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Syllabus

Course Meeting Times

Lectures: 2 sessions / week, 1.5 hours / session

Recitations: 2 sessions / week, 1 hour / session

Course Description

Quantum Physics I explores the experimental basis of quantum mechanics, including:

- Photoelectric effect
- Compton scattering
- Photons
- Franck-Hertz experiment
- The Bohr atom, electron diffraction
- deBroglie waves
- Wave-particle duality of matter and light

This class also provides an introduction to wave mechanics, via:

- Schrödinger's equation
- Wave functions
- Wave packets
- Probability amplitudes
- Stationary states
- The Heisenberg uncertainty principle
- Zero-point energies
- Solutions to Schrödinger's equation in one dimension
  - Transmission and reflection at a barrier
  - Barrier penetration
  - Potential wells
  - The simple harmonic oscillator
- Schrödinger's equation in three dimensions
  - Central potentials
  - Introduction to hydrogenic systems

Prerequisites

In order to register for 8.04, students must have previously completed Vibrations and Waves (8.03) or Electrodynamics (6.014), and Differential Equations (18.03 or 18.034) with a grade of C or higher.

Textbooks

Required

Buy at Amazon Gasiorowicz, Stephen. *Quantum Physics*. 3rd ed. Hoboken, NJ: Wiley, 2003. ISBN: 9780471057000.

Strongly Recommended

Buy at Amazon French, A. P., and Edwin F. Taylor. *Introduction to Quantum Physics*. New York, NY: Norton, 1978. ISBN: 9780393090154.

Read Again and Again

Feynman, Richard P., Robert B. Leighton, and Matthew L. Sands. *The Feynman Lectures on Physics: Commemorative Issue*. Vol. 3. Redwood City, CA: Addison-Wesley, 1989. ISBN: 9780201510058.

References

Liboff, Richard L. *Introductory Quantum Mechanics*. 4th ed. San Francisco, CA: Addison Wesley, 2003. ISBN: 9780805387148.

Eisberg, Robert Martin, and Robert Resnick. *Quantum Physics of Atoms, Molecules, Solids, Nuclei, and Particles*. New York, NY: Wiley, 1974. ISBN: 9780471873730.

Problem Sets

The weekly problem sets are an essential part of the course. Working through these problems is crucial to understanding the material deeply. After attempting each problem by yourself, we encourage you to discuss the problems with the teaching staff and with each other--this is an excellent way to learn physics! **However, you must write-up your solutions by yourself**. Your solutions should not be transcriptions or reproductions of someone else's work.

Exams

There will be two in-class exams. There will also be a comprehensive final exam, scheduled by the registrar and held during the final exam period.

Grading Policy

ACTIVITIES	PERCENTAGES
Exam 1	20%
Exam 2	20%
Final exam	40%
Problem sets	20%

Calendar

LEC #	TOPICS
1	Overview, scale of quantum mechanics, boundary between classical and quantum phenomena
2	Planck's constant, interference, Fermat's principle of least time, deBroglie wavelength
3	Double slit experiment with electrons and photons, wave particle duality, Heisenberg uncertainty
4	Wavefunctions and wavepackets, probability and probability amplitude, probability density
5	Thomson atom, Rutherford scattering
6	Photoelectric effect, X-rays, Compton scattering, Franck Hertz experiment
7	Bohr model, hydrogen spectral lines
8	Bohr correspondence principle, shortcomings of Bohr model, Wilson-Sommerfeld quantization rules
9	Schrödinger equation in one dimension, infinite 1D well
	In-class exam 1
10	Eigenfunctions as basis, interpretation of expansion coefficients, measurement
11	Operators and expectation values, time evolution of eigenstates, classical limit, Ehrenfest's theorem
12	Eigenfunctions of p and x, Dirac delta function, Fourier transform
13	Wavefunctions and operators in position and momentum space, commutators and uncertainty
14	Motion of wavepackets, group velocity and stationary phase, 1D scattering off potential step
15	Boundary conditions, 1D problems: Finite square well, delta function potential
16	More 1D problems, tunneling
17	Harmonic oscillator: Series method
	In-class exam 2

18	Harmonic oscillator: Operator method, Dirac notation
19	Schrödinger equation in 3D: Cartesian, spherical coordinates
20	Angular momentum, simultaneous eigenfunctions
21	Spherical harmonics
22	Hydrogen atom: Radial equation
23	Hydrogen atom: 3D eigenfunctions and spectrum
24	Entanglement, Einstein-Podolsky Rosen paradox
	Final exam

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Lecture Notes

The lecture notes were typed by Morris Green, an MIT student, from Prof. Vuletic's handwritten notes.

LEC #	TOPICS
1	Overview, scale of quantum mechanics, boundary between classical and quantum phenomena (PDF)
2	Planck's constant, interference, Fermat's principle of least time, deBroglie wavelength (PDF)
3	Double slit experiment with electrons and photons, wave particle duality, Heisenberg uncertainty (PDF)
4	Wavefunctions and wavepackets, probability and probability amplitude, probability density (PDF)
5	Thomson atom, Rutherford scattering (PDF)
6	Photoelectric effect, X-rays, Compton scattering, Franck Hertz experiment (PDF)
7	Bohr model, hydrogen spectral lines (PDF)
8	Bohr correspondence principle, shortcomings of Bohr model, Wilson-Sommerfeld quantization rules (PDF)
9	Schrödinger equation in one dimension, infinite 1D well (PDF)
10	Eigenfunctions as basis, interpretation of expansion coefficients, measurement (PDF)
11	Operators and expectation values, time evolution of eigenstates, classical limit, Ehrenfest's theorem (PDF)
12	Eigenfunctions of p and x, Dirac delta function, Fourier transform (PDF)
13	Wavefunctions and operators in position and momentum space, commutators and uncertainty (PDF)
14	Motion of wavepackets, group velocity and stationary phase, 1D scattering off potential step (PDF)
15	Boundary conditions, 1D problems: finite square well, delta function potential (PDF)
16	More 1D problems, tunneling (PDF)
17	Harmonic oscillator: series method (PDF)
18	Harmonic oscillator: operator method, Dirac notation (PDF)
19	Schrödinger equation in 3D: cartesian, spherical coordinates (PDF)
20	Angular momentum, simultaneous eigenfunctions (PDF)
21	Spherical harmonics (PDF)
22	Hydrogen atom: radial equation (PDF)
23	Hydrogen atom: 3D eigenfunctions and spectrum (PDF)
24	Entanglement, Einstein-Podolsky Rosen paradox (PDF)

Lecture 2

1. ✓ Natural Units

2. ✓ Degeneracy
   ↓
   No degeneracy in one dimensional bound state problem.

3. ✓ Sudden expansion

4. ✓ Spread of the wave function

5. ✓ Classical limits of simple harmonic oscillator

6. ✓ Commutator and Heisenberg's Equation of Motion.

The Art of Estimation Physics

also known as **Ph 239**

I. "Natural Units"

Patrick Diamond, George M. Fuller, Tom Murphy
***Department of Physics, University of California, San Diego,* 2012**

Richard Feynman :

“use sloppy thinking”

“never attempt a physics problem
until you know the answer”

“Natural Units”

In this system of units there is only one fundamental dimension, *energy.* This is accomplished by setting Planck’s constant, the speed of light, and Boltzmann’s constant to unity, *i.e.,*

$$\hbar = c = k_{\rm B} = 1$$

By doing this most any quantity can be expressed as powers of energy, because now we easily can arrange for

$$[\text{Energy}] = [\text{Mass}] = [\text{Temperature}] = [\text{Length}]^{-1} = [\text{Time}]^{-1}$$

To restore “normal” units we need only insert appropriate powers of of the fundamental constants above

It helps to remember the dimensions of these quantities . . .

$$[\hbar c] = [\text{Energy}] \cdot [\text{Length}]$$

$$[c] = [\text{Length}] \cdot [\text{Time}]^{-1}$$

for example, picking convenient units (*for me!*)

$$\hbar\, c \approx 197.33 \text{ MeV fm}$$

$$c \approx 2.9979 \times 10^{23} \text{ fm s}^{-1}$$

length units

$$1\,\text{fm} = 10^{-13}\,\text{cm} = 10^{-15}\,\text{m}$$

$$1\,\text{Å} = 10^{-8}\,\text{cm} = 10^{-10}\,\text{m} = 0.1\,\text{nm}$$

Figure of merit for typical visible light wavelength and corresponding energy

$$\lambda = 10^4\,\text{Å} = 10^3\,\text{nm}$$

$$E = h\nu = 2\pi\hbar\nu = 2\pi\frac{\hbar c}{\lambda}$$

$$E = 2\pi\frac{\hbar c}{\lambda} = 2\pi\frac{1.9733\times 10^3\,\text{eV}\,\text{Å}}{10^4\,\text{Å}} \approx 1.24\,\text{eV}$$

Boltzmann's constant

– from now on measure temperature in energy units

$$[k_\mathrm{B}] = \frac{[\mathrm{Energy}]}{\mathrm{Kelvin}}$$

for example . . .

$$k_\mathrm{B} = \frac{8.617 \times 10^{-5}\,\mathrm{eV}}{\mathrm{Kelvin}} \sim 10^{-4}\ \frac{\mathrm{eV}}{\mathrm{K}}$$

but I like $k_\mathrm{B} = 0.08617\ \ \mathrm{MeV}/T9$

with $T9 \equiv \dfrac{T}{10^9\,\mathrm{K}}$

Examples:

Number Density

$$n = \frac{\#}{\text{volume}} = \frac{\#}{[\text{Length}]^3} = [\text{Energy}]^3$$

$$[n] = \text{MeV}^3 = \frac{\text{MeV}^3}{(\hbar c)^3} = \frac{1}{(\text{fm})^3}$$

e.g., number density of photons in thermal equilibrium at temperature T= 1 MeV

$$n_\gamma = \frac{2\,\zeta(3)}{\pi^2} T^3 \approx \frac{2 \cdot (1.20206)}{\pi^2} T^3 \approx 0.2436\, T^3$$

$$= 0.2436\ \text{MeV}^3 = \frac{0.2436\,\text{MeV}^3}{(\hbar c)^3} = \frac{0.2436\,\text{MeV}^3}{(197.33\,\text{MeV fm})^3} = 3.170 \times 10^{-8}\,\text{fm}^{-3}$$

$$\approx 3.17 \times 10^{31}\,\text{cm}^{-3}$$

stresses

e.g., energy density, pressure, shear stress, *etc.*

$$[\mathrm{Pressure}] = \frac{[\mathrm{Force}]}{[\mathrm{Area}]} = \frac{[\mathrm{Force}]}{[\mathrm{Area}]} \cdot \frac{[\mathrm{Length}]}{[\mathrm{Length}]} = \frac{[\mathrm{Energy}]}{[\mathrm{Volume}]} = [\mathrm{Energy}]^4$$

another example . . .

A quantum mechanics text gives the Bohr radius as $a_0 = \frac{\hbar^2}{m_e e^2}$

But I see this as . . .

$$a_0 = \frac{1}{m_e e^2} = \frac{\hbar c}{e^2} \cdot \frac{\hbar c}{m_e} = (137.036) \cdot \frac{197.33\,\text{Mev fm}}{0.511\,\text{MeV}} = 0.52918\,\text{Å}$$

or whatever units you prefer . . .

$$\hbar c \approx 1.9733 \times 10^{-5}\ \mathrm{eV\ cm}$$
$$c \approx 2.9979 \times 10^{10}\ \mathrm{cm\ s^{-1}}$$

or maybe even . . .

$$\hbar c \approx 1.9733 \times 10^{3}\ \mathrm{eV\ \AA}$$
$$c \approx 2.9979 \times 10^{18}\ \mathrm{\AA\ s^{-1}}$$

OK, why not use ***ergs*** or ***Joules*** and ***centimeters*** or ***meters*** ?

You can if you want but . . .

better to be like **Hans Bethe** and use units scaled to the problem at hand

size of a nucleon/nucleus ~ 1 fm
energy levels in a nucleus ~ 1 MeV

atomic/molecular sizes $\sim$ Å
atomic/molecular energies $\sim$ eV

supernova explosion energy $1\ \mathrm{Bethe} \equiv 10^{51}\ \mathrm{erg}$

electric charge and potentials/energies

one elementary charge $1\ e \approx 1.6022 \times 10^{-19}$ Coulombs

One Coulomb falling through a potential difference of 1 Volt = 1 Joule= 10^7 erg

$$1\ \mathrm{eV} \approx 1.6022 \times 10^{-19}\ \mathrm{J} = 1.6022 \times 10^{-12}\ \mathrm{erg}$$

or

$$1\ \mathrm{MeV} \approx 1.6022 \times 10^{-6}\ \mathrm{erg}$$

$$1\ \mathrm{erg} \approx 6.241 \times 10^{5}\ \mathrm{MeV} \sim 10^{6}\ \mathrm{MeV}$$

fine structure constant α_{em}

SI $$\frac{e^2}{4\pi\epsilon_0\ \hbar c} \approx \frac{1}{137.036}$$

cgs $$\frac{e^2}{\hbar c} \approx \frac{1}{137.036}$$

particle masses, atomic dimensions, *etc.*

electron rest mass $$m_\mathrm{e} \approx 0.511\,\mathrm{MeV}$$

proton rest mass $$m_\mathrm{p} \approx 938.26\,\mathrm{MeV}$$

neutron-proton mass difference $$m_\mathrm{n} - m_\mathrm{p} \approx 1.293\,\mathrm{MeV}$$

atomic mass unit $$1\ \mathrm{amu} \approx 931.494\,\mathrm{MeV}$$

Avogadro's number $$N_\mathrm{A} \approx 6.022 \times 10^{23}\,\frac{\mathrm{amu}}{\mathrm{g}}$$

Handy Facts: Solar System

solar mass $M_{\odot} \approx 1.989 \times 10^{33}\,\mathrm{g} \approx 10^{60}\,\mathrm{MeV}$

solar radius $R_{\odot} \approx 6.9598 \times 10^{10}\,\mathrm{cm}$

solar luminosity $L_{\odot} \approx 3.9 \times 10^{33}\,\mathrm{erg\,s^{-1}}$

$1\,\mathrm{A.U.} \approx 1.4960 \times 10^{13}\,\mathrm{cm}$ radius of earth's orbit around sun

earth mass $M_{\mathrm{earth}} \approx 3 \times 10^{-6}\,M_{\odot}$ $M_{\mathrm{Jupiter}} \sim 300\,M_{\mathrm{earth}} \sim 10^{-3}\,\mathrm{M}_{\odot}$

earth radius $R_{\mathrm{earth}} \approx 6.3782 \times 10^{8}\,\mathrm{cm} \sim 10^{-2}\,R_{\odot}$

Jupiter orbital radius $\sim 5\,\mathrm{A.U.}$

solar system diameter $\sim 100\,\mathrm{A.U.}$

sidereal day $\approx 8.6164091 \times 10^{4}\,\mathrm{s} \sim 10^{5}\,\mathrm{s}$

sidereal year $\approx 3.1558 \times 10^{7}\,\mathrm{s} \sim \pi \times 10^{7}\,\mathrm{s} \sim 3 \times 10^{7}\,\mathrm{s}$

1 dog year $\approx 7.0000\,\mathrm{yr}$

We can do all this for spacetime too !

Define the Planck Mass $$m_{\rm pl} \equiv \left(\frac{\hbar c}{\rm G}\right)^{1/2}$$

$$m_{\rm pl} \approx 1.2211 \times 10^{22}\,{\rm MeV} \sim 10^{22}\,{\rm MeV}$$

. . . and now the Gravitational constant is just . . . $${\rm G} = \frac{1}{m_{\rm pl}^2}$$

The essence of General Relativity:

There is no gravitation: in *locally* inertial coordinate systems, which the Equivalence Principle guarantees are always there, the effects of gravitation are absent!

The Einstein Field equations have as their solutions global coordinate systems which cover big patches of spacetime

A convenient coordinate system for
***weak* & *static* (no time dependence) gravitational fields**
is given by the following coordinate system/metric:

$$ds^2 = -(1+2\varphi)dt^2 + (1-2\varphi)\left(dx^2 + dy^2 + dz^2\right)$$

This would be a decent description of the spacetime geometry and gravitational effects around the earth, the sun, and white dwarf stars, but not near the surfaces of neutron stars.

It turns out that in a weak gravitational field the time-time component of the metric is related to the Newtonian gravitational potential by . . .

$$g_{0\,0} \approx -1 - 2\varphi$$

Where the Newtonian gravitational potential is $\varphi \approx -\frac{G\,M}{R}$

$$G \equiv \frac{1}{m_{\rm pl}^2}$$

$$m_{\rm pl} \approx 1.221 \times 10^{22}\,\text{MeV}$$

$$\hbar\,c \approx 197.33\,\text{MeV fm}$$

$$1\,\text{fm} = 10^{-13}\,\text{cm}$$

$$1\,\text{MeV} \approx 1.6022 \times 10^{-13}\,\text{Joules}$$

$$\varphi \approx -\frac{M\,\hbar\,c}{m_{\rm pl}^2\,R}$$

dimensionless !

