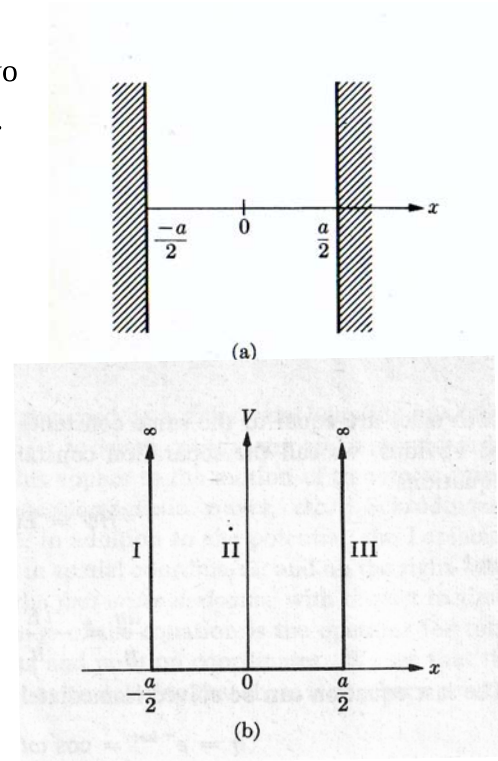
(Lecture 8) Wave Mechanics : Applications

Some of Interested Quantities in Quantum Mechanics :

Bound state's energy levels in Quantun System (atom, nucleus, etc)
Bound state's angular momentum (=spin) and parity
Barrier penetration probability
Quantum transition, decay probability (or rate)
Scattering, reaction probability (or cross section)
etc, etc.

1. The One-dimensional Square Well of Infinite Depth



A particle bouncing back and forth between two impenetrable walls → 1-dim. motion 만 고려.
One dimensional Schrödinger equation :

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

Regions : region I $x \le -a/2$
region II $-a/2 \le x \le a/2$
region III $x \ge a/2$

Region I & III : $V(x) = \infty$ → E 와 $\psi(x)$가 유한이라면 kinetic energy 에 해당되는 항이 $-\infty$이라야 등식 성립 가능 → unphysical (negative and infinite kinetic energy) → $\psi(x) = 0$ 만이 가능한 해.

Region II : $V(x) = 0$ 이므로

$$\frac{d^2\psi}{dx^2}+k^2\psi(x)=0\,, \qquad k=\frac{1}{\hbar}\sqrt{2mE} \qquad (1)$$

→ $\psi(x) = A\sin kx + B\cos kx$

A and B determined by boundary conditions and normalization conditions.

Cf. Consideration of boundary conditions for ψ(x) :

A smooth continuous $\psi(x)$ → continuous function for $d\psi(x)/dx$
A non-smooth continuous $\psi(x)$ → discontinuity in $d\psi(x)/dx$ → $d^2\psi(x)/dx^2$ =

