Quantum Mechanics I

Week 10 (Solutions)

Spring Semester 2025

1 Find the particle...

A. Consider the infinite square well that extends in the interval $0 < x < L$. A particle is in the n-th eigenstate of the Hamiltonian. What is the probability of finding the particle in the region $0 < x < aL$, where the parameter a takes a value in the interval $0 < a < 1$. Compare your results with that in Classical Physics, focusing on larger values of n.

The probability of finding the particle in the region $0 < x < aL$ is simply given by:

$$P_n(a) = \int_0^{aL} dx\, \psi_n^*(x)\psi_n(x)$$

where $\psi_n(x)$ are the wavefunctions of the infinite square well,

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin k_n x, \quad k_n = \frac{n\pi}{L}.$$

We carry out the spatial integral as follows

$$\begin{aligned} P_n(a) &= \frac{2}{L} \int_0^{aL} dx\, \sin^2 k_n x = \\ &= \frac{2}{L} \int_0^{aL} dx \left[\frac{1 - \cos 2k_n x}{2}\right] = \\ &= \frac{2}{L} \left[\frac{1}{2}x - \frac{\sin 2k_n x}{4k_n}\right]_0^{aL} = \\ &= a - \frac{\sin(2n\pi a)}{2n\pi}. \end{aligned}$$

Clearly, when $a = 1$, the probability P_n is equal to one. To provide further insights, we consider the classical analogue of this problem. In classical physics, we would be allowed to specify E since it is just the kinetic energy that the particle has inside the well, and it can be a positive quantity. The particle would just bounce around inside the well without ever changing its speed (assuming the walls were perfectly elastic and there was no friction). Therefore, the probability to find the particle in the interval x and $x + dx$ is constant, and thus

$$P_{cl}(a) = a.$$

We first plot the probability distribution for a few eigenstates of the infinite square well problem in Figure 1. The wavefunctions are presented in alternative units:

$$\tilde{\psi}_n(\tilde{x}) = \sqrt{2} \sin(n\pi\tilde{x})$$

where $\tilde{\psi}_n = \psi_n \sqrt{L}$ and $\tilde{x} = x/L$, such that $\int d\tilde{x}\, \tilde{\psi}_n^2(\tilde{x}) = 1$. As n increases, the number of nodes in the wavefunction increases.

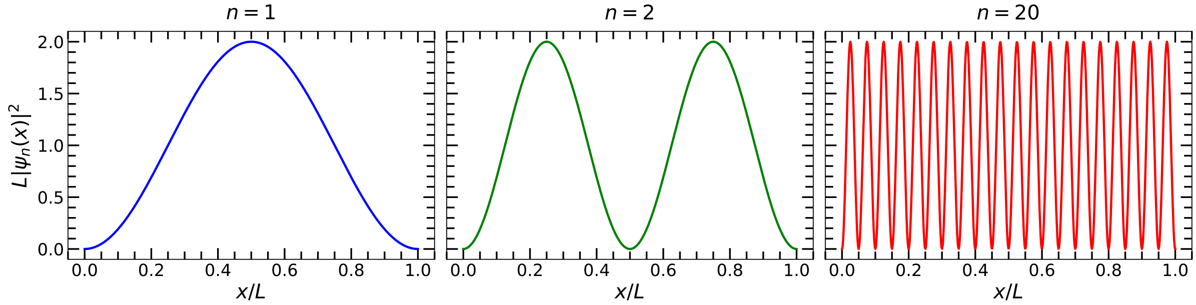

Figure 1: The probability densities of the infinite square well problem for $n = 1$, $n = 2$ and $n = 20$.

We now plot $P_n(a)$ in Figure 2 as a function of a for the eigenstates of the infinite square well we considered above, along with the classical expectation.

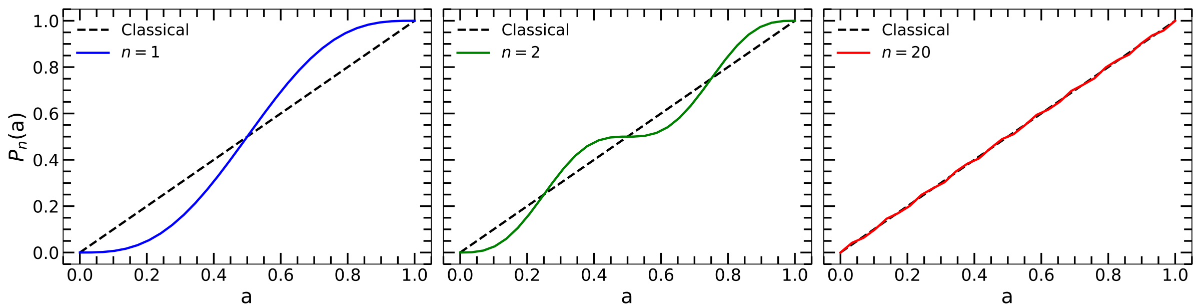

Figure 2: The probability to find the particle within the interval $0 < x < aL$ as a function of the parameter a for $n = 1$, $n = 2$ and $n = 20$.

The probability $P_n(a)$ oscillates around the classical value. In the limit of large n, the amplitude of the oscillations decreases towards zero, and we have:

$$\lim_{n\to\infty} P_n(a) = P_{cl}(a). \tag{1.1}$$

B. For the ground state of the simple harmonic oscillator, calculate the probability that the coordinate x takes a value greater than the amplitude of a classical oscillator of the same energy.