Characteristic Metric Deviation

OBJECT	MASS (solar masses)	RADIUS (cm)	Newtonian Gravitational Potential
earth	3×10^{-6}	6.4×10^{8}	$\sim 10^{-9}$
sun	1	6.9×10^{10}	$\sim 10^{-6}$
white dwarf	~1	5×10^{8}	$\sim 10^{-4}$
neutron star	~1	10^{6}	~0.1 to 0.2

Handy Facts: the Universe

$$1 \text{ parsec (pc)} \approx 3.2615 \text{ light year (l.y.)}$$

$$1 \text{ mega} - \text{parsec (Mpc)} \approx 3.0856 \times 10^{24} \text{ cm} \quad \sim 3 \times 10^{24} \text{ cm}$$

size galaxy $\sim 1\,\mathrm{Mpc}$, $10^{12}\,M_\odot$ dark matter

size galaxy (visible/baryons) $\sim 100\,\mathrm{kpc}$, $10^{11}\,M_\odot$ baryons

galaxy density (inside causal horizon) $\sim 1\,\mathrm{Mpc}^{-3}$

big galaxy clusters $\sim$ 1000 galaxies

Virgo Cluster distance $\sim 16\,\mathrm{Mpc}$

Coma Cluster distance $\sim 55\,\mathrm{Mpc}$

$$\mathrm{H_0} = \text{expansion rate of universe (current epoch)} = (100\ \mathrm{h})\ \mathrm{km\ s^{-1}\ Mpc^{-1}}$$

$$\mathrm{h} \approx 0.71 \quad \textit{e.g.},\ \text{WMAP3}$$

$$\mathrm{H_0} \approx \left(2.13 \times 10^{-39}\,\mathrm{MeV}\right)\ \mathrm{h} \approx \left(3.24 \times 10^{-18}\,\mathrm{s^{-1}}\right)\ \mathrm{h}$$

$$\mathrm{H_0^{-1}} \approx (9.78\,\mathrm{Gyr})\,\mathrm{h^{-1}} \qquad \text{age of universe} \approx 13.7\,\mathrm{Gyr}$$

$$\Omega \equiv \text{closure fraction} = \frac{\rho}{\rho_c} \qquad \Omega_{\text{Dark Matter}} \approx 0.23 \qquad \Omega_{\text{vac}} \approx 0.73 \qquad \Omega_{\text{baryon}} \approx 0.04$$

$$\rho_c = \text{closure density} = \frac{3\mathrm{H_0^2}}{8\pi G} = \frac{3}{8\pi}\,\mathrm{H_0^2}\,m_{\mathrm{pl}}^2 \approx \left(8.1 \times 10^{-35}\,\mathrm{MeV^4}\right)\ \mathrm{h^2}$$

$$\approx \left(1.054 \times 10^{4}\,\mathrm{eV\,cm^{-3}}\right)\ \mathrm{h^2} \sim 10^{-5}\ \frac{\mathrm{amu}}{\mathrm{cm^3}}$$

$$\rho_{\text{vac}} = \text{dark energy density} \approx \left(3.9\ \frac{\mathrm{keV}}{\mathrm{cm^3}}\right) \cdot \left(\frac{\mathrm{h}}{0.71}\right)^2 \cdot \left(\frac{\Omega_{\text{vac}}}{0.73}\right) \sim 4\,\mathrm{keV\,cm^{-3}}$$

Rates and Cross Sections

$$[\mathrm{Rate}] = [\mathrm{Flux}] \cdot [\mathrm{Cross\ Section}]$$

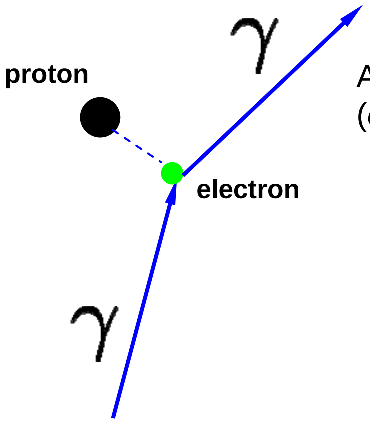
$$[\mathrm{s}^{-1}] = \left[\frac{\#}{\mathrm{cm}^2\ \mathrm{s}}\right] \cdot [\mathrm{cm}^2]$$

Eddington Luminosity

Photon scattering-induced momentum transfer rate to electrons/protons must be less than gravitational force on proton

$$\gamma + e \rightarrow e + \gamma$$

Electrons tied to protons via Coulomb force



Sir Arthur Eddington
www.sil.si.edu

At radius r where interior mass is $M(r)$ and photon energy luminosity (*e.g.*, in ergs s^{-1}) is $L_\gamma(r)$ the forces are equal when

$$\frac{L_\gamma(r)}{4\pi r^2 c} \cdot \sigma_T = \frac{G\, M(r)\, m_p}{r^2}$$

Flux of photon momentum

Gravitational force on proton with mass m_p

Thomson cross section $\sigma_T \approx 6.65 \times 10^{-25}\,\mathrm{cm}^2 \sim 10^{-24}\,\mathrm{cm}^2 = 1\,\mathrm{barn}$

$$\Rightarrow \quad L_\gamma^{\mathrm{Eddington}} = \frac{4\pi G\, M\, m_p c}{\sigma_T} = 4\pi \left[\frac{M\, m_p}{m_{pl}^2}\right] \frac{(\hbar c)c}{\sigma_T}$$

$$\approx 10^{38}\,\mathrm{erg\,s}^{-1} \left[\frac{M}{M_\odot}\right]$$

Natural units

In physics, **natural units** are physical units of measurement based only on universal physical constants. For example the elementary charge *e* is a natural unit of electric charge, and the speed of light *c* is a natural unit of speed. A purely natural system of units is defined in such a way that some set of selected universal physical constants are each normalized to unity; that is, their numerical values in terms of these units are exactly 1. While this has the advantage of simplicity, there is a potential disadvantage in terms of loss of clarity and understanding, as these constants are then omitted from mathematical expressions of physical laws.

Introduction

Natural units are intended to elegantly simplify particular algebraic expressions appearing in the laws of physics or to normalize some chosen physical quantities that are properties of universal elementary particles and are reasonably believed to be constant. However there is a choice of the set of natural units chosen, and quantities which are set to unity in one system may take a different value or even assumed to vary in another natural unit system.

Natural units are "natural" because the origin of their definition comes only from properties of nature and not from any human construct. Planck units are often, without qualification, called "natural units", although they constitute only one of several systems of natural units, albeit the best known such system. Planck units (up to a simple multiplier for each unit) might be considered one of the most "natural" systems in that the set of units is not based on properties of any prototype, object, or particle but are solely derived from the properties of free space.

As with other systems of units, the base units of a set of natural units will include definitions and values for length, mass, time, temperature, and electric charge (in lieu of electric current). Some physicists do not recognize temperature as a fundamental physical quantity, since it expresses the energy per degree of freedom of a particle, which can be expressed in terms of energy (or mass, length, and time). Virtually every system of natural units normalizes Boltzmann's constant k_B to 1, which can be thought of as simply a way of defining the unit temperature.

In the SI unit system, electric charge is a separate fundamental dimension of physical quantity, but in natural unit systems charge is expressed in terms of the mechanical units of mass, length, and time, similarly to cgs. There are two common ways to relate charge to mass, length, and time: In Lorentz–Heaviside units (also called "rationalized"), Coulomb's law is $F = q_1 q_2/(4\pi r^2)$, and in Gaussian units (also called "non-rationalized"), Coulomb's law is $F = q_1 q_2/r^2$.[1] Both possibilities are incorporated into different natural unit systems.

Notation and use

Natural units are most commonly used by *setting the units to one*. For example, many natural unit systems include the equation $c = 1$ in the unit-system definition, where c is the speed of light. If a velocity v is half the speed of light, then as $v = \frac{1}{2}c$ and $c = 1$, hence $v = \frac{1}{2}$. The equation $v = \frac{1}{2}$ means "the velocity v has the value one-half when measured in Planck units", or "the velocity v is one-half the Planck unit of velocity".

The equation $c = 1$ can be plugged in anywhere else. For example, Einstein's equation $E = mc^2$ can be rewritten in Planck units as $E = m$. This equation means "The rest-energy of a particle, measured in Planck units of energy, equals the rest-mass of a particle, measured in Planck units of mass."

Advantages and disadvantages

Compared to SI or other unit systems, natural units have both advantages and disadvantages:

- **Simplified equations:** By setting constants to 1, equations containing those constants appear more compact and in some cases may be simpler to understand. For example, the special relativity equation $E^2 = p^2c^2 + m^2c^4$ appears somewhat complicated, but the natural units version, $E^2 = p^2 + m^2$, appears simpler.
- **Physical interpretation:** Natural unit systems automatically subsume dimensional analysis. For example, in Planck units, the units are defined by properties of quantum mechanics and gravity. Not coincidentally, the Planck unit of length is approximately the distance at which quantum gravity effects become important. Likewise, atomic units are based on the mass and charge of an electron, and not coincidentally the atomic unit of length is the Bohr radius describing the orbit of the electron in a hydrogen atom.
- **No prototypes:** A prototype is a physical object that defines a unit, such as the International Prototype Kilogram, a physical cylinder of metal whose mass is by definition exactly one kilogram. A prototype definition always has imperfect reproducibility between different places and between different times, and it is an advantage of natural unit systems that they use no prototypes. (They share this advantage with other *non-natural* unit systems, such as conventional electrical units.)
- **Less precise measurements:** SI units are designed to be used in precision measurements. For example, the second is defined by an atomic transition frequency in cesium atoms, because this transition frequency can be precisely reproduced with atomic clock technology. Natural unit systems are generally *not* based on quantities that can be precisely reproduced in a lab. Therefore, in order to retain the same degree of precision, the fundamental constants used still have to be measured in a laboratory in terms of physical objects that can be directly observed. If this is not possible, then a quantity expressed in natural units can be less precise than the same quantity expressed in SI units. For example, Planck units use the gravitational constant G, which is measurable in a laboratory only to four significant digits.
- **Greater ambiguity:** Consider the equation $a = 10^{10}$ in Planck units. If a represents a length, then the equation means $a = 16 \times 10^{-25}$ m. If a represents a mass, then the equation means $a = 220$ kg. Therefore, if the variable a was not clearly defined, then the equation $a = 10^{10}$ might be misinterpreted. By contrast, in SI units, the equation would be (for example) $a = 220$ kg, and it would be clear that a represents a mass, not a length or anything else. In fact, natural units are especially useful when this ambiguity is *deliberate*: For example, in special relativity space and time are so closely related that it can be useful not to have to specify whether a variable represents a distance or a time.

Choosing constants to normalize

Out of the many physical constants, the designer of a system of natural unit systems must choose a few of these constants to normalize (set equal to 1). It is not possible to normalize just *any* set of constants. For example, the mass of a proton and the mass of an electron cannot both be normalized: if the mass of an electron is defined to be 1, then the mass of a proton has to be ≈1836. In a less trivial example, the fine-structure constant, α≈1/137, cannot be set to 1, because it is a dimensionless number. The fine-structure constant is related to other fundamental constants

$$\alpha = \frac{k_{\mathrm{e}}e^2}{\hbar c},$$

where k_e is the Coulomb constant, e is the elementary charge, $\hbar$ is the reduced Planck constant, and c is the speed of light. Therefore it is not possible to simultaneously normalize all four of the constants c, $\hbar$, e, and k_e.

Electromagnetism units

In SI units, electric charge is expressed in coulombs, a separate unit which is additional to the "mechanical" units (mass, length, time), even though the traditional definition of the ampere refers to some of these other units. In natural unit systems, however, electric charge has units of $[\text{mass}]^{1/2}$ $[\text{length}]^{3/2}$ $[\text{time}]^{-1}$.

There are two main natural unit systems for electromagnetism:

- **Lorentz–Heaviside units** (classified as a **rationalized** system of electromagnetism units).
- **Gaussian units** (classified as a **non-rationalized** system of electromagnetism units).

Of these, Heaviside-Lorentz is somewhat more common,[2] mainly because Maxwell's equations are simpler in Lorentz-Heaviside units than they are in Gaussian units.

In the two unit systems, the elementary charge *e* satisfies:

- $e = \sqrt{4\pi\alpha\hbar c}$ (Lorentz–Heaviside),
- $e = \sqrt{\alpha\hbar c}$ (Gaussian)

where $\hbar$ is the reduced Planck constant, *c* is the speed of light, and $\alpha \approx 1/137$ is the fine-structure constant.

In a natural unit system where *c*=1, Lorentz-Heaviside units can be derived from SI units by setting $\varepsilon_0 = \mu_0 = 1$. Gaussian units can be derived from SI units by a more complicated set of transformations, such as dividing all electric fields by $\sqrt{4\pi\epsilon_0}$, multiplying all magnetic susceptibilities by 4π, and so on.[3]

Systems of natural units

Planck units

Quantity	Expression	Metric value	Name
Length (L)	$l_P = \sqrt{\frac{\hbar G}{c^3}}$	1.616×10^{-35} m	Planck length
Mass (M)	$m_P = \sqrt{\frac{\hbar c}{G}}$	2.176×10^{-8} kg	Planck mass
Time (T)	$t_P = \sqrt{\frac{\hbar G}{c^5}}$	5.3912×10^{-44} s	Planck time
Temperature (Θ)	$T_P = \sqrt{\frac{\hbar c^5}{G {k_B}^2}}$	1.417×10^{32} K	Planck temperature
Electric charge (Q)	$q_P = e/\sqrt{4\pi\alpha}$ (L–H)	5.291×10^{-18} C	
	$q_P = e/\sqrt{\alpha}$ (G)	1.876×10^{-18} C	

Planck units are defined by

$$c = G = \hbar = k_B = 1$$

where *c* is the speed of light, *G* is the gravitational constant, $\hbar$ is the reduced Planck constant, and k_B is the Boltzmann constant.

Planck units are a system of natural units that is not defined in terms of properties of any prototype, physical object, or even elementary particle. They only refer to the basic structure of the laws of physics: *c* and *G* are part of the structure of spacetime in general relativity, and $\hbar$ captures the relationship between energy and frequency which is at the foundation of quantum mechanics. This makes Planck units particularly useful and common in theories of quantum gravity, including string theory.

Some may consider Planck units to be "more natural" even than other natural unit systems discussed below. For example, some other systems use the mass of an electron as a parameter to be normalized. But the electron is just one of 15 known massive elementary particles, all with different masses, and there is no compelling reason, within fundamental physics, to emphasize the electron mass over some other elementary particle's mass.

Like the other systems (see above), the electromagnetism units in Planck units can be based on either Lorentz–Heaviside units or Gaussian units. The unit of charge is different in each.

"Natural units" (particle physics)

Unit	Metric value	Derivation
1 eV^{-1} of length	1.97×10^{-7} m	$= (1\mathrm{eV}^{-1})\hbar c$
1 eV of mass	1.78×10^{-36} kg	$= (1\mathrm{eV})/c^2$
1 eV^{-1} of time	6.58×10^{-16} s	$= (1\mathrm{eV}^{-1})\hbar$
1 eV of temperature	1.16×10^{4} K	$= 1\mathrm{eV}/k_B$
1 unit of electric charge (L–H)	5.29×10^{-19} C	$= e/\sqrt{4\pi\alpha}$
1 unit of electric charge (G)	1.88×10^{-19} C	$= e/\sqrt{\alpha}$

In particle physics, the phrase "natural units" generally means:[4][5]

$$\hbar = c = k_B = 1.$$

where $\hbar$ is the reduced Planck constant, c is the speed of light, and k_B is the Boltzmann constant.

Like the other systems (see above), the electromagnetism units in Planck units can be based on either Lorentz–Heaviside units or Gaussian units. The unit of charge is different in each.

Finally, one more unit is needed. Most commonly, electron-volt (eV) is used, despite the fact that this is not a "natural" unit in the sense discussed above – it is defined by a natural property, the elementary charge, and the anthropogenic unit of electric potential, the volt. (The SI prefixed multiples of eV are used as well: keV, MeV, GeV, etc.)

With the addition of eV (or any other auxiliary unit), any quantity can be expressed. For example, a distance of 1 cm can be expressed in terms of eV, in natural units, as:[5]

$$1\,\mathrm{cm} = \frac{1\,\mathrm{cm}}{\hbar c} \approx 51000\,\mathrm{eV}^{-1}$$

Stoney units

Quantity	Expression	Metric value
Length (L)	$l_S = \sqrt{\frac{Ge^2}{c^4(4\pi\epsilon_0)}}$	1.381×10^{-36} m
Mass (M)	$m_S = \sqrt{\frac{e^2}{G(4\pi\epsilon_0)}}$	1.859×10^{-9} kg
Time (T)	$t_S = \sqrt{\frac{Ge^2}{c^6(4\pi\epsilon_0)}}$	4.605×10^{-45} s
Temperature (Θ)	$T_S = \sqrt{\frac{c^4e^2}{G(4\pi\epsilon_0){k_B}^2}}$	1.210×10^{31} K
Electric charge (Q)	$q_S = e$	1.602×10^{-19} C

Stoney units are defined by:

$$c = G = e = k_B = 1$$

$$\hbar = \frac{1}{\alpha}$$

where c is the speed of light, G is the gravitational constant, e is the elementary charge, k_B is the Boltzmann constant, $\hbar$ is the reduced Planck constant, and α is the fine-structure constant.

George Johnstone Stoney was the first physicist to introduce the concept of natural units. He presented the idea in a lecture entitled "On the Physical Units of Nature" delivered to the British Association in 1874.[6] Stoney units differ from Planck units by fixing the elementary charge at 1, instead of Planck's constant (only discovered after Stoney's proposal).

Stoney units are rarely used in modern physics for calculations, but they are of historical interest.

Atomic units

Quantity	Expression (Hartree atomic units)	Metric value (Hartree atomic units)
Length (L)	$l_A = \frac{\hbar^2(4\pi\epsilon_0)}{m_e e^2}$	5.292×10^{-11} m
Mass (M)	$m_A = m_e$	9.109×10^{-31} kg
Time (T)	$t_A = \frac{\hbar^3(4\pi\epsilon_0)^2}{m_e e^4}$	2.419×10^{-17} s
Electric charge (Q)	$q_A = e$	1.602×10^{-19} C
Temperature (Θ)	$T_A = \frac{m_e e^4}{\hbar^2(4\pi\epsilon_0)^2 k_B}$	3.158×10^{5} K

There are two types of atomic units, closely related: **Hartree atomic units**:

$$e = m_e = \hbar = k_B = 1$$

$$c = \frac{1}{\alpha}$$

Rydberg atomic units:[7]

$$\frac{e}{\sqrt{2}} = 2m_e = \hbar = k_B = 1$$

$$c = \frac{2}{\alpha}$$

These units are designed to simplify atomic and molecular physics and chemistry, especially the hydrogen atom, and are widely used in these fields. The Hartree units were first proposed by Douglas Hartree, and are more common than the Rydberg units.

The units are designed especially to characterize the behavior of an electron in the ground state of a hydrogen atom. For example, using the Hartree convention, in the Bohr model of the hydrogen atom, an electron in the ground state has orbital velocity = 1, orbital radius = 1, angular momentum = 1, ionization energy = ½, etc.

The unit of energy is called the Hartree energy in the Hartree system and the Rydberg energy in the Rydberg system. They differ by a factor of 2. The speed of light is relatively large in atomic units (137 in Hartree or 274 in Rydberg), which comes from the fact that an electron in hydrogen tends to move much slower than the speed of light. The gravitational constant is extremely small in atomic units (around 10^{-45}), which comes from the fact that the gravitational force between two electrons is far weaker than the Coulomb force. The unit length, m_A, is the Bohr radius, a_0.

The values of c and e shown above imply that $e = \sqrt{\alpha \hbar c}$, as in Gaussian units, *not* Lorentz–Heaviside units.[8] However, hybrids of the Gaussian and Lorentz–Heaviside units are sometimes used, leading to inconsistent conventions for magnetism-related units.[9]

Quantum chromodynamics (QCD) system of units

Quantity	Expression	Metric value
Length (L)	$l_{\text{QCD}} = \frac{\hbar}{m_p c}$	2.103×10^{-16} m
Mass (M)	$m_{\text{QCD}} = m_p$	1.673×10^{-27} kg
Time (T)	$t_{\text{QCD}} = \frac{\hbar}{m_p c^2}$	7.015×10^{-25} s
Temperature (Θ)	$T_{\text{QCD}} = \frac{m_p c^2}{k_B}$	1.089×10^{13} K
Electric charge (Q)	$q_{\text{QCD}} = e/\sqrt{4\pi\alpha}$ (L–H)	5.291×10^{-18} C
	$q_{\text{QCD}} = e/\sqrt{\alpha}$ (G)	1.876×10^{-18} C

$$c = m_p = \hbar = k_B = 1$$

The electron mass is replaced with that of the proton. *Strong units* are "convenient for work in QCD and nuclear physics, where quantum mechanics and relativity are omnipresent and the proton is an object of central interest".[10]

Geometrized units

$$c = G = 1$$

The geometrized unit system, used in general relativity, is not a completely defined system. In this system, the base physical units are chosen so that the speed of light and the gravitational constant are set equal to unity. Other units may be treated however desired. By normalizing appropriate other units, geometrized units become identical to Planck units.

Summary table

Quantity / Symbol	Planck (with Gaussian)	Stoney	Hartree	Rydberg	"Natural" (with L-H)	"Natural" (with Gaussian)
Speed of light in vacuum c	1	1	$\frac{1}{\alpha}$	$\frac{2}{\alpha}$	1	1
Planck's constant (reduced) $\hbar = \frac{h}{2\pi}$	1	$\frac{1}{\alpha}$	1	1	1	1
Elementary charge e	$\sqrt{\alpha}$	1	1	$\sqrt{2}$	$\sqrt{4\pi\alpha}$	$\sqrt{\alpha}$
Josephson constant $K_J = \frac{e}{\pi\hbar}$	$\frac{\sqrt{\alpha}}{\pi}$	$\frac{\alpha}{\pi}$	$\frac{1}{\pi}$	$\frac{\sqrt{2}}{\pi}$	$\sqrt{\frac{4\alpha}{\pi}}$	$\frac{\sqrt{\alpha}}{\pi}$
von Klitzing constant $R_K = \frac{2\pi\hbar}{e^2}$	$\frac{2\pi}{\alpha}$	$\frac{2\pi}{\alpha}$	2π	π	$\frac{1}{2\alpha}$	$\frac{2\pi}{\alpha}$
Gravitational constant G	1	1	$\frac{\alpha_G}{\alpha}$	$\frac{8\alpha_G}{\alpha}$	$\frac{\alpha_G}{{m_e}^2}$	$\frac{\alpha_G}{{m_e}^2}$
Boltzmann constant k_B	1	1	1	1	1	1
Electron mass m_e	$\sqrt{\alpha_G}$	$\sqrt{\frac{\alpha_G}{\alpha}}$	1	$\frac{1}{2}$	$511\,\text{keV}$	$511\,\text{keV}$

where:

- α is the fine-structure constant, approximately 0.007297,
- α_G is the gravitational coupling constant, $(m_e/m_{Planck})^2 \approx 1.752 \times 10^{-45}$,

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[2] http://books.google.com/books?id=12DKsFtFTgYC&pg=PA385 *Thermodynamics and statistical mechanics*, by Greiner, Neise, Stöcker

[3] See Gaussian units#General rules to translate a formula and references therein.

