PHYSICS
251A

QUANTUM
MECHANICS

PHYSICS 251a

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QUANTUM MECHANICS

NOTES

Professor: Dr. Furry
Room: Jefferson 250, MWF at 12

LECTURE I

Recommended Reading List:

Introductory:
- Schiff
- Bohm
- Mandl
- Pauling & Wilson

Advanced:
- Dirac
- Kemble
- Pauli in Hand. d. Phys.
- Kramers
- Landau & Lifshitz

Three Main Catagories of Problems in Physics:
1. Phenomenological (e.g., valences in chemistry)
2. Atomic & nuclear structures (Quantum Mechanics)
3. Nuclear Forces, Quantum Field Theory (Inadequate today)

Assomed Background:
1. Interference and diffraction of light and X-rays, wave nature of light.
2. Black-body spectrum, photoelectric effect, Compton effect, particle nature of light.
3. Combination Principle of Spectral States
4. Bohr theory of atomic states
5. Franck-Hertz Experiment
6. Stern-Gerlach Experiment
7. Discreet States of atomic and molecular systems

8. Electron Diffraction, wave motion of matter
9. Particle nature of matter, oil drop experiment, shot effect, etc.

Classical Idea of Objectivity:
Phenomenon is in principle independent of the means of observation. This idea is discounted by quantum mechanics, which does not say that mere knowledge affects objectivity.

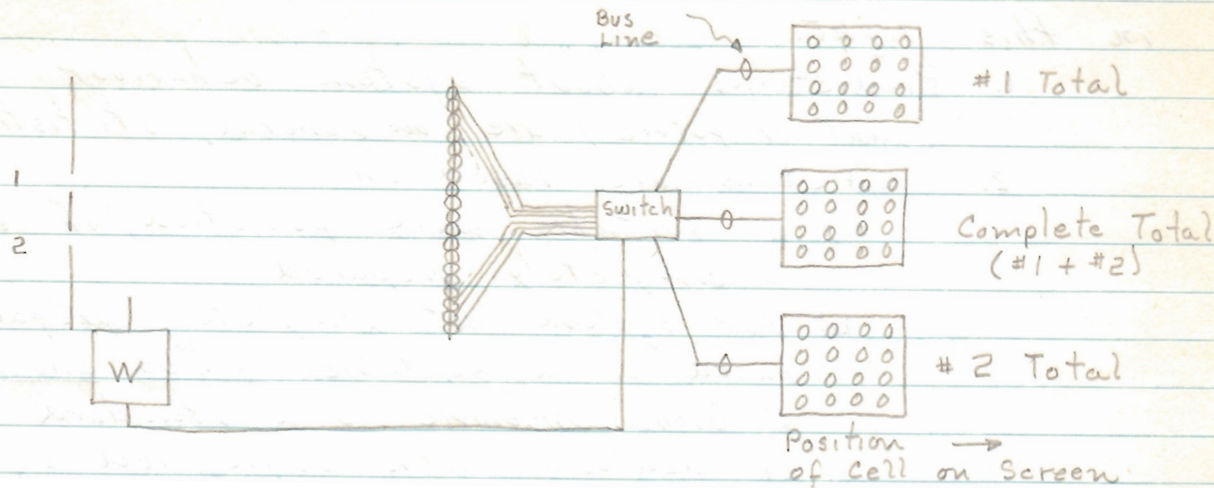
The experimental apparatus used to learn knowledge of a system may completely exclude gaining knowledge of other aspects of system - Principle of Complementarity.

LECTURE II 9/28/60

The key problem in the principle of complementarity is the solution of the wave-particle duality.

This effect includes many photons or particles. We get the usual diffraction pattern indicating the wave nature of light. It is possible to wonder if one could not count the number of photons, its velocity and direction, while passing through each slit.

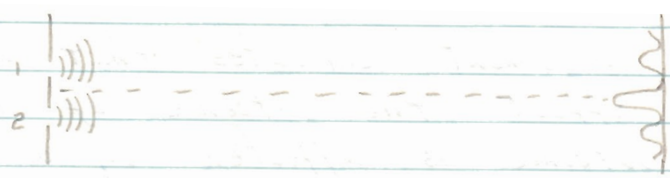
Let us envision the following "thought experiment"



We have our screen covered with minute counters of 100% efficiency which are wired into a gigantic switch controlled by a mechanism W which senses which slit a photon has passed thru and gates its return to the proper display. The display indicates the number of counts for each counter in position on the screen. Consider the following cases:

	Wave Field	Pattern

"W" not there



Case ①
"W" is there
Gives answer 1

Case ②
"W" is there
Gives answer 2

"W" there but not read
Total counts only read

We will now examine two postulates of Quantum Mechanics and examine the results in this light.

1. Predictions about system behaviour (past or future) are, in general, statistical.
2. Predictions are based on:
   a) a suitable wave function, if system is completely prepared.
   b) For system not completely prepared, based on a suitable <u>Gibbs ensemble</u>. A Gibbs ensemble is a standard way of dealing with unprepared systems, for example, the statistical mechanics of gas systems where it is not possible to know everything about each of the particles.

As can be seen from the diagrams, the presence of "W" destroys the diffraction pattern, and makes the two sources incoherent. When "W" is used but not read, we have an ensemble of 1/2 case ① and 1/2 case ② or their average. It is only when "W" is removed that the interference occurs.

This argument indicates that mere knowledge does not affect the outcome of the experiment, but the outcome is affected by a change in the apparatus.

The Quantum Mechanical situation is <u>not</u> like classical physics statistical situation, i.e., it is not decribable by a Gibbs ensemble.

Next time: Setting up of $\Psi(r,t) = \int A(\mathbf{k}) e^{i(\mathbf{k}\cdot\mathbf{r} - \omega t)} d\mathbf{k}$, Fourier analysis of wave particle that is free: $\omega = \omega(\mathbf{k})$, for photons, $\omega = c\,k$.

$\mathbf{r}, \mathbf{k}$ are vectors

r, k are scalars

LECTURE III   9-30-60

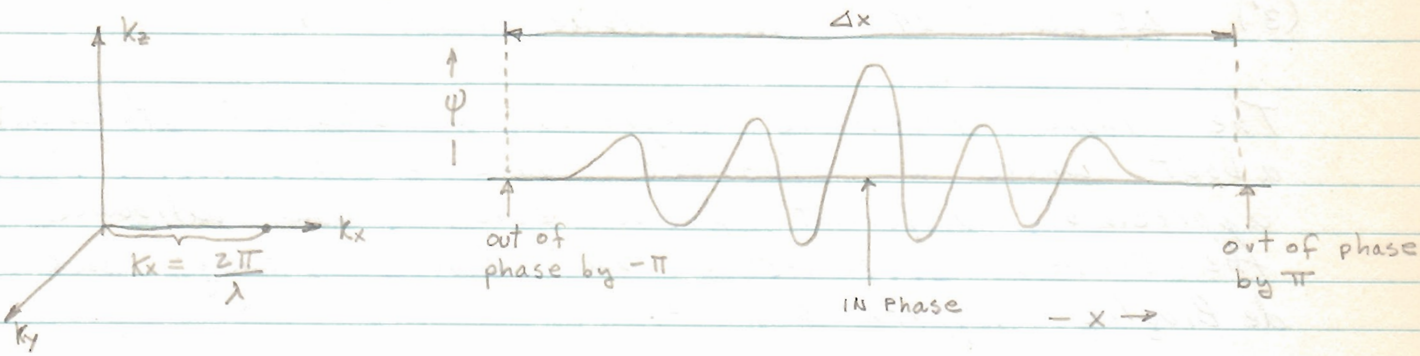
We will consider the Fourier representation of a free particle or a wave packet

(1) $\Psi(r,t) = \int A(k)\, e^{i(k\cdot r - \omega t)}\, dk$

where $A(k)$ is given by the Fourier transform

(2) $A(k) = \frac{1}{2\pi} \int \Psi(r,t)\, e^{-i(k\cdot r - \omega t)}\, dr$

for which $\omega = kc$ for the e.m. field case. We will think of $\Psi(r,t)$ as a scalar function of an e.m. field and $\Psi^2(r,t)$ as its intensity. Where Ψ is large tells us where the particle might be. Fix the z and y directions and consider motion in the x direction:



We shall limit the domain of Ψ to the interval Δx and consider it to be zero otherwise. The wave packet, as shown by equation (1), can be considered to be made up of a large number of waves with slightly different wave numbers k_x. As can be seen, outside Δx the waves interfere and the total change in phase over Δx is 2π. Now the phase factor is $k\cdot r$ in space or simply $k_x x$ for the above case. Then the spread in k_x over the interval Δx must have 2π as the result of the product of these two quantities, as its limiting value, or $\Delta x\, \Delta k_x = 2\pi$.

In reality, however, the wave packet does not vanish at the ends of the interval Δx, but in reality exists to a finite degree. Thus, there is not complete interference because the change in phase is not 2π, but is less than this value. Therefore, $\Delta x \Delta k_x \geq 2\pi$ where Δx is the whole range in which the particle may be reasonably found, and Δk_x is between two important k_x's. Thus, for each, direction in k space, at time t, we have

$$(3) \quad \begin{aligned} \Delta x \, \Delta k_x &\geq 2\pi \\ \Delta y \, \Delta k_y &\geq 2\pi \\ \Delta z \, \Delta k_z &\geq 2\pi \end{aligned}$$

The same operation can be done with the frequency and the time, viz.,

$$(3') \quad \Delta t \, \Delta \omega \geq 2\pi \quad \text{in volume element "}V\text{"}$$

The above discussion expresses a classical statement about where a classical wave field is appreciably different from zero. Now introduce the Einstein photoelectric law, Bohr frequency, and de Broglie hypothesis, viz.,

$$(4) \quad \left. \begin{aligned} h\nu &= K.E. + wk.\,fn. \\ h\nu_{nm} &= E_n - E_m \end{aligned} \right\} \text{ Deduce } \Delta E = h\,\Delta\nu = \hbar\,\Delta\omega$$

$$(5) \quad p = \frac{h}{\lambda} = \hbar k \; ; \text{ deduce } \Delta p = \hbar \Delta k$$

What suggested this to de Broglie was the four vectors of special relativity:

$$(6) \quad p_\mu = \left(\vec{p}, \frac{E}{c}\right), \text{ thus } k_\mu = \left(k, \frac{\omega}{c}\right)$$

Operating on equations (3, 3′):

(7) $\Delta x \, \Delta p_x \gtrsim h$

$\Delta y \, \Delta p_y \gtrsim h$

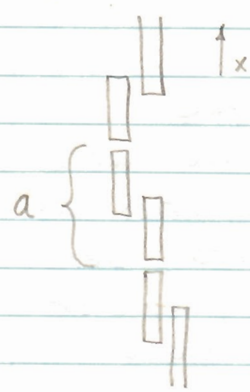
$\Delta z \, \Delta p_z \gtrsim h$

$\Delta t \, \Delta E \gtrsim h$

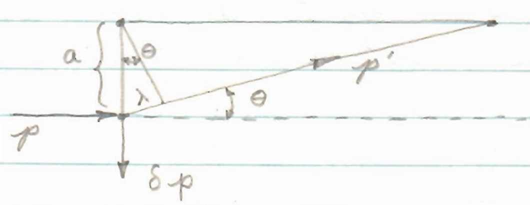
An examination of equation (2) shows that we could reverse the roles of Δx and Δk_x, etc.

The uncertainty principle applies to all bodies. If it did not, one could get a violation by considering a body for which it does not hold and use conservation laws to transmit the property between bodies.

We will now consider the mechanism W of our previous thought experiment:



When a wave changes from a plane to a circular wave, a change in momentum is produced which will react against the mechanism W.



By conservation of momentum and considering θ small:

(8) $\delta p = p\theta$ with $\theta \approx \frac{\lambda}{a}$; then $\delta p = \frac{p\lambda}{a} = \frac{h}{a}$

We require that $\Delta p < \delta p$; thus $\Delta p < \frac{h}{a}$

Upon then introducing the uncertainty condition:

(9) $\Delta x \gtrsim \frac{h}{\Delta p}$; $\Delta x > a$

Thus, if we try to measure which slit the particle went through by measuring its momentum reaction at the slit, we find an uncertainty in the position which is more than the distance between the slits, and the interference will not occur. A partially working W gives a smear at high orders where δp is large enough to make W work and gives an interference pattern in the center where δp is small.

More uncertainty discussions may be found in Bohm, pp. 91-92.

LECTURE IV 10-3-60

For background, consult a reprint by Dover publications on Einstein with article by Bohr.

As well as having a lower limit on the uncertainty of the product $\Delta p_x \Delta x$, there are also limits in some cases on the individual quantities Δx and Δp_x. For Δp_x the lower limit is zero, but for Δx the lower limit depends on whether or not the particle motion is relativistic or non-relativistic. In general:

$$(1) \quad \Delta x \gtrsim \frac{h}{mc} = \frac{h}{mv}\frac{v}{c} = \lambda \frac{v}{c} \rightarrow 0 \text{ for}$$

non-relativistic motion. For light quanta, lower limit is λ, thus we find that Non-Relativistic Quantum Mechanics (NRQM) is concerned with particles.

Non-Relativistic Wave Mechanics (NRWM):

Free Particle:

(2) $E = \frac{p^2}{2m}$, or

(3) $\hbar\omega = \frac{(\hbar k)^2}{2m}$, $\omega = \frac{\hbar}{2m} k^2$

or the frequency of the de Broglie wave is proportional to the square of the wave vector magnitude. A superposition of de Broglie waves gives the most general wave function, viz.,

(4) $\psi(r,t) = \int A(k)\, e^{i(k \cdot r - \omega t)}\, dk$

assuming that the wave functions may be added, one of the main foundations of quantum mechanics.

Apply a small change in time, Δt, and move r in the direction of k, Δr_k. $\Delta r_k = \frac{\omega}{k} \Delta t$ will eventually move back into phase.
The phase velocity would then be:

(5) $v_{ph} = \frac{\omega}{k} = \frac{\hbar}{2m} k = \frac{p}{2m} = \frac{1}{2} v_{particle}$

In special relativity:

(6) $E^2 = m^2c^4 + p^2c^2$, then,

(7) $\omega^2 = \left(\frac{mc^2}{\hbar}\right)^2 + k^2c^2$; so that $\frac{\omega^2}{k^2} = \frac{m^2c^4}{p^2} + c^2$, and

(8) $v_{ph} = \frac{\omega}{k} = \frac{E}{p}$

Now $p =$ (mass, not rest mass) $v_{particle} = \frac{E}{c^2} v_{particle}$

From this and (8)

(9) $v_{ph} = \frac{\omega}{k} = \frac{E}{p} = \frac{c^2}{v_{particle}}$

which is the result one usually sees in the de Broglie theory. Equation (9) would seem to indicate that the phase velocity is greater than that of light. However, a particular phase is not observable so no information could be transmitted faster than light. This saves us from embarrassment over the fact that $v_{ph} > c$. Only the phase difference is observable and detectable. If we expand (6) such that:

(10) $$E = mc^2 \left[1 + \frac{p^2}{(mc)^2} \right]^{1/2} \cong mc^2 + \frac{p^2}{2m} \quad \text{at small } p$$

and neglect the intrinsic energy mc^2, we see that equation (5) follows in a non-relativistic manner.

We shall build our wave function such that the result is appreciable in only one region by choosing $A(k)$ judiciously. How does this region move? We write:

(11) $A(k) = |A(k)| e^{i\epsilon(k)}$ where $\epsilon(k)$ is the phase of the particular wave coefficient $A(k)$. For one particular wave in the whole superposition of waves:

(12) $$|A(k)| e^{i[k \cdot r - \omega t + \epsilon(k)]}$$

where $k \cdot r - \omega t + \epsilon(k)$ is the particular phase of our individual wave. For motion in the x direction, we have for a stationary phase, that is, no change of phase with respect to a change in k_x; assuming that in the region of the particle, the phase is about the same for each k_x, the following:

(13) $$\frac{\partial(\text{phase})}{\partial k_x} = x - t\frac{\partial \omega}{\partial k_x} + \frac{\partial \epsilon}{\partial k_x} = 0$$

Solving for x:

(14) $$x = -\frac{\partial \epsilon}{\partial k_x} + t\frac{\partial \omega}{\partial k_x}$$

where $\frac{\partial E}{\partial k_x}$ can be thought of as x_0 and $\frac{\partial \omega}{\partial k_x}$ is defined as the group velocity. Thus we have for the velocity of motion:

(15) $(v_{group})_x = \frac{\partial \omega}{\partial k_x} = \frac{\partial E}{\partial p_x} = (v_{particle})_x$ as seen from the classical equation, $\dot{x} = \frac{\partial E}{\partial p_x}$

For the group velocity in general:

(16) $\frac{\partial \omega}{\partial k_x} = \frac{\partial \omega}{\partial k}\frac{\partial k}{\partial k_x} = \frac{\partial \omega}{\partial k}\frac{k}{k_x}$ where $\frac{k}{k_x}$ is the direction cosine of the group velocity. Thus $\frac{\partial \omega}{\partial k} = \frac{p}{m}$

Under Relativistic conditions:

(17) $2E\,dE = c^2 \cdot 2p\,dp$; $\frac{d\omega}{dk_x} = \frac{dE}{dp} = \frac{p}{E/c^2} = \frac{p}{(mass)}$

Now, for the general case of quantum-mechanical particles, we will choose the following form of the wave coefficients:

(18) $A(k) = \varphi(p,t)\, e^{i\omega t} \left(\frac{\hbar}{2\pi}\right)^{3/2}$ and $dk_x = \frac{dp_x}{\hbar}$, etc.

The exponential term will remove the time dependency of of the phase factor of the wave and $\frac{\hbar}{2\pi}$ is chosen with "foresight." Substituting in (4):

(19) $\psi(r,t) = h^{-3/2} \int \varphi(p,t)\, e^{i\frac{p}{\hbar}\cdot r}\, dp$; $dp = dp_x\, dp_y\, dp_z$

Using the Fourier Transforms, viz.,

(20) $f(x) = \frac{1}{\sqrt{2\pi}} \int e^{ikx} g(k)\, dk$

$g(k) = \frac{1}{\sqrt{2\pi}} \int e^{-ikx} f(x)\, dx$

Transforming (19):

(21) $\varphi(p,t) = h^{-3/2} \int \psi(r,t)\, e^{-i \frac{p}{\hbar} \cdot r}\, dr$

In this system the momentum and position have no lower limit independent of each other.

We now consider the probability of finding the particle. It would seem reasonable to assume that distribution of the position of the particle would take the shape of the intensity of the particle wave:

(22) $W(r)\,dr = |\psi(r,t)|^2\, dr$ thus is the probability

of finding the wave in dr. A corresponding distribution should be:

(23) $\mathcal{W}(p)\,dp = |\varphi(p,t)|^2\, dp$

Impose conditions of normality, viz.,

(24) $\int |\psi|^2 dr = 1$
(25) $\int |\varphi|^2 dp = 1$

These conditions must occur together because $\psi = \psi(\varphi)$ as seen from equation (19). Also, $\varphi = \varphi(\psi)$ from equation (21). We must also check that they are independent of time. Thus, using (20)*:

(26) $\int |\psi|^2 dr = h^{+3/2} \iint \varphi^*(p,t)\, \psi(r,t)\, e^{-i p \cdot r/\hbar}\, dp\, dr$

using (22):

(27) $\int |\varphi|^2 dp = h^{-3/2} \iint \varphi^*(p,t)\, \psi(r,t)\, e^{-i p \cdot r/\hbar}\, dr\, dp$

These are equal with the exception of the constants which may be accounted for in the normalization constant. Thus $\int |\psi|^2 dr = \int |\varphi|^2 dp$.

Check for constancy with time:
It is clear that for a free particle, $\int |\varphi|^2 dp$ is independent of time.
We will take general ψ for a free particle and see that it satisfies the Schroedinger equation.

$$(28) \quad i\hbar \frac{\partial \psi}{\partial t} = \frac{-\hbar^2}{2m} \nabla^2 \psi$$ and next time

will check that $\frac{d}{dt} \int |\psi|^2 dr = 0$

LECTURE V 10-5-60

One of the important facts of Wave Mechanics is the introduction of waves in both co-ordinate space and momentum space.

$$(1) \quad \psi(r,t) = h^{-3/2} \int e^{ip\cdot r/\hbar} \varphi(p,t)\, dp$$

$$(2) \quad \varphi(p,t) = h^{-3/2} \int e^{-ip\cdot r/\hbar} \psi(r,t)\, dr \text{ , with}$$

$$(3) \quad \int |\psi|^2 dr = \int |\varphi|^2 dp$$

The relation (3) is also constant in time. We know for the free particle:

$$(4) \quad \varphi(p,t) = c\, A(k)\, e^{-i\omega t}, \text{ with } \omega = \frac{\hbar k^2}{2m} = \frac{p^2}{2m\hbar}$$

This is one way to construct the waves. However, usually one wants to work with ψ. ψ must satisfy the Schoedinger equation for the free particle.

$$(5) \quad i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi$$

If one tried to construct a solution to the Schroedinger equation, one would get (1) constructed out of de Broglie waves. We now write (5)*.

$$(5)^* \quad -i\hbar \frac{\partial \psi^*}{\partial t} = \frac{-\hbar^2}{2m} \nabla^2 \psi^*$$

Now form $\psi^* (5) - (5)^* \psi$ and get:

$$(6) \quad i\hbar \frac{\partial}{\partial t} \psi^* \psi = -\frac{\hbar^2}{2m} \left[\psi^* \nabla^2 \psi - (\nabla^2 \psi^*) \psi \right]$$

Integrate over all space:

$$(7) \quad i\hbar \frac{d}{dt} \int |\psi|^2 dr = -\frac{\hbar^2}{2m} \int \left[\psi^* \nabla^2 \psi - (\nabla^2 \psi^*) \psi \right] dr$$

Use Green's Theorem on right side

$$(8) \quad i\hbar \frac{d}{dt} \int |\psi|^2 dr = \frac{-\hbar^2}{2m} \int_{\text{surface}} \left(\psi^* \frac{d\psi}{dn} - \frac{d\psi^*}{dn} \psi \right) ds$$

Assume that wave functions vanish at large distances. This is motivated by fact that particles are somewhere in the universe. Then let the boundaries of the surface in (8) go to infinity. Thus the integral over this surface of vanishing wave functions also vanishes. Therefore,

$$(9) \quad \frac{d}{dt} \int_{\substack{\text{all} \\ \text{space}}} |\psi|^2 dr = 0$$ and is thus independent of time.

Consider average values. Define:

$$(10) \quad \overline{F(r)} = \int F(r)\, W(r)\, dr = \int \psi^*(r,t)\, F(r)\, \psi(r,t)\, dr$$

$$(11) \quad \overline{\mathcal{F}(p)} = \int \mathcal{F}(p)\, \mathcal{W}(p)\, dp = \int \varphi^*(p,t)\, \mathcal{F}(p)\, \varphi(p,t)\, dp$$

Now, given ψ, how does one find $\overline{F(p)}$? We will assume $F(p)$ is expandable in a power series. Then the problem is finding $\overline{p_x^n}$.

$$(12) \quad \overline{p_x^n} = \int \varphi^*(p)\, p_x^n\, \varphi(p)\, dp \qquad (\text{use } \varphi = \varphi\{\psi\})$$

$$= \int \varphi^*(p)\, dp \cdot h^{-3/2} \int p_x^n\, e^{-i p \cdot r/\hbar}\, \psi(r)\, dr$$

$$= h^{-3/2} \int \varphi^*(p)\, dp \int \left\{ \left(-\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^n e^{-ip\cdot r/\hbar} \right\} \psi(r)\, dr$$

Integrate by parts n times:

$$(13) \quad \therefore \overline{p_x^n} = \underbrace{h^{-3/2} \int \varphi^*(p)\, dp \int e^{-i p\cdot r/\hbar}}_{\psi^*(r)} \left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^n \psi(r)\, dr$$

$$= \int \psi^*(r,t) \left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^n \psi(r,t)\, dr$$

In general:

$$(14) \quad \overline{p_x^l\, p_y^m\, p_z^n} = \int \psi^* \left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^l \left(\frac{\hbar}{i}\frac{\partial}{\partial y}\right)^m \left(\frac{\hbar}{i}\frac{\partial}{\partial z}\right)^n \psi\, dr$$

$$(15) \quad \overline{F(p)} = \int \psi^*\, F\left(\frac{\hbar}{i}\nabla\right) \psi\, dr$$

In Wave Mechanics, the pure state of a system is represented by a wave function and the dynamical variable is represented by an operator. In the coordinate representation, the wave function is ψ and the dynamical variable x is represented by multiplying by x. The operator p_x is represented by $\frac{\hbar}{i}\frac{\partial}{\partial x}$, or

$$(16) \quad p \rightarrow \frac{\hbar}{i}\nabla$$

The Schroedinger rule played big role in proving equivalence between Matrix Mechanics and Wave Mechanics. If one is working in momentum space with the wave function φ, interchange r and p, ψ and φ, and i to $-i$. Then the dynamical operators are:

(17)

$$p_x \rightarrow p_x \cdot \qquad x \rightarrow -\frac{\hbar}{i}\frac{\partial}{\partial p_x}$$

$$p_y \rightarrow p_y \cdot \qquad y \rightarrow -\frac{\hbar}{i}\frac{\partial}{\partial p_y}$$

$$p_z \rightarrow p_z \cdot \qquad z \rightarrow -\frac{\hbar}{i}\frac{\partial}{\partial p_z}$$

It is more common to use coordinate space. The reason is that most functions of p are expressible in power series. Many functions of r may not be (for example, $1/r$). However, this does not mean that the problem cannot be solved in momentum space.

A generalization of average value is the concept of matrix representation. However, this time we use separate states. Define the operator $\underline{A}$:

(18) $A_{ba} = \int \psi_b^* \, \underline{A} \, \psi_a \, dr$, also:

(18)′ $A_{ba} = \int \varphi_b^* \, \underline{A} \, \varphi_a \, dp$

where the A_{ba} can be taken as matrix elements. There is significance in this matrix diagonal.

$$\begin{bmatrix} A_{aa} & A_{ab} & A_{ac} & \cdots \\ A_{ba} & A_{bb} & A_{bc} & \cdots \\ \vdots & \vdots & \vdots & \end{bmatrix}$$

The matrix diagonals are the expectation values for their respective states. The main difference between Matrix Mechanics and Mathematical Matrices is that the matrices in Quantum Mechanics are infinite and elements have physical meanings.

LECTURE VI   10-7-60

Recapitulation:

(1) $\bar{x} = \int \psi^* x \psi \, d\tau$, $\bar{p}_x = \int \psi^* \left(\frac{\hbar}{i} \frac{d}{dx} \right) \psi \, d\tau$

It is important now that the order of ψ^* and ψ be preserved. Also, matrix elements are:

(2) $A_{ab} = \int \psi_a^* \underline{A} \, \psi_b \, d\tau$

Asking why there is order in the ψ's brings us to the definition of Hermitian operators.

Hermitian Operators:

(3) $A_{ab} = \int \psi_a^* \underline{A} \, \psi_b \, d\tau \equiv \int (\underline{A} \, \psi_a)^* \psi_b \, d\tau$

This will lead to:

(4) $$\|A\| = \begin{pmatrix} A_{11} & A_{12} & A_{13} & \cdots \\ A_{21} & A_{22} & A_{23} & \cdots \\ \vdots & \vdots & \vdots & \end{pmatrix}$$

Now:

(5) $A_{ba} = \int \psi_b^* \underline{A} \, \psi_a \, d\tau$, $(A_{ba})^* = \int \psi_b \, (\underline{A} \, \psi_a)^* \, d\tau$

Therefore, a Hermitian operator gives a Hermitian matrix, viz.,

(6) $A_{ab} = (A_{ba})^*$

This also means that the diagonals must be real.

Unitary Operators:

(7) $\int (U\psi_a)^* U \psi_b \, dr \equiv \int \psi_a^* \psi_b \, dr$

Definition of the Adjoint of an Operator: A^+ means the adjoint of $\underline{A}$:

(8) $\int \psi_a^* \underline{A} \psi_b \, dr = \int (\underline{A}^+ \psi_a)^* \psi_b \, dr$

For Hermitian operators: $\underline{A}^+ = \underline{A}$ or a Hermitian operator is a self-adjoint operator.

For Unitary Operators:

(9) $\int (U^+ U \psi_a)^* \psi_b \, dr \equiv \int \psi_a^* \psi_b \, dr$

(10) $\underline{U}^+ \underline{U} = \underline{1}$ or $\underline{U}^+ = \underline{U}^{-1}$

The same relations hold in momentum space.

The official definition of Hermitian and Adjoint operators:

(11) Hermitian: $(\underline{A} \psi_a)^* \psi_b - \psi_a^* \underline{A} \psi_b$ = divergence

(12) Adjoint: $(\underline{A}^+ \psi_a)^* \psi_b - \psi_a^* \underline{A} \psi_b$ = divergence

This divergence, when integrated, gives boundary terms which in our case may be dropped because $\psi = 0$ at $r = \infty$. However, one must sometimes be careful of singularities in the potential functions.

However, there is one operator we must insist is always Hermitian and that is the Hamiltonian. This operator occurs in Schroedinger's Equation:

(13) $i \hbar \frac{\partial \psi}{\partial t} = \underline{H} \psi$

For the free particle:

(14) $\underline{H} = -\frac{\hbar^2}{2m}\nabla^2 = \frac{p^2}{2m}$

We may show that it is indeed Hermitian with the following:

(15) $(\underline{H}\,\psi_a)^* \psi_b - \psi_a^* \underline{H}\,\psi_b = \frac{-\hbar^2}{2m}\left[(\nabla^2\psi_a)^*\psi_b - \psi_a^*\nabla^2\psi_b\right]$

$(\nabla^2\psi_a)^* = \nabla^2\psi_a^*$, because ∇^2 is real

$= \nabla\cdot\left[\frac{-\hbar^2}{2m}\left\{(\nabla\psi_a^*)\psi_b - \psi_a^*\nabla\psi_b\right\}\right]$

⇓ Green's Second Theorem, when integrated over boundary vanishes. Therefore, $\bar{H}$ is Hermitian.

This result, and the others using Green's Theorem, indicate that when the integrands represented in (15) are integrated over all space, their difference vanishes and they are thus equal.

It should be that the operator $\underline{x}$ is Hermitian. That is,

(16) $(\underline{x}\,\psi_a)^*\psi_b - \psi_a^*\underline{x}\,\psi_b = x^*\psi_a^*\psi_b - \psi_a^* x\,\psi_b = 0$

since x is real.

For the momentum operator:

(17) $(\underline{p_x}\cdot\psi_a)^*\psi_b - \psi_a^*\underline{p_x}\cdot\psi_b = \left(\frac{\hbar}{i}\frac{\partial\psi_a}{\partial x}\right)^*\psi_b - \psi_a^*\frac{\hbar}{i}\frac{\partial}{\partial x}\psi_b$

$= -\frac{\hbar}{i}\left[\left(\frac{\partial}{\partial x}\psi_a^*\right)\psi_b + \psi_a^*\frac{\partial}{\partial x}\psi_b\right]$

$= \frac{\partial}{\partial x}\left[-\frac{\hbar}{i}\psi_a^*\psi_b\right]$

Algebra of Wave Functions and Operators:

If ψ_1, ψ_2 are admissible, then $c_1\psi_1 + c_2\psi_2$ is acceptable. This is the rule of superposition.

The operators are linear operators, that is:

(18) $\underline{A}\,(c_1\psi_1 + c_2\psi_2) = c_1\underline{A}\,\psi_1 + c_2\underline{A}\,\psi_2$

(19) $(\underline{A} + \underline{B})\,\psi = \underline{A}\,\psi + \underline{B}\,\psi$

(20) $(c\underline{A})\,\psi = c\,\underline{A}\,\psi$

c may be +, −, or complex, but if complex, then $(c\underline{A})$ is a non-Hermitian operator.

(21) $(\underline{A}\,\underline{B})\,\psi = \underline{A}\,(\underline{B}\,\psi)$

(22) $\left.\begin{aligned} \underline{A}\,(\underline{B}+\underline{C}) &= \underline{A}\,\underline{B} + \underline{A}\,\underline{C} \\ (\underline{B}+\underline{C})\,\underline{A} &= \underline{B}\,\underline{A} + \underline{C}\,\underline{A} \end{aligned}\right\}$ Distributive Law

(23) $\underline{A}\,(\underline{B}\,\underline{C}) = (\underline{A}\,\underline{B})\,\underline{C} = \underline{A}\,\underline{B}\,\underline{C}$ Associative Law

Concerning the commutative law; in general:

(24) $\underline{A}\,\underline{B} \neq \underline{B}\,\underline{A}$

Commutating Operators are defined by:

(25) $\underline{A}\,\underline{B} = \underline{B}\,\underline{A}$, examples: (x, y) or (p_x, p_y)

For (x, p_x), however

(26) $x\,p_x\,\psi = x\,\frac{\hbar}{i}\frac{\partial\psi}{\partial x}$; $p_x\,x\,\psi = \frac{\hbar}{i}\frac{\partial}{\partial x}\,x\,\psi$

$= \frac{\hbar}{i}\left(x\frac{\partial\psi}{\partial x} + \psi\right)$

(27) $p_x\,x\,\psi - x\,p_x\,\psi = \frac{\hbar}{i}\,\psi$

LECTURE VII 10-10-60

More on Operators:

(1) $\underline{A}\,\underline{B} \neq \underline{B}\,\underline{A}$, in general

Introduce the commutator bracket notation, viz.,

(2) $[\underline{A}, \underline{B}] = \underline{A}\,\underline{B} - \underline{B}\,\underline{A}$

Pauli's Notation: $[\underline{A}, \underline{B}] = i(\underline{A}\,\underline{B} - \underline{B}\,\underline{A})$
Dirac's Notation: $i\hbar[\underline{A}, \underline{B}] = \underline{A}\,\underline{B} - \underline{B}\,\underline{A}$

Now:

(3) $\underline{p_x}\,\underline{x}\,\psi = \frac{\hbar}{i} x \frac{\partial \psi}{\partial x} + \frac{\hbar}{i}\psi$

$\underline{x}\,\underline{p_x}\,\psi = \frac{\hbar}{i} x \frac{\partial \psi}{\partial x}$

(4) Thus $[\underline{x}, \underline{p_x}] = i\hbar$

In general:

(5) $[\underline{x_j}, \underline{x_k}] = 0$; $[\underline{p_j}, \underline{p_k}] = 0$; $[\underline{x_j}, \underline{p_k}] = i\hbar\,\delta_{jk}$

Let us investigate what other physical quantities can be formed in Quantum Mechanics. It is necessary that the product of two Hermitians be a Hermitian if they commute. When:

(6) $\int \psi_1^* \underline{A}\,\underline{B}\,\psi_2\,d\tau = \int (\underline{B}^\dagger \underline{A}^\dagger \psi_1)^* \psi_2\,d\tau$

then: $(\underline{A}\,\underline{B})^\dagger = \underline{B}^\dagger \underline{A}^\dagger$

If: $\underline{A} = \underline{A}^\dagger$, $\underline{B} = \underline{B}^\dagger$; $(\underline{A}\,\underline{B})^\dagger = \underline{B}\,\underline{A}$

If one encounters two classical quantities whose operators do not commute, we may form the <u>symmeterized product.</u>

(7) $\frac{1}{2}\{\underline{A},\underline{B}\} = \frac{1}{2}(\underline{A}\underline{B} + \underline{B}\underline{A})$

the brackets $\{\ \}$ are known as the anti-commutator brackets. This would be an ordinary product if $\underline{A}, \underline{B}$ were to commute.
If $\underline{A}$ and $\underline{B}$ are Hermitian:

(8) $[\underline{A},\underline{B}]^{+} = (\underline{A}\underline{B} - \underline{B}\underline{A})^{+} = (\underline{B}\underline{A} - \underline{A}\underline{B}) = -[\underline{A},\underline{B}]$

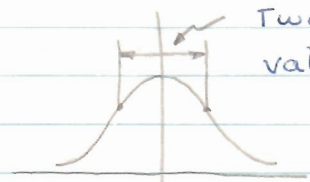
sometimes called anti-Hermitian.