Hint: The following integral may be useful:

$$\frac{1}{\sqrt{\pi}} \int_1^{\infty} e^{-\xi^2}\, d\xi = 0.0785.$$

We first find the classical turning points by considering the total energy of the oscillator,

$$E = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2.$$

The total energy remains constant due to energy conservation, since we consider a lossless system. At the highest points (turning points), the kinetic energy is zero, and thus

$$E = \frac{1}{2} m\omega^2 A^2,$$

where A is the amplitude of the oscillation. By a simple rearrangement, we find:

$$A^2 = \frac{2E}{m\omega^2}.$$

For $n = 0$, $E_0 = \hbar\omega/2$ and thus $A_0 = \sqrt{\hbar/m\omega}$. We will compute the following integral

$$\mathcal{I} = \int_{A_n}^{\infty} dx\, \psi_n^*(x)\psi_n(x),$$

and the final probability will be given by two times this integral, i.e. $P_{ncl} = 2\mathcal{I}$, because the ground state is symmetric with respect to the origin, as evident from:

$$\psi_0(x) = \left(\frac{1}{\ell_0^2 \pi}\right)^{1/4} e^{-x^2/2\ell_0^2}, \quad \ell_0 = \sqrt{\frac{\hbar}{m\omega}}.$$

This is true for any eigenstate since the product $\psi_n^*(x)\psi_n(x)$ is even for any n. For the ground state, the lowering limit of the integral $\mathcal{I}$ is simply $A_0 = \ell_0$, thus:

$$\begin{aligned}
\mathcal{I} &= \sqrt{\frac{1}{\pi\ell_0^2}} \int_{\ell_0}^{\infty} e^{-x^2/\ell_0^2}\, dx \\
&= \sqrt{\frac{1}{\pi\ell_0^2}} \ell_0 \int_1^{\infty} e^{-\xi^2}\, d\xi \\
&= \frac{1}{\sqrt{\pi}} \int_1^{\infty} e^{-\xi^2}\, d\xi. \\
&= 0.0785,
\end{aligned}$$

where in the last equality we used the hint provided. Thus the overall probability to find the particle outside the classical region is $P_{ncl} = 2\mathcal{I} = 0.157$.

C. Consider the problem of the harmonic oscillator and the corresponding wavefunctions:

$$\psi_n(x) = \left(\frac{1}{\pi\ell_0^2}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\xi) e^{-\xi^2/2}$$

where $\ell_0^2 = \hbar/m\omega$ and $\xi = x/\ell_0$, and $H_n(\xi)$ is the Hermite polynomial. Plot the probability density for $n = 5, 20, 100$ on separate diagrams and the corresponding classical probability function. Comment on your results. Hint: Use a software such as Python or Mathematica for the plots.

The probability of finding the oscillator in any spatial interval $[x, x+dx]$ is given by $P(x)dx$. In particular, it is expressed as the ratio of the time taken dt by the oscillator to travel across this interval to the time for one traversal $T/2$, i.e.

$$P(x)dx = \frac{2dt}{T}, \tag{1.2}$$

where T is the period of the oscillation. Using $v = dx/dt$, we write

$$P(x)dx = \frac{2dx}{vT}. \tag{1.3}$$

To find this probability, we need to determine v. The position of the oscillator has the following generic form:

$$x(t) = A\sin(\omega t + \phi),$$

where A, ϕ are determined by some initial conditions. The first derivative with respect to time gives the velocity:

$$v(x) = \pm\omega\sqrt{A^2 - x^2}.$$

Thus, the probability is identified as:

$$P(x) = \frac{2}{vT} = \frac{1}{\pi\sqrt{A^2 - x^2}}.$$

We consider only the positive solution since $P(x)$ will always be positive due to the symmetry of the system. The amplitude A is obtained by considering the total energy of the system at the turning points, i.e. $E = \frac{1}{2}m\omega^2 A^2$, and energy is conserved. Thus, the amplitude is found as:

$$A_n^2 = \frac{2E_n}{m\omega^2}.$$

where E_n are the energies of the (quantum) harmonic oscillator.

Now consider the quantum harmonic oscillator, whose wavefunctions are given

$$\psi_n(x) = \left(\frac{1}{\pi\ell_0^2}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\xi) e^{-\xi^2/2}$$

where $\ell_0^2 = \hbar/m\omega$ and $\xi = x/\ell_0$. The probability density, as usual, is given by the Born rule:

$$P_n(x) = |\psi_n(x)|^2.$$

For the following plots, we consider reduced units. In particular, length is measured in units of ℓ_0, the wavefunction $\psi_n(x)$ becomes $\tilde{\psi}_n(x) = \psi_n(x)\sqrt{\ell_0}$ (in accordance to the normalization condition) and hence $\tilde{P}_n(x) = P_n(x)\ell_0$.

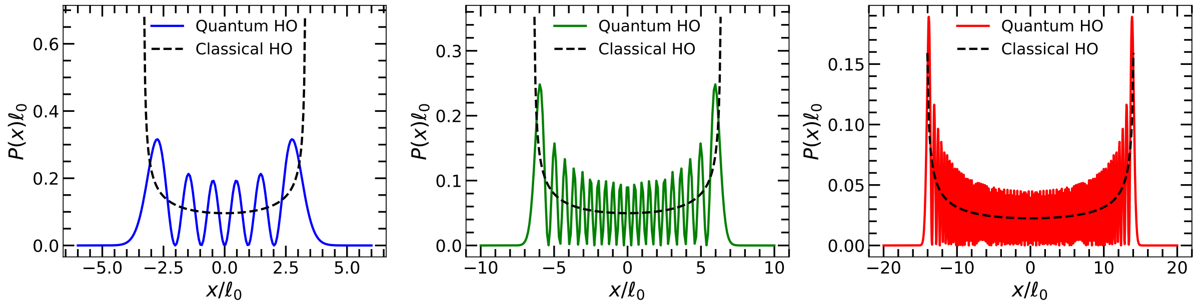

Figure 3: The classical and quantum probability functions for (a) $n = 5$, (b) $n = 20$ and (c) $n = 100$.