[4] *Gauge field theories: an introduction with applications*, by Guidry, Appendix A (http://books.google.com/books?id=kLYx_ZnanW4C&pg=PA511)

[5] *An introduction to cosmology and particle physics*, by Domínguez-Tenreiro and Quirós, p422 (http://books.google.com/books?id=OF4TCxwpcN0C&pg=PA422)

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[7] Turek, Ilja (1997). *Electronic structure of disordered alloys, surfaces and interfaces* (http://books.google.com/books?id=15wz64DPVqAC&pg=PA3) (illustrated ed.). Springer. pp. 3. ISBN 978-0-7923-9798-4.

[8] *Relativistic Quantum Chemistry: The Fundamental Theory of Molecular Science*, by Markus Reiher, Alexander Wolf, p7 [books.google.com/books?id=YwSpxCfsNsEC&pg=PA7 link]

[9] *A note on units* lecture notes (http://info.phys.unm.edu/~ideutsch/Classes/Phys531F11/Atomic Units.pdf). See the atomic units article for further discussion.
[10] Wilczek, Frank, 2007, " Fundamental Constants, (http://frankwilczek.com/Wilczek_Easy_Pieces/416_Fundamental_Constants.pdf)" *Frank Wilczek* web site.

External links

- The NIST website (http://physics.nist.gov/cuu/) (National Institute of Standards and Technology) is a convenient source of data on the commonly recognized constants.
- K.A. Tomilin: *NATURAL SYSTEMS OF UNITS; To the Centenary Anniversary of the Planck System* (http://www.ihst.ru/personal/tomilin/papers/tomil.pdf) A comparative overview/tutorial of various systems of natural units having historical use.
- Pedagogic Aides to Quantum Field Theory (http://www.quantumfieldtheory.info) Click on the link for Chap. 2 to find an extensive, simplified introduction to natural units.

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1. Natural Unit

Conversion Table for natural and MKSA Units

Natural units defined by: $\hbar = c = 1$ (and $4\pi\varepsilon_0 = 1$). Remaining unit is choosen to be Energy (eV).

Quantity	Symbol	natural units	MKSA
Length	ℓ	1/eV	$1.9732705 \cdot 10^{-7}$ m $\approx 0.2\ \mu$m
Mass	m	1 eV	$1.7826627 \cdot 10^{-36}$ kg
Time	t	1/eV	$6.5821220 \cdot 10^{-16}$ s $\approx$ .66 fs
Frequency	ν	1 eV	$1.5192669 \cdot 10^{15}$ Hz
Speed	v	1	$2.99792458 \cdot 10^{8}$ m/s
Momentum	p	1 eV	$5.3442883 \cdot 10^{-28}$ kg·m/s
Force	F	1 eV^2	$8.1194003 \cdot 10^{-13}$ N
Power	P	1 eV^2	0.24341350 mW
Energy	E	1 eV	$1.6021773 \cdot 10^{-19}$ J
Charge	q	1	$1.8755468 \cdot 10^{-18}$ C
Charge density	ρ	1 eV^3	244.10013 C/m^3
Current	I	1 eV	2.8494561 mA
Current density	J	1 eV^3	$7.3179379 \cdot 10^{10}$ A/m^2
Electric field	E	1 eV^2	432.90844 V/mm
Potential	Φ	1 eV	85.424546 mV
Polarization	P	1 eV^2	$4.8167560 \cdot 10^{-5}$ C/m^2
Conductivity	σ	1 eV	$1.6904124 \cdot 10^{5}$ S/m
Resistance	R	1	29.979246 Ω
Capacitance	C	1/eV	$2.1955596 \cdot 10^{-17}$ F
Magnetic flux	ϕ	1	$5.6227478 \cdot 10^{-17}$ Wb
Magnetic induction	B	1 eV^2	1.4440271 mT
Magnetization	M	1 eV^2	$1.4440271 \cdot 10^{4}$ A/m
Inductance	L	1/eV	$1.9732705 \cdot 10^{-14}$ H
some constants:			
Planck's quantum	$\hbar$	1	$1.05457266 \cdot 10^{-34}$ J·s
$h = 2\pi\hbar$	h	2π	$6.6260755 \cdot 10^{-34}$ J·s
Charge of electron	e	$8.5424546 \cdot 10^{-2}$	$1.60217733 \cdot 10^{-19}$ C
Bohr radius, $\hbar^2/me^2$	a_0	$2.6817268 \cdot 10^{-4}$/eV	$5.29177249 \cdot 10^{-11}$ m
Energy 1 electron Volt	eV	1 eV	$1.60217733 \cdot 10^{-19}$ J
Rydberg energy, $e^2/2a_0$	E_{Ryd}	13.605698 eV	$2.1798741 \cdot 10^{-18}$ J
Hartree energy, e^2/a_0	E_{h}	27.211396 eV	$4.3597482 \cdot 10^{-18}$ J
Speed of light	c	1	$2.99792458 \cdot 10^{8}$ m/s
Permeability of vacuum	μ_0	4π	$4\pi \cdot 10^{-7}$ H/m
Permittivity of vacuum	ε_0	$1/4\pi$	$8.854187817 \cdot 10^{-12}$ F/m
Bohr magneton	μ_B	$8.3585815 \cdot 10^{-8}$/eV	$9.2740154 \cdot 10^{-24}$ J/T
Mass of electron	m_e	510.99906 keV	$9.1093897 \cdot 10^{-31}$ kg
Mass of proton	m_p	938.27234 MeV	$1.6726231 \cdot 10^{-27}$ kg
Mass of neutron	m_n	939.56563 MeV	$1.6749286 \cdot 10^{-27}$ kg
Gravitation constant	G	$6.70711 \cdot 10^{-57}$/eV^2	$6.67259 \cdot 10^{-11}$ N·m^2/kg^2

The Rayleigh-Jeans law (1-7) (Jeans made a minor contribution to its derivation) does not agree with experiment at high frequencies, where the Wien formula works, though it does fit the experimental curve at low frequencies (Fig. 1.2). The Rayleigh-Jeans law cannot, on general grounds, be correct, since the total energy density (integrated over all frequencies) is predicted to be infinite!

In 1900, Max Planck found a formula by an ingenious interpolation between the high-frequency Wien formula and the low-frequency Rayleigh-Jeans law. The formula is

$$u(\nu, T) = \frac{8\pi h}{c^3} \frac{\nu^3}{e^{h\nu/kT} - 1} \tag{1-8}$$

where h, *Planck's constant*, is an adjustable parameter whose numerical value was found to be $h = 6.63 \times 10^{-27}$ erg sec. This law approaches the Rayleigh-Jeans form when $\nu \to 0$, and reduces to

$$\begin{aligned} u(\nu, T) &= \frac{8\pi h}{c^3} \nu^3 e^{-h\nu/kT} (1 - e^{-h\nu/kT})^{-1} \\ &\cong \frac{8\pi h}{c^3} \nu^3 e^{-h\nu/kT} \end{aligned} \tag{1-9}$$

when the frequency is large, or, more accurately, when $h\nu \gg kT$. If we rewrite the formula as a product of the number of modes [we obtain this from (1-7) by dividing the energy density by kT] and another factor that can be interpreted as the average energy per degree of freedom

$$\begin{aligned} u(\nu, T) &= \frac{8\pi\nu^2}{c^3} \frac{h\nu}{e^{h\nu/kT} - 1} \\ &= \frac{8\pi\nu^2}{c^3} kT \frac{h\nu/kT}{e^{h\nu/kT} - 1} \end{aligned} \tag{1-10}$$

we see that the classical equipartition law is altered whenever the frequencies are not small compared with kT/h. This alteration in the equipartition law shows that the modes have an average energy that depends on their frequency, and that the high frequency modes have a very small average energy. This effective cut-off removes the difficulty of the Rayleigh-Jeans density formula: the total energy in a cavity of unit volume is no longer infinite. We have

$$\begin{aligned} U(T) &= \frac{8\pi h}{c^3} \int_0^\infty d\nu \frac{\nu^3}{e^{h\nu/kT} - 1} \\ &= \frac{8\pi h}{c^3} \left(\frac{kT}{h}\right)^4 \int_0^\infty \frac{(h\nu/kT)^3 \, d(h\nu/kT)}{e^{h\nu/kT} - 1} \\ &= \frac{8\pi k^4}{h^3 c^3} T^4 \int_0^\infty dx \frac{x^3}{e^x - 1} \end{aligned} \tag{1-11}$$

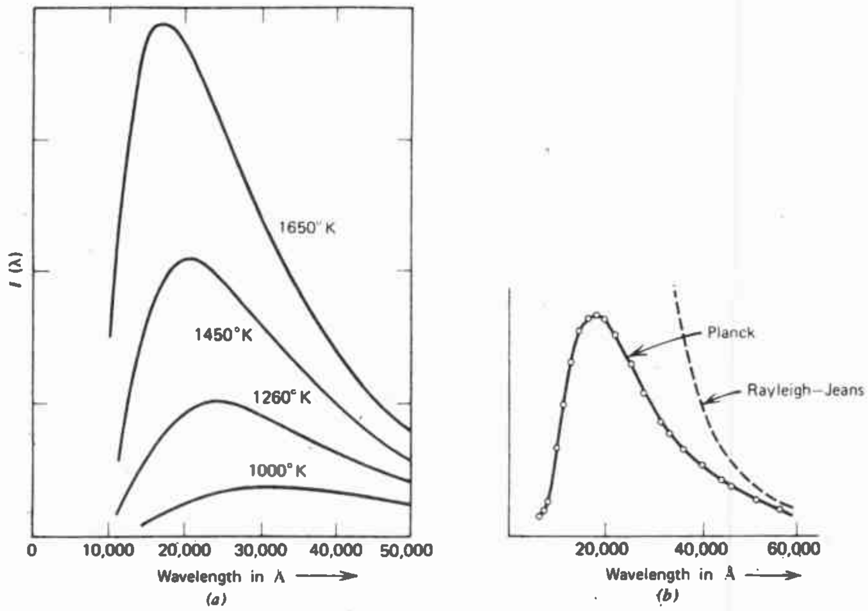


Fig. 1-2. (*a*) Distribution of power radiated by a black body at various temperatures. (*b*) Comparison of data at 1600°K with Planck formula and Rayleigh-Jeans formula.

ever, in accord with some very general notions of classical physics. Rayleigh, in 1900, derived the result

$$u(\nu, T) = \frac{8\pi\nu^2}{c^3} kT \tag{1-7}$$

where k is Boltzmann's constant, $k = 1.38 \times 10^{-16}$ erg/deg and c is the velocity of light, $c = 3.00 \times 10^{10}$ cm/sec. The ingredients that went into the derivation were (1) the classical law of equipartition of energy, according to which the average energy per degree of freedom for a dynamical system in equilibrium is, in this context,[4] kT, and (2) the calculation of the number of modes (i.e., degrees of freedom) for electromagnetic radiation with frequency in the interval $(\nu, \nu + d\nu)$, confined in a cavity.[5]

[4] The equipartition law predicts that the energy per degree of freedom is $kT/2$. For an oscillator—and the modes of the electromagnetic field are simple harmonic oscillators—a contribution of $kT/2$ from the kinetic energy is matched by a like contribution from the potential energy, giving kT.

[5] We will need this result again, and derive it in Chapter 23. The number of modes is $4\pi\nu^2/c^3$, further multiplied by a factor of 2 because transverse electromagnetic waves correspond to two-dimensional harmonic oscillators.

Example 1.1 (Wien's displacement law)

(a) Show that the maximum of the Planck energy density (1.9) occurs for a wavelength of the form $\lambda_{max} = b/T$, where T is the temperature and b is a constant whose value needs to be estimated.

(b) Use the relation derived in (a) to estimate the surface temperature of a star if the radiation it emits has a maximum wavelength of 446nm. What is the intensity radiated by the star?

(c) Estimate the wavelength and the intensity of the radiation emitted by a glowing tungsten filament whose surface temperature is 3300K.

Solution

(a) Since $\nu = c/\lambda$, we have $d\nu = |d\nu/(d\lambda)|\, d\lambda = (c/\lambda^2)d\lambda$; we can thus write Planck's energy density (1.9) in terms of the wavelength as follows:

$$\tilde{u}(\lambda, T) = \tilde{u}(\nu, T)\left|\frac{d\nu}{d\lambda}\right| = \frac{8\pi hc}{\lambda^5}\frac{1}{e^{hc/\lambda kT} - 1}. \tag{1.11}$$

The maximum of $\tilde{u}(\lambda, T)$ corresponds to $\partial\tilde{u}(\lambda, T)/\partial\lambda = 0$, which yields

$$\frac{8\pi hc}{\lambda^6}\left[-5\left(1 - e^{-hc/\lambda kT}\right) + \frac{hc}{\lambda kT}\right]\frac{e^{hc/\lambda kT}}{\left(e^{hc/\lambda kT} - 1\right)^2} = 0, \tag{1.12}$$

and hence

$$\frac{\alpha}{\lambda} = 5\left(1 - e^{\alpha/\lambda}\right), \tag{1.13}$$

[5] To integrate (1.9) over all frequencies, we need: $\int_0^{+\infty} \frac{x^3}{e^x - 1} dx = \frac{\pi^4}{15}$.

where $\alpha = hc/(kT)$. We can solve this transcendental equation either graphically or numerically by writing $\alpha/\lambda = 5 - \varepsilon$. Inserting this value into (1.13), we obtain $5 - \varepsilon = 5 - 5e^{-5+\varepsilon}$, which leads to a suggestive approximate solution $\varepsilon \approx 5e^{-5} = 0.0337$ and hence $\alpha/\lambda = 5 - 0.0337 = 4.9663$. Since $\alpha = hc/(kT)$ and using the values $h = 6.626 \times 10^{-34}\,\text{J s}$ and $k = 1.3807 \times 10^{-23}\,\text{J K}^{-1}$, we can write the wavelength that corresponds to the maximum of the Planck energy density (1.9) as follows:

$$\boxed{\lambda_{max} = \frac{hc}{4.9663k}\frac{1}{T} = \frac{2898.9 \times 10^{-6}\,\text{m K}}{T}.} \tag{1.14}$$

This relation, which shows that λ_{max} decreases with increasing temperature of the body, is called *Wien's displacement law*. It can be used to determine the wavelength corresponding to the maximum intensity if the temperature of the body is known; or, conversely, to determine the temperature of the radiating body if the wavelength of the strongest emission is known. This law can be used, in particular, to estimate the temperature of stars (or of glowing objects) from their radiation, as shown in part (b). From (1.14) we obtain

$$\boxed{\nu_{max} = \frac{c}{\lambda_{max}} = \frac{4.9663}{h}kT.} \tag{1.15}$$

This relation shows that the peak of the radiation spectrum occurs at a frequency that is proportional to the temperature

(b) If the radiation emitted by the star has a maximum wavelength of $\lambda_{max} = 446\,\text{nm}$, its surface temperature is given by

$$T = \frac{2898.9 \times 10^{-6}\,\text{m K}}{446 \times 10^{-9}\,\text{m}} \simeq 6500\,\text{K}. \tag{1.16}$$

Using Stefan's law (1.1), and assuming the star to radiate like a blackbody, we can estimate the total power per unit area emitted at the surface of the star:

$$E = \sigma T^4 = 5.67 \times 10^{-8}\,\text{W m}^{-2}\,\text{K}^{-4} \times (6500\,\text{K})^4 \simeq 101.2 \times 10^6\,\text{W m}^{-2}. \tag{1.17}$$

This an enormous intensity which will decrease as it spreads over space.

(c) The dominant wavelength of the radiation emitted by a glowing tungsten filament of temperature 3300K is

$$\lambda_{max} = \frac{2898.9 \times 10^{-6}\,\text{m K}}{3300\,\text{K}} \simeq 878.45\,\text{nm}. \tag{1.18}$$

The intensity radiated by the filament is given by

$$E = \sigma T^4 = 5.67 \times 10^{-8}\,\text{W m}^{-2}\,\text{K}^{-4} \times (3300\,\text{K})^4 \simeq 6.7 \times 10^6\,\text{W m}^{-2} = 6.7\,\text{W mm}^{-2}. \tag{1.19}$$

1.11. UNITS IN HIGH-ENERGY PHYSICS

The fundamental units in physics are of length, mass, and time, the familiar systems (MKS) expressing these in meters, kilograms, and seconds. Such units are however not very appropriate in particle physics, where lengths are typically 10^{-15} m and masses 10^{-27} kg.

Lengths in particle physics are usually quoted in terms of the *femtometer* or *fermi* (1 fm = 10^{-15} m), and cross-sections in terms of the *barn* (1 b = 10^{-28} m^2), millibarn (1 mb = 10^{-31} m^2), or microbarn (1 μb = 10^{-34} m^2). The unit of energy is based on the electron volt (1 eV = 1.6×10^{-19} joules) with the larger units MeV (=10^6 eV), GeV (=10^9 eV), and TeV (=10^{12} eV). Masses are usually measured in MeV/c^2, meaning that if the mass is M, the rest energy is Mc^2 MeV. For example, the proton has a rest energy of 938.28 MeV or 0.938 GeV. Often masses (meaning the rest-energy equivalents) are loosely quoted in MeV or GeV.

In calculations, the quantities $\hbar = h/2\pi$ and c occur frequently, and it is often advantageous to use a system of units in which $\hbar = c = 1$. We do this by choosing some standard mass m_0 (e.g., the proton mass) as the unit:

$$m_0 = 1.$$

The natural unit of length is then the Compton wavelength of the standard particle:

$$\lambda\!\!\!^{-}_0 = \frac{\hbar}{m_0 c} = 1;$$

that of time is

$$t_0 = \frac{\lambda\!\!\!^{-}_0}{c} = \frac{\hbar}{m_0 c^2} = 1,$$

and that of energy is

$$E_0 = m_0 c^2 = 1.$$

In these units, it is seen that $\hbar = c = 1$. In converting back, at the end of the calculation to the more usual units, it is useful to remember that $\hbar c = 197$ MeV fm. Thus, a particle of mass energy $m_0 c^2 = 197$ MeV has a Compton wavelength of $\hbar/m_0 c = \hbar c/m_0 c^2 = 1$ fm.

Throughout this text we shall be dealing with the coupling of charges—strong, electric and weak—to mediating bosons. In MKS units, electric charge, e, is measured in Coulombs and the fine-structure constant is then given by

$$\alpha = \frac{e^2}{4\pi\varepsilon_0 \hbar c} \simeq \frac{1}{137}.$$

For the general coupling of charges to bosons, such units are not useful and we define e in Heaviside-Lorentz units ($\varepsilon_0 = \mu_0 = 1$) so that with $\hbar = c = 1$

$$\alpha = \frac{e^2}{4\pi} \simeq \frac{1}{137},$$

as in (1.12). A similar definition is used to relate charges and coupling constants in the other interactions.

2. Degeneracy

Show that, in one-dimensional problems, the energy spectrum of the bound states is always non-degenerate.

