Lesson 8: Solutions of the Schrodinger equation (III)

Clara E. Alonso Alonso

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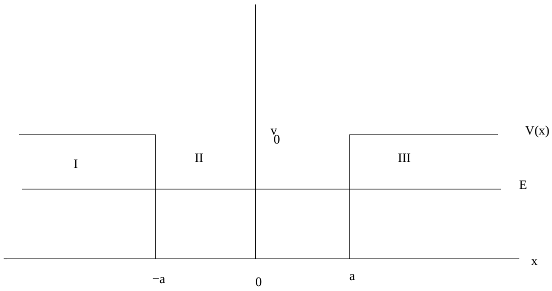

$$V(x) = \begin{cases} 0\ ; & -a < x < a \\ V_0\ ; & x < -a\ ;\ x > a \end{cases}$$

Time independent Schrodinger equation

$$-\frac{\hbar^2}{2m}\phi''(x) + V(x)\phi(x) = E\phi(x)$$

$$\phi_I(x) = Ae^{k_1 x} + Be^{-k_1 x} \quad ; \quad k_1 = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$$

$$\phi_{II}(x) = Pe^{ik_2 x} + Qe^{-ik_2 x} \quad ; \quad k_2 = \frac{\sqrt{2mE}}{\hbar}$$

$$\phi_{III}(x) = Ce^{k_3 x} + De^{-k_3 x} \quad ; \quad k_3 = k_1$$

- the wave function must vanish at $x = -\infty \rightarrow B = 0$
- the wave function must vanish at $x = \infty \rightarrow C = 0$

We require continuity of the wave function and its derivative in $-a$ and a

$$** \quad \phi_I(-a) = \phi_{II}(-a) \quad \rightarrow \quad Ae^{-k_1 a} = Pe^{-ik_2 a} + Qe^{ik_2 a} \quad (1)$$

$$\phi'_I(-a) = \phi''_{II}(-a) \quad \rightarrow \quad Ae^{-k_1 a} = i\frac{k_2}{k_1}\left(Pe^{-ik_2 a} - Qe^{ik_2 a}\right)$$

$$\rightarrow \quad Pe^{-ik_2 a} + Qe^{ik_2 a} = i\frac{k_2}{k_1}\left(Pe^{-ik_2 a} - Qe^{ik_2 a}\right) \quad (2)$$

$$** \quad \phi_{II}(a) = \phi_{III}(a) \rightarrow Pe^{ik_2 a} + Qe^{-ik_2 a} = De^{-k_1 a} \quad (3)$$

$$\phi''_{II}(a) = \phi''_{III}(a) \rightarrow -i\frac{k_2}{k_1}\left(Pe^{ik_2 a} - Qe^{-ik_2 a}\right) = De^{-k_1 a} \quad (4)$$

$$\rightarrow \quad Pe^{ik_2 a} + Qe^{-ik_2 a} = -i\frac{k_2}{k_1}\left(Pe^{ik_2 a} - Qe^{-ik_2 a}\right) \quad (5)$$

Adding (2) + (5)

$$\rightarrow (P + Q)\cos(k_2 a) = \frac{k_2}{k_1}(P + Q)\sin(k_2 a) \quad (6)$$

subtracting (5) - (2)

$$\rightarrow (P - Q)\sin(k_2 a) = -\frac{k_2}{k_1}(P - Q)\cos(k_2 a) \quad (7)$$

For arbitrary P and Q there is no solution for these two equations simultaneously. This is easily seen dividing them

$$\cot(k_2 a) = -\tan(k_2 a) \rightarrow \tan^2(k_2 a) = -1$$

However, there are two solutions for cases involving certain relative values of P and Q:

- (i) if $P = Q$ the two members of (7) are zero. We obtain from (6)

$$\cot(k_2 a) = \frac{k_2}{k_1}$$

Moreover if $P = Q$ necessarily $D = A$ (from (1) and (3))