The probability to find the particle outside the classical limits is non-zero, and this apparent for the small n case. Also notice that the probability to find the particle within the classical limits vary depending on the number of nodes, while in the classical limit remains roughly uniform (away from the edges). For large n, we observe a resemblance to the classical case. We should emphasize on one important distinction, namely that in the classical case we are talking about the distribution of positions over time for one oscillator while in the quantum case, we are talking about the distribution over an ensemble of identically prepared systems.

2 Current Conservation Implies Unitarity of Transfer Matrix

Consider a step function potential $V(x) = V\,\Theta(x)$ and particles of energy $E > V$ incident on it from both sides simultaneously. The wave function is

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx}, & x < 0 \\ Ce^{iqx} + De^{-iqx}, & x > 0 \end{cases}$$

where $k \equiv \sqrt{2mE/\hbar^2}$ and $q \equiv \sqrt{2m(E-V)/\hbar^2}$.

(a) Determine two relations among the coefficients $A, B, C,$ and D from the continuity of the wave function and of its derivative at the point $x = 0$.

We use the boundary conditions at $x = 0$. From the continuity of the wavefunction, we find:

$$A + B = C + D,$$

while from the continuity of the first derivative, we find:

$$ik(A - B) = iq(C - D).$$

(b) Determine the matrix U defined by the relation

$$\begin{pmatrix} \sqrt{q}\,C \\ \sqrt{k}\,B \end{pmatrix} = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix} \begin{pmatrix} \sqrt{k}\,A \\ \sqrt{q}\,D \end{pmatrix}$$

Show that U is a unitary matrix.

Using the relations we derived from the boundary conditions in the first question, we can show, by simple algebraic manipulation, the following relations:

$$\sqrt{q}\,C = -\left(\frac{1-q/k}{1+q/k}\right)\sqrt{q}\,D + \left(\frac{2\sqrt{q/k}}{1+q/k}\right)\sqrt{k}\,A,$$

$$\sqrt{k}\,B = \left(\frac{2\sqrt{q/k}}{1+q/k}\right)\sqrt{q}\,D + \left(\frac{1-q/k}{1+q/k}\right)\sqrt{k}\,A.$$

In these, we have expressed the amplitudes of the outgoing waves B, C in terms of the incoming ones A, D. Now, from these two relations, we can construct the matrix U:

$$U = \frac{1}{1+q/k}\begin{pmatrix} 2\sqrt{q/k} & -1+q/k \\ 1-q/k & 2\sqrt{q/k} \end{pmatrix}.$$

Unitarity requires $U^\dagger U = \mathbb{1}$, which in terms of the matrix elements, this is shown as follows

$$\begin{pmatrix} U_{11}^* & U_{21}^* \\ U_{12}^* & U_{22}^* \end{pmatrix}\cdot\begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix} = \begin{pmatrix} |U_{11}|^2+|U_{21}|^2 & U_{11}^*U_{12}+U_{21}^*U_{22} \\ U_{12}^*U_{11}+U_{22}^*U_{21} & |U_{12}|^2+|U_{22}|^2 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

and thus,

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

By carrying out the calculations for the unitary matrix of interest, we can easily show that indeed these relations are satisfied and thus U is unitary!

(c) Write down the probability current conservation and show that it is directly related to the unitarity of the matrix U.

The probability current densities in the left-hand region are

$$J_i^{(-)} = \frac{\hbar\,k}{m}\,|A|^2, \qquad J_r^{(-)} = -\,\frac{\hbar\,k}{m}\,|B|^2.$$

where the subscripts i, r denotes incident and reflected waves. Similarly, in the right-hand region, we have

$$J_i^{(+)} = -\,\frac{\hbar\,q}{m}\,|D|^2, \qquad J_r^{(+)} = \frac{\hbar\,q}{m}\,|C|^2.$$

These expressions are shown by considering the definition of the probability current as

$$J = \frac{\hbar}{m} Im\left\{\psi^*\frac{\mathrm{d}\psi}{\mathrm{d}x}\right\}.$$

Current conservation is expressed as

$$J_i^{(-)} + J_r^{(-)} \;=\; J_i^{(+)} + J_r^{(+)},$$

and substituting the current expressions we found earlier for the incident and reflected waves in the two regions (left and right), we find:

$$q\,|C|^2 + k\,|B|^2 \;=\; k\,|A|^2 + q\,|D|^2.$$

Expressing C and B in terms of the matrix U from the previous question, we have:

$$\begin{aligned}q\,|C|^2 + k\,|B|^2 = & \left(|U_{11}|^2 + |U_{21}|^2\right) k\,|A|^2 \;+\; \left(|U_{12}|^2 + |U_{22}|^2\right) q\,|D|^2 + \\ & + \sqrt{k\,q}\,A\,D^*\left(U_{11}^*\,U_{12} + U_{21}\,U_{22}^*\right) \;+\; \sqrt{k\,q}\,A^*\,D\left(U_{11}\,U_{12}^* + U_{22}\,U_{21}^*\right) \\ = & \;\; k\,|A|^2 \;+\; q\,|D|^2,\end{aligned}$$

where we have used

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

This immediately implies the unitarity relations. Thus, current conservation is directly related to the unitarity of U.