+∞ or -∞ at the joint point → permissible if V(x) = +∞ or -∞ at the joint point

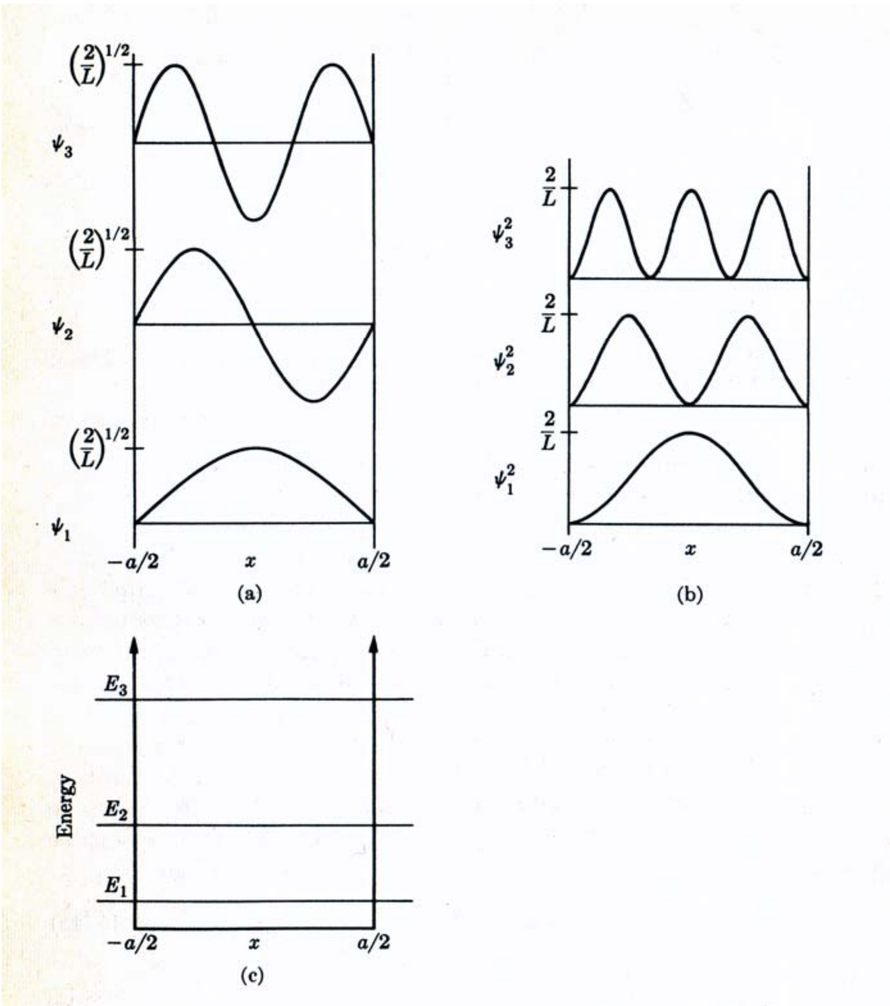
A discontinuous ψ(x) → discontinuity in probability density → no practical physical situation except such as particle creation or death at the point

Boundary conditions at x = +a/2 and –a/2 → ψ(a/2) = ψ(-a/2) = 0

→ ψ(x) = either Asinkx or Bcoskx with ka = nπ (n=integer) (2)

→ For n = odd, $\psi_n(x)$ = Bcoskx (A=0), and

for n = even, $\psi_n(x)$ = Asinkx (B=0) (3)



Eq. (2) → k (or wavelength) quantization

Using eqs. (1)&(2), $E_n = \frac{\pi^2 \hbar^2}{2ma^2} n^2$

Determination of A and B by normalization condition : $\int_{-a/2}^{a/2} \psi^*(x)\psi(x)dx = 1$

$\rightarrow \quad A = B = \sqrt{2/a}$

Expectation Values

$$\langle x \rangle = \int_{-a/2}^{a/2} \frac{2}{a} x \sin^2 kx dx = 0$$

$$\langle p_x \rangle = \int_{-a/2}^{a/2} \frac{2}{a} \sin kx \frac{\hbar}{i} k \cos kx dx = 0$$

$$\langle p_x^2 \rangle = \int_{-a/2}^{a/2} \frac{2}{a} \sin kx (-\hbar^2 k^2)(-\sin kx) dx = \hbar^2 k^2 = \frac{\pi^2 \hbar^2}{a^2} n^2$$

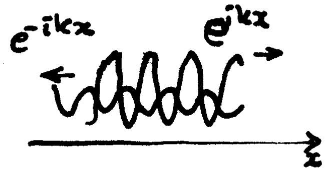
2. Momentum Eigenfunctions

Constant potential or Free space (V=0) :

- Schrödinger equation in one dimension

$$\hat{H}\psi(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\psi(x) \qquad E>0$$

let $\quad p = \sqrt{2mE} = \hbar k \quad \rightarrow \quad k = \frac{1}{\hbar}\sqrt{2mE}$



$$\psi(x) = A \sin kx + B \cos kx$$

or $\quad \psi(x) = C \exp(ikx) + D \exp(-ikx)$

↑motion to +x ↑motion to –x

In other words, these are the momentum eigenfunctions.