For the sake of argument let us suppose that the opposite is true. Let $\psi_1(x)$ and $\psi_2(x)$ then be two linearly independent eigenfunctions with the same energy eigenvalue E. From the equations

$$\psi_1'' + \frac{2m}{\hbar^2}(E-V)\psi_1 = 0, \quad \psi_2'' + \frac{2m}{\hbar^2}(E-V)\psi_2 = 0,$$

we obtain

$$\frac{\psi_1''}{\psi_1} = \frac{\psi_2''}{\psi_2} = \frac{2m}{\hbar^2}(V-E),$$

i.e.

$$\psi_1''\psi_2 - \psi_2''\psi_1 = (\psi_1'\psi_2)' - (\psi_2'\psi_1)' = 0.$$

After integrating this equation we find that

$$\psi_1'\psi_2 - \psi_2'\psi_1 = \text{a constant}.$$

Since, at infinity, $\psi_1 = \psi_2 = 0$ (bound states), we must have the constant $= 0$ and hence

$$\frac{\psi_1'}{\psi_1} = \frac{\psi_2'}{\psi_2}.$$

Integrating once more we have $\ln \psi_1 = \ln \psi_2 + \ln c$, i.e. $\psi_1 = c\psi_2$, which contradicts the assumed linear independence of the two functions.

3. Sudden Expansion

A particle is initially ($t < 0$) in the ground state of an infinite, one-dimensional potential well with walls at $x = 0$ and $x = a$.

(a) If the wall at $x = a$ is moved *slowly* to $x = 8a$, find the energy and wave function of the particle in the new well. Calculate the work done in this process.

(b) If the wall at $x = a$ is now *suddenly* moved (at $t = 0$) to $x = 8a$, calculate the probability of finding the particle in (i) the ground state, (ii) the first excited state, and (iii) the second excited state of the new potential well.

Solution

For $t < 0$ the particle was in a potential well with walls at $x = 0$ and $x = a$, and hence

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}, \qquad \psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right) \qquad (0 \le x \le a). \tag{10.76}$$

(a) When the wall is moved slowly, the adiabatic theorem dictates that the particle will be found at time t in the ground state of the new potential well (the well with walls at $x = 0$ and $x = 8a$). Thus, we have

$$E_1(t) = \frac{\pi^2\hbar^2}{2m(8a)^2} = \frac{\pi^2\hbar^2}{128ma^2}, \qquad \psi_1'(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{8a}\right) \qquad (0 \le x \le a). \tag{10.77}$$

The work needed to move the wall is $\Delta W = E_1 - E_1(t) = \pi^2\hbar^2/(2ma^2) - \pi^2\hbar^2/(2m(8a)^2) = 63\pi^2\hbar^2/(128ma^2)$.

(b) When the wall is moved rapidly, the particle will find itself instantly (at $t \ge 0$) in the new potential well; its energy levels and wave function are now given by

$$E_n' = \frac{n^2\pi^2\hbar^2}{2m(8a)^2} = \frac{n^2\pi^2\hbar^2}{128ma^2}, \qquad \psi_n'(x) = \sqrt{\frac{2}{8a}}\sin\left(\frac{n\pi x}{8a}\right) \qquad (0 \le x \le 8a). \tag{10.78}$$

The probability of finding the particle in the ground state of the new box potential can be obtained from (10.73): $P_{11} = |\langle\psi_1' \mid \psi_1\rangle|^2$ where

$$\langle\psi_1' \mid \psi_1\rangle = \int_0^a \psi_1'^*(x)\psi_1(x)\,dx = \frac{2}{\sqrt{8}a}\int_0^a \sin\left(\frac{\pi x}{8a}\right)\sin\left(\frac{\pi x}{a}\right)dx = \frac{16}{63\pi}\sqrt{4-2\sqrt{2}}, \tag{10.79}$$

hence

$$P_{11} = \left|\langle\psi_1' \mid \psi_1\rangle\right|^2 = \left(\frac{16}{63\pi}\right)^2(4-2\sqrt{2}) = 0.0077 \simeq 0.7\%. \tag{10.80}$$

The probability of finding the particle in the first excited state of the new box potential is given by $P_{12} = \left|\langle\psi_2' \mid \psi_1\rangle\right|^2$ where

$$\langle\psi_2' \mid \psi_1\rangle = \int_0^a \psi_2'^*(x)\psi_1(x)\,dx = \frac{2}{\sqrt{8}a}\int_0^a \sin\left(\frac{\pi x}{4a}\right)\sin\left(\frac{\pi x}{a}\right)dx = \frac{8}{15\pi},$$

hence

$$P_{12} = \left|\langle\psi_2' \mid \psi_1\rangle\right|^2 = \left(\frac{8}{15\pi}\right)^2 = 0.1699 \simeq 17\%.$$

A similar calculation leads to

$$P_{13} = \left|\langle\psi_3' \mid \psi_1\rangle\right|^2 = \left|\frac{2}{\sqrt{8}a}\int_0^a \sin\left(\frac{3\pi x}{8a}\right)\sin\left(\frac{\pi x}{a}\right)dx\right|^2 = \left|\frac{16}{55\pi}\sqrt{4+2\sqrt{2}}\right|^2 \simeq 24.2\%. \tag{10.83}$$

These calculations show that the particle is most likely to be found in higher excited states; the probability of finding it in the ground state is very small.

4. Spread of the Wave Function

Assume that, at time $t = 0$, the wavefunction $\psi(x, t)$ of a particle is of the form (cf. problem 16, Chapter III):

$$\psi(x, 0) = \frac{1}{(2\pi\delta^2)^{1/4}} \exp\left(-\frac{x^2}{4\delta^2}\right), \quad \delta^2 = (\Delta x)^2.$$

Investigate the change in time of this wave-packet if, for $t > 0$, no forces act on the particle.

It is necessary to determine the wavefunction $\psi(x, t)$ which satisfies the Schrödinger equation

$$i\hbar \frac{\partial\psi(x, t)}{\partial t} = H\psi(x, t),$$

and which, at time $t = 0$, is the given function $\psi(x, 0)$. With that end in view we expand $\psi(x, 0)$ in terms of the set of orthonormal time-independent eigenfunctions $\psi_n(x)$, $(H\psi_n(x) = E_n\psi_n(x))$ (see p. 204, footnote), thus:

$$\psi(x, 0) = \sum_n a_n\psi_n(x), \qquad a_n = \int \psi_n^*(x)\,\psi(x, 0)\,dx.$$

The function $\sum_n a_n\psi_n(x) \exp\left(-\frac{i}{\hbar}E_n t\right)$ then satisfies the Schrödinger equation, and, at time $t = 0$, coincides with $\psi(x, 0)$. Hence

$$\psi(x, t) = \sum_n a_n\psi_n(x)e^{-\frac{i}{\hbar}E_n t},$$

i.e.

$$\psi(x, t) = \int G(\xi, x, t)\psi(\xi, 0)\,d\xi$$

where

$$G(\xi, x, t) = \sum_n \psi_n^*(\xi)\,\psi_n(x)\,e^{-\frac{i}{\hbar}E_n t}$$

Since, in the case of free motion, the eigenfunctions are

$$\psi_p(x) = \frac{1}{(2\pi\hbar)^{1/2}} \exp\left(\frac{i}{\hbar}px\right);$$

the Green's function (8.4) becomes (with p continuous)

$$G(\xi, x, t) = \int \frac{1}{2\pi\hbar} \exp\left\{\frac{i}{\hbar}\left[p(x-\xi) - \frac{p^2 t}{2m}\right]\right\} dp$$

$$= \left(\frac{m}{2\pi i\hbar t}\right)^{1/2} e^{\frac{im}{2\hbar t}(x-\xi)^2}.$$

From (8.3) and (8a) it follows that

$$\psi(x, t) = \int \left(\frac{m}{2\pi i\hbar t}\right)^{1/2} \frac{1}{(2\pi\delta^2)^{1/4}} \exp\left\{-\frac{\xi^2}{4\delta^2} + \frac{im}{2\hbar t}(x-\xi)^2\right\} d\xi,$$

whence we obtain finally, for the wave function,

$$\psi(x, t) = \frac{1}{(2\pi\delta^2)^{1/4}\left(1+\frac{\hbar^2 t^2}{4m^2\delta^4}\right)^{1/4}} \exp\left\{-\frac{x^2}{4\delta^2\left(1+\frac{\hbar^2 t^2}{4m^2\delta^4}\right)}\left(1-\frac{i\hbar t}{2m\delta^2}\right)\right\},$$

and for the probability density

$$|\psi(x, t)|^2 = \left[2\pi\delta^2\left(1+\frac{\hbar^2 t^2}{4m^2\delta^4}\right)\right]^{-1/2} \exp\left\{-\frac{x^2}{2\delta^2\left(1+\frac{\hbar^2 t^2}{4m^2\delta^4}\right)}\right\}.$$

This expression has the same form as the initial probability density

$$|\psi(x, 0)|^2 = \frac{1}{(2\pi\delta^2)^{1/2}} \exp\left\{-\frac{x^2}{2\delta^2}\right\},$$

5 Classical limit of Harmonic Oscillator

Since the general solution of the equation of motion of a classical oscillator, $\ddot{x}+\omega^2 x = 0$, is of the form $x = C \sin(\omega t+\phi)$, the total energy

$$E_1 = T+V = \frac{m\dot{x}^2}{2}+\frac{m\omega^2}{2}x^2$$

of such an oscillator is given by $E_1 = m\omega^2 c^2/2$.

Since $T \geqslant 0$, we have $E_1 \geqslant V$, which means that, classically, the particle can be found only in the range $-a \leqslant x \leqslant +a$. At the ends of this interval, where $E_1 = V$, its kinetic energy vanishes; the points $x = \pm a$ are called "turning points". Accordingly, $C^2 = a^2 = 2E_1/m\omega^2 = 3\hbar/m\omega$. The classical probability of finding the particle in the interval $(x, x+dx)$ is proportional to the time dt which it takes to pass through this interval. If the period of oscillation is $T = 2\pi/\omega$, then

$$W_{cl}(x)\, dx = 2\frac{dt}{T} = \frac{\omega}{\pi}\frac{dx}{\dot{x}} = \frac{\omega}{\pi}\frac{dx}{a\omega\cos(\omega t+\phi)} = \frac{1}{\pi a}\left(1-\frac{x^2}{a^2}\right)^{-1/2} dx,$$

which is the required expression.

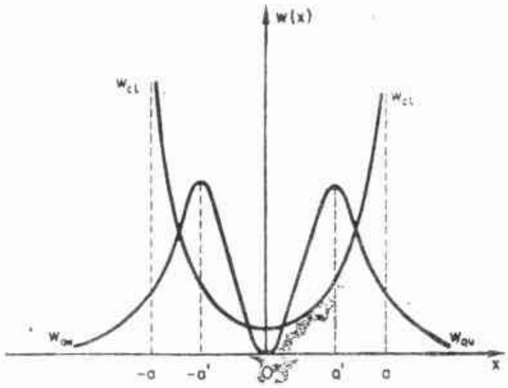


FIG. II.23.

It can be seen that this probability is greatest at the turning points $x = \pm a$ (Fig. II.23). According to quantum mechanics the probability of finding the particle in the interval $(x, x+dx)$ is

$$W_{qu}(x)\, dx = 2\pi^{-1/2} x_0^{-3} x^2 \exp\left(-\frac{x^2}{x_0^2}\right) dx.$$

It should be noted that $W_{qu}(x)$ has maxima near the classical turning points $\left(a = \sqrt{3\hbar/m\omega},\ a' = \sqrt{\hbar/m\omega}\right)$, but, in contrast with the classical case, it does not vanish beyond these points. This phenomenon, of the penetration of a particle into regions with "negative kinetic energy" $(|x| > a)$, does not lead to any contradiction because the equality $E = T+V$ in quantum mechanics is not a simple relation between numbers, but between operators; the kinetic and the potential energies cannot in fact be determined simultaneously.

For higher levels, it is found that the curve $2W_{cl}(x)$ becomes the envelope of the peaks of $W_{qu}(x)$ in the classical limit $n \to \infty$ (cf. Fig. II.24, which represents $W_{qu}(x) = |\psi_{10}(x)|^2$, $a = \sqrt{21\hbar/m\omega}$).

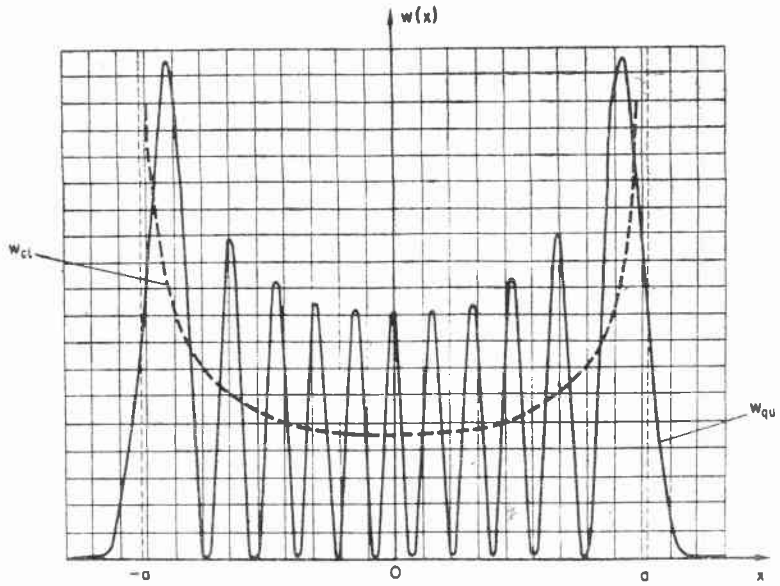


Fig. II.24

4

Operator

Linear , Hermitian.

Physical observable ⟷ Linear , Hermitian Operator

Eigenfunctions and Eigenvalues

Eigenvalues of Hermitian Operator and Real.

Eigenfunctions of Hermitian Operator with Distinct Eigenvalues are Orthogonal.

Eigenfunctions of Hermitian Operator with Identical Eigenvalues can be made to be orthogonal (through Schmidt procedure)

Eigenfunctions of a Hermitian Operator Form an Orthonormal Set. Furthermore , any wave function can be expanded as a linear combination of this orthormal set.

⇒ Completness.

Solving the Schrodinger equation with time-independent potential $V(\vec{r})$

(Here we shall restrict ourselve to the one dimensional case)

Time - dependent Schrodinger equation

→ Seperation of variable → time - independent

Schrodinger equation

Schrodinger (time-independent) equation is an eigenvalue equation for the Hamiltonian (energy operator) operator $H u_n = E_n u_n$

$\Rightarrow \quad \psi_n(x,t) = u_n e^{-\frac{i}{\hbar}E_n t}$

is a solution of time dependent Schrodinger equation.

$\psi_n(x,t) \longleftrightarrow$ stationary state (of Bohr)

- $\psi_n^*(x,t)\,\psi(x,t)$ is independent of time
- $\langle H \rangle = E_n$

  $\langle H^2 \rangle - \langle H \rangle^2 = 0$

  $\Downarrow$

  it is a state with definite energy E_n.

Initial Condition $\psi(x,0)$

General solution of time-dependent Schrodinger equation

$$\psi(x,t) = \sum_n c_n \psi_n(x,t)$$
$$= \sum_n c_n u_n e^{iE_n t/\hbar}$$

$\psi(x,0) \longleftrightarrow c_n$ (Fourier's technique)

$$\psi(x,0) = \sum_n c_n u_n$$

$$\int_{-\infty}^{\infty} u_m^* \psi(x,0)\,dx = \int_{-\infty}^{\infty} \sum_n u_m^* c_n u_n \,dx$$
$$= \sum_n c_n \delta_{nm} = c_m.$$

Physical Meaning of $\psi(x,t)$

$$\langle H \rangle = \int \psi^*(x,t)\, H\, \psi(x,t)\, dx$$

$$= \int \sum_m c_m^* u_m^* e^{i\frac{E_m t}{\hbar}} H \sum_n c_n u_n e^{-iE_n t/\hbar} dx$$

$$= \int \sum_m c_m^* \underline{u_m^*} e^{i\frac{E_m t}{\hbar}} \sum_n c_n E_n \underline{u_n} e^{-iE_n t/\hbar} \underline{dx}$$

$$= \sum_m \sum_n c_m^* c_n e^{i\frac{E_m t}{\hbar}} E_n e^{-iE_n t/\hbar} \delta_{mn}$$

↓ orthonormal conditions have been used.

$$= \sum_n |c_n|^2 E_n$$

$|c_n|^2$ that the system in state $\psi_n(x,t)$ with eigenvalue (energy E_n)

Determination of $\psi(x,0)$

If we measure a physical observable A and finding it has eigenvalue a_n, then right afterwards again measure A then we should find the state to be in a state u_{a_n} which is an eigenfunction of A with eigenvalue a_n

↓

collapse of the wave function.

分類：	
編號：	1
總號：	

Operator

Linear, Hermitian

Physical observable ⟷ Linear, Hermitian Operator

Eigenfunctions and Eigenvalues

Eigenvalues of Hermitian Operator are Real

Eigenfunctions of Hermitian Operator with Distinct Eigenvalues are Orthogonal

Eigenfunctions of Hermitian Operator with Identical Eigenvalues can be made to be Orthogonal (through Schmidt procedure)

Eigenfunctions of a Hermitian Operator Form an Orthonormal Set. Furthermore, any wave function can be expanded as a linear combination of this orthonormal set

$\Rightarrow$ completness

Solving the Schrodinger equation with time - independent potential $V(r)$

(Here we shall restrict ourself to the one dimensional case)

Time - dependent Schrodinger equation $\longrightarrow$

Seperation of Variable $\longrightarrow$ time - dependent

分類：
編號： 2
總號：

Schrodinger equation

it is an eigenvalue equation for the energy

(Hamiltonian) equation

$$H u_n = E_n u_n$$

$$\Rightarrow \quad \psi_n(x,t) = u_n e^{-\frac{i}{\hbar}E_n t}$$

is a solution of the time-dependent Schrodinger equation

$\psi_n(x,t) \longleftrightarrow$ stationary state (of Bohr)

* $\psi_n^*(x,t)\psi_n(x,t)$ is independent of time

* $\langle H_n \rangle = E_n$

$$\langle H^2 \rangle - \langle H \rangle^2 = 0$$

$\Downarrow$

it is a state with definite energy E_n

Initial condition $\psi(x,0)$

General solution of time-dependent Schrodinger equation

$$\psi(x,t) = \sum_n c_n \psi_n(x,t)$$

$$= \sum_n c_n u_n e^{-iE_n t/\hbar}$$

$$\psi(x,0) \leftrightarrow c_n$$

$$\psi(x,0) = \sum_n c_n u_n$$

$$\int_{-\infty}^{\infty} u_m^* \psi(x,0)\,dx = \int_{-\infty}^{\infty} \sum_n u_m^* c_n u_n\,dx$$

$$= \sum_n c_n \delta_{nm} = c_m$$

分類:
編號: 3
總號:

Physical Meaning of $\psi(x,t)$

$$\langle H\rangle = \langle E\rangle = \int \psi^*(x,t)\, H\, \psi(x,t)$$

$$= \int \sum_m c_m^* u_m^* e^{i\frac{E_m t}{\hbar}} \sum_n c_n E_n u_n e^{-iE_n t/\hbar} dx$$

$$= \sum_m \sum_n c_m^* c_n e^{iE_m t/\hbar} E_n e^{-iE_n t/\hbar} dx$$

↓ orthonormal conditions have been used.

$$\sum_n |c_n|^2 E_n$$

$|c_n|^2 \leftrightarrow$ probability that $\psi(x,t)$ is in $\psi_n(x,t)$ with energy E_n

Determination of $\psi(x,0)$

If we measure a physical observable A and find it has value a_n, then right afterwards again measure A then we shall definitely find the value $a_n \Rightarrow$ it must be in a state u_{a_n} which is an eigenfunction of A with eigenvalue a_n

↓

collapse of the wave function

Commutator of two Hemitian operator

$$[A, B] = AB - BA$$

$[A, B] = 0 \Rightarrow A, B$ commute

$[A, B] \neq 0 \Rightarrow A, B$ do not commute

Properties of the commute

Fundamental commutator

Commutator and Poisson bracket.

Commutator and uncertainty relation.

Commutator and simultaneous eigenfunctions.