(d) Consider the case in which incident particles move only from the left to the right, not from the right to the left (however, reflected particles in the region $x < 0$ will travel from right to left). Use the results found in the previous exercise to calculate the transmitted and reflected currents as a function of the incident current.

In the case in which incident particles are only moving from the left to the right, we must have $D = 0$. The coefficients B and C, then, represent respectively the amplitudes of the reflected beam and of the transmitted beam. If $D = 0$, the continuity equations reduce to

$$\begin{aligned}&A + B = C\ ,\\ &ik(A - B) = iqC\ .\end{aligned} \tag{2.1}$$

The solution is:

$$B = \frac{k-q}{k+q}A\ , \qquad C = \frac{2k}{k+q}A\ . \tag{2.2}$$

Let us now calculate the current propagating in the region $x > 0$. In this region, there are only transmitted particles travelling from the left to the right. The current is

$$\begin{aligned}J_t(x) &= \frac{\hbar}{2mi}\left(\psi^*\frac{d\psi}{dx} - \psi\frac{d\psi^*}{dx}\right)\\ &= \frac{\hbar|C|^2}{2mi}\left(e^{-iqx}\frac{d}{dx}e^{iqx} - e^{iqx}\frac{d}{dx}e^{-iqx}\right)\\ &= \frac{\hbar q|C|^2}{m}\ .\end{aligned} \tag{2.3}$$

This is a particular case of the result found before. The transmitted current is therefore $J_t = \hbar q|C|^2/m$.

The incident current, instead, is

$$J_i = \frac{\hbar k|A|^2}{m}\ . \tag{2.4}$$

Thus the ratio between the transmitted and the incident currents is

$$T = \frac{J_t}{J_i} = \frac{q|C|^2}{k|A|^2} = \frac{4qk^2}{k(k+q)^2} = \frac{4qk}{(k+q)^2} \ . \tag{2.5}$$

This is the "transmission coefficient" across the barrier. For a single incident electron of momentum k, it represents the probability that the electron will pass across the barrier. The reflected current is $|J_r| = \frac{\hbar k|B|^2}{m}$ so the "reflection coefficient" is:

$$R = \frac{|J_r|}{J_i} = \frac{|B|^2}{|A|^2} = \frac{(k-q)^2}{(k+q)^2} \ . \tag{2.6}$$

One can verify that $R+T=1$, which is required by the conservation of probability: $J_i - |J_r| = J_t$.

3 Positive square potential

An electron with energy E collides against a square potential barrier

$$V(x) = \begin{cases} 0 & x < -a \\ V & -a < x < a \\ 0 & x > a \end{cases} , \qquad V > 0 \ . \tag{3.1}$$

Assume that the motion is one-dimensional (only along the x axis) and that the incident electron travels from left to right.

(a) Show that the possible solutions of the time-independent Schrödinger equation in the regions $x < -a$ and $x > a$ are linear combinations of $\psi_{l,r}(x) = e^{\pm ikx}$ and calculate the corresponding momentum k as a function of the energy E. Similarly, write the forms of the stationary-state wavefunctions for $|x| < a$.

The time-independent Schrödinger equation reads:

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) + V(x)\psi(x) = E\psi(x) \ . \tag{3.2}$$

For $x < -a$ and $x > a$, where the potential $V(x)$ is zero, these equations reduce to

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) = E\psi(x) \ . \tag{3.3}$$

The general solution of this equation can be written as a linear combination of $e^{\pm ikx}$ where

$$\frac{\hbar^2 k^2}{2m} = E \ . \tag{3.4}$$

For $|x| < a$, similarly, we have $\psi = e^{\pm iqx}$ where $\hbar^2 q^2/(2m) = (E - V)$. If $V > E$, the solutions for the momenta become imaginary. In this case, the wavefunction can be written as $\psi = e^{\pm|q|x}$ where $\hbar q^2/(2m) = -(E - V)$.

(b) Since for $V > 0$ the potential is repulsive, the potential should not admit any bound states. Show this explicitly by demonstrating that there are no solutions with negative energy to the time-dependent Schrödinger equation. (Use parity to write the solutions as even or odd).

To demonstrate the absence of bound states, suppose that we had a bound-state solution. Then we could write a solution in the form

$$\psi(x) = Z \begin{cases} e^{kx} & x < -a \\ A\cosh(qx) & -a < x < a \\ e^{-kx} & x > a\ , \end{cases} \tag{3.5}$$

for states even under parity, or in the form

$$\psi(x) = Z \begin{cases} -e^{kx} & x < -a \\ A\sinh(qx) & -a < x < a \\ e^{-kx} & x > a \end{cases} . \tag{3.6}$$

Here Z are normalization factors needed to make $\int_{\infty}^{\infty} |\psi|^2 = 1$.

