Free Study Material from

All Lab Experiments

All Lab Experiments

Quantum Mechanics & Applications
Chapter - 3
General Discussion of Bound States

3 General Discussion of Bound States in an Arbitrary Potential

Syllabus: Continuity of wave function, boundary condition and energence of discrete energy levels; application to one-dimensional problem-square well potential; Quantum mechanics of simple harmonic oscillator-energy levels and energy eigen functions using Frobenius method; Hermite polynomials; ground state, zero point energy & uncertainty principle

Q 1. What are the necessary conditions for a wavefunction- continuity, boundary condition and discrete energy levels?

Ans. Continuity of the wave function and of its derivative.

We shall for the time being consider only stationary states, and we shall say "wave function" meaning the spatial wave function $u(x)$

The 1D TiSE for a particle of mass m in the potential *V(x) is*

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

or

$$u''(x)=\frac{2m}{\hbar^2}[V(x)-E]u(x)$$

where

$$u''(x)\equiv d^2u(x)/dx^2$$

Let us integrate this eqn from x_0 to x:

$$u'(x)=u'(x_0)+\frac{2m}{\hbar^2}\int_{x_0}^{x}[V(t)-E]u(t)dt$$

Now we postulate that the wave function is continuous everywhere.

This is plausible since the probability of finding the electron at two points separated by an infinitesimal distance should not change discontinuously.

Then, if the P.E. is continues in the interval $[x_0,x]$, we have

$$u'(x)=u'(x_0)+\frac{2m}{\hbar^2}[V(x_0+\theta\Delta x)-E]u(x_0+\theta x)\Delta x$$

where

$$\theta\in[0,1] \text{ and } \Delta x = x-x_0$$

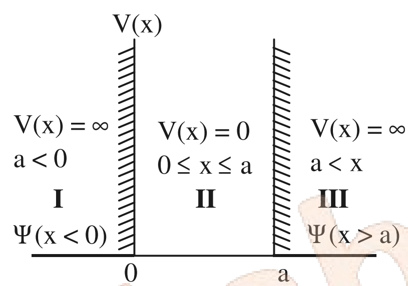
and taking the limit $x \to x_{0+} i.e \Delta x \to 0$ we get

$$\lim_{x \to x_{0+}} \left[u'(x) - u'(x_0)\right] = 0$$

i.e. the derivative of the wfn is also contiuous.

Only at points of infinite discontinuity of the P.E. function does the derivative of the wavefunction exhibit a discontinuity. Such as in the case of particle in a box we can't apply continuity at its boundaries because the potential outside the box is infinity.

Q 2. Derive an expression for particle in a box.



Ans. Schrodinger equation:

In region I and III:

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

$$\Rightarrow \qquad \psi(x) = Ae^{\sqrt{\frac{2m}{\hbar^2}(V-E)x}} + Be^{-\sqrt{\frac{2m}{\hbar^2}(V-E)x}}$$

$$\Rightarrow \qquad \psi(x) = \begin{cases} Ae^{\sqrt{\frac{2m}{\hbar^2}(V-E)x}} & \text{(For region } I, x<0) \\ Be^{-\sqrt{\frac{2m}{\hbar^2}(V-E)x}} & \text{(For region } II, x>a) \end{cases}$$

But V(x)=∞,

$\therefore \psi(x) = 0$ for both cases.

Now work on region II with V(x)=0

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi + V\psi = E\psi \Rightarrow \frac{\partial^2}{\partial x^2}\psi = -\frac{2m}{\hbar^2}E\psi \qquad (\because V=0)$$

$$\Rightarrow \psi(x) = Ae^{i\sqrt{\frac{2mE}{\hbar^2}}x} + Be^{-i\sqrt{\frac{2mE}{\hbar^2}}x}$$

Let $$K = \sqrt{\frac{2mE}{\hbar^2}}$$

Continuity at x=0 :

$$\psi_I(0) = \psi_{II}(0) \Rightarrow 0 = A + B \Rightarrow B = -A$$

Continuity at x=a :

$$\psi_I(a) = \psi_{II}(a) \Rightarrow 0 = Ae^{ika} + Be^{-ika}$$

$$\Rightarrow \quad 0 = Ae^{ika} - Ae^{-ika} \qquad (\because B = -A)$$

$$\Rightarrow \quad A \sin ka = 0$$

$$\Rightarrow \quad Ka = n\pi \qquad n = 1, 2, 3, ..., 4$$

1. $n \neq 0$, because $\psi(x)$ will be trivial (i.e. $\psi(x) = 0$) if $n = 0$
2. Take only positive n because negative n represents the same wave function

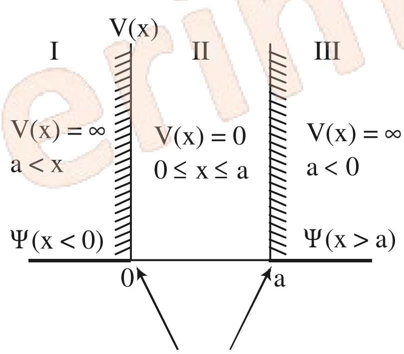
$$\Rightarrow \quad K_n = \frac{n\pi}{a}$$

E_1 is the lowest energy state, so n = 1 is the ground state.

