on time, i.e. $\psi(x, t_2) = \hat{U}_{t_2, t_1} \psi(x, t_1)$. The composition rule then says, $\hat{U}_{t_1+t_2, 0} = \hat{U}_{t_1+t_2, t_1} \hat{U}_{t_1, 0}$. Time-translation invariance then says that $\hat{U}_{t_o+t, t_o} = \hat{U}_{t, 0} \equiv \hat{U}_t$.

and since the latter Equation holds for any $\psi(x, 0)$, we can write

$$\partial_t \hat{U}_t = -\frac{i}{\hbar} \hat{E} \hat{U}_t. \quad (16)$$

(d) **(5 points)** The most general solution to Equation (16) is

$$\hat{U}_t = e^{-\frac{i}{\hbar} \hat{E} t} \hat{C}, \quad (17)$$

where \hat{C} is a constant operator. Unitarity requires

$$\hat{\mathbb{1}} = \hat{C}^\dagger e^{\frac{i}{\hbar} \hat{E} t} e^{-\frac{i}{\hbar} \hat{E} t} \hat{C} = \hat{C}^\dagger \hat{C} \quad (18)$$

thus \hat{C} has to be unitary. From part (b), we require that

$$\hat{U}_{t_2} = \hat{U}_{t_1+t_2} \hat{U}_{t_1}^\dagger, \quad (19)$$

thus

$$e^{-\frac{i}{\hbar} \hat{E} t_2} \hat{C} = e^{-\frac{i}{\hbar} \hat{E} (t_1+t_2)} \hat{C} \hat{C}^\dagger e^{\frac{i}{\hbar} \hat{E} t_1}, \quad (20)$$

which requires $\hat{C} = \hat{\mathbb{1}}$. Thus there is only one solution which satisfies properties (a) and (b):

$$\hat{U}_t = e^{-\frac{i}{\hbar} \hat{E} t}, \quad (21)$$

note that $\hat{U}_0 = \hat{\mathbb{1}}$, which is important – evolving for zero time should do nothing to the state.

(e) **(3 points)** In the case of the harmonic oscillator, we have

$$\hat{E} = \hbar\omega \left(\hat{N} + \frac{1}{2} \right), \quad (22)$$

thus

$$\hat{U}_t = e^{-\frac{i}{\hbar} t \hat{E}} = e^{-i\omega t \left(\hat{N} + \frac{1}{2} \right)}. \quad (23)$$

Problem 3. (20 points) Getting a Sense for T

(a) (4 points) The scattering potential is defined as:

$$V(x) = \begin{cases} 0 & x < 0 \\ V_0 & x > 0 \end{cases}. \quad (24)$$

Let's analyze the two energy cases separately. When $E > V_0$ the wavefunction takes the form:

$$\psi(x) = \begin{cases} Ae^{ik_1x} + Be^{-ik_1x} & x < 0 \\ Ce^{ik_2x} & x > 0 \end{cases}, \quad (25)$$

with $k_1 = \frac{1}{\hbar}\sqrt{2mE}$ and $k_2 = \frac{1}{\hbar}\sqrt{2m(E - V_0)}$. The wavefunction and its first derivative continuity conditions at $x = 0$ requires that:

$$A + B = C, \quad (26a)$$

$$ik_1(A - B) = ik_2C. \quad (26b)$$

The set of equations (26) can be easily solve for B and C in terms of A :

$$B = \frac{k_1 - k_2}{k_1 + k_2}A \Rightarrow r = \frac{B}{A} = \frac{k_1 - k_2}{k_1 + k_2}, \quad (27a)$$

$$C = \frac{2k_1}{k_1 + k_2}A \Rightarrow t = \frac{C}{A} = \frac{2k_1}{k_1 + k_2}. \quad (27b)$$

To compute the transmission probability T and the reflection probability R we use their definitions:

$$R = \frac{|j_B|}{|j_A|} = \frac{|B|^2 \frac{k_1}{m}}{|A|^2 \frac{k_1}{m}} = \frac{|B|^2}{|A|^2} = |r|^2 = \left| \frac{k_1 - k_2}{k_1 + k_2} \right|^2, \quad (28a)$$

$$T = \frac{|j_C|}{|j_A|} = \frac{|C|^2 \frac{k_2}{m}}{|A|^2 \frac{k_1}{m}} = \frac{|B|^2 k_2}{|A|^2 k_1} = |t|^2 \frac{k_2}{k_1} = \frac{4k_1 k_2}{(k_1 + k_2)^2}, \quad k_1, k_2 \in \mathbb{R} \quad (28b)$$

For the case in which $E < V_0$, k_2 becomes complex. We don't need to change the previous equations for r , t , and R as long as we take k_2 to be the positive complex root, i.e. $k_2 \rightarrow +i|k_2|$. For T there is a different story; j_C it is no longer given by the expression used in Eq. 28b since the associated speed is complex. For this case we

have to use the actual definition of the current probability (or the result from Problem 3, Pset 6):

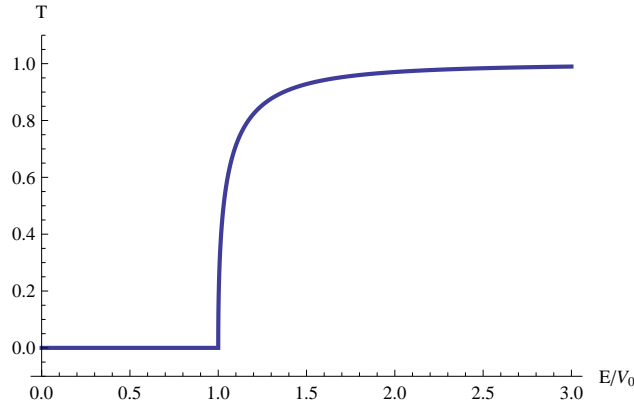
$$j_C = |C|^2 \frac{i}{2m} \left[e^{-|k_2|x} \frac{\partial (e^{-|k_2|x})}{\partial x} - e^{-|k_2|x} \frac{\partial (e^{-|k_2|x})}{\partial x} \right] = 0 \quad (29)$$

So in this case:

$$T = 0, \quad (30a)$$

$$R = \frac{k_1 - i|k_2|}{k_1 + i|k_2|} \times \frac{k_1 + i|k_2|}{k_1 - i|k_2|} = 1 = 1 - T. \quad (30b)$$

Shown below is a plot of transmission T as function of energy E (in units of V_0).



