COURSE CODE: PHS412
COURSE TITLE: QUANTUM MECHANICS II
NUMBER OF UNITS: 3
COURSE DURATION: 3 HOURS PER WEEK

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COURSE DETAILS

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COURSE CONTENT

PHS 412: Time-dependent and time-independent perturbation theory. Scattering theory, elastic potential scattering. Green's function and partial wave methods. Selected phenomena from each of Atomic Physics, Molecular Physics, Solid state physics and Nuclear Physics are described using quatum mechanical models.

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COURSE REQUIREMENT

This e-lecture note is not the totality teahing-learning requirement. Attendance at lectures and participation in class work are essential.

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READING LIST

1. Quantum Mechanics by L. I. Schiff

2. Quantum Mechanics by E. Merzbacher

3. Schaum's Outline of Theory and Problems of Quantum Mechanics by Y. Peleg, R. Pnini and E. Zaatur

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LECTURE NOTES

Chapter 1

APPROXIMATION METHODS

1.1 VARIATIONAL METHOD

This method is applicable to conservative systems. Consider a physical system with time-independent Hamiltonian H. We assume for simplicity that the entire spectrum of H is discrete and non degenerate

$$(H|\phi_n\rangle = E_n|\phi_n\rangle), \quad n = 1, 2, 3... \tag{1.1}$$

Let E_o be the smallest eigenvalue of H (i.e, the smallest energy of the system). An arbitrary state $|\psi\rangle$ can be written in the form

$$|\psi\rangle = \sum_n c_n|\phi_n\rangle \tag{1.2}$$

Then

$$\langle\psi|H|\psi\rangle = \sum_n |c_n|^2 E_n \geq E_o \sum_n |c_n|^2 \tag{1.3}$$

On the other hand,

$$\langle\psi|\psi\rangle = \sum_n |c_n|^2 \tag{1.4}$$

Thus, we can conclude that for every ket,

$$\langle H \rangle = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} \geq E_o \tag{1.5}$$

Eq.(6.5) is the basis of the variational method. A family of kets $|\psi(\alpha)\rangle$ is chosen, the so called trial kets. The mean value of H in the states $|\psi(\alpha)\rangle$ is calculated, and the expression $\langle H \rangle(\alpha)$ is minimized with respect to the parameter α. The minimum value obtained is an approximation of the ground state energy E_o.

Equation (6.5) is actually a part of a more general result called the Ritz theorem. The mean value of the Hamiltonian H is stationary in the neighborhood of its discrete eigenvalues.

The variational problem can therefore be generalized to provide an estimation for other energy levels based on the ground state. If the function $\langle H \rangle(\alpha)$ obtained from the trial kets $|\psi(\alpha)\rangle$ has several extrema, they give approximate values of some of its energies E_n.

Examples *1. Consider a 1D harmonic oscillator*

$$H = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}mw^2x^2$$

(a) For the one-parameter family of wave functions $\psi_\alpha(x) = e^{-\alpha x^2} (\alpha > 0)$, find a wave function that minimizes $\langle H \rangle$. What is the value of $\langle H \rangle$ min?
(b) For another one parameter family of wave functions $\psi_\beta(x) = xe^{-\beta x^2}(\beta > 0)$, find a wave function that minimizes $\langle H \rangle$ and compute the value of $\langle H \rangle$ min.
(c) Repeat the same procedure for

$$\psi_\gamma(x) = \frac{1}{x^2 + \gamma} \quad (\gamma > 0)$$

<u>Solution</u>

(a) We begin by considering $\langle H \rangle$.

$$\langle H \rangle = \frac{\int_{-\infty}^{\infty} \psi_\alpha^* \left[\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}mw^2x^2\right]\psi_\alpha(x)dx}{\int_{-\infty}^{\infty} \psi_\alpha^*(x)\psi_\alpha(x)dx}$$

$$= \frac{\hbar^2}{2m}\alpha + \frac{1}{8}\frac{mw^2}{\alpha}$$

We differentiate $\langle H \rangle$ with respect to α

$$\frac{d\langle H \rangle}{d\alpha} = \frac{\hbar^2}{2m} - \frac{1}{8}\frac{mw^2}{\alpha^2}$$

From the condition $\frac{d\langle H \rangle}{d\alpha}\Big|_{\alpha=\alpha_o} = 0$, we have

$$\frac{\hbar^2}{2m} - \frac{mw^2}{8\alpha_o^2} = 0 \Rightarrow \alpha_o = \frac{mw}{2\hbar};$$

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thus α_o gives the minimum value of $\langle H \rangle$. The wave function that minimizes $\langle H \rangle$ is $\psi_{\alpha_o}(x) = e^{-\frac{mwx^2}{2\hbar}}$ and

$$\langle H \rangle_{min} = \frac{\hbar^2}{2m}\alpha_o + \frac{mw^2}{8\alpha_o} = \frac{1}{2}\hbar w$$

Thus $\langle H \rangle_{min}$ coincides with the energy of the n=0 level of a 1D harmonic oscillator. Note that the family of functions we are studying coincides with the ground state wave function of the harmonic oscillator.

(b) We proceed with the same method as in part (a).

$$\langle H \rangle = \frac{\int_{-\infty}^{\infty} \psi_\beta^* \left[\frac{-\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2}mw^2x^2 \right] \psi_\beta(x)dx}{\int_{-\infty}^{\infty} \psi_\beta^*(x)\psi_\beta(x)dx}$$

$$= 3\frac{\hbar^2}{m}\beta + \frac{3}{8}\frac{mw^2}{\beta}$$

and

$$\frac{d\langle H \rangle}{d\beta} = \frac{3\hbar^2}{2m} - \frac{3mw^2}{8}\frac{1}{\beta^2} = 0$$

We obtain $\beta_o = \frac{1}{2}\frac{mw}{\hbar}$ and $\psi_{\beta_o}(x) = xe^{-mwx^2/2\hbar}$; so $\langle H \rangle_{min}$ equals the energy of the n = 1 level of the one-dimensional harmonic oscillator.

(c) Applying the procedures of parts (a) and (b), we obtain

$$\langle H \rangle = \frac{\int_{-\infty}^{\infty} \psi_\gamma^* \left[\frac{-\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2}mw^2x^2 \right] \psi_\gamma(x)dx}{\int_{-\infty}^{\infty} \psi_\gamma^*(x)\psi_\gamma(x)dx}$$

$$= \frac{\hbar^2}{2m}\frac{1}{\gamma} + \frac{1}{2}mw^2\gamma$$

and

$$\psi_{\gamma_o}(x) = \frac{1}{x^2 + \hbar^2/\sqrt{2}mw} \qquad \gamma_o = \frac{1}{\sqrt{2}}\frac{\hbar}{mw}$$

2. Consider a particle in a one-dimensional potential $V(x)$ - λx^4. Using the variational method, find an approximate value for the energy of the ground state. Compare it to the exact value $E_o = 1.06\frac{\hbar^2}{2m}k^{\frac{1}{3}}$ where $k = 2m\lambda/\hbar^2$. Choose as a trial function $\psi = (2\alpha/\pi)^{\frac{1}{4}}e^{-\alpha x^2}$.

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Solution: First note that the trial function $\psi = (2\alpha/\pi)^{\frac{1}{4}} e^{-\alpha x^2}$ is normalized to unity; that is $\int_{-\infty}^{\infty} |\psi|^2 dx = 1$. The Hamiltonian is $H = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + \lambda x^4$; thus

$$\langle H \rangle = \frac{\int_{-\infty}^{\infty} \psi^* \left[\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + \lambda x^4\right] \psi(x) dx}{\int_{-\infty}^{\infty} \psi^*(x)\psi(x) dx}$$

The denominator equals one since $\psi(x)$ is normalized; thus

$$\langle H \rangle = \int_{-\infty}^{\infty} \left(\frac{2\alpha}{\pi}\right)^{\frac{1}{4}} e^{-\alpha x^2} \left(-\frac{\hbar^2}{2m}\right)\frac{d^2}{dx^2}\left(\frac{2\alpha}{\pi}\right)^{\frac{1}{4}} e^{-\alpha x^2} dx + \int_{-\infty}^{\infty} \left(\frac{2\alpha}{\pi}\right)^{\frac{1}{4}} e^{-\alpha x^2}\lambda x^4 \left(\frac{2\alpha}{\pi}\right)^{\frac{1}{4}} e^{-\alpha x^2} dx$$

$$= -\frac{\hbar^2}{2m}\sqrt{\frac{2\alpha}{\pi}} \int_{-\infty}^{\infty} e^{-2\alpha x^2} 2\alpha[2\alpha x^2 - 1] dx + \lambda\sqrt{\frac{2\alpha}{\pi}} \int_{-\infty}^{\infty} x^4 e^{-2\alpha x^2} dx$$

$$= -\frac{\hbar^2(4\alpha^2)}{2m}\sqrt{\frac{2\alpha}{\pi}} \int_{-\infty}^{\infty} x^2 e^{-2\alpha x^2} dx + \frac{\hbar^2(2\alpha)}{2m}\sqrt{\frac{2\alpha}{\pi}} \int_{-\infty}^{\infty} e^{-2\alpha x^2} dx + \lambda\sqrt{\frac{2\alpha}{\pi}} \int_{-\infty}^{\infty} x^4 e^{-2\alpha x^2} dx$$

The first integral is

$$I_1 \equiv -\frac{\hbar^2(4\alpha^2)}{2m}\sqrt{\frac{2\alpha}{\pi}} \int_{-\infty}^{\infty} e^{-2\alpha x^2} x^2 dx = -\frac{\hbar^2(4\alpha^2)}{2m}\sqrt{\frac{2\alpha}{\pi}}\frac{1}{4\alpha}\sqrt{\frac{\pi}{2\alpha}} = -\frac{\hbar^2\alpha}{2m}$$

The second integral is:

$$I_2 \equiv \frac{\hbar^2(2\alpha)}{2m}\sqrt{\frac{2\alpha}{\pi}} \int_{-\infty}^{\infty} e^{-2\alpha x^2} dx = \frac{\hbar^2(2\alpha)}{2m}\sqrt{\frac{2\alpha}{\pi}}\sqrt{\frac{\pi}{2\alpha}} = \frac{\hbar^2\alpha}{m}$$

and the third integral is:

$$I_3 \equiv \lambda\sqrt{\frac{2\alpha}{\pi}} \int_{-\infty}^{\infty} x^4 e^{-2\alpha x^2} dx = \lambda\sqrt{\frac{2\alpha}{\pi}}\frac{3}{4(2\alpha)^2}\sqrt{\frac{\pi}{2\alpha}} = \frac{3\lambda}{16\alpha^2}$$

Substituting these integrals we obtain

$$\langle H \rangle = -\frac{\hbar^2\alpha}{2m} + \frac{\hbar^2\alpha}{m} + \frac{3\lambda}{16\alpha^2} = \frac{\hbar^2}{2m}\alpha + \frac{3}{16}\frac{\lambda}{\alpha^2} \quad \dagger$$

Hence, $\frac{d\langle H \rangle}{d\alpha} = \frac{\hbar^2}{2m} - \frac{3}{8}\frac{\lambda}{\alpha^3}$. Since $\left.\frac{d\langle H \rangle}{d\alpha}\right|_{\alpha=\alpha_0} = 0$, we obtain $\frac{\hbar^2}{2m} - \frac{3}{8}\frac{\lambda}{\alpha_o^3} = 0 \rightarrow$

$\alpha_o = \left(\frac{3m\lambda}{4\hbar^2}\right)^{\frac{1}{3}}$. In terms of k $= 2m\lambda/\hbar^2$, we have $\alpha_o = (3/8)^{\frac{1}{3}} k^{\frac{1}{3}}$. Substituting this value in $\dagger$, we obtain

$$\langle H \rangle_{min} = \frac{3}{4}3^{\frac{1}{3}}\frac{\hbar^2}{2m}k^{\frac{1}{3}} = 1.082\frac{\hbar^2}{2m}k^{\frac{1}{3}}$$

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Comparing the last result to the exact value of E_o we see that we have quite a good approximation. The error is approximately 2 percent.