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

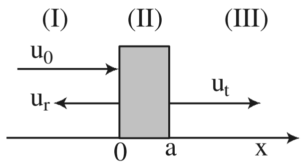
or

$$\psi_n(x) = A \sin\frac{n\pi}{a}x$$



We require Ψ to be continuous at these two points, but not the first derivative Ψ, because V(x) is not continuous at these two points.

Q 3. Derive an expression for potential barrier.



$$V(x)=\begin{cases} 0 & \text{for } x\le 0 \quad (I) \\ V_o>0 & \text{for } 0\le x\le a\ (II) \\ 0 & \text{for } x\ge 0 \quad (III) \end{cases}$$

u_0 is the incident wave

u_r is the reflected wave

u_t is the transmitted wave

Two cases are of interest:

(i) $E<V_o$

(ii) $E>V_o$

(i) Case 1: $E<V_o$

Tise : $u''_I(x)+k^2u_I(x)=0,\ k^2=2mE/\hbar^2$

$$u''_{II}(x)-k^2u_{II}(x)=0,\ k^2=2m(V_0-E)/\hbar^2$$

$$u''_{III}(x)+k^2u_{III}(x)=0$$

General solution: $u_I(x)=Ae^{ikx}+Be^{-ikx}$

$$u_{II}(x)-Ce^{kx}+De^{-kx}$$

$$u_{III}(x)=Fe^{ikx}+Ge^{-ikx}$$

No wave incident from the right: G=0

Continuity at x=0 and x=a:

$$u_I(0)=u_{II}(0) \qquad u_{II}(a)=u_{III}(a)$$
$$u'_I(0)=u'_{II}(0) \qquad u'_{II}(a)=u'_{III}(a)$$

$$A+B=C+D \qquad Ce^{ka}+De^{-ka}=Fe^{ika}$$

$$ik(A-B)=k(c+D) \qquad k(Ce^{ka}-De^{-ka})-ikFe^{ika}$$

i.e we have 4 equations for 5 coefficients (amplitudes).

Our strategy will be to express B and F in terms of A:

B is the amplitude of the reflected wave,

F is the amplitude of the transmitted wave

C and D are of no interest; we shall eliminate them

After solving these equations we get -

$$R = \frac{B^2}{A} = \frac{V_0^{\,2}\sinh^2 ka}{4E(V_0 - E) + V_0^{\,2}\sinh^2 ka}$$

$$T = \frac{F^2}{A} = \frac{4E(V_0 - E}{4E(V_0 - E) + V_0^{\,2}\sinh^2 ka}$$

R is the *reflection coefficient*

T is the *transmission coefficient*

$T+R=1$

R is the probability of the particle being reflected

T is the probability of the particle being transmitted

Contrary to classical expectation, the particle is not completely reflected by the barrier:

Partly it is reflected and partly it is transmitted.

(ii) Case 2: $E>V_0$

for $E>V_0$ we can similarly find the formulae for R and T (Exercise):

$$R = \left|\frac{B}{A}\right|^2 = \frac{V_0^{\,2}\sin^2 Ka}{4E(E - V_0) + V_0^{\,2}\sin^2 Ka};\; K^2 = 2m(E - V_0)/\hbar^2$$

But we do not need to retrieve the formulae: just note that they are related by the transformation $K^2 \to -K^2$

(iii) Case 3: $E = V_0$

Exercise: derive the formulae for this case (a) and (b) from the results of cases 1 and 2 by taking the appropriate limit.

Q 4. Derive an expression for Potential step.