The easiest way to analyze the downhill scattering is to invert our scattering potential (24):

$$V(x) = \begin{cases} V_0 & x < 0 \\ 0 & x > 0 \end{cases}. \quad (31)$$

Then we can reuse all the equations 25 through 28 from part (a), except that k_1 and k_2 interchange roles: $k_1 \rightarrow k_2$ and $k_2 \rightarrow k_1$. Thus we see that the amplitude scattering coefficients r and t are different, while the probability scattering coefficients T and R remain the same.

- (b) **(4 points)** We first write the transmission coefficients in terms of the dimensionless variables E/V_0 and $g_0 = \frac{L}{\hbar} \sqrt{2mV_0}$. For $E < V_0$ we have

$$T = \frac{1}{1 + \frac{V_0^2}{4E(V_0 - E)} \sinh^2(\alpha L)} = \frac{1}{1 + \frac{1}{4\left(\frac{E}{V_0}\right)\left(1 - \frac{E}{V_0}\right)} \sinh^2\left(g_0 \sqrt{1 - \frac{E}{V_0}}\right)}, \quad (32)$$

whereas for $E > V_0$ we get

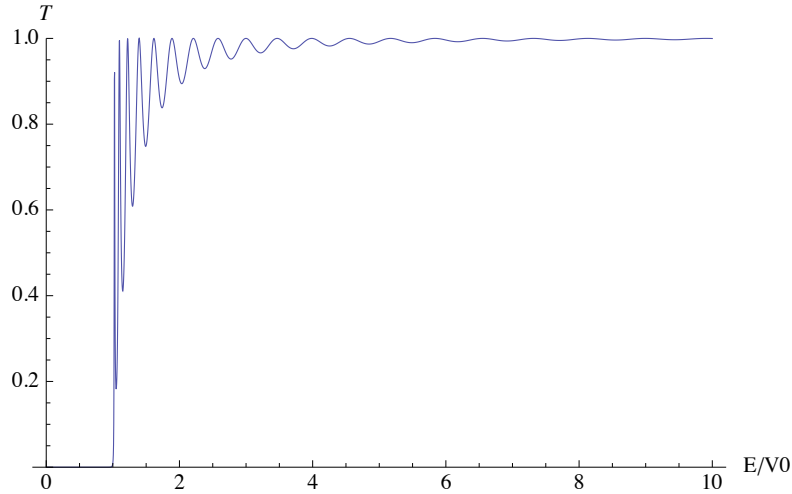
$$T = \frac{1}{1 + \frac{V_0^2}{4E(V_0-E)} \sinh^2(\alpha L)} = \frac{1}{1 + \frac{1}{4\left(\frac{E}{V_0}\right)\left(\frac{E}{V_0}-1\right)} \sin^2\left(g_0\sqrt{\frac{E}{V_0}-1}\right)}. \quad (33)$$

As $E \rightarrow V_0$, the argument of either the sine or the hyperbolic sine (depending on whether we're approaching V_0 from above or below) becomes very small. It thus becomes appropriate to Taylor expand the expressions. In particular, $\sin x \approx \sinh x \approx x$ for small x , so $\sin^2 g_0\sqrt{\frac{E}{V_0}-1} \approx g_0^2\left(\frac{E}{V_0}-1\right)$ and $\sinh^2\left(g_0\sqrt{1-\frac{E}{V_0}}\right) \approx g_0^2\left(1-\frac{E}{V_0}\right)$. Substituting into our equations for T gives

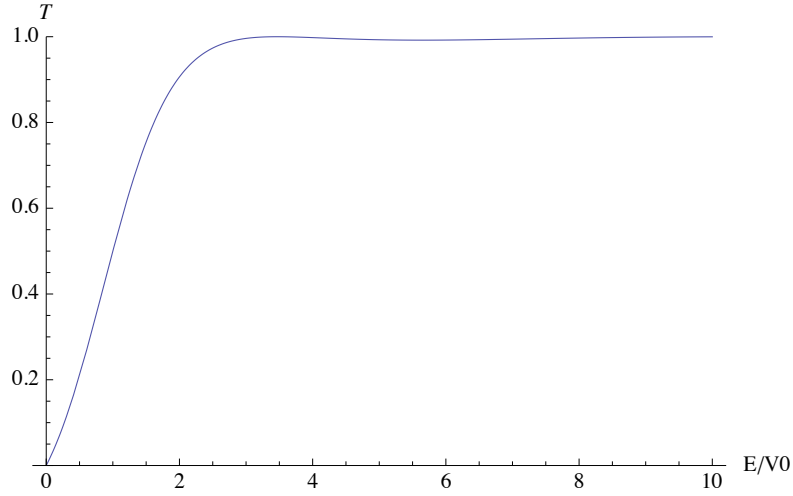
$$\lim_{E \rightarrow V_0} T = \frac{1}{1 + \frac{g_0^2}{4\left(\frac{E}{V_0}\right)}} = \frac{1}{1 + \frac{g_0^2}{4}}, \quad (34)$$

for both cases, just like we expect. Shown below are plots for:

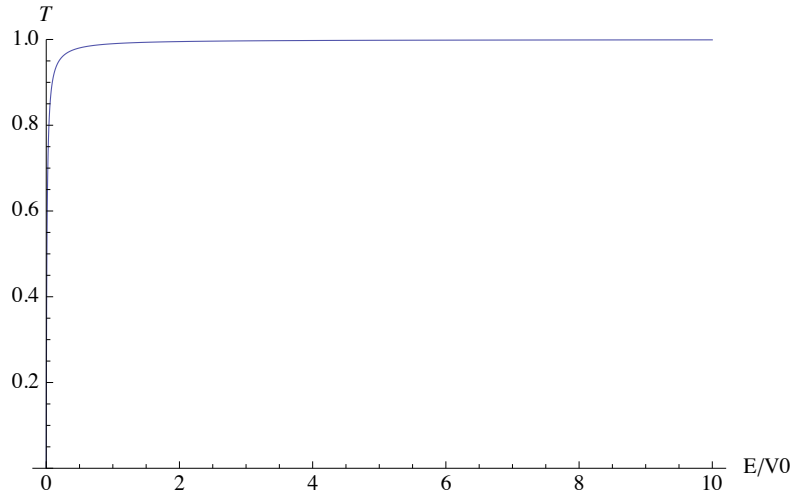
- A very wide barrier ($g_0 = 20$):



- A medium barrier ($g_0 = 2$):



- A thin barrier ($g_0 = 0.2$):



- (c) **(3 points)** For a high, wide barrier, $V_0 > E$ and $g_0 \gg 1$. Thus, the argument in the sinh function is very large, and since

$$\sinh x \equiv \frac{e^x - e^{-x}}{2} \approx \frac{e^x}{2}, \quad (35)$$

our transmission coefficient becomes

$$T \approx \left[1 + \frac{\exp\left(2g_0\sqrt{1 - \frac{E}{V_0}}\right)}{16\left(\frac{E}{V_0}\right)\left(1 - \frac{E}{V_0}\right)} \right]^{-1} \approx 16\left(\frac{E}{V_0}\right)\left(1 - \frac{E}{V_0}\right) \exp\left(-2g_0\sqrt{1 - \frac{E}{V_0}}\right), \quad (36)$$

where in the last step we used the fact that the exponential factor is likely to be much greater than 1. The transmission probability is exponentially suppressed (notice

the minus sign in the exponential), and thus the goldfish is unlikely to tunnel after hitting the wall of its bowl. (Note that this argument relies on the factor of \hbar in the denominator of g_0 . If \hbar weren't such a tiny number, we *would* see the tunneling classical objects like goldfish).