3.(a) Taking a trial wave function proportional to $\exp(-\beta r)$, where β is a variable parameter, use the variational method to obtain an upper limit for the energy of the ground state of the hydrogen atom in terms of atomic constants.

(a) The upper limit of the ground state is the minimum value of the expectation value of the energy as β varies. Denote the trial wave function by

$$\psi = A \exp(-\beta r)$$

where A is a constant. Its value is obtained from the normalizing condition. Since ψ depends only on r, we put $d^3r = 4\pi r^2 dr$. Therefore, the normalization condition yields,

$$4\pi A^2 \int_0^\infty r^2 \exp(-2\beta r) dr = \frac{8\pi A^2}{(2\beta)^3} = 1$$

Thus

$$A^2 = \frac{\beta^3}{\pi} \qquad (1)$$

The Hamiltonian for the hydrogen atom is

$$H = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_o}\frac{1}{r} \qquad (2)$$

The expectation value of the energy for the function ψ is

$$\langle E \rangle = 4\pi A^2 \int_0^\infty \exp(-\beta r)\left(-\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_o}\frac{1}{r}\right)\exp(-\beta r)r^2 dr \qquad (3)$$

Since $\exp(-\beta r)$ depends only on r, we need only the r- dependent part of the operator

$$\nabla^2 \exp(-\beta r) = \left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right)\exp(-\beta r \qquad (4)$$

Inserting (1) and (4) in (3) gives

$$\langle E \rangle = \quad 4\beta^3\Big\{\frac{\hbar^2}{2m}\beta^2 \int_0^\infty r^2 \exp(-2\beta r) dr$$
$$+ \left(\frac{\beta\hbar^2}{m} - \frac{e^2}{4\pi\epsilon_o}\right)\int_0^\infty r \exp(-2\beta r) dr\Big\}$$
$$= \quad -\frac{\hbar^2}{2m}\beta^2 + \frac{\hbar^2}{m}\beta^2 - \frac{e^2}{4\pi\epsilon_o}\beta$$
$$= \quad \frac{\hbar^2}{2m}\beta^2 - \frac{e^2}{4\pi\epsilon_o}\beta$$

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Then

$$\frac{d\langle E\rangle}{d\beta} = \frac{\hbar^2\beta}{m} - \frac{e^2}{4\pi\epsilon_o}$$

which is

$$0, \quad when \quad \beta = \frac{me^2}{4\pi\epsilon_o\hbar^2}$$

Inserting this in the expression for $\langle E\rangle$ gives

$$\langle E\rangle_{min} = -\frac{m_e}{2\hbar^2}\left(\frac{e^2}{4\pi\epsilon_o}\right)^2$$

$$= -\frac{e^2}{8\pi\epsilon_o}\frac{1}{a_o}$$

Where a_o is the Bohr radius.

(b) The expression obtained above is the correct value of the ground-state energy of the hydrogen atom. The expression is correct because the rtrial function is the correct form of the ground-state wave function.

1.2 THE WKB APPROXIMATION (or Semiclassical Approximation)

WKB stands for the names of the proponents: Wentzel, Kramer and Brillouin. The method is suitable for obtaining solutions of the one-dimensional Schrödinder equation as well as the 3-dimensional problems, if the potential is spherically symmetric and a radial defferential equation can be separated. That is, it is applicable to situations in which the wave can be separated into one or more total differential equations each of which involves a single independent variable.

Consider the Schrödinger equation in one-dimention:

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}[E - V(x)]\psi(x) = 0 \tag{1}$$

Let

$$\begin{cases} k(x) = \frac{1}{\hbar}\sqrt{2m[E - V(x)]} & \text{for } E \rangle V(x) \\ \\ \kappa(x) = \frac{-i}{\hbar}\sqrt{2m[E - V(x)]} & \text{for } E \langle V(x) \end{cases} \tag{2}$$

If $V(x)$ is constant eq.(1) has solution $\psi \sim e^{\pm ikx}$

However if $V(x)$ varies slowly with x we assume a solution of the form

$$\psi = Ae^{iu(x)/\hbar} \tag{3}$$

Subsituting this solution in eq.(1) we find that $u(x)$ satisfies the equation

$$i\hbar\frac{d^2u}{dx^2} - \left(\frac{du}{dx}\right)^2 + [\hbar k(x)]^2 = 0 \tag{4}$$

In the WKB approximation we expand $u(x)$ in power series of $\hbar$ as follows:

$$u(x) = u_0 + \hbar u_1 + \hbar^2 u_2 + \ldots \tag{5}$$

where $u_n, \quad n = 0, 1, 2, \ldots$ are approximate solutions of eq.(4). Neglecting expansion terms of order $\hbar^2$ and putting eq.(5) in eq.(4) we have

$$\hbar\left\{i\frac{d^2u_0}{dx^2} + 2\left(\frac{du_0}{dx}\right)\left(\frac{du_1}{dx}\right)\right\} - \left(\frac{du_0}{dx}\right)^2 + [\hbar k(x)]^2 = 0 \tag{6}$$

where again the expansion terms of order $\hbar^2$ are neglected and the terms in eq.(6) are grouped in powers of $\hbar$. Now equating equal powers of $\hbar$ we have

$$-u_0'^2 + [\hbar k(x)]^2 = 0 \tag{7}$$

$$iu_0'' - 2u_0'u_1' = 0 \tag{8}$$

Integrating eqs.(7) and (8) we have

$$u_0(x) = \pm\hbar \int^x k(x')dx' + c_1 \tag{9}$$

$$u_1(x) = \frac{1}{2}i \ln k(x) + c_2 \tag{10}$$

where c_1 and c_2 are arbitrary constants of integration. Substituting eqs.(9) and (10) into eq.(5) and sustituting eq.(5) in eq.(3) one gets

$$\psi(x) = Ak^{-\frac{1}{2}}(x)\exp(\pm i \int^x k(x')dx') \quad \text{for } E > V \tag{11}$$

where c_1 and c_2 are absorbed into A. In a similar fashion, the case $E\langle V$ gives

$$\psi(x) = B\kappa^{-\frac{1}{2}}(x)\exp(\pm \int^x \kappa(x')dx') \quad \text{for } E\langle V \tag{12}$$

The region in which $E > V(x)$ is called a *classically allowed region* of motion, while a region in which $E\langle V(x)$ is called *classically inaccessible*. The points in the boundary between these 2 kinds of regions are called *turning points* [where $E = V(x)$].

Applicability condition: The WKB approximation is based on the condition

$$\frac{1}{2}\left|\frac{dk}{dx}\right| \ll |k^2(x)| \tag{13}$$

(i.e. V(x)varies very slowly with x). $k(x)$ is the wave number so $k(x) = \frac{2\pi}{\lambda}$, where λ is the wavelength. We can then write eq.(13) as

$$\frac{1}{2}\left|\frac{dk}{dx}\right| \ll \frac{2\pi}{\lambda}k(x)$$

$$\text{or} \quad \frac{\lambda}{4\pi}\left|\frac{dk}{dx}\right| \ll k(x) \tag{14}$$

Solution near a turning point: Adjacent to the turning points for which $k(x_0)$, we have $k \approx \frac{dk}{dx}|_{x0}(x - x_0)$. Thus the WKB approximation is applicable for a distance from the turning point satisfying the condition

$$|x - x_0| \gg \frac{\lambda}{4\pi} \tag{15}$$

The connection formulas

The connection formulas at the turning point depends on whether the classical region is to the left (p_1) or to the right (p_2) of it.

In the first case we have $x > a$:

$$\psi_1(x) = \frac{A_1}{\sqrt{k}} \cos(\int_a^x k(x')dx' - B_1\pi) \tag{16}$$

while in the second case, for $x \langle b$

$$\psi_2(x) = \frac{A_2}{\sqrt{k}} \cos(\int_x^b k(x')dx' - B_2\pi) \tag{17}$$

(The results in eqs.(16 and 17) are quoted)

Application to the bound state: The WKB approximation can be applied to derive an equation for the energies of a bound state. Since the wave function is zero at the boundaries the argument of the cosine in the connection formulas eqs.(16 and 17) is given by

$$\int_a^b k(x)dx - B\pi = (n + \frac{1}{2})\pi \quad n = 0, 1, 2\ldots \tag{18}$$

$$\text{or} \qquad \int_a^b k(x)dx = (n + \frac{1}{2})\pi \quad n = 0, 1, 2\ldots \tag{19}$$

if the initial phase is chosen to be zero, i.e. $B = 0$.

$$\int p(x)dx = 2\pi\hbar(n + \frac{1}{2}) \quad n = 0, 1, 2\ldots \tag{20}$$

where $p(x) = \hbar k(x)$ Eq.(20) is called the Bohr-Sommerfeld quantization rule.
Barrier potential: For a potential barrier V(x) between $x = a$ and $x =$

b and a particle of energy E, the transmission coefficient T in the WKB approximation is (quoted)

$$T = \exp\left\{\frac{-2}{\hbar}\int_a^b \sqrt{2m[V(x) - E]dx}\right\}\tag{21}$$

Solved examples:

1. *Using the WKB approximation find the bounded states for a one-dimensional infinite potential well. Compare your result with the exact solution.*

Suppose that the boundaries of the potential well are at $x = \pm a$. At the boundaries the wave function has value zero and $k(a) = 0$. From eqs.(16) and (17) we have

$$\begin{cases} 0 = \cos(-B_1\pi) \\ \\ 0 = \cos(-B_2\pi) \end{cases}$$

and therefore $B_1 = B_2 = \frac{1}{2}$. Thus we get, according to eq.(18)

$$\int_{-a}^a K_n dx - \frac{1}{2}\pi = (n + \frac{1}{2})\pi$$

i.e. $\qquad 2ak_n = (n+1)\pi \qquad \Rightarrow \qquad k_n = \frac{(n+1)\pi}{2a}$

