# Quantum Mechanics

## Solutions to the Problems in Homework Assignment 04

### Fall, 2019

1. **[C-T Exercise 1-7]** Consider a particle of mass $m$ placed in the one-dimensional potential

$$V(x) = \begin{cases} \infty, & x < 0, \\ -V_0, & 0 \le x < a, \\ 0, & x \ge a. \end{cases}$$

Let $\varphi(x)$ be a wave function associated with a stationary state of the particle.

(a) Show that $\varphi(x)$ can be extended to give an odd wave function which corresponds to a stationary state for a square well of width $2a$ and depth $V_0$.

(b) Discuss, with respect to $a$ and $V_0$, the number of bound states of the particle. Is there always at least one such state as for the symmetric square well?

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The potential is depicted in Fig. 1.

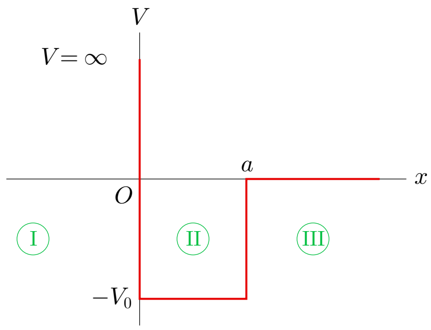


FIG. 1: One-dimensional square potential well in half space.

The jumps in the potential divide the one-dimensional space into three regions. Region I is for $x \le 0$; region II is for $0 < x < a$; region III is for $x \ge a$. Because the potential in infinite in region I, the wave function of a stationary state is identically zero in this region, $\varphi_{\rm I}(x) = 0$.

Here we only consider bound states. The stationary Schrödinger equations for bound states in the regions II and III are respectively given by

$$\frac{d^2\varphi_{\rm II}(x)}{dx^2} + k^2\varphi_{\rm II}(x) = 0,$$
$$\frac{d^2\varphi_{\rm III}(x)}{dx^2} - \kappa^2\varphi_{\rm III}(x) = 0,$$

where

$$k = \sqrt{\frac{2m(V_0+E)}{\hbar^2}}, \quad \kappa = \sqrt{-\frac{2mE}{\hbar^2}}$$

with $-V_0 < E < 0$.

The general solutions to the above two equations are respectively given by

$$\varphi_{\rm II}(x) = A\sin(kx) + B\cos(kx),$$
$$\varphi_{\rm III}(x) = Ce^{-\kappa x} + De^{\kappa x}.$$

The boundary condition at $x = 0$ is given by $\varphi_{\mathrm{II}}(0) = 0$. The boundary condition at $x = \infty$ is given by $\varphi_{\mathrm{III}}(x \to \infty) = 0$. The matching conditions at $x = a$ are given by

$$\varphi_{\mathrm{II}}(a) = \varphi_{\mathrm{III}}(a),$$
$$\varphi'_{\mathrm{II}}(a) = \varphi'_{\mathrm{III}}(a).$$

From $\varphi_{\mathrm{II}}(0) = 0$, we have $B = 0$. From $\varphi_{\mathrm{III}}(x \to \infty) = 0$, we have $D = 0$. The expressions for the bound-state wave functions then become

$$\varphi_{\mathrm{II}}(x) = A\sin(kx),$$
$$\varphi_{\mathrm{III}}(x) = Ce^{-\kappa x}.$$

Inserting the above bound-state wave functions into the matching conditions at $x = a$, we have

$$\sin(ka)A - e^{-\kappa a}C = 0,$$
$$k\cos(ka)A + \kappa e^{-\kappa a}C = 0.$$

The above two equations are homogeneous linear algebraic equations for $A$ and $C$. The necessary and sufficient condition for the existence of nontrivial solutions is that the determinant of the coefficients vanishes. From this condition, we obtain

$$\begin{vmatrix} \sin(ka) & -e^{-\kappa a} \\ k\cos(ka) & \kappa e^{-\kappa a} \end{vmatrix} = 0$$

from which the secular equation follows

$$\tan(ka) = -k/\kappa.$$

(a) Comparing the above-obtained secular equation for the present problem, $\tan(ka) = -k/\kappa$, with the secular equation $\tan\bigl(ka/2\bigr) = -k/\kappa$ for the bound states with odd wave functions in the problem of a symmetric square well about $x = 0$ of width $a$, we see that, if the wave function of a bound state is extended to give an odd wave function, we will obtain the wave function of a bound state with an odd wave function for a square well of width $2a$ and depth $V_0$.
That this can be done is because the wave function in the present problem vanishes at $x = 0$ so that the extension to an odd wave function can be achieved.

(b) To see how the number of bound states varies with $a$ and $V_0$, we rewrite the secular equation in the form

$$|\sin(ka)| = k/k_0 \text{ with } \tan(ka) < 0.$$

Here $k_0 = \sqrt{2mV_0/\hbar^2}$. The functions $|\sin(ka)|$ with $\tan(ka) < 0$ and $k/k_0$ are plotted in Fig. 2.

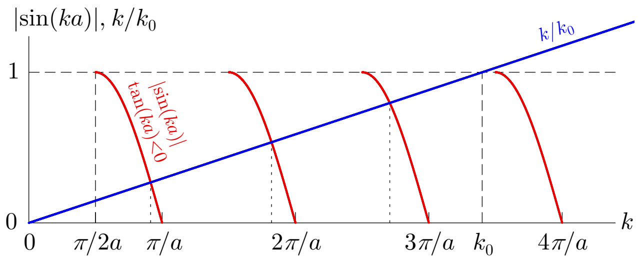


FIG. 2: Graphical solution of $|\sin(ka)| = \dfrac{k}{k_0}$ with $\tan(ka) < 0$.

The solutions to the secular equation are given by the intersections of the two curves in Fig. 2 from which we see that, at a fixed value of $V_0$, the number of bound states increases as $a$ increases as long as $V_0 \geq \dfrac{\pi^2\hbar^2}{8ma^2}$.
We can also see that, at a fixed value of $a$, the number of bound states increases as $V_0$ increases for $V_0 \geq \dfrac{\pi^2\hbar^2}{8ma^2}$.
From Fig. 2, we see that the two curves do not intersect if $k_0 < \pi/2a$. Thus, no bound states exist for the particle if $V_0 < \dfrac{\pi^2\hbar^2}{8ma^2}$.

2. Consider a particle of mass $m$ placed in the one-dimensional potential

$$V(x) = \begin{cases} \lambda\delta(x), & |x| < a, \\ \infty, & |x| \geq a. \end{cases}$$

Here $\lambda > 0$. Find the energies and wave functions of the stationary states for the particle. The wave functions are not required to be normalized.

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The potential is depicted in Fig. 3.

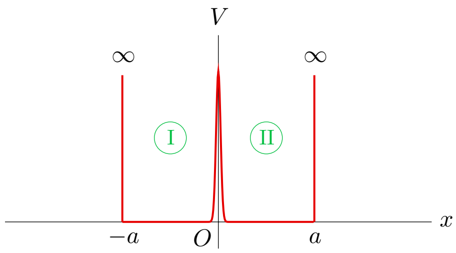


FIG. 3: One-dimensional square potential well of infinite depth with a $\delta$-function potential barrier at the center.