- (d) **(4 points)** To obtain the transmission probability on a potential well of depth $-V_o$ we just need to flip the sign of V_o inside the formula for T we already have. Because $E > 0$, we just have one case here, which is $E > V_o$. Thus,

$$k_2^2 = \frac{2m}{\hbar^2}(E - (-V_o)) = \frac{2m}{\hbar^2}(E + V_o), \quad (37)$$

$$T = \frac{1}{1 + \frac{V_o^2}{4E(E - (-V_o))} \sin^2(k_2L)} = \frac{1}{1 + \frac{V_o^2}{4E(E + V_o)} \sin^2(k_2L)}. \quad (38)$$

Which is the same expression we obtained in lecture. The reason why this works is that the kinematic is the same in both cases. In other words, in the first case, we have to solve the eigenstate equation

$$\left(-\frac{\hbar^2}{2m} \partial_x^2 + V_o \right) \psi = E\psi, \quad (39)$$

and in the second case we have to solve the equation

$$\left(-\frac{\hbar^2}{2m} \partial_x^2 - V_o \right) \psi = E\psi. \quad (40)$$

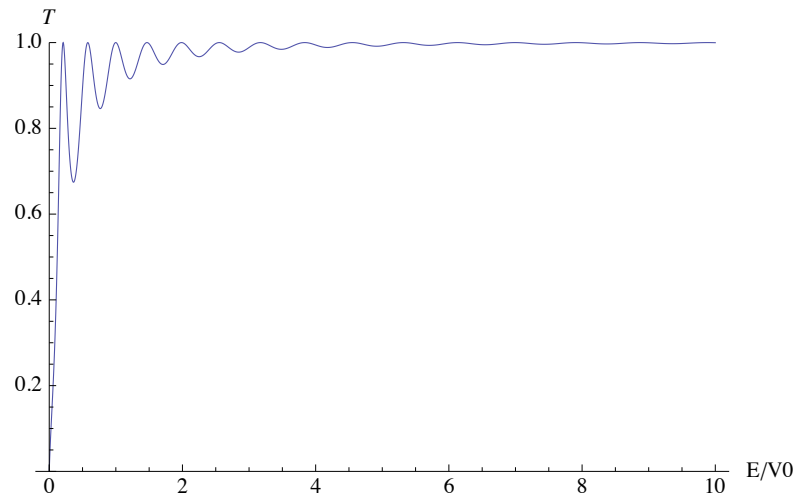
Since there is only a sign difference in the coefficient V_o , it is reasonable to expect that the expression for T can be obtained by extending V_o to $-V_o$, as in the procedure to derive T there is no assumption on the sign of V_o .

Performing the same non-dimensionalization as before, we get

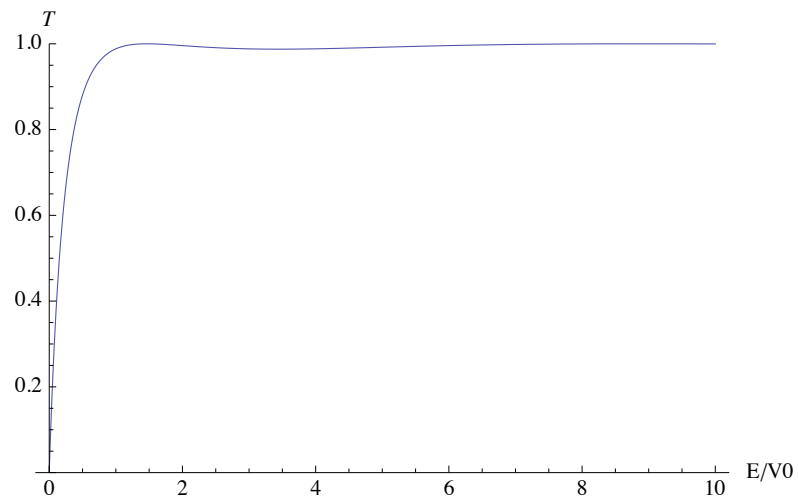
$$T = \frac{1}{1 + \frac{1}{4\frac{E}{V_o}(1+\frac{E}{V_o})} \sin^2\left(g_0\sqrt{1 + \frac{E}{V_o}}\right)}. \quad (41)$$

Again, we show plots for various values of g_0 :

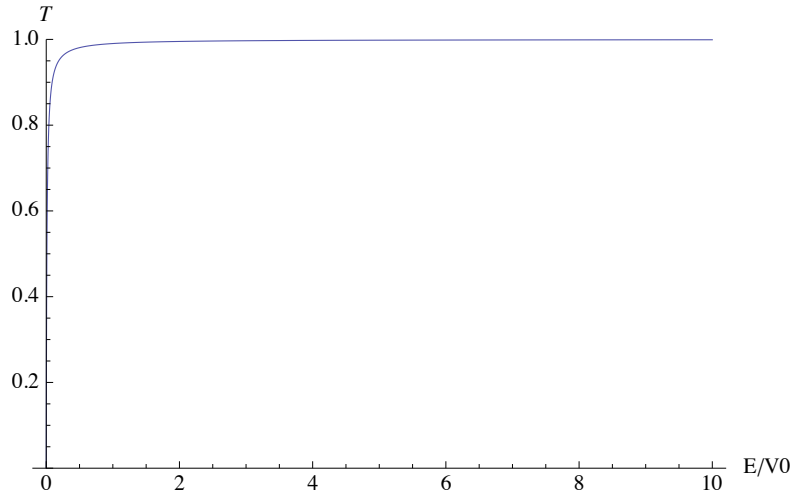
- A very wide barrier ($g_0 = 20$):



- A medium barrier ($g_0 = 2$):



- A thin barrier ($g_0 = 0.2$):