From eq.(2) we get $\qquad E_n = \frac{1}{2}\frac{\hbar^2 k_n^2}{m} = \frac{\pi^2\hbar^2(n+1)^2}{8ma^2}$

Recall that the exact solution is $\frac{\pi^2\hbar^2 n^2}{8ma^2}$

2. *Use the WKB approximation to obtain the energy levels of a harmonic oscillator.*

Consider the Bohr-Sommerfeld quantization rule:

$$\int_a^b p(x)dx = \hbar\pi(n + \frac{1}{2}) \quad (n = 0, 1, 2, \ldots)\tag{i}$$

where $p(x) = \sqrt{2m[E - V(x)]}$ is the momentum of the oscillator, $V(x) = \frac{1}{2}m\omega^2 x^2$. Since $\int pdx = 2\int_a^b pdx$ holds for a linear harmonic oscillator we can use eq.(i). The points a and b are the turning points that are determined by the condition $p(a) = p(b) = 0$ or $E - V = 0$; thus $E - \frac{1}{2}m\omega^2 x^2 = 0$ so we have
$a = -\sqrt{\frac{2E}{m\omega^2}}, \quad b = \sqrt{\frac{2E}{m\omega^2}}$. We introduce the new variable $z = x\sqrt{\frac{m\omega^2}{2E}}$, and obtain

$$\int_a^b p(x)dx = \frac{2E}{\omega}\int_{-1}^1 \sqrt{1 - z^2}dz = \frac{\pi E}{\omega}\tag{ii}$$

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Comparing eqs.(ii) and (i) we obtain $E_n = \hbar\omega(n + \frac{1}{2})$ which is the exact solution.

1.3   TIME-INDEPENDENT PERTURBATION THEORY

(FOR BOUND STATES) OR STATIONARY PERTURBATION THEORY (SPT)

Time-independent perturbation theory is widely used in Physics. Perturbation theory is appropriate when the Hamiltonian H of the system can be put in the form

$$H = H_0 + \lambda h \tag{1}$$

where λ is a small parameter such that the perturbation (or disturbance) $\lambda h \ll H_0$, i.e., $\lambda \ll 1$; and the matrix elements of the operator h are comparable in magnitude to those of H_0. The eigenstates u_n and eigenvalues E_n of the unperturbed Hamiltonian, H_0 must be known. The SPT is concerned with finding the changes in discrete energy levels and eigenfunctions of a system when a small disturbance (perturbation) is applied.

In the **unperturbed state**

$$H_0 u_n = E_n u_n \tag{2}$$

$$\text{or } H_0|n\rangle = E_n|n\rangle \tag{2}$$

where u_n or $|n\rangle$ form an orthonormal basis of the state space.

(i.e., $\langle m|n\rangle = \delta_{mn}$ and $\sum_n |n\rangle\langle n| = 1$).

In the **perturbed state** $H = H(\lambda)$ as in eq.(1) and its nth eigenstate $\psi_n(\lambda)$ and the corresponding eigenvalue $E_n(\lambda)$ are also functions of λ. Therefore

$$H(\lambda)\psi_n(\lambda) = E_n(\lambda)\psi_n(\lambda) \tag{3}$$

We assume that $E_n(\lambda)$ and $\psi_n(\lambda)$ can be expanded as a power series of λ in the form

$$E_n(\lambda) = \epsilon_0 + \lambda\epsilon_1 + \lambda^2\epsilon_2 + \ldots \tag{4}$$

$$\psi_n(\lambda) = \phi_0 + \lambda\phi_1 + \lambda^2\phi_2 + \ldots \tag{5}$$

Substituting eqs.(4) and (5) into eq.(3) we obtain

$$(H_0 + \lambda h)(\phi_0 + \lambda\phi_1 + \lambda^2\phi_2 + \ldots) = (\epsilon_0 + \lambda\epsilon_1 + \lambda^2\epsilon_2 + \ldots)(\phi_0 + \lambda\phi_1 + \lambda^2\phi_2 + \ldots) \tag{6}$$

Expanding eq.(6) and equating equal powers of λ we have for

$$\lambda^0 : \qquad (H_0 - \epsilon_0)\phi_0 = 0 \tag{7}$$

$$\lambda^1: \qquad (H_0 - \epsilon_0)\phi_1 = (\epsilon_1 - h)\phi_0 \tag{8}$$

$$\lambda^2: \quad (H_0 - \epsilon_0)\phi_2 = (\epsilon_1 - h)\phi_1 + \epsilon_2\phi_0 \tag{9}$$

$$\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots$$

Note the following:

1. As $\lambda \to 0$, we have $\epsilon_0 = E_n$ (the unperturbed eigenvalue of the nth level) and eq.(7) means that ϕ_0 is the corresponding unperturbed eigenfunction. We, therefore put

$$\phi_0 = u_n, \quad \epsilon_0 = E_n \tag{10}$$

2. any arbitrary multiple of ϕ_0 can be added to any of the functions ϕ_s without affecting the RHS of eqs.(7) to (9) and the determination of ϕ_s in terms of lower order functions. Hence we choose the arbitrary multiple such that

$$(\phi_0, \phi_s) = 0 \quad s > 0 \tag{11}$$

3. Using the result

$$\Omega_{\alpha\beta} = \int \phi_\alpha^*(r)\Omega\phi_\beta(r)d^3r = \int [\Omega^\dagger\phi_\alpha(r)]^*\phi_\beta(r)d^3r = \langle\alpha|\Omega|\beta\rangle \tag{12}$$

(where $\Omega_{\alpha\beta}$ is the matrix element of Ω in the states α, β) the inner product of ϕ_0 and the LHS of eqs.(7) to (9) is zero in each case, and it follows, with the help of eqs.(10) and (11) that

$$\epsilon_s = \frac{(\phi_0, h\phi_{s-1})}{(\phi_0, \phi_0)} = (u_n, \phi_{s-1}) \tag{13}$$

First-order perturbation theory: Eq.(13) with $s = 1$ shows that

$$\epsilon_1 = (u_n, hu_n) \text{ or } \langle n|h|n\rangle \tag{14}$$

which is the expectation value of h for the unperturbed state u_n or $|n\rangle$. Any function can be written as a linear combination of the orthonormal basis functions u_m so

$$\phi_1 = \sum_m a_m^{(1)} u_m \tag{15}$$

Substituting eq.(15) into eq.(8) we have

$$\sum_m a_m^{(1)}(H_0 - E_n)u_m = (\epsilon_1 - h)u_n$$

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where $a_n^{(1)} = 0$ because of eq.(11) (*free choice*). Now replace $H_0 u_m$ by $E_m u_m$, multiply by u_k^* and sum over all m making use of the orthonormality of the $u's$ (only terms $k = m$ survive) to have

$$a_k^{(1)} = \frac{(u_k, h u_n)}{E_n - E_k} \text{ or } \frac{\langle k|h|n\rangle}{E_n - E_k} \qquad k \neq n \tag{16}$$

$$\text{i.e. } a_m^{(1)} = \frac{\langle m|h|n\rangle}{E_n - E_m} \qquad m \neq n \tag{17}$$

$$\text{Hence } \phi_1 = \sum_m \frac{\langle m|h|n\rangle}{E_n - E_m}|m\rangle \qquad m \neq n \tag{18}$$

The first-order solutions are

$$E_n(\lambda) = \epsilon_0 + \lambda\epsilon_1 = E_n + \lambda\langle n|h|n\rangle \tag{19}$$

$$\psi_n(\lambda) = \phi_0 + \lambda\phi_1 = u_n + \lambda\sum_m \frac{\langle m|h|n\rangle}{E_n - E_m}|m\rangle \qquad m \neq n \tag{20}$$

Usually we set $\lambda = 1$

Second-order perturbation

When $s = 2$ eq.(13) gives

$$\epsilon_2 = (u_n, h\phi_1) = (u_n, h\sum_m a_m^{(1)} u_m) = \sum_m a_m^{(1)}(u_n, h u_m) = \sum_m a_m^{(1)}\langle n|h|n\rangle$$

$$= \sum_m \frac{\langle m|h|n\rangle}{E_n - E_m}\langle n|h|m\rangle = \sum_m \frac{|\langle n|h|m\rangle|^2}{E_n - E_m} \qquad m \neq n \tag{21}$$

since h is assumed to be hermitian. Eq.(21) is the second-order approximation of the eigenvalue.

The second-order approximation of the eigenfunction ϕ_2 is calculated by expanding it in terms of u_m:

$$\phi_2 = \sum_m a_m^{(2)} u_m, \qquad a_n^{(2)} = 0 \tag{22}$$

Substituting eq.(22) into eq.(9) we obtain

$$\sum_m a_m^{(2)}(H_0 - E_n)u_m = \sum_m a_m^{(1)}(\epsilon_1 - h)u_m + \epsilon_2 u_n$$

Again, replace $H_0 u_m$ by $E_m u_m$, multiply by u_k^* and sum over all m making use of the orthonormality of the $u's$ (only terms $k = m$ survive) to have

$$a_k^{(2)}(E_k - E_n) = a_k^{(1)}\epsilon_1 - \sum_m a_m^{(1)}(u_k, h u_m) \text{ or } a_k^{(1)}\epsilon_1 - \sum_m a_m^{(1)}\langle k|h|m\rangle \qquad k \neq n$$

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This gives, with the help of eqs.(14) and (17),

$$a_k^{(2)} = -\frac{\langle k|h|n\rangle\langle n|h|n\rangle}{(E_n - E_k)^2} + \sum_m \frac{\langle k|h|m\rangle\langle m|h|n\rangle}{(E_n - E_k)(E_n - E_m)} \qquad \begin{matrix} m\neq n \\ n\neq k \end{matrix} \qquad (23)$$

Inserting eq.(23) into eq.(22) we have

$$\phi_2 = \sum_k \left[-\frac{\langle k|h|n\rangle\langle n|h|n\rangle}{(E_n - E_k)^2} + \sum_m \frac{\langle k|h|m\rangle\langle m|h|n\rangle}{(E_n - E_k)(E_n - E_m)} \right] |m\rangle \qquad \begin{matrix} m\neq n \\ n\neq k \end{matrix} \qquad (24)$$