Because $V(x) = \infty$ for $|x| \geq a$, the wave function of a stationary state of the particle is identically zero for $|x| \geq a$. We therefore concentrate on the solution of the stationary Schrödinger equation in regions I and II indicated in Fig. 3. The stationary Schrödinger equation reads in these two regions

$$\frac{d^2\varphi_{\mathrm{I}}(x)}{dx^2} + k^2\varphi_{\mathrm{I}}(x) = 0,$$
$$\frac{d^2\varphi_{\mathrm{II}}(x)}{dx^2} + k^2\varphi_{\mathrm{II}}(x) = 0,$$

where $k = \sqrt{2mE/\hbar^2}$. The general solutions to the above two equations are given by

$$\varphi_{\mathrm{I}}(x) = A\sin(kx) + B\cos(kx),$$
$$\varphi_{\mathrm{II}}(x) = C\sin(kx) + D\cos(kx).$$

From the boundary condition $\varphi_{\mathrm{I}}(-a) = 0$, we have

$$-A\sin(ka) + B\cos(ka) = 0.$$

From the boundary condition $\varphi_{\mathrm{II}}(a) = 0$, we have

$$C\sin(ka) + D\cos(ka) = 0.$$

From the matching conditions at $x = 0$,

$$\varphi_{\mathrm{I}}(0) = \varphi_{\mathrm{II}}(0),$$
$$\varphi'_{\mathrm{II}}(0) - \varphi'_{\mathrm{I}}(0) = \frac{2m\lambda}{\hbar^2}\varphi_{\mathrm{I}}(0),$$

we have

$$B = D,$$
$$kC - kA = \frac{2m\lambda}{\hbar^2}B.$$

Collecting the above-obtained equations from the boundary and matching conditions, we have

$$\begin{aligned} -\sin(ka)A \;+\; & \cos(ka)B & & = 0, \\ & \cos(ka)B \;+\; \sin(ka)C & & = 0, \\ -kA \;-\; & (2m\lambda/\hbar^2)B \;+\; kC & & = 0, \end{aligned}$$

where $D = B$ has been used. The above equations constitute a set of homogeneous linear algebraic equations for $A$, $B$, and $C$. The condition for the existence of nontrivial solutions is that the determinant of the coefficients vanishes. We have

$$\begin{vmatrix} -\sin(ka) & \cos(ka) & 0 \\ 0 & \cos(ka) & \sin(ka) \\ 1 & 2m\lambda/\hbar^2 k & -1 \end{vmatrix} = 0.$$

Evaluating the determinant, we obtain

$$\sin(ka)\left[\cos(ka) + \frac{m\lambda}{\hbar^2 k}\sin(ka)\right] = 0$$

from which it follows that

$$\sin(ka) = 0 \text{ or } \tan(ka) = -\frac{\hbar^2 k}{m\lambda}.$$

We thus have two sets of energy eigenvalues. In the following, we separately discuss these two sets of energy eigenvalues as well as the corresponding energy eigenfunctions.

**Case** $\sin(ka) = 0$.

From $\sin(ka) = 0$, we have

$$k_n = \frac{n\pi}{a},\ n = 0, \pm 1, \pm 2, \pm 3, \cdots.$$

Whether or not all the values of $n = 0, \pm 1, \pm 2, \pm 3, \cdots$ are allowed will be clear after we have obtained the corresponding energy eigenfunctions. For $\sin(k_n a) = 0$, from the equations for $A$, $B$, and $C$, we obtain $D = B = 0$ and $C = A$. The energy eigenfunctions in the two regions are of the same form in this case and are given by

$$\varphi_n(x) = A\sin(k_n x) = A\sin\left(\frac{n\pi x}{a}\right),\ -a < x < a.$$

For $n = 0$, $\varphi_{n=0}(x) \equiv 0$, which is physically unacceptable. Thus, $n = 0$ is not allowed. For negative values of $n$, the energy eigenfunctions are negatives of those for positive values of $n$ and are thus not independent solutions. Therefore, the allowed values of $n$ are $1, 2, 3, \cdots$. The energy eigenvalues are then given by

$$E_n = \frac{\hbar^2 k^2}{2m} = \frac{n^2\pi^2\hbar^2}{2ma^2},\ n = 1, 2, 3, \cdots.$$

The normalization constants of the energy eigenfunctions can be evaluated as follows

$$1 = \int_{-a}^{a} dx\ |\varphi_n(x)|^2 = |A|^2 \int_{-a}^{a} dx\ \sin^2\left(\frac{n\pi x}{a}\right) = a|A|^2.$$

Thus, $|A| = 1/\sqrt{a}$. We choose $A = 1/\sqrt{a}$. The normalized energy eigenfunctions are then given by

$$\varphi_n(x) = \frac{1}{\sqrt{a}}\sin\left(\frac{n\pi x}{a}\right),\ -a < x < a,\ n = 1, 2, 3, \cdots.$$

Note that the energy eigenfunctions in this case possess a definite parity (the odd parity). This is because the energy eigenfunctions in a symmetric potential with respect to the origin possess a definite parity (either an odd parity or an even parity). The energy eigenvalues and eigenfunctions in this case are identical with those of odd parity for a particle in a symmetric infinite-depth square potential well of width $2a$. This is due to the fact that the $\delta$-function at $x = 0$ does not affect the eigenstates of odd parity because the eigenfunctions vanish at $x = 0$. From these discussions, we expect that the energy eigenfunctions in the other case possess an even parity.

**Case** $\tan(ka) = -\dfrac{\hbar^2 k}{m\lambda}$.

For $\tan(ka) = -\dfrac{\hbar^2 k}{m\lambda}$, from the equations for $A$, $B$, and $C$, we obtain

$$A = -C,$$
$$D = B = \frac{\hbar^2 k}{m\lambda}C.$$

The energy eigenfunctions in this case are given by

$$\varphi(x) = \begin{cases} C\left[-\sin(kx) + \dfrac{\hbar^2 k}{m\lambda}\cos(kx)\right], & -a < x < 0, \\ C\left[\sin(kx) + \dfrac{\hbar^2 k}{m\lambda}\cos(kx)\right], & 0 < x < a. \end{cases}$$

Thus, the energy eigenfunctions in this case are indeed even functions. The energy eigenvalues in this case can be solved from $\tan(ka) = -\dfrac{\hbar^2 k}{m\lambda}$ by a graphical or numerical method. Introducing the variable $\xi = ka$ and the parameter $\alpha = \dfrac{\hbar^2}{m\lambda a}$, we can cast the equation $\tan(ka) = -\dfrac{\hbar^2 k}{m\lambda}$ into the following form

$$\tan(\xi) = -\alpha\xi.$$

The graphical solution of the above equation is given in Fig. 4 for $\alpha = \dfrac{1}{4}$.

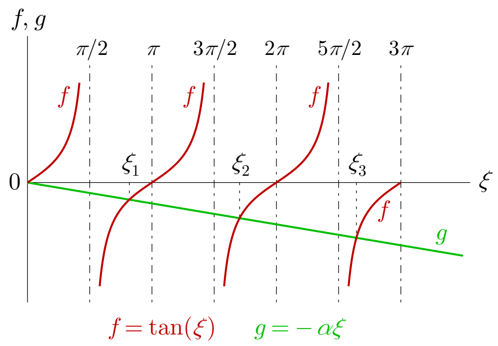


FIG. 4: Graphical solution of the equation $\tan(\xi) = -\alpha\xi$ for $\alpha = \dfrac{1}{4}$.

The solutions to the equation $\tan(\xi) = -\alpha\xi$ are given by the intersections of the curve $f(\xi) = \tan(\xi)$ and the straight line $g(\xi) = -\alpha\xi$ excluding the intersection at $\xi = 0$ because $\xi = ka$ is greater than zero. For $k = 0$, the energy eigenfunction is identically zero, which is physically unacceptable. The displayed intersections of $f(\xi) = \tan(\xi)$ and $g(\xi) = -\alpha\xi$ are indicated with vertical dotted lines and labeled with $\xi_1$, $\xi_2$, and $\xi_3$ in Fig. 4. The first three solutions for $\alpha = \dfrac{1}{4}$ are

$$\xi_1 \approx 2.570,\ \xi_2 \approx 5.354,\ \xi_3 = 8.303.$$

The energy eigenvalues corresponding to these solutions are respectively given by

$$E_1 \approx 6.607\frac{\hbar^2}{2ma^2},\ E_2 \approx 28.666\frac{\hbar^2}{2ma^2},\ E_3 \approx 68.939\frac{\hbar^2}{2ma^2}.$$

3. Consider a particle of mass $m$ placed in the one-dimensional potential

$$V(x) = \begin{cases} V_1, & x \leq 0, \\ 0, & 0 < x < a, \\ V_2, & x \geq a. \end{cases}$$

Here $V_1 > V_2$. Find the equation that determines the energies of the bound states of the particle.

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The potential is depicted in Fig. 5.

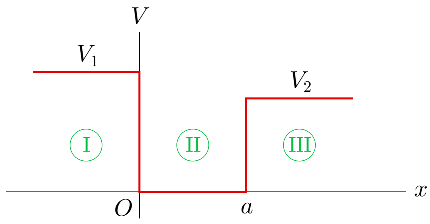


FIG. 5: Asymmetrical potential well.