The continuity conditions on the wavefunctions and its derivative imply

$$\begin{cases} e^{-ka} = A\cosh(qa) \\ -ke^{-ka} = Aq\sinh(qa) \end{cases} , \qquad \begin{cases} e^{-ka} = A\sinh(qa) \\ -ke^{-ka} = Aq\cosh(qa) \end{cases} , \tag{3.7}$$

for even and off wavefunctions respectively. Taking the ratio of these equations gives however $q\tanh(qa) = -k$ and $q/\tanh(qa) = -k$. The equations have no solutions because $q\tanh(qa)$ and $q/\tanh(qa)$ are always positive, whereas $-k$ is always negative.

(c) Consider an electron incident from the left to the right. Show that the electron has a nonzero probability of being transmitted across the barrier even if its energy is smaller than V ($E < V$) (the "tunnel" effect). Calculate the transmission probability as a function of E and V. Hint: For $E < V$ the wavefunction in the region $|x| < a$ is of the form $Ae^{-qx} + Be^{qx}$. In the final result, analyze the limit in which the potential barrier is very wide.

The full wavefunction can be taken in the form

$$\psi(x) = Z \begin{cases} e^{ikx} + re^{-ikx} & x < -a \\ Ae^{-qx} + Be^{qx} & |x| < a \\ te^{ikx} & x > a \end{cases} , \tag{3.8}$$

with Z a normalization factor. The coefficients r, A, B, and t have to be determined from the condition that the wavefunction and its derivative are continuous at the interfaces $x = -a$ and $x = a$. q and k are related to the total energy E via $E = \hbar^2 k^2/(2m)$ and $E = -\hbar^2 q^2/(2m) + V$.

At $x = -a$ we find

$$\begin{cases} e^{-ika} + re^{ika} = Ae^{qa} + Be^{-qa} \\ ik(e^{-ika} - re^{ika}) = -q(Ae^{qa} - Be^{-qa}) \ . \end{cases} \tag{3.9}$$

At $x = a$ we find instead:

$$\begin{cases} te^{ika} = Ae^{-qa} + Be^{qa} \\ ikte^{ika} = -q(Ae^{-qa} - Be^{qa}) \end{cases} . \tag{3.10}$$

From the second set of relations we get

$$Ae^{-qa} = \frac{1}{2}\left(1 - \frac{ik}{q}\right) te^{ika} , \qquad Be^{qa} = \frac{1}{2}\left(1 + \frac{ik}{q}\right) te^{ika} . \tag{3.11}$$

Substituting in the first set of equations we find:

$$\begin{cases} e^{-ika} + re^{ika} = \frac{1}{2}\left(1 - \frac{ik}{q}\right) te^{ika+2qa} + \frac{1}{2}\left(1 - \frac{ik}{q}\right) te^{ika-2qa} \\ ik\left(e^{-ika} - re^{ika}\right) = -\frac{1}{2}(q - ik)te^{ika+2qa} + \frac{1}{2}(q + ik)te^{ika-2qa} . \end{cases} \tag{3.12}$$

Combining the two relations gives

$$\begin{aligned} e^{-ika} = \frac{1}{4}\Bigg[& \left(1 - \frac{ik}{q}\right) e^{ika+2qa} + \left(1 - \frac{ik}{q}\right) e^{ika-2qa} \\ & + \left(1 + \frac{iq}{k}\right) e^{ika+2qa} - \left(1 - \frac{iq}{k}\right) e^{ika-2qa} \Bigg] t , \end{aligned} \tag{3.13}$$

or equivalently

$$e^{-2ika} = \frac{1}{4}\left[\left(2 + \frac{iq}{k} - \frac{ik}{q}\right) e^{2qa} + \left(2 + \frac{iq}{k} - \frac{ik}{q}\right) e^{-2qa}\right] t . \tag{3.14}$$

The transmission coefficient, determining the ratio between the transmitted and the incident current, is

$$T = |t|^2 = \left| \frac{4}{\left(2 + \frac{iq}{k} - \frac{ik}{q}\right) e^{2qa} + \left(2 + \frac{iq}{k} - \frac{ik}{q}\right) e^{-2qa}} \right|^2 . \tag{3.15}$$

When the barrier is very wide we can neglect the term proportional to e^{-2qa} in comparison with that proportional to e^{2qa}. We then obtain

$$\begin{aligned} T &= \frac{16e^{-4qa}}{\left|2 + \frac{iq}{k} - \frac{ik}{q}\right|^2} = \frac{16q^2k^2e^{-4qa}}{4k^2q^2 + (q^2 - k^2)^2} = \frac{16q^2k^2e^{-4qa}}{(q^2 + k^2)^2} \\ &= \frac{16E(V - E)}{V^2} e^{-4qa} . \end{aligned} \tag{3.16}$$

The tunneling probability is exponentially small for large a, but is never exactly zero. There is always a finite probability that the electron passes through the barrier, despite $E < V$.

4 The Double-Delta potential

Consider a potential consisting of two delta functions:

$$V(x) = \frac{\hbar^2 g_1}{2m}\,\delta(x+a) + \frac{\hbar^2 g_2}{2m}\,\delta(x-a). \tag{4.1}$$

where g_1, g_2 are constants.

In this problem, we will consider the two boundary conditions at $x = \pm a$, namely the continuity of the wavefunction and the first derivative. However, because the potential is singular at these points, the first derivative is not continuous, and an additional term arises. The discontinuity condition reads:

$$\psi'(x_0+\epsilon) - \psi'(x_0-\epsilon) = \frac{2m}{\hbar^2}\int_{x_0-\epsilon}^{x_0+\epsilon} V(x)\,\psi(x)\,dx. \tag{4.2}$$

and it was derived in the lecture. Here, x_0 is the point at which the potential becomes singular and $\epsilon > 0$ is a very small quantity.