The second-order solutions are:

$$E_n(\lambda) = \epsilon_0 + \lambda\epsilon_1 + \lambda^2\epsilon_2 = E_n + \lambda\langle n|h|n\rangle + \lambda^2 \sum_m \frac{|\langle n|h|m\rangle|^2}{E_n - E_m} \qquad m\neq n \qquad (25)$$

$$\psi_n(\lambda) = \phi_0 + \lambda\phi_1 + \lambda^2\phi_2 = u_n + \lambda\sum_m \frac{\langle m|h|n\rangle}{E_n - E_m}|m\rangle$$

$$+\lambda^2 \sum_k \left[-\frac{\langle k|h|n\rangle\langle n|h|n\rangle}{(E_n - E_k)^2} + \sum_m \frac{\langle k|h|m\rangle\langle m|h|n\rangle}{(E_n - E_k)(E_n - E_m)} \right] |m\rangle \qquad \begin{matrix} m\neq n \\ n\neq k \end{matrix} \qquad (26)$$

Example 1: *The effect of the finite size of the nucleus is to raise the energies of the electronic states from the theoretical values based on a point nucleus. Show from first-order perturbation theory that, if the proton is regarded (for simplicity) as a thin uniform spherical shell of charge of radius b, the fractional change in the energy of the ground state is $\frac{4b^2}{3a_0^2}$ where the ground state eigenfunction for Hydrogen is $u_s = (\frac{1}{\pi a_0^3})^{\frac{1}{2}} \exp(-r/a_0)$ and $b/a_0 = 10^{-5}$.*
Solution: For a point nucleus the potential is

$$V_0 = -\frac{e^2}{4\pi\epsilon_0 r} \qquad (i)$$

For this uniform spherical shell the potential is

$$V = \begin{cases} \frac{e^2}{4\pi\epsilon_0 r} & r > b \\ \\ -\frac{e^2}{4\pi\epsilon_0 b} & r \langle b \end{cases} \qquad (ii)$$

The perturbation potential is therefore

$$V_1 = V - V_0 = \begin{cases} \frac{e^2}{4\pi\epsilon_0}(\frac{1}{r} - \frac{1}{b}) & r \langle b \\ \\ 0 & r > b \end{cases} \qquad (iii)$$

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The first order correction to the energies of the ground state is

$$\epsilon_1 = \int u_0^* V_1 u_0 d\tau \qquad (iv)$$

where $d\tau = 4\pi r^2 dr$ is the volume element and $u_0 = (\frac{1}{\pi a_0^3})^{\frac{1}{2}} \exp(-r/a_0)$

$$\text{Thus} \quad \frac{4}{a_0^3} \frac{e^2}{4\pi\epsilon_0} \int_0^b r^2 (\frac{1}{r} - \frac{1}{b}) \exp(-2r/a_0) dr \qquad (v)$$

Since $b/a_0 \approx 10^{-5}$, the exponential term may be replaced by unity over the range of integration, and the integral becomes

$$\int_0^b (r - \frac{r^2}{b}) dr = \frac{1}{6} b^2 \qquad (vi)$$

The ground-state energy for a point nucleus is

$$E_0 = -\frac{e^2}{8\pi\epsilon_0 a_0} \qquad (vii)$$

From eqs.(v), (vi) and (vii)

$$\frac{E_1}{E_0} = -\frac{4b^2}{3a_0^2}$$

Example 2: *Consider a 3 dimensional problem. In a given orthonormal basis, the Hamiltonian is represented by the matrix*

$$H = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & -2 \end{pmatrix} + \begin{pmatrix} 0 & c & 0 \\ c & 0 & 0 \\ 0 & 0 & c \end{pmatrix}$$

Here, $H = H^o + H'$ and c is a constant, $c \ll 1$.

1. Find the exact eigenvalues of H.

2. Use second order perturbation to determine the eigenvalues.

3. Compare the results of 1 and 2.

Solution 1. The eigenvalue of H are roots of the equation $\det(H-\lambda I) = 0$.

$$\begin{vmatrix} 1-\lambda & c & 0 \\ c & 3-\lambda & 0 \\ 0 & 0 & c-2-\lambda \end{vmatrix} = (c-2-\lambda) \begin{vmatrix} 1-\lambda & c \\ c & 3-\lambda \end{vmatrix} = (c-2-\lambda)[\lambda^2 - 4\lambda + 3 - c^2]$$

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Therefore, $\lambda = c - 2, 2 \pm \sqrt{1 + c^2}$.

2. The second order correction to the energy may be written as: $E_n = E_n^{(0)} + E_n^{(1)} + E_n^{(2)}$ or

$$(E)_i = (H^o)_{ii} + (H')_{ii} + \sum_{k \neq i} \frac{H'_{ik} H'_{ki}}{E_i^{(0)} - E_k^{(0)}}$$

It can be seen that $(H^o)_{ii} = 1, 3$ and -2. The first order energy correction is given by $H'_{11} = 0, H'_{22} = 0$ and $H'_{33} = c$. For the second correction, we have

$$E_1^{(2)} = \frac{H'_{12} H'_{21}}{E_1^{(0)} - E_2^{(0)}} + \frac{H'_{13} H'_{31}}{E_1^{(0)} - E_3^{(0)}} = \frac{c^2}{-2} + \frac{0}{3} = -\frac{c^2}{2}$$

$$E_2^{(2)} = \frac{H'_{21} H'_{12}}{E_2^{(0)} - E_1^{(0)}} + \frac{H'_{23} H'_{32}}{E_2^{(0)} - E_3^{(0)}} = \frac{c^2}{3 - 1} + \frac{0.0}{3} = \frac{c^2}{2}$$

and

$$E_3^{(2)} = \frac{H'_{31} H'_{13}}{E_3^{(0)} - E_1^{(0)}} + \frac{H'_{32} H'_{23}}{E_3^{(0)} - E_2^{(0)}} = 0 + 0 = 0$$

Thus $E_1 = 1 - \frac{c^2}{2}$, $E_2 = 3 + \frac{c^2}{2}$; $E_3 = -2 + c$.

3. Expand $2 \pm \sqrt{1 + c^2}$ in a binomial series

$$2 \pm \sqrt{1 + c^2} = 2 \pm (1 + \frac{1}{2}c^2 + ...) = 3 + \frac{c^2}{2}, 1 - \frac{c^2}{2}(c^2 \ll 1).$$

This gives the same result as the second order corrections.

Example 3: Consider a perturbation of the form $\frac{1}{2}bx^2$ to the linear harmonic oscillator problem. Thus,

$$H_o = \frac{-\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2}kx^2$$

and $H' = \frac{1}{2}bx^2$. The eigenvalues and eigenfunctions of H_o are well known

$$H_o u_n = E_n u_n$$

where

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega; \quad n = 0, 1, 2, 3...$$

$$u_n = N_n H_n(\xi) \exp(-\frac{1}{2}\xi^2)$$

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$$\omega = \sqrt{\frac{k}{m}}, \quad N_n = \left[\frac{\gamma}{\sqrt{\pi}2^n n!}\right]^{\frac{1}{2}}$$

$$\xi = \gamma x, \quad \gamma = \sqrt{\frac{m\omega}{\hbar}} = \left[\frac{mk}{\hbar^2}\right]^{1/4}$$

Notice that the exact solution can easily be obtained; all that one has to do is replace k by k+b. Thus if we write

$$H\psi_n = E_n \psi_n$$

where $\qquad H = H_o + H'$

then $\qquad E_n = \left(n + \frac{1}{2}\right)\hbar\sqrt{\frac{k}{m}}\left[1 + \frac{b}{k}\right]^{1/2}$

or $\qquad E_n = \left(n + \frac{1}{2}\right)\hbar\sqrt{\frac{k}{m}}\left[1 + \frac{1}{2}\frac{b}{k} - \frac{1}{8}\frac{b^2}{k^2} + \dots\right]\dots **$

the binomial expansion been valid when $\frac{b}{k}\langle 1$. If we compare (**) with equation (4), we obtain

$$\epsilon_o = \left(n + \frac{1}{2}\right)\hbar\sqrt{\frac{k}{m}}\dots\dots\dots(*)$$

$$\epsilon_1 = \frac{1}{2}\left(n + \frac{1}{2}\right)\hbar\sqrt{\frac{k}{m}}\frac{b}{k}\dots\dots\dots(**)$$

$$\epsilon_2 = -\frac{1}{8}\left(n + \frac{1}{2}\right)\hbar\sqrt{\frac{k}{m}}\frac{b^2}{k^2}\dots\dots\dots(***)$$

where ϵ_o represents the unperturbed eigenvalue, and ϵ_1 and ϵ_2 represent the first and second order perturbations respectively. We can now apply perturbation theory to compute ϵ_1 and ϵ_2 etc. Now,

$$\epsilon_1 = \frac{1}{2}b\int_{-\infty}^{\infty} u_n^*(x)x^2 u_n(x)dx = \frac{1}{2}b\langle n|x^2|n\rangle$$

$$= \frac{1}{2}\left(n + \frac{1}{2}\right)\hbar\sqrt{\frac{k}{m}}\frac{b}{k}\dots\dots\dots(i*)$$

Equation (i*) agrees with eqn. (**). In order to calculate ϵ_2, we note that

$$H'_{mn} = \langle m|H'|n\rangle = \frac{1}{2}b\langle m|x^2|n\rangle$$

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and this is non zero , only when m=n-2, m=n or m=n+2. Thus

$$\epsilon_2 = \sum_m{}' \frac{|H'_{mn}|^2}{E_n - E_m} = \left(\frac{1}{2}b\right)^2\left[\frac{|\langle n-2|x^2|n\rangle|^2}{E_n - E_{n-2}} + \frac{|\langle n+2|x^2|n\rangle|^2}{E_n - E_{n+2}}\right]$$

$$= -\frac{1}{8}b^2\frac{\hbar}{m^2\omega^2}\left(n + \frac{1}{2}\right)$$

which agrees with eqn (***).

