Lecture 6 Particle Waves in One Dimension (cont.)

SCPY152, Second Semester 2021-22

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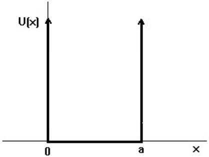
Topics

1. Infinite potential well
2. Finite potential well
3. Harmonic potential well

Infinite potential well

In case of infinite potential well

$$U(x) = \begin{cases} \infty, & x < 0 \\ 0, & 0 < x < x \\ \infty, & x > a \end{cases} \quad (1)$$



A particle wave is confined within o rigid walls in a region of $0 < x < a$. SE in side the walls is

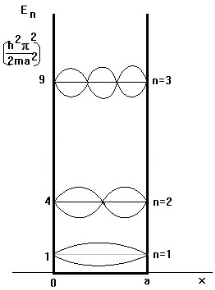
$$\varphi''(x) + k^2\varphi(x) = 0,\ k^2 = \frac{2mE}{\hbar^2} \qquad (2)$$

The particle wave must be standing wave so that we can write solution of the above equation immediately as

$$\varphi(x) = A\sin(kx);\ \sin(0) = 0,\ \sin(ka) = 0 \mapsto ka = n\pi,\ n = 1, 2, \ldots \quad (3)$$

$$\mapsto k_n = \frac{n\pi}{a} \to E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2\pi^2}{2ma^2} n^2 \quad (4)$$

What we get is n^{th}-order of standing waves with discrete energies of $E_n = (\hbar^2\pi^2/2m)n^2$, with $n = 1, 2, 3, ...$



For real standing particle waves, its energy will become discrete quantum energies, identify with running quantum number n.
This is characteristic of any quantum system.
$n = 1$ is called ground state
$n = 2, 3, ...$ are excited states

The normalized particle wave function is

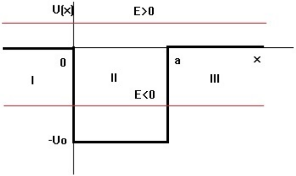
$$\varphi_n(x) = C\sin(n\pi x/a) \mapsto \int_0^a |\varphi_n(x)|^2 dx = 1$$

$$= |C|^2 \int_0^a \sin^2(n\pi x/a)dx = |C|^2 \frac{a}{2} \mapsto C = \sqrt{\frac{2}{a}} \qquad (5)$$

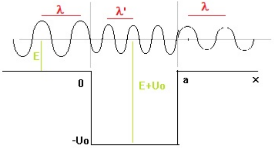
Finite potential well

In case of finite potential well

$$U(x) = \begin{cases} 0, & x < 0 \\ -U_0, & 0 < x < a \\ 0, & x > a \end{cases} \quad (6)$$



- In case of $E > 0$, we have the same problem as the case of potential barrier for the case of $E > U_0$. You just change $k'^2 = \frac{2m(E-U_0)}{\hbar^2}$ to $k'^2 = \frac{2m(E+U_0)}{\hbar^2}$ $(k = 2\pi/\lambda)$

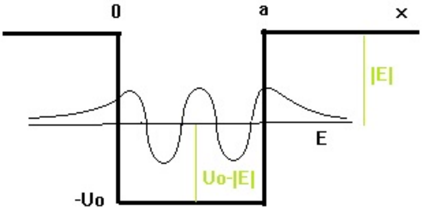


We also have resonance tunneling through the potential well (see lecture 5/ eq.(23))

- In case of $0 < E < -U_0$, i.e., $E = -|E|$, SE in three regions will be

$$
\begin{aligned}
I: &\quad \varphi_I'' - \kappa^2 \varphi_I = 0 \mapsto \varphi_I(x) = Ae^{\kappa x} && (7)\\
II: &\quad \varphi_{II}'' + k^2 \varphi_{II} = 0 \mapsto \varphi_{II}(x) = Be^{ikx} + Ce^{-ikx} && (8)\\
III: &\quad \varphi_{III}'' - \kappa^2 \varphi_{III} = 0 \mapsto \varphi_{III}(x) = De^{-\kappa x} && (9)
\end{aligned}
$$

where we have defined $\kappa^2 = \frac{2m|E|}{\hbar^2}$ and $k^2 = \frac{2m(U_0 - |E|)}{\hbar^2}$. We have ignored particle waves growing into region I ($e^{-\kappa x}$)and region III ($e^{\kappa x}$)



Connection of these waves at $x = 0$ and $x = a$ results to

$$A = B + C \tag{10}$$

$$\kappa A = ik(B - C) \tag{11}$$

$$De^{-\kappa a} = Be^{ika} + Ce^{-ika} \tag{12}$$

$$-\kappa De^{-\kappa a} = ik(Be^{ika} - Ce^{-ika}) \tag{13}$$

Solving these equations for E

$$B + C = \frac{ik}{\kappa}(B - C) \mapsto (1 - ik/\kappa)B = -(1 + ik/\kappa)C$$

$$C = \frac{ik - \kappa}{ik + \kappa}B \tag{14}$$

$$(Be^{ika} + Ce^{-ika}) = -\frac{ik}{\kappa}(Be^{ika} - Ce^{-ika})$$

$$\left(e^{ika} + \frac{ik - \kappa}{ik + \kappa}e^{-ika}\right) = -\frac{ik}{\kappa}\left(e^{ika} - \frac{ik - \kappa}{ik + \kappa}e^{-ika}\right)$$

$$(ik + \kappa)e^{ika} + (ik - \kappa)e^{-ika} = -\frac{ik}{\kappa}((ik + \kappa)e^{ika} - (ik - \kappa)e^{-ika})$$