(a) Find the bound-state spectrum in the case $g_1 = g_2 < 0$. *Hint: Since the potential is even, look for even and odd solutions.*

In the case of equal (attractive) couplings, i.e. $g_1 = g_2 \equiv -g^2 < 0$, the system is parity-even and we can exploit this symmetry to look for even and odd solutions.

An even candidate wave function is ($E = -\hbar^2 k^2/(2m)$),

$$\psi_+(x) = \begin{cases} A\,e^{k\,x}, & x < -a, \\ B\,\cosh\big(k\,x\big), & -a < x < a, \\ A\,e^{-k\,x}, & x > a, \end{cases}$$

where we have chosen the hyperbolic cosine function which is an even function with respect to the origin. From the continuity and discontinuity conditions, we obtain:

$$B = \frac{A\,e^{-k\,a}}{\cosh\big(k\,a\big)}, \quad 1 + \tanh\big(k\,a\big) = \frac{g^2\,a}{k\,a}. \tag{4.3}$$

In Figure 4, we plot the left- and right-hand sides of the second condition. We can read off that there is always one (even) solution. We can also verify the intersection (of the LHS and RHS functions) from the two limiting cases of each side:

$$\lim_{ka\to 0} \text{LHS} = 1, \quad \lim_{ka\to\infty} \text{LHS} = 2$$

and

$$\lim_{ka\to 0} \text{RHS} = \infty, \quad \lim_{ka\to\infty} \text{RHS} = 0.$$

For low ka the RHS is greater, while for larger ka the LHS is. Thus, we must expect that the two curves will intersect no matter the value of $g^2 a$.

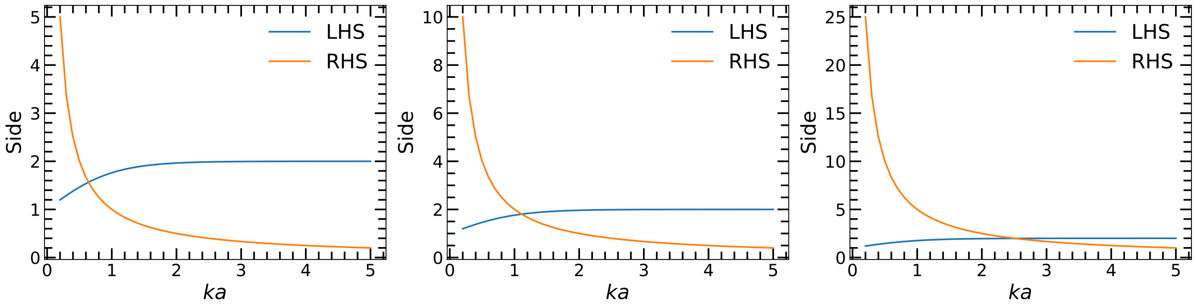

Figure 4: Solutions for even bound states for (a) $g^2a = 1$, (b) $g^2a = 2$ and (c) $g^2a = 5$.

An odd candidate wave function is

$$\psi_-(x) = \begin{cases} -A\,e^{k\,x}, & x < -a, \\ B\,\sinh\big(k\,x\big), & -a < x < a, \\ A\,e^{-k\,x}, & x > a, \end{cases}$$

where now we have chosen the hyperbolic sine function which has odd parity. From the continuity and discontinuity conditions, we obtain:

$$B = \frac{A\,e^{-k\,a}}{\sinh\big(k\,a\big)}, \quad 1 + \coth\big(k\,a\big) = \frac{g^2\,a}{k\,a}. \tag{4.4}$$

The graphical solution of the last condition is given in Figure 5. It is clear that an odd solution does not always exist. In order to guarantee the presence of a bound state with odd-parity wave function we need a strong enough attractive coupling. It can be seen from the plot that $g^2 > 1/a$ is required.

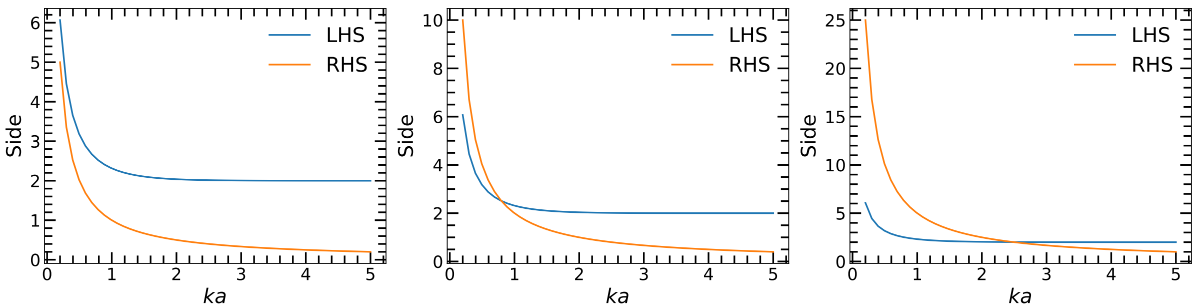

Figure 5: Solutions for odd bound states for (a) $g^2a = 1$, (b) $g^2a = 2$ and (c) $g^2a = 5$.

We cannot tell from the limiting cases of $ka \to 0$ and $ka \to \infty$ whether they will cross or not, since for the former limit, both functions tend to infinity. However, the possibility of intersection will be dictated by the value of g^2a of the RHS. It must be large enough so that it will decay slower than the LHS, and thus achieve an intersection.