1.4 TIME-DEPENDENT PERTURBATION THEORY

The time-dependent perturbation theory, which is sometimes called the method of variation of constants, assumes as in the last section that

$$H(t) = H_0 + \lambda h(t) \tag{1}$$

$$H_0 u_k = E_k u_k \tag{2}$$

where H_0 is the unperturbed Hamiltonian with known eigenvalues E_k and eigenstates u_k, and h (the perturbation) is small, (i.e., $\lambda \ll 1$) and depends on time t. h has the effect of causing transitions between eigenstates of H_0 that would be stationary in the absence of h. We use the adiabatic approximation which assumes that $H(t)$ contains parameters which change very slowly with time. For time-dependent perturbation we work with the time-dependent Schrödinger equation. The time-dependent Schrödinger equation for the unperturbed state is

$$i\hbar \frac{\partial u_k(t)}{\partial t} = H_0 u_k(t) = E_k u_k(t)$$

$$\text{i.e.} \quad \frac{\partial u_k(t)}{\partial t} = -\frac{i}{\hbar} E_k u_k(t)$$

$$\Rightarrow \quad u_k(t) = u_k(0) e^{-\frac{iE_k t}{\hbar}} \tag{3}$$

$u_k(0)$ is the solution of the unperturbed time-independent Schrödinger eq.(2). The time-dependent Schrödinger equation for the perturbed state is

$$i\hbar \frac{\partial \psi}{\partial t} = H(t)\psi \tag{4}$$

We express ψ as an expansion in the eigenfunctions $u_k e^{-\frac{iE_k t}{\hbar}}$ with coefficients $a_k(t)$ that depend on time.

$$\psi = \sum_n a_n(t) u_n e^{-\frac{iE_n t}{\hbar}} \tag{5}$$

$$\Rightarrow \quad a_k(t) = u_k^* \psi \tag{6}$$

$a_k(t)$ is the probability amplitude for state u_k, $|a_k(t)|^2$ is the probability that the system is in the state u_k. Substituting eq.(5) into eq.(4) we have

$$\sum_n i\hbar \, \dot{a}_n \, u_n e^{-\frac{iE_n t}{\hbar}} + \sum_n a_n E_n u_n e^{-\frac{iE_n t}{\hbar}} = \sum_n a_n (H_0 + \lambda h(t)) u_n e^{-\frac{iE_n t}{\hbar}}$$

where $\dot{a}_n = \frac{da_n}{dt}$. We replace $H_0 u_n$ by $E_n u_n$ on the RHS, multiply through on the left by u_k, and sum over all k, making use of the orthonormality of the u's to have

$$i\hbar\, \dot{a}_k\, e^{-\frac{iE_k t}{\hbar}} = \lambda \sum_n a_n(t) e^{-\frac{iE_n t}{\hbar}} \langle k|h(t)|n \rangle \tag{7}$$

where $\langle k|h(t)|n \rangle = \int_{\substack{all \\ space}} u_k^* h(t) u_n d\tau$. We define the Bohr (angular) frequency

$$\omega_{kn} = \frac{E_k - E_n}{\hbar} \tag{8}$$

and eq.(7) becomes

$$\dot{a}_k = \frac{\lambda}{i\hbar} \sum_n \langle k|h(t)|n \rangle a_n(t) e^{i\omega_{kn} t} \tag{9}$$

First-order Perturbation

We express the $a_n(t)$ in eq.(9) as a power series in λ:

$$a_n(t) = a_n^{(0)}(t) + \lambda a_n^{(1)}(t) + \lambda^2 a_n^{(2)}(t) + \dots \tag{10}$$

Substitute eq.(10) into eq.(9), equate the coefficients of corresponding powers of λ, and set $\lambda = 1$ in final result to have the set of equations

$$\dot{a}_k^{(0)}(t) = 0 \tag{11a}$$

$$\dot{a}_k^{(s+1)}(t) = \frac{1}{i\hbar} \sum_n \langle k|h(t)|n \rangle a_n^{(s)}(t) e^{i\omega_{kn} t} \tag{11b}$$

Eq.(11) can be integrated successively to obtain approximate solutions to any desired order in the perturbation. For first-order perturbation $s = 0$ and

$$\dot{a}_k^{(1)}(t) = \frac{1}{i\hbar} \sum_n \langle k|h(t)|n \rangle a_n^{(0)}(t) e^{i\omega_{kn} t} \tag{12}$$

where $a_n^{(0)}(t)$ are the solution of eq.(11a), the zero-order coefficients $a_k^{(0)}$, which are constant with time. The $a_k^{(0)}$ are the initial conditions of the system before the perturbation is applied.

Assuming, for simplicity, that all except one of the $a_k^{(0)}$ are zero, so that the system is initially in a definite unperturbed energy state $|m\rangle$.

$$\text{We thus put} \qquad a_k^{(0)} = \langle k|m \rangle = \delta_{km} \tag{13}$$

Put eq.(13) into eq.(12) to have

$$\dot{a}_k^{(1)}(t) = \frac{1}{i\hbar}\langle k|h(t)|m\rangle e^{i\omega_{km}t}$$

$$\Rightarrow \quad a_k^{(1)}(t) = \frac{1}{i\hbar}\int_{\substack{-\infty \\ or\ 0}}^{t}\langle k|h(t')|m\rangle e^{i\omega_{km}t'}dt'$$

$a_k^{(1)}(t)$ is the first-order probability amplitude at any time $t > 0$ for state $|k\rangle$, $|a_k^{(1)}(t)|^2$ is the first-order probability of finding the system in the state $|k\rangle$ i.e. the transition probability from state $|m\rangle$ to $|k\rangle$ after time $t > 0$.

Examples

1. *A system of hydrogen atoms in the ground state is contained between the plates of a parallel-plate capacitor. A voltage pulse is applied to the capacitor so as to produce a homogeneous electric field*

$$E = \begin{cases} 0 & t\langle 0 \\ e\epsilon_0\exp(-t/\tau) & t > 0 \end{cases}$$

Show that, after a long time, the fraction of atoms in the 2p ($m = 0$) state is, to first order

$$\frac{2^{15}}{3^{10}}\frac{a_0^2 e^2 \epsilon_0^2}{\hbar^2(\omega^2 + \frac{1}{\tau^2})}$$

where a_0 is the Bohr radius, and $\hbar\omega$ is the energy difference between the 2p and the ground state.

Solution: First-order time-dependent perturbation theory gives the result that if a Hamiltonian $h(t)$ is applied at $t = 0$ to a system in an initial state $|m\rangle$ with energy E_m, the probability that a transition has occurred to a state $|k\rangle$, with energy E_k at time t is $|a_k|^2$, where

$$a_k = \frac{1}{i\hbar}\int_0^t \langle k|h(t')|m\rangle\exp(i\omega t')dt', \quad \hbar\omega = E_k - E_m \qquad (i)$$

In this problem $h(t')$ is the potential of the electron in the applied field, whose direction we take as the z-axis, i.e.

$$h(t') = e\epsilon_0 z\exp(-t'/\tau), \quad t' > 0 \qquad (ii)$$

For $t = \infty$, eq.(i) becomes

$$a_k = \frac{e\epsilon_0}{i\hbar}\langle k|z|m\rangle\int_0^{\infty}\exp\{(i\omega - 1/\tau)t'\}dt' \qquad (iii)$$

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The time integral is

$$\int_0^\infty \exp\{(i\omega - 1/\tau)t'\}dt' = \frac{1}{i\omega - 1/\tau}[\exp\{(i\omega - 1/\tau)t'\}]_0^\infty = \frac{1}{i\omega - 1/\tau} \quad (iv)$$

$$\text{Therefore,} \quad a_k = \frac{e\epsilon_0}{\hbar(\omega + i/\tau)}\langle k|z|m\rangle \quad (v)$$

The initial state is the ground state of the hydrogen atom, i.e., the quantum numbers are $n = 1, \; l = 0, \; m = 0$ and the final state has $n = 2, \; l = 1 \; m = 0$. We evaluate the matrix element in spherical polar coordinates r, θ, ϕ using the relation $z = r\cos\theta$. Then

$$\langle k|z|m\rangle = \int_{\substack{all \\ space}} u_{210}^* r\cos\theta u_{100}dv \quad (vi)$$

$$\text{where} \quad dv = r^2 dr \sin\theta d\theta d\phi \quad (vii)$$

$$u_{100} = R_{10}Y_{00} = \frac{2}{\sqrt{4\pi}}\frac{1}{a_0^{3/2}}\exp(-r/a_0) \quad (viii)$$

$$u_{210} = R_{21}Y_{10} = \frac{1}{\sqrt{4\pi}}\frac{1}{(2a_0)^{3/2}}\frac{r}{a_0}\exp(-r/2a_0)\cos\theta \quad (ix)$$

$$\text{Thus} \quad \langle k|z|m\rangle = \frac{1}{2^{3/2}}\frac{1}{a_0^4}\int_0^\infty r^4\exp(-\frac{3r}{2a_0})dr\int_0^\pi \cos^2\theta\sin\theta d\theta \quad (x)$$

$$= \frac{4!}{2^{3/2}}\left(\frac{2}{3}\right)^6 a_0 \quad (xi)$$

(We have used the result $\int_0^\infty r^4\exp(-\beta r)dr = \frac{4!}{\beta^5}$). From eqs.(v) and (xi) the probability of a transition is

$$|a_k|^2 = \frac{2^{15}}{3^{10}}\frac{a_0^2 e^2 \epsilon_0^2}{\hbar^2(\omega^2 + \frac{1}{\tau^2})}$$

2. *A time-varying Hamiltonian $h(t')$ brings about transition of a system from a state $|k\rangle$ at $t' = 0$ to $|j\rangle$ at $t' = t$ with probability $p_{kj}(t)$. Use first-order time-dependent perturbation theory to show that, if $p_{jk}(t)$ is the probability that the same Hamiltonian brings about the transition $j \to k$ in the same time interval, then $p_{jk}(t) = p_{kj}(t)$.*
Solution: The probability of a transition from $|k\rangle$ (at time zero) to $|j\rangle$ (at time t) is

$$p_{kj}(t) = |a_{kj}(t)|^2 \quad (i)$$

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where the first-order expression for $a_{kj}(t)$ is

$$a_{kj}(t) = \frac{1}{i\hbar} \int_0^t \langle j|h(t')|k \rangle \exp(i\omega_{jk}t')dt' \qquad (ii)$$

Similarly, $\qquad a_{jk}(t) = \frac{1}{i\hbar} \int_0^t \langle k|h(t')|j \rangle \exp(i\omega_{kj}t')dt' \qquad (iii)$

Now $h(t')$ is a Hermitian operator. Therefore

$$\langle k|h(t')|j \rangle = \langle j|h(t')|k \rangle^* \qquad (iv)$$

$$\text{Also} \qquad \hbar\omega_{kj} = E_k - E_j = -\hbar\omega_{jk} \qquad (v)$$

Therefore the integral in eq.(iii) is the complex conjugate of the one in eq.(ii). Thus

$$a_{jk}(t) = -\{a_{kj}(t)\}^*$$

$$\text{giving} \qquad p_{jk}(t) = |a_{kj}(t)|^2 = p_{kj}(t)$$

Comment: It is in general true that the probability of transition between two states, due to an external stimulus represented by $h(t)$, is the same for transition in either direction. The result is known as the *principle of detailed balancing*

3. *Consider a one-dimensional harmonic oscillator with angular frequecy ω_0 and electric charge q. At time $t = 0$ the oscillator is in ground state. An electric field is applied for time τ, so the perturbation is*

$$h(t) = \begin{cases} -q\epsilon x & 0 \leq t \leq \tau \\ 0 & otherwise \end{cases}$$

where ϵ is a field strength and x is a position operator. Using first-order perturbation theory, calculate the probability of transition to the state $n = 1$.

Chapter 2

SCATTERING THEORY

Introduction: Much of what we know about the forces and interactions in atoms and nuclei has been learnt from scattering experiments, in which atoms in a target are bombarded with beams of particles whose nature are known. Theoretically, the most significant aspect of scattering processes is that of the continuous part of energy spectrum. Here intensities are the objects of measurement and prediction. These intensities, being measures of the likelihood of finding a particle at certain places, are related to the eigenfunctions. Establishing this relation is the first problem of scattering theory.