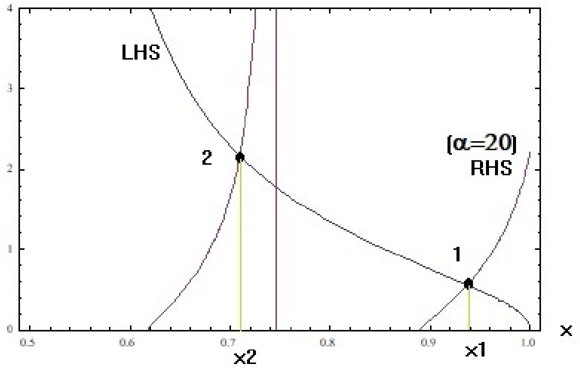
$$
\begin{aligned}
k\cos(ka) - \kappa\sin(ka) &= \frac{k}{\kappa}(k\sin(ka) - \kappa\cos(ka)) \\
k\kappa - \kappa^2\tan(ka) &= k^2\tan(ka) - k\kappa \\
\frac{2k\kappa}{(k^2-\kappa^2)} &= \tan(ka) \qquad (15)
\end{aligned}
$$

In term of $|E|$, we have

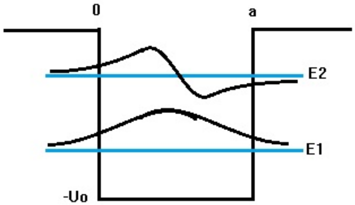
$$
\frac{2\sqrt{|E|(U_0-|E|)}}{(2|E|-U_0)} = \tan\left(\sqrt{\frac{2m|E|a^2}{\hbar^2}}\right) \qquad (16)
$$

$$
x = \frac{|E|}{U_0} \mapsto \frac{2\sqrt{x(1-x)}}{2x-1} = tan\left(\alpha\sqrt{x}\right),\ \alpha^2 = \frac{2mU_0a^2}{\hbar^2} \qquad (17)
$$

We can solve this equation for $|E|$ by using graphical method, i.e., graph the left and wright hand functions, the crossing points are our solutions.
We will observe that the possible solutions for $|E|$ will have finite numbers, this corresponds to finite energy levels inside the well.



4
3
2
1
0
0.5
0.6
0.7
0.8
0.9
1.0
LHS
2
1
(α=20)
RHS
x
x2
x1



0
a
E2
E1
-Uo

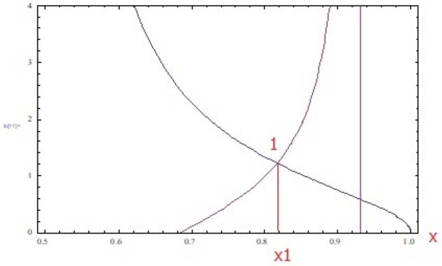
Example:

Energy level of an electron inside finite potential of depth $U_0 = 10eV$ and width $a = 0.7nm$ is, see the figure below,

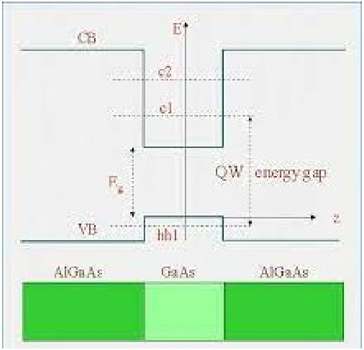
$$\alpha^2 = \frac{2(mc^2)U_0a}{(\hbar c)^2} = \frac{2(0.512 \times 10^6 eV)(10eV)(7 \times 10^{-10}m)^2}{(1.97 \times 10^{-7} eV \cdot m)^2}$$

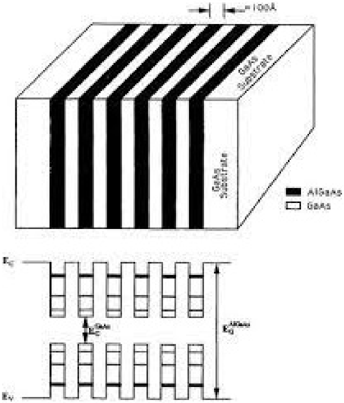
$$= 1.29 \times 10^2 \mapsto \alpha = 11.4$$

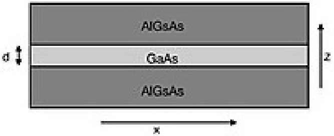
$$x_1 = 0.82 \mapsto |E_1| = 0.82U_0 = 8.2eV \mapsto E_1 = -8.2eV \quad (18)$$