(b) Do the same in the case of $g_1 = -g_2 > 0$.

This choice of parameters correspond to an asymmetric potential

$$V(x) = \frac{g^2 \hbar^2}{2m} \left[\delta(x+a) \; - \; \delta(x-a)\right].$$

The candidate bound-state wave function is:

$$\psi(x) = \begin{cases} A\, e^{k\,x}, & x < -a, \\ B\, e^{k\,x} + C\, e^{-k\,x}, & -a < x < a, \\ D\, e^{-k\,x}, & x > a, \end{cases} \tag{4.5}$$

Solving the algebraic system from the continuity and discontinuity conditions at $x = \pm a$, we get the energy eigenvalue condition

$$e^{4\,k\,a} = \frac{g^4}{g^4 - 4\,k^2}.$$

which, in terms of $\xi \equiv \; k\,a$ and $\lambda^2 \equiv g^4\,a^2$, is

$$e^{4\xi} \;=\; \frac{1}{1 - 4\xi^2/\lambda^2}, \tag{4.6}$$

and can be solved graphically as in the previous cases to show that one bound state exists. We demonstrate this one solution in Figure 6 by plotting the LHS and RHS of Eq. (4.6).

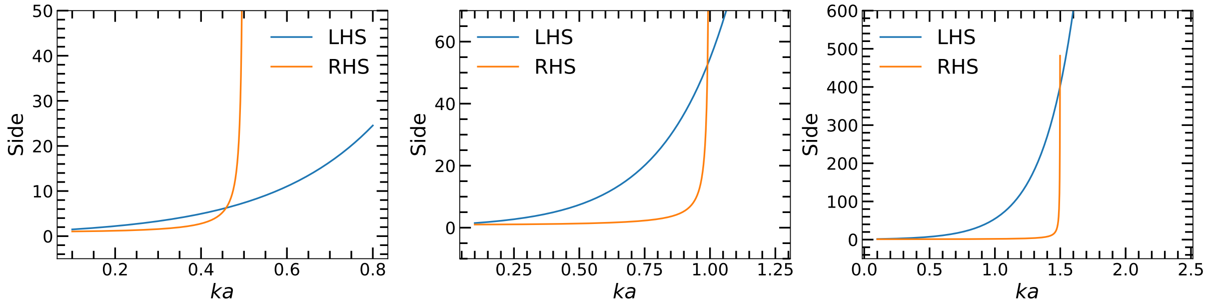

Figure 6: Bound state solutions to the asymmetric potential for (a) $g^2 a = 1$, (b) $g^2 a = 2$ and (c) $g^2 a = 3$. Only one of the two branches of the RHS of Eq. (4.6) is shown.

(c) Let us now look for scattering states. Consider the incidence (from the left hand side) of particles of energy $E > 0$ at this potential. Show that the transmission coefficient for arbitrary g_1, g_2 is:

$$\mathcal{T} = |F|^2 = \left\{ \left[1 - \frac{g_1 g_2}{4\,k^2}\left(1 - \cos(4\,k\,a)\right)\right]^2 + \left(\frac{g_1 g_2}{4\,k^2}\sin(4\,k\,a) + \frac{g_1+g_2}{2\,k}\right)^2 \right\}^{-1}. \tag{4.7}$$

The wave function will be

$$\psi(x) = \begin{cases} e^{ikx} + B\,e^{-\,ikx}, & x < -\,a, \\ C\,e^{ikx} + D\,e^{-\,ikx}, & -\,a < x < a, \\ F\,e^{ikx}, & x > a, \end{cases} \tag{4.8}$$

We consider now the boundary conditions at $x = -a, x = a$. First, we start by considering the continuity of the wavefunction at $x = -a$, from which we find

$$\mu^{-1} + \mu B = C\mu^{-1} + D\mu \tag{4.9}$$

where $\mu = e^{ika}$. We also impose the same condition at $x = a$ and find:

$$F\mu = C\,\mu + D\mu^{-1}. \tag{4.10}$$

We move on by considering the discontinuity equation at the two singular points:

$$\psi'(\,\pm a + \epsilon\,)\;-\;\psi'(\,\pm a - \epsilon\,)\;=\;g_{2,1}\,\psi(\pm a). \tag{4.11}$$

Thus, for the wavefunction of Eq. (4.8), the discontinuity condition at $x = -a$ gives:

$$i\,k\,F\,\mu\;-\;i\,k\,C\,\mu + i\,k\,D\,\mu^{-1}\;=\;g_2\,F\,\mu \tag{4.12}$$

while the one at $x = a$ gives:

$$i\,k\,C\,\mu^{-1}\;-\;i\,k\,D\;-\;i\,k\,\mu^{-1} + i\,k\,B\,\mu\;=\;g_1\big(\mu^{-1} + \mu\,B\big). \tag{4.13}$$

From Eqs. (4.10) and (4.12), we obtain:

$$F\;=\;D\Big(\tfrac{2\,i\,k}{g_2}\Big)\,\mu^{-2},\quad C\;=\;i\,\mu^{-2}\left(\tfrac{2\,k + i\,g_2}{g_2}\right)D \tag{4.14}$$

Canceling B from the other two conditions, i.e. Eqs. (4.9) and (4.13), we find for the coefficient D:

$$D\;=\;-\,2\,i\,\mu^{-2}\,\frac{g_2\,k}{g_1 g_2\,\mu^4\;+\;(2\,k + i\,g_1)(2\,k + i\,g_2)} \tag{4.15}$$

and finally for F we find:

$$F\;=\;\frac{4\,k^2}{\mu^4\,g_1 g_2\;+\;(2\,k + i\,g_1)(2\,k + i\,g_2)}. \tag{4.16}$$