Derivation of the General Uncertainty Principle:

We must specify:

(9) Average or Expectation: $\overline{\underline{A}}$
Mean squared deviation, Variance: $\overline{(\underline{A} - \overline{\underline{A}})^2} = \overline{(\Delta A)^2}$
Standard Deviation: $\left[\overline{(\Delta A)^2}\right]^{1/2}$

Before we had: $\Delta x \, \Delta p_x \gtrsim h$
Now we are going to get: $\left[\overline{(\Delta x)^2}\right]^{1/2}\left[\overline{(\Delta p)^2}\right]^{1/2}$ which may lead to a smaller uncertainty than before.



Two important values of k.

Given two Hermitian operators, $\underline{A}, \underline{B}$, we define:

(10) $\underline{\alpha} = \underline{A} - \overline{\underline{A}}$; $\underline{\beta} = \underline{B} - \overline{\underline{B}}$; $\overline{(\Delta A)^2} = \overline{\underline{\alpha}^2} = \int \psi^* \underline{\alpha}^2 \psi \, d\tau$

$= \int (\underline{\alpha}\psi)^* \underline{\alpha} \psi \, d\tau = \int |\underline{\alpha}\psi|^2 \, d\tau$

Consider an integral assumed to be positive:

(11) $\int |f - \xi e^{i\gamma} g|^2 \, d\tau \geq 0$

where ξ is real and $|f - \xi e^{i\gamma} g|^2 = (f^* - \xi e^{-i\gamma} g^*)(f - \xi e^{i\gamma} g)$

Then:

$$(12) \quad \int |f|^2 d\tau - 2\xi \, Re\left\{ e^{i\gamma} \int f^* g \, d\tau \right\} + \xi^2 \int |g|^2 d\tau \geq 0$$

Thus we have a quadratic in ξ, with the condition that, since ξ is real:

$$(13) \quad \int |f|^2 d\tau \cdot \int |g|^2 d\tau - \left[Re\left\{ e^{i\gamma} \int f^* g \, d\tau \right\} \right]^2 \geq 0$$

In Schwartz' Inequality, we pick γ to give 0 phase factor, i.e., make { } real and get:

$$(14) \quad \int |f|^2 d\tau \cdot \int |g|^2 d\tau \geq \left[\left| \int f^* g \, d\tau \right| \right]^2$$

which means: $|\vec{A}|^2 \cdot |\vec{B}|^2 \geq |\vec{A} \cdot \vec{B}|^2$ or $1 \geq \cos^2(\vec{A}, \vec{B})$

Returning to Variance:

$$(15) \quad \overline{(A - \overline{A})^2} = \overline{A^2} - \overline{A}^2$$

$$(16) \quad \int |f|^2 d\tau \cdot \int |g|^2 d\tau \geq \left[\cos\gamma \cdot \frac{1}{2} \int (f^* g + f g^*) \, d\tau \right.$$

$$\left. + i \sin\gamma \cdot \frac{1}{2} \int (f^* g - g^* f) \, d\tau \right]^2$$

Take $f = \alpha \psi$; $g = \beta \psi$

If $\gamma = 0$:

$$(17) \quad \left\{ \frac{1}{2} \int \left[(\alpha\psi)^* \beta\psi + (\beta\psi)^* \alpha\psi \right] d\tau \right\}^2 = \left\{ \frac{\overline{\alpha\beta + \beta\alpha}}{2} \right\}^2$$

which is a symmeterized product.

For $\gamma = \pi/2$:

(18) $$\left[\frac{i}{2}\int\left\{(\alpha\psi)^*\,\underline{\beta}\,\psi - (\beta\psi)^*\,\underline{\alpha}\,\psi\right\}d\tau\right]^2 = \left[\frac{i\,\overline{(\underline{\alpha}\,\underline{\beta} - \underline{\beta}\,\underline{\alpha})}}{2}\right]^2$$

Then ; $$\overline{(\Delta A)^2}\cdot\overline{(\Delta B)^2} \geq \left\{\frac{i\,\overline{[\underline{A},\underline{B}]}}{2}\right\}^2$$

Final Result;

(19) $$\sqrt{\overline{(\Delta A)^2}}\cdot\sqrt{\overline{(\Delta B)^2}} \geq \frac{\left|\,\overline{[A,B]}\,\right|}{2}$$

(20) $$\sqrt{\overline{(\Delta x)^2}}\cdot\sqrt{\overline{(\Delta P_x)^2}} \gtrsim \frac{\hbar}{2}$$

LECTURE VIII 10-14-60

More on General Uncertainty Principle (See Bohm):

(1) $$\int|f|^2 d\tau\cdot\int|g|^2 d\tau \geq \left|\int f^* g\, d\tau\right|^2$$

with $f = \underline{\alpha}\,\psi$, $g = \underline{\beta}\,\psi$;

(2) $$\overline{\alpha^2}\cdot\overline{\beta^2} \geq |\overline{\alpha\beta}|^2$$

Now :

(3) $$\alpha\beta = \tfrac{1}{2}(\alpha\beta + \beta\alpha) + \tfrac{1}{2}(\alpha\beta - \beta\alpha)$$, then:

(4) $$\overline{\alpha^2}\cdot\overline{\beta^2} \geq \left|\,\tfrac{1}{2}\overline{\{\alpha,\beta\}} + \tfrac{1}{2}\overline{[\alpha,\beta]}\,\right|^2$$

Bohm comments that since α and β are Hermitian, the anti-commutator is real, but the commutator is imaginary. Thus, we must take the magnitude of the right hand side of (4).

(5) $\overline{\alpha^2} \cdot \overline{\beta^2} \geq \left(\overline{\frac{\alpha\beta + \beta\alpha}{2}}\right)^2 + \left(\overline{\frac{\alpha\beta - \beta\alpha}{2}}\right)^2$

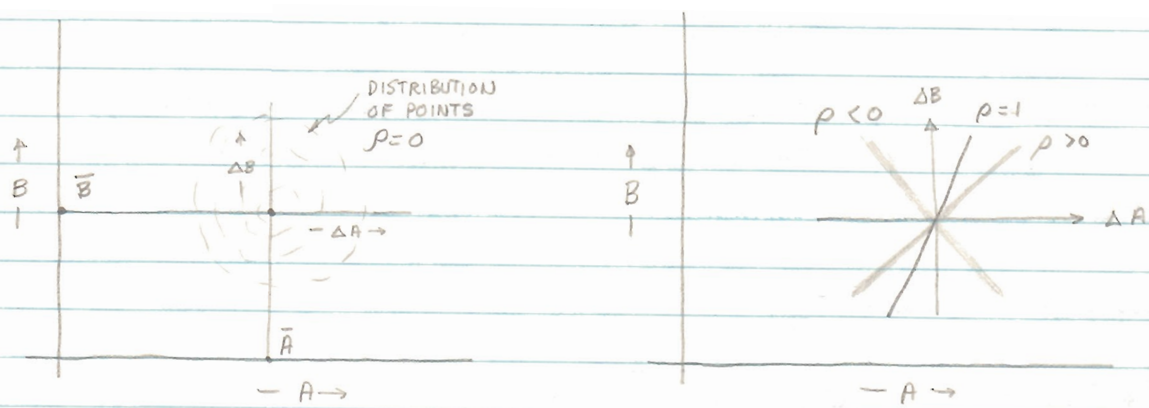
Classically $\overline{\alpha^2} \cdot \overline{\beta^2} \geq |\overline{\alpha\beta}|^2$ means that the correlation factor is less than one.

Finally,

(6) $\overline{(\Delta A)^2} \cdot \overline{(\Delta B)^2} \geq \left(\overline{\frac{\Delta A \cdot \Delta B + \Delta B \cdot \Delta A}{2}}\right)^2 + \frac{1}{4}\left[A, B\right]^2$

from $\Delta A = A - \overline{A}$.

Plot a Classical Distribution: ρ = correlation factor



However, we can always choose a state to make $\rho = 0$. However, in Quantum Mechanics, we have $1/4\,[A, B]^2$ left over. Therefore, at the very least:

(7) $\sqrt{\overline{(\Delta A)^2}}\sqrt{\overline{(\Delta B)^2}} \geq \frac{1}{2}\left|\,[A, B]\,\right|$

In particular:

(8) $\sqrt{\overline{(\Delta x)^2}}\sqrt{\overline{(\Delta p_x)^2}} \geq 1/2\,\hbar$

This is not the same as the heuristic derivation result because standard deviations are used.

We will now attack the question as to what is the form of the optimum wave packet that satisfy the equal sign in the uncertainty principle. Let $\bar{x}$ and $\bar{p}_x$ be zero. Take:

(9) $\int |f - \xi e^{i\gamma} g|^2 \, dr \geq 0$

The discriminant will vanish (see equation (1)) by choosing properly $f \propto g$ and the Schwartz Inequality will have the equal sign. Thus choose arbitrarily:

(10) $x\psi = C p_x \psi = C \frac{\hbar}{i} \frac{\partial \psi}{\partial x} = K \frac{d\psi}{dx}$, ∴

(11) $\psi = c' e^{\frac{x^2}{2K}}$, take $\frac{1}{2K}$ to be real and negative, then $\frac{1}{2K} = -\kappa^2$ and

(12) $\psi = c' e^{-\kappa^2 x^2}$

We demand normality:

(13) $\int |\psi|^2 dx = 1$: $|c'|^2 \int_{-\infty}^{\infty} e^{-2\kappa^2 x^2} dx = 1$

Now: $\Gamma(q) = \int_0^{\infty} e^{x} x^{q-1} dx$

$q\Gamma(q) = \Gamma(q+1)$; $\Gamma(1/2) = \sqrt{\pi}$

Let $y = 2\kappa^2 x^2$, then $2|c'|^2 \int_0^{\infty} e^{-y} \frac{dy}{2\kappa\sqrt{2y}} = 1$

and find $|c'|^2 \cdot \frac{1}{\kappa\sqrt{2}} \cdot \sqrt{\pi} = 1$

(14) ∴ $\psi = \frac{\kappa^{1/2} 2^{1/4}}{\pi^{1/4}} e^{-\kappa^2 x^2}$

thus $\bar{x} = 0$ and $\bar{p}_x = 0$

Now:

(15) $\overline{(\Delta x)^2} = \overline{x^2} = \kappa \sqrt{\frac{2}{\pi}} \int_{-\infty}^{\infty} x^2 e^{-2\kappa^2 x^2} dx \quad \left(\propto \int_0^{\infty} y^{1/2} e^{-y} dy \right)$

$= \frac{1}{4\kappa^2}$

Then finally:

(16) $$\psi = \frac{1}{(2\pi \overline{x^2})^{1/4}} e^{-x^2/4\overline{x^2}}$$

which is the square root of the Gaussian distribution. Let us now calculate $\overline{p_x^2}$.

(17) $$\overline{p_x^2} = \int_{-\infty}^{\infty} \psi^* p_x^2 \psi \, dx$$

$$p_x^2 \psi = -\hbar^2 \frac{d^2\psi}{dx^2} = -\hbar^2 \frac{d}{dx} \frac{1}{(2\pi \overline{x^2})^{1/4}} \left(-\frac{x}{2\overline{x^2}}\right) e^{-x^2/4\overline{x^2}}$$

$$= \hbar^2 \left(\frac{1}{2\overline{x^2}} - \frac{x^2}{4\overline{x^2}}\right) e^{-x^2/4\overline{x^2}} \frac{1}{(2\pi \overline{x^2})^{1/4}} \text{ ; then}$$

(18) $$\overline{p_x^2} = \hbar^2 \left(\frac{1}{2\overline{x^2}} - \frac{1}{4\overline{x^2}}\right) = \frac{\hbar^2}{4\overline{x^2}} \text{ ; thus}$$

(19) $$\overline{(\Delta x)^2}\ \overline{(\Delta p_x)^2} = \overline{x^2}\ \overline{p_x^2} = \frac{\hbar^2}{4}$$ and we have the ideal wave packet.

Let us examine the correlation factor which should indeed vanish.

(20) $$x p_x + p_x x = 2 x p_x + \frac{\hbar}{i} = 2x p_x + [p_x, x]$$

$$2x p_x \frac{e^{-x^2/4\overline{x^2}}}{(2\pi \overline{x^2})^{1/4}} = 2x \frac{\hbar}{i} \frac{\partial}{\partial x} \frac{e^{-x^2/4\overline{x^2}}}{(2\pi \overline{x^2})^{1/4}} = -\frac{4x^2}{4\overline{x^2}} \frac{\hbar}{i} \frac{e^{-x^2/4\overline{x^2}}}{(2\pi \overline{x^2})^{1/4}}$$

Now $\overline{2x p_x} = -\frac{\hbar}{i}$, and we get $\rho = 0$

Time Derivatives of Operators:

In classical mechanics, the time derivative of a function is the value of the function at two ends of a vanishingly small time interval divided by this time interval. In quantum mechanics we may not use this limiting method because the first measurement will destroy the validity of the second measurement. A first precise measurement of x will destroy the accuracy of p_x, hence v_x, the very quantity trying to be measured.

In Quantum Mechanics, we can prepare a great many specimens in a system and measure state at time t after the preparation. Prepare another system and measure at $t + \Delta t$. Do this many times and divide the average of the difference between the states at the two different times by Δt. In the mathematical limit, we have the definition:

$$(21) \quad \overline{\frac{dA}{dt}} = \frac{d}{dt}\overline{A}$$

LECTURE IX 10-17-60

Time Derivatives of Operators:

Given A, we define $\frac{dA}{dt}$ such that:

$$(1) \quad \overline{\left(\frac{dA}{dt}\right)} = \frac{d\overline{A}}{dt}$$

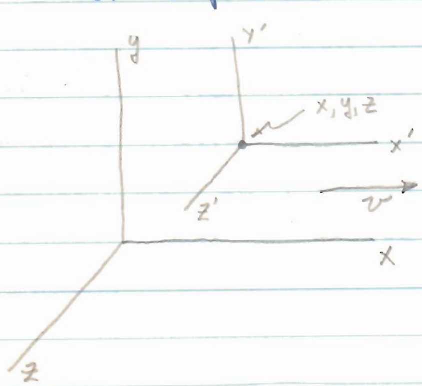
Now:

$$(2) \quad \frac{d}{dt}\overline{A} = \frac{d}{dt}\int \psi^* A \psi \, d\tau = \int \psi^* \frac{\partial A}{\partial t}\psi \, d\tau$$

$$+ \int \frac{\partial \psi^*}{\partial t} A \psi \, d\tau + \int \psi^* A \frac{\partial \psi}{\partial t} \, d\tau$$

since the limits on the integrals are independent of time.

The operators may depend explicitly on time, for example:



Now, $x' = x - v_x t$ and involves time.

However, it is very common to find $\frac{\partial A}{\partial t} = 0$.

Using the Schroedinger Equation;

(3) $$i\hbar \frac{\partial \psi}{\partial t} = \underline{H}\,\psi \quad , \quad -i\hbar \frac{\partial \psi^*}{\partial t} = (\underline{H}\,\psi)^*$$

we have:

(4) $$\frac{d}{dt}\overline{A} = \int \left\{ \psi^* \frac{\partial \underline{A}}{\partial t} \psi + \frac{i}{\hbar} (\underline{H}\psi)^* \underline{A}\, \psi - \frac{i}{\hbar}\psi^* \underline{A}\, \underline{H}\, \psi \right\} dr$$

$$= \int \left\{ \psi^* \frac{\partial \underline{A}}{\partial t} \psi + \frac{i}{\hbar} \psi^* [\underline{H}, \underline{A}]\, \psi \right\} dr$$

since $\underline{H}$ is a Hermitian operator. Finally,

(5) $$\frac{d\overline{A}}{dt} = \overline{\frac{\partial A}{\partial t} + \frac{i}{\hbar}[\underline{H}, \underline{A}]}$$

(6) $$\frac{d\underline{A}}{dt} = \frac{\partial \underline{A}}{\partial t} + \frac{i}{\hbar}[\underline{H}, \underline{A}]$$

We have made no distinction between the states on ψ so (6) is good for any matrix element. In the general case of no explicit time dependence of A on time:

(7) $$\frac{d\underline{A}}{dt} = \frac{i}{\hbar}[\underline{H}, \underline{A}]$$

We show that time differentiation of a product is similar to commutation of three operators:

(8) $$\frac{d}{dt}\underline{A}\,\underline{B} = \frac{d\underline{A}}{dt}\underline{B} + \underline{A}\frac{d\underline{B}}{dt}$$

(9) $$[\underline{A}, \underline{B}\,\underline{C}] = [\underline{A}, \underline{B}]\underline{C} + \underline{B}[\underline{A}, \underline{C}]$$

(10) $$[\underline{B}\,\underline{C}, \underline{A}] = [\underline{B}, \underline{A}]\underline{C} + \underline{B}[\underline{C}, \underline{A}]$$

Consider:

(11) $[f(r), p_x]\psi = f p_x \psi - p_x (f\psi)$

$= f p_x \psi - p_x f \psi - f p_x \psi$

$= - p_x f \psi$

Therefore,

(12) $[f(r), p_x] = -\frac{\hbar}{i}\frac{\partial f}{\partial x}$, and

(13) $[x, F(p)] = -\frac{\hbar}{i}\frac{\partial F}{\partial p_x}$

We can show:

(14) $[x, p_x^n] = -\frac{\hbar}{i} n p_x^{n-1}$; $n \geq 1$

by the commutation rules (9) and (10), viz.

(15) $[x, p_x^n] = [x, p_x p_x^{n-1}] = [x, p_x] p_x^{n-1} + p_x [x, p_x p_x^{n-2}]$

$= [x, p_x] p_x^{n-1} + p_x [x, p_x] p_x^{n-2} + \ldots + p_x^{n-1} [x, p_x]$

$= \sum_{k=1}^{n} p_x^{k-1} [x, p_x] p_x^{n-k} = i\hbar n p_x^{n-1}$

This demonstrates that this rule holds regardless of the representation space.

Results Applied to the Free Particle:

(16) $\dot{x} = \frac{i}{\hbar}[H, x] = \frac{i}{\hbar \cdot 2m}[p_x^2, x] = \frac{p_x}{m}$

then $\dot{\bar{x}} = \bar{\dot{x}} = \frac{1}{m}\bar{p}_x$

We see that the velocity of the centroid of the particle is equal to the average momentum over mass or just what one would expect classically.

Also, $\dot{p}_x = 0$ for a free particle, therefore:

(17) $\overline{\dot{p}_x} = 0$

That is, the acceleration is zero.

Calculate: $\frac{d}{dt}\overline{(x - \bar{x})^2} = \overline{(\dot{x} - \dot{\bar{x}})(x-\bar{x})} + \overline{(x-\bar{x})(\dot{x} - \dot{\bar{x}})}$

$= \frac{1}{m}\overline{(p_x - \bar{p}_x)(x-\bar{x})} + \frac{1}{m}\overline{(x-\bar{x})(p_x - \bar{p}_x)}$

$\frac{d^2}{dt^2}\overline{(x-\bar{x})^2} = \frac{2}{m^2}\overline{(p_x - \bar{p}_x)^2}$

Now, by MacLaurin Series:

(18) $\overline{(x-\bar{x})^2} = \overline{[(x-\bar{x})^2]}_{t=0} + \frac{1}{m}\overline{\{(p - \bar{p}_x), (x-\bar{x})\}}_{t=0}\, t$

$+ \frac{1}{m^2}\overline{[(p_x - \bar{p}_x)^2]}_{t=0}\, t^2$

This means that the wave packet spreads out as time increases because the variance increases. We could eliminate the middle term by using a taylor expansion around $t = t_0$ which we would have in a classical ensemble. This whole problem is analogous to a string of cars on a highway which are moving at constant velocity and which would disperse after a period of time.

LECTURE X 10-19-60

Resumé of Previous Work:

Generally Valid Statements:

$$\psi(r,t) = h^{-3/2} \int e^{i p\cdot r/\hbar} \varphi(p,t)\, dp$$

$$\varphi(p,t) = h^{-3/2} \int e^{-i p\cdot r/\hbar} \psi(r,t)\, dr$$

$$\int |\psi|^2 dr = \int |\varphi|^2 dp = 1$$

$$W(r)\,dr = |\psi|^2 dr \; ; \; \mathcal{W}(p)\,dp = |\varphi|^2 dp$$

Coordinate Representation: $\underline{x} = x \cdot \cdots \; ; \; \underline{p_x} = \frac{\hbar}{i}\frac{\partial}{\partial x} \cdots$

Momentum Representation: $\underline{x} = -\frac{\hbar}{i}\frac{\partial}{\partial p_x} \cdots \; ; \; \underline{p_x} = p_x \cdot \cdots$

$$\frac{d}{dt}\int |\psi|^2 dr = 0 \; ; \; i\hbar \frac{\partial \psi}{\partial t} = \underline{H}\psi \quad \text{with } \underline{H} \text{ Hermitian}$$

$$[x_j, p_k] = i\hbar\,\delta_{jk} \; ; \; [x_j, x_k] = [p_j, p_k] = 0$$

$$\overline{(\Delta A)^2}\;\overline{(\Delta B)^2} \geq \tfrac{1}{4}\overline{[A,B]}^2 \; ; \; \sqrt{\overline{(\Delta x)^2}}\sqrt{\overline{(\Delta p_x)^2}} \geq \tfrac{1}{2}\hbar$$

$$\overline{\frac{dA}{dt}} = \dot{\bar{A}} = \bar{\dot{A}} = \frac{d}{dt}\bar{A} \quad \text{by definition}$$

$$\frac{dA}{dt} = \frac{\partial A}{\partial t} + \frac{i}{\hbar}[\underline{H}, \underline{A}]$$

Definitions:

- Adjoint
- Hermitian
- Unitary
- Commutator
- Symmeterized Product
- Algebraic Rules of Operators

Particle Subject to Conservative, Non-Velocity Dependent Forces

It is a Quantum Mechanical Postulate that ψ obeys:

(1) $i\hbar \frac{\partial \psi}{\partial t} = \underline{H}\,\psi$, with

(2) $\underline{H} = \frac{p^2}{2m} + V(r) = -\frac{\hbar^2}{2m}\nabla^2 + V(r)$

This choice was a key point in Schroedingers early work on simple classical problems of central forces.

In Classical Theory: Hamiltonian function is $H(p, q)$
In Wave Mechanics: Hamiltonian operator is $H\left(\frac{\hbar}{i}\frac{\partial}{\partial q}, q\right)$

Ambiguities that may arise in other coordinate systems are taken care of when using the proper Laplacian in that system. Here notice can be taken that one of the essential features of non-relativistic Quantum Mechanics is that it leans on classical mechanics on the form of its Hamiltonian.

Let us now consider once again time diffentiation of $\int |\psi|^2 dr$ in a more general sense.

$$\frac{d}{dt}\int |\psi|^2 dr = \int \frac{\partial}{\partial t}\psi^*\psi\, dr \quad \text{with}$$

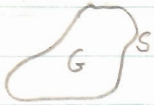
$$\frac{\partial}{\partial t}\psi^*\psi = \frac{1}{i\hbar}\left[\psi^*\underline{H}\,\psi - (H\psi)^*\psi\right] \quad \text{from the}$$

Schroedinger equation. When this is integrated over all space, the integral will vanish since $\underline{H}$ is Hermitian. Now consider the integral over a fixed boundary S enclosing a volume G. First we may, using the above form of the Hamiltonian, write:

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

The potential term drops out on expanding the Hamiltonian in the above equations.

Now:



$$\frac{d}{dt}\int_G \psi^* \psi \, dr = \frac{i\hbar}{2m}\int_G \nabla \cdot (\psi^* \nabla \psi - \psi \nabla \psi^*) \, dr$$

Using the divergence theorem:

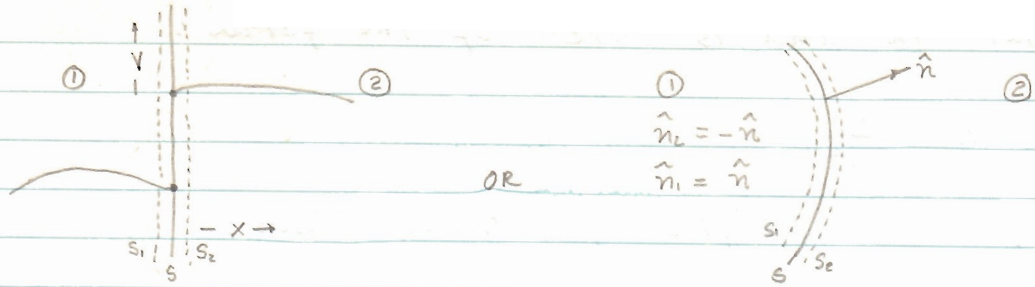
(3) $$\frac{d}{dt}\int_G \psi^* \psi \, dr = -\int_S J_n \, dS$$, where

(4) $$\vec{J} = -\frac{i\hbar}{2m}(\psi^* \nabla \psi - \psi \nabla \psi^*)$$

Now this gives the change with respect to time of the probability of a particle in the region G. Therefore $\vec{J}$ is the probability per unit area per unit time going through S which is called the probability flux vector. The mathematical definition of Hermiticity is that $\psi^* \underline{H} \psi - (H\psi)^* \psi$ be a divergence. However, we would desire to define "physical" Hermiticity as a vanishing integral over a surface surrounding the divergence. There are conditions where the space may be not infinite and the integral will still vanish. Suppose ψ to be confined in a box and ψ to be zero on the wall. Also the normal derivative $\frac{\partial \psi}{\partial n} = 0$. This makes H "physically" Hermitian and the integral vanishes. Also, in general, the Hermiticity of $\underline{H}$ must be preserved for different states, that is:

$$\int (\psi_a^* \underline{H} \psi_b - (H\psi_a)^* \psi_b) \, dr = 0$$

Let us now consider some cases of where the potential is discontinuous and examine the boundary conditions of ψ at these points.



Let the distance between S_1 and S_2 become vanishingly small. We want to require:

$$\frac{d}{dt}\int_{\substack{all\\space}} |\psi|^2 dr = \frac{d}{dt}\int_{G_1} |\psi_1|^2 dr + \frac{d}{dt}\int_{G_2} |\psi_2|^2 dr$$

$$= \int_S dS \left\{ \vec{J}_1 \cdot \hat{n}_1 + \vec{J}_2 \cdot \hat{n}_2 \right\} = \int dS \left\{ \vec{J}_1 \cdot \hat{n} - \vec{J}_2 \cdot \hat{n} \right\}$$

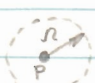
$$= \int_S dS \left\{ \left[\psi_a^* \nabla \psi_b - \psi_b \nabla \psi_a^* \right]_1 \cdot \hat{n}_1 - \left[\psi_a^* \nabla \psi_b - \psi_b \nabla \psi_a^* \right]_2 \cdot \hat{n}_2 \right\} = 0$$

The only way this can be zero is for:

(6) $\psi_2 = \psi_1$ and $\left(\frac{\partial \psi}{\partial n}\right)_1 = \left(\frac{\partial \psi}{\partial n}\right)_2$

and it will be this regardless of ψ_a, so the integral will vanish.

What about points where $V \to \infty$? Suppose a singular point P in the potential V.



Choose this singular point as the origin, thus permitting any integration to be over a sphere, which has an element of surface $dS = r^2 d\Omega$.

We want to require:

$$\lim_{r \to 0} r^2 \int d\Omega \left[\psi_a^* \left(-\frac{\partial \psi_b}{\partial r} \right) - \psi_b \left(-\frac{\partial \psi_a^*}{\partial r} \right) \right] = 0$$

Let us say that ψ_a and ψ_b are of the form:

$$\psi_a = \frac{f}{r^\alpha} \quad ; \quad \psi_b = \frac{g}{r^\alpha}$$

where f and g are analytic functions. Thus:

$$\lim_{r\to 0} r^2 \int \left[\frac{f^*}{r^\alpha}\left(\frac{\alpha g}{r^{\alpha+1}} - \frac{\frac{\partial g}{\partial r}}{r^\alpha}\right) - \frac{g}{r^\alpha}\left(\frac{\alpha f^*}{r^{\alpha+1}} - \frac{\frac{\partial f^*}{\partial r}}{r^\alpha}\right)\right] d\Omega$$

$$= \lim_{r\to 0} \frac{\left(g\frac{\partial f^*}{\partial r} - f^*\frac{\partial g}{\partial r}\right)}{r^{2\alpha-2}} \int d\Omega = 0$$

Thus a singularity of ψ of the form $\psi \sim \frac{1}{r^\alpha}$ must have $\alpha < 1$. For two dimensions, use the relation between a surface integral and a line integral. For one dimension ψ cannot have singularities stronger than the logarithmic type.

LECTURE XI 10-21-60

Static Potential Fields Continued:
From before:

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

(2) $\underline{H} = \frac{p^2}{2m} + V(r) = \frac{-\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + V(r)$

In the absence of explicit time dependence:

(3) $\dot{\underline{A}} = \frac{i}{\hbar}[\underline{H}, \underline{A}]$

$$\dot{x} = \frac{i}{\hbar}[\underline{H}, x] = \frac{p_x}{m}$$

$$\dot{p}_x = \frac{i}{\hbar}[\underline{H}, p_x] = \frac{i}{\hbar}[V(r), p_x] = \left[V(r), \frac{\partial}{\partial x}\right]$$

$$= -\frac{\partial V(r)}{\partial x} = m\ddot{\underline{x}} = \underline{f_x}$$

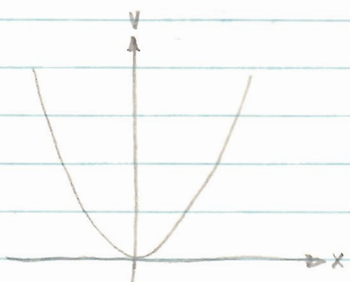
therefore:

$$(4) \quad \dot{\bar{x}} = \frac{\bar{p}_x}{m} \; ; \quad \dot{\bar{p}}_x = m\ddot{\bar{x}} = \bar{f}_x \text{ (mean value of } f_x \text{ over wave packet)}$$

This is known as Ehrenfests' Theorem. We must remark, however, that in general:

$$(5) \quad \bar{f}_x \neq f_x(\bar{x}).$$

The equality would be approximately true for a narrow wave packet because the change in f_x over the width of the packet would be small. There is a good correspondence between classical and wave mechanics during the time the wave packet stays small. It is this inequality that prevents wave mechanics from reducing completely to classical mechanics. Is it possible to have the wave packet stay small with time or will it spread indefinitely? The answer is that the particle can be confined in a potential "box" and will have a constant wave packet shape. Let us examine the problem in its one-dimensional aspects.



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

The particle is confined in the well and its wave packet will spread to the walls

Consider:

$$(6) \quad \frac{d}{dt}\overline{(x-\bar{x})^2} = \frac{1}{m}\left\{\overline{(p-\bar{p})(x-\bar{x})} + \overline{(x-\bar{x})(p-\bar{p})}\right\}$$

which is the correlation factor between position and momentum. Choose the initial shape of the wave packet such that:

$$(7) \quad \left[\frac{d}{dt}\overline{(x-\bar{x})^2}\right]_{t=0} = 0$$

Such a choice makes the wave packet shape Gaussian.

Now take:

$$(8)\quad \frac{d^2}{dt^2}(x-\bar{x})^2 = \frac{2}{m^2}(p-\bar{p})^2 + \frac{1}{m}\left\{(f-\bar{f})(x-\bar{x}) + (x-\bar{x})(f-\bar{f})\right\}$$

Now choose the shape of the well, that of the harmonic oscillator potential $f \propto x$, $f = -sx$. Then:

$$(9)\quad \frac{d^2}{dt^2}(x-\bar{x})^2 = \frac{2}{m^2}(p-\bar{p})^2 - \frac{2s}{m}(x-\bar{x})^2$$

Already considerable simplification has taken place. Now take the initial Gaussian packet so that $\left[d^2/dt^2\,(x-\bar{x})^2\right]_{t=0} = 0$ by choosing properly the ratio of momentum and position variances; which ratio will be independent of the uncertainty conditions. This ratio is:

$$(10)\quad \frac{s}{2}\,\overline{(x-\bar{x})^2} = \frac{1}{2m}\,\overline{(p-\bar{p})^2}$$

Now take:

$$(11)\quad \frac{d^3}{dt^3}(x-\bar{x})^2 = \frac{2}{m^2}\left\{(p-\bar{p}),(f-\bar{f})\right\} - \frac{2s}{m^2}\left\{(x-\bar{x}),(p-\bar{p})\right\}$$

Substitute $f = -sx$, $\bar{f} = -s\bar{x}$:

$$(12)\quad \frac{d^3}{dt^3}(x-\bar{x})^2 = -\frac{2s}{m}\frac{d}{dt}(x-\bar{x})^2$$

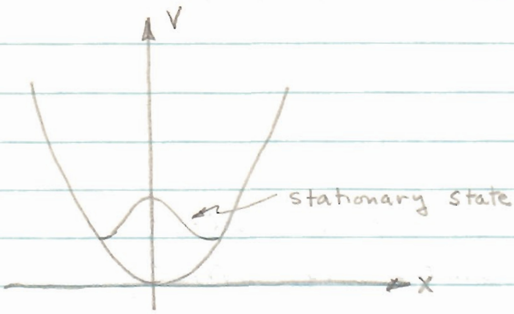
$$\frac{d^4}{dt^4}(x-\bar{x})^2 = -\frac{2s}{m}\frac{d^2}{dt^2}(x-\bar{x})^2$$

Thus all derivatives will vanish upon $t=0$ and upon expansion into a MacLaurin series all coefficients of t^n will vanish. For the case when $\bar{x}=0$, $\bar{p}=0$, $t=0$, $V = -s/2\, x^2$:

$$(13)\quad \overline{PE} = \overline{KE}$$

$$\frac{s}{2}\overline{x^2} = \frac{\overline{p^2}}{2m}$$

For this case, not only will the packet not spread, it will not move as can be seen from equation (4). This is called a stationary state.



If we position the packet off center, $\dot{x} = \frac{\bar{p}}{m}$; $\ddot{x} = -\frac{s\bar{x}}{m}$, the packet center will just move back and forth in the usual harmonic manner.

The above analysis leads directly to the proper shape of the wave packet and well. This result could also have been obtained from a superposition of the Hermite polynomial wave functions for the Harmonic Oscillator.