$\because \quad \hat{p} \exp(ikx) = -i\hbar \frac{d}{dx} \exp(ikx) = \hbar k \exp(ikx) \quad and \quad \hat{p} \exp(-ikx) = -\hbar k \exp(-ikx)$

Normalization in (-∞, ∞) is not easy !!

$$\because \quad |\exp(ikx)| = |\exp(-ikx)| = 1$$

Box normalization (boundary at $x = \pm L$)

Many particle interpretation :

$|\psi|^2 \quad = \quad$ probabilty density for a single particle

or $\quad = \quad$ average number density of particles

$\psi(x) = C \exp(ikx) \quad \rightarrow \quad |C|^2 \quad$ number density of particles

with velocity $\quad v = \frac{p_x}{m} = \frac{\hbar k}{m}$

$\psi(x) = D\exp(-ikx) \quad \to \quad |D|^2$ number density of particles

with velocity $v = \frac{p_x}{m} = -\frac{\hbar k}{m}$

입자들의 속도가 동일하다면, x-축에 수직인 단위 면적 당, 단위 시간 당 통과하는 입자수 (particle current density **j**):

$+x$ 방향 : $|C|^2 v$ $\qquad$ $-x$ 방향 : $|D|^2 v$

3. Barrier Penetration

non-zero probabilty of existence in the classically forbidden region
(exponentially decaying wave functions)

→ Potential barrier of finite width : probability of barrier penetration 존재

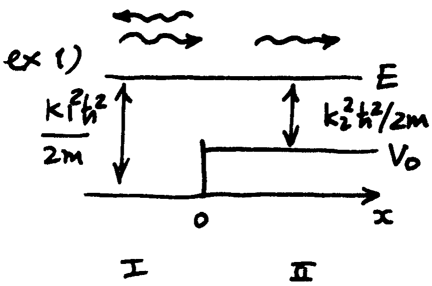
(ex 1) Step Barrier

Classical particle description :

all transmission ($E > V_0$)

Wave mechanics :

partial reflection at potential step ($x > 0$)



왼쪽에서 $S_1 = k_1\hbar/m$ (particles/area·time) 입사

→ 시간 경과 후 정상상태 도달 (Reflected wave and Transmitted wave) 형성

∴ Region-I : $\psi_1(x) = \exp(ik_1x) + R\exp(-ik_1x)$

Region-II : $\psi_2(x) = T\exp(ik_2x)$

$$\text{where} \quad k_1^2 = \frac{2mE}{\hbar^2}, \quad k_2^2 = \frac{1}{\hbar^2}2m(E - V_0)\,.$$

Boundary condition : $\psi_1(0) = \psi_2(0), \quad \psi_1'(0) = \psi_2'(0)$

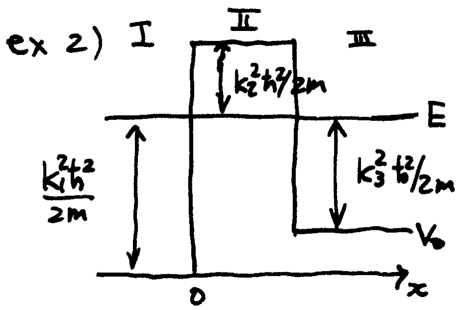
→ $1 + R = T, \quad k_1 - k_1R = k_2T$

$$T = \frac{2k_1}{k_1 + k_2}, \qquad R = \frac{k_1 - k_2}{k_1 + k_2}$$

$$\text{Reflection probability} = \frac{|R|^2(k_1\hbar/m)}{(k_1\hbar/m)} = R^2$$

Transmission prob. $= \dfrac{|T|^2 (k_2 \hbar / m)}{(k_1 \hbar / m)} = \dfrac{k_2}{k_1} T^2$ (transmission coefficient)

(ex 2) Barrier with different ground level



$\psi_1(x) = \exp(ik_1 x) + R\exp(-ik_1 x)$

$\psi_2(x) = C\exp(k_2 x) + D\exp(-k_2 x)$

$\psi_3(x) = T\exp(ik_3 x)$

barrier penetration factor B

= transmission coefficient

$= |T|^2 \dfrac{k_3}{k_1}$

(ex 1)의 경우처럼 유도해 보면,

$$T = \frac{4ik_1 k_2 \exp(-k_2 a)}{(k_1 + ik_2)(k_3 + ik_2) - (k_1 - ik_2)(k_3 - ik_2)\exp(-2k_2 a)},$$