For bound states, the energy $E$ of the particle is in the range $(0, V_2)$. That is, $0 < E < V_2$. For the convenience of solving the problem, we introduce the following parameters

$$\kappa_1 = \sqrt{\frac{2m(V_1 - E)}{\hbar^2}}, \ \kappa_2 = \sqrt{\frac{2m(V_2 - E)}{\hbar^2}}, \ k = \sqrt{\frac{2mE}{\hbar^2}}.$$

The stationary Schrödinger equations in the three regions are

$$\begin{aligned} &\frac{d^2\varphi_{\rm I}(x)}{dx^2} - \kappa_1^2 \varphi_{\rm I}(x) = 0, \\ &\frac{d^2\varphi_{\rm II}(x)}{dx^2} + k^2 \varphi_{\rm II}(x) = 0, \\ &\frac{d^2\varphi_{\rm III}(x)}{dx^2} - \kappa_2^2 \varphi_{\rm III}(x) = 0. \end{aligned}$$

The general solutions to the above three equations are

$$\begin{aligned} \varphi_{\rm I}(x) &= Ae^{\kappa_1 x} + Be^{-\kappa_1 x}, \\ \varphi_{\rm II}(x) &= C\sin(kx) + D\cos(kx), \\ \varphi_{\rm III}(x) &= Fe^{\kappa_2 x} + Ge^{-\kappa_2 x}. \end{aligned}$$

The boundary condition at $x = -\infty$ is $\lim\limits_{x \to -\infty} \varphi_{\rm I}(x) = 0$. The boundary condition at $x = \infty$ is $\lim\limits_{x \to \infty} \varphi_{\rm III}(x) = 0$. The matching conditions at $x = 0$ are

$$\begin{aligned} \varphi_{\rm I}(0) &= \varphi_{\rm II}(0), \\ \varphi_{\rm I}'(0) &= \varphi_{\rm II}'(0). \end{aligned}$$

The matching conditions at $x = a$ are

$$\begin{aligned} \varphi_{\rm II}(a) &= \varphi_{\rm III}(a), \\ \varphi_{\rm II}'(a) &= \varphi_{\rm III}'(a). \end{aligned}$$

From the boundary condition at $x = -\infty$, $\lim\limits_{x \to -\infty} \varphi_{\rm I}(x) = 0$, we have $B = 0$. From the boundary condition at $x = \infty$, $\lim\limits_{x \to \infty} \varphi_{\rm III}(x) = 0$, we have $F = 0$. The solutions in regions I and III have thus been simplified. The solutions now become

$$\begin{aligned} \varphi_{\rm I}(x) &= Ae^{\kappa_1 x}, \\ \varphi_{\rm II}(x) &= C\sin(kx) + D\cos(kx), \\ \varphi_{\rm III}(x) &= Ge^{-\kappa_2 x}. \end{aligned}$$

From the matching conditions at $x = 0$ and $x = a$, we have

$$\begin{aligned}
&A - D = 0,\\
&\kappa_1 A - kC = 0,\\
&\sin(ka)C + \cos(ka)D - e^{-\kappa_2 a}G = 0,\\
&k\cos(ka)C - k\sin(ka)D + \kappa_2 e^{-\kappa_2 a}G = 0.
\end{aligned}$$

From the first two equations, we have $D = A$ and $C = \kappa_1 A/k$. Inserting these two relations into the last two equations yields

$$\begin{aligned}
&\big[(\kappa_1/k)\sin(ka) + \cos(ka)\big]A - e^{-\kappa_2 a}G = 0,\\
&\big[\kappa_1\cos(ka) - k\sin(ka)\big]A + \kappa_2 e^{-\kappa_2 a}G = 0.
\end{aligned}$$

The above two equations are homogeneous linear algebraic equations for $A$ and $G$. The necessary and sufficient condition for the existence of nontrivial solutions reads

$$\begin{vmatrix} (\kappa_1/k)\sin(ka) + \cos(ka) & -e^{-\kappa_2 a} \\ \kappa_1\cos(ka) - k\sin(ka) & \kappa_2 e^{-\kappa_2 a} \end{vmatrix} = 0.$$

Evaluating the determinant, we obtain

$$\tan(ka) = \frac{\kappa_1/k + \kappa_2/k}{1 - \kappa_1\kappa_2/k^2}.$$

The trigonometric identity $\tan(\alpha+\beta) = \dfrac{\tan\alpha + \tan\beta}{1 - \tan\alpha\tan\beta}$ suggests that we write

$$\tan\alpha = \frac{\kappa_1}{k} = \sqrt{\frac{V_1}{E} - 1},\ \tan\beta = \frac{\kappa_2}{k} = \sqrt{\frac{V_2}{E} - 1}.$$

We then have

$$\tan(ka) = \tan(\alpha+\beta)$$

from which it follows that

$$ka = n\pi + \alpha + \beta,\ n = 0, 1, 2, \cdots.$$

From

$$\tan\alpha = \frac{\kappa_1}{k} = \sqrt{\frac{V_1}{E} - 1},\ \tan\beta = \frac{\kappa_2}{k} = \sqrt{\frac{V_2}{E} - 1},$$

we have

$$\begin{aligned}
&\cos\alpha = \sqrt{\frac{E}{V_1}} = \frac{\hbar k}{\sqrt{2mV_1}},\ \cos\beta = \sqrt{\frac{E}{V_2}} = \frac{\hbar k}{\sqrt{2mV_2}},\\
&\alpha = \arccos\frac{\hbar k}{\sqrt{2mV_1}},\ \beta = \arccos\frac{\hbar k}{\sqrt{2mV_2}},\\
&\alpha = \frac{\pi}{2} - \arcsin\frac{\hbar k}{\sqrt{2mV_1}},\ \beta = \frac{\pi}{2} - \arcsin\frac{\hbar k}{\sqrt{2mV_2}}.
\end{aligned}$$

Making use of the above expressions of $\alpha$ and $\beta$, we can put the equation for the energy eigenvalues into the following form

$$ka = n\pi - \arcsin\frac{\hbar k}{\sqrt{2mV_1}} - \arcsin\frac{\hbar k}{\sqrt{2mV_2}},\ n = 1, 2, 3, \cdots.$$

Recall that the parameter $k$ is related to the energy eigenvalue $E$ through $k = \sqrt{2mE/\hbar^2}$.

4. Consider a particle of mass $m$ placed in a one-dimensional infinite-depth potential well with the potential energy given by

$$V(x) = \begin{cases} 0, & 0 < x < a, \\ \infty, & x \le 0, x \ge a. \end{cases}$$

The particle is in a state described by the wave function $\psi(x) = Ax(x-a)\theta(x)\theta(a-x)$ with $A = \sqrt{30}\, a^{-5/2}$.

(a) If the energy of the particle is measured, what are the possible results? What are the probabilities of obtaining these results?

(b) What is the mean of all possible experimental results when the energy of the particle is measured? What is the standard deviation?

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The energy eigenvalues and normalized eigenfunctions of a particle in the one-dimensional infinite-depth potential well are given by

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2},\ \varphi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right),\ n = 1, 2, 3, \cdots.$$

We first expand the given state wave function of the particle in terms of its energy eigenfunctions. The expansion reads

$$\psi(x) = \sum_{n=1}^{\infty} c_n\varphi_n(x)$$

with $c_n$ given by

$$\begin{aligned} c_n = (\varphi_n, \psi) &= \frac{\sqrt{60}}{a^3}\int_0^a dx\ x(x-a)\sin\left(\frac{n\pi x}{a}\right) = -\frac{\sqrt{60}}{n\pi a^2}\int_0^a d\cos\left(\frac{n\pi x}{a}\right)\ x(x-a) \\ &= \frac{\sqrt{60}}{n\pi a^2}\int_0^a dx\ (2x-a)\cos\left(\frac{n\pi x}{a}\right) = \frac{\sqrt{60}}{n^2\pi^2 a}\int_0^a d\sin\left(\frac{n\pi x}{a}\right)\ (2x-a) \\ &= -\frac{2\sqrt{60}}{n^2\pi^2 a}\int_0^a dx\ \sin\left(\frac{n\pi x}{a}\right) = \frac{2\sqrt{60}}{n^3\pi^3}\cos\left(\frac{n\pi x}{a}\right)\Big|_0^a \\ &= -\frac{2\sqrt{60}}{n^3\pi^3}\left[1-(-1)^n\right],\ n = 1, 2, 3, \cdots. \end{aligned}$$