<u>Stationary States:</u>

$W(r)$ = constant in time
$\mathcal{W}(p)$ = constant in time
$\vec{J}(r)$ = constant in time

Only the phase of the waves can be changed with time.
Again:

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

Introduce the stationary state: $\psi(r,t) = T(t) \cdot u(r)$, then:

(15) $i\hbar\, \dot{T} u = \left(-\frac{\hbar^2}{2m} \nabla^2 + V(r) \right) T \cdot u$

$\frac{i\hbar \dot{T}}{T} = \frac{Hu}{u} = E$, the constant of separation. Finally,

(16) $i\hbar \ln T = Et + \text{constant}$

$T = e^{-iEt/\hbar}$

$\underline{H}\, u = Eu$

LECTURE XII   10-24-60

Stationary States:

There is no dependency on time, therefore, from the uncertainty principle,

$$\sqrt{\overline{(\Delta E)^2}}\,\sqrt{\overline{(\Delta t)^2}} \geq \frac{1}{2}\hbar$$

we see that if there is no dependency on time, $\Delta t = 0$, and the energy of the stationary states is strictly defined. We obtain stationary states for non-time dependent Hamiltonians. Then:

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

(2) $\underline{H}\, u = E u$

Justification of Symbol E:

A. Bohr frequency condition, $E_{n'} - E_{n''} = \hbar\omega$, transitions

B. E is additive. The ψ functions can be multiplied together to form probabilities when ψ's are independent.

C. $E = \overline{\underline{H}}$ where H is the Hamiltonian.

Also, if:

(3) $\int \psi^* \psi \, dr = 1$; $\int u^*(r)\, u(r)\, dr = 1$, and:

(4) $\overline{\underline{H}} = \int u^* \underline{H}\, u \, dr = E \int u^* u \, dr = E$

(5) $\overline{\underline{H}^2} = \int u^* \underline{H}\,\underline{H}\, u \, dr = E^2 \int u^* u \, dr = E^2$

Then:

(6) $\overline{(\Delta H)^2} = \overline{(H - \overline{H})^2} = \overline{H^2} - \overline{H}^2 = E^2 - E^2 = 0$

Thus showing that E is perfectly defined.

However, stationary states are really a fiction because transitions may occur with time from higher to lower states in an isolated system. Then, given an atom in an excited state with a lifetime around $\Delta t \sim 10^{-(7\text{ or }8)}$ sec, the uncertainty principle gives:

$$\Delta E \sim \frac{10^{-27}\text{ erg}\cdot\text{sec}}{10^{-7\text{ or }8}\text{ sec}} \sim 10^{-(19\text{ or }20)}\text{ ergs} \sim 10^{-(7\text{ or }8)}\text{ ev.}$$

However, the usual distance or difference between stationary states is 1 to 2 ev, hence the uncertainty is negligible. Thus we can consider excited states as stationary.

Consider the following equation, called an Eigenvalue equation:

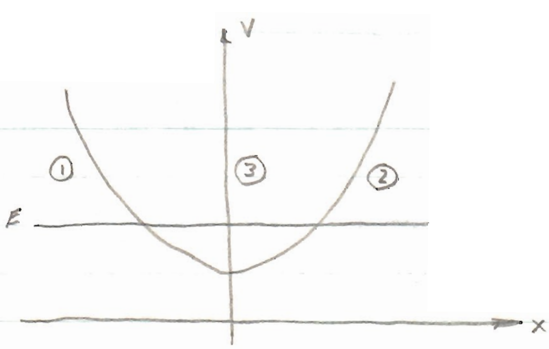
(7) $\underline{H}\,u = E u$

where $u \rightarrow$ eigenfunction, characteristic function
$E \rightarrow$ eigenvalue, eigenwerte, characteristic value.

The eigenvalues of an operator represent possible physical states of a system, They may be discrete or continuous or mixed. An example of a continuous operator would be the position x.

Many 3-D problems can be reduced to 1-D problems by separation of variables, thus we shall consider examples of the latter.

Harmonic Oscillator:



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

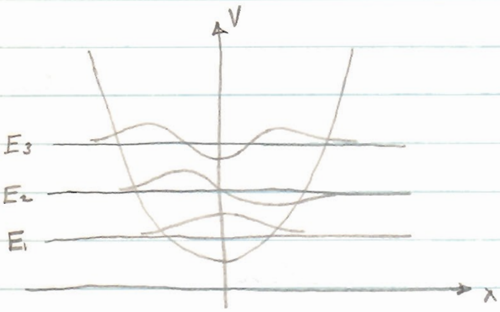
or: $$\frac{d^2u}{dx^2} = \frac{2m}{\hbar^2}(V-E)\,u$$

In region ① : $V-E$ is +, and if u is + ; u ∪
if u is − ; u ∩

In region ② : $V-E$ is +, same as ①

In region ③ : $V-E$ is −, and if u is + ; u ∩
if u is − ; u ∪

We desire u to vanish at $\pm\infty$. Thus we must choose the proper value of E to prevent blowing up of u at ∞. See this argument in Pauling - Wilson which brings out discreet nature of eigenvalues.

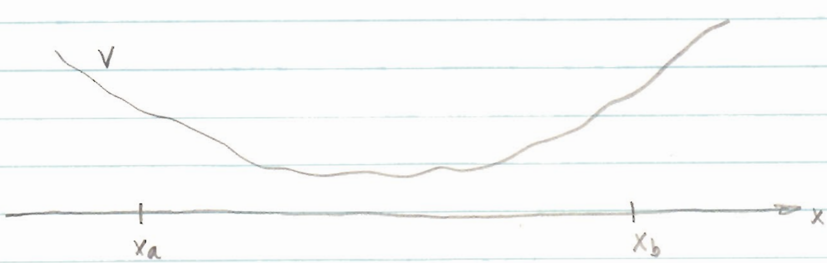


Number of nodes:

0: in lowest state
1: next lowest
2: next state above

LECTURE XIII 10-26-60

Harmonic Oscillator:
Consider the following potential:



$V(x) > E$ for $x < x_a$ and $x > x_b$ is considered.

Let $u_-^{(1)}(x,E) \to 0$ for $x \to -\infty$ and $u_-^{(1)}(x_a, E) = 1$

Now there is another possibility:

Choose:

$u_-^{(2)}(x,E)$ such that the Wronskian is:

$$\begin{vmatrix} u_-^{(2)} & u_-^{(1)} \\ u_-^{(2)\prime} & u_-^{(1)\prime} \end{vmatrix} = 1$$

We see that $u_-^{(2)}$ is not a multiple of $u_-^{(1)}$ because the Wronskian will vanish.

Now let $u_+^{(1)}(x,E) \to 0$ for $x \to +\infty$ and $u_+^{(1)}(x_b, E) = 1$

Choose $u_+^{(2)}(x,E)$ such that the Wronskian is unity as above. Now, all this holds for differential equations of the form:

$$u'' = K(V-E)\,u$$

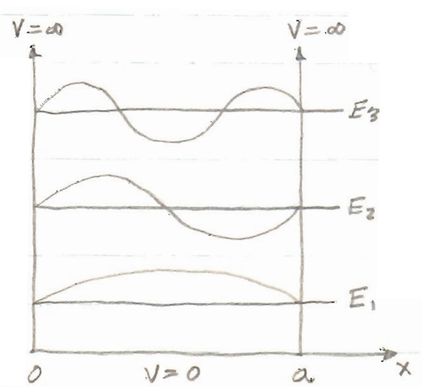
where the absence of u' means the Wronskian is a constant. Thus we can form independent solutions as follows:

$$u_-^{(1)}(x,E) = A\,u_+^{(1)}(x,E) + B\,u_+^{(2)}(x,E)$$

$$u_-^{(2)}(x,E) = C\,u_+^{(1)}(x,E) + D\,u_+^{(2)}(x,E)$$

where $A = A(E)$ and $B = B(E)$ with $B(E) = 0$ at the eigenvalues.

Particle in a Box:



Boundary Conditions:

$u = 0$ at $x = 0, a$

Then:

$$u'' = -\frac{2m}{\hbar^2} E u$$

$$u = C \sin \sqrt{\frac{2mE}{\hbar^2}}\, x$$

In case V is merely large, $u'' = q^2 u$, $\frac{u}{u'} = -\frac{1}{q}$

As $q \to \infty$, $\frac{u}{u'} \to 0$, but $u' \neq \infty$, so $u = 0$

Since $u(a) = 0$, $\sin \sqrt{\frac{2mE}{\hbar^2}}\, a = 0$

then $\sqrt{\frac{2mE}{\hbar^2}}\, a = n\pi$, $n = 1, 2, 3, \ldots$

and :

$$E = \frac{n^2 \pi^2 \hbar^2}{2ma^2}$$

$$\int u^2 dx = 1 = c^2 \int_0^a \sin^2 \sqrt{\frac{2mE}{\hbar^2}}\, x \, dx = c^2 \frac{a}{2}, \therefore \; c = \sqrt{\frac{2}{a}}$$

and $u_n(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}$

Note that we could expand any function, $f(x)$, as

$$f(x) = \sum_{n=1}^{\infty} u_n(x) \cdot C_n$$

with the result a Fourier series.

As a matter of fact, any well behaved quantity can be expressed as an expansion of orthogonal functions (eigenfunctions). However, this cannot be proved in general. For Sturm-Liouville problems when the variables can be separated, we have:

$$(p(x)u')' + q(x)u + \lambda \rho(x) u = 0$$

λ ↓ eigenvalue

Boundary Condition: $Au' + Bu = 0$ (homogeneous)

For two different eigenfunctions and eigenvalues, when available, we can form:

$$\int_a^b dx \left\{ \underbrace{u_2 (p u_1')' - u_1 (p u_2')'}_{\frac{d}{dx}\left[u_2 p u_1' - u_1 p u_2'\right]} + (\lambda_1 - \lambda_2) \rho u_1 u_2 = 0 \right.$$

$$= \left[u_2 \, p \, u_1' - u_1 \, p \, u_2' \right]_a^b + (\lambda_1 - \lambda_2) \int_a^b \rho \, u_1 u_2 \, dx = 0$$

(the bracketed term $= 0$ if BC satisfied at limits)

then $\int_a^b \rho \, u_1 u_2 \, dx = 0$, $\lambda_2 \neq \lambda_1$

and thus u_1, u_2 are orthogonal. However, this is also assumed to be true if variables cannot be separated. The same thing can be done with the Schroedinger equation by forming:

$$u_2^* \Big\} \; \underline{H} \, u_1 = E_1 u_1 \quad ; \quad (\underline{H} \, u_2)^* = E_2 u_2^* \; \Big\} - u_1$$

Then: $\int \left(u_2^* \underline{H} \, u_1 - (\underline{H} \, u_2)^* u_1 \right) d\tau = (E_1 - E_2) \int u_2^* u_1 \, d\tau$

(the left-hand integral $= 0$)

$$\therefore \int u_2^* u_1 \, d\tau = 0 \quad , \quad E_2 \neq E_1$$

In many dimensions, we can have degeneracy, that is, for a given eigenvalue, there are several different eigenfunctions. If we use only linearly independent wave functions, then for f-fold degeneracy, there are f linearly independent functions for the same eigenvalue.

Example: $E_a \rightarrow u_1^{(a)}$
$E_b \rightarrow u_1^{(b)} \; u_2^{(b)} \; u_3^{(b)}$

Are degenerate functions orthogonal within themselves?

Introduce the notation $(f, g) = \int f^* g \, d\tau$ and consider the degenerate set of wave functions $w_1, w_2, w_3, \ldots, w_f$, which are not orthonormal.

We then form:

$$u_1 = \frac{v_1}{\sqrt{(v_1, v_1)}} \quad ; \quad v_1 = w_1$$

$$u_2 = \frac{v_2}{\sqrt{(v_2, v_2)}} \quad ; \quad v_2 = w_2 - (u_1, w_2)\, u_1$$

$$u_3 = \frac{v_3}{\sqrt{(v_3, v_3)}} \quad ; \quad v_3 = w_3 - (u_1, w_3)\, u_1 - (u_2, w_3)\, u_2$$

and in general:

$$u_n = \frac{v_n}{\sqrt{(v_n, v_n)}} \quad ; \quad v_n = w_n - \sum_{k=1}^{n-1} (u_k, w_n)\, u_k$$

and so forth to w_f and u_f. This is called the Schmidt orthogonalization procedure.

LECTURE XIV 10-28-60

Recapitulation:

Linear Independence

Schmidt Procedure:

Given w_k, $(k = 1, \dots, f)$

We form orthonormal functions via:

$$u_k = \frac{v_k}{\sqrt{(v_k, v_k)}} \quad , \quad v_k = w_k - \sum_{j=1}^{k-1} (u_j, w_k)\, u_j$$

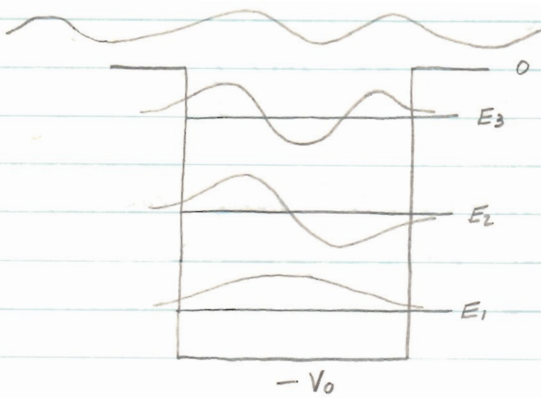
$$(f, g) = \int f^* g \, d\tau \cdot \rho$$

Expansion Theorem: We can expand a function f as a series in orthogonal functions, viz.,

$$f = \sum_{n=1}^{\infty} c_n u_n \quad , \quad c_n = (u_n, f)$$

This expansion will converge to the function in the mean, but may not at certain points. For example, Fourier series at discontinuities in the function where it then converges to the mean.

Consider, now, the potential well:



It is hard to expand in only three functions. We must include the continuous spectrum also. These functions are not quadratically integrable, that is, the integral:

$$\int u^* u \, dx \quad \text{diverges.}$$

The worst case is, of course, for free particles. We can expand in terms of these functions, except that we use an $\int$ sign instead of the Σ sign.

$$f(x) = \int_{-\infty}^{\infty} a(k) \frac{e^{ikx}}{\sqrt{2\pi}} \, dk$$

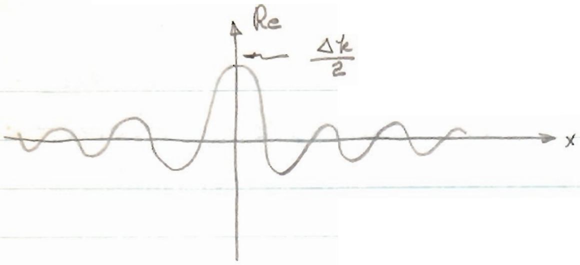
$$a(k) = \int_{-\infty}^{\infty} f(x) \frac{e^{-ikx}}{\sqrt{2\pi}} \, dx$$

where we see $u_k(x) = \frac{e^{ikx}}{\sqrt{2\pi}}$, then:

$$a(k) = \int_{-\infty}^{\infty} u_k^*(x) f(x) \, dx \quad \text{analogous to} \quad a_n = \int u_n^*(x) f(x) \, dx$$

Now let us take these functions and form a wave packet:

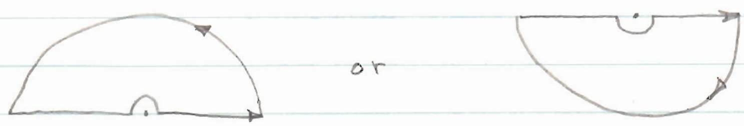
$$u(x; k, \Delta k) = \underbrace{\int_{k-\frac{\Delta k}{2}}^{k+\frac{\Delta k}{2}} u_k(x) \, dk}_{\text{quadratically integrable}} = \underbrace{\frac{e^{ikx}}{\sqrt{2\pi}} \cdot \frac{2 \sin \frac{\Delta k}{2} x}{x}}_{\text{this gives shape of packet}}$$



Now study:

$$\int_{-\infty}^{\infty} u_{k'}^{+}(x)\, u(x; k, \Delta k)\, dx = \frac{1}{2\pi i}\int_{-\infty}^{\infty}\frac{dx}{x}\left\{e^{i(k+\frac{\Delta k}{2}-k')x} - e^{i(k-\frac{\Delta k}{2}-k')x}\right\}$$

We will use contour integration. Integrate along the real axis, but exclude $x=0$. Two paths possible:



Consider the following theorems from Phillips, p. 125., supposing $Q(x)$ to have only simple poles on the real axis:

$$P\int_{-\infty}^{\infty} Q(x)\, e^{mix}\, dx = 2\pi i \sum R^{+} + \pi i \sum R^{0} \quad ; \quad m>0$$

$$P\int_{-\infty}^{\infty} Q(x)\, e^{-mix}\, dx = -2\pi i \sum R^{-} - \pi i \sum R^{0} \quad ; \quad m>0$$

Then, if $Q(x) = \frac{1}{x}$, there are no residues either in the upper or lower half plane and the only singular point is on the real axis at the origin.

$$\therefore \quad R^{0} = \lim_{z\to 0}\left\{e^{\pm miz}\right\} = 1$$

Therefore it is clear that, for:

$k' > k + \frac{\Delta k}{2}$: $m<0$, and C is: , $\int_{-1+1} \to 0$

$k' < k + \frac{\Delta k}{2}$: $m>0$, and c is: , $\int_{1-1} \to 0$

And, for, $k - \frac{\Delta k}{2} < k' < k + \frac{\Delta k}{2}$:

First term: C:  ; $\frac{1}{2\pi i}\int \rightarrow \frac{\pi i}{2\pi i} = \frac{1}{2}$

Second term: C:  ; $\frac{1}{2\pi i}\int \rightarrow \frac{-\pi i}{2\pi i} = -\frac{1}{2}$

and $\int_{-\infty}^{\infty} u_{k'}^*(x)\, u(x; k, \Delta k)\, dx = 1$

Finally:

$$\int_{-\infty}^{\infty} u_{k'}^*(x)\, u(x; k, \Delta k)\, dx = \begin{cases} 0 & \text{if } k' \text{ not in } \Delta k \\ 1/2 & \text{if } k' \text{ on boundary} \\ 1 & \text{if } k' \text{ in } \Delta k \end{cases}$$

This is called normalization on the scale of k:

Therefore an expansion in terms of continuous eigenfunctions will use $\int$ instead of Σ and be normalized in the scale of k.

We are two-fold degenerate in the continuous spectrum, as we can see from the two different starting points of $u = 0$, or $u' = 0$. If we have complete symmetry, (in potential) then if $u(x)$ is an eigenvalue, $u(-x)$ also is an eigenvalue.

For the discrete spectrum: $u(-x) = c\, u(x)$

$u(x) = c\, u(-x) = c^2 u(x)$, $\therefore c = \pm 1$

For continuous spectrum:

$$\frac{u(x) + u(-x)}{2} = u_e(x), \quad e \rightarrow \text{even}$$

$$\frac{u(x) - u(-x)}{2} = u_o(x), \quad o \rightarrow \text{odd}$$

Then the complete set of states for the symmetrical potential well is:

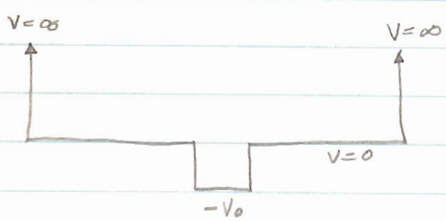
$$u_1(x),\ u_2(x),\ u_3(x),\ u_{ek}(x),\ u_{ok}(x)$$

and the expansion theorem takes the form:

$$f(x) = a_1 u_1 + a_2 u_2 + a_3 u_3 + \int_0^\infty dk\, a_e(k)\, u_{ek}(x) + \int_0^\infty dk\, a_o(k)\, u_{ok}(x)$$

where $a_n = \int_{-\infty}^{\infty} u_n^* f\, dx$; $a_{\substack{e\\o}}(k) = \int u^*_{\substack{e\\o}k}(x)\, f\, dx$

Hueristic Argument:



Using the diagram, we would get discreet states for $E > V_0$, expand a function as a sum and then let $x \to \infty$ and $\Sigma \to \int$.

LECTURE XV 10-31-60

Recapitulation:

Normalization of discreet spectrum:

Build packets around k: $u(x; k, \Delta k) = \int_{\Delta k} u_k(x)\, dk$

Then: $\int u^*_{k'}(x)\, dx \int_{\Delta k} u_k(x)\, dk = \begin{cases} 0 & k' \text{ not in } \Delta k \\ 1 & k' \text{ in } \Delta k \end{cases}$

Although this was shown for the free particle, it holds in the general case.

Another approach to this problem is to use a convergence factor.

Example: $1 + x + x^2 + x^3 + \cdots = \frac{1}{1+x}$, $|x| < 1$

For $x = 1$, the sum of the series is $1/2$, that is, we take the limit as $x \to 1$. In the same way:

$$\lim_{\alpha \to 0+} \int_{-\infty}^{\infty} e^{-\alpha |x|} u_{k'}^*(x)\, u_k(x)\, dx = 0 \quad , \quad k' \neq k$$

↑ converging factor

For $k' = k$, nothing can be done, the integral diverges. Let's see what free particle gives, using $e^{-\alpha^2 x^2}$ as the converging factor:

$$\lim_{\alpha \to 0} \int_{-\infty}^{\infty} e^{-\alpha^2 x^2} u_{k'}^*(x)\, u_k(x)\, dx = \lim_{\alpha \to 0} \underbrace{\int_{-\infty}^{\infty} e^{-\alpha^2 x^2} \frac{e^{i(k-k')x}}{2\pi} dx}_{I(\alpha)}$$

In the exponent:

$$-\alpha^2 \left(x^2 - \frac{i(k-k')x}{\alpha^2} \right) = -\alpha^2 \underbrace{\left(x - \frac{i(k-k')}{2\alpha^2} \right)^2}_{y} - \frac{(k-k')^2}{4\alpha^2}$$

Then: $$I(\alpha) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-\alpha^2 y^2} \cdot e^{-\frac{(k-k')^2}{4\alpha^2}} dy$$

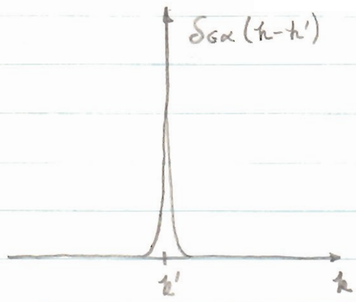
$$= \frac{1}{2\sqrt{\pi}\,\alpha} e^{-\frac{(k-k')^2}{4\alpha^2}}$$

Now: $$\lim_{\alpha \to 0} I(\alpha) = 0 \quad , \text{ if } k' \neq k$$
$$= \infty \quad , \text{ if } k' = k$$

Then define: $$\delta_{G\alpha}(k-k') = \frac{1}{2\sqrt{\pi}\,\alpha} e^{-\frac{(k-k')^2}{4\alpha^2}}$$

with, obviously, $\int_{-\infty}^{\infty} \delta_{G\alpha}(k-k')\, dk = 1$

Consider, now, the following limit:



$$\lim_{\alpha \to 0} \delta_{G\alpha}(k-k') = \delta(k-k')$$

which is called the Dirac Delta Function.

This function has the following properties:

$$\delta(x) = 0 \quad , \quad x \neq 0$$
$$= \infty \quad \text{otherwise}$$

$$\int_a^b \delta(x)\, dx = 1 \quad , \quad a < 0 < b$$
$$= 0 \quad , \quad \text{otherwise}$$

The Dirac Delta Function plays the same role in integrals as the Kronecker delta plays in sums.

$$\int_a^b f(x)\, \delta(x-x_0)\, dx = \begin{cases} f(x_0) & , \; a < x_0 < b \\ 0 & , \; \text{otherwise} \end{cases}$$

and corresponds to:

$$\sum_{m=k}^{l} A_m \delta_{mn} = \begin{cases} A_n & , \; k \leq n \leq l \\ 0 & , \; \text{otherwise} \end{cases}$$

Then the normalization scheme for orthogonal functions is:

$$\int u_m^* u_n \, d\tau = \delta_{mn} \quad \text{(discrete)}$$

$$\int u_{k'}^* u_k \, d\tau = \delta(k-k') \quad \text{(continuous, normalization on } k \text{ scale)}$$

We could also normalize on an energy scale.

To show this, simply consider:

$$\int_{\substack{\text{contains}\\ x_0}} F(y(x))\,\delta(x-x_0)\,dx = F(y(x_0))$$

and

$$\int_{\substack{\text{contains}\\ y_0}} F(y)\,\delta(y-y_0)\,dy = F(y(x_0))$$

$y_0 = y(x_0)$

Now $dy = \frac{dy}{dx}\,dx$, then $\delta(y-y_0)\left|\frac{dy}{dx}\right| = \delta(x-x_0)$

($\frac{dy}{dx}$ could possibly be $-$.)

and finally: $$\delta(y-y_0) = \frac{1}{\left|\frac{dy}{dx}\right|}\,\delta(x-x_0)$$

Therefore: $$\int u_{E'}^{*}\,u_E\,dr = \delta(E-E') \qquad (E \text{ scale})$$

$$\int u_{k'}^{*}\,u_k\,dr = \delta(k-k') \qquad (k \text{ scale})$$

Then $$u_E(r) = \frac{1}{\left|\frac{dE}{dk}\right|^{1/2}}\,u_k(r)$$

What is the method of forming the normalization of non-free problems? Use the asymptotic expansion where $V \to 0$ for large r. For example, cutting off orthogonal functions at a finite number of terms. We always get a form of trig function for the asymptotic expansion in the first term.

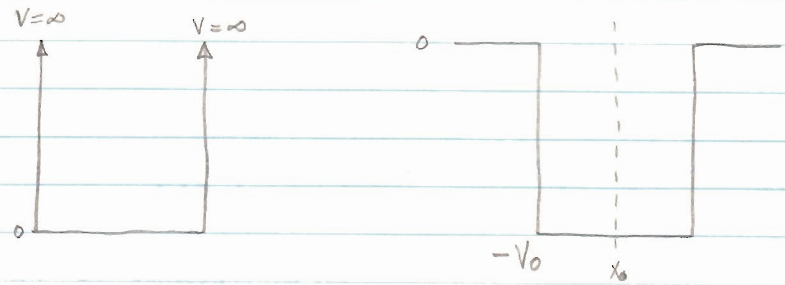
Useful Relation:

$$\int_{-\infty}^{\infty} e^{ikx}\,dx = 2\pi\,\delta(x)$$

LECTURE XVI   11-2-60

Solvable Problems:

Rectangular Potentials:



We usually consider the bound states only, and thus impose the following conditions:

1) $u \to 0$, $x \to \pm\infty$
2) $\frac{u'}{u}$ is continuous where V is discontinuous
3) Symmetrical Well, $V(x) = V(-x)$

Now, when the above is the case, we can define a reflection operator such that:

$$\underline{R}\, f(x) = f(-x)$$

and also, $[\underline{R}, \underline{H}] = 0$ when $V(x) = V(-x)$, that is:

$$\underline{R}\, \underline{H}\, u(x) = \underline{H}\, \underline{R}\, u(x)$$

Suppose we have stationary states:

$$\underline{H}\, u(x) = E\, u(x)$$

$$\underline{H}\, \underline{R}\, u(x) = \underline{R}\, \underline{H}\, u(x) = E\, \underline{R}\, u(x)$$

and $\underline{H}\, u(-x) = E\, u(-x)$

This means that in one-dimension:

$$\underline{R}\, u(x) = u(-x) = c\, u(x)$$
$$u(x) = c\, u(-x) = c^2 u(x)$$
$$\therefore \quad c^2 = 1, \quad c = \pm 1$$

and either $u(-x) = u(x)$
or $u(-x) = -u(x)$

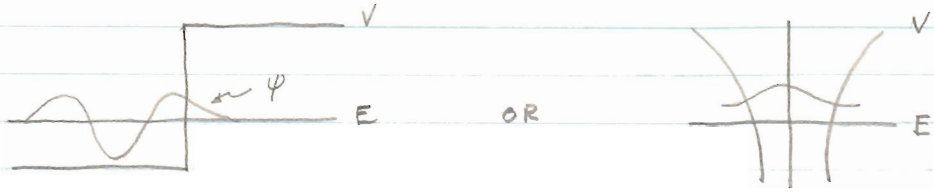
This property is called parity of state.

This property also holds in 3 dimensions. Define vector $\bar{r}$. If we have $\underline{R}\, f(\bar{r}) = f(-\bar{r})$, we have inversion symmetry.

Physical Appearance of Well Wave Functions:

When we consider the well, whose sides are not of infinite potential, we have a tunneling effect which is classically not possible, because the particle would have to have negative kinetic energy.

Consider:



We actually find from smears in the x-ray pattern, a finite probability of being outside the box. In this region, the wave function is usually of the form:

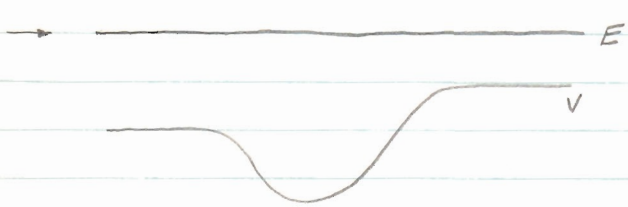
$$\psi \sim e^{-\kappa x}, \quad \kappa = \sqrt{\frac{2m(V-E)}{\hbar^2}}$$

For measurement outside, $\Delta x < \frac{1}{\kappa}$. Now $\Delta x\, \Delta p_x \gtrsim \hbar$, then $\Delta p_x > \hbar\kappa$ and $\frac{(\Delta p_x)^2}{2m} = V - E$.

Thus, for a particle at rest outside the well needs an X-ray of energy V−E to reveal its presence.

Loops and nodes are not predicted classically either, as one would expect an uniform distribution. However, waves in stationary states are analogous in complementarity to particles and a uniform distribution could be built up from a superposition of stationary states.

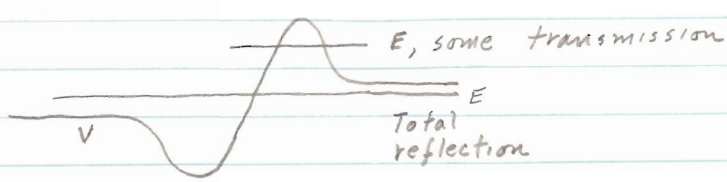
Reflection and Transmission:



What is the chance of reflection or transmission of an electron coming in from left with a given kinetic energy?

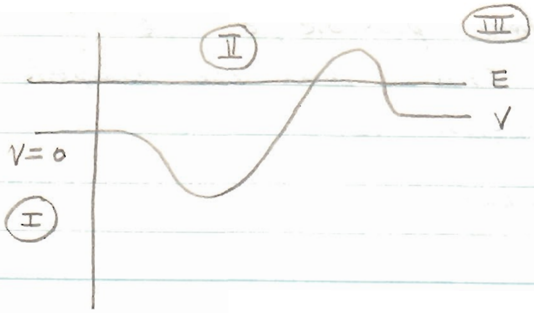
Classically, if KE is larger than highest PE, the electron will be completely transmitted.

Another Case:



We can talk about reflection and transmission coefficients R and T.

We now examine the mathematical methods of finding these coefficients.



R and T are functions of the amplitudes of unnormalizable plane waves which we assume to be incident on our model.

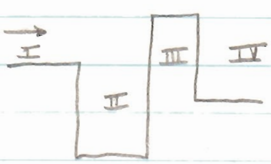
Boundary Conditions: Particles are streaming from left to right with none incident from the right, so that we can write:

In region III: $u = e^{ik'x}$, $k' = \sqrt{\dfrac{2m(E - V_{III})}{\hbar^2}}$

In region I: $u = Ae^{ikx} + Be^{-ikx}$,

$$k = \sqrt{\frac{2m(E - V_I)}{\hbar^2}}$$

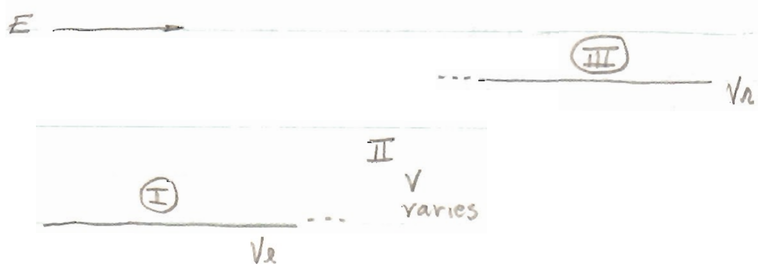
The number of equations we arrive at is dependent on the number of potential regions.



We would have 6 equations in 6 unknowns.

LECTURE XVII 11-4-60

Collision Problems:



For incidence from the left, the BC for fixed E is:

$u = e^{ik_R x}$ in III

with $\hbar^2 k_R^2 = 2m(E - V_R)$

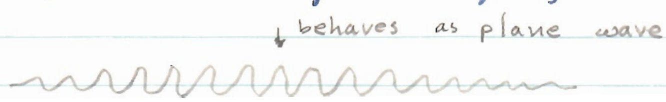
In region I: there are two solutions possible, $e^{ik_e x}$, $e^{-ik_e x}$ from $u'' = \frac{2m}{\hbar^2}(V-E)u$. Then the complete solution in this region is:

$$u = Ae^{ik_e x} + Be^{-ik_e x}$$

and the complete solution is:

$$\psi = \begin{cases} e^{ik_r x}\, e^{-iEt/\hbar} & \text{in III} \\ (Ae^{ik_e x} + Be^{-ik_e x})e^{-iEt/\hbar} & \text{in I} \end{cases}$$

Although we are using plane waves, they can be considered as part of a slowly decaying wave packet



Probabilities calculated with plane waves are proportional to actual probabilities. Now, the probability current density is:

$$j = \frac{\hbar}{2mi}\left(\psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx}\right)$$

In III: $j = \frac{\hbar}{2mi}(2ik_r) = \frac{\hbar k_r}{m} = v_r$

In I: $$j = \frac{\hbar}{2mi}\left(|A|^2 2ik_e - |B|^2 2ik_e\right) + \frac{\hbar}{2mi} A^*B\,(-ik_e + ik_e)\,e^{-2k_e x} + \frac{\hbar}{2mi} BA^*\,(-ik_e + ik_e)\,e^{-2k_e x}$$

Then: $j = (|A|^2 - |B|^2)\,v_e$: $\begin{cases} |A|^2 v_e & \text{to right} \\ |B|^2 v_e & \text{to left} \end{cases}$

and $v_e = \frac{\hbar k_e}{m}$

Transmission Coefficient:

$$T \equiv \frac{\text{transmitted flux}}{\text{incident flux}} = \frac{v_r}{v_\ell}\frac{1}{|A|^2} = \frac{k_r}{k_\ell}\frac{1}{|A|^2}$$

$$R \equiv \frac{\text{reflected flux}}{\text{incident flux}} = |B|^2/|A|^2$$

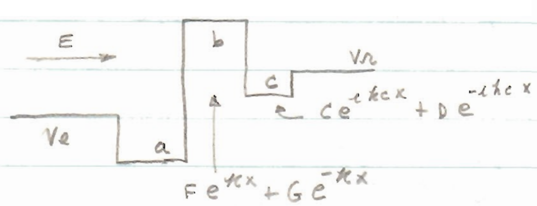
f is constant in position as can be seen from the fact that f is proportional to the Wronskian:

$$\begin{vmatrix} u^* & u \\ u'^* & u' \end{vmatrix} = W \;; \quad W' = 0 + \begin{vmatrix} u^* & u \\ u''^* & u'' \end{vmatrix} = 0$$

, because $u^{*''}$ is proportional to u'' since the potential is real.

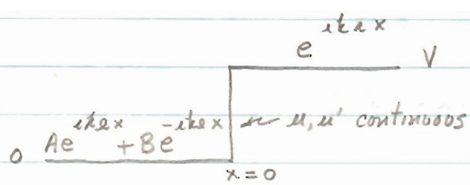
Therefore, as $W'=0$, then f is constant in position.

Solvable Problems:



By taking u, u' continuous at the boundaries, we can find T and R by simultaneous solution of all the equations.