Commutator and conservation law

Physical argument for the uncertainty relation

Wave packet and uncertainty relation.

Application of uncertainty relation.

Dirac

Postulational Form of Quantum Mechanics.

Commutator and Poisson bracket.

Fundamental Commutator.

$$[P_x, x] = \frac{\hbar}{i}$$

1925 Dirac

$$\{\ ,\ \}_{P.B.} \rightarrow \frac{[\ ,\ ]}{i\hbar}$$

Orbital Angular Momentum Operator

$L_x, L_y, L_z, \vec{L}^2$

Simultaneous eigenfunctions of A, B

$\Leftrightarrow [A, B] = 0$ Example orbital angular momentum

Relations to Uncertainty Principle.

Uncertainty Relation $\leftrightarrow$ Commutator.

6. Commutator, Heisenberg's Equation of Motion.

$$\langle Q \rangle_t = \int \psi^*(x,t)\, \hat{Q}\, \psi(x,t)\, dx$$

$$\hat{H}\psi = i\hbar \frac{\partial}{\partial t}\psi \qquad \text{Schrodinger equation}$$

$$\frac{d\langle Q\rangle_t}{dt} = \int \frac{\partial \psi^*}{\partial t}\hat{Q}\,\psi\, dx + \int \psi^* \hat{Q}\frac{\partial \psi}{\partial t}\, dx + \int \psi^* \frac{\partial \hat{Q}}{\partial t}\psi\, dx$$

$$H\psi = i\hbar\frac{\partial}{\partial t}\psi \Rightarrow \frac{\partial \psi}{\partial t} = \frac{1}{i\hbar}\hat{H}\psi$$

$$(H\psi)^* = -i\hbar\frac{\partial \psi^*}{\partial t} \Rightarrow \frac{\partial \psi^*}{\partial t} = \frac{1}{-i\hbar}(H\psi)^*$$

$$\frac{d\langle \hat{Q}\rangle}{dt} = \int \frac{\partial \psi^*}{\partial t}\hat{Q}\,\psi\, dx + \int \psi^* \hat{Q}\frac{\partial \psi}{\partial t}\, dx + \int \psi^* \frac{\partial \hat{Q}}{\partial t}\psi\, dx$$

$$= \frac{1}{-i\hbar}\int (\hat{H}\psi)^*\hat{Q}\psi\, dx + \frac{1}{i\hbar}\int \psi^*\hat{Q}\hat{H}\psi\, dx + \int \psi^* \frac{\partial Q}{\partial t}\psi\, dx$$

Look at

$$\int (\hat{H}\psi)^*\hat{Q}\psi\, dx$$

Definition of Hermitian adjoint $\hat{A}^+$

$$\int (\hat{A}\psi_2)^*\psi_1\, dx = \int \psi_2^*\hat{A}^+\psi_1\, dx$$

$\hat{H} \leftrightarrow A \qquad \psi_2 \to \psi$

$(\hat{Q}\psi) \to \psi_1$

$$\int (\hat{H}\psi)^*\hat{Q}\psi\, dx = \int \psi^*\hat{H}^+\hat{Q}\psi\, dx$$

$\hat{H} \rightarrow$ Hamiltonian operator

Energy operator $\longleftrightarrow$ physical observerable

↓

$\hat{H}$ is Hermitian, i.e., $\hat{H} = \hat{H}^+$

$$\int (H\psi)^*\hat{Q}\psi\, dx = \int \psi^* H Q \psi\, dx$$

Put it all together

$$\frac{d\langle \hat{Q}\rangle}{dt} = \frac{1}{i\hbar}\int \psi^*(\hat{Q}\hat{H} - \hat{H}\hat{Q})\psi\, dx + \left\langle \frac{\partial \hat{Q}}{\partial t}\right\rangle$$

$$= \frac{1}{i\hbar}\int \psi^* [\hat{Q}, \hat{H}]\psi\, dx + \left\langle \frac{\partial \hat{Q}}{\partial t}\right\rangle$$

$$\underline{\underline{\frac{d\langle \hat{Q}\rangle}{dt} = \frac{i}{\hbar}\langle [\hat{H}, \hat{Q}]\rangle + \left\langle \frac{\partial \hat{Q}}{\partial t}\right\rangle}}$$

This is one of the most useful equation in quantum mechanics

(1) Example ; $\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V}(x)$, $\hat{Q} \to \hat{x}$ does not explicitly depend on t

$$[\hat{H}, x] = [\frac{\hat{p}^2}{2m} + \hat{V}(x), \hat{x}]$$

$[\hat{V}(x), \hat{x}] = 0$; commutes

$$= [\frac{\hat{p}^2}{2m}, \hat{x}]$$

↓ examination problem

$$\Rightarrow \frac{d\langle \hat{x}\rangle}{dt} = \frac{\langle \hat{p}\rangle}{m}.$$

Now identify $\hat{Q} \to \hat{p}$

$$[\frac{\hat{p}^2}{2m} + V(x), \hat{p}]$$

$$= [\frac{\hat{p}^2}{2m}, \hat{p}] + [V(x), \hat{p}]$$

$[\frac{\hat{p}^2}{2m}, \hat{p}]$ ↓ 0 ; $[V(x), \hat{p}]$ ↓ examination problem

$$\Rightarrow \quad \frac{d\langle p\rangle}{dt} = -\left\langle \frac{\partial V}{\partial x} \right\rangle$$

(ii) If $[\hat{H}, \hat{Q}] = 0$ and $\frac{\partial \hat{Q}}{\partial t} = 0$

then $\frac{d}{dt}\langle Q\rangle_t = 0$

$\langle Q\rangle_t$ is independent of time, i.e., it is constant of motion, it is conserved.

Example. For a central force problem

$\hat{V}(r)$, it can be shown that

↓ independent of θ, ϕ.

$[\hat{H}, \hat{\vec{L}}] = 0$

↳ angular momentum operator

then $\frac{d\langle\hat{\vec{L}}\rangle}{dt} = 0$

$\langle \hat{\vec{L}} \rangle$ is conserved.

Next topics

Angular momentum

Spherical coordinate

Angular momentum operator in spherical coordinates

Hydrogen atom.

Physics

Natural Unit

Degeneracy → nondegeneracy in one dimension.

Momentum Representation

Angular Momentum operator

Expectation Value

Heisenberg's Equation of Motion.

Barrier and Wells

Spread of the wave function

Summary

Mathematics

Hermitian Operator

Orthogonal

Fourier Transformation

δ - function

Seperation of Variable

Commutator

Spherical Coordinate

Eigenfunction, Eigenvalue

分類：
編號：8 - 1
總號：

Chapter 8

Barriers and Wells

The quantum mechanical nature of matter has some surpising consequences

The behaviors seen in realistic experiments and applications can be illustrated in highly simplified systems which contains one - dimensional potentials with sharp edges

General Discussions

Time - dependent Schrodinger equation

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V(x)\psi \qquad (A)$$

$V(x)$ is assumed to be real and independent of time.

$$-i\hbar \frac{\partial \psi^*}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi^*}{\partial x^2} + \underset{V(x)}{\overset{}{\overset{*}{V}(x)}}\,\psi^* \qquad (B)$$

$\psi^* \cdot (A) - \psi \cdot (B)$

$$\Rightarrow \quad i\hbar\left[\psi^*\frac{\partial}{\partial t}\psi + \psi\frac{\partial}{\partial t}\psi^*\right] = -\frac{\hbar^2}{2m}\left[\psi^*\frac{\partial^2\psi}{\partial x^2} - \psi\frac{\partial^2\psi^*}{\partial x}\right]$$

$$\frac{\partial}{\partial t}\psi^*\psi = \frac{1}{i\hbar}\left(\frac{\hbar^2}{2m}\frac{\partial^2\psi^*}{\partial x^2}\psi - \frac{\hbar^2}{2m}\psi^*\frac{\partial^2\psi}{\partial x^2}\right)$$

$$= -\frac{\partial}{\partial x}\left[\frac{\hbar}{2im}\left(\psi^*\frac{\partial\psi}{\partial x} - \frac{\partial\psi^*}{\partial x}\psi\right)\right]$$

Define the probability flux $S(x,t) = \frac{\hbar}{2im}\left(\psi^*\frac{\partial\psi}{\partial x} - \frac{\partial\psi^*}{\partial x}\psi\right)$

$$\Rightarrow \quad \frac{\partial}{\partial t}P(x,t) + \frac{\partial}{\partial x}S(x,t) = 0$$

[Going to three dimensional case

$$\frac{\partial}{\partial t}P(\vec{r},t) + \nabla\cdot\vec{S}(\vec{r},t) = 0 \qquad (C)$$

$$\vec{S}(\vec{r},t) = \frac{\hbar}{2im}\left[\psi^*(\vec{r},t)\nabla\psi(\vec{r},t) - \nabla\psi^*(\vec{r},t)\psi(\vec{r},t)\right]$$

It is similar to the continuity equation

$$\frac{\partial\rho}{\partial t} + \nabla\cdot\vec{j} = 0 \quad \leftrightarrow \quad \text{conseration of charge}$$

Equation (C) $\rightarrow$ conservation of probability.]

$$\frac{\partial}{\partial t}\int_a^b dx\, P(x,t) = -\int_a^b dx \frac{\partial}{\partial x} S(x,t)$$

$$= S(a,t) - S(b,t)$$

$\Rightarrow$ $S(x,t) \rightarrow$ probability flux.
(probability / time cross point x)

Remark. (C) is a consequence of $V(x)$ is real.

When $V(x)$ is independent of time $\rightarrow$ seperation of variable method can be used.

$$\psi(x,t) = \psi_E(x)\, e^{-iEt/\hbar} = \psi_E(x)\, e^{-\omega t}$$

with

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

↳ time independent Schrodinger equation.

$$\psi_E(x) \equiv \psi(x)$$

Requirements for acceptible solutions

(i) $\psi(x)$ is square integrable* — *for unbound motion, we shall discuss this point further

(ii) (a) $\psi(x)$ must be finite
(b) $\psi(x)$ must be continuous
(c) $\frac{d\psi(x)}{dx}$ must be finite
(d) $\frac{d\psi(x)}{dx}$ must be continuous

(a), (c) follows from the requirement that $P(x,t)$, $S(x,t)$ are well-defined

(b) follows from requirement (c)

Requirement (d) $\leftrightarrow$ Schrodinger equation

Time-independent Schrodinger equation

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

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

Integrate the above equation from $a-\epsilon$ to $a+\epsilon$

$$\left(\frac{d\psi}{dx}\right)_{a+\epsilon} - \left(\frac{d\psi}{dx}\right)_{a-\epsilon} = \int_{a-\epsilon}^{a+\epsilon}\frac{2m}{\hbar^2}[V(x)-E]\psi(x)dx$$

$\rightarrow 0$ as $\epsilon \rightarrow 0$
if V is finite

Note: If potential V has an infinite discontinuity, then the right-hand side may or may not vanish

Example $\quad V(x) = V_0 \delta(x-a)$

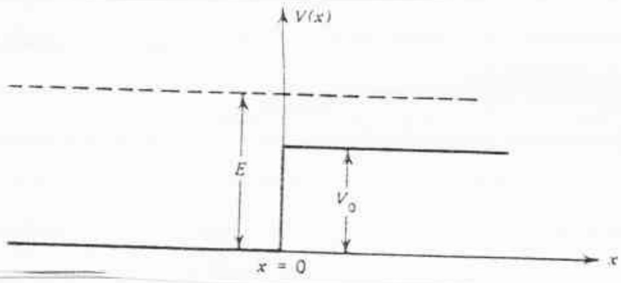
$$\Rightarrow \quad \left(\frac{d\psi}{dx}\right)_{a+\epsilon} - \left(\frac{d\psi}{dx}\right)_{a-\epsilon} = \int_{a-\epsilon}^{a+\epsilon} \frac{2m}{\hbar^2}\left[V_0 \delta(x-a) - E\right]\psi(x)\,dx$$

$$= \frac{2m}{\hbar^2} V_0 \psi(a)$$

The Potential Step

$E > V_0 > 0$

$$V(x) = \begin{cases} 0 & \text{for } x<0 \\ V_0 & \text{for } x>0 \end{cases}$$



The Schrodinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_1 = E\psi_1 \quad \text{in I } (x<0)$$

$$\Rightarrow \frac{d^2}{dx^2}\psi_1 = -\frac{2mE}{\hbar^2}\psi_1 = -k_1^2\psi_1$$

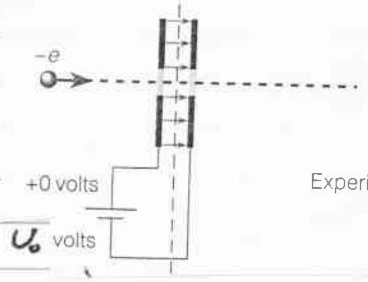
$$k_1 = \sqrt{2mE}/\hbar$$

$$\Rightarrow \psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x}$$

$$\psi_1(x,t) = \psi_1 e^{-i\omega t}$$

$$= Ae^{ik_1x - i\omega t} + Be^{-ik_1x - i\omega t}$$

($Ae^{ik_1x-i\omega t}$ ↓ incident plane wave; $Be^{-ik_1x-i\omega t}$ ↓ reflected plane wave)



Experimental setup

$V_0 = eU_0$

Experimental setup

The Schrodinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_2}{dx^2} + V_0\psi_2(x) = E\psi_2(x) \quad \text{in II } (x>0)$$

$$\Rightarrow \frac{d^2}{dx^2}\psi_2 = -\frac{2m}{\hbar^2}(E-V_0)\psi_2 = -k_2^2\psi_2$$

$$k_2 = \frac{\sqrt{2m(E-V_0)}}{\hbar}$$

$$\Rightarrow \psi_2(x) = Ce^{ik_2x} + De^{-ik_2x}$$

$D = 0$ (no new potential to reflect the wave from the right)

$$\psi(x) = \begin{cases} \psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x}, & x<0 \\ \psi_2(x) = Ce^{ik_2x}, & x>0 \end{cases}$$

Continuity equation at $x=0$

$\psi_1(x=0) = \psi_2(x=0) \Rightarrow A+B=C$

$\left(\frac{d\psi_1}{dx}\right)_{x=0} = \left(\frac{d\psi_2}{dx}\right)_{x=0} \Rightarrow k_1(A-B) = k_2 C$

$$\Rightarrow \quad B = \frac{k_1-k_2}{k_1+k_2} A$$

$$C = \frac{2k_1}{k_1+k_2} A$$

$$\Rightarrow \quad \psi(x) = \begin{cases} A e^{ik_1x} + A \frac{k_1-k_2}{k_1+k_2} e^{-ik_1x} & x<0 \\ A \frac{2k_1}{k_1+k_2} e^{ik_2x} & x \geq 0 \end{cases}$$

$$\psi(x,t) = \psi(x) e^{-i\omega t}$$

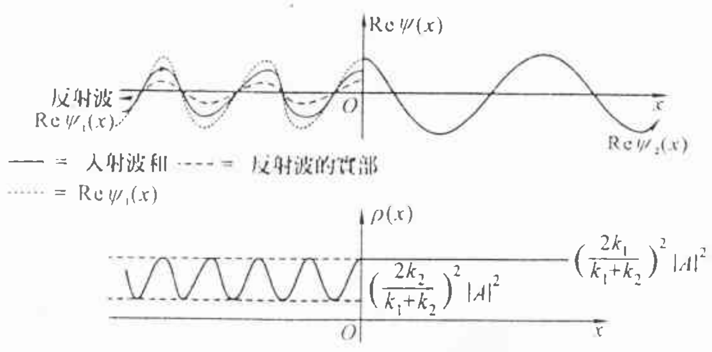
$$\rho(x,t) = \psi^*(x,t)\,\psi(x,t)$$

$$= \begin{cases} \frac{4}{(k_1+k_2)^2} |A|^2 (k_1\cos k_1x - ik_2\sin k_1x)(k_1\cos k_1x + ik_2\sin k_1x) & [x \leq 0] \\ \frac{2k_1}{(k_1+k_2)^2} |A|^2 & x \geq 0 \end{cases}$$

$\rho(x,t)$ is positive definite and independent of time.

$$\rho_I(x) = \frac{4|A|^2}{(k_1+k_2)^2}(k_1^2\cos^2 k_1x + k_2^2\sin^2 k_1x)$$

$$\rho_{II}(x) = \frac{4k_1^2}{(k_1+k_2)^2}|A|^2$$



$\rho(x<0) = \frac{4|A|^2}{(k_1+k_2)^2}(k_1^2\cos^2 k_1x + k_2^2\sin^2 k_1x)$ $\qquad$ $\rho(x \geqslant 0) = \frac{4k_1^2}{(k_1+k_2)^2}|A|^2$

$\psi(x)$= 能量本徵函數， $\rho(x)$= 機率密度

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Reflection Coefficient and Transmission Coefficient

R (reflection coefficient) $= \dfrac{\text{reflected probability flux}}{\text{incident probability flux}}$

$$= \frac{\left(\frac{k_1-k_2}{k_1+k_2}\right)^2 |A|^2 \frac{\hbar}{2im}\left(e^{ik_1x}\frac{d}{dx}e^{-ik_1x} - e^{-ik_1x}\frac{d}{dx}e^{ik_1x}\right)}{|A|^2 \frac{\hbar}{2im}\left(e^{-ik_1x}\frac{d}{dx}e^{ik_1x} - e^{ik_1x}\frac{d}{dx}e^{-ik_1x}\right)}$$

$$= \left(\frac{k_1-k_2}{k_1+k_2}\right)^2 = \left\{\frac{1-\sqrt{1-\frac{V_0}{E}}}{1+\sqrt{1-\frac{V_0}{E}}}\right\}^2$$

$T = \dfrac{\text{transmitted probability flux}}{\text{incident probability flux}}$

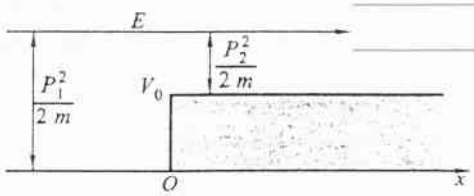
$$= \frac{\left(\frac{2k_1}{k_1+k_2}\right)^2 |A|^2 \frac{\hbar}{2im}\left(e^{-ik_2x}\frac{d}{dx}e^{ik_2x} - e^{ik_2x}\frac{d}{dx}e^{-ik_2x}\right)}{|A|^2 \frac{\hbar}{2im}\left(e^{-ik_1x}\frac{d}{dx}e^{ik_1x} - e^{ik_1x}\frac{d}{dx}e^{-ik_1x}\right)}$$

$$= \frac{4k_1k_2}{(k_1+k_2)^2}$$

Remarks

- For classical mechanics, when $E > V_0$, the particle only change its momentum at $x=0$

  $R \neq 0$, the presence of reflected wave, is due to the wave property of particle
  ↓
  quantum effect.