AlGaAs-GaAs quantum well device (QW Laser Diode/Detector)







Harmonic potential well

The harmonic potential well is

$$U(x) = \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2 x^2,\ \omega^2 = \frac{k}{m} \tag{19}$$

SE in the region $x \in (-\infty, \infty)$ will be

$$\varphi''(x) + \left(\frac{2mE}{\hbar^2} - \frac{m^2\omega^2}{\hbar^2}x^2\right)\varphi(x) = 0 \tag{20}$$

Multiply through by $\hbar/m\omega$, and define

$$y = \sqrt{\frac{m\omega}{\hbar}}x \mapsto \varphi = \varphi(y),\ \epsilon = \frac{2E}{\hbar\omega}$$

From (18) we have

$$\varphi''(y) + (\epsilon - y^2)\varphi(y) = 0 \tag{21}$$

Trial solution

$$\varphi(y) = e^{-y^2/2}H(y) \mapsto \varphi' = -ye^{-y^2/2}H + e^{-y^2/2}H'$$
$$\varphi'' = -e^{-y^2/2}H + y^2e^{-y^2/2}H - 2ye^{-y^2/2}H' + e^{-y^2/2}H''$$
$$(19) \mapsto H'' - 2yH' + (\epsilon - 1)H = 0 \quad (22)$$

When compare to *Hermite equation* (Wolfram Alpha)

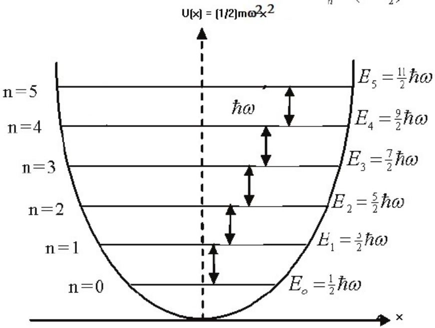
$$f''(x) - 2xf'(x) + 2nf(x) = 0$$

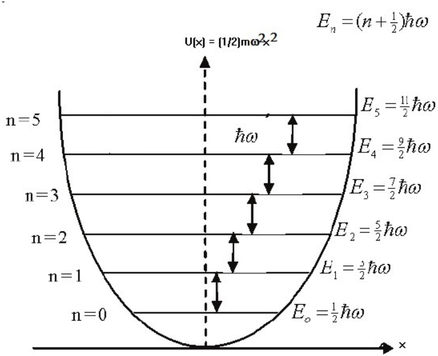
We observe that our equation (21) is a kind of Hermite equation with

$$\epsilon - 1 = 2n \mapsto \epsilon = \frac{2E}{\hbar\omega} = 2(n + 1/2)$$
$$\mapsto E_n = (n + 1/2)\hbar\omega, \;\; n = 0, 1, 2, 3, ... \quad (23)$$

We derive the quantum energy of the system E_n runs with the quantum numbers (integer) $n = 0, 1, 2, ...$

$$E_n = (n + \tfrac{1}{2})\hbar\omega$$





Solution of Hermite equation is called *Hermite polynomial*

$$H_n(y) = H_n(\sqrt{m\omega/\hbar}x)$$

when

$$H_n(y) = (-1)^n e^{y^2} \frac{d^n}{dy^n} e^{-y^2} \tag{24}$$

Hermite polynomials $H_n(x)$

$$
\begin{aligned}
H_0(x) &= 1 \\
H_1(x) &= 2x \\
H_2(x) &= 4x^2 - 2 \\
H_3(x) &= 8x^3 - 12x \\
H_4(x) &= 16x^4 - 48x^2 + 12 \\
H_5(x) &= 32x^5 - 160x^3 + 120x \\
H_6(x) &= 64x^6 - 480x^4 + 720x^2 - 120 \\
H_7(x) &= 128x^7 - 1344x^5 + 3360x^3 - 1680x
\end{aligned}
$$

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\end{aligned}
$$

Solution of SE (19)

$$\varphi_n(x) = C_n e^{-m\omega x^2/2\hbar} H_n(\sqrt{m\omega/\hbar}\,x) \tag{25}$$

$$\int_{-\infty}^{\infty} |\varphi_n(x)|^2 dx = 1 \mapsto C_n = \left(\frac{1}{2^n n!} \sqrt{\frac{m\omega}{\pi\hbar}} \right)^{1/2} \tag{26}$$

$$\varphi 0 = \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-y^2/2}$$

$$\varphi 1 = \left(\frac{\alpha}{\pi}\right)^{1/4} \sqrt{2} y\, e^{-y^2/2}$$

$$\varphi 2 = \left(\frac{\alpha}{\pi}\right)^{1/4} \frac{1}{\sqrt{2}}(2y^2 - 1) e^{-y^2/2}$$

$$\varphi 3 = \left(\frac{\alpha}{\pi}\right)^{1/4} \frac{1}{\sqrt{3}}(2y^3 - 3y) e^{-y^2/2}$$

$$\alpha = \frac{m\omega}{\hbar} \qquad y = \sqrt{\alpha}\, x$$