Simplest Example:



Using boundary conditions on u, u':

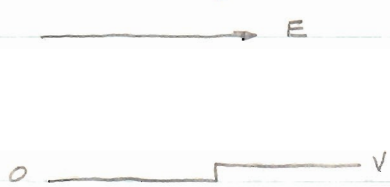
$A + B = 1$

$ik_\ell A - ik_\ell B = ik_r$

$$\therefore\; A = \frac{k_\ell + k_r}{2k_\ell} \;;\quad B = \frac{k_\ell - k_r}{2k_\ell}$$

$$T = \frac{k_r}{k_\ell}\frac{4k_\ell^2}{(k_\ell + k_r)^2} = \frac{4k_r k_\ell}{(k_\ell + k_r)^2} \;;\quad R = \left(\frac{k_\ell - k_r}{k_\ell + k_r}\right)^2$$

Consider only a small step in Potential: $V \ll E$



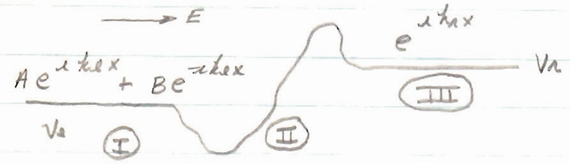
$$\text{Now } R = \left(\frac{\sqrt{E} - \sqrt{E-V}}{\sqrt{E} + \sqrt{E-V}}\right)^2$$

with $\sqrt{E-V} = \sqrt{E}\sqrt{1-\frac{V}{E}} \approx \sqrt{E}\left(1 - \frac{V}{2E}\right)$

$$\text{Then } R \approx \left(\frac{1-\left(1-\frac{V}{2E}\right)}{1+\left(1-\frac{V}{2E}\right)}\right)^2 = \left(\frac{V}{2E}\right)^2$$

This relation holds for either a step up or a step down because of the fact that V comes in squared.

Consider the general case:



We can choose:

$u = e^{ik_r x}$ in III, wave coming from left

$v = e^{-ik_l x}$ in I, wave coming from right

We can show that u and v are orthogonal and we will normalize in the k scale.

$$\int_{-\infty}^{\infty} u^*(x, k_r') \, u(x, k_r) \, dx = \int_{-\infty}^{0} \left\{ |A|^2 e^{i(k_l - k_l')} + |B|^2 e^{-i(k_l - k_l')x} \right\} dx$$

$$+ \int_0^{\infty} e^{i(k_r - k_r')x} \, dx$$

Notice $k_l^2 = k_r^2 + (V_r - V_l)\frac{2m}{\hbar^2}$; $k_l'^2 = k_r'^2 + (V_r - V_l)\frac{2m}{\hbar^2}$

and $2k_l(k_l - k_l') \simeq 2k_r(k_r - k_r')$, near $k_{r,l} = k_{r,l}'$

Let $x \simeq \frac{k_l}{k_r} x'$ and $x' = x''$

Then $\frac{k_l}{k_r}|A|^2 \int_{-\infty}^{0} e^{i(k_r - k_r')x} dx - \frac{k_l}{k_r}|B|^2 \int_{\infty}^{0} e^{i(k_r - k_r')x''} dx''$

$$+ \int_0^{\infty} e^{i(k_r - k_r')x} dx = \frac{k_l}{k_r}|A|^2 \int_{-\infty}^{0} e^{i(k_r - k_r')x} dx + \left(\frac{k_l}{k_r}|B|^2 + 1\right) \int_0^{\infty} e^{i(k_r - k_r')x} dx$$

$$= \frac{k_l}{k_r}|A|^2 \int_{-\infty}^{\infty} e^{i(k_r - k_r')x} dx = \frac{2\pi}{T} \delta(k_r - k_r')$$

Hence $u_{k_r} = \sqrt{\frac{T}{2\pi}}\, u$ (u normalized in the k_r scale)

We could normalize v in the k_l scale and get:

$$v_{k_l} = \sqrt{\frac{T}{2\pi}}\, v$$

We can expand any function then as:

$$f(x) = \sum_n (u_n, f)\, u_n(x) + \int_{\kappa}^{\infty} (u_{k_r}, f)\, u_{k_r}(x)\, dx$$

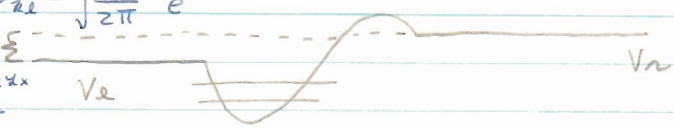
$$+ \int_{\kappa'}^{\infty} (v_{k_l}, f)\, v_{k_l}(x)\, dk_l$$

LECTURE XVIII   11-7-60

Errata:

$$v_{k_\ell} = \sqrt{\frac{T}{2\pi}}\, e^{-i k_\ell x} \qquad u_{k_r} = e^{i k_r x}\sqrt{\frac{T}{2\pi}}$$

$$w_k = \frac{e^{i k x} + e^{i\delta} e^{-i k x}}{\sqrt{2\pi}}$$



Now: $$f(x) = \sum_{n=1}^{N} (u_n, f)\, u_n(x) + \int_K^{\infty} (v_{k_\ell}, f)\, v_{k_\ell}(x)\, dk_\ell$$

(Discreet terms)

$$+ \int_0^{\infty} (u_{k_r}, f)\, u_{k_r}(x)\, dk_r + \int_0^{K} (w_k, f)\, w_k(x)\, dk$$

(For E greater than V_r)
(degenerate & continuous)

(non-degenerate continuous spectrum)

$$K = \sqrt{\frac{2m(V_r - V_\ell)}{\hbar}}$$

The Hydrogen Atom:

We will treat this problem by the polynomial method.

Schroedinger Equation:

$$(1) \quad \nabla^2 u + \frac{2m}{\hbar^2}(E - V\{r\})\, u = 0$$

where $V(r) = -\dfrac{Ze^2}{r}$

Choose suitable units: $\hbar = 1$, $2m = 1$, $Ze^2 = 2$

Then:

unit of length: $\dfrac{\hbar^2}{mZe^2} = \dfrac{a_0}{Z}$ where a_0 is Bohr radius

unit of energy: $\dfrac{Z^2 me^4}{2\hbar^2} = Z^2 R h c$

Another system of units that are used are due to Hartree: $\hbar = 1$, $m = 1$, $e^2 = 1$.

Substituting:

$$(2) \quad \nabla^2 u + \left(E + \frac{Z}{r}\right) u = 0$$

$$\downarrow$$

$$V(r)$$

Consider general case of potential as function of r. We can separate the variables and obtain spherical harmonics:

$$(3) \quad u = R(r)\, Y_l^m(\theta, \varphi) = R(r) \cdot C_{lm} P_l^{|m|}(\cos\theta)\, e^{im\varphi}$$

with $\int |Y_l^m|^2 \, d\Omega = 1$; $l = 0, 1, 2, \ldots$

$m = -l, -l+1, \ldots, l-1, l$

Form of $e^{im\varphi}$ comes from assumption that wave functions are single-valued. If m is not integer, we get branch lines. Now, we must preserve the property that the wave functions are isotropic in space, thus, if we change the co-ordinates we get new branch line so we must say m is an integer and the wave functions are single valued. Now, our radial equation is:

$$(4) \quad R'' + \frac{2}{r} R' + \left(E - V\{r\} - \frac{l(l+1)}{r^2}\right) R = 0$$

We have no m in the equation and the radial wave functions are $(2l+1)$ fold degenerate.

Define a rotator operator $R_{\alpha, \hat{n}}$ which commutes with the Hamiltonian. Now take $Hu = Eu$ and operate with R : $H R_{\alpha,\hat{n}} u = E R_{\alpha\hat{n}} u$.
Thus there is a finite degeneracy in which a rotation can be expressed with a sum of other spherical harmonics. We have here a <u>natural symmetry</u> which leads to a <u>natural degeneracy</u>.

when form of V is substituted, we find an accidental degeneracy such that the energy does not depend on l. Upon substituting $V = \frac{Z}{R}$

(5) $R'' + \frac{2}{r} R' + \left(E + \frac{2}{r} - \frac{l\{l+1\}}{r^2} \right) R = 0$

(this term can be thought of as the centripetal force potential)

Now $\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} = \frac{1}{r}\frac{d^2}{dr^2} r$, then:

(6) $(rR)'' + \left(Er + z - \frac{l\{l+1\}}{r} \right) rR = 0$

The boundaries are $r = 0$ and $r = \infty$

Look at asymptotic solution; $r \to \infty$; $R'' + ER \simeq 0$
with:

$$R \sim e^{\pm\sqrt{-E}\,r}$$

Take: $R \sim e^{-\sqrt{-E}\,r}$

Now, we have a singularity at $r = 0$, which is also regular if the coefficient of the first derivative is not stronger than $\frac{1}{r}$ and the coefficient of R not stronger than $\frac{1}{r^2}$ and such is the case here.
We make the solution of the form:

(7) $\sum_{n=0}^{\infty} C_n r^{\beta+n}$

For $n = 0$: $r^{-2+\beta}$: $c_0 \beta(\beta-1) + c_0 2\beta - c_0 l(l+1)$

we get indicial equation: $\beta(\beta+1) - l(l+1) = 0$; $\beta = l$, $\beta = -l-1$

We through out $\beta = -l-1$ because $r^{-2+\beta}$ will be worse than r^{-2}. We shall find for R

(8) $R = r^l e^{-\sqrt{-E}\,r} v$

LECTURE XIX 11-9-60

Continuation of Hydrogen-Like Model:

(1) $u = R(r)\, Y_\ell^m(\theta, \varphi)$

(2) $(rR)'' + \left(E + \frac{2}{r} - \frac{\ell\{\ell+1\}}{r^2} \right)(rR) = 0$

$\frac{\ell(\ell+1)}{r^2}$ is centripetal potential; classically, $\frac{M \text{ (angular momentum)}}{r^2}$

(3) $rR = r^{\ell+1} e^{-\sqrt{-E}\, r}\, v$

from asymptotic solution and indicial equation. Substituting (3) into (2):

(4) $v'' + 2\left(\frac{\ell+1}{r} - \sqrt{-E} \right) v' + \frac{2}{r}\left(1 - \{\ell+1\}\sqrt{-E} \right) v = 0$

Make definitions:
$2r\sqrt{-E} = x$
$2\ell + 2 = b$
$\ell + 1 = a$

and get:

(5) $\frac{d^2 v}{dx^2} + \left(\frac{b}{x} - 1 \right) \frac{dv}{dx} - \frac{a}{x} v = 0$

which gives one of the confluent hypergeometric functions, The Laguerre polynomials. We now solve by the polynomial method:

(6) $v = \sum_{k=0}^{\infty} C_k x^k$

Substituting in (5):

(7) $\sum_{k=0}^{\infty} C_k \left\{ \left[k(k-1) + bk \right] x^{k-2} - \left[k + a \right] x^{k-1} \right\} = 0$

Rearranging:

$$(8) \quad \sum_{k=0}^{\infty} x^{k-1} \left\{ C_{k+1}(k+1)(k+b) - C_k(k+a) \right\} = 0$$

then: $$C_{k+1} = \frac{k+a}{(k+1)(k+b)} C_k$$

$$(9) \quad v = 1 + \frac{a}{1 \cdot b} x + \frac{a(a+1)}{1 \cdot 2\, b(b+1)} x^2 + \frac{a(a+1)(a+2)}{1 \cdot 2 \cdot 3\; b(b+1)(b+2)} x^3 + \cdots$$

$$= {}_1F_1(a, b, x)$$

These type of functions derive from the so-called Gaussian hypergeometric series:

$${}_2F_1(a, \beta; b; z) = 1 + \frac{a \cdot \beta}{1 \cdot b} z + \frac{a(a+1)\beta(\beta+1)}{1 \cdot 2\, b(b+1)} z^2 + \cdots$$

We have for the special case above: ${}_1F_1(a,b,x) = \lim_{\substack{z \to 0 \\ \beta \to \infty \\ \beta z \to x}} {}_2F_1(a,\beta,b,z)$

We have finally for the complete solution:

$$(10) \quad rR = C r^{l+1} e^{-\sqrt{-E}\, r}\; {}_1F_1\left(l+1 - \frac{1}{\sqrt{-E}},\; 2l+2,\; 2\sqrt{-E}\, r\right)$$

As x becomes large, ${}_1F_1$ approaches an exponential and wave functions become unbounded. Therefore, we cut off series at some term:

For $\underline{E < 0}$: $$a = l + 1 - \frac{1}{\sqrt{-E}} = -n', \quad n' = 0, 1, 2, 3, \ldots$$

$$\frac{1}{\sqrt{-E}} = +(l+1+n') = +n, \quad n = l+1,\ l+2$$

Therefore:

$$(11) \quad E = -\frac{1}{n^2} \longrightarrow E = -\frac{1}{n^2} Z^2 Rhc$$

We have for given n: $l = n-1, n-2, \ldots 0$.

For $\underline{E>0}$: Define $\sqrt{E} = \kappa$, then $\sqrt{-E} = i\kappa$

We get for solution:

(12) $$rR = C r^{l+1} e^{-i\kappa r} {}_1F_1 \left(l+1+\frac{i}{\kappa};\ 2l+2;\ 2i\kappa r\right)$$

or $$rR = C r^{l+1} e^{i\kappa r} {}_1F_1 \left(l+1-\frac{i}{\kappa};\ 2l+2,\ -2i\kappa r\right)$$

where C's are the same in each. We do the above by Kummer's First Formula:

$$e^{-x} {}_1F_1(a,b,x) = {}_1F_1(b-a,b,-x)$$

We now can write:

(13) $$rR = C r^{l+1} e^{-r/n} {}_1F_1 (l+1-n,\ 2l+2,\ 2r/n)$$

or $$rR = C r^{l+1} e^{+r/n} {}_1F_1 (l+1+n,\ 2l+2,\ -2r/n)$$

LECTURE XX 11-14-60

Problems 12-15 (inclusive) due Monday Nov. 21.

Continuation of Hydrogenic Wave Equation:

(1) $$(rR)'' + \left(E + \frac{2}{r} - \frac{l(l+1)}{r^2}\right)(Rr) = 0$$

Found that

(2) $$rR = r^{l+1} e^{-\sqrt{-E}\,r} {}_1F_1 \left(l+1-\frac{1}{\sqrt{-E}},\ 2l+2,\ 2\sqrt{-E}\,r\right)$$

or $$rR = r^{l+1} e^{+\sqrt{-E}\,r} {}_1F_1 \left(l+1+\frac{1}{\sqrt{-E}};\ 2l+2;\ -2\sqrt{-E}\,r\right)$$

We cut off series; and get

(3) $E = -\frac{1}{n^2}$ for energy levels.

and we can then write:

(4) $rR = C r^{l+1} e^{-r/n} \, {}_1F_1 (l+1-n; 2l+2; 2r/n)$

$rR = C r^{l+1} e^{+r/n} \, {}_1F_1 (l+1+n; 2l+2; -2r/n)$

Note: $l+1+n - (2l+2) = n-l-1 = 0$ or + int., then

$${}_1F_1 (b+c; b; x)$$
$$\uparrow$$
$$0, 1, 2, \ldots$$

Expanding: ${}_1F_1 (b; b; x) = 1 + x + \frac{x^2}{2!} + \ldots = e^x$

$${}_1F_1 (b+1; b; x) = \frac{1}{b} x^{-b+1} \frac{d}{dx} \left(x^b + \frac{x^{b+1}}{1} + \frac{x^{b+2}}{2!} + \frac{x^{b+3}}{3!} + \ldots \right)$$

$$= \frac{1}{b} x^{-b+1} \frac{d}{dx} x^b e^x$$

from ${}_1F_1 (b+1; b; x) = \frac{1}{b} \left(1 \cdot b + \frac{b \cdot (b+1)}{1 \cdot b} x + \frac{b(b+1)(b+2)}{1 \cdot 2 \cdot b \, (b+1)} x + \ldots \right)$

Generally:

$${}_1F_1 (b+c; b; x) = \frac{1}{b(b+1) \cdots (b+c-1)} \Big(b(b+1) \cdots (b+c-1)$$

$$+ \frac{b \cdots (b+c-1)}{1 \cdot b} x + \frac{b(b+1)(b+2) \cdots (b+c)(b+c+1)}{1 \cdot 2 \; b(b+1)} x^2$$

$$+ \ldots + \frac{b(b+1) \cdots (b+c-1)(b+c)(b+c+1) \cdots (b+2c)}{(c+1)! \; b(b+1) \cdots (b+c)} x^{c+1} + \ldots$$

$$= \frac{1}{b \cdots (b+c-1)} x^{-b+1} \left(\frac{d}{dx} \right)^c x^{b+c-1} e^x$$

Then; because of demensionality of ${}_1F_1(b+c; b; x)$

(5) $$rR = c\,\frac{(2l+1)!}{(n+l)!}\, r^{-l} e^{r/n} \left(\frac{d}{dr}\right)^{n-l-1} r^{n+l} e^{-2r/n}$$

we now wish to normalize (rR) : $\int_0^\infty |rR|^2\,dr = 1$

(6) $$1 = |c|^2 \frac{(2l+1)!}{(n+l)!} \int_0^\infty r\,{}_1F_1(l+1-n;\ 2l+2;\ 2r/n) \left(\frac{d}{dr}\right)^{n-l-1} r^{n+l} e^{-2r/n}\,dr$$

Integrate by parts; to form

$$\left(-\frac{d}{dr}\right)^{n-l-1} r\,{}_1F_1 = \left(-\frac{d}{dr}\right)^{n-l-1} \left(-\frac{n}{2}\right)\Big\{\left(-\frac{2r}{n}\right) + \frac{l+1-n}{1!\,(2l+2)}\left(-\frac{2r}{n}\right)^2$$

$$+ \cdots + \frac{(n-l-1)!\,(2l+1)!}{(n-l-2)!\,(n+l-1)!}\left(-\frac{2r}{n}\right)^{n-l-1}$$

$$+ \frac{(n-l-1)!\,(2l+1)!}{(n-l-1)!\,(n+l)!}\left(-\frac{2r}{n}\right)^{n-l}\Big]$$

$$= \left(\frac{2}{n}\right)^{n-l-2} \frac{(n-l-1)!\,(2l+1)!}{(n+l)!}\left[-(n+l)(n-l-1) + (n-l)\cdot\frac{2r}{n}\right]$$

Then we have:

(7) $$|c|^{-2} = \left[\frac{(2l+1)!}{(n+l)!}\right]^2 (n-l-1)!\left(\frac{n}{2}\right)^{2l+3}\Big[-(n+l)(n-l-1)(n+l)!$$

$$+ (n-l)(n+l+1)(n+l)!\Big]$$ from $\int_0^\infty e^{-x} x^m\,dx = m!$

(8) $$|c|^{-2} = \left[(2l+1)!\right]^2 \cdot \frac{(n-l-1)!}{(n+l)!} \cdot 4\left(\frac{n}{2}\right)^{2l+4}$$

from $[\ ] = (n+l)!\left[-(n+l)(n-l-1) + (n+l+1)(n-l)\right]$

Finally:

(9) $$r R_{nl} = \frac{1}{2}\left(\frac{2}{n}\right)^{l+2}\left\{(n-l-1)!\,(n+l)!\right\}^{-1/2} r^{-l}\, e^{r/n}\left(\frac{d}{dr}\right)^{n-l-1} r^{n+l}\, e^{-2r/n}$$

$$\bar{V} = 2E\,; \quad V = -\frac{2}{r}\,, \quad E = -\frac{1}{n^2}$$

$$\text{from } \overline{\left(\frac{1}{r}\right)} = \frac{1}{n^2}$$

LECTURE XXI 11-16-60

Continuation of Hydrogenic Model:

Summary: Using atomic constants:

(1) $$u_{nlm} = R_{nl}\, Y_l^m$$

(2) $$R_{nl} = \frac{1}{2}\left(\frac{2}{n}\right)^{l+2}\left\{(n+l)!\,(n-l-1)!\right\}^{1/2} \cdot r^{-l-1}\, e^{r/n}\left(\frac{d}{dr}\right)^{n-l-1} r^{n+l}\, e^{-2r/n}$$

(3) $$Y_l^m = \left[\frac{2l+1}{4\pi}\right]^{1/2}\left[\frac{(l-|m|)!}{(l+|m|)!}\right]^{1/2} P_l^{|m|}(\cos\theta)\, e^{im\varphi}$$

$$P_l^{|m|}(\mu) = (1-\mu^2)^{|m|/2}\frac{d^{|m|}}{d\mu^{|m|}} P_l(\mu)$$

$$P_l(\mu) = \frac{1}{2^l\, l!}\frac{d^l}{d\mu^l}(\mu^2-1)^l$$

Using cgs units: $r \to r \cdot \frac{Z}{a_0}$; $R \to \left(\frac{Z}{a_0}\right)^{3/2} R$

First Few States:

$$u_{100} = \frac{1}{\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0} \quad : \quad E_1 = -Z^2 Rhc$$

$$u_{200} = \frac{1}{4\sqrt{2\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\left(2 - \frac{Zr}{a_0}\right) e^{-Zr/2a_0}$$

$$u_{210} = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \frac{Zr}{a_0} e^{-Zr/2a_0} \cos\theta$$

$$u_{21\pm1} = \frac{1}{8\sqrt{2\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \frac{Zr}{a_0} e^{-Zr/2a_0} \sin\theta \; e^{\pm i\varphi}$$

$$E_2 = -\frac{1}{4} Z^2 Rhc$$

with the following rules:

$l = 0, \ldots, n-1$

$1 + 3 + \cdots + (2n-1) = n^2$

each energy level is n^2 degenerate.

Continuous Spectrum : $E > 0$: l unrestricted.

(4) $R = \text{constant} \cdot r^l e^{-\sqrt{-E}\, r} \; {}_1F_1\left(l+1-\frac{1}{\sqrt{-E}} ; 2l+2 ; 2\sqrt{-E}\, r\right)$

In cgs units: $E \rightarrow \dfrac{E}{Z^2 Rhc}$, $r \rightarrow r \dfrac{Z}{a_0}$

Make $\sqrt{-E}\, r = \pm i \sqrt{E}\, r$ into a pure number.

$\pm i \sqrt{E}\, r = \pm i k r$, and get $k = \dfrac{\sqrt{2mE}}{\hbar}$

then $\dfrac{1}{\sqrt{-E}} = \dfrac{\mp i}{\sqrt{E}} \longrightarrow \dfrac{\mp i Z}{k a_0} = \mp i \nu$ (imaginary quantum #)

Now we can write:

(5) $R_{k,l} = C' r^l e^{ikr} \; {}_1F_1\left(l+1-i\nu ; 2l+2 ; -2ikr\right)$

We want to normalize in the k scale. Look up asymptotic expansion in M & O. For $-\frac{3}{2}\pi < \arg z < \frac{1}{2}\pi$,

(6) $${}_1F_1(a; b; z) \sim e^{-i\pi a} \frac{\Gamma(b)}{\Gamma(b-a)} z^{-a} \left\{1 + O\left(\frac{1}{z}\right)\right\}$$

$$+ \frac{\Gamma(b)}{\Gamma(a)} e^{z} z^{a-b} \left\{1 + O\left(\frac{1}{z}\right)\right\}$$

$$(7) \quad R \sim c'(2l+1)! \left\{ \frac{e^{-\pi\nu/2}}{\Gamma(l+1+i\nu)} \left(\frac{-i}{2k}\right)^{l+1} \frac{e^{ikr + i\nu \ln 2kr}}{r} \right.$$

$$\left. + \frac{e^{-\pi\nu/2}}{\Gamma(l+1-i\nu)} \left(\frac{i}{2k}\right)^{l+1} e^{-ikr - i\nu \ln 2kr} \right\} \text{, and}$$

$$(8) \quad r R_{kl} \sim A_{kl}\, e^{ikr + i\nu \ln 2kr} + A_{kl}^{*}\, e^{-ikr - i\nu \ln 2kr}$$

Normalizing in the k scale:

$$(9) \quad \int_0^\infty (r R_{k'l})^* r R_{kl}\, dr \longrightarrow |A_{lk}|^2 \int_{-\infty}^{\infty} e^{i(k-k')r}\, dr = 2\pi |A_{lk}|^2 \delta(k-k')$$

$$\text{"} \\ 1$$

We finally get,

$$(10) \quad \frac{(2k)^{l+1} e^{\pi\nu/2} |\Gamma(l+1+i\nu)|}{(2\pi)^{1/2} (2l+1)!} \cdot r^l e^{ikr} {}_1F_1(l+1-i\nu;\, 2l+2,\, -2ikr)$$

$$= R_{kl}$$

Thus we have discrete and continuous spectrum for $V = \dfrac{-Ze^2}{r}$.

LECTURE XXII 11-18-60

Harmonic Oscillator:

$$(1) \quad \underline{H} = \frac{p^2}{2m} + \frac{S}{2} q^2 \text{, satisfying } \underline{H}u = Eu$$

We will use ladder method to solve this problem rather than the usual polynomial method. Define the following quantities and convert to natural units:

$$(2) \quad \omega = \sqrt{\frac{S}{m}} \;; \quad \frac{p^2}{2m\hbar\omega} + \frac{m\omega}{2\hbar} q^2 = \frac{H}{\hbar\omega} = \underline{K}$$

$$\underline{q} = \sqrt{\frac{2\hbar}{m\omega}}\, \underline{Q} \,, \quad \underline{p} = \sqrt{2m\hbar\omega}\, \underline{P} \quad \text{(Defined)}$$

Then we have:

(3) $P^2 + Q^2 = K$ satisfying $\underline{K}u = \eta u$

$$Q = \sqrt{\frac{m\omega}{2\hbar}}\, q \quad , \quad P = \frac{p}{\sqrt{2m\hbar\omega}}$$

(4) $[Q,P] = \frac{1}{2\hbar}[q,p] = \frac{i}{2}$ (evidently $k = \frac{1}{2}$)

In Q representation $\underline{Q} \to Q$, $\underline{P} \to \frac{1}{2i}\frac{d}{dQ}$

Define: New operators:

(5) $$\left.\begin{aligned} a &= Q + iP \\ a^+ &= Q - iP \end{aligned}\right\} \quad [a, a^+] = -2i[Q,P] = 1$$

$$a a^+ = K - i[Q,P] = K + \tfrac{1}{2}$$

$$a^+ a = K - \tfrac{1}{2}$$

(6) $[K,a] = [aa^+, a] = a[a^+,a] = -a$

$$[K; a^+] = a^+$$

Consider $Ku = \eta u$:

(7) $Kau = aKu + [K,a]u = (\eta - 1)\,au$

To show that all eigenvalues are positive, show $\bar{K}$ is positive:

(8) $\bar{K} = \int u^* \left(-\frac{1}{4}\frac{d^2}{dQ^2} + Q^2\right) u \, dQ = \int \left(\frac{1}{4}\left|\frac{du}{dQ}\right|^2 + Q^2 |u|^2\right) dQ$

must be > 0, obviously.

Thus, to keep eigenvalues positive, we stipulate that in $Hu = Eu \rightarrow Ku = \eta u$, $u \neq 0$ and we have a lowest eigenfunction u_0 such that:

(9) $a u_0 = 0$; $\left(Q + \frac{1}{2}\frac{d}{dQ}\right) u_0 = 0$

$\frac{1}{2} u_0' = -Q u_0$ with solution $u_0 = C e^{-Q^2}$ which is our gaussian wave packet for the lowest wave state of the harmonic oscillator.

(10) $C^{-2} = \int_{-\infty}^{\infty} e^{-2Q^2}\, dQ = \sqrt{\frac{\pi}{2}}$, then $u_0 = \left(\frac{2}{\pi}\right)^{1/4} e^{-Q^2}$

We can now find lowest eigenvalue

(11) $K u_0 = \left(a^+ a + \frac{1}{2}\right) u_0 = \frac{1}{2} u_0$

Now consider:

(12) $K a^+ u = a^+ K u + [K, a^+] u = (\eta + 1) a^+ u$, then

(13) $u_1 = c_1 a^+ u_0$, $K u_1 = \left(1 + \frac{1}{2}\right) u_1$

and in general

(14) $u_n = c_n (a^+)^n u_0$, $K u_n = \left(n + \frac{1}{2}\right) u_n$

To find C_n:

(15) $C_n^{-2} = \int_{-\infty}^{\infty} \left[(a^+)^n u_0\right]^* (a^+)^n u_0 \, dQ$

Use definition of Adjoint operators; viz.

$$\int u^* A v \, dQ \equiv \int (A^+ u)^* v \, dQ$$

(16) $C_n^{-2} = \int_{-\infty}^{\infty} \left\{(a^+)^{n-1} u_0\right\}^* a (a^+)^n u_0 \, dQ$

with $a (a^+)^n u_0 = [a, (a^+)^n] u_0 = n (a^+)^{n-1} [a, a^+]$

Therefore $C_n^{-2} = n\, C_{n-1}^{-2}$, $C_n = \frac{1}{\sqrt{n}}\, C_{n-1}$

$C_0 = 1$ $\qquad C_3 = \frac{1}{\sqrt{3 \cdot 2}}$

$C_1 = 1$ $\qquad \vdots$

$C_2 = \frac{1}{\sqrt{2}} \cdot 1$ $\qquad C_n = \frac{1}{\sqrt{n!}}$

Finally:

$$(17) \quad u_n = \frac{1}{\sqrt{n!}} \left(\frac{2}{\pi}\right)^{1/4} (a^+)^n e^{-Q^2} \qquad n = 0, 1, 2, 3, \ldots$$

$$K\, u_n = \left(n + \tfrac{1}{2}\right) u_n$$

Would like to know matrix form of operators:

$$(18) \quad a^+ u_n = \sqrt{n+1}\, u_{n+1} \quad ; \quad a\, u_n = \sqrt{n}\, u_{n-1}$$

Multiplying by $\int_{-\infty}^{\infty} u_m^* \, dQ$, then

$$a^+_{m,n} = \sqrt{n+1}\, \delta_{m,\,n+1}$$

$$a_{m,n} = \sqrt{n}\, \delta_{m,\,n-1}$$

(19) Now $Q = \frac{a + a^+}{2}$ then

$$q_{mn} = \sqrt{\frac{\hbar}{2m\omega}} \left\{ \sqrt{n+1}\, \delta_{m,n+1} + \sqrt{n}\, \delta_{m,n-1} \right\}$$

$$P = \frac{a - a^+}{2i}$$

$$p_{mn} = \sqrt{\frac{m\hbar\omega}{2}} \left\{ i\sqrt{n+1}\, \delta_{m,n+1} - i\sqrt{n}\, \delta_{m,n-1} \right\}$$

Note that solution is exactly the same if one works in P space, since $Q = -\frac{1}{2i}\frac{d}{dP}$ and $K = P^2 + Q^2$. We would get

$$(20) \quad w_0(P) = \left(\frac{2}{\pi}\right)^{1/4} e^{-P^2} = u_0(P) \quad , \quad w_n(P) = u_n(P)\,(-i)^n$$

$F_2\, u(P) = \int_{-\infty}^{\infty} e^{-2iPQ}\, u(Q)\, dQ$, which is a Fourier transform acting as an operator.

LECTURE XXIII   11-21-60

Continuation of Harmonic Oscillator:

(1) $Q = \sqrt{\frac{m\omega}{2\hbar}}\, q \quad ; \quad P = \sqrt{\frac{1}{2m\omega\hbar}}\, p$

$H = (P^2 + Q^2)\hbar\omega \quad ; \quad E = (n+\frac{1}{2})\hbar\omega, \quad n = 0, 1, 2, 3, \ldots$

(2) $u_n(Q) = \left(\frac{2}{\pi}\right)^{1/4} (n!)^{-1/2} (a^+)^n e^{-Q^2}$

$a^+ = Q - iP \rightarrow Q - \frac{1}{2}\frac{d}{dQ} \quad ; \quad \int u_n^2\, dQ = 1$

Determine a new u_n in terms of q such that $\int u_n^2\, dq = 1$.

(3) $u_n(q) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} (n!)^{-1/2}\, 2^{-n/2} \left(y - \frac{d}{dy}\right)^n e^{-y^2/2}$

where $y = \sqrt{2}\, Q \quad ; \quad a^+ = \frac{1}{\sqrt{2}}\left(y - \frac{d}{dy}\right) \quad ; \quad y = \sqrt{\frac{m\omega}{\hbar}}\, q$

(4) Notice: $\left(y - \frac{d}{dy}\right) f = e^{y^2/2}\left(-\frac{d}{dy}\right) e^{-y^2/2} f$, then

(5) $u_n(q) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} (n!)^{-1/2}\, 2^{-n/2} H_n(y)\, e^{-y^2/2}$

where $H_n(y)$ are the Hermite polynomials:

$H_n(y) = e^{y^2}\left(-\frac{d}{dy}\right)^n e^{-y^2}$

We can form the generating equation for $H_n(y)$ thus:

(6) $\sum_{n=0}^{\infty} H_n(y)\frac{t^n}{n!} = e^{y^2} e^{-(y-t)^2} = e^{2yt - t^2}$

Two Dimensional Harmonic Oscillator:

(7) $$H = \frac{|\bar{p}|^2}{2m} + \frac{m\omega_1^2}{2}x^2 + \frac{m\omega_2^2}{2}y^2$$

(8) $$\left[-\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right] + \frac{m\omega_1^2}{2}x^2 + \frac{m\omega_2^2}{2}y^2 - E\right]u = 0$$

Separating the variables: $u = U(x)V(y)$:

$$-\frac{\hbar^2}{2m}\frac{1}{U}\frac{d^2U}{dx^2} + \frac{m\omega_1^2}{2}x^2 - E = \frac{\hbar^2}{2m}\frac{1}{V}\frac{d^2V}{dy^2} - \frac{m\omega_2^2}{2}y^2$$

Make the traditional arguments putting $E = E_1 + E_2$:

(9) $$-\frac{\hbar^2}{2m}\frac{d^2U}{dx^2} + \left(\frac{m\omega_1^2}{2}x^2 - E_1\right)U = 0$$

$$-\frac{\hbar^2}{2m}\frac{d^2V}{dy^2} + \left(\frac{m\omega_2}{2}y^2 - E_2\right)V = 0$$

We get for solutions:

(10) $$E_1 = (n_1 + \tfrac{1}{2})\hbar\omega_1 \quad ; \quad E_2 = (n_2 - \tfrac{1}{2})\hbar\omega_2$$

Special Case: $\omega = \omega_1 = \omega_2$, $PE = \frac{m\omega^2}{2}r^2$

$E = (n+1)\hbar\omega$; $u_n = u_{n_1}(x)\, u_{n_2}(y)$

$n = 0$: $n_1 = 0$, $n_2 = 0$

$n = 1$: $n_1 = 1$, $n_2 = 0$

$n_1 = 0$, $n_2 = 1$

In general, each level is $(n+1)$ fold degenerate.

Three Dimensional Case:

We get the results: $E = (n_1 + 1/2)\hbar\omega_1 + (n_2 + 1/2)\hbar\omega_2 + (n_3 + 1/2)\hbar\omega_3$

For isotropic case: $E = (n + 3/2)\hbar\omega$

$n = 0$: 0 0 0

$n = 1$: $\left\{\begin{matrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{matrix}\right\}$

$n = 2$: $\left\{\begin{matrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \\ 1 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{matrix}\right\}$

The degree of degeneracy is a combinatorial problem:

x x | x x x | x x x ← indistinguishable

We can divide the objects in $\frac{(n+2)!}{n!\,2!} = \frac{(n+1)(n+2)}{2}$ ways. Therefore, the levels have a deneracy of degree $\frac{(n+1)(n+2)}{2}$

Another Way: The coefficient of x^n in

$$(1 + x + x^2 + \cdots)(1 + x + x^2 + \cdots)(1 + x + x^2 + \cdots) = \frac{1}{(1+x)^3}$$

$$= \frac{1}{2}\frac{d^2}{dx^2}\frac{1}{1-x} = \frac{1}{2}\frac{d^2}{dx^2}(1 + x + x^2 + \cdots)$$

$$= \frac{1}{2}(1\cdot 2x^0 + 2\cdot 3x + 3\cdot 4x^2 + \cdots)$$

This concludes the discussion of exactly solvable problems.