(a) If the energy of the particle is measured, the possible results are

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2},\ n = 1, 2, 3, \cdots.$$

The probabilities of obtaining these results are respectively given by

$$|c_n|^2 = \frac{240}{n^6\pi^6}\left[1-(-1)^n\right]^2 = \frac{480}{n^6\pi^6}\left[1-(-1)^n\right],\ n = 1, 2, 3, \cdots.$$

(b) The mean of all possible experimental results when the energy of the particle is measured is given by

$$\langle E\rangle = \sum_{n=1}^{\infty} E_n|c_n|^2 = \frac{240\hbar^2}{\pi^4 ma^2}\sum_{n=1}^{\infty}\frac{1-(-1)^n}{n^4} = \frac{480\hbar^2}{\pi^4 ma^2}\sum_{k=1}^{\infty}\frac{1}{(2k-1)^4}.$$

Utilizing

$$\sum_{k=1}^{\infty}\frac{1}{(2k-1)^4} = \frac{\pi^4}{96},$$

we have

$$\langle E\rangle = \frac{480\hbar^2}{\pi^4 ma^2}\times\frac{\pi^4}{96} = \frac{5\hbar^2}{ma^2}.$$

To obtain the standard deviation, we need to evaluate the average of the square of the energy. We have

$$\langle E^2\rangle = \sum_{n=1}^{\infty} E_n^2|c_n|^2 = \frac{120\hbar^4}{\pi^2 m^2a^4}\sum_{n=1}^{\infty}\frac{1-(-1)^n}{n^2} = \frac{240\hbar^4}{\pi^2 m^2 a^4}\sum_{k=1}^{\infty}\frac{1}{(2k-1)^2}.$$

Utilizing

$$\sum_{k=1}^{\infty}\frac{1}{(2k-1)^2} = \frac{\pi^2}{8},$$

we have

$$\langle E^2\rangle = \frac{240\hbar^4}{\pi^2 m^2a^4}\times\frac{\pi^2}{8} = \frac{30\hbar^4}{m^2a^4}.$$

The standard deviation is given by

$$\Delta E = \sqrt{\langle E^2\rangle - \langle E\rangle^2} = \sqrt{\frac{30\hbar^4}{m^2a^4} - \frac{25\hbar^4}{m^2a^4}} = \frac{\sqrt{5}\,\hbar^2}{ma^2}.$$

5. **[C-T Exercise 1-5]** Consider a particle of mass $m$ whose potential energy is $V(x) = -\alpha\delta(x) - \alpha\delta(x-\ell)$, where $\alpha$ is greater than zero and $\ell$ is a constant length.

   (a) Calculate the bound states of the particle, setting $E = -\dfrac{\hbar^2\rho^2}{2m}$. Show that the possible energies are given by the relation $e^{-\rho\ell} = \pm\left(1-\dfrac{2\rho}{\mu}\right)$ with $\mu = \dfrac{2m\alpha}{\hbar^2}$. Give a graphic solution of this equation.

   i. *Ground state.* Show that this state is even (invariant with respect to reflection about the point $x = \ell/2$), and that its energy $E_S$ is less than the energy $-E_L = -\dfrac{m\alpha^2}{2\hbar^2}$. Interpret this result physically. Represent graphically the corresponding wave function.

   ii. *Excited state.* Show that, when $\ell$ is greater than a value which you are to specify, there exists an odd excited state of energy $E_A$ greater than $-E_L$. Find the corresponding wave function.

   iii. Explain how the preceding calculations enable us to construct a model which represents an ionized diatomic molecule ($H_2^+$, for example) whose nuclei are separated by a distance $\ell$. How do the energies of the two levels vary with respect to $\ell$? What happens at the limit where $\ell \to 0$ and at the limit where $\ell \to \infty$? If the repulsion of the two nuclei is taken into account, what is the total energy of the system? Show that the curve which gives the variation with respect to $\ell$ of the energies thus obtained enables us to predict in certain cases the existence of bound states of $H_2^+$, and to determine the value of $\ell$ at equilibrium. In this way we obtain a very elementary model of the chemical bond.

   (b) Calculate the reflection and transmission coefficients of the system of two delta function barriers. Study their variations with respect to $\ell$. Do the resonances thus obtained occur when $\ell$ is an integral multiple of the de Broglie wavelength of the particle? Why?

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(a) The potential is depicted in Fig. 6.

For bound states, the energy $E$ of the particle lies in the range $-\infty < E < 0$. For the convenience of solving the problem, we introduce the following parameter

$$\rho = \sqrt{-\frac{2mE}{\hbar^2}}.$$

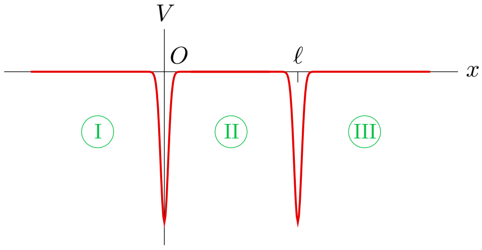


FIG. 6: Double $\delta$-function potential.

The stationary Schrödinger equation in the three regions reads, respectively,

$$\frac{d^2\varphi_{\rm I}(x)}{dx^2} - \rho^2\varphi_{\rm I}(x) = 0,$$
$$\frac{d^2\varphi_{\rm II}(x)}{dx^2} - \rho^2\varphi_{\rm II}(x) = 0,$$
$$\frac{d^2\varphi_{\rm III}(x)}{dx^2} - \rho^2\varphi_{\rm III}(x) = 0.$$

The general solutions to the above three equations are

$$\varphi_{\rm I}(x) = Ae^{\rho x} + Be^{-\rho x},$$
$$\varphi_{\rm II}(x) = Ce^{\rho x} + De^{-\rho x},$$
$$\varphi_{\rm III}(x) = Fe^{\rho x} + Ge^{-\rho x}.$$

The boundary condition at $x = -\infty$ is $\lim_{x\to-\infty}\varphi_{\rm I}(x) = 0$. The boundary condition at $x = \infty$ is $\lim_{x\to\infty}\varphi_{\rm III}(x) = 0$. The matching conditions at $x = 0$ are

$$\varphi_{\rm I}(0) = \varphi_{\rm II}(0),$$
$$\varphi'_{\rm II}(0) - \varphi'_{\rm I}(0) = -\frac{2m\alpha}{\hbar^2}\varphi_{\rm I}(0).$$

The matching conditions at $x = \ell$ are

$$\varphi_{\rm II}(\ell) = \varphi_{\rm III}(\ell),$$
$$\varphi'_{\rm III}(\ell) - \varphi'_{\rm II}(\ell) = -\frac{2m\alpha}{\hbar^2}\varphi_{\rm II}(\ell).$$

From the boundary condition at $x = -\infty$, $\lim_{x\to-\infty}\varphi_{\rm I}(x) = 0$, we have $B = 0$. From the boundary condition at $x = \infty$, $\lim_{x\to\infty}\varphi_{\rm III}(x) = 0$, we have $F = 0$. The solutions in regions I and III have thus been simplified. The solutions now become

$$\varphi_{\rm I}(x) = Ae^{\rho x},$$
$$\varphi_{\rm II}(x) = Ce^{\rho x} + De^{-\rho x},$$
$$\varphi_{\rm III}(x) = Ge^{-\rho x}.$$

From the matching conditions at $x = 0$, we have

$$A = C + D,$$
$$\rho(C - D - A) = -\frac{2m\alpha}{\hbar^2}A.$$

Expressing $C$ and $D$ in terms of $A$ using the above equations, we obtain

$$C = \left(1 - \frac{m\alpha}{\hbar^2\rho}\right)A,$$
$$D = \frac{m\alpha}{\hbar^2\rho}A.$$

The solutions now become

$$\varphi_{\rm I}(x) = Ae^{\rho x},$$
$$\varphi_{\rm II}(x) = A\left[\left(1-\frac{m\alpha}{\hbar^2\rho}\right)e^{\rho x}+\frac{m\alpha}{\hbar^2\rho}e^{-\rho x}\right],$$
$$\varphi_{\rm III}(x) = Ge^{-\rho x}.$$