- (e) **(5 points)** The most robust way of analyzing this data is to consider the *peaks* in the transmission function, where $T = 1$. From the expressions above, we can see that this occurs whenever the argument of the sine function is a multiple of π . We need not consider the $E < V_0$ transmission function for the potential barrier (where we have a hyperbolic sine instead of sine), because the transmission function can only reach 1 for $E > V_0$. This happens when we have

$$g_0 \sqrt{\frac{E_{max}}{V_0} \pm 1} = n\pi, \quad (42)$$

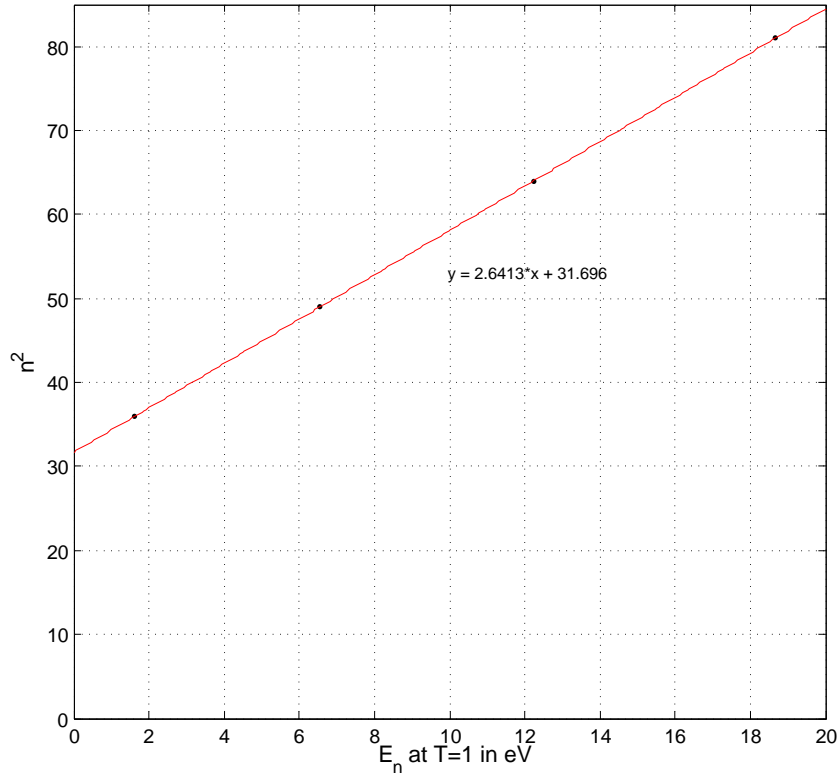
where g_0 is as defined above, E_{max} is some energy at which $T = 1$, n is an integer, and the sign is determined by whether we have a barrier (minus) or a well (plus). Rearranging this gives us

$$n^2 = \frac{g_0^2}{\pi^2 V_0} E_{max} \pm \frac{g_0^2}{\pi^2}. \quad (43)$$

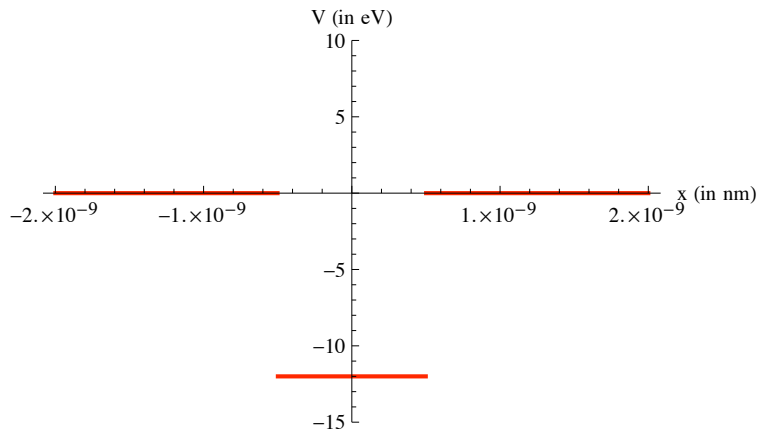
This means that if we read off the various E_{max} 's from the graph and plot them against n^2 , the sign of the intercept will tell us whether we have a well or a barrier, the value of the intercept will give us g_0 , and the slope will allow us to solve for V_0 . The only subtlety here is that we do not know *a priori* what value of n to associate with a given E_{max} . It is incorrect, for example, to assume that the first point at which $T = 1$ corresponds to $n = 1$, because the left hand side of Equation 42 can get no smaller than g_0 , so if $g_0 > \pi$ then n begins at some integer greater than 1. Fortunately, we can determine what n to begin at by making a guess and plotting the data, because Equation 43 predicts a linear relationship *only* if we choose the correct starting n (the relationship is quadratic otherwise). On the next page we show a plot of E_{max} against n , where the starting n was determined to be 6. The plot is clearly linear.

The intercept is positive, so we conclude that we have a potential *well*. From Equation 43 we see that the intercept occurs at g_0^2/π^2 , giving $g_0 \approx 17.7$. The slope, on the other

hand, equals $\frac{g_0^2}{\pi^2 V_0}$, so $V_0 = 12.0 \text{ eV}$. Since we know that $g_0 = \frac{\hbar}{L} \sqrt{2mV_0}$, this allows us to solve for L as well, and we get $L = 10^{-9} \text{ m} = 1 \text{ nm}$.



The potential thus looks like this:



Problem 4. (20 points) Properties of the S-Matrix

(a) (4 points) By definition the scattering matrix S is:

$$\begin{pmatrix} B \\ C \end{pmatrix} = \begin{pmatrix} r & \tilde{t} \\ t & \tilde{r} \end{pmatrix} \begin{pmatrix} A \\ D \end{pmatrix}. \quad (44)$$

If we have particles incoming only from the left then $D = 0$:

$$\begin{pmatrix} B \\ C \end{pmatrix} = \begin{pmatrix} r & \tilde{t} \\ t & \tilde{r} \end{pmatrix} \begin{pmatrix} A \\ 0 \end{pmatrix}, \quad (45)$$

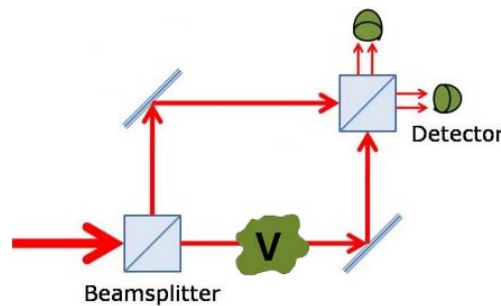
and if we divide both sides by A we get:

$$\begin{pmatrix} \frac{B}{A} \\ \frac{C}{A} \end{pmatrix} = \begin{pmatrix} r & \tilde{t} \\ t & \tilde{r} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} r \\ t \end{pmatrix} \quad (46)$$

This tells us that $|r|^2$ is the probability that a particle sent from left will reflect left, and $|t|^2$ is the probability that a particle from left is transmitted to the right of the potential. A similar reasoning goes with $|\tilde{r}|^2$ and $|\tilde{t}|^2$, but with beams coming from the right.