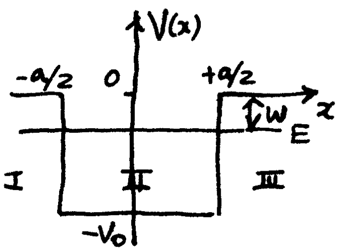
여기서 a 는 Region II Potential 의 width

a가 상당한 두께에 해당할 경우 ($2k_2 a >> 1$), B는 간단하게 근사 표현 가능 → $\exp(-2k_2 a) << 1$ 로서 T의 분모의 두번째 항은 생략 →

$$B = |T|^2 \frac{k_3}{k_1} \approx \frac{16 k_1 k_2^2 k_3}{(k_1^2 + k_2^2)(k_2^2 + k_3^2)} \exp(-2k_2 a) \quad \approx \exp(-2k_2 a),$$

여기서 B의 첫째항은 최대 4 이며 대부분의 경우 1 근방의 값을 가지므로, B값의 크기를 지배하는 항은 $\exp(-2k_2 a) << 1$ 로서 order-of-magnitude 계산에서는 $B \approx \exp(-2k_2 a)$로 충분해 진다.

4. The One-dimensional Square Well Potential



particle is bound → energy E < 0

binding energy W → E = -W (W>0)

classical motion : -a/2 ≤ x ≤ a/2

quantum mechanical motion : -∞ < x < ∞

smaller probabilty in the region x > a/2 and x< -a/2

Regions : region I x ≤ -a/2

region II -a/2 ≤ x ≤ a/2

region III x ≥ a/2

In region II : $V(x) = -V_0, \quad \psi = \psi_{II}(x), \quad E = -W$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_{II}}{dx^2} - V_0\psi_{II}(x) = -W\psi_{II}(x)$$

$$-\frac{d^2\psi_{II}}{dx^2} = \frac{2m}{\hbar^2}(V_0 - W)\psi_{II}(x)$$

$V_0 > W$ 이므로, $\frac{2m}{\hbar^2}\underbrace{(V_0 - W)}_{E_k} \equiv k^2$ 으로두면 (k: wave number in region II)

$$\frac{d^2\psi_{II}}{dx^2} = -k^2\psi_{II}(x) \quad \rightarrow \quad \psi_{II}(x) = A\sin kx + B\cos kx$$

In region I & III : $V(x) = 0, \quad E = -W$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = -W\psi(x) \quad or \quad \frac{d^2\psi}{dx^2} = \frac{2mW}{\hbar^2}\psi(x)$$

앞서와 같이, $\frac{2mW}{\hbar^2} \equiv \gamma^2 \ (>0)$ 으로 놓으면

$$\frac{d^2\psi}{dx^2} - \gamma^2\psi(x) = 0 \quad \rightarrow \quad \psi(x) = C\exp(\gamma x) + D\exp(-\gamma x)$$

Boundary conditions :

region I 에서 $x \rightarrow -\infty$ 일때 $\psi(x) \rightarrow 0$ $\therefore$ D=0 $\quad \psi_I(x) = C\exp(\gamma x)$

region III 에서 $x \rightarrow \infty$ 일때 $\psi(x) \rightarrow 0$ $\therefore$ C=0 $\quad \psi_{II}(x) = D\exp(-\gamma x)$

region II 와의 경계에서 $\psi(x)$는 연속이며 smooth(1 차 미분 연속)

Otherwise, $V(x) \rightarrow \pm\infty$ at the discontinuous point or unsmooth(kinking) point.

$$\psi_I(-a/2) = \psi_{II}(-a/2), \qquad \left.\frac{d\psi_I}{dx}\right|_{x=-a/2} = \left.\frac{d\psi_{II}}{dx}\right|_{x=-a/2}$$

or simply by using logarithmic derivative

$$\left.\frac{1}{\psi_I}\frac{d\psi_I}{dx}\right|_{x=-a/2} = \left.\frac{1}{\psi_{II}}\frac{d\psi_{II}}{dx}\right|_{x=-a/2}$$

$$\rightarrow \quad \gamma = k\cot(-\frac{ka}{2}) \quad \text{if B=0}$$

$$\rightarrow \quad \gamma = -k\tan(-\frac{ka}{2}) \quad \text{if A=0}$$

유사하게 x=a/2 에서 $\left.\frac{1}{\psi_{II}}\frac{d\psi_{II}}{dx}\right|_{x=a/2}=\left.\frac{1}{\psi_{III}}\frac{d\psi_{III}}{dx}\right|_{x=a/2}$