From the matching conditions at $x=\ell$, we have

$$\left[\left(1-\frac{m\alpha}{\hbar^2\rho}\right)+\frac{m\alpha}{\hbar^2\rho}e^{-2\rho\ell}\right]A-e^{-2\rho\ell}G=0,$$
$$\left[\left(1-\frac{m\alpha}{\hbar^2\rho}\right)-\frac{m\alpha}{\hbar^2\rho}e^{-2\rho\ell}\right]A+e^{-2\rho\ell}\left(1-\frac{2m\alpha}{\hbar^2\rho}\right)G=0.$$

The above two equations are homogeneous linear algebraic equations for $A$ and $G$. The necessary and sufficient condition for the existence of nontrivial solutions reads

$$\begin{vmatrix} \left(1-\frac{m\alpha}{\hbar^2\rho}\right)+\frac{m\alpha}{\hbar^2\rho}e^{-2\rho\ell} & -e^{-2\rho\ell} \\ \left(1-\frac{m\alpha}{\hbar^2\rho}\right)-\frac{m\alpha}{\hbar^2\rho}e^{-2\rho\ell} & e^{-2\rho\ell}\left(1-\frac{2m\alpha}{\hbar^2\rho}\right) \end{vmatrix}=0.$$

Evaluating the determinant, we obtain $e^{-2\rho\ell}=\left(1-\dfrac{\hbar^2\rho}{m\alpha}\right)^2$. Taking the square roots of both sides of this equation yields

$$e^{-\rho\ell}=\pm\left(1-\frac{\hbar^2\rho}{m\alpha}\right)=\pm\left(1-\frac{2\rho}{\mu}\right),$$

where $\mu=\dfrac{2m\alpha}{\hbar^2}$. The above equation is the equation for the energy eigenvalues. In term of the dimensionless variable $\xi=\rho\ell$, the above result is written as

$$e^{-\xi}=\pm\left(1-\frac{2\xi}{\mu\ell}\right)=\pm\big(1-\beta\xi\big),$$

where $\beta=\dfrac{2}{\mu\ell}=\dfrac{\hbar^2}{m\alpha\ell}$. The three functions $e^{-\xi}$ and $\pm\big(1-\beta\xi\big)$ in the above equation are plotted in Fig. 7. The intersections of the curve $e^{-\xi}$ vs $\xi$ with the straight lines $\pm\big(1-\beta\xi\big)$ vs $\xi$ give the solutions to the equation for the energy eigenvalues.

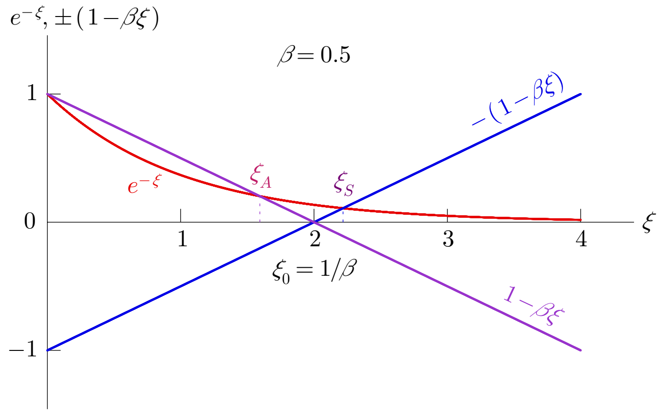


FIG. 7: Graphical solution of the energy eigenvalues for a particle in the double $\delta$-function potential.

Note that the curve $e^{-\xi}$ and the straight line $-(1-\beta\xi)$ always have a nonzero intersection as long as $\beta$ is finite, which is a physically reasonable condition. However, the curve $e^{-\xi}$ and the straight line $1-\beta\xi$ do not always has a nonzero intersection even if $\beta$ is finite. If the slope of the straight line $1-\beta\xi$ at $\xi=0$ is more negative than that of the curve $e^{-\xi}$ at $\xi=0$, then they do not have a nonzero intersection. The slope of the straight line $1-\beta\xi$ at $\xi=0$ is given by

$$\left.\frac{d(1-\beta\xi)}{d\xi}\right|_{\xi=0}=-\beta.$$

The slope of the curve $e^{-\xi}$ at $\xi=0$ is given by

$$\left.\frac{de^{-\xi}}{d\xi}\right|_{\xi=0}=-1.$$

Thus, the condition for the existence of a nonzero intersection for the curve $e^{-\xi}$ and the straight line $1-\beta\xi$ is given by

$$\beta<1.$$

From $\beta=\dfrac{2}{\mu\ell}=\dfrac{\hbar^2}{m\alpha\ell}$, we have

$$\ell>\frac{\hbar^2}{m\alpha}.$$

If the two $\delta$-function peaks are closer than $\dfrac{\hbar^2}{m\alpha}$, then there exists no nonzero intersection for the curve $e^{-\xi}$ and the straight line $1-\beta\xi$. If $\ell<\dfrac{\hbar^2}{m\alpha}$, then there exists only one bound state. If $\ell>\dfrac{\hbar^2}{m\alpha}$, then there exist two bound states.

Here we discuss the $\ell>\dfrac{\hbar^2}{m\alpha}$ case. In Fig. 7, the intersection of $e^{-\xi}$ with $1-\beta\xi$ is denoted by $\xi_A$ and that of $e^{-\xi}$ with $-(1-\beta\xi)$ by $\xi_S$. The intersection of $1-\beta\xi$ and $-(1-\beta\xi)$ is denoted by $\xi_0$. Note that the intersection of $1-\beta\xi$ and $-(1-\beta\xi)$ is also the intersection of $1-\beta\xi$ with the $\xi$-axis and the intersection of $-(1-\beta\xi)$ with the $\xi$-axis. From $\pm\big(1-\beta\xi\big)=0$, we have $\xi_0=1/\beta$. Note that $\xi_A<\xi_0<\xi_S$.

We denote the energy corresponding to $\xi_0$ by $-E_L$. From

$$\rho=\sqrt{-\frac{2mE}{\hbar^2}},\ \xi=\rho\ell,\ \xi_0=\frac{1}{\beta},\ \beta=\frac{2}{\mu\ell}=\frac{\hbar^2}{m\alpha\ell},$$

we have

$$-E_L=-\frac{\hbar^2\rho^2}{2m}=-\frac{\hbar^2\xi_0^2}{2m\ell^2}=-\frac{\hbar^2}{2m\beta^2\ell^2}=-\frac{\hbar^2}{2m\ell^2}\left(\frac{m\alpha\ell}{\hbar^2}\right)^2=-\frac{m\alpha^2}{2\hbar^2}.$$

i. *Ground state.* From Fig. 7, we see that there exist two bound states in this potential for $\ell>\dfrac{\hbar^2}{m\alpha}$. Note that $\xi=0$ is physically unacceptable because the corresponding energy eigenfunction does not satisfy the boundary conditions at $x=\pm\infty$ unless the energy eigenfunction is identically zero.
From

$$\rho=\sqrt{-\frac{2mE}{\hbar^2}},\ \xi=\rho\ell,$$

we obtain the following expression of the energy eigenvalue in terms of $\xi$

$$E=-\frac{\hbar^2\rho^2}{2m}=-\frac{\hbar^2\xi^2}{2m\ell^2}.$$

Because $\xi_A<\xi_0<\xi_S$, in consideration of the above expression of $E$ in terms of $\xi$, we see that the energy eigenvalue corresponding to $\xi_S$ is lower than that corresponding to $\xi_A$. Thus, the energy eigenvalue corresponding to $\xi_S$ is the energy of the ground state.