To measure $|t|^2$, we simply need a measurement of the fraction of a beam which transmit forward from left to right.

To measure the phase of t , we can consider the experiment represented by the picture below.



First we split the beam, then we send one beam through the potential and the other along a free path of the same length, then we interfere the two beams to compare the phase.

Alternatively, we can measure the time required for a wavepacket to arrive without the

potential, then again for a wavepacket to arrive with the potential — this last only really measures $d\phi/dk$, but that's close enough.²

(b) **(4 points)** Let's compute the left and right current:

$$j_{\text{left}} = \frac{\hbar k}{m} (|A|^2 - |B|^2), \quad (47a)$$

$$j_{\text{right}} = \frac{\hbar k}{m} (|C|^2 - |D|^2). \quad (47b)$$

Conservation of probability tells us that

$$\frac{d}{dt}\rho(x, t) = -\partial_x j_x$$

For an energy eigenstate, however, $\rho = |\psi(x, t)|^2$ is time-independent, so

$$j_{\text{left}} = j_{\text{right}} \Rightarrow |A|^2 - |B|^2 = |C|^2 - |D|^2 \Leftrightarrow |B|^2 + |C|^2 = |A|^2 + |D|^2, \quad (48)$$

But from the definition of S we get:

$$|B|^2 + |C|^2 = \begin{pmatrix} B^* & C^* \end{pmatrix} \begin{pmatrix} B \\ C \end{pmatrix} = \begin{pmatrix} A^* & D^* \end{pmatrix} S^\dagger S \begin{pmatrix} A \\ D \end{pmatrix}, \quad (49)$$

So we see that the probability conservation requires $S^\dagger S = I$.

(c) **(2 points)** From the definition of S ,

$$S^\dagger S = I \Leftrightarrow \begin{pmatrix} r^* & t^* \\ \tilde{t}^* & \tilde{r}^* \end{pmatrix} \begin{pmatrix} r & \tilde{t} \\ t & \tilde{r} \end{pmatrix} = \begin{pmatrix} |r|^2 + |t|^2 & \tilde{t}r^* + \tilde{r}t^* \\ t\tilde{r}^* + r\tilde{t}^* & \tilde{r}^2 + \tilde{t}^2 \end{pmatrix} = I$$

Thus, $|r|^2 + |t|^2 = |\tilde{r}|^2 + |\tilde{t}|^2 = 1$ and $t\tilde{r}^* + r\tilde{t}^* = 0$.

(d) **(5 points)** The Scattering matrix S is defined such that,

$$\begin{pmatrix} B \\ C \end{pmatrix} = S \begin{pmatrix} A \\ D \end{pmatrix} \quad (50)$$

Now, under Parity, $x \rightarrow -x$, the region on the left of the potential is swapped for the region on the right, while $A \leftrightarrow D$ and $B \leftrightarrow C$. However, if the system is invariant under Parity, we must have that $S \rightarrow S$. Thus,

$$\begin{pmatrix} C \\ B \end{pmatrix} = S \begin{pmatrix} D \\ A \end{pmatrix} \quad (51)$$

Using the fact that

$$\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \beta \\ \alpha \end{pmatrix} \quad (52)$$

²This last also requires running the experiment many times in order to get a good measure, while the first experiment is much more clean.

we can rewrite this as,

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} B \\ C \end{pmatrix} = S \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} A \\ D \end{pmatrix} \quad (53)$$

Multiplying by $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ then gives,

$$\begin{pmatrix} B \\ C \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} S \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} A \\ D \end{pmatrix} \quad (54)$$

Comparing to the definition of S , we see that Parity invariance implies that,

$$S = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} S \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (55)$$

Plugging in the component expression for S then gives

$$\begin{pmatrix} r & \tilde{t} \\ t & \tilde{r} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} r & \tilde{t} \\ t & \tilde{r} \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (56)$$

or, multiplying everything out,

$$\begin{pmatrix} r & \tilde{t} \\ t & \tilde{r} \end{pmatrix} = \begin{pmatrix} \tilde{r} & t \\ \tilde{t} & r \end{pmatrix} \quad (57)$$

Thus we see that Parity invariance implies

$$\boxed{r = \tilde{r} \quad t = \tilde{t}}$$

(e) **(3 points)** From the last relation in Eq. (50) for a symmetric potential we have:

$$tr^* + rt^* = 0. \quad (58)$$

If we rewrite r as $r = |r|e^{i\theta}$ the above equation becomes:

$$|t|e^{-i\phi}|r|e^{-i\theta} + |t|e^{i\phi}|r|e^{i\theta} = 0 \Rightarrow e^{2i\theta} = -e^{-2i\phi} \Rightarrow e^{i\theta} = \pm ie^{-i\phi}, \quad (59)$$

and $r = \pm i|r|e^{-i\phi}$.

(f) **(2 points)** The phase tells us how the phase of the wavefunction is shifted upon reflection or transmission with respect to the incident wavefunction. In the interference experiment we described in part (a), we get the experimental proof of this effect, and we would obtain a different phase depending on the shape of the potential to which the particle is subject.

Such a phase shift should be familiar from 8.03 where you saw, for example, that a light wave incident on a mirror reflects back with a phase shift of π (i.e. a minus sign). When light bounces off a non-perfect mirror, however, the phase shift is not exactly π , but depends on the detail of the surface.