Variation Method:

Consider the solutions to $(H - E_n) u_n = 0$. We can expand in series of these solutions, viz.,

(11) $u = \sum_n a_n u_n$; with $\int |u|^2 d\tau = 1$

Then: $Hu = \sum_n a_n E_n u_n$

(12) $\overline{H} = \int u^* H u \, d\tau = \int \sum_m a_m^* u_m^* \sum_n a_n E_n u_n \, d\tau$

or $\overline{H} = \sum_m \sum_n a_m^* a_n E_n \delta_{mn} = \sum_n |a_n|^2 E_n$

(13) $\overline{H} - E_0 = \sum_n |a_n|^2 (E_n - E_0) \geq 0$

LECTURE XXIV 11-23-60

Variation Method:

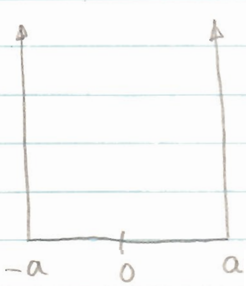
(1) $\overline{H} = \dfrac{\int u^* H u \, d\tau}{\int |u|^2 d\tau} \geq E_0$

One dimensional Example:

u' discontinuous at x_0:

when taking $\frac{d^2}{dx^2}$ we have the usual second derivative plus $\delta(x - x_0)\left[u'(x_0^+) - u'(x_0^-)\right]$

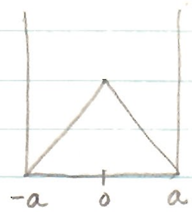
Take potential box:



$H = -\dfrac{\hbar^2}{2m}\dfrac{d^2}{dx^2}$

$u_0 = \sqrt{\dfrac{2}{a}} \cos\dfrac{\pi x}{2a}$; $E_0 = \dfrac{\pi^2 \hbar^2}{8ma^2}$

Try various approximations:



$$u = c\,(a - |x|)\,, \quad |x| < a$$

$$Hu = \frac{+\hbar^2}{2m} \cdot 2c\,\delta(x)$$

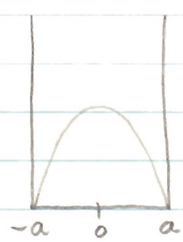
Normalizing: $2c^2 \int_0^a (a-x)^2\,dx = 2c^2 \cdot \frac{a^3}{3} = 1$

Now: $\int u^* H u\,dx = \frac{\hbar^2}{2m}\, 2 \cdot c \cdot ca = \dfrac{\frac{\hbar^2 a}{m}}{\frac{2a^3}{3}}$

$$= \frac{\hbar^2}{ma^2} \cdot \frac{3}{2} = E_0 \left(\frac{12}{\pi^2} = 1.216 \right)$$

or this approximation leads to about a 20% error

Now try parabolic approximation:



$$u = c\,(a^2 - x^2)$$

$$\int_{-a}^{a} u^2\,dx = 2c^2 \int_0^a (a^2-x^2)^2\,dx$$

$$= 2c^2 a^5 \left(1 - \frac{2}{3} + \frac{1}{5}\right) = \frac{16}{15} c^2 a^5 = 1$$

Now: $\int u^* H u\,dx = \frac{\hbar^2}{m} c^2 \cdot 2 \int_0^a (a^2 - x^2)\,dx = 2c^2 \frac{\hbar^2}{m} a^3 \left(1 - \frac{1}{3}\right)$

$$= \frac{4}{3} c^2 \frac{\hbar^2}{m} a^3 = \frac{\hbar^2}{ma^2} \frac{5}{4} = E_0 \left(\frac{10}{\pi^2} = 1.013 \right)$$

better!

Now we try a function which involves a parameter:

$$u = c\,(a^n - |x|^n)$$

$$Hu = \frac{\hbar^2}{2m}\, n(n-1)\, x^{n-2}$$, break in first derivative when $n = 1$

Normalizing: $\int u^2\,dx = 2c^2 \int_0^a (a^n - x^n)^2\,dx = \frac{4n^2}{(n+1)(2n+1)} c^2 = 1$

$$\int u^* H u\,dx = \frac{(n+1)(2n+1)}{4(2n-1)} \frac{\hbar^2}{ma^2} = \overline{H}$$

We wish to minimize $\overline{H}$ by differentiating with respect to the prameter n.

$$\frac{d}{dn} \ln \overline{H} = \frac{1}{n+1} + \frac{1}{2n+1} - \frac{1}{2n-1} = 0$$

or $4n^2 - 4n - 5 = 0$, $n = \frac{1+\sqrt{6}}{2}$

We get $\overline{H} = E_0 \left(\frac{2\sqrt{6}+5}{\pi^2} = 1.0030 \right)$ or about .3% error.

Check wave functions:

$$\overline{H} = \sum |a_n|^2 E_n$$

$$\overline{H} > |a_0|^2 E_0 + \underbrace{\sum_{n>1} |a_n|^2}_{1-|a_0|^2} 9E_0$$

$$\overline{H} > E_0 - (1-|a_0|^2) E_0 + (1-|a_0|^2)\, 9E_0$$

$$1 - |a_0|^2 = \sum_{n>0} |a_n|^2 = \frac{1}{8} \left(\frac{H}{E_0} - 1 \right)$$

Wave function may be quite different from real wave functions yet still give a good approximation to the energy.

Application : He I - like

$$H = -\frac{\hbar^2}{2m}\nabla_1^2 - \frac{\hbar^2}{2m}\nabla_2^2 - \frac{Ze^2}{r_1} - \frac{Ze^2}{r_2} + \frac{e^2}{r_{12}}$$

operating on $u(r_1, r_2)$.

Introduce: $\hbar = 1$, $2m = 1$, $e^2 = 2$

length: $a_0 = \frac{\hbar^2}{me^2}$

Energy: $Rhc = \frac{me^4}{2\hbar^2}$

Then $$H = \underbrace{-\nabla_1^2 - \nabla_2^2 - \frac{2Z}{r_1} - \frac{2Z}{r_2}}_{H_0} + \underbrace{\frac{2}{r_{12}}}_{H'}$$

Thus H_0 now splits up into two H-like cases:

$H = -\nabla^2 - \frac{2Z}{r}$ with ground state as : $\sqrt{\frac{Z^3}{\pi}}\, e^{-Zr}$; $-Z^2$

Transfering to He I-like case :

$$u = \frac{\mathfrak{z}^3}{\pi} e^{-\mathfrak{z}(r_1 + r_2)}$$

LECTURE XXV 11-25-60

Continuation of He I Problem :

We take for the trial function :

$$(1) \quad u = \frac{\mathfrak{z}^3}{\pi} e^{-\mathfrak{z}(r_1 + r_2)}$$

This would be product of spherically symmetric wave functions of two non-interacting electrons.

We can split Hamiltonian into $\overline{H} = \overline{H_0} + \overline{H'}$

(2) $H_0 = H_0(\zeta) - Z(Z-\zeta)\cdot\left(\frac{1}{r_1} + \frac{1}{r_2}\right)$

$H_0(\zeta)\, u = -2\zeta^2 u \quad , \quad \overline{H_0(\zeta)} = -2\zeta^2$

(3) $\overline{\left(\frac{1}{r_1}\right)}_{\zeta} = \int_0^\infty \frac{\zeta^3}{\pi}\frac{1}{r_1} e^{-2\zeta r_1}\, 4\pi r_1^2\, dr_1$

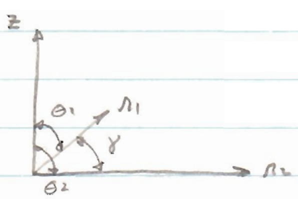
$= 4\int_0^\infty \zeta^3 r_1\, dr_1\, e^{-2\zeta r_1} = \zeta \int_0^\infty x\, dx\, e^{-x} = \zeta$

Therefore:

(4) $\overline{H_0} = -2\zeta^2 - Z(Z-\zeta)\cdot 2\zeta = -2\zeta(2Z - \zeta)$

We can expand $\frac{1}{r_{12}}$ because of spherical symmetry into Legendre Functions:

(5) $\frac{1}{r_{12}} = \sum_{l=0}^{\infty} \frac{r_<^l}{r_>^{l+1}} P_l(\cos\gamma)$



Now: $P_l(\cos\gamma) = \sum_{m=-l}^{l} \frac{(l-|m|)!}{(l+|m|)!} P_l^{|m|}(\cos\theta_1)\, P_l^{|m|}(\cos\theta_2)\, e^{im(\varphi_2-\varphi_1)}$

Since wave functions are independent of any angles, and Legendre functions are orthogonal and all terms except $l=0$ vanish. Thus:

(6) $\overline{\frac{Z}{r_{12}}} = \int u^2 \frac{Z}{r_{12}}\, dr_1\, dr_2 = \frac{2\zeta^6}{\pi^2}\int e^{-2\zeta(r_1+r_2)} \frac{1}{r_>} 4\pi r_1^2 dr_1\, 4\pi r_2^2 dr_2$

$= 2\zeta \int_0^\infty e^{-x_1} x_1^2\, dx_1 \int_{x_1}^\infty e^{-x_2} x_2\, dx_2$

considering first $x_1 < x_2$ and then times two because of possibility $x_1 > x_2$.

(7) $\overline{\left(\frac{Z}{r_{12}}\right)} = \frac{5}{4} \mathfrak{z}$

Finally:

(8) $\bar{H} = -2\mathfrak{z}(2Z - \mathfrak{z}) + \frac{5}{4}\mathfrak{z}$

Taking the minimum:

(9) $\frac{d\bar{H}}{d\mathfrak{z}} = -4Z + 4\mathfrak{z} + \frac{5}{4} = 0 \quad ; \quad \mathfrak{z} = Z - \frac{5}{16}$

with $\bar{H}_{min} = -2\left(Z - \frac{5}{16}\right)^2$

We check this against the ionization energy: He$^+$I :

(10) $E_{ion} = -\bar{H}_{min} - Z^2 = 2\left(Z - \frac{5}{16}\right)^2 - Z^2 = \frac{217}{128}$ (Rydberg units)

= 22.95 ev } 6% (not too bad)

Experimentally 24.46 ev

For Li II : E_{ion} : 2% ; $\bar{H}$: 1.1% } Be4: E_{ion}: ~ 1% ; $\bar{H}$: .5%

We could try another wave function:

(11) $u = c\left\{e^{-\mathfrak{z}_1 r_1 - \mathfrak{z}_2 r_2} + e^{-\mathfrak{z}_1 r_2 - \mathfrak{z}_2 r_1}\right\}$

which leads for He I to: 3% in E_{ion}
1% in $\bar{H}$

The wave functions we have been using have the following properties:

$u(r_1, r_2) = u(r_2, r_1)$ (symmetric)

spectroscopically ^3S

If $u = c\left(e^{-z_1 r_1 - z_2 r_2} - e^{-z_2 r_1 - z_1 r_2}\right)$

$u(r_1, r_2) = -u(r_2, r_1)$ (antisymmetric)

spectroscopically 'S.

Now: $(u_s, u_a) = \int u_s^*(r_1, r_2)\, u_a(r_1, r_2)\, dr_1\, dr_2$

must equal $-\int u_s^*(r_2, r_1)\, u_a(r_2, r_1)\, dr_2\, dr_1$

and thus $(u_s, u_a) = 0$

If one can find this property between successive states, the minimum level for any state can be found.

LECTURE XXVI 11-28-60

Perturbation Theory:

We will use the traditional Schroedinger perturbation theory for stationary states.

(1) $\underline{H}\, u_E = E\, u_E$

Expand u_E in terms of some function v_E;

(2) $u_E = \sum_n C_n(E)\, v_n$

(3) $\sum_n C_n(E)\, \underline{H}\, v_n = E \sum_n C_n(E)\, v_n$

Now perform the operation $\int v_m^* (3)\, d\tau$:

(4) $\sum_n H_{mn} C_n(E) = E\, C_m(E)$

(5) where $H_{mn} = \int v_m^* H v_n \, d\tau$

(6) $C_m(E) = \int v_m^* u_E \, d\tau$

Now:

(7) $\int u_{E'}^* u_E \, d\tau = 0, \quad E' \neq E$ and substituting from (3)

$$\int \sum_{mn} C_m^*(E')\, v_m^* \cdot C_n(E)\, v_n \, d\tau = 0 , \quad E \neq E'$$

or $\sum_n C_n^*(E')\, C_n(E) = 0, \quad E \neq E'$

The C's can be thought of as wave functions in a new representation satisfying equation (4).
In equation (4), we can think of $C_n(E)$ as a column matrix and of H_{mn} as a square matrix and the sum on n as their product.
Recall $\sum_\ell A_{i\ell} B_{\ell j} = C_{ij}$.

Continuing; for discrete spectra, (7) becomes:

(8) $\sum_n C_n^*(E_k)\, C_n(E_\ell) = \delta_{k\ell}$

which is analog of $\int u_{E_k}^* u_{E_\ell} \, d\tau = \delta_{k\ell}$

For degenerate case: $\sum_n C_n^*(E_k, k)\, C_n(E_\ell, \ell) = \delta_{k\ell}$

We then introduce:

(9) $C_n(E_k, k) = \delta_{nk}$

Then (8) becomes:

(8') $\sum_n S^*_{nk} S_{nl} = \delta_{kl}$

(10) or $\sum_n S^+_{kn} S_{nl} = \delta_{kl}$

or $S^+ = S^{-1}$, $S^+ S = 1$

That is, S is a unitary matrix. Sometimes $S^+S \neq SS^+$ but in this case it holds for infinite matrices. We know that H is hermitian and (4) takes the form:

(11) $\sum_n H_{mn} S_{nk} = E_k S_{mk}$

Performing $\sum_m S^+_{lm} \cdot (4)$:

(12) $\sum_{mn} S^+_{lm} H_{mn} S_{nk} = E_k \delta_{kl}$

or $(S^+ H S)_{lk} = E_k \delta_{lk}$

where $E = \begin{pmatrix} E_1 & 0 & 0 & \cdots \\ 0 & E_2 & & \\ 0 & & & \\ \vdots & & & \end{pmatrix}$

or $S^+ H S = E$

which is just the diagonalization of the Hamiltonian.

In the new notation, (2) becomes:

(13) $u_k = \sum_n v_n S_{nk}$

and (6) becomes:

(14) $S_{mk} = \int v^*_m u_k \, dr$

We now go to perturbation theory and take for v_n solutions of an unperturbed problem. Hamiltonian is called $\underline{H}_0$:

(15) $\underline{H_0}\, v_n = E_n^{(0)} v_n$

Case where $E_n^{(0)}$'s are all different:

(16) $\underline{H} = \underline{H_0} + \underline{V}$ where $\underline{V}$ is small compared to the energy of the unperturbed state.

However, we will find that it is easy to expand in terms of a dummy parameter λ which we consider small instead of V

(16') $\underline{H} = \underline{H_0} + \lambda \underline{V}$ (λ called tag)

Expanding E_k as a sum in terms of λ.

(17) $E_k = E_k^{(0)} + \lambda E_k^{(1)} + \lambda^2 E_k^{(2)} + \ldots$

(18) $S_{nk} = \delta_{nk} + \lambda C_{nk}^{(1)} + \lambda^2 C_{nk}^{(2)} + \ldots$

(19) $H_{mn} = E_n^{(0)} \delta_{mn} + \lambda V_{mn}$

Plugging in (11):

(20) $$\sum_n \left(E_n^{(0)} \delta_{mn} + \lambda V_{mn}\right)\left(\delta_{nk} + \lambda C_{nk}^{(1)} + \ldots\right)$$

$$= \left(E_k^{(0)} + \lambda E_k^{(1)} + \ldots\right)\left(\delta_{mk} + \lambda C_{mk}^{(1)} + \ldots\right)$$

We now equate equal powers of λ:

$$E_m^{(0)} \delta_{mk} = E_k^{(0)} \delta_{mk} \qquad (\lambda^0)$$

(21) $$E_m^{(0)} C_{mk}^{(1)} + V_{mk} = E_k^{(0)} C_{mk}^{(1)} + E_k^{(1)} \delta_{mk} \qquad (\lambda^1)$$

(22) $$E_m^{(0)} C_{mk}^{(2)} + \sum_n V_{mn} C_{nk}^{(1)} = E_k^{(0)} C_{mk}^{(2)} + E_k^{(1)} C_{mk}^{(1)} + E_k^{(2)} \delta_{mk}$$

for (λ^2)

These are key equations in the perturbation theory.

LECTURE XXVII 11-30-60

Perturbation Theory:

(11) $$\sum_n H_{mn} S_{nk} = E_k S_{mk}$$

(16) $$H = H_0 + V$$

We are considering non-degenerate perturbation theory.

Putting $m = k$ in (21):

(23) $$E_k^{(1)} = V_{kk}$$ First order correction

For $m \neq k$ in (21):

(24) $$C_{mk}^{(1)} = \frac{V_{mk}}{E_k^{(0)} - E_k^{(0)}}$$

or $$u_k = v_k + \sum_{m \neq k} v_m \frac{V_{mk}}{E_k^{(0)} - E_m^{(0)}}$$

We form the normalization integral:

(25) $$\int u_k^* u_k \, d\tau = \int \left(v_k^* + \sum_m C_{mk}^{*(1)} v_m^* + \cdots\right)\left(v_k + \sum_m C_{mk}^{(1)} v_m + \cdots\right) d\tau = 1$$

(26) $1 + C_{kk}^{(1)} + C_{kk}^{*(1)} = 1$, Thus $C_{kk}^{(1)}$ is pure imaginary

and $u_k = v_k(1 + i\delta) + \sum_{m \neq k} \sim\!\sim + \cdots$

(27) We can then stipulate $C_{kk}^{(1)} = 0$

Consider $m = k$ in (22):

(28) $$E_k^{(2)} = \sum_{n \neq k} \frac{V_{kn} V_{nk}}{E_k^{(0)} - E_n^{(0)}}$$

If $E_n^{(0)}$ below $E_k^{(0)}$ then (28) is negative and $E_k^{(0)}$ tends to rise. If $E_n^{(0)}$ above $E_k^{(0)}$, opposite effect occurs.

We see that the levels seem to repel each other in second order perturbation theory.

Degenerate Perturbation Theory:

(15') $H_0 v_{n,\alpha} = E_n^{(0)} v_{n,\alpha}$, $\alpha = 1, 2, \cdots g_n$

(11') $$\sum_{n,\beta} H_{m,\alpha;n,\beta} S_{n,\beta;k,\gamma} = E_{k,\gamma} S_{m,\alpha;k,\gamma}$$

(18') $$S_{n,\beta;k,\gamma} = \delta_{nk} S_{\beta\gamma}(k) + \lambda C_{n,\beta;k,\gamma}^{(1)} + \cdots$$

(17') $$E_{k,\gamma} = E_{k,\gamma}^{(0)} + \lambda E_{k,\gamma}^{(1)} + \lambda^2 E_{k,\gamma}^{(2)} + \cdots$$

(19') $$H_{m,\alpha;n,\beta} = E_m^{(0)} \delta_{mn} \delta_{\alpha\beta} + \lambda V_{m,\alpha;n,\beta}$$

$$\sum_{n,\beta} \left[E_m^{(0)} \delta_{mn} \delta_{\alpha\beta} + \lambda V_{m,\alpha;n,\beta} \right] \left[\delta_{nk} S_{\beta\gamma}(k) + \lambda C^{(1)}_{n,\beta;k\gamma} + \cdots \right]$$

$$= \left(E_k^{(0)} + \lambda E^{(1)}_{k,\gamma} + \cdots \right) \left(\delta_{mk} S_{\alpha\gamma}(k) + \lambda C^{(1)}_{m,\alpha;k,\gamma} + \cdots \right)$$

0th order: $E_m^{(0)} \delta_{mk} S_{\alpha\gamma}(k) = E_k^{(0)} \delta_{mk} S_{\alpha\gamma}(k)$

(21') 1st order: $E_m^{(0)} C^{(1)}_{m,\alpha;k,\gamma} + \sum_\beta V_{m,\alpha;k,\beta} S_{\beta\gamma}(k)$

$$= E_k^{(0)} C^{(1)}_{m,\alpha;k,\gamma} + \delta_{mk} S_{\alpha\gamma}(k) E^{(1)}_{k,\gamma}$$

Set $m = k$:

(29) $$\sum_{\beta=1}^{g_k} \left\{ V_{k,\alpha;k,\beta} - E^{(1)}_{k,\gamma} \delta_{\alpha\beta} \right\} S_{\beta\gamma}(k) = 0, \quad \alpha = 1, 2, 3, \cdots g_k$$

For fixed γ: we have g_k equations in g_k unknowns which are homogeneous and linear, thus determinant vanishes.

(30) $$\begin{vmatrix} V_{k,1;k,1} - E^{(1)}_{k,\gamma} & V_{k,1;k,2} & V_{k,1;k,3} & \cdots \\ V_{k,2;k,1} & V_{k,2;k,2} - E^{(1)}_{k,\gamma} & V_{k,2;k,3} & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{vmatrix} = 0$$

This is the secular equation. If all roots are unequal, the perturbation has removed the degeneracy.

LECTURE XXVIII   12-2-60

Continuation of Perturbation Theory:

Additional Equation:

(22') $E_m^{(0)} C_{m,\alpha;k\gamma}^{(2)} + \sum_{n\beta} V_{m,\alpha;n,\beta} C_{n,\beta;k,\gamma}^{(1)}$

$$= E_k^{(0)} C_{m,\alpha;k,\gamma}^{(2)} + E_{k,\gamma}^{(1)} C_{m,\alpha;k,\gamma}^{(1)} + \delta_{mk} E_{k,\gamma}^{(2)} S_{\alpha\gamma}(k)$$

If some roots of the secular equation are equal, the first order perturbation has not completely removed the degeneracy. Suppose the original degeneracy of $E_k^{(0)}$ is g_k, with f remaining degeneracy of level k, $\left\{ \begin{matrix} \gamma = 1 \\ \gamma = 2 \\ \gamma = f \end{matrix} \right\}$. We can form $E_{k,\gamma,A}^{(1)}$ independent of A, $A = 1, \ldots f$.

Solving (21') with $m \neq k$

(31) $$C_{m,\alpha;k,\gamma}^{(1)} = \frac{\sum_\beta V_{m\alpha;k\beta} S_{\beta\gamma}}{E_k^{(0)} - E_m^{(0)}}$$

Examine: $\sum_\beta \int v_{m\alpha}^* V v_{k,\beta} S_{\beta\gamma} \, dr$

$w_{k\gamma}$ = right linear combination

If we choose right combinations to begin with, the secular equation will be diagonal. How is this done? Examine symmetry, since this is what gives rise to degeneracy originally.

Second Order Degenerate Perturbation Correction:

Use (22') with $m = k$

(32) $$\sum_{n,\beta} \left\{ V_{k,\alpha;\,n,\beta} - \delta_{kn}\delta_{\alpha\beta} E^{(1)}_{k,\gamma} \right\} C^{(1)}_{n\beta;\,k\gamma} = E^{(2)}_{k,\gamma} S$$

(33) $$\sum_{\beta} \left\{ V_{k,\alpha;\,k,\beta} - \delta_{\alpha\beta} E^{(1)}_{k,\gamma} \right\} C^{(1)}_{k\beta;\,k\gamma}$$

$$= - \sum_{\substack{n \neq k \\ \beta\,\delta}} \frac{V_{k,\alpha;\,n\beta} V_{n\beta;\,k\delta} S_{\delta\gamma}(k)}{E^{(0)}_{k} - E^{(0)}_{n}} + E^{(2)}_{k\gamma} S_{\alpha\gamma}(k)$$

In trying to solve this by determinential methods, we find that the determinant is zero. That is:

$$\sum a_{ik} x_k = b_i \quad \text{with} \quad |a_{ik}| = 0$$

There is a general algebraic theorem that states that in general no solution exists except in special cases which we might have here. Consider transposed equation:

$$\sum y_i a_{il} = 0, \quad \text{thus the condition } \sum_i b_i y_i = 0$$

for all y_i is necessary.

Proof: $$\sum_i y_i \sum a_{ik} x_k = \sum_i b_i y_i = 0$$

Notice that if a is Hermitian, then we could write:

$$\sum_i a^*_{li} y_i = 0, \quad \sum_i a_{li} y_i^* = 0$$

We write:

$$\sum_{\alpha} S^{\dagger}_{\gamma'\alpha} \sum_{\delta} \left\{ \sum_{\substack{n \neq k \\ \beta}} \frac{V_{k\alpha;\,n\beta} V_{n\beta;\,k\delta}}{E^{(0)}_{k} - E^{(0)}_{n}} - E^{(2)}_{k\gamma} \delta_{\alpha\delta} \right\} S_{\delta\gamma}(k) = 0$$

because all degeneracy may not have been removed

all γ' with $E^{(1)}_{k\gamma'} = E^{(1)}_{k\gamma}$

If there is only one such γ', that is $\gamma' = \gamma$, we have when the first order has removed all degeneracies:

$$E^{(2)}_{k\gamma} = \sum_{\alpha\beta\delta} \sum_{n\neq k} \frac{S_{\gamma\alpha}(k)\, V_{k,\alpha;n,\beta}\, V_{n\beta;k\delta}\, S_{\delta\gamma}(k)}{E_k^{(0)} - E_n^{(0)}}$$

which reduces to the second order non-degenerate upon choosing proper combinations.

If some degeneracy remains, we have a second order secular equation: First of all, change notation:

$$\gamma \rightarrow \gamma, A \quad , \quad S_{\delta\gamma}(k) \Rightarrow S_{\delta;\gamma A}(k) \longrightarrow \sum_B S_{\delta;\gamma B}(k)\, S_{BA}(k,\delta)$$

since there might still be some degeneracy left. Thus we have:

$$\sum_{\substack{\alpha\beta \\ C}} S^{+}_{AB}(k,\gamma)\, S^{+}_{\gamma,\beta;\alpha}(k) \sum_{\delta} \left\{ \quad \right\} S_{\delta,\gamma C}(k)\, S_{CD}(k,\gamma)$$

which gives the secular equation: Define $\sum_{\delta} v_{k\delta} S_{\delta\gamma C} = \omega_{k(\gamma,C)}$

$$\begin{vmatrix} \sum_{\substack{n\neq k \\ \beta}} \frac{V_{k(\gamma,1);n\beta}\, V_{n\beta;k(\gamma,1)}}{E_k^{(0)} - E_n^{(0)}} - E^{(2)}_{k,\gamma A} & \sum_{\substack{n\neq k \\ \beta}} \frac{V_{k,(\gamma,1);n,\beta}\, V_{n,\beta;k(\gamma,2)}}{E_k^{(0)} - E_n^{(0)}} & \cdots \\ \vdots & \vdots & \end{vmatrix} = 0$$

LECTURE XXIX   12-5-60

Applications of Perturbation Theory:

Example: Perturbed Harmonic Oscillator:

(1) $H_0 = -\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} + x^2 + y^2$

Consider $-\frac{d^2}{dx^2} + x^2$; $n = 0, 1, 2$
$E^{(0)} = 1, 3, 5$

$$\left(-\frac{d^2}{dx^2} + x^2\right) e^{-x^2/2} = e^{-x^2/2}$$

with $x_{n,m} = \sqrt{\frac{n}{2}}\, \delta_{m,n-1} + \sqrt{\frac{n+1}{2}}\, \delta_{m,n+1}$

Extending to two dimensions, we have:

$v_{kl} = v_k(x)\, v_l(y)$ (unperterbed wave functions)

with $E^{(0)} = 2, 4, 6, \ldots$

- 2: v_{00}
- 4: 2 fold deg. → v_{01}, v_{10}
- 6: 3 fold deg. → v_{20}, v_{11}, v_{02}

(2) Consider perturbing potential $V = axy$
Then:

$V_{00;00} = 0$; $E^{(1)}_{00} = 0$

$$E^{(2)}_{00} = \sum_{mn} \frac{|V_{00;mn}|^2}{E^{(0)}_{00} - E^{(0)}_{mn}}$$

where: $V_{00;mn} = \iint v_m(x)\, v_n(y) \cdot axy \cdot v_0(x)\, v_0(y)\, dx\, dy$

$$= a \int v_m(x)\, x\, v_0(x)\, dx \cdot \int v_n(y)\, y\, v_0(y)\, dy$$

where $\int v_m(x)\, x\, v_0(x)\, dx \to x_{m,0}$ and $\int v_n(y)\, y\, v_0(y)\, dy \to y_{n,0}$

Then $E_{00}^{(2)} = \dfrac{a^2 \left| \sqrt{\frac{1}{2}} \sqrt{\frac{1}{2}} \right|^2}{2-6} = -\dfrac{a^2}{16}$

We then have so far: $E_{0,0} = 2 - \dfrac{a^2}{16} + \cdots$

Going to the next state: (2 fold degenerate)

$V_{10,10} = V_{01,01} = 0$

$V_{10,01} = V_{01,10} = \dfrac{a}{2}$

Then the secular equation is

$$\begin{vmatrix} -E^{(1)} & \frac{a}{2} \\ \frac{a}{2} & -E^{(1)} \end{vmatrix} = 0$$

; $\therefore$ $E^{(1)} = \frac{a}{2}, -\frac{a}{2}$, thus the degeneracy is removed in the first order, giving the levels: $E = 4 + \frac{a}{2}$; $E = 4 - \frac{a}{2}$

What are the proper combination of wave functions?
The equations which gave the determinant are:

(3) $-E^{(1)} S^{\beta}_{10,\gamma} + \frac{a}{2} S_{01,\gamma} = 0$

(4) $\frac{a}{2} S_{10,\gamma} - E^{(1)} S_{01,\gamma} = 0$

The correct wave functions will be of the form:
$w_\gamma = v_{10} S_{10,\gamma} + v_{01} S_{01,\gamma}$

Plug in $E^{(1)} = \frac{a}{2}$ in (3) and (4) and see that

$S_{10,\gamma} = S_{10,\gamma}$

Then $w_{\{0,1\}} = \dfrac{1}{\sqrt{2}} (v_{10} + v_{01})$

Now using $E^{(1)} = -\frac{a}{2}$; $S_{01,\gamma} = -S_{10,\gamma}$

we get $\omega_{[0,1]} = \frac{1}{\sqrt{2}}(v_{10} - v_{01})$

The $\{\ \}$, $[\ ]$ denote anti-commutation and comutation symbology respectively. Thus the energies are :

$$E_{\{0,1\}} = 4 + \frac{a}{2} \quad ; \quad E_{[0,1]} = 4 - \frac{a}{2}$$

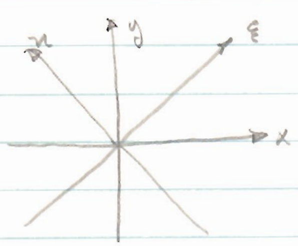
Now $$E^{(2)}_{\{0,1\}} = \sum_{mn}{}' \frac{|V_{\{0,1\};mn}|^2}{4 - E^{(0)}_{mn}} = \frac{2\left|\frac{1}{\sqrt{2}}\sqrt{\frac{2}{2}}\sqrt{\frac{1}{2}}\right|^2 a^2}{4-8} = -\frac{a^2}{8}$$

$$\therefore E_{\{0,1\}} = 4 + \frac{a}{2} - \frac{a^2}{8} \quad ; \quad E_{[0,1]} = 4 - \frac{a}{2} - \frac{a^2}{8}$$

No splitting as degeneracy is completely removed in first order

Exact Solution:

We have : $$x^2 + y^2 + axy = \left(1+\tfrac{a}{2}\right)\underbrace{\frac{(x+y)^2}{2}}_{\xi} + \underbrace{\frac{(x-y)^2}{2}}_{\eta}\left(1 - \frac{a}{2}\right)$$



We can solve in ξ and η co-ordinates and get for the energy:

$$E = \sqrt{1+\tfrac{a}{2}}\,(2n_\xi + 1) + \sqrt{1-\tfrac{a}{2}}\,(2n_\eta + 1)$$

with $$\sqrt{1+\tfrac{a}{2}} = 1 + \frac{a}{4} - \frac{a^2}{32} + \dots$$

$$\sqrt{1-\tfrac{a}{2}} = 1 - \frac{a}{4} - \frac{a^2}{32} - \dots$$

$\left.\begin{matrix} n_\xi = 1 \\ n_\eta = 0 \end{matrix}\right\}$ $4 + \frac{a}{2} - \frac{a^2}{8}$

so we get in the first few terms the same energy as obtained by perturbation treatment.

Now consider example where first order perturbation does not completely remove the degeneracy:

(5) $H_0 = -\nabla^2 + r^2 = H_x + H_y + H_z$

with $E^{(0)} =$

3	5	7
000	100, 010, 001	200, 020, 002 110, 101, 011

Choose for perturbing potential:

(6) $V = 2a\,(xy + yz)$

and we have: $E_{000} = 3 + 0 + \cdots$

thus we consider second order:

(7) $E^{(2)}_{\substack{000\\110\\011}} = 2\,\dfrac{|2a \cdot \frac{1}{2}|^2}{-4} = -\dfrac{a^2}{2}$

so that $E_{000} = 3 + 0 - \dfrac{a^2}{2}$

Now consider next states We set up secular equation:

	100	010	001
100	$-E^{(1)}$	a	0
010	a	$-E^{(1)}$	a
001	0	a	$-E^{(1)}$

$= 0$; $E^{(1)}\left(2a^2 - E^{(1)2}\right) = 0$,

$E^{(1)} = 0,\ +\sqrt{2a^2},\ -\sqrt{2a^2}$

Thus for this level, the first order removes the degeneracy

We now form the proper wave functions:
Using the same procedure as before, we have:

$0: \quad c_{010} = 0 \quad ; \quad w_{(100)} = \dfrac{1}{\sqrt{2}}\left(v_{100} - v_{001}\right)$

$+\sqrt{2}\,a$: $-\sqrt{2}\,c_{100} + c_{010} = 0$

$c_{010} - \sqrt{2}\,c_{001} = 0$

then: $\omega_{(1\sqrt{2}a))} = \frac{1}{2}\left(v_{100} + \sqrt{2}\,v_{010} + v_{001}\right)$

$-\sqrt{2}\,a$: $\omega_{(1-\sqrt{2}a))} = \frac{1}{2}\left(v_{100} - \sqrt{2}\,v_{010} + v_{001}\right)$

LECTURE XXX   12-7-60

Recall for one dimension:

$$H_x = -\frac{d^2}{dx^2} + x^2$$

eigenvalues: $2n+1$
matrix elements: $\sqrt{\frac{n_>}{2}}$

In three dimensions:

$$H_0 = H_x + H_y + H_z \quad ; \quad V = 2a\,(xy + yz)$$

eigenvalues: 3, 5, 7, ...