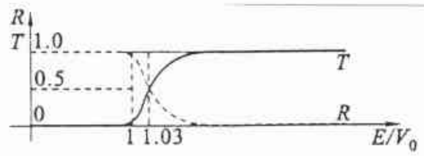


- Probability density $\rho(x)$ is real, positive-definite.
  $\rho(x)\,dx \sim$ probability of finding the particle in the interval dx
- $\rho(x,t)$ is independent of time
  Probability conservation

$$\frac{\partial S}{\partial x} + \frac{\partial \rho}{\partial t} = 0$$

$\Rightarrow S(x)$ is a constant

Furthermore, $R + T = 0$
↓
can be seen from the following figure
(R, T are plotted as a function of $\frac{V_0}{E}$)



$E < V_0$

In region (I)

$$\psi_1(x) = A e^{ik_1 x} + B e^{-ik_1 x}$$

$$k_1 = \frac{\sqrt{2mE}}{\hbar}$$

In region (II)

Schrodinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_2 + V_0\psi_2 = E\psi_2$$

$$\Rightarrow \frac{d^2}{dx^2}\psi_2 = \frac{2m(V_0-E)}{\hbar^2}\psi_2 = k_2^2\psi_2$$

$$k_2 = \frac{\sqrt{2m(V_0-E)}}{\hbar}$$

$$\Rightarrow \psi_2(x) = Ce^{k_2 x} + De^{-k_2 x}$$

↓ cannot increase exponentially as $x \to \infty$

$\Rightarrow C = 0$

$$\Rightarrow \psi_2(x) = De^{-k_2 x}$$

Continuity equation at $x = 0$

$$\psi_1(x=0) = \psi_2(x=0) \Rightarrow A + B = D$$

$$\left(\frac{d\psi_1}{dx}\right)_{x=0} = \left(\frac{d\psi_2}{dx}\right)_{x=0} \Rightarrow ik_1(A-B) = -k_2 D$$

$$\Rightarrow A = \frac{D}{2}\left(1 + \frac{ik_2}{k_1}\right)$$

$$B = \frac{D}{2}\left(1 - \frac{ik_2}{k_1}\right)$$

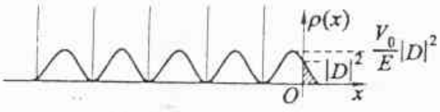
$$\Rightarrow \psi(x,t) = \psi(x)e^{-i\omega t}$$

$$= \begin{cases} \left(D\cos k_1 x - D\frac{k_2}{k_1}\sin\frac{k_2}{k_1}\sin k_1 x\right)e^{-i\omega t} & x<0 \\ De^{-k_2 x}e^{-i\omega t} & x>0 \end{cases}$$

$$\rho(x,t) = \begin{cases} |D|^2\left(\cos k_1 x - \frac{k_2}{k}\sin k_1 x\right)^2 & x<0 \\ |D|^2 e^{-2k_2 x} & x>0 \end{cases}$$

$\rho(x,t)$ is independent of time, positive - definite

The $\rho(x)$ can be plotted



Penetrating depth.

$$\rho(x>0) = |D|^2 e^{-2k_2 x}$$

The particle can penerate into $x>0$ region (classically forbidden region)

The penetrating depth

$$\Delta x = \frac{1}{2k_2} \sim \frac{1}{k_2} = \frac{\hbar}{\sqrt{2m(V_0-E)}}$$

$$\Delta p \sim \frac{\hbar}{\Delta x} = \sqrt{2m(V_0-E)}$$

$$\Rightarrow \quad \Delta E \sim \frac{(\Delta p)^2}{2m} = V_0 - E$$

↳ the energy deficit

Reflection coefficient

$$R = \frac{\text{reflected probability flux}}{\text{incident probability flux}}$$

$$= \frac{\frac{1}{4}|D|^2 (1+\frac{ik_2}{k_1})(1-\frac{ik_2}{k_1})}{\frac{1}{4}|D|^2 (1-\frac{ik_2}{k_1})(1+\frac{ik_2}{k_1})} = 1$$

Transmission coefficient

$$T = \frac{\text{transmitted probability flux}}{\text{incident probability flux}}$$

Transmitted probability flux $= \frac{\hbar}{2im}|D|^2 (e^{-k_2 x}\frac{d}{dx}e^{-k_2 x} - e^{-k_2 x}\frac{d}{dx}e^{-k_2 x})$
$= 0$

$\Rightarrow \quad T = 0 \qquad \Rightarrow \qquad T + R = 1$

Furthermore $\quad S = 0$ for all x

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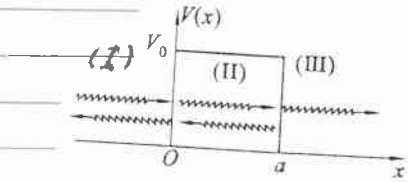
The Potential Barrier



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

$E < V_0$

Region I

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_1}{dx^2} = E\psi_1$$

$$\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x}$$

$$k_1 = \frac{\sqrt{2mE}}{\hbar}$$

Region II

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_2}{dx^2} + V_0\psi_2 = E\psi_2$$

$$\psi_2(x) = Fe^{-k_2x} + Ge^{k_2x}$$

$$k_2 = \frac{\sqrt{2m(V_0-E)}}{\hbar}$$

Region III

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_3}{dx^2} = E\psi_3$$

$$\psi_3(x) = Ce^{ik_3x} + De^{-ik_3x}$$

$$k_3 = \frac{\sqrt{2mE}}{\hbar} = k_1$$

Tunneling problem
↓
Incident wave is partially reflected and partially transmitted.

[Note, only the origin is shifted between the two figures]

In classical mechanics, the particle cannot be transmitted.

A particle may transmit through a potential barrier is due to the wave property of particle
↓
quantum effect

[Furthermore, a "whole" particle (electron) is transmitted with probability, related to T

This quantum effect is known as tunneling phenomena.

Matching the boundary condition at $x=0$ and $x=a$.

$$\psi_1(x=0) = \psi_2(x=0) \qquad A+B = F+G$$

$$\left.\frac{d\psi_1}{dx}\right|_{x=0} = \left(\frac{d\psi_2}{dx}\right)_{x=0} \qquad ik_1(A-B) = k_2(G-F)$$

$$\psi_2(x=a) = \psi_3(x=a) \qquad Ge^{k_2 a} + Fe^{-k_2 a} = Ce^{ik_1 a}$$

$$\left(\frac{d\psi_2}{dx}\right)_{x=a} = \left(\frac{d\psi_3}{dx}\right)_{x=a} \qquad k_2(Ge^{k_2 a} - Fe^{-k_2 a}) = ik_1 C e^{ik_1 a}$$

There are 5 unknowns (A, B, G, F, C) and 4 equations

$\Rightarrow$ A, B, G, F can be solved in terms of C.

$$A = C\left\{\cosh(k_2 a) + i\frac{k_2^2 - k_1^2}{2k_1 k_2}\sinh(k_2 a)\right\}e^{ik_1 a}$$

$$B = -i\left(C\frac{k_1^2+k_2^2}{2k_1k_2}\sinh k_2 a\right)e^{ik_1 a}$$

$$F = \frac{C}{2}\left(1 - i\frac{k_1}{k_2}\right)e^{(k_2+k_1)a}$$

$$G = \frac{C}{2}\left(1 + i\frac{k_1}{k_2}\right)e^{(-k_2+ik_1)a}$$

$\psi(x,t)$ is given (up to a constant C)

$$\psi_1(x,t) = \psi_1(x)e^{-i\omega t} = iC\frac{k_1^2+k_2^2}{2k_1k_2}\sinh(k_2 a)\left(e^{i(k_1 x+\omega t)} + e^{i(k_1 x - \omega t)}\right)e^{ik_1 a} + C\left(\cosh k_2 a + i\frac{k_2}{k_1}\sinh(k_2 a)\right)e^{ik_1 a}\, e^{i(k_1 x - \omega t)}$$

$$\psi_2(x,t) = \psi_2(x)e^{-i\omega t}$$

$$= C\left\{\cosh[k_2(x-a)] + i\frac{k_1}{k_2}\sinh[k_2(x-a)]\right\}e^{i(k_1 a - \omega t)}$$

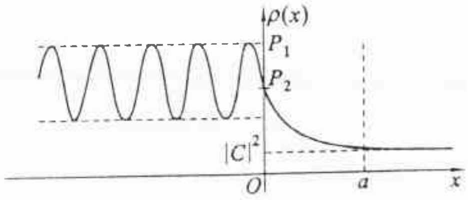
$$\psi_3(x,t) = \psi_3(x)e^{-i\omega t} = Ce^{i(k_1 x - \omega t)}$$

Using $\rho(x,t) = \psi^*(x,t)\,\psi(x,t)$, $\rho(x,t)$ can be calculated.

$\downarrow$

$\rho(x,t)$ is positive definite and independent of time.

$\rho(x,t) = \rho(x)$



The most interesting quantity for tunneling problem is the transmission coefficent T

$$T = \frac{\text{transmitted probability flux}}{\text{incident probability flux}}$$

$$= \frac{\left|\frac{\hbar}{2im}\left\{e^{-ik_1x}\frac{d}{dx}e^{ik_1x} - e^{ik_1x}\frac{d}{dx}e^{-ik_1x}\right\}\right| |C|^2}{\left|\frac{\hbar}{2im}\left\{e^{-ik_1x}\frac{d}{dx}e^{ik_1x} - e^{ik_1x}\frac{d}{dx}e^{-ik_1x}\right\}\right| |A|^2}$$

$$= \frac{\frac{\hbar k_1}{m}|C|^2}{\frac{\hbar k_1}{m}|A|^2} = \frac{|C|^2}{|A|^2}$$

$$\Rightarrow \quad T = \left[\cosh^2(k_2a) + \frac{1}{4}\left(\frac{k_2^2-k_1^2}{k_1k_2}\right)^2\sinh^2(k_2a)\right]^{-1}$$

$$= \left[1 + (\sinh^2(k_2a))\left(1 + \frac{1}{4}\frac{(k_2^2-k_1^2)^2}{k_1^2k_2^2}\right)\right]^{-1}$$

$$= \left[1 + \frac{\sinh^2 k_2a}{4\frac{E}{V_0}(1-\frac{E}{V_0})}\right]^{-1} = \left[1 + \frac{(e^{k_2a} - e^{-k_2a})^2}{16\frac{E}{V_0}(1-\frac{E}{V_0})}\right]^{-1}$$

$$= \left[1 + \frac{e^{2k_2a}(1 - 2e^{-2k_2a} + e^{-4k_2a})}{16\frac{E}{V_0}(1-\frac{E}{V_0})}\right]^{-1}$$

T is a function of E, V_0 and a.

↓

This is the fundamental equation for discussing the tunneling problem.

If $k_2a \gg 1$, then

$$T \sim \left[\frac{e^{2k_2a}}{16\frac{E}{V_0}(1-\frac{E}{V_0})}\right]^{-1} = 16\frac{E}{V_0}\left(1-\frac{E}{V_0}\right)e^{-2k_2a}$$

$$= 16\frac{E}{V_0}\left(1-\frac{E}{V_0}\right)e^{-2\sqrt{2m(V_0-E)}\,a/\hbar}$$

Usually, the exponential is the dominating factor.

Potential barrier with $E > V_0$ can be carried out with the same method. (with appropriate changes in region II

$$R = \frac{\sin^2\left[\frac{\sqrt{2m(E-V_0)}}{\hbar} a\right]}{\sin^2\left[\frac{\sqrt{2m(E-V_0)}}{\hbar} a + 4\frac{E}{V_0}\left(\frac{E}{V_0}-1\right)\right.}$$

$$T = \frac{4\frac{E}{V_0}\left(\frac{E}{V_0}-1\right)}{\sin^2\left[\frac{\sqrt{2m(E-V_0)}}{\hbar} + 4\frac{E}{V_0}\left(\frac{E}{V_0}-1\right)\right.}$$

Although the reflection and transmission probabilities are in general non-zero, the numerator of the reflection probability involve a sine. When the sine is zero, there is no reflection
↓
resonant transmission.

The condition is

$$\frac{\sqrt{2m(E-V_0)}}{\hbar} a = n\pi \quad \Rightarrow \quad E = V_0 + \frac{n^2\pi^2\hbar^2}{2ma^2}$$

↳ n: integer

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Compare with the formula in the textbook (where the detail has not been worked out)

$k_2 a \gg 1$

$$T \cong \left[\frac{1}{4}\left(\frac{k_2^2+k_1^2}{k_1 k_2}\right)^2 \frac{1}{4} e^{2k_2 a}\right]^{-1}$$

$$= \frac{16 k_1^2 k_2^2}{k_1^2+k_2^2} e^{-2k_2 a}$$

[$\cosh k_2 a \sim \sinh k_2 a \sim \frac{1}{2} e^{k_2 a}$ as $ka \gg 1$]

With the identification

	our notation	notation of the textbook
	k_1	k
	k_2	κ
width	a	$2a$
	T	$\lvert T\rvert^2$

$\Rightarrow$ we recover the equation (8-18)

$$T = \frac{16 k^2 \kappa^2}{k^2+\kappa^2} e^{-4\kappa a}.$$

[Our notation follow that of 林清凉 "近代物理" I 第十章]

In general, the barriers that encounter in physical phenomena are not square

⇒ we want to oblain an approximate exp ession for the transmission coefficient $|T|^2$ through irregular barrier

Proper way: WKB method will not be discussed here
(WKB: still an approximate method)

The most important factor $e^{-4\kappa a} = e^{-2\kappa(2a)}$ (2a: width)

Other factors are slowly varying compared with this factor

For a square barrier

$$\ln|T|^2 = -2\kappa(2a) + 2\ln\frac{2(ka)(\kappa a)}{(ka)^2+(\kappa a)^2}$$

(will neglect this term)

Approximate a smooth barrier by a juxaposition of square potential barrier (See the following figure

$$\ln|T|^2 = \sum_{\substack{\text{partial}\\\text{barrier}}} \ln|T_{\substack{\text{partial}\\\text{barrier}}}|^2$$

$$\simeq -2\sum \Delta x \langle \kappa \rangle$$

(Δx: width of the barrier; $\langle \kappa \rangle$: average κ in the inverval)

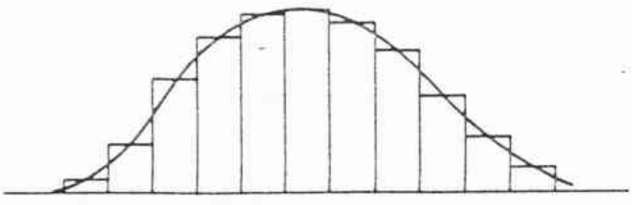
$$\simeq -2\int dx \sqrt{\frac{2m}{\hbar^2}[V(x)-E]}$$

$$\Rightarrow |T|^2 \simeq e^{-2\int dx \sqrt{\frac{2m}{\hbar^2}[V(x)-E]}}$$

The equation requires for each partial barrier $2\Delta x \cdot \kappa \gg 1$

⇒ (i) the above approximation is poor near the turning point (i.e., $V(x) = E \Rightarrow \kappa = 0$)

(ii) $V(x)$ must be smooth so that one can approximate a curved barrier by a stack of sufficient large width square barrier

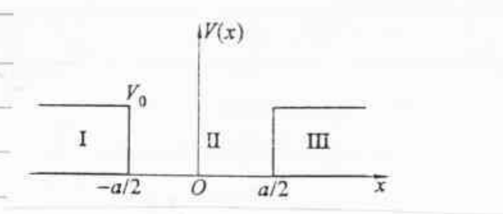


Approximation of smooth barrier by a juxta-position of square potential barriers.

Potential Well

We have already discussed the problem of infinite potential well.

In this section, we shall discuss the finite potential well problem.



$E < V_0$

Region I

$x < -\frac{a}{2}$

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_0\right)\psi_1(x) = E\psi_1(x)$$

$$\Rightarrow \psi_1(x) = Ce^{k_1 x} + De^{-k_1 x}$$

$$k_1 = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$$

The wave function is finite at $x = -\infty$

$\Rightarrow D = 0$

Region II

$-\frac{a}{2} < x < \frac{a}{2}$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_2(x) = E\psi_2(x)$$

$$\Rightarrow \psi_2(x) = A'e^{ik_2 x} + B'e^{-ik_2 x}$$

$$= A\sin k_2 x + B\cos k_2 x$$

$$k_2 = \frac{\sqrt{2mE}}{\hbar}$$

we use sin and cos because we want to take advantage of the symmetry property

Region III

$\frac{a}{2} < x$

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_0\right)\psi_3(x) = E\psi_3(x)$$

$$\Rightarrow \psi_3(x) = Fe^{k_1 x} + Ge^{-k_1 x}$$

The wave function must be finite at $x = \infty$

$\Rightarrow F = 0$

$$\psi(x) = \begin{cases} \psi_1(x) = Ce^{k_1 x} & x < -\frac{a}{2} \\ \psi_2(x) = A\sin k_2 x + B\cos k_2 x & -\frac{a}{2} < x < \frac{a}{2} \\ \psi_3(x) = Ge^{-k_1 x} & \frac{a}{2} < x \end{cases}$$

Symmetry of the potential

$$V(x) = V(-x)$$

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

Let $x \to -x$ (we just rename our variable

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

With $V(x) = V(-x)$, the equation becomes

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

If $\psi(x)$ is eigenfunction of the Schrodinger equation with eigenvalue E, then $\psi(-x)$ is also an eigenfunction of the same Schrodinger equation with the same eigenvalue E.

From superposition principle

$$\psi_{\substack{even \\ odd}}(x) = \frac{1}{\sqrt{2}}\left(\psi(x) \pm \psi(-x)\right)$$

are also eigenfunctions of the Schrodinger equation with eigenvalue E

$$\psi_{even}(x) = \psi_{even}(-x)$$

$$\psi_{odd}(x) = -\psi_{odd}(-x)$$

$\Rightarrow$ With $V(x) = V(-x)$, we can solve the problem by looking for even, odd eigenfunction.

Even solution

~~$\psi_1(x) = C e^{k_1 x}$~~ $\quad x < -\frac{a}{2}$

$\psi_2(x) = B\cos k_2 x \quad -\frac{a}{2} < x < \frac{a}{2}$

$\psi_3(x) = C e^{-k_1 x} \quad x > \frac{a}{2}$

Matching the boundary condition at $x = -\frac{a}{2}$

$$\psi_1\left(x = -\frac{a}{2}\right) = \psi_2\left(x = -\frac{a}{2}\right)$$

$$B\cos\frac{k_2 a}{2} = C e^{-k_1\frac{a}{2}}$$

$$\left(\frac{d\psi_1}{dx}\right)_{x=-\frac{a}{2}} = \left(\frac{d\psi_2}{dx}\right)_{x=-\frac{a}{2}}$$

$$-Bk_2\sin\left(k_2\left(\frac{-a}{2}\right)\right) = Ck_1 e^{k_1\left(-\frac{a}{2}\right)}$$

~~$\Rightarrow \quad k_2 \tan k_2 a = k_1$~~

Compare our notation with that used in the textbook

Our notation	Notation of the textbook
k_2	q
k_1	κ

We recover the equation (8-35) of the textbook, i.e.,

$$q \tan qa = \kappa \qquad (A)$$

· With V_0, a given, (A) is an equation for E

$\downarrow$

only certain values of E will satisfy (A)

$\downarrow$

only discrete energies are allowed.

· The boundary conditions at $x = \frac{a}{2}$, can be shown, are satified automatically

· Equation (A) is solved graphically

From Equation (A), we have

$$\sqrt{\frac{2mE}{\hbar}} \tan \sqrt{\frac{mEa^2}{2\hbar^2}} = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

Eigenvalue of E can be found by solving above equation.

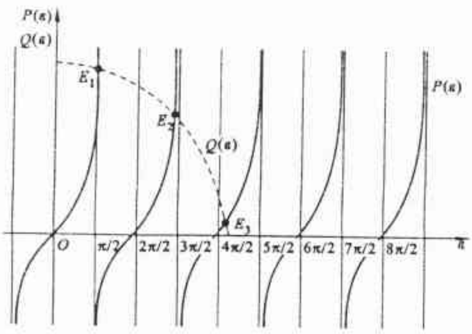
Analytic solutions are difficult to find, we usually solved it using graphic method, i.e., plot LHS, RHS as function of E. The intersection $\Rightarrow$ eigenvalues of E

Define $\epsilon = \sqrt{\frac{mEa^2}{2\hbar^2}}$

Equation (A) becomes $\underbrace{\epsilon \tan\epsilon}_{P(\epsilon)} = \underbrace{\sqrt{\frac{mV_0a^2}{2\hbar^2} - \epsilon^2}}_{Q(\epsilon)}$

$$Q(\epsilon) = \sqrt{\frac{mV_0a^2}{2\hbar^2} - \epsilon^2} \quad \Rightarrow \quad Q^2 + \epsilon^2 = \frac{mV_0a^2}{2\hbar^2}$$

(a circle when Q is plotted against ϵ.)