We now look at the properties of the energy eigenfunctions. For the energy eigenfunction corresponding to the energy eigenvalue $E_S$, inserting $e^{-\rho\ell} = -(1 - \hbar^2\rho/m\alpha)$ into

$$\left[\left(1 - \frac{m\alpha}{\hbar^2\rho}\right) + \frac{m\alpha}{\hbar^2\rho}e^{-2\rho\ell}\right]A - e^{-2\rho\ell}G = 0,$$
$$\left[\left(1 - \frac{m\alpha}{\hbar^2\rho}\right) - \frac{m\alpha}{\hbar^2\rho}e^{-2\rho\ell}\right]A + e^{-2\rho\ell}\left(1 - \frac{2m\alpha}{\hbar^2\rho}\right)G = 0,$$

we obtain $G = e^{\rho\ell}A$. Inserting

$$G = e^{\rho\ell}A,\ \frac{m\alpha}{\hbar^2\rho} = \frac{1}{e^{-\rho\ell}+1},\ 1 - \frac{m\alpha}{\hbar^2\rho} = \frac{e^{-\rho\ell}}{e^{-\rho\ell}+1}$$

into the energy eigenfunction

$$\begin{aligned}\varphi_{\rm I}(x) &= Ae^{\rho x},\\ \varphi_{\rm II}(x) &= A\left[\left(1 - \frac{m\alpha}{\hbar^2\rho}\right)e^{\rho x} + \frac{m\alpha}{\hbar^2\rho}e^{-\rho x}\right],\\ \varphi_{\rm III}(x) &= Ge^{-\rho x},\end{aligned}$$

we obtain

$$\begin{aligned}\varphi_{\rm I}(x) &= Ae^{\rho x},\\ \varphi_{\rm II}(x) &= A\frac{\cos[\rho(\ell/2 - x)]}{\cos(\rho\ell/2)},\\ \varphi_{\rm III}(x) &= Ae^{\rho(\ell - x)}.\end{aligned}$$

To infer the symmetry property of the above energy eigenfunction with respect to $x = \ell/2$, we transform the origin of the coordinate system to $\ell/2$. In the new coordinate system, the coordinate $x'$ is related to $x$ through $x' = x - \ell/2$. Setting $x = x' + \ell/2$ in the above energy eigenfunction, we have

$$\begin{aligned}\varphi_{\rm I}(x') &= Ae^{\rho\ell/2}e^{\rho x'},\\ \varphi_{\rm II}(x') &= A\frac{\cos(\rho x')}{\cos(\rho\ell/2)},\\ \varphi_{\rm III}(x') &= Ae^{\rho\ell/2}e^{-\rho x'}.\end{aligned}$$

The energy eigenfunction is obviously an even function of $x'$. Therefore, the wave function of the ground state is even (invariant with respect to reflection about the point $x = \ell/2$). We already argued in the above that the energy eigenvalue corresponding to $\xi_S$ is lower than that corresponding to $\xi_A$. Thus, the energy eigenvalue corresponding to $\xi_S$ is the ground-state energy as concluded in the above. In terms of $\xi_S$, the value of $E_S$ is given by

$$E_S = -\frac{\hbar^2\xi_S^2}{2m\ell^2}.$$

Because $\xi_S > \xi_0$, we have

$$E_S = -\frac{\hbar^2\xi_S^2}{2m\ell^2} < -\frac{\hbar^2\xi_0^2}{2m\ell^2} = -E_L.$$

That the wave function of the ground state is even (invariant with respect to reflection about the point $x = \ell/2$) is because the potential is symmetric about the point $x = \ell/2$. It can be shown that the energy eigenfunctions of a particle in a symmetric one-dimensional potential can be chosen to be either even or odd functions. That is, each energy eigenfunction can be chosen to possess a definite parity. The proof goes as follows.

Assume that the one-dimensional potential $V(x)$ is an even function of $x$, $V(-x) = V(x)$. The stationary Schrödinger equation reads

$$-\frac{\hbar^2}{2m}\frac{d^2\varphi(x)}{dx^2} + V(x)\varphi(x) = E\varphi(x).$$

Replacing $x$ with $-x$ in the above equation yields

$$-\frac{\hbar^2}{2m}\frac{d^2\varphi(-x)}{dx^2}+V(-x)\varphi(-x)=E\varphi(-x).$$

Making use of $V(-x)=V(x)$, we have

$$-\frac{\hbar^2}{2m}\frac{d^2\varphi(-x)}{dx^2}+V(x)\varphi(-x)=E\varphi(-x)$$

which indicates that $\varphi(-x)$ is also a solution corresponding to the same energy eigenvalue as $\varphi(x)$. If $\varphi(x)$ does not possess a definite parity, we can construct energy eigenfunctions of definite parity through the following combinations

$$\varphi(x)+\varphi(-x),\ \varphi(x)-\varphi(-x)$$

with the first combination an even function and the second combination an odd function.
If the energy eigenvalue is nondegenerate, we then have $\varphi(-x)=C\varphi(x)$. Because the normalization constant can be determined only within a phase factor of unit modulus, we can choose $C=\pm 1$. Thus, the energy eigenfunction corresponding to a nondegenerate energy eigenvalue possesses a definite parity. In the present problem, the ground state is nondegenerate so that the ground-state wave function possesses a definite parity (an even parity). The ground-state wave function is plotted in Fig. 8 for $\beta=0.5$.

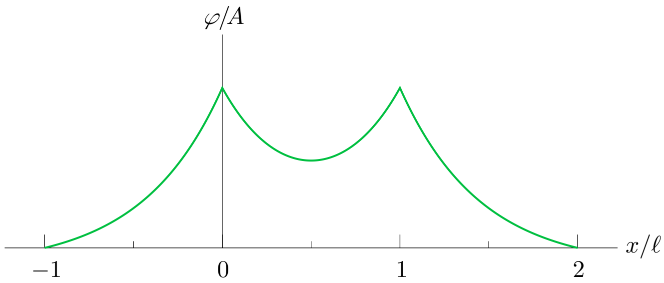


FIG. 8: Plot of the ground-state wave function in the double $\delta$-function potential as a function of $x$. The value of 0.5 for $\beta$ is used here.

ii. As discussed in the above, the second solution exists for $\ell>\dfrac{\hbar^2}{m\alpha}$. That is, an excited state exists if $\ell>\dfrac{\hbar^2}{m\alpha}$. We assume this is the case. The solution to

$$e^{-\rho\ell}=1-\frac{\hbar^2\rho}{m\alpha}\ \text{or}\ e^{-\xi}=1-\beta\xi$$

gives the energy of the excited state. The solution is indicated with $\xi_A$ in Fig. 7. Because $\xi_A<\xi_0$, the energy $E_A$ of this excited state is greater than $-E_L$,

$$E_A=-\frac{\hbar^2\xi_A^2}{2m\ell^2}>-\frac{\hbar^2\xi_0^2}{2m\ell^2}=-E_L.$$

We now examine the symmetry property of the wave function of this excited state. Inserting $e^{-\rho\ell}=1-\hbar^2\rho/m\alpha$ into

$$\left[\left(1-\frac{m\alpha}{\hbar^2\rho}\right)+\frac{m\alpha}{\hbar^2\rho}e^{-2\rho\ell}\right]A-e^{-2\rho\ell}G=0,$$
$$\left[\left(1-\frac{m\alpha}{\hbar^2\rho}\right)-\frac{m\alpha}{\hbar^2\rho}e^{-2\rho\ell}\right]A+e^{-2\rho\ell}\left(1-\frac{2m\alpha}{\hbar^2\rho}\right)G=0,$$

we obtain $G = -e^{\rho\ell}A$. Inserting

$$G = -e^{\rho\ell}A,\ \frac{m\alpha}{\hbar^2\rho} = \frac{e^{\rho\ell}}{e^{\rho\ell}-1},\ 1 - \frac{m\alpha}{\hbar^2\rho} = -\frac{1}{e^{\rho\ell}-1}$$

into the energy eigenfunction

$$\begin{aligned}
\varphi_{\mathrm{I}}(x) &= Ae^{\rho x},\\
\varphi_{\mathrm{II}}(x) &= A\left[\left(1 - \frac{m\alpha}{\hbar^2\rho}\right)e^{\rho x} + \frac{m\alpha}{\hbar^2\rho}e^{-\rho x}\right],\\
\varphi_{\mathrm{III}}(x) &= Ge^{-\rho x},
\end{aligned}$$

we obtain

$$\begin{aligned}
\varphi_{\mathrm{I}}(x) &= Ae^{\rho x},\\
\varphi_{\mathrm{II}}(x) &= -A\frac{\sin[\rho(\ell/2 - x)]}{\sin(\rho\ell/2)},\\
\varphi_{\mathrm{III}}(x) &= -Ae^{\rho(\ell - x)}.
\end{aligned}$$

Replacing $x$ with $\ell/2 + x'$ yields

$$\begin{aligned}
\varphi_{\mathrm{I}}(x) &= Ae^{\rho\ell/2}e^{\rho x'},\\
\varphi_{\mathrm{II}}(x) &= -A\frac{\sin(\rho x')}{\sin(\rho\ell/2)},\\
\varphi_{\mathrm{III}}(x) &= -Ae^{\rho\ell/2}e^{-\rho x'}.
\end{aligned}$$

From the above expression, we see clearly that the wave function of the excited state is an odd function with respect to $x = \ell/2$. That is, the excited state is of odd parity.

iii. ***Variation of $E_S$ with $\ell$.*** The dependence of $E_S$ on $\ell$ can be inferred from the following two equations

$$E_S = -\frac{\hbar^2\rho^2}{2m},\ e^{-\rho\ell} = \frac{\hbar^2\rho}{m\alpha} - 1.$$

At a given value of $\ell$, the value of $\rho$ can be solved numerically from the second equation. Then the value of $E_S$ is evaluated from the first equation. We thus obtain the dependence of $E_S$ on $\ell$ which is shown in Fig. 9 together with the to-be-discussed dependence of $E_A$ on $\ell$.