$\rightarrow \quad -\gamma = k\cot(\frac{ka}{2})$ if B=0

$\rightarrow \quad -\gamma = -k\tan(\frac{ka}{2})$ if A=0

위와 동일한 식.

And if both the A and B are nonzero, $\psi_{II}(x) = A'\sin(kx-\delta)$

where $A'\cos\delta = A, \quad -A'\sin\delta = B$

i.e. $A' = \sqrt{A^2+B^2}, \quad \tan\delta = -B/A$

Then, the boundary conditions at x = ±a/2 are

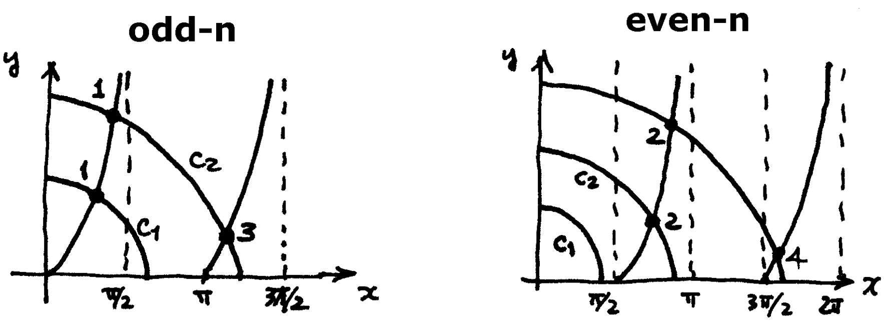
$$\gamma = k\cot(-\frac{ka}{2}-\delta) \quad \text{and} \quad -\gamma = k\cot(\frac{ka}{2}-\delta)$$

i.e. $\cot(-\frac{ka}{2}-\delta) = -\cot(\frac{ka}{2}-\delta) = \cot(-\frac{ka}{2}+\delta)$

이는 $\delta = \frac{n\pi}{2} \quad (n = 1,2,3,\cdots)$ 일때만 성립

→ n = odd means A = 0 (tanδ → +∞ or -∞), ψ(x) : even(symmetric function)

n=even means B = 0 (tanδ=0), ψ(x) : odd(antisymmetric function)



Odd-n solution : $\gamma = k\tan(\frac{ka}{2})$ where $\gamma = \sqrt{\frac{2mW}{\hbar^2}}$ and $k = \sqrt{\frac{2m(V_0-W)}{\hbar^2}}$

are unknown before the solution for W is acquired.

Equations to solve :

$$\frac{\gamma a}{2} = \frac{ka}{2}\tan(\frac{ka}{2}) \quad \text{and} \quad \left(\frac{\gamma a}{2}\right)^2 + \left(\frac{ka}{2}\right)^2 = \left(\frac{a}{2\hbar}\sqrt{2mV_0}\right)^2$$

let $y = \frac{\gamma a}{2}$, $x = \frac{ka}{2}$, then

$$y = x\tan x \quad and \quad x^2 + y^2 = c^2$$

transcendental equation (초월방정식) ← numerical solution

small c(=radius) ↔ shallow potential V_0 ↔ one solution (n=1) only

large c ↔ deep V_0 ↔ n=1, n=3 solutions etc.