In an idealized scattering experiment a single fixed scattering center is bombarded by particles (projectiles) incident along the z-axis. In the classical limit each particle can be assigned an *impact parameter, ρ* and an *azimuth angle, ϕ*, which together with z define its position in cylindrical coordinates.

Let $d\sigma/d\Omega$ be the area which, when placed at right angles to the incident beam, would be traversed by as many particles as are scattered into the unit solid angle around a direction characterized by the angles θ and ϕ (fig.

above). If the scattering potential is spherically symmetric, $V = V(r)$ the scattering becomes independent of ϕ. Therefore, classically it can be shown that the *differential cross-section* is

$$\frac{d\sigma}{d\Omega} = \frac{\rho}{\sin\theta}\left|\frac{d\rho}{d\theta}\right| \tag{1}$$

The impact parameter ρ is a function of θ. To determine this function from Newton's second law is the problem of classical scattering theory. Eq.(1) is valid if the de Broglie wavelength of the projectile is much smaller than the dimension of the scattering region. As the wavelength increases quantum features appear. Quantum Mechanics represents the particles in the beam by wave packets. That is, the particles do not have sharp boundaries. Therefore, in Quantum Mechanics particles need not actually touch each other as they can do in Classical Mechanics. When two particles are near each other they feel the influence of each other by the *degree of freedom* which is common to both. E.g., an electron has the degrees of freedom (mass, charge, spin) while a neutron has (mass, spin). So an electron and a neutron can feel or relate with each other by (mass, spin) which is common to both.

Elastic Scattering

It is scattering without energy loss or gain by the projectile, i.e. kinetic energy of projectile is conserved. In elastic scattering the scattering center on the particles can be represented by a potential energy $V(r)$ of finite range d such that $V(r) = 0$, if $r > d$. The disc of radius d is called the scattering cross-section. Scattering cross-section is a measure of the probability of scattering of the projectile by the target.

Definition of differential cross-section: A beam of particles of mass m travelling along the z-direction with velocity v is scattered by a short-range potential $V(r)$ centred on the origin O (fig. below). We use spherical polar coordinates r, θ, ϕ taking z as the polar axis. The Schrödinger equation is used to calculate the probability of a particle being scattered into a small solid angle $d\Omega$ in the direction θ, ϕ. The probability is expressed in terms of a *differential cross-section, $d\sigma/d\Omega$*, which is defined as the ratio of the number of scattered particles $dn(\theta, \phi)$ per unit time within the solid angle $d\Omega$ to the incident flux F;

$$d\sigma/d\Omega = dn(\theta, \phi)/Fd\Omega \tag{2}$$

where $d\sigma/d\Omega$ has dimension of surface. We assume:
1. Any interaction between the scattered particles themselves is negligible

2. Possible multiple scattering processes are negligible. (A multiple scattering process is a process in which a scattered particle can be scattered multiple times in the same target range)

3. The incident beam width is much larger than a typical range of the scattering potential, so that the particle will have a well-defined momentum. The total scattering cross-section σ_{sc} =(total number of particles scattered per second)$/F = \int \frac{d\sigma}{d\Omega} d\Omega$. Absorption cross-section σ_{ab} = (total number of particles absorbed per second)$/F$.

The Schrödinger equation for scattering

1. Ignore the center of mass motion

2. Consider only the motion in the center of mass frame i.e. relative motion which is important for collision.

$$\left[-\frac{\hbar^2}{2\mu} \nabla^2 + V(r) \right] \psi(r) = E\psi(r) \tag{3}$$

where μ = reduced mass. This is the equation for the projectile; it is not an eigenvalue equation. E is positive and is the energy given to the projectile by the experimenter. Therefore, it is arbitrary. Divide (3) through by $\hbar^2/2\mu$ to obtain

$$\left[-\nabla^2 + \frac{2\mu V}{\hbar^2} - \frac{2\mu E}{\hbar^2} \right] \psi$$

$$\text{or} \quad [\nabla^2 + k^2]\psi = U\psi \tag{4}$$

where $E = \frac{\hbar^2 k^2}{2\mu}$ and $U = \frac{2\mu V}{\hbar^2}$

Green's function method: We seek solution $\psi(r) = \Phi(r) \exp(-i\omega t)$ that satisfies the boundary conditions that

$\psi(r)$ is finite at $r = 0$ and $\psi(r) \to 0$ as $r \to \infty$. In that case

$$\Phi(r) = \exp(ikz) + \frac{f(\theta, \phi)}{r} \exp(ikr) \tag{5}$$

This result is obtained by Green's function method applied to (4) (details deferred). Therefore,

$$\psi(r) = \exp i(kz - \omega t) + \frac{f(\theta, \phi)}{r} \exp i(kr - \omega t) \tag{6}$$

The first term represents the incident particles moving along the z-axis, and the second term, which is a spherical wave travelling outwards from the origin, represents the scattered particles. We are confining the dicussion to elastic scattering hence the value of k is the same in the incident and scattered terms in (6). The function $f(\theta, \phi)$ is known as the *scattering amplitude*. The differential cross-section is related to $f(\theta, \phi)$ by

$$d\sigma/d\Omega = |f(\theta, \phi)|^2 \tag{7}$$

Proof: The area dA subtends a solid angle $d\Omega$ at the origin, where

$$d\Omega = dA/r^2 \tag{i}$$

The term $u_i = \exp(ikz)$ in the wave function (6) represents the incident particles with density

$$G_i = |u_i|^2 = 1 \tag{ii}$$

While the term $u_s = \frac{1}{r} f(\theta, \phi) \exp(ikr)$ represents the scattered particles with density

$$G_s = |u_s|^2 = |f(\theta, \phi)|^2/r^2 \tag{iii}$$

The number of scattered particles passing through dA in unit time = (density of particles at $\vec{r}$)$\times v \times dA = \frac{|f(\theta,\phi)|^2}{r^2} = |f(\theta, \phi)|^2 v d\Omega$ (iv)
where v is the velocity of the incident and scattered particles. The incident flux is $F = G_i \times v = v$ (v).
Inserting (iv) and (v) into the definition of $d\sigma/d\Omega$, eq.(2) we have (7)

Born Approximation

This is a first-order perturbation calculation, valid for fast particles and a weak potential, which means that the incident wave function is only slightly perturbed by the potential. The approximation gives

$$f(\theta, \phi) = -\frac{m}{2\pi\hbar^2} \int_{\substack{all \\ space}} V(r) \exp(i\vec{\kappa}.\vec{r}) dv \tag{8}$$

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where the quantity $\vec{\kappa}$, known as the scattering vector, is defined by $\vec{\kappa} = \vec{k} - \vec{k'}$, where k is the wave vector of the incident particles, and k' that of the scattered particles. The angle between $\vec{k}$ and $\vec{k'}$ is the scattering angle θ. For elastic scattering

$$|\vec{k}| = |\vec{k'}|, \text{ and } \kappa = 2k \sin \frac{\theta}{2} \tag{9}$$

Example 1: *Show that for a spherically symmetric potential*

$$\int_{-\infty}^{\infty} V(\vec{r}) \exp(i\vec{k}.\vec{r}) = \frac{4\pi}{k} \int_0^{\infty} V(r) \sin kr dr$$

Solution: Since the potential is spherically symmetric, it depends only on the magnitude of $\vec{r}$, thus we have

$$\int V(\vec{r}) \exp(\vec{k}.\vec{r}) d^3r = 2\pi \int_0^{\infty} V(r) r^2 dr \int_0^{\pi} \exp(ikr cos\theta) \sin\theta d\theta \tag{i}$$

where θ is the angle between $\vec{r}$ and the polar axis. Put $u = \cos\theta$. Then

$$du = -\sin\theta$$

and

$$\int_0^{\pi} \exp(ikr \cos\theta) \sin\theta d\theta = \int_{-1}^{1} \exp(ikru) du = \frac{2}{kr} \sin kr \tag{ii}$$

Inserting (ii) in (i), we have the expected result.

Example 2: a) *Particles are incident on a spherically symmetric potential $V(r) = \frac{\beta}{r} \exp(-\gamma r)$, where β and γ are constants. Show that, in the Born approximation, the differential scattering cross-section for the scattering vector $\vec{\kappa}$ is given by $d\sigma/d\Omega = \left\{ \frac{2m\beta}{\hbar^2(\kappa^2+\gamma^2)} \right\}^2$*
b) *Use this result to derive the Rutherford formula for the scattering of α-particles, namely, that for α-particles of energy E incident on nuclei of atomic number Z, the differential scattering cross-section for scattering at an angle θ to the incident direction is $d\sigma/d\Omega = \left\{ \frac{Ze^2}{8\pi\epsilon_0 E \sin^2(\frac{\theta}{2})} \right\}$*
Solution: a) The Born approximation gives the amplitude

$$f(\theta) = -\frac{mI}{2\pi\hbar^2} \tag{i}$$

$$\text{where} \quad I = \int_{\substack{all \\ space}} V(r) \exp(i\vec{\kappa}.\vec{r}) dv \tag{ii}$$

Using the result that

$$I = \int_{\substack{all \\ space}} V(r) \exp(i\vec{\kappa}.\vec{r}) dv = \frac{4\pi}{k} \int_0^\infty V(r) r \sin \kappa r dr \qquad (example1)$$

$$\text{with} \quad V(r) = (\beta/r) \exp(-\gamma r) dr$$

$$I = \frac{4\pi\beta}{\kappa} \int_0^\infty \sin \kappa r \exp(-\gamma r) dr \qquad (iii)$$

The integral is easily evaluated expressing the sine function as

$$\sin \kappa r = \frac{1}{2i} \{\exp(i\kappa r) - \exp(-i\kappa r)\} \qquad (iv)$$

and noting that the integrated expression vanishes at $r = \infty$ due to the factor $\exp(-\gamma r)$. The result is

$$I = \frac{4\pi\beta}{\kappa^2 + \gamma^2} \qquad (v)$$

Thus from (i) and (v)

$$d\sigma/d\Omega = |f(0)|^2 = \left\{ \frac{2m\beta}{\hbar^2(\kappa^2 + \gamma^2)} \right\}^2 \qquad (vi)$$

b) α-particles are scattered by the electrostatic interaction between the charge $2e$ on the α-particle and the charge Ze on the nucleus. The potential is

$$V(r) = \frac{2Ze^2}{4\pi\epsilon_0} \frac{1}{r} \qquad (vii)$$

This is represented by the potential in part (a), with

$$\beta = \frac{2Ze^2}{4\pi\epsilon_0}, \quad \gamma = 0 \qquad (viii)$$

Inserting these values in (vi) gives

$$d\sigma/d\Omega = \left\{ \frac{mZe^2}{\pi\epsilon_0\hbar^2(\kappa^2} \right\}^2 \qquad (ix)$$