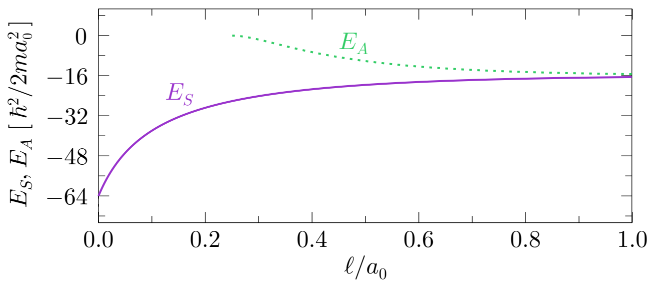


FIG. 9: Plots of $E_S$ and $E_A$ as functions of $\ell$. Here $\hbar^2/m\alpha a_0 = 0.25$ is used.

For the convenience of our discussions, the distance $\ell$ is measured in the Bohr radius $a_0 = 4\pi\varepsilon_0\hbar^2/me^2$ and the energies $E_S$ and $E_A$ are measured in $\hbar^2/2ma_0^2$.
From Fig. 9, we see that $E_S$ takes on a negative value at $\ell = 0$ and tends monotonically to a less negative value as $\ell \to \infty$. We can easily find the values of $E_S(\ell = 0)$ and $E_S(\ell = \infty)$. At $\ell = 0$, from the equation $e^{-\rho\ell} = \hbar^2\rho/m\alpha - 1$, we have $\rho = 2m\alpha/\hbar^2$ which leads to the following value of $E_S$ at $\ell = 0$

$$E_S(\ell = 0) = -\frac{\hbar^2}{2m}\left(\frac{2m\alpha}{\hbar^2}\right)^2 = -\frac{2m\alpha^2}{\hbar^2} = -4E_L.$$

At $\ell = \infty$, $e^{-\rho\ell} = 0$ since $\rho$ must be finite as can be seen from $e^{-\rho\ell} = \hbar^2\rho/m\alpha - 1$, we have $\rho = m\alpha/\hbar^2$ which leads to the following value of $E_S$ at $\ell = \infty$

$$E_S(\ell = \infty) = -\frac{\hbar^2}{2m}\left(\frac{m\alpha}{\hbar^2}\right)^2 = -\frac{m\alpha^2}{2\hbar^2} = -E_L.$$

***Variation of*** $E_A$ ***with*** $\ell$. Similarly to the case for $E_S$, the dependence of $E_A$ on $\ell$ can be inferred from the following two equations

$$E_A = -\frac{\hbar^2\rho^2}{2m},\ e^{-\rho\ell} = 1 - \frac{\hbar^2\rho}{m\alpha}.$$

At a given value of $\ell$, the value of $\rho$ can be solved numerically from the second equation. Then the value of $E_A$ is evaluated from the first equation. We thus obtain the dependence of $E_A$ on $\ell$ which is shown in Fig. 9.
From Fig. 9, we see that the curve for $E_A$ does not start from $\ell = 0$. This is because the excited state does not exist for $\ell < \hbar^2/m\alpha$ as previously discussed. $E_A$ is equal to zero at $\ell = \hbar^2/m\alpha$. It then deceases monotonically as $\ell$ increases and tends to a constant value as $\ell \to \infty$. We can easily find the value of $E_A(\ell = \infty)$. At $\ell = \infty$, $e^{-\rho\ell} = 0$ since $\rho$ is finite, we then have $\rho = m\alpha/\hbar^2$ which leads to the following value of $E_A(\ell = \infty)$

$$E_A(\ell = \infty) = -\frac{\hbar^2}{2m}\left(\frac{m\alpha}{\hbar^2}\right)^2 = -\frac{m\alpha^2}{2\hbar^2} = -E_L.$$

Note that $E_S$ and $E_A$ have the same value at $\ell = \infty$.
***A model of*** $\boldsymbol{H_2^+}$. We assume that the electron is in the ground state. With the repulsion of the two nuclei taken into account, the total energy of the system is given by

$$E_{\rm tot} = -\frac{\hbar^2\rho^2}{2m} + \frac{e^2}{4\pi\varepsilon_0\ell}$$

with $\rho$ determined from the following equation for a given value of $\ell$

$$e^{-\rho\ell} = \frac{\hbar^2\rho}{m\alpha} - 1.$$

It has been found that a minimum exists in the $E_{\rm tot}$-vs-$\ell$ curve only if $\dfrac{\hbar^2}{m\alpha a_0}$ is smaller than about 0.43816. Here $a_0$ is the Bohr radius, $a_0 = \dfrac{4\pi\varepsilon_0\hbar^2}{me^2}$. The dependence of $E_{\rm tot}$ on $\ell$ is illustrated in Fig. 10 for $\dfrac{\hbar^2}{m\alpha a_0} = \dfrac{1}{4}$.

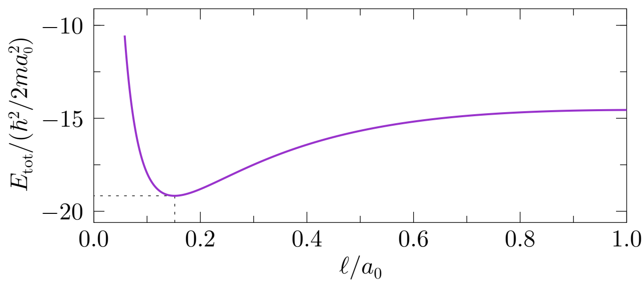


FIG. 10: Plot of the total energy of the model system for $H_2^+$ as a function of the distance between the two nuclei for $\hbar^2/m\alpha a_0 = 1/4$.

For a given value of $\dfrac{\hbar^2}{m\alpha a_0}$ with the existence of a minimum in $E_{\rm tot}$, the system is in a stable state if the distance between the two nuclei is equal to the value of $\ell$ at the minimum. That is, there exist

bound states of $H_2^+$ in certain cases. The length of the chemical bond in $H_2^+$ is given by the separation of the nuclei at the minimum of the total energy.
For $\hbar^2/m\alpha a_0 = 1/4$ as used in Fig. 10, the length of the chemical bond in $H_2^+$ is given by $\ell \approx 0.1514 a_0$ and the minimum value of $E_{\text{tot}}$ is given by

$$E_{\text{tot}}^{\text{min}} \approx -19.1676 \frac{\hbar^2}{2ma_0^2}.$$

(b) The two $\delta$-function barriers are depicted in Fig. 11.

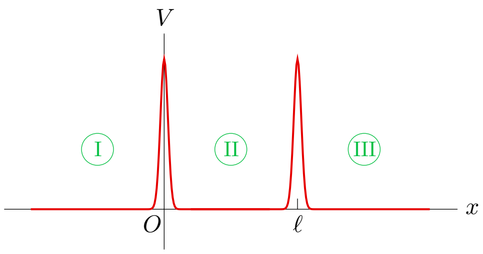


FIG. 11: Two $\delta$-function barriers.