The energy eigenvalues: $E_{even,0}, E_{even,1}, \cdots$ can be found.
$\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \| \qquad\quad \|$
$\qquad\qquad\qquad\qquad\qquad\qquad\qquad E_{e0} \qquad E_{e1}$

Odd solution.

$$\psi_1(x) = C e^{k_1 x} \qquad x < -\frac{a}{2}$$

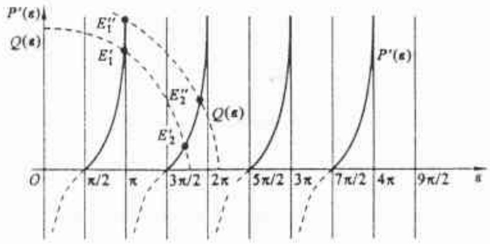
$$\psi_2(x) = A \sin k_2 x \qquad -\frac{a}{2} < x < \frac{a}{2}$$

$$\psi_3(x) = -C e^{-k_1 x} \qquad x > \frac{a}{2}$$

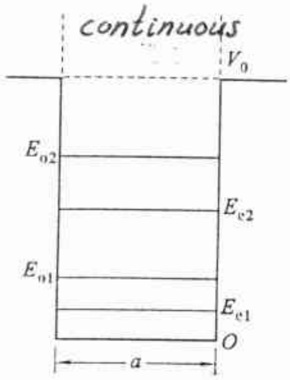
$k_2 \cot \frac{k_2 a}{2} = -k_1$ (from matching the boundary conditions)

$$\Rightarrow \sqrt{\frac{2mE}{\hbar^2}} \cot \sqrt{\frac{mEa^2}{2\hbar^2}} = -\sqrt{\frac{2m(V_0-E)}{\hbar^2}}$$

Again, graphic method can be used to find $E_{01}, E_{02}, \cdots$



From these calculation, we find the energy spectrum of this finite square well problem.



With eigenvalue E given, the wave function is now determined

- k_1, k_2 are known
- the only free parameter is C, can be determined through normalization.

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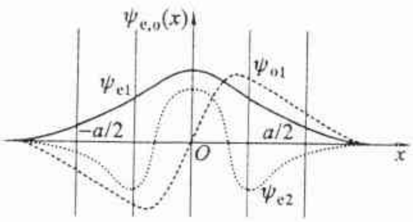
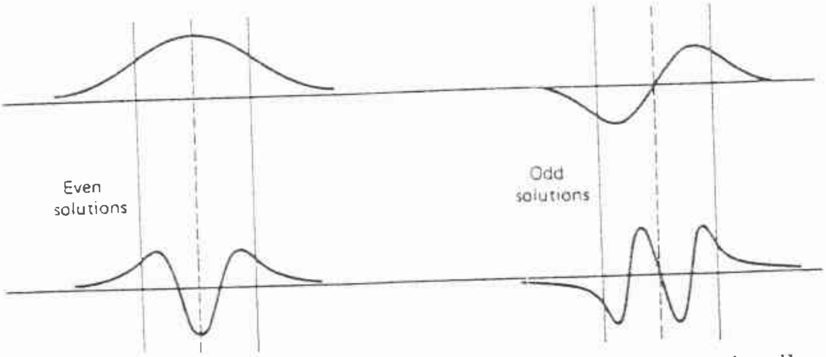
The wave functions (eigenfunctions) corresponding to the first few lowest eigenvalues (energy) E_{e1}, E_{e2}, E_{o1}, E_{o2} are given in the following figure.





Solutions for discrete spectrum in attractive potential well.

The more nodes, the higher are the energies of the bound states.

This can be understood as follows

· $p \propto \frac{d\psi}{dx}$

roughly speaking, the more a wave function wiggles, the higher is the average value of the slope, and accordingly the higher is the average kinetic energy

· The sign of the slope is not important, since the kinetic energy involves the square of the momentum.

Single and Double δ-Function Potential

Single δ-Function Potential

$V(x) = -V_0\,\delta(x) \qquad V_0 > 0$ → attractive potential

The Schrodinger equation is

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}u(x) - V_0\,\delta(x)\,u(x) = E\,u(x)$$

$$\Rightarrow \frac{d^2}{dx^2}u(x) + \frac{2mE}{\hbar^2}u(x) = -\frac{2mV_0}{\hbar^2}\delta(x) = -\lambda\,\delta(x)$$

$$\lambda \equiv \frac{2mV_0}{\hbar^2}$$

$E<0 \qquad \frac{d^2u}{dx^2} - \kappa^2 u(x) = 0$ for $x \neq 0$

$$\kappa^2 = \frac{2m|E|}{\hbar^2}$$

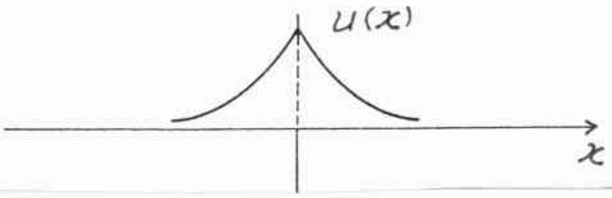
$u(x) = A e^{-\kappa x} + A' e^{\kappa x}$ for $x>0$

$A' = 0$ required by normalization condition

$u(x) = B e^{\kappa x} + B' e^{-\kappa x}$ for $x<0$

$B' = 0$ required by normalization condition

The wave function must be continuous at $x=0 \Rightarrow A = B$



The derivative of the wave function has a discontinuity at $x=0$

$$\left(\frac{du}{dx}\right)_{x=0^+} - \left(\frac{du}{dx}\right)_{x=0^-} = -\lambda\,u(0)$$

$$-\kappa A - \kappa a = -\lambda A$$

$$\Rightarrow \kappa = \frac{\lambda}{2} \Rightarrow \frac{\lambda^2}{4} = \frac{2m|E|}{\hbar^2}$$

$\Rightarrow$ only at $|E| = \frac{\hbar^2\lambda^2}{8m}$ there exists solution

Normalization $|A|^2\left[\int_0^\infty e^{-2\kappa x}dx+\int_{-\infty}^0 e^{2\kappa x}dx\right]=1$

$\Rightarrow |A|^2\frac{1}{2\kappa}\cdot 2=1 \Rightarrow |A|^2=\kappa$

$\Rightarrow A=\frac{1}{\sqrt{\kappa}}$

Double δ - Function Potential

$V(x)=-V_0\,\delta(x+a)-V_0\,\delta(x-a)$

$V(-x)=V(x)$, the potential is symmetric under $x\to -x$.
The solution should be either even or odd
We shall discuss the case : $E<0$

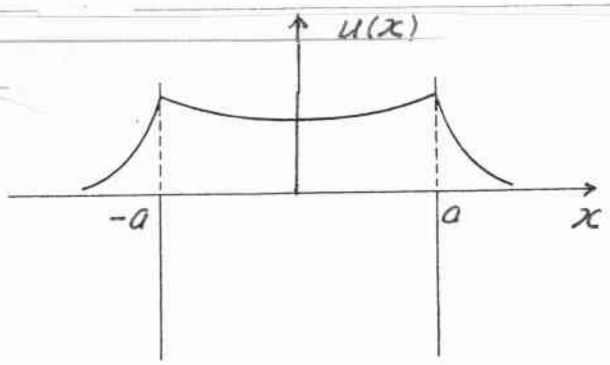
Even solution.

We are looking for the eigenvalue of the problem, we may leave the overall normalization to be open.

$u(x)=e^{-\kappa x}$ for $x>a$ ($e^{\kappa x}$ term is absent due to normalization requirement)

$u(x)=A\cosh\kappa x$ for $a>x>-a$ (originally, it is a linear combination of $e^{\kappa x}$ and $e^{-\kappa x}$, even solution requirement makes it possible to write it as $\cosh\kappa x$)

$u(x)=e^{\kappa x}$ for $x<-a$ (from even solution requirement)



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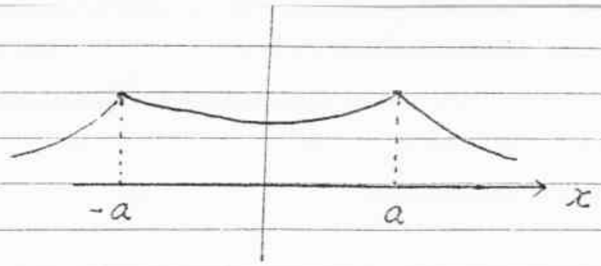


Wave function is continuous at $x = a$

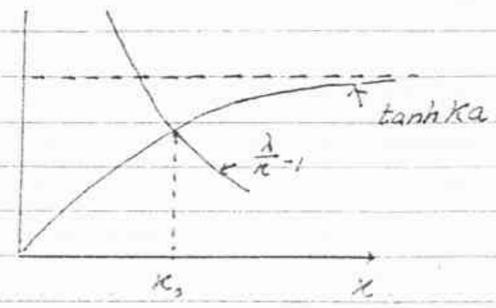
$$e^{-\kappa a} = A\cosh \kappa a$$

Derivative of the wave function has a discontinuity at $x = a$

$$-\kappa e^{-\kappa a} - \kappa A \sinh \kappa a = -\lambda \underbrace{e^{-\kappa a}}_{u(a)} \qquad \lambda = \frac{2mV_0}{\hbar^2}$$

Due to symmetry requirement, the boundary condition at $x = -a$ will give no new result.

$$\Rightarrow \quad \tanh \kappa a = \frac{\lambda}{\kappa} - 1 \quad \text{eigenvalue equation}$$



$$\kappa = \sqrt{\frac{2m|E|}{\hbar^2}}$$

$\kappa_0 \rightarrow$ eigenvalue of energy

Discussion

$\tanh \kappa a > 0 \qquad \frac{\lambda}{\kappa_0} - 1 > 0 \quad \Rightarrow \quad \lambda > \kappa_0$

$\tanh \kappa a < 1 \qquad \frac{\lambda}{\kappa_0} - 1 < 1 \quad \Rightarrow \quad \frac{\lambda}{2} < \kappa_0$

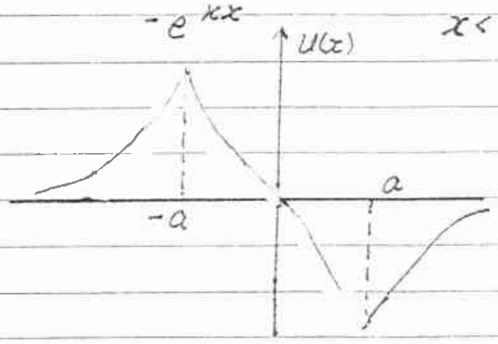
$\Rightarrow \qquad \lambda > \kappa_0 > \frac{\lambda}{2} \qquad\qquad \kappa = \frac{\lambda}{2}$ for single δ function

Energy of the double well is a larger negative number than that of a single δ function potential with the same strength

In real world, an electron bound to two nuclei seperated by a small distance (similar to a double δ-function potential) will have lower energy than bound to a single nuclei (similar to a single δ-function potential)

Odd solution

$$u(x) = \begin{cases} e^{-\kappa x} & x > a \\ A \sinh \kappa x & a > x > -a \\ -e^{\kappa x} & x < -a \end{cases}$$



Boundary condition at $x = a$

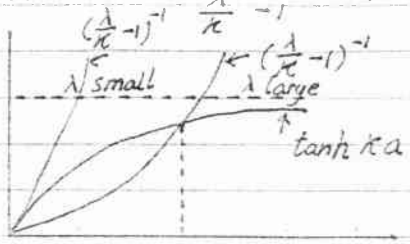
$$A \sinh \kappa a = e^{-\kappa a}$$

$$-\kappa e^{-\kappa a} - \kappa a \cosh \kappa a = -\lambda e^{-\kappa a}$$

$$\Rightarrow \quad \coth \kappa a = \frac{\lambda}{\kappa} - 1 \qquad \Rightarrow \quad \tanh \kappa a = \frac{1}{\left(\frac{\lambda}{\kappa} - 1\right)}$$

$$\tanh \kappa a > 0 \quad \Rightarrow \quad \frac{\lambda}{\kappa} - 1 > 0 \quad \Rightarrow \quad \frac{\lambda}{\kappa} > 1 \quad \Rightarrow \quad \lambda > \kappa$$

$$\tanh \kappa a < 1 \quad \Rightarrow \quad \frac{1}{\frac{\lambda}{\kappa} - 1} < 1 \quad \Rightarrow \quad 1 < \frac{\lambda}{\kappa} - 1 \quad \Rightarrow \quad \kappa < \frac{\lambda}{2}$$



⇒ The odd solution, if there is a bound state, is less strongly bound than the even solution.
The wave function, which has to go through zero, is forced to be steep because the wells, and thus can only accommodate to a less rapidly falling exponential.
Depending on the size of λ, there may or may not exist an odd bound state.

Chapter 9

Schrodinger Equation in Three Dimension. (Hydrogen Atom)

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi(x,y,z,t)+V(x,y,z,t)\psi(x,y,z,t)$$

$$= i\hbar\frac{\partial}{\partial t}\psi(x,y,z,t)$$

$\psi(x,y,z,t)$ = wave function.

$|\psi(x,y,z,t)|^2\,dx\,dy\,dz$ = probability of finding the "electron" in the volume element between x and $x+dx$, y and $y+dy$, z and $z+dz$ at time t

$$= |\psi|^2 d^3r = |\psi|^2 dV$$

In more compact notation, it can be written as

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r},t)+V(\vec{r},t)\psi(\vec{r},t)=i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t)$$

$$\Rightarrow \quad H\psi = i\hbar\frac{\partial\psi}{\partial t}$$

$$H = -\frac{\hbar^2}{2m}\nabla^2+V$$

For $V(\vec{r},t)=V(\vec{r})$ time independent potential, the problem can be solved by the method of seperation of variable

$$\psi(\vec{r},t) = u(\vec{r})\,e^{-iEt/\hbar}$$

with $u(\vec{r})$ satisfies the time-independent Schrodinger equation

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)u(x,y,z)+V(x,y,z)\,u(x,y,z)$$

$$= E\,u(x,y,z)$$

If $V(x,y,z)=V_1(x)+V_2(y)+V_3(z)$, then

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)u(x,y,z)+\left(V_1(x)+V_2(y)+V_3(z)\right)$$

$$u(x,y,z) = E\,u(x,y,z)$$

Ansatz : $\quad u(x,y,z) = X(x)\,Y(y)\,Z(z)$

Substitute into the above equation

$$-\frac{\hbar^2}{2m}YZ\frac{d^2}{dx^2}X-\frac{\hbar^2}{2m}XZ\frac{d^2}{dy^2}Y-\frac{\hbar^2}{2m}XY\frac{d^2}{dz^2}Z$$

$$+ V_1(x) XYZ + V_2(y) XYZ + V_3(z) XYZ = E XYZ$$

Divide through by XYZ and rearrange

$$-\frac{\hbar^2}{2m}\frac{1}{X}\frac{d^2}{dx^2}X + V_1(x) = \frac{\hbar^2}{2m}\frac{1}{Y}\frac{d^2}{dy^2}Y + \frac{\hbar^2}{2m}\frac{1}{Z}\frac{d^2}{dz^2}Z - V_2(y)$$
$$- V_3(z) + E$$

LHS is function of x only
RHS is function of y, z only

$$\Rightarrow \quad -\frac{\hbar^2}{2m}\frac{1}{X}\frac{d^2}{dx^2}X + V_1(x) = E_x$$

$$+\frac{\hbar^2}{2m}\frac{d^2}{dy^2}Y + \frac{\hbar^2}{2m}\frac{1}{Z}\frac{d^2}{dz^2}Z - V_2(y) - V_3(z) + E = E_x$$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dy^2}Y + V_2(y) = \frac{\hbar^2}{2m}\frac{1}{Z}\frac{d^2}{dz^2} - V_3(z) + E - E_x$$

LHS is function of y only
RHS is function of z alone

$$\Rightarrow \quad -\frac{\hbar^2}{2m}\frac{1}{Y}\frac{d^2}{dy^2}Y + V_2(y) = E_y$$

and $-\frac{\hbar^2}{2m}\frac{1}{Z}\frac{d^2}{dz^2} + V_3(z) = E - E_x - E_y = E_z$

$$\Rightarrow \quad -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}X(x) + V_1(x)X(x) = E_x X(x)$$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}Y(y) + V_2(y)Y(y) = E_y X(x)$$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}Z(z) + V_3(z)Z(z) = E_z Z(z)$$

with $E = E_x + E_y + E_z$

The problem is reduced to solve three one dimensional Schrodinger equations.

Example: three dimensional infinite well problem

$$V_1(x) = \begin{cases} 0 & \text{for } 0 < x < L_1 \\ \infty & \text{for } x > L_1, \ x < 0 \end{cases}$$

$$V_2(y) = \begin{cases} 0 & \text{for } 0 < y < L_2 \\ \infty & \text{for } y > L_2, \ y < 0 \end{cases}$$

$$V_3(z) = \begin{cases} 0 & \text{for } 0<z<L_3 \\ \infty & \text{for } z>L_3,\ z<0 \end{cases}$$

$$X(x) = A_1 \sin kx + B \cos kx \quad \text{in} \quad 0<x<L_1$$

$$\frac{\hbar^2 k^2}{2m} = E_x$$

$$= 0 \quad \text{in} \quad x<0,\ x>L_1$$

Boundary condition $X(0)=0 \Rightarrow B=0$
$X(L_1)=0 \Rightarrow k_n L_1 = n\pi$

$$\Rightarrow k_n = \frac{n\pi}{L_1} \qquad n_x = \text{integers.}$$

$$\Rightarrow X(x) = A_n \sin \frac{n\pi}{L_1} x \quad \text{with } n_x = \text{integrals in } 0<x<L_1$$

Normalization $|A_n|^2 \int_0^{L_1} \sin^2 \frac{n\pi}{L_1} x \, dx = 1.$

$$A_n = \sqrt{\frac{2}{L_1}}$$

$$E_{x,n_x} = \frac{\hbar^2 n_x^2 \pi^2}{2mL_1^2}$$

The same method can be used to solve the y, z equation

$$\Rightarrow u_{n_x,n_y,n_z}(x,y,z) = \sqrt{\frac{2^3}{L_1L_2L_3}} \sin \frac{n_x \pi x}{L_1} \sin \frac{n_y \pi y}{L_2} \sin \frac{n_z \pi z}{L_3}$$

$$\Rightarrow \psi_{n_x,n_y,n_z}(x,y,z,t) = u_{n_x,n_y,n_z}(x,y,z)\, e^{-i\frac{E}{\hbar}t}$$

$$E = E_{n_x} + E_{n_y} + E_{n_z} = \frac{\hbar^2\pi^2 n_x^2}{2mL_1^2} + \frac{\hbar^2\pi^2 n_y^2}{2mL_2^2} + \frac{\hbar^2\pi^2 n_z^2}{2mL_3^2}$$

Degeneracy : different number wave functions with same energy
↓
linear independent

Example : for the case $L_1 = L_2 = L_3 = L$

$$E = \frac{\hbar^2\pi^2}{2mL^2}(n_x^2 + n_y^2 + n_z^2)$$

Clearly, $n_x=2,\ n_y=1,\ n_z=1$, $n_x=1,\ n_y=2,\ n_z=1$ and $n_x=1,\ n_y=1,\ n_z=2$ will have the

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⇒ these three states are said to be degenerate.
the number of degeneracy = 3.

· This is an important concept that we shall encount ofter
· From this example, it can be seen the concept of degeneracy is closely related to symmetry.