Problem 5. (25 points) Scattering off an Attractive δ -function Well

- (a) **(4 points)** Our first step is to solve the energy eigenvalue equation for our potential $V(x) = -V_0\delta(x)$. In the regions away from the delta-function well (*i.e.* in all regions but $x = 0$), we have

$$\hat{E}\phi_E(x) = E\phi_E(x) \quad \Rightarrow \quad \frac{d^2\phi_E}{dx^2} = -k^2\phi_E, \quad (60)$$

where $k \equiv \sqrt{2mE}/\hbar$ because we are dealing with the $E > 0$ states. Solving this differential equation allows us to write a general solution for both $x < 0$ and $x > 0$:

$$\phi_E(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & \text{for } x < 0 \\ Ce^{ikx} + De^{-ikx} & \text{for } x > 0 \end{cases} \quad (61)$$

In this problem we are considering a beam of particles incident from the *left*. This means that $D = 0$, since the De^{-ikx} term describes incoming particles from the *right*. To fix the other constants, we require that the wavefunction be continuous at $x = 0$:

$$\phi_E(0^-) = \phi_E(0^+) \quad \Rightarrow \quad A + B = C, \quad (62)$$

and that the *slope* of the wavefunction jumps by the right amount at the δ -function:

$$\left. \frac{d\phi_E}{dx} \right|_{0^+} - \left. \frac{d\phi_E}{dx} \right|_{0^-} = -\frac{2mV_0}{\hbar^2}\psi(0) \quad \Rightarrow \quad ik(C + B - A) = -\frac{2mV_0}{\hbar^2}C. \quad (63)$$

We thus only have two equations for three unknowns (A , B , and C), which means we can solve for B and C in terms of A but not for A , B , and C individually. This is, however, to be expected — recall that the Ae^{ikx} part of the wavefunction represents the incoming beam of particles from the left, while the Be^{-ikx} and Ce^{ikx} pieces represent the reflected and transmitted particles respectively. Since we have not specified the intensity of the incoming beam, A is a free parameter and intuitively we expect that the intensity of the reflected and transmitted beams to be dependent on A . It therefore makes sense that in addition to constants like \hbar^2 , our results for B and C will involve A .

Solving Equations 62 and 63 simultaneously gives

$$\frac{B}{A} = \frac{\frac{imV_0}{\hbar^2 k}}{1 - \frac{imV_0}{\hbar^2 k}} \quad \text{and} \quad \frac{C}{A} = \frac{1}{1 - \frac{imV_0}{\hbar^2 k}}. \quad (64)$$

To find the reflection coefficient R , we need to find the probability current carried by the incoming and reflected waves. Recall that the reflection coefficient is given by

$$R \equiv \frac{\mathcal{J}_{\text{refl.}}}{\mathcal{J}_{\text{inc.}}}, \quad (65)$$

where the probability current is computed in the usual manner:

$$\mathcal{J}(x, t) = \frac{i}{2m} \left(\psi \frac{\partial \psi^*}{\partial x} - \psi^* \frac{\partial \psi}{\partial x} \right). \quad (66)$$

For a generic plane wave $Ge^{\pm ikx}$, we have $\mathcal{J} = \frac{k}{m}|G|^2$. This means that our reflection coefficient becomes

$$R \equiv \frac{\mathcal{J}_{\text{refl.}}}{\mathcal{J}_{\text{inc.}}} = \frac{|B|^2}{|A|^2} = \frac{B^2}{A^2} = \frac{1}{1 + \frac{2k}{mV_0}} = \frac{1}{1 + \frac{2^2 E}{mV_0^2}}, \quad (67)$$

where in the last equality we used the fact that $k \equiv \sqrt{2mE}/\hbar$.

In the limit $V_0 \rightarrow 0$, we expect no reflection, and this borne out by our expression for R : the denominator goes to infinity, and R correspondingly goes to zero. As $E \rightarrow 0$, on the other hand, the incident waves do not have enough energy to transmit across the barrier, as we saw in the finite well, too, so we expect $R \rightarrow 1$, which is precisely what we find.

- (b) **(3 points)** Since the potential is symmetric under reflection and from Eq. (64), the scattering matrix is:

$$S = \begin{pmatrix} \frac{imV_0}{\hbar^2 k} & \frac{1}{1 - \frac{imV_0}{\hbar^2 k}} \\ \frac{1}{1 - \frac{imV_0}{\hbar^2 k}} & \frac{imV_0}{\hbar^2 k} \end{pmatrix}. \quad (68)$$

Verifying that S is Unitary is then a simple matter of taking a transpose, complex conjugating, multiplying and simplifying,

$$\begin{aligned} & \begin{pmatrix} \frac{imV_0}{k^2 \left(1 - \frac{imV_0}{\hbar^2 k}\right)} & \frac{1}{1 - \frac{imV_0}{\hbar^2 k}} \\ \frac{1}{1 - \frac{imV_0}{\hbar^2 k}} & \frac{imV_0}{k^2 \left(1 - \frac{imV_0}{\hbar^2 k}\right)} \end{pmatrix} \cdot \begin{pmatrix} -\frac{imV_0}{k^2 \left(1 + \frac{imV_0}{\hbar^2 k}\right)} & \frac{1}{1 + \frac{imV_0}{\hbar^2 k}} \\ \frac{1}{1 + \frac{imV_0}{\hbar^2 k}} & \frac{-imV_0}{k^2 \left(1 + \frac{imV_0}{\hbar^2 k}\right)} \end{pmatrix} \\ &= \begin{pmatrix} \frac{1}{\left(1 - \frac{imV_0}{\hbar^2 k}\right)\left(1 + \frac{imV_0}{\hbar^2 k}\right)} + \frac{m^2 V_0^2}{k^2 \left(1 - \frac{imV_0}{\hbar^2 k}\right)\left(1 + \frac{imV_0}{\hbar^2 k}\right)} & 0 \\ 0 & \frac{1}{\left(1 - \frac{imV_0}{\hbar^2 k}\right)\left(1 + \frac{imV_0}{\hbar^2 k}\right)} + \frac{m^2 V_0^2}{k^2 \left(1 - \frac{imV_0}{\hbar^2 k}\right)\left(1 + \frac{imV_0}{\hbar^2 k}\right)} \end{pmatrix} \\ &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \end{aligned} \quad (69)$$

In these situations, it is very useful to check your result against Mathematica.