The resulting transmission coefficient is

$$\mathcal{T} = |F|^2 = \left\{\left[1 - \frac{g_1 g_2}{4\,k^2}\big(1 - \cos(4\,k\,a)\big)\right]^2 + \left(\frac{g_1 g_2}{4\,k^2}\sin(4\,k\,a) + \frac{g_1 + g_2}{2\,k}\right)^2\right\}^{-1}. \tag{4.17}$$

(d) Consider the case $g_1 = -g_2$ and show that there exist special values of the energy for which transmission is perfect and there is no reflection.

In the case $g_1 = -\, g_2 \equiv g$, the transmission coefficient simplifies to:

$$\mathcal{T} = \left\{ \left[1 + \frac{g^2}{4\,k^2} \big(1 - \cos(4\,k\,a)\big) \right]^2 + \frac{g^4}{16\,k^4} \sin^2\!\big(4\,k\,a\big) \right\}^{-1} .$$

It is obvious that for $4ka = 2n\pi$ the transmission is perfect, i.e.

$$E_n = \frac{\hbar^2\, n^2\, \pi^2}{8\,m\,a^2} \quad (n = 1, 2, \dots) \quad \Longrightarrow \quad T = 1, \quad R = 0.$$

In Figure 7, the transmission is plotted as a function of ka for $\lambda_1 = g_1 a = 1$ and $\lambda_2 = g_2 a = -1$. The first three solutions for perfect transmission are shown, and these correspond to $ka = \pi/2, \pi, 3\pi/2$.

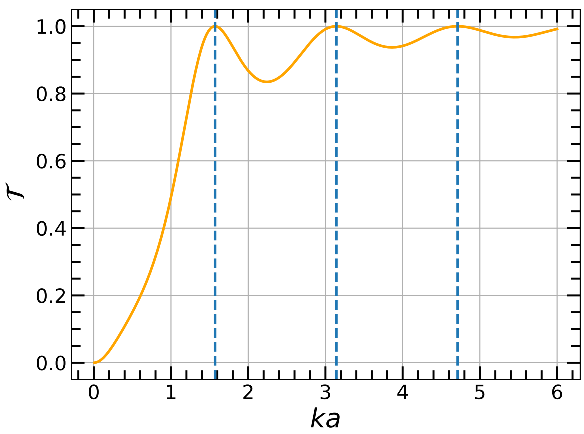

Figure 7: The transmission as a function of ka for $\lambda_1 = -\lambda_2 = 1$ (orange solid line), with the first three solutions (blue dashed lines) for perfect transmission.

(e) Compare the low-energy behavior ($E \to 0$) and high-energy behavior ($E \to \infty$) in the three cases $g_1 = g_2$, $g_1 = -g_2$ and $g_1 \neq 0, g_2 = 0$.

The qualitative behavior in all these three cases is the same. In detail, we have the following results:

- For the case $g_1 = g_2 \equiv g$:

$$\lim_{k \to 0} \{T\} \sim \frac{k^2}{g^2 \big(1 + a\, g^2\big)}, \qquad \lim_{k \to \infty} \{T\} \sim 1 - \frac{g^2}{k^2} \cos^2(2\,k\,a).$$

- For the case $g_1 = -\, g_2 \equiv g$:

$$\lim_{k \to 0} \{T\} \sim \frac{k^2}{g^4\, a^2}, \qquad \lim_{k \to \infty} \{T\} \sim 1 - \frac{g^2}{k^2} \sin^2(2\,k\,a).$$

- For the case $g_1 \equiv g \neq 0,\ g_2 = 0$,

$$\lim_{k\to 0}\{T\} \sim \frac{4\,k^2}{g^2}, \quad \lim_{k\to\infty}\{T\} \sim 1 - \frac{g^2}{4\,k^2}.$$

In all of these cases, the transmission scales with the second power of k (with different coefficients) for low k. On the other hand, in the high-k limit, the transmission approaches unity, but in a different fashion for each of the three cases. A highly energetic electron, incident from the left, will have a high transmission probability.

In Figure 8, we visualize the three cases we examined above, and in which clearly we can see their respective limits for low and high ka. The parameters λ_1, λ_2 are defined as:

$$\lambda_1 = g_1 a, \quad \lambda_2 = g_2 a.$$

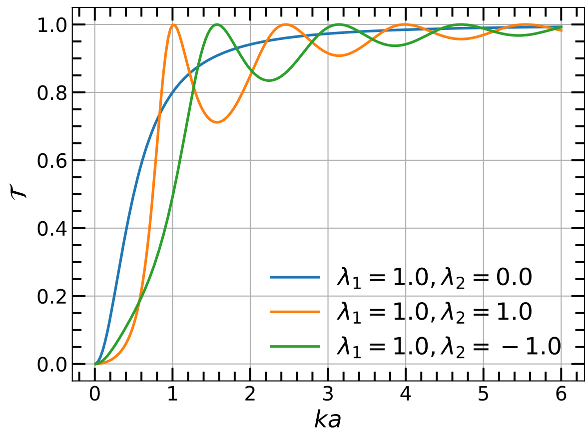

Figure 8: The transmission as a function of ka for different pair of values for (λ_1, λ_2).