Central force problem. $V(x,y,z) = V(r)$

$$r = \sqrt{x^2+y^2+z^2}$$

Obviously, it is more convenient to use the spherical coordinate

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi$$

$$\Rightarrow -\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\left(\frac{\partial^2\psi}{\partial\phi^2}\right)\right]$$

$$+ V(r)\psi = E\psi$$

[$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}$
are proved in various books on mathematical physics. In the Appendix A]

Since $V(r)$ is a function of r only, we shall try to solve the problem using the method of seperation of variable

$\psi(r,\theta,\phi)$ → time independent wave function

[$\psi(r,\theta,\phi,t) = \psi_E(r,\theta,\phi)e^{-iEt/\hbar}$]

$$\psi(r,\theta,\phi) = R(r)Y(\theta,\phi)$$

Substitute into the time-independent Schrodinger equation

$$-\frac{\hbar^2}{2m}\left[\frac{Y}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{R}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{R^2}{r^2\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right]$$

$$+ V(r)RY = ERY$$

Divide by YR and rearrange. (multiple $-\frac{2mr^2}{\hbar^2}$)

$$\Rightarrow \left\{\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{2mr^2}{\hbar^2}[V(r)-E]\right.$$

$$= -\frac{1}{Y}\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right.$$

LHS is function of r only

RHS is function of θ, φ

⇒ must be constant

For reasons that will appear in the due course, we shall choose the "seperation constant" to be $\ell(\ell+1)$

$$\Rightarrow \frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)-\frac{2mr^2}{\hbar^2}[V(r)-E]=\ell(\ell+1)$$

↓ radial equation, depend on V(r)

$$\frac{1}{Y}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right]=-\ell(\ell+1)$$

↓ angular equation, independent of V(r)

Multiply $Y\sin^2\theta$

$$\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right)+\frac{\partial^2 Y}{\partial\phi^2}=-\ell(\ell+1)\sin^2\theta\, Y.$$

Again, try seperation of variables

Ansatz $\quad Y(\theta,\phi)=\Theta(\theta)\Phi(\phi)$

Put it into above equation, divide through by $\Theta\Phi$, and rearrange

$$\Rightarrow \frac{1}{\Theta}\left[\sin\theta\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+\ell(\ell+1)\sin^2\theta\right]$$
$$=-\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2}$$

LHS is function of θ only
RHS is function of φ only

$$\Rightarrow \frac{1}{\Theta}\left[\sin\theta\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)\right]+\ell(\ell+1)\sin^2\theta=m^2$$

↓ θ equation

$$\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2}=-m^2$$

↓ φ equation

$$\frac{d^2\Phi}{d\phi^2} = -m^2\Phi$$

$\Rightarrow \quad \Phi(\phi) = e^{im\phi}$

$\Phi(\phi + 2\pi) = \Phi(\phi)$

↓

single-valueness of the wave function

$\Rightarrow \quad e^{2\pi i m} = 1 \Rightarrow m$ must be integer.

· This is closely related to the quantization of angular momentum.

· m is known as magnetic quantum number.

θ - equation

$$\sin\theta \frac{d}{d\theta}\left(\sin\theta \frac{d\Theta}{d\theta}\right) + [l(l+1)\sin^2\theta - m^2]\Theta = 0$$

Note: $m = 0, \pm 1, \pm 2, \cdots$

Change variable $x = \cos\theta$

[using the chain rule

$$\frac{d}{d\theta} = \frac{dx}{d\theta}\frac{d}{dx} = -\sin\theta \frac{d}{dx} = -\sqrt{1-x^2}\frac{d}{dx}$$

$\sin^2\theta = 1 - x^2$]

The above equation becomes

$$(1-x^2)\frac{d^2\Theta}{dx^2} - 2x\frac{d\Theta}{dx} + \left[l(l+1) - \frac{m^2}{1-x^2}\right]\Theta = 0$$

↓

associated Legendre equation.

Physical requirement:

$\Theta(x)$ must be well-behaved at $x = \pm 1$

$\Rightarrow \quad l$ must be integers, i.e. $l = 0, 1, 2, \cdots$

m must be from $-l$ to l, i.e.,

$m = -l, -l+1, -l+2, \cdots -1, 0, +1, \cdots l-2, l-1, l$

Θ is labelled by l, m

$\Theta(x) \propto P_l^m(x) \rightarrow$ associated Legendre polynomial.

A more general discussion of Legendre equation, Legendre polynomial is given in Appendix. B.

Radial equation depends on the $V(r)$ given, and will be discussed later.

分類：
編號： 16
總號：

(Orbital) Angular Momentum

$$\vec{L} = \vec{r} \times \vec{p} \rightarrow -i\hbar \, \vec{r} \times \nabla$$

In Cartesian coordinate

$$\vec{L} = \begin{vmatrix} i & j & k \\ x & y & z \\ P_x & P_y & P_z \end{vmatrix}$$

$$L_x = yP_z - zP_y = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$$

$$L_y = zP_x - xP_z = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)$$

$$L_z = xP_y - yP_y = -i\hbar\left(z\frac{\partial}{\partial y} - y\frac{\partial}{\partial z}\right)$$

Commutators between the angular momentum components

$$L_x L_y - L_y L_x = i\hbar L_z$$

$$L_y L_z - L_z L_y = i\hbar L_x$$

$$L_z L_x - L_x L_z = i\hbar L_y$$

Write in compact form

$$[L_i, L_j] = i\hbar \epsilon_{ijk} L_k$$

$$\epsilon_{ijk} = \begin{cases} +1 & \text{if } i,j,k \text{ is even permutation of } 1,2,3 \\ -1 & \text{if } i,j,k \text{ is odd permutation of } 1,2,3 \\ 0 & \text{if two or more indices are equal} \end{cases}$$

Fundamental commutator

$$[x, P_x] = [y, P_y] = [z, P_z] = i\hbar$$

$$[x, P_y] = [x, P_z] = [y, P_x] = [y, P_z] = [z, P_x] = [z, P_y] = 0$$

Theorem $[A+B, C+D]$

$$= (A+B)(C+D) - (C+D)(A+B)$$

$$= AC + BC + AD + BD - CA - DA - CB - DB$$

$$= [A, C] + [B, C] + [A, D] + [B, D]$$

Theorem $[AB, C] = A[B, C] + [A, C]B$

$$[AB, C] = ABC - ACB + ACB - CAB$$

$$-ACB = A[B, C] \qquad ACB - CAB = [A, C]B$$

Theorem $[A, BC] = [A, B]C + B[A, C]$

$$[A, BC] = ABC - BAC + BAC - BCA$$

$$ABC - BAC = [A, B]C \qquad BAC - BCA = B[A, C]$$

$$[L_x, L_y] = [yP_z - zP_y, zP_x - xP_z]$$

$$= \underbrace{[yP_z, zP_x]}_{(I)} - \underbrace{[zP_y, zP_x]}_{(II)} - \underbrace{[zP_y, zP_x]}_{(III)} + \underbrace{[zP_y, xP_z]}_{(IV)}$$

$$(I) = [yP_z, zP_x]$$

$$= y[P_z, zP_x] + [y, zP_x]P_z$$

$$y[P_z, zP_x] = y\left([P_z, z]P_x + z\underbrace{[P_z, P_x]}_{0}\right)$$

$$[y, zP_x]P_z = \underbrace{[y, z]}_{0}P_x P_z - z\underbrace{[y, P_x]}_{0}P_z$$

$$\downarrow$$

$$y[P_z, z]P_x$$

$$= y(-i\hbar P_x)$$

$$= -i\hbar\, yP_x$$

(II), (III) are obviously zero

$$(IV) = [z P_y, x P_z]$$

$$= z \underbrace{[P_y, x P_z]}_{0} + \underbrace{[z, x P_z]}_{} P_y$$

$$[z, x P_z] = \underbrace{[z, x]}_{0} P_z P_y + x \underbrace{[z, P_z]}_{i\hbar} P_y$$

$$[L_x, L_y] = i\hbar (x P_y - y P_x) = i\hbar L_z$$

Use similar method, we can show

$$[L_y, L_z] = i\hbar L_x$$

$$[L_z, L_x] = i\hbar L_y$$

$$\vec{L}^2 = L_x^2 + L_y^2 + L_z^2$$

$$[\vec{L}^2, L_z] = [L_x^2 + L_y^2 + L_z^2, L_z]$$

$$= [L_x^2, L_z] + [L_y^2, L_z] + \underbrace{[L_z^2, L_z]}_{0}$$

$$[L_x^2, L_z] = L_x \underbrace{[L_x, L_z]}_{} + \underbrace{[L_x, L_z]}_{} L_x$$

$$L_x(-i\hbar L_y) \qquad -i\hbar L_y L_x$$

$$[L_y^2, L_z] = L_y \underbrace{[L_y, L_z]}_{} + \underbrace{[L_y, L_z]}_{} L_y$$

$$i\hbar L_y L_x \qquad i\hbar L_x L_y$$

$$\Rightarrow [L^2, L_z] = 0$$

分類:
編號: 19
總號:

Angular Momentum in Spherical Coordinate

$$L_x = yP_z - zP_y = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$$

$$\frac{\partial}{\partial y} = \frac{\partial r}{\partial y}\frac{\partial}{\partial r} + \frac{\partial \theta}{\partial y}\frac{\partial}{\partial \theta} + \frac{\partial \phi}{\partial y}\frac{\partial}{\partial \phi}$$

$$= \sin\theta\sin\phi\frac{\partial}{\partial r} + \frac{\cos\theta\sin\phi}{r}\frac{\partial}{\partial \theta} + \frac{\cos\phi}{r\sin\theta}\frac{\partial}{\partial \phi}$$

$$\underset{r\cos\theta}{\overset{z}{\shortparallel}}\frac{\partial}{\partial y} = r\cos\theta\sin\theta\sin\phi\frac{\partial}{\partial r} + \cos^2\theta\sin\phi\frac{\partial}{\partial \theta} + \frac{\cos\theta\cos\phi}{\sin\theta}\frac{\partial}{\partial \phi}$$

$$\frac{\partial}{\partial z} = \frac{\partial r}{\partial z}\frac{\partial}{\partial r} + \frac{\partial \theta}{\partial z}\frac{\partial}{\partial \theta} + \frac{\partial \phi}{\partial z}\frac{\partial}{\partial \phi}$$

$$= \cos\theta\frac{\partial}{\partial r} + \left(-\frac{\sin\theta}{r}\right)\frac{\partial}{\partial \theta} + 0$$

$$y\frac{\partial}{\partial z} = r\sin\theta\sin\phi\left[\cos\theta\frac{\partial}{\partial r} - \frac{\sin\theta}{r}\frac{\partial}{\partial \theta}\right]$$

$$= r\cos\theta\sin\theta\sin\phi\frac{\partial}{\partial r} - \sin^2\theta\sin\phi\frac{\partial}{\partial \theta}$$

Put it together

$$L_x = i\hbar\left(\sin\phi\frac{\partial}{\partial \theta} + \cot\theta\cos\phi\frac{\partial}{\partial \phi}\right)$$

$$L_y = zP_x - xP_z = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)$$

$$\frac{\partial}{\partial x} = \frac{\partial r}{\partial x}\frac{\partial}{\partial r} + \frac{\partial \theta}{\partial x}\frac{\partial}{\partial \theta} + \frac{\partial \phi}{\partial x}\frac{\partial}{\partial \phi}$$

$$= \sin\theta\cos\phi\frac{\partial}{\partial r} + \frac{\cos\theta\cos\phi}{r}\frac{\partial}{\partial \theta} + \left(-\frac{\sin\phi}{r\sin\theta}\right)\frac{\partial}{\partial \phi}$$

$$z\frac{\partial}{\partial x} = r\cos\theta\left(\sin\theta\cos\phi\frac{\partial}{\partial r} + \frac{\cos\theta\cos\phi}{r}\frac{\partial}{\partial \theta} - \frac{\sin\phi}{r\sin\theta}\frac{\partial}{\partial \phi}\right)$$

$$= r\cos\theta\sin\theta\cos\phi\frac{\partial}{\partial r} + \cos^2\theta\cos\phi\frac{\partial}{\partial \theta} - \frac{\cos\theta\sin\phi}{\sin\theta}\frac{\partial}{\partial \phi}$$

$$\frac{\partial}{\partial z} = \frac{\partial r}{\partial z}\frac{\partial}{\partial r} + \frac{\partial \theta}{\partial z}\frac{\partial}{\partial \theta} + \frac{\partial \phi}{\partial z}\frac{\partial}{\partial \phi}$$

$$= \cos\theta\frac{\partial}{\partial r} + \left(-\frac{\sin\theta}{r}\right)\frac{\partial}{\partial \theta} + 0$$

$$x\frac{\partial}{\partial z} = r\sin\theta\cos\phi\left(\cos\theta\frac{\partial}{\partial r} - \frac{\sin\theta}{r}\frac{\partial}{\partial \theta}\right)$$

分類：
編號： 20
總號：

$$= r\cos\theta\sin\theta\cos\phi\frac{\partial}{\partial r} - \sin^2\theta\cos\phi\frac{\partial}{\partial\theta}$$

Put it together

$$L_y = i\hbar\left(-\cos\phi\frac{\partial}{\partial\theta} + \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right)$$

$$L_z = xP_y - yP_x = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$$

$$\frac{\partial}{\partial y} = \frac{\partial r}{\partial y}\frac{\partial}{\partial r} + \frac{\partial\theta}{\partial y}\frac{\partial}{\partial\theta} + \frac{\partial\phi}{\partial y}\frac{\partial}{\partial\phi}$$

$$= \sin\theta\sin\phi\frac{\partial}{\partial r} + \frac{\cos\theta\cos\phi}{r}\frac{\partial}{\partial\theta} + \frac{\cos\phi}{r\sin\theta}\frac{\partial}{\partial\phi}$$

$$x\frac{\partial}{\partial y} = r\sin\theta\cos\phi\left(\sin\theta\sin\phi\frac{\partial}{\partial r} + \frac{\cos\theta\cos\phi}{r}\frac{\partial}{\partial\theta} + \frac{\cos\phi}{r\sin\theta}\frac{\partial}{\partial\phi}\right)$$

$$= r\sin^2\theta\cos\phi\sin\phi\frac{\partial}{\partial r} + \sin\theta\cos\phi\cos\theta\sin\phi\frac{\partial}{\partial\theta} + \cos^2\phi\frac{\partial}{\partial\phi}$$

$$\frac{\partial}{\partial x} = \frac{\partial r}{\partial x}\frac{\partial}{\partial r} + \frac{\partial\theta}{\partial x}\frac{\partial}{\partial\theta} + \frac{\partial\phi}{\partial x}\frac{\partial}{\partial\phi}$$

$$y\frac{\partial}{\partial x} = r\sin^2\theta\cos\phi\sin\phi\frac{\partial}{\partial r} + \sin\theta\cos\theta\cos\phi\sin\phi\frac{\partial}{\partial\theta} - \sin^2\phi\frac{\partial}{\partial\phi}$$

Put it together

$$L_z = -i\hbar\frac{\partial}{\partial\phi} = \frac{\hbar}{i}\frac{\partial}{\partial\phi}$$

分類：	
編號：	21
總號：	

$$L_x = i\hbar\left(\sin\phi \frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right)$$

$$L_x^2 = -\hbar^2\left(\sin\phi\frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right)\left(\sin\phi\frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right)$$

$$\sin\phi\frac{\partial}{\partial\theta}\sin\phi\frac{\partial}{\partial\theta} = \sin^2\phi\frac{\partial^2}{\partial\theta^2}.$$

$$\cot\theta\cos\phi\frac{\partial}{\partial\phi}\left(\sin\phi\frac{\partial}{\partial\theta}\right) = \cot\theta\cos\phi\sin\phi\frac{\partial^2}{\partial\theta\partial\phi}$$

$$+ \cot\theta\cos\phi\cos\phi\frac{\partial}{\partial\theta}$$

$$\sin\phi\frac{\partial}{\partial\theta}\cot\theta\cos\phi\frac{\partial}{\partial\phi}$$

$$= \sin\phi\cos\phi\cot\theta\frac{\partial^2}{\partial\theta\partial\phi} + \sin\phi\cos\phi(-\csc^2\theta)\frac{\partial}{\partial\phi}$$

$$\cot\theta\cos\phi\frac{\partial}{\partial\phi}\cot\theta\cos\phi\frac{\partial}{\partial\phi}$$

$$= \cot^2\theta\cos\phi(-\sin\phi)\frac{\partial}{\partial\phi} + \cot^2\theta\cos^2\phi\frac{\partial^2}{\partial\phi^2}$$

$$L_y = i\hbar\left(-\cos\phi\frac{\partial}{\partial\theta} + \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right)$$

$$L_y^2 = -\hbar^2\left(-\cos\phi\frac{\partial}{\partial\theta} + \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right)\left(-\cos\phi\frac{\partial}{\partial\theta} + \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right)$$

$$-\cos\phi\frac{\partial}{\partial\theta}\left(-\cos\phi\frac{\partial}{\partial\theta}\right) = \cos^2\phi\frac{\partial^2}{\partial\theta^2}.$$

$$\cot\theta\sin\phi\frac{\partial}{\partial\phi}\left(-\cos\phi\frac{\partial}{\partial\theta}\right) = -\cot\theta\sin\phi\cos\phi\frac{\partial^2}{\partial\theta\partial\phi}$$

$$+ \cot\theta\sin^2\phi\frac{\partial}{\partial\theta}$$

$$-\cos\phi\frac{\partial}{\partial\theta}\left(\cot\theta\sin\phi\frac{\partial}{\partial\phi}\right) = -\cos\phi\sin\phi\cot\theta\frac{\partial^2}{\partial\theta\partial\phi}$$

$$-\cos\phi(\sin\phi)(-\csc^2\theta)\frac{\partial}{\partial\phi}$$

$$\cot\theta\sin\phi\frac{\partial}{\partial\phi}\left(\cot\theta\sin\phi\frac{\partial}{\partial\phi}\right) = \cot^2\theta\sin\phi\cos\phi\frac{\partial}{\partial\phi}$$

$$+ \cot^2\theta\sin^2\phi\frac{\partial^2}{\partial\phi^2}$$

$L_x^2 + L_y^2 \qquad -\hbar^2 \, [\; A \;]$

A

Coefficient of $\frac{\partial^2}{\partial\theta^2}$: $\sin^2\phi + \cos^2\phi = 1$

Coefficient of $\frac{\partial^2}{\partial\theta\partial\phi}$: $\cot\theta\cos\phi\sin\phi - \cot\theta\sin\phi\cos\phi$
$= 0$

Coefficient of $\frac{\partial}{\partial\theta}$ $\cot\theta\cos^2\phi + \cot\theta\sin^2\phi$
$= \cot\theta$

Coefficient of $\frac{\partial}{\partial\phi}$ $-\csc^2\theta\sin\phi\cos\phi - \cot^2\theta\cos\phi\sin\phi$
$+ \csc^2\theta\sin\phi\cos\phi + \cot^2\theta\sin\phi\cos\phi$
$= 0$

Coefficient of $\frac{\partial^2}{\partial\phi^2}$ $\cot^2\theta\cos^2\phi + \cot^2\theta\sin^2\phi$
$= \cot^2\theta$

$$\Rightarrow \quad L_x^2 + L_y^2 = \frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \cot^2\theta\frac{\partial^2}{\partial\phi^2}$$

$$L_z = -i\hbar\frac{\partial}{\partial\phi}$$

$$\Rightarrow \quad L_z^2 = -\hbar^2\frac{\partial^2}{\partial\phi^2}$$

$$L^2 = L_x^2 + L_y^2 + L_z^2$$

$$= -\hbar^2\left[\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \cot^2\theta\frac{\partial^2}{\partial\phi^2} + \frac{\partial^2}{\partial\phi^2}\right]$$

$$= -\hbar^2\left[\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \csc^2\theta\frac{\partial^2}{\partial\phi^2}\right]$$

$$* \quad \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} = \frac{1}{\sin\theta}\sin\theta\frac{\partial^2}{\partial\theta^2} + \frac{1}{\sin\theta}\cos\theta\frac{\partial}{\partial\theta}$$

$$= \frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta}$$

$$** \quad \csc^2\theta\frac{\partial^2}{\partial\phi} = \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}$$

$$\Rightarrow \quad L^2 = L_x^2 + L_y^2 + L_z^2$$

$$= -\hbar^2\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]$$