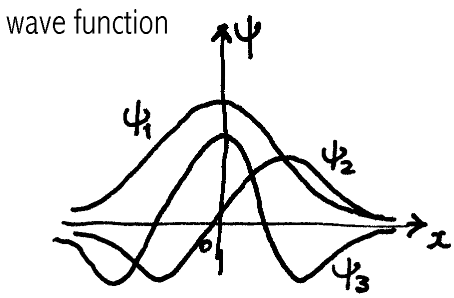
Even-n solution : 위와 같이 진행하면

$$y = -x\cot x \quad and \quad x^2 + y^2 = c^2$$

small c_1 ($<\pi/2$) → no solution (no even-n)

larger c_1 → one or more solution depending on the size of c_1

(n=2 or n=2, 4 or n=2,4,6 etc)



5. The Harmonic Oscillator (HO)

One dimensional HO : $F = -\beta x$, β: spring constant

$$V(x) = (1/2)\beta x^2$$

- Classical solution → $x(t) = A\sin(\omega t+\delta_0)$, $\omega = \sqrt{\beta / m}$ ang. freq.

  Planck's quantization of energy exchange between the HO in the isothermal cavity wall and the EM radiation field : $\Delta E = \hbar\omega$

  ← HO energy levels in steps of $\Delta E = \hbar\omega$?

- Quantum mechanical solution → Schrödinger equation

$$\hat{H}\psi(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + \frac{1}{2}\beta x^2\psi(x) = E\psi(x) \qquad (0)$$

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - \frac{1}{2}\beta x^2)\psi = 0 \qquad (1)$$

change of variables : $\alpha^2 = m\omega/\hbar, \quad \gamma = 2mE/\hbar^2, \quad \xi = \alpha x$

(α^2, γ는 length^{-2} 단위, ξ는 무차원)

$$\frac{d^2\psi}{d\xi^2} + (\frac{\gamma}{\alpha^2} - \xi^2)\psi = 0 \qquad (2)$$

asymptotic behaviour : $\xi^2 \to \infty$, (2) $\to$ $\frac{d^2\psi}{d\xi^2} - \xi^2\psi = 0$

$$\psi_{asym} = B\exp(-\frac{\xi^2}{2})$$

For finite ξ region, try a solution of the type $\psi(\xi) = \exp(-\frac{\xi^2}{2})H(\xi)$

where $H(\xi)$ satisfies

$$H'' - 2\xi H' + (\frac{\gamma}{\alpha^2} - 1)H = 0 \qquad (3)$$

Solution of eq. (3) in the form of power series

$$H(\xi) = a_0 + a_1\xi + a_2\xi^2 + a_3\xi^3 + \cdots \qquad (4)$$

$$H'' = 2a_2 + 3\cdot 2a_3\xi + 4\cdot 3a_4\xi^2 + 5\cdot 4a_5\xi^3 + \cdots$$

$$-2\xi H' = -2\cdot 1a_1\xi - 2\cdot 2a_2\xi^2 - 2\cdot 3a_3\xi^3 - \cdots$$

$$(\frac{\gamma}{\alpha^2} - 1)H = (\frac{\gamma}{\alpha^2} - 1)\left[a_0 + a_1\xi + a_2\xi^2 + a_3\xi^3 + \cdots\right]$$

ξ의 각 지수항 계수들을 정돈하여 0 으로 두면

$$1\cdot 2a_2 + (\frac{\gamma}{\alpha^2} - 1 - 2\cdot 0)a_0 = 0$$

$$2\cdot 3a_3 + (\frac{\gamma}{\alpha^2} - 1 - 2\cdot 1)a_1 = 0$$

$$3\cdot 4a_4 + (\frac{\gamma}{\alpha^2} - 1 - 2\cdot 2)a_2 = 0$$

$$4\cdot 5a_5 + (\frac{\gamma}{\alpha^2} - 1 - 2\cdot 3)a_3 = 0$$

$\cdots \qquad \cdots \qquad \cdots$

$$a_{l+2} = -\frac{(\frac{\gamma}{\alpha^2} - 1 - 2l)}{(l+1)(l+2)}a_l, \qquad l = 0, 1, 2, \text{etc.}$$

All a_l's in terms of a_0, a_1. The a_0, a_1 are determined by b.c.

$$\text{For large } \xi, \quad H(\xi) \rightarrow \xi^{-(\gamma/2\alpha^2+\frac{1}{2})} \exp(\xi^2)$$

$$\psi(\xi) \rightarrow \xi^{-(\gamma/2\alpha^2+\frac{1}{2})} \exp(\frac{\xi^2}{2}) \qquad \text{diverge.}$$