Then $\phi_{II}(x) = P(e^{ik_2 x} + e^{-ik_2 x}) = 2P\cos(k_2 x)$

$$\phi_{even}(x) = \begin{cases} A\ e^{k_1 x} & x < -a \quad \text{(I)} \\ 2P\cos k_2 x & -a < x < a \quad \text{(II)} \\ A\ e^{-k_1 x} & x > a \quad \text{(III)} \end{cases}$$

The relation between A and P is obtained, for example, from equation (1)
$\phi_I(-a) = \phi_{II}(-a)$

$$A = 2P\cos(k_2 a)\ e^{k_1 a}$$

$\phi_{even}(x)$ is an even function $\rightarrow$ (i) **even solutions**

P is determined by normalization

- (ii) If $P = -Q$ both sides of (6) are zero. We obtain from (7)

$$\tan(k_2 a) = -\frac{k_2}{k_1}$$

Moreover if $P = -Q$ necessarily $D = -A$ (from (1) and (3))

Then $\phi_{II}(x) = 2iP\sin(k_2 x)$

$$\phi_{odd}(x) = \begin{cases} A\ e^{k_1 x} & x < -a \quad \text{(I)} \\ 2iP\sin k_2 x & -a < x < a \quad \text{(II)} \\ -A\ e^{-k_1 x} & x > a \quad \text{(III)} \end{cases}$$

Equation (1) gives the relation between A and P

$$A = -2iP\sin(k_2 a)e^{k_1 a}$$

P is determined by normalization

$\phi_{odd}(x)$ is an odd wave function $\rightarrow$ (ii) **odd solutions**

Eigenvalues

(i) **even solutions**: $\cot(k_2 a) = \frac{k_2}{k_1}$

therefore $k_2 a\ \tan(k_2 a) = k_1 a$

we define $\xi = k_2 a$ and $\eta = k_1 a$ (dimensionless)

$$\xi = \frac{\sqrt{2mE}}{\hbar}\,a \quad ; \quad \eta = \frac{\sqrt{2m(V_0 - E)}}{\hbar}\,a$$

$$\xi^2 + \eta^2 = \frac{2mV_0}{\hbar^2}a^2 = r^2 \quad ; \quad r = \frac{\sqrt{2mV_0}}{\hbar}\,a \ \text{(dimensionless)}$$

The even solution (i) must fulfill simultaneously

$$\xi\tan\xi = \eta \quad \text{and}$$

$$\xi^2 + \eta^2 = r^2 \ \text{(circumference of radius } r \text{ in the plane } \eta\ \xi)$$

In order to solve them we can use **numerical or graphical** methods

Graphical solution

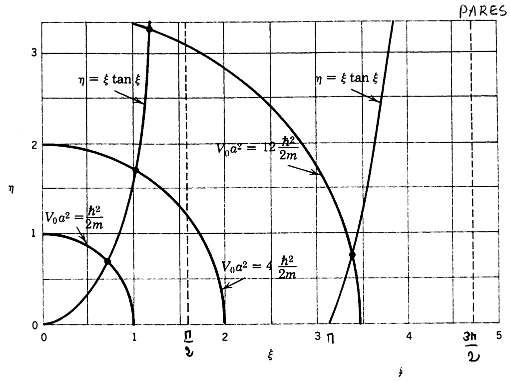

Fig. 8 Graphical solution of Eq. (9.7) for three values of $V_0 a^2$; the vertical dashed lines are the first two asymptotes of $\eta = \xi \tan \xi$.

The infinite well is a special case with $r = \infty$, you can also get their solutions $\xi_n = n \, \frac{\pi}{2}; \quad n = 1, 3...$

Make a table with entries ξ / $\sqrt{r^2 - \xi^2}$ / $\xi \tan \xi$ (numerical method)

Ex. if $V_0 \, a^2 = 25 \, \frac{\hbar^2}{2m} \rightarrow r = 5$

after obtaining approximate values for ξ and η which are solutions, by the graphical method, one can get more accurate values of ξ and η. η.