The energy of the α-particle is

$$E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} \qquad (x)$$

where p is the momentum. Since $\kappa = 2k \sin(\frac{\theta}{2})$

$$\hbar^2 \kappa^2 = 8mE \sin^2 \left(\frac{\theta}{2}\right) \qquad (xi)$$

Inserting (xi) in (ix) gives the required result

Partial waves and phase shifts

We look for solutions of the Schrödinger equation

$$-\frac{\hbar^2}{2\mu} \nabla^2 \psi + V(r)\psi = \frac{\hbar^2 k^2}{2\mu} \psi \qquad (10)$$

(where ∇^2 is the Laplacian in spherical polar coordinates and $V(r)$ is a spherically symmetric potential $\Rightarrow$ elastic scattering) which have the asymptotic form

$$\psi_k^{(+)} = e^{ikr\cos\theta} + f_k(\theta)\frac{e^{ikr}}{r} \qquad (11)$$

We establish the connection between these solutions and

$$\psi(r, \theta, \phi) = R_{l,k}(r)Y_l^m(\theta, \phi) = \frac{u_{l,k}(r)}{r}Y_l^m(\theta, \phi) \qquad (12)$$

which are simultaneous (common) eigenfunctions of H, L^2 and L_z. The radial functions $R_{l,k}$ and $u_{l,k}$ satisfy the differential equations

$$\left[-\frac{1}{r^2}\frac{d}{dr}(r^2\frac{d}{dr}) + \frac{l(l+1)}{r^2} + \frac{2\mu}{\hbar^2}V(r) - k^2\right] R_{l,k}(r) = 0 \qquad (13)$$

$$\left[-\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} + \frac{2\mu}{\hbar^2}V(r) - k^2\right] u_{l,k}(r) = 0 \qquad (14)$$

respectively as well as the boundary condition that $R_{l,k}$ be finite at the origin
$\Rightarrow u_{l,k} = 0$ \qquad (15)

For the region $r > d$, $V(r) = 0$

$$\left[-\frac{1}{r^2}\frac{d}{dr}(r^2\frac{d}{dr}) + \frac{l(l+1)}{r^2} - k^2\right] R_{l,k}(r) = 0 \qquad (16)$$

The asymptotic solution of (16) for large kr is (quoted)

$$R_{l,k}(r) = \frac{u_{l,k}(r)}{r} \sim A_l\frac{\sin(kr - l\pi/2)}{kr} - B_l\frac{\cos(kr - l\pi/2)}{kr} \qquad (17)$$

The first term of (17) is called the *regular* solution while the second term is the *irregular* solution. The magnitude of B_l/A_l is a measure of the intensity scattering.

$$B_l/A_l = -\tan\delta_l \tag{18}$$

where δ_l is called *scattering phase shift*. Hence (17) can be written as

$$\frac{u_{l,k}(r)}{r} \sim C_l\frac{\sin(kr - l\pi/2 + \delta_l)}{kr}$$

$$\text{or} \quad \frac{u_{l,k}(r)}{r} \sim \frac{\sin(kr - l\pi/2 + \delta_l)}{kr} \tag{19}$$

(where $C_l = 1$ in order to fix the normalization). If we expand $\psi_k^{(+)}$ in terms of the separable solution of (12) (i.e. Legendre polynomials) we get

$$\psi_k^{(+)}(r,\theta) = \sum_{l=0}^{\infty} a_l(k)p_l(\cos\theta)\frac{u_{l,k}(r)}{r} \tag{20}$$

where $\psi_k^{(+)}$ depends only on the angle between $\vec{k}$ and $\vec{r}$ but not on their directions. The asymptotic expansion of the plane wave e^{ikz} gives

$$e^{ikz} = e^{ikr\cos\theta} \sim \sum_{l=0}^{\infty}(2l + 1)i^l\frac{\sin(kr - l\pi/2)}{kr}p_l(\cos\theta) \tag{21}$$

Substituting (21) into (11), and (19) into (20) and comparing coefficients of the terms of the form $p_l(\cos\theta)\frac{\exp(-ikr+il\pi/2)}{kr}$ we have

$$a_l = \frac{(2l + 1)i^l}{(2\pi)^{3/2}}e^{i\delta_l} \tag{22}$$

Hence asymptotically, (i.e. using (22) and (19) in (20))

$$\psi_k^{(+)}(r,\theta) \sim \sum_{l=0}^{\infty}(2l + 1)i^l e^{i\delta_l}\frac{\sin(kr - l\pi/2 + \delta_l)}{(2\pi)^{3/2}kr}p_l(\cos\theta) \tag{23}$$

Eq.(23) differs from a plane wave by the presence of δ and is called *distorted plane waves*. Put (21) into (11) and compare the coefficients of $\frac{e^{ikr}}{r}$ in (11) and (23) to have

$$f_k(\theta) = \sum_{l=0}^{\infty}(2l + 1)\frac{e^{2i\delta_l} - 1}{2ik}p_l(\cos\theta) \tag{24}$$

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$$\text{or} \quad f_k(\theta) = \frac{1}{k} \sum_{l=0}^{\infty} (2l+1) e^{i\delta_l(k)} \sin \delta_l(k) p_l(\cos \theta) \tag{25}$$

Each l term in (24) or (25) is known as a *partial wave*. The $l = 0$ wave is termed an *s*-wave, the $l = 1$ a *p*-wave, the $l = 2$ a *d*-wave and so on (same nomenclature as for atomic states). The lth wave, being an eigenfunction of the operator L^2, is a state in which the particle has orbital angular momentum about the origin of magnitude $\sqrt{\{l(l+1)\}}\hbar \approx l\hbar$. Since the linear momentum of the particle is $\hbar k$, a classical picture of the lth wave is that it corresponds to the particle passing the potential at a distance ρ_l from its centre, where $\hbar k \rho_l = l\hbar$, i.e.

$$\rho_l = l/k \tag{26}$$

Eq.(25) shows that, if $\delta_l = 0$, that partial wave gives no contribution to $f(\theta)$. If ρ_l, the distance of closest approach, is much larger than d, the range of the potential, the particle passes outside the potential and is not scattered, so $\delta_l = 0$ for that partial wave. It follows from (26) that only those partial waves with $l \leq dk$ have non-zero values of δ_l, and contribute to the scattering. If $dk \ll 1$, as in the case for nuclear scattering at low energy all the $\delta_l = 0$, except δ_0. Since $k = 2\pi/\lambda$ the condition $dk \ll 1 \Rightarrow 2\pi d/\lambda \ll 1 \Rightarrow \lambda \gg d$ i.e. the wavelength λ of the particle is large compared to the range of the potential. In this situation, when only the *s*-wave is disturbed, the angular dependence of $f(\theta)$ is given by the Legendre polynomial $p_0(\cos \theta) = 1$ so the scattering is spherically symmetric. As $k \to 0$, $\tan \delta_0$ is proportional to k, i.e. $\delta_0 \to 0$ or $n\pi$ and the limiting value of $-\tan \delta_0/k$, is termed *scattering length*. the concept is most commonly applied to the scattering of thermal neutrons.

Example: 1. *a) Verify that, outside the range of a short-range potential, the wave function*

$$\psi(r, \theta) = \frac{1}{r} \left(1 + \frac{i}{kr}\right) \exp(ikr) \cos \theta$$

represents an outgoing p-wave.

b) A beam of particles represented by the plane wave $e^{(ikz)}$ is scattered by an impenetrable sphere of radius d, where $kd \ll 1$. By considering only s and p components in the scattered wave, show that, to order $(kd)^2$, the differential scattering cross-section for scattering at an angle θ is

$$d\sigma/d\Omega = d^2\{1 - \frac{1}{3}(kd)^2 + 2(kd)^2 \cos \theta\}$$

[The value of $\cos^2 \theta$ averaged over all directions is 1/3]

Solution: a) The dependence on θ for a p-wave ($l = 1$) is given by the Legendre polynomial $p_1(\theta) = \cos \theta$. So the angular part of the given function $\psi(r, \theta)$ has the required form for a p-wave. It remains to show that the radial part $R(r)$ has the correct form. Put $R(r) = u(r)/r$. From (14), outside the range of the potential, $u(r)$ satisfies

$$\frac{d^2 u}{dr^2} + \left\{ k^2 - \frac{l(l+1)}{r^2} \right\} u = 0, \tag{i}$$

with $l = 1$. For the given $\psi(r, \theta)$,

$$u(r) = \left(1 + \frac{i}{kr} \right) \exp(ikr). \tag{ii}$$

Differentiating this twice with respect to r and substituting in (i) shows that the equation is satisfied with $l = 1$.

b) Outside the range of the potential, the wave function for s and p waves has the form

$$\psi = \exp(ikz) + \frac{A}{r} \exp(ikr) + \frac{B}{r} \left(1 + \frac{i}{kr} \right) \exp(ikr) \cos \theta, \tag{iii}$$

where A and B are constants. The term in A is the spherically symmetric s-wave, and the term in B is the p-wave. As $r \to \infty$

$$\psi = \exp(ikz) + \frac{f(\theta)}{r} \exp(ikr) \tag{iv}$$

Equating terms in $(1/r) \exp(ikr)$ in (iii) and (iv) gives

$$f(\theta) = A + B \cos \theta \tag{v}$$

Since the scattering object is an impenetrable sphere, the wave function vanishes on the surface $r = d$. Thus

$$\exp(ikd \cos \theta) + \frac{A}{d} \exp(ikd) + \frac{B}{d} \left(1 + \frac{i}{kd} \right) \exp(ikd) \cos \theta = 0. \tag{vi}$$

The terms on the RHS that are independent of θ must sum to zero, and similarly the terms proportional to $\cos \theta$. Expanding $exp(ikd \cos \theta)$ in powers of kd we have

$$\exp(ikd \cos \theta) = 1 + ikd \cos \theta - \frac{1}{2}(kd)^2 \cos^2 \theta + 0(k^3 d^3). \tag{vii}$$

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We cannot make the terms in $\cos^2 \theta$ sum to zero in (vi), because that would require the contribution from d-waves, which are excluded. However, we need to take into account the *average* value of $\cos^2 \theta$, which is $1/3$. Summing the terms in (6) which are independent of θ gives

$$1 - \frac{1}{6}(kd)^2 + \frac{A}{d}\exp(ikd) = 0 \qquad (viii)$$

$$\text{whence} \quad A = -d\{1 - \frac{1}{6}(kd)^2\}\exp(-ikd). \qquad (ix)$$

Summing the terms in $\cos \theta$ gives

$$ikd + \frac{B}{d}\left(1 + \frac{i}{kd}\right)\exp(ikd) = 0. \qquad (x)$$

Since $kd \ll 1$, $i/kd \gg 1$. Therefore to terms in $(kd)^2$

$$B = -d(kd)^2. \qquad (xi)$$

From (v),(ix), and (xi), the differential scattering cross-section is

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 = |A + B\cos\theta|^2 = d^2\{1 - \frac{1}{3}(kd)^2 + 2(kd)^2\cos\theta\}, \qquad (xii)$$

to terms in $(kd)^2$

Example 2 *A particle of mass μ and momentum $\vec{P} = \hbar\vec{k}$ is scattered by the potential $V(\vec{r}) = \frac{e^{-r/a}}{r}V_o a$, where V_o and $a>0$ are real constants (Yukawa potential).*
(a) Using the Born approximation, calculate the differential cross section (b) obtain the total cross section.