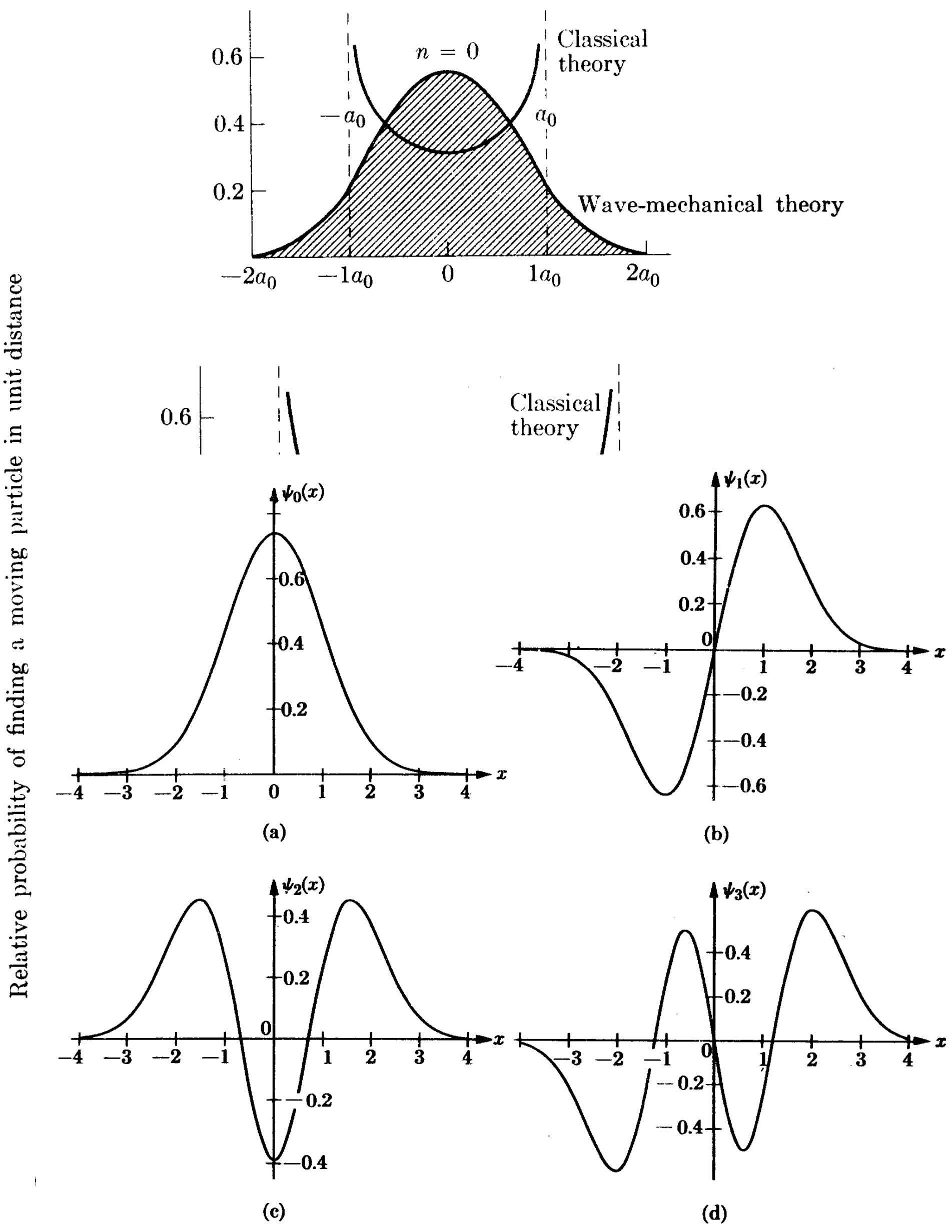


Fig. 6–8 Normalized harmonic-oscillator wave functions for the quantum numbers 0, 1, 2, and 3. [Cf. J. B. Russell, "A Table of Hermite Functions," *J. Math. Phys.* 12, 291 (1933).]