- (c) **(3 points)** From Equation (68) we have

$$t = \frac{1}{1 - \frac{imV_0}{2k}}, \quad (70)$$

thus,

$$\text{Re } t = \frac{1}{1 + \left(\frac{mV_0}{2k}\right)^2}, \quad \text{Im } t = \frac{\frac{mV_0}{2k}}{1 + \left(\frac{mV_0}{2k}\right)^2}, \quad (71)$$

and we obtain

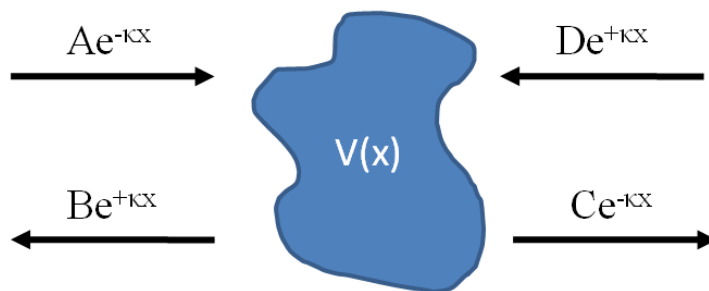
$$\phi = \arctan\left(\frac{\text{Im } t}{\text{Re } t}\right) = \arctan\left(\frac{mV_0}{2k}\right) = \arctan\left(\frac{V_0}{\hbar} \sqrt{\frac{m}{2E}}\right). \quad (72)$$

(d) **(2 points)** S has one pole when $\frac{imV_0}{k} = 1$, or:

$$k = i\sqrt{\frac{-2mE}{2}} = \frac{imV_0}{2} \Rightarrow -\frac{2mE}{2} = \left(\frac{mV_0}{2}\right)^2 \Leftrightarrow E = -\frac{mV_0^2}{2}. \quad (73)$$

This is the same result as the one we obtained the lecture.

(e) **(5 points)** Bound states of localized potentials correspond to energy eigenstates with negative energy, $E < 0$. The wavefunction for such a state is again of the form given at the start of this problem, but with $k = \sqrt{\frac{2m}{2}E} \rightarrow \sqrt{\frac{2m}{2}(-E)} = i\kappa$:



The arrows can now be interpreted as indicating the direction in which the function is exponentially *decaying*.

Now, whatever the energy of the state, the matching conditions satisfied by the wavefunction take the same form (continuity of the wavefunction, continuity of its derivative), so we again have a simple relation between A , B , C and D of the form,

$$\begin{pmatrix} B \\ C \end{pmatrix} = S_b(E) \begin{pmatrix} A \\ D \end{pmatrix}, \quad (74)$$

where $S_b = S|_{\substack{E \rightarrow -E \\ k \rightarrow i\kappa}}$ and we include the argument of $S_b(E)$ to emphasize that the S -matrix depends on the energy E .

Meanwhile, for our bound state to be normalizable, it must be true that $A = 0$ and $D = 0$. Thus the S -matrix equation becomes,

$$\begin{pmatrix} B \\ C \end{pmatrix} = S_b(E) \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \quad (75)$$

Thus the only way to have a non-trivial bound state with energy $E_n < 0$ (which must necessarily have $B, C \neq 0$) is for $S_b(E)$ to diverge at the bound state's energy

$$S_b \sim \frac{1}{E - E_n} \quad (76)$$

Thus the S -matrix must have a pole at every bound state energy,

$$S_b(E) \sim \sum_n \frac{s_n}{E - E_n} + \dots \quad (77)$$

- (f) **(5 points)** The double δ potential splits the problem up into three regions, $x < -L$, $-L < x < L$, and $x > L$. Solving the energy eigenvalue equation in these three regions gives us the form of the wavefunction:

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & \text{for } -\infty < x < -L \\ Fe^{ikx} + Ge^{-ikx} & \text{for } -L < x < L \\ Ce^{ikx} + De^{-ikx} & \text{for } L < x < \infty, \end{cases} \quad (78)$$

where $k \equiv \sqrt{2mE}$. Continuity of the wavefunction requires

$$Ae^{-ikL} + Be^{ikL} = Fe^{-ikL} + Ge^{ikL} \quad \text{and} \quad Fe^{ikL} + Ge^{-ikL} = Ce^{ikL} + De^{-ikL}. \quad (79)$$

The slope, on the other hand, suffers from discontinuities at $x = \pm L$, because of the presence of the delta function wells:

$$\left. \frac{d\psi}{dx} \right|_{a^+} - \left. \frac{d\psi}{dx} \right|_{a^-} = -\frac{2mV_0}{2} \psi(a) \quad (80)$$

This gives

$$ik [(F - A)e^{-ikL} - (G - B)e^{ikL}] = -\frac{2mV_0}{2} (Ae^{-ikL} + Be^{ikL}). \quad (81)$$

and

$$ik [(C - F)e^{ikL} - (D - G)e^{-ikL}] = -\frac{2mV_0}{2} (Ce^{ikL} + De^{-ikL}). \quad (82)$$

We thus have four simultaneous equations and six unknowns. A little algebra (checked against Mathematica) then gives,

$$S = \begin{pmatrix} \frac{e^{2ikL} \left(i \frac{\hbar^2 k}{mV_0} - 1 + e^{-2ikL} \left(i \frac{\hbar^2 k}{mV_0} + 1 \right) \right)}{e^{4ikL} - \left(i \frac{\hbar^2 k}{mV_0} + 1 \right)^2} & \frac{\left(\frac{\hbar^2 k}{mV_0} - 2 \right)}{e^{4ikL} - \left(i \frac{\hbar^2 k}{mV_0} + 1 \right)^2} \\ \frac{\left(\frac{\hbar^2 k}{mV_0} - 2 \right)}{e^{4ikL} - \left(i \frac{\hbar^2 k}{mV_0} + 1 \right)^2} & \frac{e^{2ikL} \left(i \frac{\hbar^2 k}{mV_0} - 1 + e^{-2ikL} \left(i \frac{\hbar^2 k}{mV_0} + 1 \right) \right)}{e^{4ikL} - \left(i \frac{\hbar^2 k}{mV_0} + 1 \right)^2} \end{pmatrix}. \quad (83)$$

Unitarity follows from:

$$S^\dagger S = \begin{pmatrix} \frac{e^{-2ikL} \left(-1 - \frac{ik\hbar^2}{mV_0} + e^{2ikL} \left(1 - \frac{ik\hbar^2}{mV_0} \right) \right)}{e^{4ikL} - \left(1 - \frac{ik\hbar^2}{mV_0} \right)^2} & \frac{k^2 - 4}{m^2 \left(e^{-4ikL} - \left(1 - \frac{ik\hbar^2}{mV_0} \right)^2 V_0^2 \right)} \\ \frac{k^2 - 4}{m^2 \left(e^{-4ikL} - \left(1 - \frac{ik\hbar^2}{mV_0} \right)^2 V_0^2 \right)} & \frac{e^{2ikL} \left(-1 - \frac{ik\hbar^2}{mV_0} + e^{2ikL} \left(1 - \frac{ik\hbar^2}{mV_0} \right) \right)}{e^{-4ikL} - \left(1 - \frac{ik\hbar^2}{mV_0} \right)^2} \end{pmatrix} \\ = \begin{pmatrix} \frac{e^{-2ikL} \left(-1 - \frac{ik\hbar^2}{mV_0} + e^{2ikL} \left(1 - \frac{ik\hbar^2}{mV_0} \right) \right)}{e^{-4ikL} - \left(1 - \frac{ik\hbar^2}{mV_0} \right)^2} & \frac{k^2 - 4}{m^2 \left(e^{-4ikL} - \left(1 - \frac{ik\hbar^2}{mV_0} \right)^2 V_0^2 \right)} \\ \frac{k^2 - 4}{m^2 \left(e^{-4ikL} - \left(1 - \frac{ik\hbar^2}{mV_0} \right)^2 V_0^2 \right)} & \frac{e^{-2ikL} \left(-1 - \frac{ik\hbar^2}{mV_0} + e^{2ikL} \left(1 - \frac{ik\hbar^2}{mV_0} \right) \right)}{e^{-4ikL} - \left(1 - \frac{ik\hbar^2}{mV_0} \right)^2} \end{pmatrix} \\ = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (84)$$