Ans. Potential Step

Consider a potential step described by

$V(x) = V_0$ for $x > 0$ and $V(x) = 0$ for $x < 0$ ...(1)

We will first consider $E > V_0$ and the region of negative x by I and positive x by II and the corresponding wave functions $\psi_I(x)$ and $\psi_{II}(x)$ respectively equation reads

$$\frac{d^2\psi_I}{dx^2} = -k^2\psi_I \text{ where } k = \sqrt{\frac{2mE}{\hbar^2}} \quad ...(2)$$

$$\frac{d^2\psi_{II}}{dx^2} = -q^2\psi_{II} \text{ where } q = \sqrt{\frac{2m(E - V_0)}{\hbar^2}} \quad ...(3)$$

The solution are simple and are linear combination of oscillating exponentials . Recal that if $\psi = (\pm ikx)$, the expectation value of the momentum is $\pm\hbar k$ yielding particle moving to the right and left respectively. Imagine performing an experiment in which we fire particles with energy E from the left only; i.e. there are no particles incident from the right. The particles will be scattered by the potential and yield a part transmitted to $x > 0$ and another reflected back to $x < 0$. Since there are no particles incident from the tight (moving t the left), the term e^{-iqx} will not be present in region II. So we write

$$\psi_{II}(x) = te^{iqx} \quad x > 0\,. \qquad \ldots(4)$$

In the region $x < 0$

$$\psi_I(x) = e^{iqx} + re^{-ikx} \qquad \ldots(5)$$

Where we have set the coefficient of the incident wave to be 1. There is no loss of generality in this since will see that rations of current densities are measured. (Note again that e^{ikx} is traveling to the right and is thus incident on the potential discontinuity) and r and t are the coefficients(amplitudes) of the reflected and transmitted waves respectively. The unknown quantities r and t are determined by using the continuity of ψ and $d\psi/dx$ (denoted by ψ') at $x = 0$. Matching boundary conditions we have

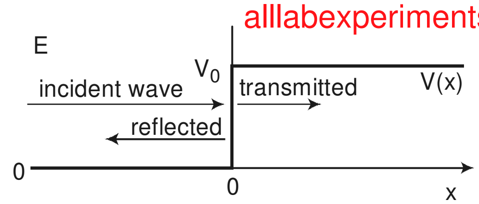
$$\psi_I(x=0): \quad 1 + r = t \quad : \psi_{II}(x=0) \qquad \ldots(6)$$

$$\psi'_I(x=0) \; : \; ik(1-r) = iqt \; : \; \psi'_{II}(x=0) \qquad \ldots(7)$$

which can be solved to obtain

$$r = \frac{k-q}{k+q} \qquad (8)$$

$$t = \frac{2k}{k+q} \qquad (9)$$



Q 5. Find the Eigen values and energy eigen functions of a simple harmonic oscillators using Frobenius method.

Ans. Find this solution in 2017 solved paper.

Q 6. Explain the terms like ground state, zero point energy and uncertainty principle.

Ans. Quantum Harmonic Oscillator: Energy Minimum from uncertainty principle

The ground state for the quantum harmonic oscillator can be shown to be the minimum energy allowed by the uncertainty principle.

The energy of the quantum harmonic oscillator must be at least

$$E = \frac{(\Delta p)^2}{2m} + \frac{1}{2}m\omega^2(\Delta x)^2 \quad \Delta x = \text{position uncertainty}$$

$$\Delta p = \text{momentum uncertainty}$$

Taking the lower limit from the uncertainty principle

$$\Delta x \Delta p = \frac{\hbar}{2}$$

Then the energy in terms of the position uncertainty can be written

$$E = \frac{\hbar^2}{8m(\Delta x)^2} + \frac{1}{2}m\omega^2(\Delta x)^2$$

Minimizing this energy by taking the derivative with respect to the position uncertainty and setting it equal to zero gives

$$-\frac{\hbar^2}{4m(\Delta x)^3} + m\omega^2 \Delta x = 0$$

Solving for the position uncertainty gives

$$\Delta x = \sqrt{\frac{\hbar}{2m\omega}}$$

Substituting gives the minimum value of energy allowed.

$$E_0 = \frac{\hbar}{8m(\Delta x)^2} + \frac{1}{2}m\omega^2(\Delta x)^2 = \frac{\hbar\omega}{4} + \frac{\hbar\omega}{4} = \frac{\hbar\omega}{2}$$

This is a very significant physical result because it tells us that the energy of a system described by a harmonic oscillator potential cannot have zero energy. Physical systems such as arms in a solid lattice or in polygamic in a gas cannot have zero energy even at absolute zero temperature. The energy of the ground vibrational state soften referred to as "zero point vibration." The zero point energy is sufficient to prevent liquid helium-4 from freezing at atmospheric pressure, no matter how low the temperature.

Key Points- Heisenberg's Uncertainty principle doesn't allow to have a zero energy at n = 0 energy level. This state is its ground state and this energy is its Zero point energy.

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