<div align="center">Solution</div>

(a) The range of the Yukawa potential is characterized by the distance a. We assume that $V_o a^2 \ll \hbar^2/\mu$, so that the Born approximation is valid for all values of ka. The scattering amplitude is then given by:

$$f(\theta, \phi) = -\frac{1}{4\pi}\frac{2\mu V_o a}{\hbar^2}\int e^{-i\vec{q}.\vec{r}}\frac{e^{-r/r_o}}{r}d^3r$$

Since the potential has spherical symmetry $V(\vec{r}) = V(r)$, we can carry out the integration using the relation

$$\int r^2 e^{-i\vec{q}.\vec{r}}V(r)drd\Omega = \frac{4\pi}{q}\int_0^\infty \sin(qr)V(r)rdr$$

where r $=|\vec{r}|$ and $d\Omega = \sin\theta d\theta d\phi$. Therefore,

$$f(\theta) = -\frac{2\mu V_o a}{\hbar^2 k}\int_0^\infty r\sin(kr)e^{-r/a}dr = -\frac{2\mu V_o a^3}{\hbar^2}\frac{1}{1+q^2 a^2}$$

$$= -\frac{2\mu V_o a^3}{\hbar^2}\frac{1}{1+[2ka\sin\frac{\theta}{2}]^2}$$

Finally, the differential cross section $\frac{d\sigma}{d\Omega} = |f(\theta)|^2$ is:

$$\frac{d\sigma(\theta)}{d\Omega} = \frac{4\mu^2 V_o^2 a^6}{\hbar^4}\frac{1}{[1+4k^2 a^2\sin^2\frac{\theta}{2}]^2} \qquad *$$

Note that due to spherical symmetry, the cross section does not depend on the azimuthal angle.

(b) The total cross section is obtained by integration

$$\sigma = \int\frac{d\sigma(\theta)}{d\Omega}d\Omega = \frac{4\mu^2 V_o^2 a^6}{\hbar^4}\frac{4\pi}{1+4k^2 a^2}$$

Note that the infinite range limit (a $\to\infty$, $V_o \to 0$ and $V_o a = Z_1 Z_2 e^2$=constant of the Yukawa potential corresponds to the Coulomb interaction between two ions of charges $Z_1 e$ and $Z_2 e$. At this point (*) reduces to the well -known Rutherford formula

$$\frac{d\sigma}{d\Omega} = \frac{4\mu^2}{\hbar^4}\frac{Z_1^2 Z_2^2 e^4}{16K^4\sin^4\frac{\theta}{2}} = \frac{Z_1^2 Z_2^2 e^4}{16E^2\sin^4\frac{\theta}{2}}$$

where $E = \frac{\hbar^2 k^2}{2\mu}$ is the energy of the particle in the center of mass frame and μ is their reduced mass.

Example 3: *A point particle is scattered by a second particle with rigid core; that is, the scattering potential is $V(r) = 0$ for r> a and $V(r) = \infty$ for $r < a$. The energy of the scattered particle satisfies ka = 1. (a) Find the expression for δ_l. Complete the table below (express δ_l in radians).*

	$\tan\delta_l$	δ_l	$\sin\delta_l$
$l = 0$			
$l = 1$			
$l = 2$			

(b) Calculate the differential cross section $d\sigma/d\Omega$ for angles 0 and π, taking into account only the waves l =0 and l =1. (c) Compute the total cross

section σ_T taking into account only the waves $l = 0$ and $l = 1$. (d) What is the accuracy of part (c)?

<div align="center">Solution</div>

(a) The phase shifts for a rigid sphere is given by the equation:

$$\tan \delta_l = \frac{j_l(ka)}{n_l(ka)}$$

Using the known expressions for the Spherical Bessel functions:

$$j_o(x) = \frac{\sin x}{x} \qquad\qquad n_o(x) = -\frac{\cos x}{x}$$

$$j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x} \qquad n_1(x) = -\frac{\cos x}{x^2} - \frac{\sin x}{x}$$

$$j_2(x) = \left(\frac{3}{x^2} - \frac{1}{x}\right) \sin x - 3\frac{\cos x}{x^2} \quad n_2(x) = -\left(\frac{3}{x^2} - \frac{1}{x}\right) \cos x - 3\frac{\sin x}{x^2}$$

and substituting x=ka =1, we find $\tan \delta_o$ = -1.56, $\tan \delta_1$= -0.22 and $\tan \delta_2$ = -0.02. Therefore

	$\tan \delta_l$	δ_l	$\sin \delta_l$
$l = 0$	-1.56	-1.00	-0.84
$l = 1$	-0.22	-0.22	-0.22
$l = 2$	-0.02	-0.02	-0.02

(b) The differential cross section is given by:

$$\frac{d\sigma}{d\Omega} = \frac{1}{k^2}|\sum_{l=0}^{\infty}(2l + 1)e^{i\delta_l} \sin \delta_l P_l(\cos \theta)|^2$$

For l =0, 1 and k =a^{-1}

$$\frac{d\sigma}{d\Omega} = a^2|\sin \delta_o e^{i\delta_o} + 3 \sin \delta_1 e^{i\delta_1} \cos \theta|^2$$
$$= a^2[\sin^2 \delta_o + 6 \sin \delta_o \sin \delta_1 \cos(\delta_o - \delta_1) \cos \theta$$
$$+9 \sin^2 \delta_1 \cos^2 \theta]$$

Substituting $\theta = 0, \pi$, we obtain:

$$\frac{d\sigma}{d\Omega}|_{0,\pi} = a^2|\sin^2 \delta_o \pm 6 \sin \delta_o \sin \delta_1 \cos(\delta_0 - \delta_1) + 9 \sin^2 \delta_1|$$

with δ_1 and δ_0 given in the table above.

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(c) The total cross section is given by:

$$\sigma_T = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2 \delta_l$$

for l =0, 1 and k =1/a

$$\sigma_T = 4\pi a^2 [\sin^2 \delta_o + 3 \sin^2 \delta_1] \approx 0.854\pi a^2.$$

(d) A rough estimate on the accuracy of the calculation in part (c) is given by calculating the additional term l =2.

$$\sigma_T \approx (0.85 + 0.002)4\pi a^2$$

Example 4: *(a) Consider scattering from a spherical symmetric potential. The solution of the Schrodinger equation is given by the expansion $\phi(r, \theta) = \Sigma_{l=0}^{\infty} R_l(r) P_l(\cos \theta)$, where $R(r)$ is the solution of the radial wave equation and $P_l(\cos \theta)$ is the Legendre polynomial of order l. In the limit $r \to \infty$ the asymptotic form of the wave function is:*

$$\phi(r, \theta)_{r\to\infty} \approx e^{ikz} + \frac{1}{r} f(\theta) e^{ikr} \qquad (1)$$

where $f(\theta)$ is the scattering amplitude. Similarly, the asymptotic form of $R(r)$ is

$$R(r)_{r\to\infty} \approx \frac{A_l \sin\left(kr - \frac{\pi}{2}l + \delta_l\right)}{kr} \qquad (2)$$

where δ_l are phase shifts. (i) use expressions (1) and (2) to obtain the Legendre expansion of $f(\theta)$
(b) Show that the total cross section is given by

$$\sigma_T = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2 \delta_l$$

Solution (a) The asymptotic form of the wave function is as given above:

$$\phi(r, \theta)_{r\to\infty} \approx \sum_{l=0}^{\infty} A_l \frac{\sin\left(kr - \frac{\pi}{2}l + \delta_l\right)}{kr} P_l(\cos \theta) = e^{ikr} + \frac{1}{r} f(\theta) e^{ikr}$$

Using the Legendre expansion of e^{ikz},

$$e^{ikz} = e^{ikr\cos\theta} = \sum_{l=0}^{\infty} (2l+1) i^l j_l(kr) P_l(\cos \theta)$$

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we find that

$$\sum_{l=0}^{\infty} A_l \frac{\sin\left(kr - \frac{\pi}{2}l + \delta_l\right)}{kr} P_l(\cos\theta) = e^{ikr} + \frac{1}{r}f(\theta)e^{ikr}$$

$$= \sum_{l=0}^{\infty}\left[(2l+1)i^l\frac{\sin\left(kr - \frac{\pi}{2}l + \delta_l\right)}{kr} + \frac{1}{r}f_l(\theta)e^{ikr}\right]P_l(\cos\theta)$$

where $f(\theta) = \sum_{l=0}^{\infty} f_l P_l(\cos\theta)$. Now, we write $\sin x = \frac{e^{ix}-e^{-ix}}{2i}$, and obtain

$$I \quad A_l e^{i\left(kr - \frac{\pi}{2}l + \delta_l\right)} - (2l+1)i^l e^{i\left(kr - \pi\frac{l}{2}\right)} = 2ikf_l e^{ikr}$$

$$II \qquad A_l e^{-ikr - \pi\frac{l}{2} + \delta_l} - 2l + i^l e^{-ikr - \pi\frac{l}{2}} = 0$$

Therefore from (II), we obtain $A_l = (2l+1)i^l e^{i\delta_l}$ and then by subst back in (II), we have

$$f(\theta) = (2ik)^{-1}\sum_{l=0}^{\infty}(2l+1)(e^{2i\delta_l} - 1)P_l(\cos\theta)$$

(b) The total cross section is

$$\sigma_T = \int |f(\theta)|^2 d\Omega = 2\pi\int_{-1}^{1}\frac{d(\cos\theta)}{4k^2}|\sum_{l=0}^{\infty}(2l+1)(e^{2i\delta_1} - 1)P_l(\cos\theta)|^2$$

$$= \frac{\pi}{2k^2}\int_{-1}^{1}d(\cos\theta)\sum_{l,l'=0}^{\infty}(2l'+1)(2l+1)(e^{2i\delta_{l'}} - 1)(e^{2i\delta_l} - 1)P_{l'}(\cos\theta)P_l(\cos\theta)$$

Now,

$$\int_{-1}^{1}d(\cos\theta)P_{l'}(\cos\theta)P_l(\cos\theta) = \frac{2}{(2l+1)}\delta_{ll'}.$$

Therefore

$$\sigma_T = \frac{\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)(2 - e^{2i\delta_l} - e^{-2i\delta_l}) = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l$$