For the eigenvalue 7:

$$\sum_{\Sigma n'=2} \left\{ V_{n_x n_y n_z;\, n_x' n_y' n_z'} - E^{(1)}_{(7)\gamma}\, \delta^{(3)}_{nn'} \right\} \underbrace{S_{n_x' n_y' n_z';\,\gamma}}_{C_{n_x' n_y' n_z'}} = 0$$

from equation (29) of the general treatment. The c's form:

$$\omega = \sum_{\Sigma n=2} v_{n_x n_y n_z}\, C_{n_x n_y n_z}$$

with $v_{n_x n_y n_z} = u_{n_x}(x)\, u_{n_y}(y)\, u_{n_z}(z)$

	011	101	110	200	020	002
011	$-E^{(1)}$	a	0	0	$\sqrt{2}\,a$	$\sqrt{2}\,a$
101	a	$-E^{(1)}$	a	0	0	0
110	0	a	$-E^{(1)}$	$\sqrt{2}\,a$	$\sqrt{2}\,a$	0
200	0	0	$\sqrt{2}\,a$	$-E^{(1)}$	0	0
020	$\sqrt{2}\,a$	0	$\sqrt{2}\,a$	0	$-E^{(1)}$	0
002	$\sqrt{2}\,a$	0	0	0	0	$-E^{(1)}$

$= 0$

Operations: $-\sqrt{2} \times$ 2nd column + 5th column

$$\begin{vmatrix} -E^{(1)} & a & 0 & 0 & 0 & \sqrt{2}\,a \\ a & -E^{(1)} & a & 0 & \sqrt{2}\,E^{(1)} & 0 \\ 0 & a & -E^{(1)} & \sqrt{2}\,a & 0 & 0 \\ 0 & 0 & \sqrt{2}\,a & -E^{(1)} & 0 & 0 \\ \sqrt{2}\,a & 0 & \sqrt{2}\,a & 0 & -E^{(1)} & 0 \\ \sqrt{2}\,a & 0 & 0 & 0 & 0 & -E^{(1)} \end{vmatrix}$$

$\sqrt{2} \times$ 5th row + (2nd row)

$$-E^{(1)} \begin{vmatrix} -E^{(1)} & a & 0 & 0 & \sqrt{2}\,a \\ 3a & -E^{(1)} & 3a & 0 & 0 \\ 0 & a & -E^{(1)} & \sqrt{2}\,a & 0 \\ 0 & 0 & \sqrt{2}\,a & -E^{(1)} & 0 \\ \sqrt{2}\,a & 0 & 0 & 0 & -E^{(1)} \end{vmatrix}$$

$\frac{\sqrt{2}\,a}{E_{(1)}}$ (5th row) + (1st row)

$$-E^{(1)2} \begin{vmatrix} \frac{2a^2}{E^{(1)}} - E^{(1)} & a & 0 & 0 \\ 3a & -E^{(1)} & 3a & 0 \\ 0 & a & -E^{(1)} & \sqrt{2}\,a \\ 0 & 0 & \sqrt{2}\,a & -E^{(1)} \end{vmatrix}$$

$\frac{\sqrt{2}\,a}{E^{(1)}}$ (4 th row) + (3rd row)

$$- E^{(1)3} \begin{vmatrix} \frac{2a^2}{E^{(1)}} - E^{(1)} & a & 0 \\ 3a & -E^{(1)} & 3a \\ 0 & a & \frac{2a^2}{E^{(1)}} - E^{(1)} \end{vmatrix}$$

with the result that:

$$E^{(1)2} \left(2a^2 - E^{(1)2}\right)\left[2a^2 - E^{(1)2} + 6a^2\right] = 0$$

$$E^{(1)} = 0,\ 0,\ \sqrt{2}\,a,\ -\sqrt{2}\,a,\ 2\sqrt{2}\,a,\ -2\sqrt{2}\,a$$

so that the first order perturbation has not completely removed the degeneracy. We now examine the c's:

$E^{(1)} = 0$: $c_{011} = 0$ $\quad c_{110} = 0$ (6th and 4th)

nothing (2nd and 5th)

$c_{101} + \sqrt{2}\,c_{020} + \sqrt{2}\,c_{002} = 0$ (1st and 3rd)

$c_{101} + \sqrt{2}\,c_{200} + \sqrt{2}\,c_{020} = 0$ "

or $c_{002} = c_{200}$ "

We now have one equation left in three unknowns so we choose two of them.

Choose: $c_{101} = 0$:

$$\varphi_1 = \frac{1}{\sqrt{3}}\left(v_{200} - v_{020} + v_{002}\right)$$

Choose: $c_{020} = 0$:

$$\varphi_2 = \frac{1}{2}\left(\sqrt{2}\,v_{101} - v_{200} - v_{002}\right)$$

However φ_1, φ_2 although normal, are not orthogonal.

Take $\psi_1 = \varphi_1$

$$\varphi_2 - (\varphi_1, \varphi_2)\,\varphi_1 = \frac{\sqrt{2}}{2} v_{101} - \frac{1}{2} v_{200} - \frac{1}{2} v_{002} + \frac{1}{3}\left(v_{200} - v_{020} + v_{002}\right)$$

or $\varphi_2 = \sqrt{\frac{3}{4}}\, v_{101} - \sqrt{\frac{1}{24}}\, v_{200} - \sqrt{\frac{1}{6}}\, v_{020} - \sqrt{\frac{1}{24}}\, v_{002}$

upon normalizing $\varphi_2 - (\varphi_1, \varphi_2)\varphi_1$ with $\sqrt{\frac{3}{2}}$

We can now form from equation (39) in the general treatment the determinant for $E^{(2)}$.

Combinations of φ and v:

	211	112	310	013	130	031
101	$\sqrt{2}a$	$\sqrt{2}a$	0	0	0	0
$\frac{1}{\sqrt{3}}$ 200	a	0	$\sqrt{3}a$	0	0	0
$-\frac{1}{\sqrt{3}}$ 020	0	0	0	0	$\sqrt{3}a$	$\sqrt{3}a$
$\frac{1}{\sqrt{3}}$ 002	0	a	0	$\sqrt{3}a$	0	0
φ_1	$\frac{a}{\sqrt{3}}$	$\frac{a}{\sqrt{3}}$	a	a	$-a$	$-a$
Similarly, φ_2	$5a/\sqrt{24}$	$5a/\sqrt{24}$	$-a/\sqrt{8}$	$-a/\sqrt{8}$	$-a/\sqrt{2}$	$-a/\sqrt{2}$

Then:

$$\sum_n |V_{n;(\varphi_1)}|^2 = 4\tfrac{2}{3}a^2 \qquad \times -\tfrac{1}{4}: \quad -\tfrac{7}{6}a^2$$

$$\sum_n |V_{n;(\varphi_2)}|^2 = \frac{10}{3}a^2 \qquad -\frac{5}{6}a^2$$

$$\sum (\text{cross products}) = \frac{8a^2}{3\sqrt{2}} \qquad -\frac{2a^2}{3\sqrt{2}}$$

so:

$$\begin{vmatrix} -\frac{7}{6}a^2 - E^{(2)} & -\frac{\sqrt{2}a^2}{3} \\ -\frac{\sqrt{2}a^2}{3} & -\frac{5}{6}a^2 - E^{(2)} \end{vmatrix} = 0 \qquad (\text{columns } c_1, c_2)$$

$E^{(2)} = -\frac{3}{2}a^2,\ -\frac{1}{2}a^2$, degeneracy removed

The correct wave functions $(c_1\varphi_1 + c_2\varphi_2)$ are:

$$u_{7,0;1} = \frac{\sqrt{2}\,\varphi_1 + \varphi_2}{\sqrt{3}}\ ; \quad u_{7,0;2} = \frac{-\varphi_1 + \sqrt{2}\,\varphi_2}{\sqrt{3}} = \varphi_2!$$

LECTURE XXXI 12-9-60

Exact solution:

$$H = -\nabla^2 + \underbrace{x^2 + y^2 + z^2 + 2axy + 2ayz}_{Q}$$

We now diagonalize Q

$$\begin{vmatrix} 1-\lambda & a & 0 \\ a & 1-\lambda & a \\ 0 & a & 1-\lambda \end{vmatrix} = 0$$

$$(1-\lambda)\left[(1-\lambda)^2 - 2a^2\right] = 0$$

$$\lambda = 1 \,,\; 1+\sqrt{2}\,a \,,\; 1-\sqrt{2}\,a$$

We can now separate the variables in the Schroedinger Equation and get:

$$E = 2n_1+1 + (2n_2+1)\left[1+\sqrt{2}\,a\right]^{1/2} + (2n_3+1)\left[1-\sqrt{2}\,a\right]^{1/2}$$

which will give perturbation results on expansion of radicals.

The perturbation theory presented here is that of Schroedinger's but others can be developed.

Recall: $\sum_n H_{mn} S_{nk} = E_k S_{mk}$

or $(S^{+} H S)_{\ell k} = E_k \delta_{\ell k}$

We wanted to find E_k's that diagonalized H.

If there were a finite number of states, one could set the determinant equal to zero. However, here we have infinite determinants:

$$\begin{vmatrix} H_{11} - E & H_{12} & \cdots \\ H_{21} & H_{22} - E & \\ \vdots & \vdots & \end{vmatrix} = 0$$

We can split off segments if the process has a limit. We can use this if we are discussing peretorbations between close levels.

The WKB Method (Wentzel, Kramers, Brillouin)

Really discovered by Jeffrey's and Poincaré.

Landau-Lifshitz call this the quasi-classical method. We can look a wave function and estimate its wavelength, writing,

$$\lambda = \frac{\hbar}{p} \quad , \text{ still having } \quad p = \sqrt{2m(E-V)}$$

where $E-V$ does not change much over the wave function's wavelength λ.

$$\lambda = \frac{\hbar}{p} = \frac{h}{\sqrt{2m(E-V)}}$$

(1) The condition we need is $\frac{|\nabla\lambda|}{\lambda} \cdot \lambda = |\nabla\lambda| << 1$

Consider the general wave equation:

(2) $$H\left(q, \frac{\hbar}{i}\frac{\partial}{\partial q}\right)\psi + \frac{\hbar}{i}\frac{\partial\psi}{\partial t} = 0$$

Now focus attention of phase of wave function:

(3) $\psi = e^{iS}$, S_0 is Hamilton's principle function.

Now suppose this approximation can be expanded in powers of $\hbar$ if $\hbar$ is sufficiently small.

(4) $S = \hbar^{-1} S_0 + \frac{1}{i} S_1 + \frac{\hbar}{i^2} S_2 + \cdots$, S's are real

Now substitute in ψ and then in wave equation:
Take coefficients of $\hbar^0$:

(5) $H\left(q, \frac{\partial S_0}{\partial q}\right) + \frac{\partial S_0}{\partial t} = 0$ (Hamilton-Jacobi Equation)

We can now do this for other powers of $\hbar$.
First, write:

(6) $-\frac{\hbar^2}{2m} \nabla^2 \psi + V\psi + \frac{\hbar}{i} \frac{\partial \psi}{\partial t} = 0$

For $\hbar^0$:

(7) $\frac{1}{2m} (\nabla S_0)^2 + V + \frac{\partial S_0}{\partial t} = 0$ (H-J equation again)

Now for $\hbar^1$:

(8) $-\frac{i}{2m} \nabla^2 S_0 + \frac{1}{im} (\nabla S_0)\cdot(\nabla S_1) + \frac{1}{i} \frac{\partial S_1}{\partial t} = 0$

(9) In classical mechanics, S_0 is unit of action, and $\nabla S_0 \rightarrow \bar{p}$

In quantum mechanics, for the probability density:

(10) $\rho = |\psi|^2 \simeq e^{2S_1}$

Now form $2i e^{2S_1}$ (8)

(11) $\frac{1}{m} \rho \nabla \cdot \bar{p} + \frac{\bar{p}}{m} \cdot \nabla \rho + \frac{\partial \rho}{\partial t} = 0$

Now this equation reduces to:

(12) $$\nabla\cdot(\rho\bar{v}) + \frac{\partial\rho}{\partial t} = 0$$

which is the equation of continuity of probability flow. Hamilton first used this to approximate physical optics with geometric optics and the analogy carries over.

LECTURE XXXII 12-12-60

Continuation of WKB Method:

(13) $$-\frac{\hbar^2}{2m}\frac{d^2u}{dx^2} + (V-E)u = 0$$, for stationary states.

$$u = e^{iS/\hbar}$$

This method gives classical mechanics in the 0th approximation, Bohr-Sommerfeld in the 1st, and corrections leading to wave mechanics in higher orders.

(14) $$S = S_0 + \frac{\hbar}{i}S_1 + \cdots$$

(15) $$\frac{1}{2m}\left(\frac{dS_0}{dx}\right)^2 + (V-E) = 0$$ (Hamilton-Jacobi Equation)

or $$\frac{dS_0}{dx} = \pm\sqrt{2m(E-V)}$$, or $$\frac{dS_0}{dx} = \pm p$$

For $E > V$:

(16) $$S_0 = \text{constant} \pm \int\sqrt{2m(E-V)}\,dx$$

For $E < V$:

(17) $$S_0 = \text{constant} \pm i\int\sqrt{2m(V-E)}\,dx$$

The WKB method is not good near the turning point as V-E varies rapidly. This shows up as a singularity in the solution.

In the next approximation:

(18) $$-\frac{i}{2m}\frac{d^2S_0}{dx^2} - \frac{i}{2m}2\frac{dS_0}{dx}\cdot\frac{dS_1}{dx} = 0$$

We get:

(19) $$\frac{S_0''}{S_0'} = -2S_1'$$

$$-\tfrac{1}{2}\log S_0' + \text{constant} = S_1$$

or $$-\tfrac{1}{4}\log 2m|(E-V)| + \text{constant} = S_1$$

for $E > V$, or $E < V$ since the $i\pi$ goes into the constant. We can even through the $2m$ into the constant or write it any way we please, such as:

$$S_1 = -\tfrac{1}{4}\log \frac{2|E-V|}{m} + \text{constant}$$

Thus:

(20) $$e^{S_1} = \frac{\text{constant}}{\left(\frac{2|E-V|}{m}\right)^{1/4}} \; ; \; u = e^{\frac{iS_0}{\hbar} + S_1}$$

(21) $$u = \left[\frac{2(E-V)}{m}\right]^{-1/4} \left\{ A e^{\left(\frac{i}{\hbar}\right)\int^x \sqrt{2m(E-V)}\,dx} + B e^{-\left(\frac{i}{\hbar}\right)\int^x \sqrt{2m(E-V)}\,dx} \right\}$$

for $E > V$.

For $V > E$:

(22) $$u = \left[\frac{2(V-E)}{m}\right]^{-1/4} \left\{ C e^{\frac{1}{\hbar}\int^x \sqrt{2m(V-E)}\,dx} + D e^{-\frac{1}{\hbar}\int^x \sqrt{2m(V-E)}\,dx} \right\}$$

Consider:

(23) $$j = \frac{\hbar}{2mi}\left(u^* \frac{d}{dx} u - u \frac{d}{dx} u^*\right)$$

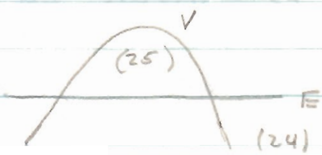
Upon substitution of (21) into (23); we get, after tedious calculation:

(24) $j = |A|^2 - |B|^2$

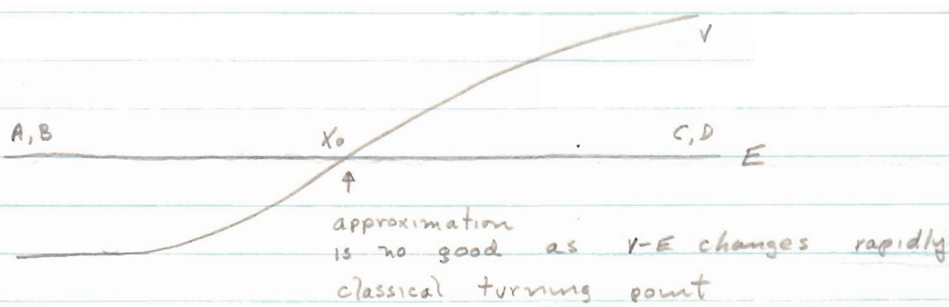
The amount of flux to left and right are constant. This means that in this approximation there is no reflection for smooth, slowly changing potentials. Analogous to slowly changing index of refraction in optics, where bending of light occurs.

Upon substitution of (22) into (23):

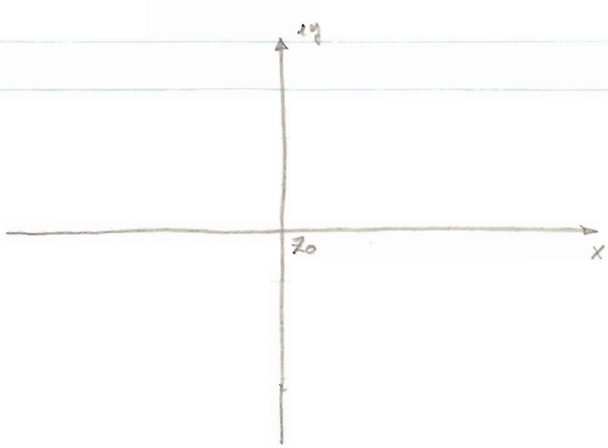
(25) $j = i\left(C^*D - CD^*\right)$



The problem is now to find the relation between A, B, C, D:



Consider manipulation in the complex plane:



Although x_0 is a singular point of the approximation, it is not in the actual solution. The fact that the constants change over the plane is called Stoke's phenomenon.

We write:

$$\frac{d^2u}{dz^2} + k^2 [y(z) + \lambda] u = 0$$

where $k^2 = \frac{2m}{\hbar^2} E_0$, $y(z) = -\frac{V}{E_0}$, $\lambda = \frac{E}{E_0}$

where the approximation is now for k^2 large or $|kw| >> 1$, where w is the distance from the turning point.

Now $y(z_0) + \lambda = 0$ at the turning point.
w is given by:

$$w = \int_{z_0}^{z} (y + \lambda)^{1/2} dz$$

$(y + \lambda)^{1/2} > 0$ on the real axis near z_0, where $y + \lambda > 0$. Then u is:

$$u \sim \frac{A e^{ikw} + B e^{-ikw}}{(y+\lambda)^{1/4}}$$

LECTURE XXXIII 12-14-60

Recall:

$$\frac{d^2u}{dz^2} + k^2 [y(z) + \lambda] u = 0$$

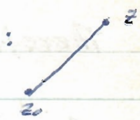
$$k^2 = \frac{2m}{\hbar^2} E_0 , \quad y = -\frac{V}{E_0} , \quad \lambda = \frac{E}{E_0}$$

giving in the asymptotic solution:

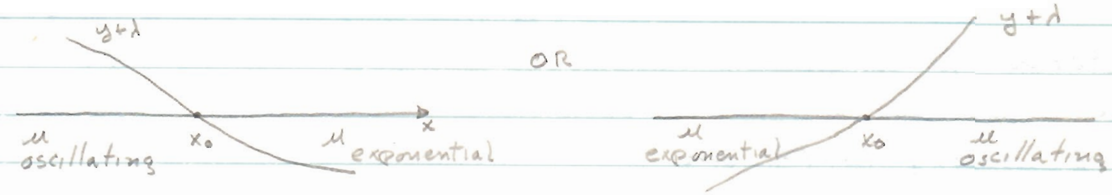
$$u \sim (y + \lambda)^{-1/4} (A e^{ikw} + B e^{-ikw})$$

(far from z_0: $y(z_0) + \lambda = 0$)

where $\omega = \pm\int_{z_0}^{z} (y+\lambda)^{1/2}\, dz$ along a straight line:

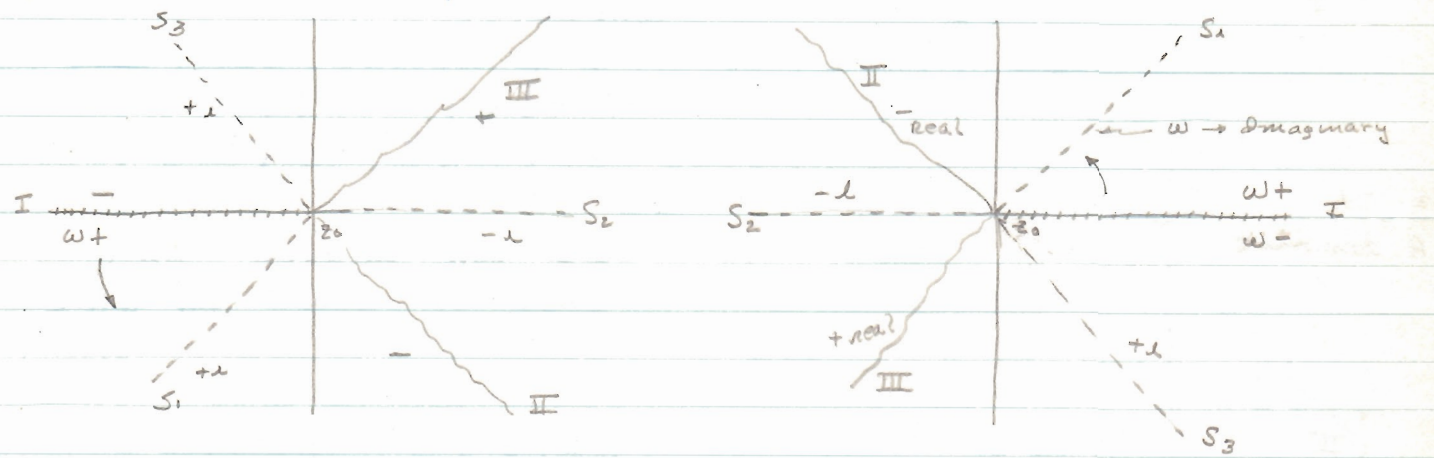


Now the plot of $y+\lambda$ vs x gives two curves:



do not confuse these diagrams with behavior of V.

Now go into the complex z plane. the following diagrams indicate the behaviour of ω as one circumvents the branch point z_0.



We pick the sign of the square root in ω to make ω positive. We write $\omega+$ above and below the real axis because the plane must be cut. We make the cut as shown. Expand $y+\lambda$ in Taylor series about z_0:

$$y+\lambda = 0 + y'(z_0)(z-z_0) + \cdots$$

$$(y+\lambda)^{1/2} = \left(y'(z_0)\right)^{1/2} (z-z_0)^{1/2} + \cdots$$

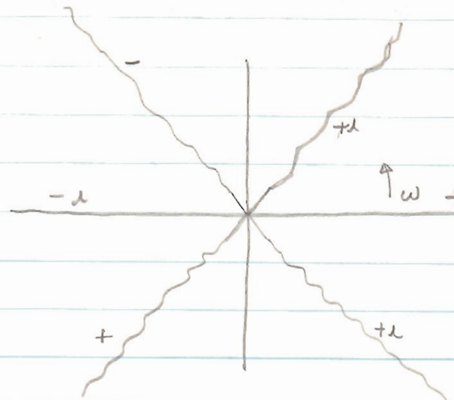
Then:

$$\omega = \int_{z_0}^{z} \left[(y'(z_0))^{1/2} (z-z_0)^{1/2} + \cdots \right] dz$$

$$= \frac{2}{3} \left(y'(z_0)\right)^{1/2} (z-z_0)^{3/2} + \cdots$$

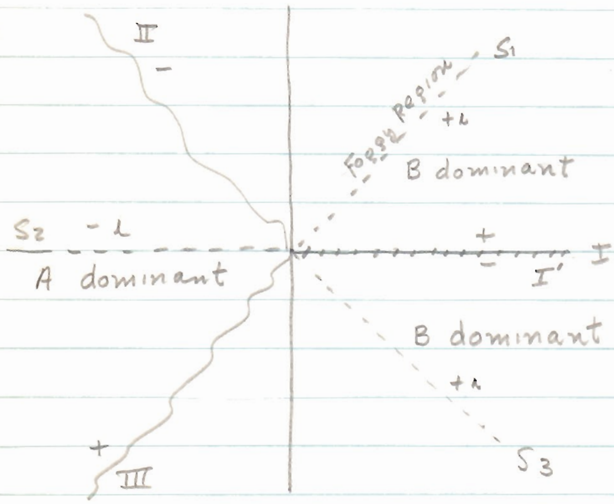
Therefore near z_0:

The function changes from real to imaginary every 60°.



$w \sim r^{3/2} e^{i\frac{3}{2}\theta}$ in its principle value as we have cut the plane. It is seen that as we circumvent z_0, w goes real and imaginary about every 60°. Higher order terms in the series will cause variations in this angle.

Now return to original diagram. We see we can work solely with one diagram.



Consider:

$$\begin{pmatrix} A_{II} \\ B_{II} \end{pmatrix} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} A_I \\ B_I \end{pmatrix}$$

We can deduce some properties about the above matrix:

$$\begin{pmatrix} A_{II} \\ B_{II} \end{pmatrix} = \begin{pmatrix} 1 & \alpha \\ 0 & 1 \end{pmatrix} \begin{pmatrix} A_I \\ B_I \end{pmatrix}$$

The one's appear because of the possibility of $B_I = 0$. Also, using the same reasoning:

$$\begin{pmatrix} A_{III} \\ B_{III} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ \beta & 1 \end{pmatrix} \begin{pmatrix} A_{II} \\ B_{II} \end{pmatrix} \quad ; \quad \begin{pmatrix} A_{I'} \\ B_{I'} \end{pmatrix} = \begin{pmatrix} 1 & \gamma \\ 0 & 1 \end{pmatrix} \begin{pmatrix} A_{III} \\ B_{III} \end{pmatrix}$$

$$= \begin{pmatrix} 1 & \gamma \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ \beta & 1 \end{pmatrix} \begin{pmatrix} 1 & \alpha \\ 0 & 1 \end{pmatrix} \begin{pmatrix} A_I \\ B_I \end{pmatrix}$$

with the result that:

$$\begin{pmatrix} A_{I'} \\ B_{I'} \end{pmatrix} = \begin{pmatrix} 1+\gamma\beta & \alpha+\gamma+\alpha\beta\gamma \\ \beta & 1+\alpha\beta \end{pmatrix} \begin{pmatrix} A_I \\ B_I \end{pmatrix}$$

Now the correct expression is, from the fact that the exponentials change sign on going around the plane:

$$\begin{pmatrix} A_I' \\ B_I' \end{pmatrix} = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} \begin{pmatrix} A_I \\ B_I \end{pmatrix}$$

giving: $1 + \gamma\beta = 0$, $\alpha + \gamma + \alpha\beta\gamma = i$

$\beta = i$, $1 + \alpha\beta = 0$

Then
$$\begin{pmatrix} A_{II} \\ B_{II} \end{pmatrix} = \begin{pmatrix} 0 & i \\ 0 & 1 \end{pmatrix} \begin{pmatrix} A_I \\ B_I \end{pmatrix}$$

Now set $A_{II} = 0$: Then $B_I = i A_I$

We want these real on I : $A_I = e^{i\pi/4}$

$B_I = e^{i\pi/4} = A_I^*$

which gives for u: $u \sim 2(y+\lambda)^{-1/4} \cos(kw - \pi/4)$ in I.

On S_2 : $u \sim |y+\lambda|^{-1/4} e^{-k|w|}$

So $|y+\lambda|^{-1/4} e^{-k|w|} \longrightarrow 2(y+\lambda)^{-1/4} \cos(kw - \pi/4)$

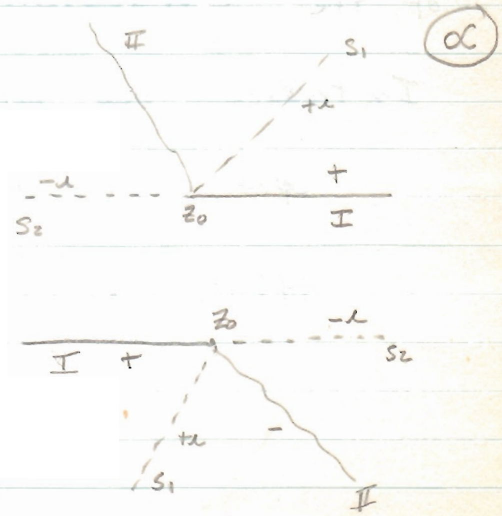
LECTURE XXXIV 12-16-60

Recapitulation:

$$u \cong (y+\lambda)^{-1/4} \left\{ A e^{ikw} + B e^{-ikw} \right\}$$

$$\begin{pmatrix} A_{II} \\ B_{II} \end{pmatrix} = \begin{pmatrix} 1 & i \\ 0 & 1 \end{pmatrix} \begin{pmatrix} A_I \\ B_I \end{pmatrix}$$

with $w = \pm \int_{z_0}^{z} (y+\lambda)^{1/2}\, dz$



Final connection formulae: $A_I = e^{-i\pi/4}$, $B_I = e^{+i\pi/4}$

$$|y+d|^{-1/4} e^{-k|\omega|} \longrightarrow 2(y+d)^{-1/4} \cos\left(k\omega - \frac{\pi}{4}\right)$$

on S_2 on I

This is the first connection formula.

Choose some other phase: $A_I = e^{+i(\pi/4 - \theta)}$, $B_I = e^{-i(\pi/4 - \theta)}$

On I: $2(y+d)^{-1/4} \cos\left(k\omega + \frac{\pi}{4} - \theta\right)$, $\theta \neq \pi/2$

What is this on S_2?

$$A_{II} = A_I + i B_I = e^{i\pi/4}\left(e^{-i\theta} + e^{i\theta}\right)$$

Thus on S_2: $2 \cos\theta \, |y+d|^{-1/4} e^{k|\omega|}$

or:

$$\cos\theta \, |y+d|^{-1/4} e^{k|\omega|} \longleftarrow (y+d)^{-1/4} \cos\left(k\omega + \frac{\pi}{4} - \theta\right)$$

on S_2 On I

Take $\theta = 0$: $|y+d|^{-1/4} e^{k|\omega|} \longleftarrow (y+d)^{-1/4} \cos\left(k\omega + \frac{\pi}{4}\right)$

This is the second form, called the canonical form, of the connection formula.

Introduce new notation: Refered to diagram (α)

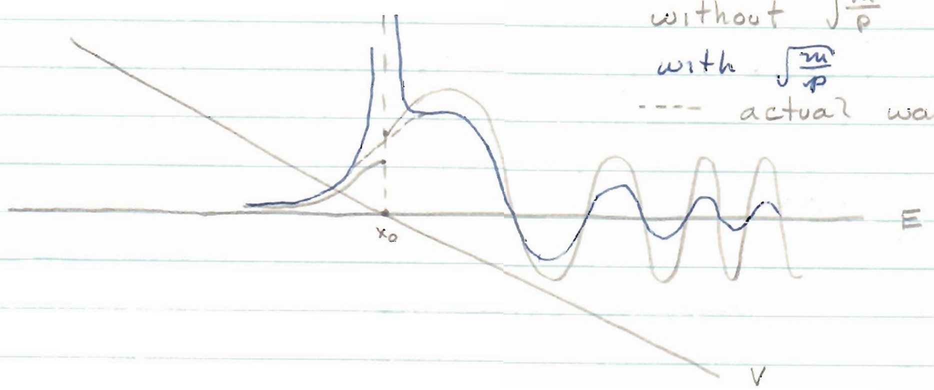
$$p = +\sqrt{2m(E-V)} \qquad E > V$$

$$|p| = +\sqrt{2m(V-E)} \qquad E < V$$

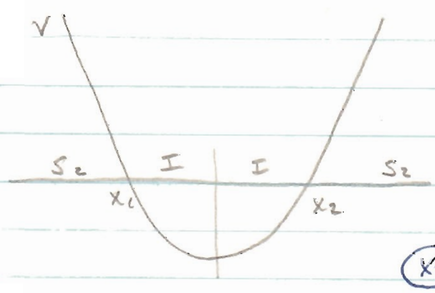
then:

First: $\sqrt{\frac{m}{|p|}}\, e^{-\frac{1}{\hbar}\int_x^{x_0} |p|\,dx} \longrightarrow 2\sqrt{\frac{m}{p}} \cos\left[\frac{1}{\hbar}\int_{x_0}^{x} p\,dx - \frac{\pi}{4}\right]$

Second: $\sqrt{\frac{m}{|p|}}\, e^{+\frac{1}{\hbar}\int_x^{x_0} |p|\,dx} \longleftarrow \sqrt{\frac{m}{p}} \cos\left[\frac{1}{\hbar}\int_{x_0}^{x} p\,dx + \frac{\pi}{4}\right]$



Application: Oscillator



(x_1) u: $C\sqrt{\frac{m}{|p|}}\, e^{-\frac{1}{\hbar}\int_x^{x_1} |p|\,dx} \longrightarrow 2C\sqrt{\frac{m}{p}} \cos\left[\frac{1}{\hbar}\int_{x_1}^{x} p\,dx - \frac{\pi}{4}\right]$

$x < x_1$ $\qquad$ $x_2 > x > x_1$

(x_2) v: $C'\sqrt{\frac{m}{|p|}}\, e^{-\frac{1}{\hbar}\int_{x_2}^{x} |p|\,dx} \longrightarrow 2C'\sqrt{\frac{m}{p}} \cos\left[\frac{1}{\hbar}\int_{x}^{x_2} p\,dx - \frac{\pi}{4}\right]$

$x > x_2$ $\qquad$ $x_1 < x < x_2$

The unallowed forms would be made from the second connection formula so that the total solution is:

$u = Av + Bv_2$, however $B = 0$ for behaved solution.

Calling $C' = 1$; we can write for u : change signs for A, B constant

$$\underbrace{\cos\left[\frac{1}{\hbar}\int_{x_1}^{x} p\,dx - \frac{\pi}{4}\right]}_{\varphi} = A \underbrace{\cos\left[-\frac{1}{\hbar}\int_{x_1}^{x_2} p\,dx + \frac{\pi}{4}\right]}_{\psi} + B \underbrace{\cos\left[\frac{-1}{\hbar}\int_{x}^{x_2} p\,dx + \frac{\pi}{4}\right]}_{\psi + \pi/2}$$

Problems 26-30
due Jan 13 (Friday)

Therefore : $\cos\varphi = \cos(\psi + \{\varphi - \psi\})$

$$= \cos\psi \cos(\varphi-\psi) - \sin\psi \sin(\varphi-\psi)$$

and for $B = 0$:

$$\sin\left[\frac{1}{\hbar}\int_{x_1}^{x} p\,dx + \frac{1}{\hbar}\int_{x}^{x_2} p\,dx - \frac{\pi}{2}\right] = 0$$

or $\frac{1}{\hbar}\int_{x_1}^{x_2} p\,dx - \frac{\pi}{2} = n\pi, \quad n = 0, 1, 2, \ldots$

and $\int_{x_1}^{x_2} p\,dx = (n+\frac{1}{2})\pi\hbar$

Somerfeld - Wilson integral is

$$\oint p\,dx = (n+\tfrac{1}{2})\,h$$

LECTURE XXXV 12-19-60

Recapitulation:

$2m(E-V)$ real , $\sqrt{2m(E-V)} = p$

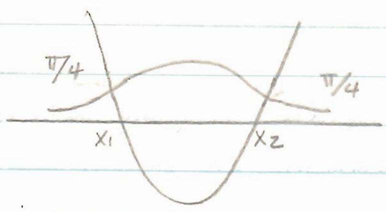
The first connection formula gives:

(I) $$\sqrt{\frac{m}{|p|}}\, e^{-\left|\frac{1}{\hbar}\int_{x_0}^{x} p\,dx\right|} \longrightarrow 2\sqrt{\frac{m}{p}}\cos\left(\left|\frac{1}{\hbar}\int_{x_0}^{x} p\,dx\right| - \frac{\pi}{4}\right)$$

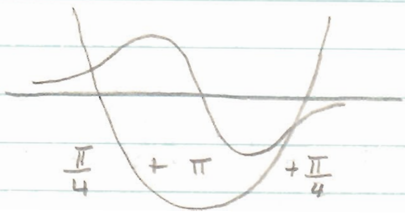
and the second connection formula gives:

(II) $$\sqrt{\frac{m}{|p|}}\, e^{+\left|\frac{1}{\hbar}\int_{x_0}^{x} p\,dx\right|} \longleftarrow \sqrt{\frac{m}{p}}\cos\left(\left|\frac{1}{\hbar}\int_{x_0}^{x} p\,dx\right| + \frac{\pi}{4}\right)$$

Application to Oscillator:



$\frac{\pi}{4} + \frac{\pi}{4}$



Somerfeld Theory gives:

$$\int_{x_1}^{x_2} p\, dx = \left(n+\tfrac{1}{2}\right)\frac{h}{2}$$

which must be satisfied.