With this approximate value of ξ compute $\sqrt{r^2 - \xi^2}$ and $\xi \tan \xi$. If they differ, vary slightly ξ.

Recalculate $\sqrt{r^2 - \xi^2}$ and $\xi \tan \xi$ $\rightarrow$ it can be seen the direction in which ξ has to be varied so that $\sqrt{r^2 - \xi^2}$ and $\xi \tan \xi$ approach each other (if in two successive tests $\sqrt{r^2 - \xi^2}$ has gone from being larger than $\xi \tan \xi$ to be smaller, the value of ξ that makes them equal is between the two we have used for the test).

Successive **iterations** are performed until the difference between $\sqrt{r^2 - \xi^2}$ and $\xi \tan \xi$ is smaller than a preset value

For $\phi_{even_3}(x)$ (second excited state), when $r = 5$ we get values $\xi = 3.8375$ and $\eta = 3.205$

There are two even bound solutions: $\phi_{even_1}(x)$ (with $\lambda_2 > 4a$) and $\phi_{even_3}(x)$ (with $\frac{4a}{3} < \lambda_2 < 2a$)

The eigenvalues of $\widehat{H}$ are

$$E_n = \frac{\hbar^2}{2m} \left(\frac{\xi_n}{a} \right)^2$$

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(ii) **odd solutions**: $\tan(k_2 a) = -\frac{k_2}{k_1}$

$k_2 a \cot(k_2 a) = -k_1 a$

Using the above definitions of ξ and η, the odd solutions (ii) must satisfy simultaneously

$$\xi \cot \xi = -\eta$$

$$\xi^2 + \eta^2 = r^2$$

For its solution one can use numerical or graphical methods

In the previous example $V_0 \, a^2 = 25 \frac{\hbar^2}{2m} \rightarrow r = 5$ there are two odd solutions: $\phi_{odd_2}(x)$ y $\phi_{odd_4}(x)$

For this example there are 4 bound solutions : 2 even and 2 odd

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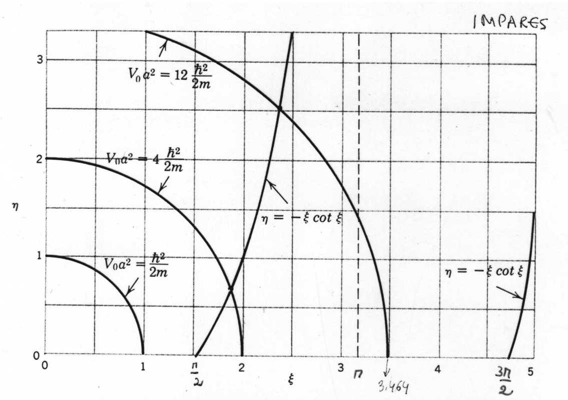
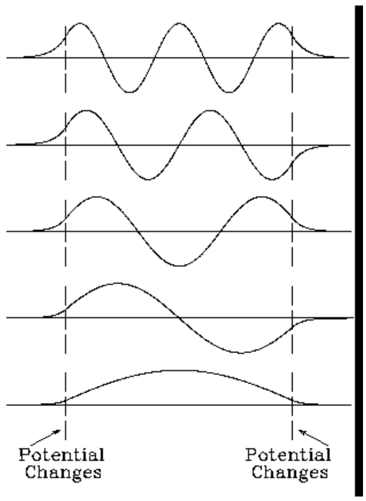


Fig. 9 Graphical solution of Eq. (9.6) for three values of V_0a^2; the vertical dashed line is the first asymptote of $\eta = -\xi \cot \xi$.