(g) **(3 points)** From the expression (83) we see that the S-matrix has poles when:

$$e^{4ikL} - \left(i \frac{2k}{mV_0} + 1 \right)^2 = 0 \Leftrightarrow e^{2ikL} = \pm \left(i \frac{2k}{mV_0} + 1 \right). \quad (85)$$

Since for bound states $k = i\sqrt{\frac{-2mE}{2}} = i\kappa$, the above expression (85) takes the form:

$$e^{-2\kappa L} = \pm \left(-\frac{2\kappa}{mV_0} + 1 \right) \\ \Rightarrow \tanh(\kappa L) = \frac{1 - e^{-2\kappa L}}{1 + e^{-2\kappa L}} = \frac{1 \mp \left(1 - \frac{2\kappa}{mV_0} \right)}{1 \pm \left(1 - \frac{2\kappa}{mV_0} \right)} = \begin{cases} \left(\frac{2mV_0}{2\kappa} - 1 \right)^{-1} & + \\ \left(\frac{2mV_0}{2\kappa} - 1 \right) & - \end{cases} \quad (86)$$

which are exactly the same results obtained in Problem 4 Pset 6.

(Aside) *It is tempting to guess that S-matrix for the 2-well system is given by the square of that for the 1-well system, $S_2 \stackrel{?}{=} S_1 S_1$. Sadly, this is not the case. However, this is almost true of the M-matrix we defined at the beginning! Recall that M is defined by*

$$\begin{pmatrix} C \\ D \end{pmatrix} = M \begin{pmatrix} A \\ B \end{pmatrix}. \quad (87)$$

For a single δ function at the origin, our results above imply that

$$M_\delta = \frac{1}{4k^2} \begin{pmatrix} 2k + imV_o & imV_o \\ -imV_o & 2k - imV_o \end{pmatrix}. \quad (88)$$

Now, suppose we have two delta functions separated by a width $2L$, as in the problem above. M_δ tells us how the coefficients of the components of the wavefunction change as we step immediately across either δ from left to right. Between the two δ 's, however, both components of the wavefunction pick up additional phases due to the $e^{\pm ikx}$ factors. We can encode this by saying that the change in the coefficients of the two components from the right of the first δ to the left of the right δ is given by the diagonal matrix,

$$M_{2L} = \begin{pmatrix} e^{2ikL} & 0 \\ 0 & e^{-2ikL} \end{pmatrix}. \quad (89)$$

Meanwhile, the coefficients of the two components at the initial delta function are not just A and B , but Ae^{-ikL} and Be^{ikL} ; similarly for C and D .

Putting the pieces together, the change in the coefficients of the two components of the energy eigenstate as we cross from the left of the first δ to the right of the second is given by,

$$M_L \begin{pmatrix} C \\ D \end{pmatrix} = M_\delta M_{2L} M_\delta M_{-L} \begin{pmatrix} A \\ B \end{pmatrix} \quad (90)$$

or, in other words,

$$M_{2\delta} = M_{-L} M_{\delta} M_{2L} M_{\delta} M_{-L} \quad (91)$$

Performing the straightforward matrix multiplication, this gives,

$$M_{2\delta} = \left(\frac{mV_o}{2k} \right)^2 \begin{pmatrix} e^{-4ikL} - \left(i \frac{2k}{mV_o} - 1 \right)^2 & 2i \frac{2k}{mV_o} \cos(2kL) - 2i \sin(2kL) \\ -2i \frac{2k}{mV_o} \cos(2kL) + 2i \sin(2kL) & e^{4ikL} - \left(i \frac{2k}{mV_o} + 1 \right)^2 \end{pmatrix} \quad (92)$$

To compare to our earlier results, we should reorganize this into an S -matrix³. A little more algebra gives,

$$S_{2\delta} = \begin{pmatrix} \frac{e^{2ikL} \left(i \frac{\hbar^2 k}{mV_0} - 1 \right) + e^{-2ikL} \left(i \frac{\hbar^2 k}{mV_0} + 1 \right)}{e^{4ikL} - \left(i \frac{\hbar^2 k}{mV_0} + 1 \right)^2} & \frac{\left(\frac{\hbar^2 k}{mV_0} \right)^2}{e^{4ikL} - \left(i \frac{\hbar^2 k}{mV_0} + 1 \right)^2} \\ \frac{\left(\frac{\hbar^2 k}{mV_0} \right)^2}{e^{4ikL} - \left(i \frac{\hbar^2 k}{mV_0} + 1 \right)^2} & \frac{e^{2ikL} \left(i \frac{\hbar^2 k}{mV_0} - 1 \right) + e^{-2ikL} \left(i \frac{\hbar^2 k}{mV_0} + 1 \right)}{e^{4ikL} - \left(i \frac{\hbar^2 k}{mV_0} + 1 \right)^2} \end{pmatrix}. \quad (93)$$

which is precisely our result by direct analysis. Nice!

³ M and S are both determined from, and faithfully encode, the conditions relating A, B, C and D . Thus, the components of S can always be expressed in terms of the components of M , and vice versa. Indeed, a short bit of algebra gives the explicit map,

$$S = \frac{1}{M_{22}} \begin{pmatrix} -M_{21} & 1 \\ \det M & M_{12} \end{pmatrix}.$$

Similarly, M can be expressed in terms of S as,

$$M = \frac{1}{\tilde{t}} \begin{pmatrix} t\tilde{t} - r\tilde{r} & \tilde{r} \\ -r & 1 \end{pmatrix}.$$

Note that, for a system which respects Parity, and using Unitarity of S , this becomes,

$$M = \begin{pmatrix} \frac{1}{t^*} & \frac{r}{\tilde{t}} \\ \frac{r^*}{t^*} & \frac{1}{\tilde{t}} \end{pmatrix}.$$

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