Total phase change will be, from diagrams, $(n+\frac{1}{2})\pi$, where n is number of zero crossings.

Now: $V = \frac{1}{2} m\omega^2 x^2$

then: $$\int_{x_1}^{x_2} \sqrt{2mE - m^2\omega^2 x^2}\, dx = \left(n+\tfrac{1}{2}\right)\pi\hbar$$

or $$\int_{x_1}^{x_2} \sqrt{\frac{2E}{m\omega^2} - x^2}\, dx = \left(n+\tfrac{1}{2}\right)\frac{\pi\hbar}{m\omega}$$

This integral is of the form $\int \sqrt{r^2 - x^2}\, dx$ or the area of semicircle:

Therefore: $\frac{\pi}{2}\,\frac{2E}{m\omega^2} = \left(n+\frac{1}{2}\right)\frac{\pi\hbar}{m\omega}$, or $E = \left(n+\frac{1}{2}\right)\hbar\omega$

which is exactly for the harmonic oscillator. For other oscillators, the approximation is very good even near the turning points which one would not expect from the setting up of the problem. This is because one may encircle both turning points with a path as large as desired as there are no singularities in the z plane.

What is normalization?

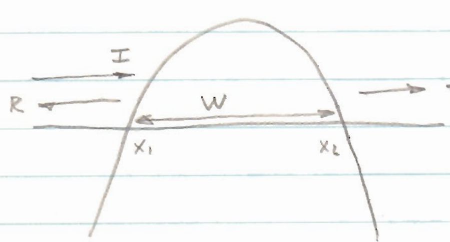
$$1 \cong 4C^2 \int_{x_1}^{x_2} \frac{m}{p}\, dx \; \underbrace{\cos^2\left(\frac{1}{\hbar}|S| - \frac{\pi}{4}\right)}_{=\frac{1}{2} \text{ since rapidly varying inside.}}$$

Therefore: $C^{-2} \cong 4 \int_{x_1}^{x_2} \frac{m}{2p}\, dx$, thus:

Inside: $$u \cong \frac{1}{\sqrt{\int_{x_1}^{x_2} \frac{m}{2p}\, dx}} \cos\left(\frac{1}{\hbar}|S| - \frac{\pi}{4}\right) \cdot \sqrt{\frac{m}{p}}$$

Outside: $$u \approx \frac{1}{2\sqrt{\int_{x_1}^{x_2} \frac{m}{2p}\, dx}} e^{-\frac{1}{\hbar}|S|} \cdot \sqrt{\frac{m}{|p|}}$$

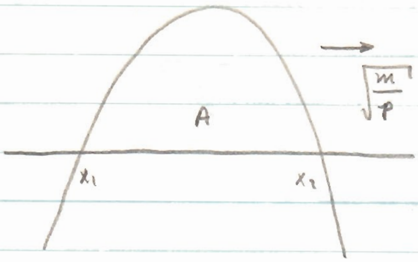
Application: Penetration of Boundary:
This is a classic application of this method.



This method is good for:

$$\frac{1}{\hbar}\int_{x_1}^{x_2} |p|\, dx = W \gg 1$$

We can induce that T will be of the form $T \sim e^{-2W}$



$\rightarrow \sqrt{\frac{m}{p}}\, e^{\frac{i}{\hbar}\int_{x_2}^{x} p\,dx + i\varphi}$

We want to choose the phase factor such that the imaginary part decays to the left of x_2.

Expanding:

$$\sqrt{\frac{m}{p}}\left\{\cos\left(\frac{1}{\hbar}\int_{x_2}^{x} px\,dx + \varphi\right) + i\sin(\ ) + i\cos\left(\frac{1}{\hbar}\int_{x_2}^{x} p\,dx + \varphi - \frac{\pi}{2}\right)\right.$$

$\varphi = \frac{\pi}{4}$; choose $-\frac{\pi}{4}$

Thus in A: real part $= \sqrt{\frac{m}{|p|}}\, e^{\frac{1}{\hbar}\int_{x}^{x_2} |p|\,dx}$

$$= \sqrt{\frac{m}{|p|}}\, e^{W - \frac{1}{\hbar}\int_{x_1}^{x} |p|\,dx}$$

Then, in $x < x_1$, real part $= 2\sqrt{\frac{m}{p}}\, e^{W}\left(\frac{1}{\hbar}\int_{x}^{x_1} p\,dx - \frac{\pi}{4}\right)$

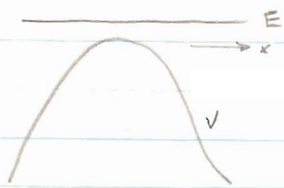
which goes to $e^{+i(\,)} + e^{-i(\,)}$

Incident Reflected

under these conditions, the transmitted is 1 and the incident and reflected are e^{W}. The consideration of the imaginary part will make the incident & reflected such that the transmission will be

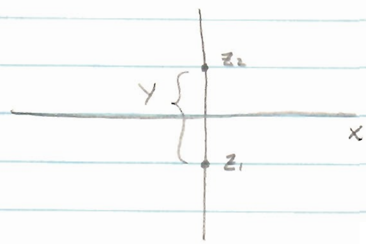
$$T \cong \frac{1}{e^{2W} + 1}$$

Consider case of no turning points:



$$E + \frac{s}{2}x^2 = 0 \;,\quad E = \pm i\sqrt{\frac{2E}{s}}$$

Thus in "z" plane:



$$Y = \left| \int_{z_1}^{z_2} \frac{|p|}{\hbar}\, dz \right|$$

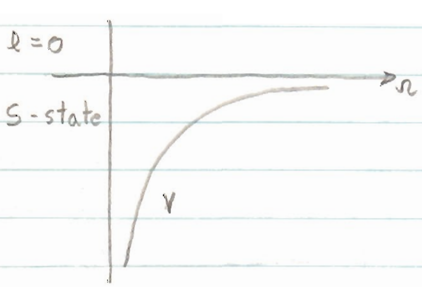
and we get:

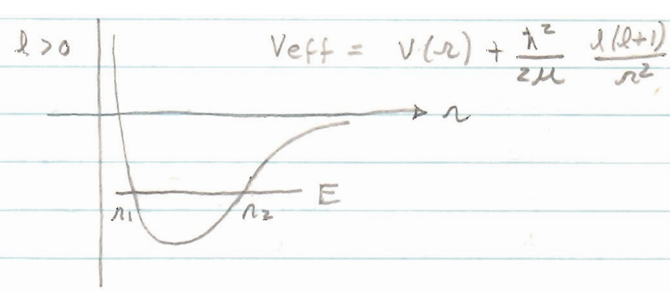
$$T = \frac{1}{e^{-2Y} + 1} \;,\quad \text{for tangent case } T = \frac{1}{2}$$

LECTURE XXXVI   12-21-60

Central Field Problems: Phase Integral Method

Inverse field: Trouble occurs when potential vanishes.





$$\frac{1}{\hbar}\int_{r_1}^{r_2} \sqrt{2m\,(E - V'_{eff})}\; dr = (n + \tfrac{1}{2})\pi$$

Kramer's Rule: $\frac{l(l+1)}{r^2} \rightarrow \frac{(l+\frac{1}{2})^2}{r^2}$ and we will get precise solution.

Langer Substitution:

$$u'' + \frac{2m}{\hbar^2}\left(E - V - \frac{\hbar^2}{2m}\left(\frac{l(l+1)}{r^2}\right)\right) u = 0$$

To make a variable run continuously, we make the change

$r = e^{x}$, $u = e^{x/2}\, y$ and get:

$$\frac{d^2y}{dx^2} + \frac{2m}{\hbar^2}\left[e^{2x}E - e^{2x}V - \frac{\hbar^2}{2m}\left(l + \tfrac{1}{2}\right)^2\right] y = 0$$

where x now ranges from $-\infty$ to $+\infty$, which gives us an oscillator situation:

Then the phase integral method gives:

$$\frac{1}{\hbar}\int \sqrt{2m[\,]}\, dx = (n' + \tfrac{1}{2})\pi$$

$$\frac{1}{\hbar}\int \sqrt{2m(E - V_{eff})}\, dr = (n' + \tfrac{1}{2})\pi$$

In the old quantum theory:

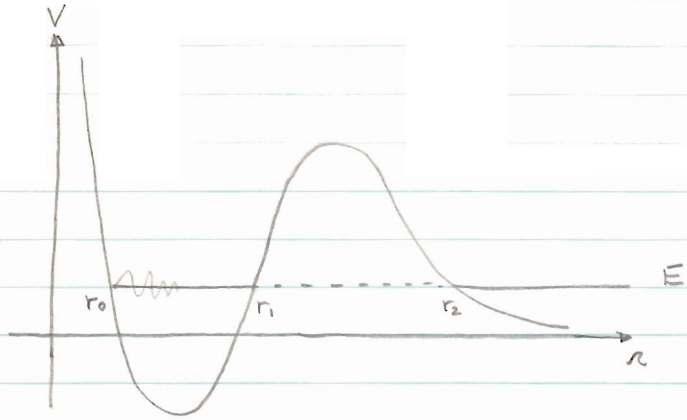
$$\frac{1}{\hbar}\int \sqrt{2m\left(E - V - \frac{\hbar^2}{2m}\cdot\frac{k^2}{r^2}\right)}\, dr = n'\pi \quad , \quad k = 1, 2, 3, \ldots$$

In W.K.B method:

$$\frac{1}{\hbar}\int \sqrt{2m\left(E - V - \frac{(l+\frac{1}{2})^2}{r^2}\,\frac{\hbar^2}{2m}\right)}\, dr = (n' + \tfrac{1}{2})\pi$$

$l = 0, 1, 2, 3, \ldots$

α Decay:



From previous lecture,

$$T = e^{-2W}$$

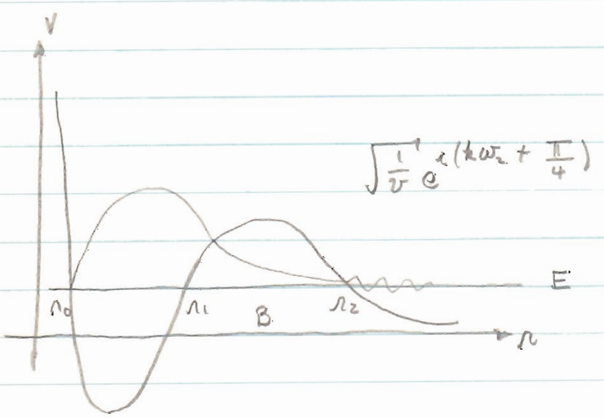
$$W = \frac{1}{\hbar}\int_{r_1}^{r_2} \sqrt{2m\left(V_{eff}' - E\right)}\, dr$$

To get particle bouncing in state, we must assume state is high enough such superposition can form packets. Now:

$$\frac{\text{decay probability}}{\text{unit time}} = \gamma = \frac{e^{-2W}}{2\int_{r_0}^{r_1} \frac{dr}{v}}$$

where $v = \sqrt{\frac{2(E - V_{eff}')}{m}}$, and then, $N = e^{-\gamma t} N_0$, where N is the number of decays/unit time.

However, this picture does not correspond to physical reality. Really have no packets formed.



We require the imaginary part to decay to the left

$$\rightarrow i \sin\left(k w_2 + \frac{\pi}{4}\right)$$
$$= i \cos\left(k w_2 - \frac{\pi}{4}\right) + \cos\left(k w_2 + \pi/4\right)$$

In B: $\frac{1}{\sqrt{|v|}}\, e^{k|w_2|}$

Now: $W = k\,|w_2(r_1)|$

where $k|w_2| = \int_r^{r_2} = \int_{r_1}^{r_2} - \int_{r_1}^{r} = W - k|w_1|$

or, in B; for real part only:

$$\frac{1}{\sqrt{|v|}} e^{k|w_2|} = \frac{1}{\sqrt{|v|}} e^{W - k|w_1|}$$

The connection formula is then:

$$2 \frac{e^W}{\sqrt{v}} \cos\left(k|w_1| - \frac{\pi}{4}\right) \longleftarrow \frac{e^W}{\sqrt{|v|}} e^{-k|w_1|}$$

for real part.

E is found from $\frac{1}{\hbar} \int_{r_0}^{r_1} \sqrt{2m(E - V'_{eff})}\, dr = (n + \frac{1}{2})\pi$

Now the imaginary part has $i \frac{e^{-W}}{\sqrt{|v|}} \cos\left(k|w_1| + \frac{\pi}{4}\right)$

However, the imaginary part will blow up to the left of r_1. Gamow's approximation is to consider E not as purely real. That is, we define:

$$E = E_0 - i\hbar \frac{\gamma}{2}$$

and $e^{-iEt/\hbar} = e^{-iE_0 t/\hbar} e^{-\frac{\gamma}{2}t}$

We now write:

$$u'' + k^2 (y + \lambda) u = 0$$

$$u^{*''} + k^2 (y + \lambda^*) u^* = 0$$

and: $(u^* u' - u u^{*'})' = k^2 \underbrace{(\lambda - \lambda^*)}_{2i \, \mathrm{Im}\, \lambda} u u^*$

then $(u^* u' - u u^{*'})\Big|_{r_0}^{r_2} = k^2 (\lambda - \lambda^*) \int_{r_0}^{r_2} u u^* \, dr$

which gives:

$$2\epsilon k = \lambda^2 (\lambda - \lambda^*) \, 4 \int_{r_0}^{r_1} \frac{1}{2} \frac{dr}{v} \, e^{2W}$$

making the approximation of $\cos\theta \sim \frac{1}{2}$ and neglecting the tail in the barrier. One will find that we get the same answer with the packet approximation.

This concludes the formal lectures. See reading period assignment.

Physics 251a Reading Period Assignment

1960-61

All in Schiff's *Quantum Mechanics*, *either* edition (they are identical):

Center-of-mass and relative coordinates in wave mechanics —

First subsection of Sect. 16 ($1\frac{1}{2}$ pages)

Definition of scattering cross-section — introductory passage and first subsection of Sect. 18 (2 pages)

Time-dependent perturbation theory and applications —

Section 29 (10 pages)

Section 31 (7 pages)

READING PERIOD ASSIGNMENT

REDUCED MASS

We are concerned with solving the Schroedinger equation for a system of two particles, viz:

(1) $i\hbar \frac{\partial}{\partial t} \psi(x_1, y_1, z_1, x_2, y_2, z_2, t)$

$$= \left[-\frac{\hbar^2}{2m_1}\left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial y_1^2} + \frac{\partial^2}{\partial z_1^2}\right) - \frac{\hbar^2}{2m_2}\left(\frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial y_2^2} + \frac{\partial^2}{\partial z_2^2}\right) \right.$$

$$\left. + V(x_1, y_1, z_1, x_2, y_2, z_2) \right] \psi(x_1, y_1, z_1, x_2, y_2, z_2)$$

If the potential depends only on the relative coordinates, such that $V = V(x_1 - x_2, y_1 - y_2, z_1 - z_2)$, we find we can separate the equation into two equations, one depending on the relative coordinates x, y, z and the other on the coordinates of the center of mass, $X\,Y\,Z$. We define these coordinates as:

(2) $x = x_1 - x_2 \quad , \quad y = y_1 - y_2 \quad , \quad z = z_1 - z_2$

$$MX = m_1 x_1 + m_2 x_2 \quad , \quad MY = m_1 y_1 + m_2 y_2 \quad , \quad MZ = m_1 z_1 + m_2 z_2$$

where $M = m_1 + m_2$ is the total mass of the system. We can now rewrite equation (1) as:

(3) $$i\hbar \frac{\partial \psi}{\partial t} = \left[-\frac{\hbar^2}{2M}\left(\frac{\partial^2}{\partial X^2} + \frac{\partial^2}{\partial Y^2} + \frac{\partial^2}{\partial Z^2}\right) - \frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) \right.$$

$$\left. + V(x, y, z) \right] \psi$$

where $\mu = \frac{m_1 m_2}{m_1 + m_2}$ is called the reduced mass.

This equation can be separated by the usual straightforward technique.

The result is:

(4) $$\Psi(x,y,z,X,Y,Z,t) = u(x,y,z)\,U(X,Y,Z)\,e^{-\frac{i(E+E')t}{\hbar}}$$

$$-\frac{\hbar^2}{2\mu}\nabla^2 u + Vu = Eu$$

$$-\frac{\hbar^2}{2M}\nabla^2 U = E'U$$

where the ∇^2 represent the Laplacian operator with respect to the appropriate coordinates. The first differential equation represents the usual stationary Schroedinger equation, except the mass used is the reduced mass. The second equation describes the motion of the system as a whole which behaves as a free particle.

READING PERIOD ASSIGNMENT

TIME DEPENDENT PERTURBATION THEORY

Reference: Schiff, Sections 29, 31

It is generally impossible to obtain solutions of Schroedinger's equation when the Hamiltonian is time dependent, hence the need for a perturbation treatment. We take the time dependent part to be small compared to the stationary part and write.

(1) $H = H_0 + H'$, $H_0 u_n = E_n u_n$

where $H_0 u_n = E_n u_n$ is the usual stationary "known" solution with the unperturbed Hamiltonian and H' is the time dependent perturbing part and is taken small. We must now work with the time dependent Schroedinger equation:

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

We make the usual expansion in terms of the unperturbed wave functions where now the coefficients depend upon the time:

(3) $\psi = \sum_n a_n(t)\, u_n\, e^{-iE_n t/\hbar}$

Substitution into (2) yields:

(4) $$\sum_n i\hbar \frac{da_n}{dt} u_n e^{-iE_n t/\hbar} + \sum_n a_n E_n u_n e^{-iE_n t/\hbar}$$

$$= \sum_n a_n (H_0 + H') u_n e^{-iE_n t/\hbar}$$

Using $H_0 u_n = E_n u_n$ and forming matrix elements, we obtain; using $|n\rangle = u_n$ and $\langle k| = u_k^*$:

(5) $$i\hbar \frac{da_k}{dt} e^{-iE_k t/\hbar} = \sum_n \langle k|H'|n\rangle a_n e^{-iE_n t/\hbar}$$

We now define the Bohr frequency as:

(6) $$\omega_{kn} = \frac{E_k - E_n}{\hbar}$$

and obtain:

(7) $$\frac{da_k}{dt} = \frac{1}{i\hbar} \sum_n \langle k|H'|n\rangle e^{i\omega_{kn} t} a_n$$

We now go to perturbation methods by writing $H' = \lambda H'$ and expanding a_n in a power series in λ:

(8) $$a_n = a_n^{(0)} + \lambda a_n^{(1)} + \lambda^2 a_n^{(2)} + \dots$$

and take the series analytic between 0 and 1. We get upon equating coefficients of equal powers in λ:

(9) $$\frac{da_k^{(0)}}{dt} = 0 \quad , \quad \frac{da_k^{(s+1)}}{dt} = \frac{1}{i\hbar} \sum_n \langle k|H'|n\rangle a_n^{(s)} e^{i\omega_{kn} t}$$

$s = 0, 1, 2, \dots$

The coefficients $a_k^{(0)}$ are constant in time and represent therefore initial conditions. We take only one of the $a_k^{(0)}$ to be non-zero at $t=0$ assuming that we begin with the system in a well defined state and can write the very important initial relation:

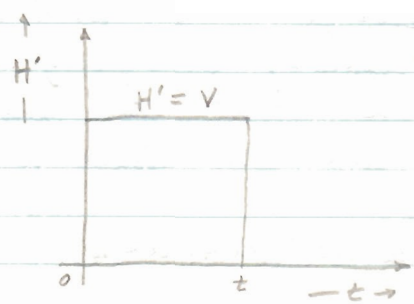
(10) $$a_k^{(0)} = \delta_{km}$$

We now have for the first order correction:

(11) $$\frac{d a_k^{(1)}}{dt} = \frac{1}{i\hbar} \langle k | H' | m \rangle e^{i\omega_{km} t} \quad , \text{ or}$$

(12) $$\boxed{a_k^{(1)}(t) = \frac{1}{i\hbar} \int_{-\infty}^{t} \langle k | H' | m \rangle e^{i\omega_{km} t} \, dt}$$

where the lower limit is chosen to make $a_k^{(1)}$ initially zero (before the perturbation is applied). If the perturbation is constant except for being applied at $t = 0$ and being turned off at $t = t$, that is:

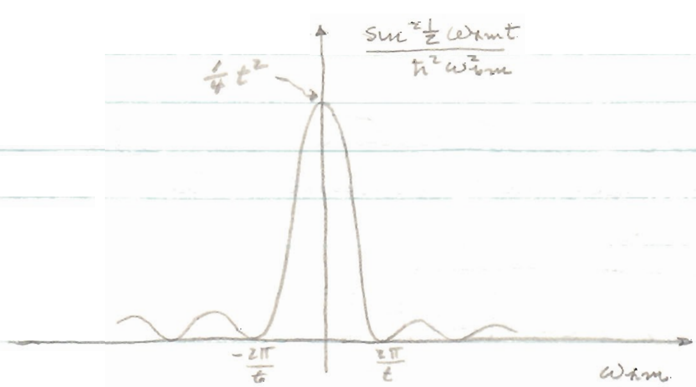


Now we can easily perform the integration and obtain:

(13) $$a_k^{(1)}(t) = -\langle k | V | m \rangle \left\{ \frac{e^{i\omega_{km} t} - 1}{\hbar \omega_{km}} \right\}$$

Thus the probability of finding the system in the state k at time t is:

(14) $$\left| a_k^{(1)}(t) \right|^2 = 4 \left| \langle k | V | m \rangle \right|^2 \left\{ \frac{\sin^2 \frac{1}{2} \omega_{km} t}{\hbar^2 \omega_{km}^2} \right\}$$



For states E_k near those initially E_m, the height increases as t^2 while the breadth goes as t^{-1}, so that the area (probability of transition) goes as t.

This is the physically interesting case, that is, the case where the transitions are to neighboring states.

thus the probability that a transition has taken place after the perturbation has been on for a time t is proportional to t.

Transition Probability

We desire to derive a transition probability per unit time, w. It is convenient to assume Born-von Karman boundary conditions. We consider the group of final states close to the initial state E_m, assuming that the matrix element $\langle k|V|m\rangle$ is a slowly varying function of k. We define a density of final states $\rho(k)$ so that $\rho(k)\,dE_k$ is the number of states in the range dE_k and also assume that $\rho(k)$ is a slowly varying function of k. Since we have shown that the probability is linear function of time, we can then write:

$$(15) \quad w = t^{-1} \sum_k |a_k^{(1)}(t)|^2 \Rightarrow t^{-1} \int |a_k^{(1)}(t)|^2 \rho(k)\, dE_k$$

The sum becomes an integral upon letting the BVK boundary become large. Using (14), recalling that $\langle k|V|m\rangle$, $\rho(k)$ are practically independent of k:

$$(16) \quad w = \frac{1}{t} \frac{4\,|\langle k|V|m\rangle|^2}{\hbar} \rho(k) \int_{-\infty}^{\infty} \frac{\sin^2 \frac{1}{2} \omega_{km} t}{\omega^2_{km}}\, d\omega_{km}$$

where the major contribution to the integral will be the region around E_m. Integrating, we finally have:

$$(17) \quad \boxed{w = \frac{2\pi}{\hbar} \rho(k)\, |\langle k|V|m\rangle|^2}$$

which is independent of time as expected.

Scattering Cross Section

We now calculate w when the initial and final states are free particle plane waves, viz.,

(18) $$u_m(r) = L^{-3/2} e^{i k_0 \cdot r}, \quad u_k(r) = L^{-3/2} e^{i k \cdot r}$$

where k_0, k are propagation vectors. Now the number of available states in a certain energy range follows from the usual considerations:

(19) $$\rho(k)\, dE_k = \left(\frac{L}{2\pi}\right)^3 k^2 dk \sin\theta \, d\theta \, d\varphi$$

For the free particle, $E_k = \frac{\hbar^2 k^2}{2m}$, $dE_k = \frac{2\hbar^2 k\, dk}{2m}$ so that:

(20) $$\rho(k) = \frac{m L^3}{8\pi^3 \hbar^2} k \sin\theta \, d\theta \, d\varphi$$

Now, assuming a perturbing potential of the form $V(r)$, we have for the matrix element:

(21) $$\langle k | V | m \rangle = L^{-3} \int V(r) e^{i K \cdot r} d^3 r$$

where $K = k_0 - k$

We define as the scattering cross-section:

(22) $$\sigma(\theta, \varphi) \sin\theta \, d\theta \, d\varphi = \frac{m L^3}{\hbar k} w$$

which, upon substitution of (21), (20) and (17) becomes:

(23) $$\sigma(\theta, \varphi) = \left(\frac{m}{2\pi \hbar^2}\right)^2 \left| \int V(r) e^{i K \cdot r} d^3 r \right|^2$$

Thus we see that cross-section of scattering is in part determined by the probability of transitions upon collision.

Harmonic Perturbation

We now assume that the perturbing term is harmonically time dependent, that is:

(24) $\langle k|H'|m\rangle = \langle k|V|m\rangle \sin\omega t \quad , \quad 0 \le t \le t$

Then the first order amplitudes at time t are:

(25) $$a_k^{(1)}(t) = -\frac{\langle k|V|m\rangle}{2i\hbar}\left\{\frac{e^{i(\omega_{km}+\omega)t}-1}{\omega_{km}+\omega} - \frac{e^{i(\omega_{km}-\omega)t}-1}{\omega_{km}-\omega}\right\}$$

We will only have an appreciable probability of finding the system in the state k if $\omega_{km} \approx \pm\omega$ or when one of the denominators vanish providing the matrix element does not vanish at the time also. The energy conservation relation subject to the uncertainty condition is then:

(26) $E_k \approx E_m \pm \hbar\omega$

Thus we see that the electromagnetic (possibly) perturbation is to impart to or recieve from the system the energy $\hbar\omega$ which we would expect from the results of such well known experiments as the photoelectric effect.

Second Order Perturbation

We can readily find the second order correction from equation (9) letting $s=1$:

(27) $$\frac{da_k^{(2)}}{dt} = \frac{1}{i\hbar}\sum_n \langle k|H'|n\rangle a_n^{(1)} e^{i\omega_{kn}t}$$

By substituting in (12) for $a_n^{(1)}(t)$, we arrive at:

$$(28)\quad a_k^{(2)} = -\frac{1}{\hbar^2}\int_{-\infty}^{t}\int_{-\infty}^{t''} \sum_n \langle k|H'(t'')|n\rangle\langle n|H'(t')|m\rangle e^{i(\omega_{nm}t' + \omega_{kn}t'')}\, dt'\, dt''$$

If we now suppose $H'(t') = V$, $0 \le t' \le t$, we arrive at:

$$(29)\quad a_k^{(2)}(t) = \frac{1}{\hbar^2}\sum_n \frac{\langle k|V|n\rangle\langle n|V|m\rangle}{\omega_{nm}}\left\{\frac{e^{i\omega_{km}t}-1}{\omega_{km}} - \frac{e^{i\omega_{kn}t}-1}{\omega_{kn}}\right\}$$

Comparing with (13) shows that for either $\omega_{km} \simeq 0$ or $\omega_{kn} \simeq 0$ are transitions for which the probability increases with time linearly. The first transition $\omega_{km} \simeq 0$ between the initial state m and the final state k conserves energy while the second does not. It is between some intermediate state n and the final state k. The reason is that the Fourier components, which are not marked in the first order transition, are strong enough in the second order. Thus the turning on of the perturbation suddenly is a mathematical artifice which is not met physically. Actually the system has been undergoing the perturbation for a long time and is usually always present.

Adiabatic and Sudden Approximations

If the Hamiltonian changes very slowly with time, we can approximate solutions of the Schroedinger equation by means of stationary energy eigenfunctions of the instantaneous Hamiltonian so one particular eigenfunction changes over continuously into another eigenfunction at a later time. This is the adiabatic approximation.

If the Hamiltonian changes from one form to another almost instantaneously, the wave function can be expected not to change much, although the expansion of this function in eigenfunctions of the initial and final Hamiltonian may be quite different. This is the sudden approximation.

Adiabatic Approximations

The appropriate Schroedinger equation is:

$$(1) \quad i\hbar \frac{\partial \psi}{\partial t} = H(t)\,\psi$$

in which $H(t)$ varies slowly with the time. The solutions at any instant are assumed known.

$$(2) \quad H(t)\,u_n(t) = E_n(t)\,u_n(t)$$

where the u_n are orthonormal, nondegenerate, and discrete. If we assume that the solutions at $t=0$ are known, we may take for the appropriate expansion for ψ:

$$(3) \quad \psi = \sum_n a_n(t)\,u_n(t)\,\exp\left[-\frac{i}{\hbar}\int_0^t E_n(t')\,dt'\right]$$

Substituting into (1):

$$(4) \quad i\hbar \sum_n \left(\frac{da_n}{dt} u_n + a_n \frac{\partial u_n}{\partial t} - \frac{i}{\hbar} a_n u_n E_n \right)$$

$$\cdot \exp\left[-\frac{i}{\hbar}\int_0^t E_n(t')\,dt'\right] = H \sum_n a_n u_n \exp\left[-\frac{i}{\hbar}\int_0^t E_n(t')\,dt'\right]$$

We note that $H u_n = E_n u_n$ so that the last term on the LHS cancels the term on the RHS.

We now form matrix elements in the usual manner:

$$(5) \quad \sum_n' \left\{ \langle k|n\rangle \frac{da_n}{dt} + \langle k|\frac{\partial}{\partial t}|n\rangle a_n \right\} \exp\left[-\frac{i}{\hbar}\int_0^t E_n(t')dt'\right] = 0$$

or:

$$(6) \quad \frac{da_k}{dt} = -\sum_n' a_n \langle k|\frac{\partial}{\partial t}|n\rangle \exp\left[-\frac{i}{\hbar}\int_0^t \omega_{kn}(t')dt'\right]$$

We desire a simpler form for the matrix element $\langle k|\frac{\partial}{\partial t}|n\rangle$. Take the time derivative of (2):

$$(7) \quad \frac{\partial H}{\partial t} u_n + H \frac{\partial u_n}{\partial t} = \frac{\partial E_n}{\partial t} u_n + E_n \frac{\partial u_n}{\partial t}$$

Forming matrix elements:

$$(8) \quad \langle k|\frac{\partial H}{\partial t}|n\rangle + \langle k|H\frac{\partial}{\partial t}|n\rangle = E_n \langle k|\frac{\partial}{\partial t}|n\rangle, \quad k \neq n$$

Using the Hermitian nature of H we have:

$$(9) \quad \langle k|\frac{\partial H}{\partial t}|n\rangle + E_k \langle k|\frac{\partial}{\partial t}|n\rangle = E_n \langle k|\frac{\partial}{\partial t}|n\rangle$$

$$\text{or} \quad \langle k|\frac{\partial}{\partial t}|n\rangle = -\frac{\langle k|\frac{\partial H}{\partial t}|n\rangle}{E_k - E_n}, \quad k \neq n$$

We must now develop an expression for $\langle n|\frac{\partial}{\partial t}|n\rangle$. We differentiate the normalization integral:

$$(10) \quad 0 = \frac{\partial}{\partial t}\langle n|n\rangle = \left(\frac{\partial}{\partial t}\langle n|\right)|n\rangle + \langle n|\frac{\partial}{\partial t}|n\rangle$$

Now the two matrix elements on the RHS are complex conjugates and must hence be pure imaginary as their sum is zero, that is, $\langle n|\frac{\partial}{\partial t}|n\rangle = i\alpha(t)$. We now change the phase of u_n by an amount $\gamma(t)$ which is permissible since the phases of the eigenfunctions are arbitrary at each instant of time.

Thus we form the new eigenfunction $u_n' \equiv u_n e^{i\gamma(t)}$.

(11) $\langle n' | \frac{\partial}{\partial t} | n' \rangle = \int u_n^* e^{-i\gamma} \frac{\partial}{\partial t} (u_n e^{i\gamma}) d\tau$

$= i\alpha(t) + i \frac{d}{dt} \gamma(t)$

It is easily seen that the choice

(12) $\gamma(t) = -\int_0^t \alpha(t')\,dt'$ will make the

matrix element vanish. We now remove the prime and substitute (9) into (6) and get:

(13) $$\frac{da_k}{dt} = \sum_n{}' \frac{a_n \langle k | \frac{\partial H}{\partial t} | n \rangle}{\hbar \omega_{kn}} \left[\exp \left(i \int_0^t \omega_{kn}\, dt' \right) \right]$$

Up to now our treatment has been completely general. We now introduce the adiabatic approximation by assuming that the quantities a_n, ω_{kn}, u_n, and $\partial H/\partial t$ are constant in time. If we further assume that the system is in the state m at $t=0$ we can put $a_n = \delta_{nm}$. Thus:

(14) $$\frac{da_k}{dt} \simeq \frac{1}{\hbar \omega_{km}} \langle k | \frac{\partial H}{\partial t} | m \rangle \exp(i \omega_{km} t), \quad k \neq m$$

or:

(15) $$a_k(t) \simeq \frac{1}{i\hbar \omega_{km}^2} \langle k | \frac{\partial H}{\partial t} | m \rangle \left(e^{i\omega_{km} t} - 1 \right), \quad k \neq m$$

Under these approximations, we have that the probability amplitude for the state k oscillates in time with no net change over a long period of time. If the change in H is small over a Bohr period as compared with the energy difference ω_{km}, that is, $\frac{\partial H}{\partial t} \ll \hbar \omega_{km}^2$, then the transition is unlikely to occur.

The change in amplitude of the state k after a long time is of the order of the ratios of these two energies:

$$(16) \quad |a_k| \sim \left| \frac{(1/\omega_{km})(\partial H/\partial t)}{E_k - E_m} \right|$$

If we assume that the Hamiltonian oscillates periodically with time, then the assumption $\partial H/\partial t$ = constant is no longer valid. If we write:

$$(17) \quad H = H_0 + V \sin \omega t$$

where V is small compared to H_0 and substitute in (14):

$$(18) \quad \frac{d a_k}{dt} \simeq \frac{\omega \langle k|V|m\rangle \cos \omega t}{\hbar \omega_{km}} e^{i \omega_{km} t}$$

Integration gives:

$$(20) \quad a_k(t) \simeq \frac{\omega \langle k|V|m\rangle}{2i \hbar \omega_{km}} \left[\frac{e^{i(\omega_{km}+\omega)t} - 1}{\omega_{km} + \omega} + \frac{e^{i(\omega_{km}-\omega)t} - 1}{\omega_{km} - \omega} \right]$$

We see that for ω close to ω_{km}, transitions are very probable and these results agree with the previous perturbation treatment.

Sudden Approximation

Let us consider the case in which the Hamiltonian changes discontinuously from one form to another.

$$(1) \quad H = H_0, \; t < 0 \quad \text{and} \quad H = H_1, \; t > 0$$

$$(2) \quad \text{now} \quad H_0 u_n = E_n u_n \quad \text{and} \quad H_1 v_m = E_m v_m$$

We take the u's and v's to be complete orthonormal sets of eigenfunctions. The general solutions are:

$$(3) \quad \psi = \sum_n a_n u_n e^{-iE_n t/\hbar}, \quad t < 0$$

$$\psi = \sum_m b_m v_m e^{-iE_m t/\hbar}, \quad t > 0$$

where a's and b's are independent of the time. Now the Schroedinger equation is of first order in the time, the wave function must be continuous in time at all points at t=0 even though its derivative is not. We can equate the equations (2) at t = 0 and express the b's in terms of the a's. We multiply through by v_m^* and integrate:

$$(4) \quad b_m = \sum_n a_n \int v_m^* u_n \, d\tau$$

The appearance of final states m that do not have the same energy as the initial state is a consequence of the non-zero Fourier components of the Hamiltonian.