For the infinite well $\xi_n = \frac{n}{2}\,\pi; \quad n = 2, 4, \ldots$

Bound eigenfunctions of the finite well

In the well **cosine** and **sine** functions alternate (even and odd), starting with an even function



Number of bound solutions = next integer to q

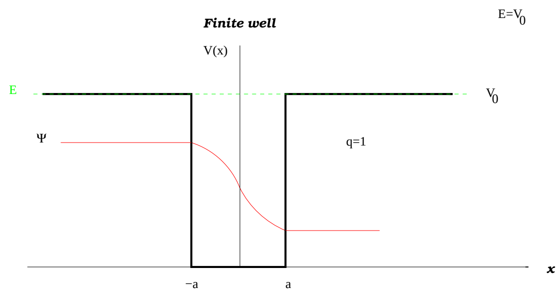
$$q = \frac{2r}{\pi}$$

If $r = 5 \rightarrow q = 3.18 \rightarrow 4$ bound solutions

- **Exception**: when q is an integer number, this is the number of bound solutions. There is the solution $\eta = 0$ and $\xi = \frac{q\pi}{2}$. If q is even it corresponds to an even solution and if it is odd to an odd one

  $\eta = 0 \rightarrow k_1 = 0$ ($\rightarrow E = V_0$) that makes that in forbidden regions the wave function is constant, so that it is not normalizable and is no longer a bound state. The state with $E = V_0$ is not bound

For $q = 1 \rightarrow 2a = \frac{\lambda}{2}$. At $x = -a$ the wave function has a maximum and at $x = a$ the wave function has a minimum (or vice versa). At these points the derivative of the wave function is zero



- Potential **with bound states**
- We take its minimum at $V = 0$

  Let's see that $\widehat{H}$ cannot have eigenvalue $E = 0$, corresponding to a bound state

  $$E = 0 \rightarrow p = 0 \rightarrow \Delta p = 0 \rightarrow \Delta x = \infty$$

  it is not possible. Δx must be of the order of the classically allowed distance

  The ground state has $E > 0$. It's called **zero point energy**
- This is a purely quantum phenomenon (classically the particle can have $E = 0$, it is still)

Example: infinite square well (width $2a$ from $-a$ to a)

$$E_1 = \frac{\hbar^2\pi^2}{2m(2a)^2}$$

$$\phi_1(x) = A\cos\frac{\pi}{2a}x$$

$$(\Delta p)_1 = \sqrt{< p^2 > - < p >^2} = \sqrt{< p^2 >} = \frac{\hbar\pi}{2a}$$

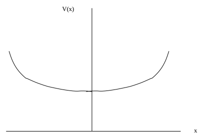
$$(\Delta x)_1 = \sqrt{< x^2 > - < x >^2} = \sqrt{0.13\ a^2} = 0.36\ a$$

$$(\Delta x)_1\ (\Delta p)_1 = 0.57\hbar \geq \frac{\hbar}{2}$$

for $E = 0 \rightarrow a = \infty \rightarrow (\Delta p)_1 = 0\ ;\ (\Delta x)_1 = \infty$

with $a = \infty$ the particle becomes free, without bound states

Parity of the eigenfunctions



Let $V(x) \ = \ V(-x)$. T. I. Schrödinger equation in one dimension

$$-\frac{\hbar^2}{2m}\phi''(x) \ + \ V(x)\phi(x) = \ E\phi(x)$$

change $x \ \to \ -x$

$$-\frac{\hbar^2}{2m}\phi''(-x) \ + \ V(x)\phi(-x) = \ E\phi(-x)$$

$\phi(x)$ and $\phi(-x)$ are solutions of the same differential equation with the same eigenvalue E

- in **bound systems in one dimension** there is no degeneration, therefore

$$\phi(x) \ = \ \alpha \ \phi(-x)$$

change of variable $x \ \to \ -x$

$$\phi(-x) \ = \ \alpha \ \phi(x)$$

$$\phi(x) \ = \ \alpha^2 \ \phi(x) \ \to \ \ \alpha \ = \ \pm 1$$

$$\phi(x) \ = \ \pm \phi(-x)$$

the eigenfunctions of $\widehat{H}$ are even or odd

(examples: infinite well, finite well, harmonic oscillator... If you choose properly the origin $V(x) \ = \ V(-x)$ and the eigenfunctions of $\widehat{H}$ are even or odd in x, for bound states)

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