Mathematically, the potential is given by

$$V(x) = \alpha\delta(x) + \alpha\delta(x-\ell).$$

For scattering states, the stationary Schrödinger equation reads in the three regions

$$\begin{aligned}
&\frac{d^2\varphi_{\text{I}}(x)}{dx^2} + k^2\varphi_{\text{I}}(x) = 0, \\
&\frac{d^2\varphi_{\text{II}}(x)}{dx^2} + k^2\varphi_{\text{II}}(x) = 0, \\
&\frac{d^2\varphi_{\text{III}}(x)}{dx^2} + k^2\varphi_{\text{III}}(x) = 0,
\end{aligned}$$

where

$$k = \sqrt{\frac{2mE}{\hbar^2}}.$$

The general solutions to the above three equations are

$$\begin{aligned}
\varphi_{\text{I}}(x) &= Ae^{ikx} + Be^{-ikx}, \\
\varphi_{\text{II}}(x) &= Ce^{ikx} + De^{-ikx}, \\
\varphi_{\text{III}}(x) &= Fe^{ikx} + Ge^{-ikx}.
\end{aligned}$$

We assume that the particle is from $x = -\infty$. Then the boundary condition at $x = \infty$ is given by $\varphi_{\text{III}}(x \to \infty) \propto e^{ikx}$.
The matching conditions at $x = 0$ are

$$\begin{aligned}
&\varphi_{\text{I}}(0) = \varphi_{\text{II}}(0), \\
&\varphi_{\text{II}}'(0) - \varphi_{\text{I}}'(0) = \frac{2m\alpha}{\hbar^2}\varphi_{\text{I}}(0).
\end{aligned}$$

The matching conditions at $x = \ell$ are

$$\begin{aligned}
&\varphi_{\text{II}}(\ell) = \varphi_{\text{III}}(\ell), \\
&\varphi_{\text{III}}'(\ell) - \varphi_{\text{II}}'(\ell) = \frac{2m\alpha}{\hbar^2}\varphi_{\text{II}}(\ell).
\end{aligned}$$

From the boundary condition at $x = \infty$, $\varphi_{\rm III}(x \to \infty) \propto e^{ikx}$, we have $G = 0$. The wave functions in the three regions are now given by

$$\begin{aligned}
\varphi_{\rm I}(x) &= Ae^{ikx} + Be^{-ikx},\\
\varphi_{\rm II}(x) &= Ce^{ikx} + De^{-ikx},\\
\varphi_{\rm III}(x) &= Fe^{ikx}.
\end{aligned}$$

From the matching conditions at $x = 0$, we have

$$\begin{aligned}
&A + B = C + D,\\
&(C - D) - (A - B) = -\frac{i2m\alpha}{\hbar^2 k}(A + B)
\end{aligned}$$

from which we obtain

$$\begin{aligned}
C &= \big(1 - i\gamma\big)A - i\gamma B,\\
D &= i\gamma A + \big(1 + i\gamma\big)B,
\end{aligned}$$

where

$$\gamma = \frac{m\alpha}{\hbar^2 k}.$$

The wave functions in the three regions are now given by

$$\begin{aligned}
\varphi_{\rm I}(x) &= Ae^{ikx} + Be^{-ikx},\\
\varphi_{\rm II}(x) &= \big[\,\big(1 - i\gamma\big)A - i\gamma B\,\big]e^{ikx} + \big[\,i\gamma A + \big(1 + i\gamma\big)B\,\big]e^{-ikx},\\
\varphi_{\rm III}(x) &= Fe^{ikx}.
\end{aligned}$$

From the matching conditions at $x = \ell$, we have

$$\begin{aligned}
&\big[\,\big(1 - i\gamma\big)A - i\gamma B\,\big] + \big[\,i\gamma A + \big(1 + i\gamma\big)B\,\big]e^{-2ik\ell} = F,\\
&\big[\,\big(1 - i\gamma\big)A - i\gamma B\,\big] - \big[\,i\gamma A + \big(1 + i\gamma\big)B\,\big]e^{-2ik\ell} = (1 + 2i\gamma)F.
\end{aligned}$$

Solving for $B$ and $F$ in terms of $A$, we obtain

$$\begin{aligned}
B &= -\frac{i\gamma\big[\,(1 - i\gamma) + (1 + i\gamma)e^{-2ik\ell}\,\big]}{\gamma^2 + (1 + i\gamma)^2 e^{-2ik\ell}}A,\\
F &= \frac{e^{-2ik\ell}}{\gamma^2 + (1 + i\gamma)^2 e^{-2ik\ell}}A.
\end{aligned}$$

The reflectivity is given by

$$\begin{aligned}
R = \left|\frac{B}{A}\right|^2 &= \frac{\gamma^2\big|(1 - i\gamma) + (1 + i\gamma)e^{-2ik\ell}\big|^2}{\big|\gamma^2 + (1 + i\gamma)^2 e^{-2ik\ell}\big|^2}\\
&= \gamma^2\frac{\big[\,1 + \cos(2k\ell) + \gamma\sin(2k\ell)\,\big]^2 + \big[\,\gamma - \gamma\cos(2k\ell) + \sin(2k\ell)\,\big]^2}{\big[\,\gamma^2 + \big(1 - \gamma^2\big)\cos(2k\ell) + 2\gamma\sin(2k\ell)\,\big]^2 + \big[\,\big(1 - \gamma^2\big)\sin(2k\ell) - 2\gamma\cos(2k\ell)\,\big]^2}\\
&= \frac{2\gamma^2\big[\,1 + \gamma^2 + (1 - \gamma^2)\cos(2k\ell) + 2\gamma\sin(2k\ell)\,\big]}{1 + 2\gamma^2\big[\,1 + \gamma^2 + (1 - \gamma^2)\cos(2k\ell) + 2\gamma\sin(2k\ell)\,\big]}.
\end{aligned}$$

The transmissivity is given by

$$T = \left|\frac{F}{A}\right|^2 = \frac{1}{1 + 2\gamma^2\big[\,1 + \gamma^2 + (1 - \gamma^2)\cos(2k\ell) + 2\gamma\sin(2k\ell)\,\big]}.$$

From the expressions of $R$ and $T$, we see that

$$R + T = 1.$$

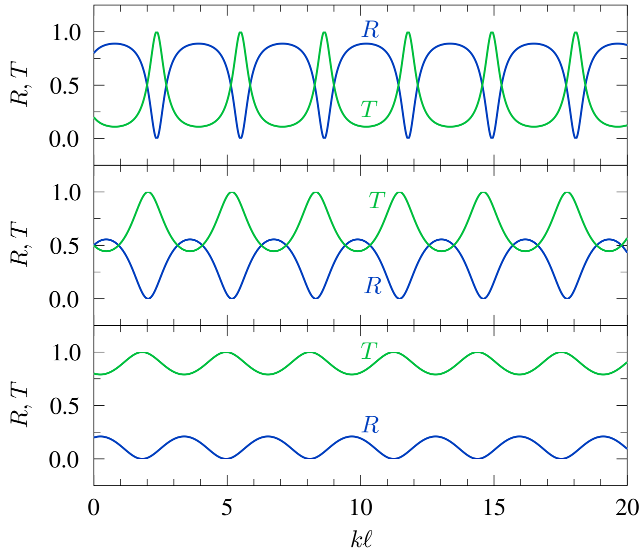


FIG. 12: Dependence of $R$ and $T$ on $k\ell$. From the bottom panel to the top panel, the values of $\gamma$ are respectively 0.25, 0.5, and 1.

$R$ and $T$ are plotted in Fig. 12 as functions of $k\ell$ for three different values of $\gamma$, $\gamma = 0.25, 0.5$, and 1.

From Fig. 12, we see that the resonances occur in transmission. These resonances do not occur at $k\ell = 2\pi n$ with $n = 1, 2, 3, \cdots$. Therefore, these resonances do not occur when $\ell$ is an integral multiple of the de Broglie wavelength of the particle. This is because the particle is not in a bound state and the wave associated with the particle is not a standing wave. The wave associated with the particle does not need to fit between the two $\delta$-function potentials.

The values of $\ell$ at which the resonances occur can also be found analytically. From the expression of $T$, we see that the values of $\ell$ at which $T = 1$ can be determined from

$$1 + \gamma^2 + (1 - \gamma^2)\cos(2k\ell) + 2\gamma\sin(2k\ell) = 0.$$

Note that $\gamma = m\alpha/\hbar^2 k = 0$ is excluded.