Displacement of the particle

Fig. 6–9 Each diagram shows the relative probability of finding a harmonic oscillator at various displacements both classically and wave-mechanically. Four different energies are shown, corresponding to quantum numbers $n = 0, 1, 2,$ and 5. The classical amplitudes are a_2 for $n = 2$, etc. Thus $2a_0$ is twice the classical amplitude for $n = 0$. Reprinted with permission from Blackwood, Osgood, and Ruark, *An Outline of Atomic Physics*, 3rd ed.

6. Parity (공간 반전 대칭성)

Potential 이 반전 대칭성(=원점 대칭성)을 갖는 경우, 상태 함수 ψ(x)의 특성

- $V(x) = V(-x)$ 대칭 (1)

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

$x \to -x$ 일때 $-\frac{\hbar^2}{2m}\frac{d^2}{d(-x)^2}\psi(-x)+V(-x)\psi(-x)=E\psi(-x)$

즉, $-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(-x)+V(x)\psi(-x)=E\psi(-x)$ (3)

(3)식은 $\psi(-x)$도 eigenvalue E 인 Schrödinger 방정식 해에 해당됨.
따라서 주어진 energy E 의 상태 (선형 독립인 해)가 유일한 경우

$\psi(x) = c\psi(-x)$ (4)

로서 $\psi(x)$, $\psi(-x)$는 상수 factor 로만 다를 수 있는 동일한 상태.

(4) → $\psi(-x) = c\psi(x) = c\cdot c\psi(-x) = c^2\psi(-x)$

$c^2 = 1$ → $c = +1$ or -1 만이 가능.

즉, 원점 대칭 potential 에 대한 상태함수 $\psi(x)$는

$\psi(x) = \psi(-x)$ even function

또는 $\psi(x) = -\psi(-x)$ odd function 만이 가능.

각각의 경우를 positive parity 함수(상태), negative parity 함수(상태)라 하며, 원점에 대해 symmetric wave function, antisymmetric wave function 이라고 각각 일컬음.

Bibliography :

(Basic)

1. R.H. Dicke and J.P. Wittke, Introduction to Quantum Mechanics, Reading, Addison-Wesley Publishing Company, Inc., 1960
2. P.T. Matthews, Introduction to Quantum Mechanics, New York, McGraw-Hill Publishing Company, 1963
3. R.L. White, Basic Quantum Mechanics, New York, McGraw-Hill Publishing Company, 1966

(Intermediate)

4. R. Eisberg and R. Resnick, Quantum Physics of Atoms, Molecules, Solids,

Nuclei and Particles, 2nd Ed., New York, John Wiley & Sons Inc., 1974, 1985
5. L.I. Schiff, Quantum Mechanics, 3rd Ed., Tokyo, McGraw-Hill Kogakusha, Ltd, 1955, 1968
6. A. Messiah, Quantum Mechanics, Vol. I, II, Amsterdam, North-Holland Publishing Company, 1962
7. J.J. Sakurai, Modern Quantum Mechanics, Menlo Park, The Benjamin/ Cummings Publishing Company, Inc., 1985
8. R.P. Feynman, R.B. Leighton, M. Sands, The Feynman Lectures on Physics, Vol. III Quantum Mechanics, Reading, Addison-Wesley Publishing Company, 1965

(Advanced)

9. J.J. Sakurai, Advanced Quantum Mechanics, Menlo Park, Addison-Wesley Publishing Company, Inc., 1967
10. L.D. Landau and E.M. Lifshitz, Quantum Mechanics Non-Relativistic Theory, 3rd Ed., Transl. by J.B. Sykes and J.S. Bell, Oxford, Pergamon Press, 1977
11. P.A.M. Dirac, The Principles of Quantum Mechanics, 4th Ed., Oxford, Clarendon Press, 1958
12. J. von Neumann, Mathematische Grundlagen der Quantenmechanik, Berlin, Julius Springer-Verlag, 1932, (English translation : Mathematical Foundations of Quantum Mechanics, transl. by R. T. Beyer, Princeton, Princeton University Press, 1955)
13. H. Weyl, Gruppentheorie und Quantenmechanik, 2nd Ed., Hirzel, Leipzig, 1930 (English translation : The Theory of Groups and Quantum Mechanics, transl. by H. P. Robertson, New York, Dover Publication, Inc., 1950)