The sudden approximation consists in using equation (4) when the change in the Hamiltonian is short but finite in time. Suppose that:

$$(5) \quad H = H_0, \; t < 0 \quad \text{and} \quad H = H_1, \; t > t_0 \quad \text{and} \quad H = H_i, \; 0 < t < t_0.$$

Now H_i, which we take to be constant in time, satisfies its own Schroedinger equation:

$$(6) \quad H_i w_k = E_k w_k$$

the true solution is, in terms of these eigenfunctions:

$$(7) \quad \psi = \sum_k c_k w_k e^{-iE_k t/\hbar}$$

and the continuity at $t=0$ gives:

$$(8) \quad c_k = \sum_n a_n \int w_k^* u_n \, d\tau$$

Now, the continuity condition at t_0 gives:

$$(9) \quad b_m = \sum_k c_k \int v_m^{*\prime} w_k' \, d\tau' \cdot e^{-i(E_k - E_m)t_0/\hbar}$$

$$= \sum_{nk} a_n \int w_k^* u_n \, d\tau \int v_m^{*\prime} w_k' \, d\tau \cdot e^{-i(E_k - E_m)t_0/\hbar}$$

$$= \sum_n a_n \iint v_m^{*\prime} \left[\sum_k w_k' w_k^* e^{-i(E_k - E_m)t_0/\hbar} \right] u_n \, d\tau \, d\tau'$$

Now the difference between (9) and (4) is the closeness of $\exp\{-i(E_k - E_m)t_0/\hbar\}$ and one. In other words, we should have:

$$(10) \quad t_0 \ll \frac{\hbar}{E_k - E_m}$$

for all the states of interest involved. Thus, to use relation (4) the change in the Hamiltonian should be quite a bit faster than the period of the Bohr orbit.

A special case is that in which the initial and final Hamiltonians are the same, that is, $H_0 = H_1$, $v_m = u_m$. If t_0 is short enough to satisfy the validity criterion above, we can expand the exponential in (9) and retain only the first two terms:

$$(11) \quad b_m \simeq \iint u_m^{*\prime} \sum_k w_k' w_k^* \left[1 - \frac{i t_0}{\hbar} (E_k - E_m) \right] u_n \, d\tau \, d\tau'$$

$$= \iint u_m^{*\prime} \sum_k w_k' w_k^* \left[1 - \frac{i t_0}{\hbar} (H_i - E_m) \right] u_n \, d\tau \, d\tau'$$

We use the closure relation, the orthogonality of u_m and u_n when $n \neq m$, $H_0 u_m^* = E_m u_m^*$, we can reduce this to:

$$(12) \quad b_m \approx -\frac{i t_0}{\hbar} \int u_m^* (H_1 - H_0) u_n \, d\tau \quad , m \neq n$$

Note that this is useful even when H_1 is large as long as the condition on t_0 is satisfied. On the other hand the time perturbation theory is useful when a small time dependent perturbation is added to the Hamiltonian and applied for a long time. Thus we have covered the two extreme cases.

As an example of the adiabatic approximation, consider the linear harmonic oscillator in which the equilibrium point depends on the time. The Hamiltonian is:

$$(13) \quad H(t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}K\left[x - a(t)\right]^2$$

The instantaneous eigenfunctions and eigenvalues follow immediately:

$$(14) \quad u_n(x) = N_n H_n\left[\alpha(x-a)\right] e^{-\frac{1}{2}\alpha^2(x-a)^2} , \quad E_n = (n+\tfrac{1}{2})\hbar\omega_0$$

Now the time derivative of the Hamiltonian is:

$$(15) \quad \frac{\partial H}{\partial t} = -K(x-a)\frac{da}{dt}$$

We use the well known relation for the matrix elements of the harmonic oscillator, assuming the oscillator initially in its 0 state and find:

$$(16) \quad \langle 1 | \frac{\partial H}{\partial t} | 0 \rangle = -\frac{(\frac{1}{2}\hbar)^{1/2} K}{(Km)^{1/4}}$$

We now substitute into the adiabatic approximation equation, viz:

(17) $$a_k(t) = \frac{1}{i\hbar\omega_{km}^2} \langle k | \frac{\partial H}{\partial t} | m \rangle \left(e^{i\omega_{km}t} - 1 \right)$$

and find for the magnitude of the coefficient:

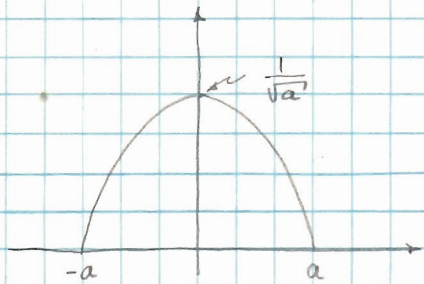
(18) $$\frac{da/dt}{(2\hbar\omega_c/m)^{1/2}}$$

We interpret physically by noting that the denominator is of the order of the maximum speed of a classical harmonic oscillator that has the zero point energy. Thus the adiabatic approximation is good if the equilibrium point moves slowly in comparison with the classical oscillator speed.

The sudden approximation can be applied to an oscillator in its ground state when the time required to move the equilibrium point from one steady position to another is small in comparison with $1/\omega_c$.

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

Variation: $u = c \cos\frac{\pi x}{2a}$; $|x| > a$, 0 otherwise



(1) $2c^2\int_0^a \cos^2\frac{\pi x}{2a}\,dx = \frac{4a}{\pi}c^2\int_0^{\pi/2}\cos^2\theta\,d\theta$

$= \frac{4a}{\pi}c^2\left(\frac{1}{2}\theta + \frac{1}{4}\sin 2\theta\right)\Big|_0^{\pi/2} = \frac{2a}{\pi}c^2\cdot\frac{\pi}{2} = 1$

$\therefore\ c = \frac{1}{\sqrt{a}}$

(2) $u = \frac{1}{\sqrt{a}}\cos\frac{\pi x}{2a}$

(3) $\frac{du}{dx} = -\frac{\pi}{2a\sqrt{a}}\sin\frac{\pi x}{2a}$; $\frac{d^2u}{dx^2} = -\frac{\pi^2}{4a^2\sqrt{a}}\cos\frac{\pi x}{2a}$

$Tu = \frac{\hbar^2}{2m}\cdot\frac{\pi^2}{4a^2\sqrt{a}}\cos\frac{\pi x}{2a}$

(4) $\int uTu\,dx = \frac{2\cdot\hbar^2\pi^2}{8ma^3}\int_0^a\cos^2\frac{\pi x}{2a}\,dx = \frac{\hbar^2\pi^2}{8ma^2}$

(5) $\int uVu\,dx = \frac{m\omega^2}{a}\int_0^a x^2\cos^2\frac{\pi x}{2a}\,dx = \frac{m\omega^2}{a}\left(\frac{2a}{\pi}\right)^3\int_0^{\pi/2}\theta^2\cos^2\theta\,d\theta$

$= \frac{m\omega^2}{a}\left(\frac{2a}{\pi}\right)^3\left[\frac{\theta^3}{6} + \left(\frac{\theta^2}{4} - \frac{1}{8}\right)\sin 2\theta + \frac{\theta\cos 2\theta}{4}\right]_0^{\pi/2}$

$= \frac{m\omega^2}{a}\left(\frac{2a}{\pi}\right)^3\left[\frac{\pi^3}{48} - \frac{\pi}{8}\right] = a^2 m\omega^2\left[\frac{1}{6} - \frac{1}{\pi^2}\right]$

$= a^2 m\omega^2\left(\frac{\pi^2 - 6}{6\pi^2}\right)$

(6) $\therefore\ \bar{H} = \frac{\hbar^2\pi^2}{8ma^2} + a^2 m\omega^2\left(\frac{\pi^2-6}{6\pi^2}\right)$

(7) $\frac{d\bar{H}}{da} = -\frac{\hbar^2\pi^2}{4ma^3} + 2a\,m\omega^2\left(\frac{\pi^2-6}{6\pi^2}\right) = 0$

$a^4 = \left(\frac{6\pi^2}{\pi^2-6}\right)\frac{\hbar^2\pi^2}{8m^2\omega^2}$; $a^2 = \left(\frac{3\pi^2}{\pi^2-6}\right)^{1/2}\frac{\hbar\pi}{2m\omega}$

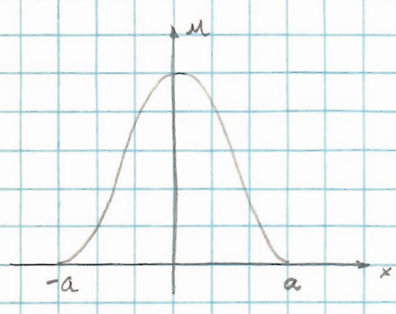
(8) $$H_{min} = \frac{\hbar^2\pi^2}{8m}\cdot\left(\frac{\pi^2-6}{3\pi^2}\right)^{1/2}\frac{2m\omega}{\hbar\pi} + \frac{m\omega^2}{2}\left(\frac{\pi^2-6}{3\pi^2}\right)\cdot\left(\frac{3\pi^2}{\pi^2-6}\right)^{1/2}\frac{\hbar\pi}{2m\omega}$$

$$= \left[\frac{\pi}{4}\left(\frac{\pi^2-6}{3\pi^2}\right)^{1/2} + \frac{\pi}{4}\left(\frac{\pi^2-6}{3\pi^2}\right)\cdot\left(\frac{3\pi^2}{\pi^2-6}\right)^{1/2}\right]\hbar\omega$$

$$= \frac{\pi}{2}\left(\frac{\pi^2-6}{3\pi^2}\right)^{1/2}\hbar\omega = \left(\frac{\pi^2-6}{3}\right)^{1/2}\frac{\hbar\omega}{2} = \left(\frac{\pi^2-6}{3}\right)^{1/2}E_0$$

$$= \left(\frac{3.8696}{3}\right)^{1/2}E_0 = 1.14\ E_0$$, differs by about 14% error.

Try the variation function: $u = C\cos^2\frac{\pi x}{2a}$, $|x| < a$, 0 otherwise



(1) $$2C^2\int_0^a \cos^4\frac{\pi x}{2a}\,dx = \frac{4C^2a}{\pi}\int_0^{\pi/2}\cos^4\theta\,d\theta$$

$$= \frac{4C^2a}{\pi}\cdot\frac{1\cdot3}{2\cdot4}\cdot\frac{\pi}{2} = \frac{3}{4}aC^2 = 1$$

(2) $$C = \frac{2}{\sqrt{3a}}\ ; \quad u = \frac{2}{\sqrt{3a}}\cos^2\frac{\pi x}{2a}$$

(3) $$\frac{du}{dx} = -\frac{\pi}{a\sqrt{3a}}\cdot 2\cos\frac{\pi x}{2a}\sin\frac{\pi x}{2a}$$

$$\frac{d^2u}{dx^2} = \frac{-\pi^2}{a^2\sqrt{3a}}\cos^2\frac{\pi x}{2a} + \frac{\pi^2}{a^2\sqrt{3a}}\sin^2\frac{\pi x}{2a}$$

$$= \frac{\pi^2}{a^2\sqrt{3a}}\left[1 - 2\cos^2\frac{\pi x}{2a}\right]$$

(4) $$\int uTu\,dx = -\frac{\hbar^2}{2m}2\cdot\frac{\pi^2\cdot2}{3a^3}\int_0^a\left(\cos^2\frac{\pi x}{2a} - 2\cos^4\frac{\pi x}{2a}\right)dx$$

$$= \frac{\hbar^2 8\pi}{2m\cdot3a^2}\int_0^{\pi/2}(2\cos^4\theta - \cos^2\theta)\,d\theta$$

$$= \frac{4\hbar^2\pi}{3ma^2}\left[2\cdot\frac{1\cdot3}{2\cdot4}\frac{\pi}{2} - \frac{\pi}{4}\right] = \frac{\hbar^2\pi^2}{6ma^2}$$

(5) $$\int uVu\,dx = \frac{4}{3a}\cdot2\cdot\frac{1}{2}m\omega^2\int_0^a x^2\cos^4\frac{\pi x}{2a}\,dx$$

$$= \frac{4}{3a}m\omega^2\left(\frac{2a}{\pi}\right)^3\int_0^{\pi/2}\theta^2\cos^4\theta\,d\theta$$

(6) $\cos 4\theta = 8\cos^4\theta - 8\cos^2\theta + 1$; $\cos 4\theta = 8\cos^4\theta - 4\cos 2\theta - 3$

$8\cos^2\theta = 4\cos 2\theta + 4$; $8\cos^4\theta = \cos 4\theta + 4\cos 2\theta + 3$

(7) $$\int_0^{\pi/2}\theta^2\cos^4\theta\, d\theta = \frac{1}{8}\int_0^{\pi/2}\theta^2\cos 4\theta\, d\theta + \frac{1}{2}\int_0^{\pi/2}\theta^2\cos 2\theta\, d\theta + \frac{3}{8}\int_0^{\pi/2}\theta^2\, d\theta$$

$$= \frac{1}{8\cdot 4^3}\int_0^{2\pi}\theta^2\cos\theta\, d\theta + \frac{1}{16}\int_0^{\pi}\theta^2\cos\theta\, d\theta + \frac{1}{8}\left(\frac{\pi}{2}\right)^3$$

$$= \left(-\frac{1}{4^4} + \frac{1}{4^2}\right)\int_0^{\pi}\theta^2\cos\theta\, d\theta + \frac{1}{8}\left(\frac{\pi}{2}\right)^3$$

$$= \frac{1}{8}\left(\frac{\pi}{2}\right)^3 + \frac{1}{16}\left(\frac{15}{16}\right)\Big[2\theta\cos\theta + (\theta^2-2)\sin\theta\Big]_0^{\pi}$$

$$= \frac{1}{8}\left(\frac{\pi}{2}\right)^3 - \frac{\pi}{8}\left(\frac{15}{16}\right) = \frac{1}{64}\left(\pi^3 - \frac{15\pi}{2}\right)$$

(8) $$\therefore \int u V u\, dx = \frac{4}{3}m\omega^2 a^2\,\frac{1}{8}\left(1 - \frac{15}{2\pi^2}\right) = \frac{m\omega^2 a^2}{12\pi^2}(2\pi^2 - 15)$$

(9) $$\therefore \bar{H} = \frac{\hbar^2\pi^2}{6ma^2} + \frac{m\omega^2 a^2}{12\pi^2}(2\pi^2 - 15)$$

(10) $$\frac{d\bar{H}}{da} = -\frac{\hbar^2\pi^2}{3ma^3} + \frac{m\omega^2 a}{6\pi^2}(2\pi^2 - 15) = 0$$

$$a^4 = \frac{2\hbar^2\pi^4}{m^2\omega^2}\cdot\frac{1}{(2\pi^2-15)^{1/2}} \;;\quad a^2 = \frac{\hbar\pi}{m\omega}\left(\frac{2\pi^2}{2\pi^2-15}\right)^{1/2}$$

(11) $$\bar{H}_{min} = \frac{\hbar^2\pi^2}{6m}\cdot\frac{m\omega}{\hbar\pi}\left(\frac{2\pi^2-15}{2\pi^2}\right)^{1/2} + \frac{m\omega^2}{6}\left(\frac{2\pi^2-15}{2\pi^2}\right)\cdot\frac{\hbar\pi}{m\omega}\left(\frac{2\pi^2}{2\pi^2-15}\right)^{1/2}$$

$$= \frac{\hbar\omega}{6}\cdot 2\left(\frac{2\pi^2-15}{2}\right)^{1/2} = \frac{2}{3}\left(\frac{2\pi^2-15}{2}\right)^{1/2}\frac{\hbar\omega}{2}$$

$$= \frac{2}{3}\left(\frac{2\pi^2-15}{2}\right)^{1/2}E_0 = \frac{2}{3}\left(\frac{4.74}{2}\right)^{1/2}E_0$$

$$= \frac{2}{3}(1.54)\,E_0 = 1.02\,E_0$$, differs by about 2%, good.

1960 - 61

HARVARD UNIVERSITY

Physics 251a

Answer **FIVE** questions

1. Use the principle of stationary phase to calculate the group velocity of de Broglie waves, and show that, for a 'well-formed' group, it agrees with the classical particle velocity (free-particle case).

   Explain how one obtains from the operator corresponding to a physical variable the operator corresponding to the time derivative of the variable. For the case of a particle subject to a force $-\nabla V$, calculate the time derivatives of $\bar{x}$ and $\bar{p}$. Discuss the extent to which this result (Ehrenfest's theorem) gives correspondence between the classical and wave-mechanical motions.

2. (a) Which of the following operators are Hermitian, and which are not?

   (1) $x^2p_x^2$ (2) xp_x+p_xx (3) p_xxp_x

   (4) $i(xp_y-yp_x)$ (5) $x^3p_xx-x^2p_xx^2+xp_xx^3$

   (6) z^2p_x

   (b) State reasons for the requirement that the Hamiltonian operator be Hermitian.

   (c) Explain the general criterion for fixing the permissible behavior of the wave function at places where the potential energy is discontinuous or singular. Apply this criterion to derive the rule for continuing the wave function across a surface where the potential energy V is discontinuous.

3. Use the ladder method to determine the eigenvalues E_n, the normalized eigenfunctions $u_n(x)$, and the matrix elements of the operators x and $-i\frac{d}{dx}$ for the harmonic oscillator with Hamiltonian operator $-\frac{d^2}{dx^2}+x^2$

Physics 251a

4. The unperturbed system has Hamiltonian

$$H_0 = H_x + H_y = -\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + x^2 + y^2$$

and energies $2n_x + 2n_y + 2$. The total Hamiltonian is

$$H = H_0 + V = H_0 + ax^2y^2$$

To save you computation, it is stated that for the one-dimensional problem with Hamiltonian H_x and energies $2n+1$ the only nonvanishing matrix elements of x^2 are

$$(x^2)_{n,n} = n+\tfrac{1}{2}$$

$$(x^2)_{n,\,n+2} = (x^2)_{n+2,n} = \tfrac{1}{2}\sqrt{(n+1)(n+2)}$$

(a) Find the energy corrections $E^{(1)}_{00}$ and $E^{(2)}_{00}$ for the ground state.

(b) Show that for the next level, with $E^{(0)}=4$, the degeneracy is not removed in the first order, and is also not removed in the second order; but do not calculate the energy corrections.

(c) For the level with $E^{(0)}=6$ determine the values of $E^{(1)}$ for the states into which this degenerate level splits, and also find the corresponding 'right linear combinations' of the original product functions $u_m(x)u_n(y)$.

5. (a) Define the transmission coefficient T and the reflection coefficient R for the case in which V has some constant value for $x < -a$ and also some (perhaps different) constant value for $x > +a$.

(b) In the sense of the phase-integral method, define T and R for the case in which for $|x| > a$ one has

$$V(x) < E; \quad \left|\frac{dV}{dx}\right| << m^{\frac{1}{2}}h^{-1}(E - V(x))^{3/2} .$$

Explain the significance of the stated condition on $\frac{dV}{dx}$.

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5. (c) For the rectangular potential step,

$$V = -V_0 < 0,\ x < 0; \quad V = 0,\ x > 0$$

calculate R as function of E.

6. Given a system with unperturbed Hamiltonian H_0, and with states labelled m, n, ... having eigenvalues and eigenfunctions such that

$$H_0 u_n = E_n u_n .$$

Suppose a set of states labelled with numbers k have closely spaced eigenvalues E_k covering a range that overlaps the value E_m for a state m that does not belong to the set k. For the case of a perturbation H' that is constant in time, give the time-dependent-perturbation-theory argument that leads to the formula

$$w = \frac{2\pi}{\hbar} \rho(k) \, |H'_{km}|^2$$

for the probability per unit time of transition from state m to the set k. ($\rho(k) dE_k$ is the number of states k in the energy range dE_k near E_m.)

Final, January 1960

$$(x + ip)(x - ip) = x^2 - ixp + ipx + p^2$$

$$(x - ip)(x + ip) = x^2 + ixp - ipx + p^2$$

$$= -2ixp + 2ipx = 2i(px - xp) = -2$$

$$\left(\frac{d}{dx} + x\right)\left(\frac{d}{dx} + x\right) = \frac{d^2}{dx^2} + 1 + x\frac{d}{dx} + x^2$$

$$\frac{d^2 u_0}{dx^2} + x\frac{du_0}{dx} + (x^2 + 1)u_0 = 0$$

Due · Mon 10-24

PROBLEM SET # 1

Physics 251a problems, 1960

1. Using the same sort of argument (Fourier transformation) as was used to find the coordinate-space form of the operator p_x, show that the mean value of $x^n p_x^m$ is the same when calculated with the momentum-space function φ as when calculated with the position-space function ψ. Prove this same equivalence for $p_x^n x^m$. Is the same true of a product arbitrarily arranged, $x^a p_x^b x^c p_x^d \ldots$?

2. Given the one-dimensional normalized Gaussian wave function (for a particular instant of time, t = 0)

$$\psi(x,0) = (2\pi\sigma^2)^{-1/4} \exp(-x^2/4\sigma^2)$$

$$(\sigma^2 = \overline{(\Delta x)^2} = \overline{x^2};\ \overline{x} = 0)$$

carry out the Fourier transformation to obtain the momentum-space wave function $\varphi(p_x,0)$. Verify that φ automatically turns out to be normalized, and find from it the value of $\overline{p_x^2}$.

3. Find a wave-function $\psi(x,0)$ that makes $\overline{(\Delta x)^2}\ \overline{(\Delta p_x)^2}$ a minimum, with $\overline{x}$ and $\overline{p}_x$ having given non-vanishing values. (Obtain it by suitable modification of the function given in Problem 2.)

4. Find the result of applying the operator $\exp(iap_x/\hbar)$ to the wave function $\psi(x,y,z,t)$. (Assume ψ is an analytic function.)

5. Express the commutator $[x^2, p_x^2]$ as an imaginary multiple of a symmetrized product. Express $[x^5, p_x^3]$ as an imaginary multiple of a sum of symmetrized products.

6. Given the three functions 1, x, x^2 on the interval $0 < x < 1$.
(a) Form linear combinations, of degrees 0, 1, 2 in x, that are orthogonal to each other on this interval (with weight factor 1, or 'ordinary orthogonal' functions).
(b) Carry out the corresponding construction, requiring orthogonality with the weight factor $\rho = x$.

7. Write the wave equation of a free particle

$$\nabla^2 u + k^2 u = 0$$

in cylindrical coordinates, $\rho = \sqrt{x^2 + y^2}$, $\varphi = \arctan \frac{y}{x}$, z. Separate the variables, and obtain the general single-valued product solution, for any given k, in
terms of
terms of $e^{\pm iKz}$ and Bessel functions of $\alpha\rho$, with $\alpha^2 + K^2 = k^2$. Which solution of Bessel's equation must be used? Why is the other inadmissible? Carry out the normalization of a typical product solution,

$$u = U(\rho)\, V(z)\, W(\varphi)$$

by normalizing each factor; normalize V in the scale of K, U in the scale of α.

3. Multiply the product $u^*_{k_2}(x)u_{k_1}(x)$ of two one-dimensional free-particle functions normalized in the scale of k
by the convergence
by the convergence factor $e^{-\beta|x|}$, and integrate. Call the result $\delta_{C\beta}(k_1-k_2)$. Discuss its behavior for various values of k_1-k_2 and β, and show that it can be thought of as giving the Dirac δ-function in the limit $\beta \to 0$.

9. Given the symmetrical rectangular potential well in one dimension,

$$V = 0, \quad |x| > a; \quad V = -V_o, \quad |x| < a$$

show that no matter how small the values of the positive quantities V_o and a may be, there is always one discrete bound state.

15. In the potential field of Problem 14, there are two independent wave functions (two-fold degeneracy) for any energy E greater than both V_e and V_r. In setting up a system for expansion of an arbitrary function, we need to pick two solutions u and v, that are orthogonal. The practical test for this is that $\int_{-\infty}^{\infty} v^* u \, dx$ shall not give any delta function (i.e. the coefficient of the integral that would give a delta function must be zero). Show that the functions u and v defined by

$$u = C \exp(ik_r x), \quad x > b$$

$$(\hbar k_r)^2 = 2m(E - V_r)$$

and

$$v = C' \exp(-ik_e x), \quad x < -a$$

$$(\hbar k_e)^2 = 2m(E - V_e)$$

satisfy this test.

16. For convenience, write u for the product rR(r). Then for the hydrogen atom, in natural units, u satisfies

$$H_\ell u = Eu \tag{1}$$

with

$$H_\ell = \frac{\ell(\ell + 1)}{r^2} - \frac{2}{r} - \frac{d^2}{dr^2} \tag{2}$$

and, for $E < 0$, $u \to 0$ exponentially for $r \to \infty$, $u(0) = 0$. Consider the operators

$$A_\ell = \frac{\ell}{r} - \frac{1}{\ell} + \frac{d}{dr}$$

$$A_\ell^+ = \frac{\ell}{r} - \frac{1}{\ell} - \frac{d}{dr}$$

Evaluate the products $A_\ell^+ A_\ell$ and $A_\ell A_\ell^+$. If u satisfies Eq.(1) and the boundary conditions, find functions Au and A^+u (with suitable subscripts on the operators) that satisfy analogous differential equations. Show that these new functions also satisfy the boundary conditions.

10. For the well of Problem 9, what is the condition on V_o and $\underline{a}$ for there to exist at least one more bound state besides the lowest one? The condition for just one more state besides the lowest one?

11. Consider the well of Problem 9 with V_o = 15 Mev and $\underline{a}$ equal to the largest value for which there is still only one bound state. Calculate the energy of this state to the nearest Mev.

12. Let the potential in a one-dimensional collision problem be given by

$$V = 0, \quad |x| > a; \quad V = V_o, \quad |x| < a$$

Find formulas for T and R, using notation
(a) For $E > V_o$, $(\hbar k)^2 = 2mE$, $(\hbar\beta)^2 = 2m(E-V_o)$

(b) For $E < V_o$, $(\hbar k)^2 = 2mE$, $(\hbar\gamma)^2 = 2m(V_o-E)$

For $ka = \pi$, plot roughly the behavior of T for values of V_o from $-4E$ to $+2E$.

13. An electron of energy $E = (\hbar k)^2/2m$ is incident from the left on the following potential distribution:

$$V = -35E, \quad x < -a$$

$$V = -15E, \quad -a < x < 0$$

$$V = 0, \quad x > 0$$

Find the reflection coefficient as function of the quantity $\theta = 4ka$. How does its minimum value compare with its value for $\theta = 0$? (The latter is the value for a single jump from $V = -35E$ to $V = 0$).

14. Let V(x) be an arbitrary potential which takes constant values outside a certain region, say

$$V = V_\ell \quad \text{for } x < -a, \text{ and } V = V_r \text{ for } x > +b$$

Apart from this the only restriction on V is that it possess no such singularities as might prevent the wave equation from having two independent single-valued solutions bounded for $-a \leq x \leq +b$; then for E greater than both V_ℓ and V_r both solutions are admissible in treating one-dimensional collision problems. Under these circumstances prove:
(a) The reflection coefficient is the same whether particles are incident from the right or the left.
(b) The sum of the reflection and transmission coefficients is always unity.

17. (Continuation). Show that for a fixed negative value of E, ℓ cannot be indefinitely large. From this and the results of Problem 16, find the possible negative values of E and the values of ℓ corresponding to each.

Using the A and A^+ operators, construct and normalize the functions $u_{n,n-1}$, $u_{n,n-2}$, and $u_{n,n-3}$. Check that they are the same as the functions rR found in class.

18. By the formula found in class, the radial factor of the wave function, normalized in the k scale, for a particle of mass m and charge ze moving in the field of a fixed point charge Ze is

$$R_{\ell k}(r) = (2k)^{\ell+1} e^{-\pi\nu/2} \left| \Gamma(\ell+1+i\nu) \right| \cdot$$
$$\cdot (2\pi)^{-\frac{1}{2}} \left[(2\ell+1)!\right]^{-1} r^{\ell} e^{-ikr} F(\ell+1-i\nu; 2\ell+2; 2ikr)$$

where $\nu = zZ/k a_0$, $a_0 = \hbar^2/me^2$.

By the nature of continuous normalization, the amplitude of R_{1k} at large distances is independent of ν. Because of the factor r^{ℓ}, only $\ell=0$ gives non-vanishing probability for the particle to be at the center of force. The effect of the charge on this probability is given by the factor

$$C = \left|R_{0k}(0)\right|^2 / \left|R_{0k}(0)\right|^2_{\nu=0}$$

This factor has an important bearing on the probabilities of many nuclear processes.

Calculate C in terms of ν and $e^{\pi\nu}$.

19. For the harmonic oscillator express $q^2 u_n$ and $p^2 u_n$ as linear combinations of the u_m. Evaluate $\overline{q^2}$ and $\overline{p^2}$ for the state u_n, and show that these are the same values as classical theory gives for a state of vibration with energy $(n + \frac{1}{2})\hbar\omega$. How could this same conclusion be reached with less calculation?

20. Using the generating function

$$e^{-t^2+2ty} = \sum_{n=0}^{\infty} H_n(y) \frac{t^n}{n!}$$

show that $H_n(y)$ satisfies the differential equation

$$v'' - 2yv' + (\epsilon - 1)v = 0$$

with $\epsilon = 2n + 1$.

17. (Continuation). Show that for a fixed negative value of [illegible] $\mathcal{l}$ cannot be indefinitely large. From this and the results of Problem 16, find the possible negative values of [illegible] and the valu[illegible] of $\mathcal{l}$ corresponding to each.

Using the A and A^+ operators, construct and normalize the functions $u_{n,n-1}$, $u_{n,n-2}$, and $u_{n,n-3}$. Check that they are the same as the functions rk found in class.

18. By the formula found in class, the radial factor of the wave function, normalized in the k scale, for a particle of mas[illegible] m and charge ze moving in the field of a fixed point charge Ze is

$$R_{\mathcal{l}k}(r) = (2k)^{\mathcal{l}+1} e^{-\pi u/2} \left| \Gamma(\mathcal{l}+1+iu) \right|$$

$$\cdot (\pi)^{-\frac{1}{2}} \left[(2\mathcal{l}+1)! \right]^{-1} r^{\mathcal{l}} e^{-ikr} F(\mathcal{l}+1-iu; 2\mathcal{l}+2; 2ikr)$$

where $u = zZ/k a_0$, $a_0 = \hbar^2/me^2$.

By the nature of continuous normalization, the amplitud[illegible] R_{lk} at large distances is independent of u. Because of the factor $r^{\mathcal{l}}$, only $\mathcal{l} = 0$ gives non-vanishing p[illegible] ticle to be at the center of force. The e[illegible] on this probability is given by the factor

$$C = \left| R_{0k}(0) \right|^2 / \left| R_{0k}(0) \right|^2_{u=0}$$

This factor has an important bearing on the probabilities of many nuclear processes.

Calculate C in terms of u and $e^{\pi u}$.

19. For the harmonic oscillator express q [illegible] combinations of the u_n. Evaluate $\overline{q^2}$ and $\overline{p}$[illegible] and show that these are the same values as [illegible] gives for a state of vibration with energy [illegible] this same conclusion be reached with less [illegible]

20. Using the generating function

$$e^{-t^2+2t\xi} = \sum_{n=0}^{\infty} H_n(\xi) \frac{t^n}{n!}$$

show that $H_n(\xi)$ satisfies the [illegible]

$$v'' - 2\xi v' + (\epsilon - 1)v = 0$$

with $\epsilon = 2n$

21. Put the wave equation of the two-dimensional isotropic harmonic oscillator into polar coordinates, and obtain the 'radial wave equation', including the term containing the quantum number m from the angular factor $e^{im\varphi}$. From the indicial equation and the requirement that the series terminate, obtain the relation $E = (n+1)\hbar\omega$, and show what values of m can occur for each value of n. Show that the number of independent wave functions for each value of n is the same as found using rectangular coordinates.

22. Carry out the same analysis for the three-dimensional harmonic oscillator; here one is concerned with the quantum numbers ℓ and n, and $E = (n+3/2)\hbar\omega$. Find what values of ℓ can go with each value of n, and by summing $(2\ell+1)$ show that the degree of degeneracy is that found in class by using rectangular coordinates. (The differential-equation work in this problem is closely analogous to that of Problem 21. Try to transfer results rather than repeat work.)

23. Use the variation method to estimate the ground-state energy of the harmonic oscillator with Hamiltonian

$$H = T + V = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \tfrac{1}{2} m\omega^2 x^2 ,$$

employing in succession the two forms of trial function:

a) $u = Ce^{-\alpha |x|}$

b) $u = C(a - |x|), \quad |x| < a; \quad u = 0, \quad |x| > a$

For each function, carry out the following steps:

a) Sketch the shape of the function.

b) Evaluate C so that $\int_{-\infty}^{\infty} u^2 dx = 1.$

c) Evaluate $Tu = -\frac{h^2}{2m}\frac{d^2u}{dx^2}$ as a function of x.

Note that where $u'(x)$ has a discontinuity Tu contains a δ-function.

d) Evaluate $\bar{H} = \int_{-\infty}^{\infty} u\, H\, u\, dx$ as a function of α or a. The δ-function contributions must not be forgotten.

e) Calculate $E_{o\ est} = \bar{H}_{min}$ by choosing the optimum value of α or a. Express each result as a 3-place decimal times $\hbar\omega$, so that the results can readily be compared with each other and with the true value, $E_o = 0.500\ \hbar\omega$.

f) Set an upper limit on the sum $\sum_{n=1}^{\infty} a_n^2$, for $u = \sum_{n=0}^{\infty} a_n u_n$, u_n being the normalized eigenfunctions of the oscillator. Note that $a_1 = 0$ because $u_1(-x) = -u_1(x)$.

24. The one-dimensional problem

$$\frac{d^2}{dx^2} v(x) + (E^{(o)} - x^2)\, v(x) = 0$$

has eigenvalues $E_n^{(o)} = 2n + 1$

and matrix elements $x_{mn} = \sqrt{\frac{m}{2}}\, \delta_{m,n+1} + \sqrt{\frac{n}{2}}\, \delta_{m+1,n}$

Use perturbation theory to find the terms in α and α^2 in the eigenvalues of

$$\frac{d^2u}{dx^2} + (E - x^2 - \alpha x)\, u = 0$$

Determine the eigenvalues exactly, and compare with your perturbation theory answer.

25. The unperturbed wave functions for Problem ~~23~~ 24 are

$$v_n = \frac{H_n(x)\, e^{-x^2/2}}{\sqrt{2^n n!\, \sqrt{\pi}}}$$

Find the terms in α by which u_n differs from v_n. Compare the approximate u_n with the Taylor series in α for the exact solution, and thus obtain a recurrence relation for H_n and H'_n.

26. Consider the states with $E^{(o)} = 6$, in the two dimensional oscillator problem discussed in class. Using perturbation theory, with $V = axy$ as in class, find the terms in a and a^2 in the energies. Check these results against the exact values.

27. Use the phase-integral method to find approximately the two smallest characteristic values of E for

$$\frac{d^2u}{dx^2} + (E - |x|)\, u = 0$$

Compute to three decimal places, and compare with the exact values 1.019..., 2.338... Can you explain why the phase-integral method works fairly well for these low states, even though the 'potential energy' is not a smooth function?

$$\frac{35}{128} a^2 \pi E^2 - \frac{3}{16} a \sqrt{\pi} \sqrt{E}^{2} + \frac{\pi}{2} E - \left(n + \frac{1}{2}\right) \pi = 0$$

28. Suppose the potential energy is

$$V = -8.0 \times 10^{16}\ x^2 \quad \text{(V in electron-volts, x in cm)}$$

For electrons with $E < 0$, this is a potential barrier. Find the approximate transmission coefficient for electrons of energy $E = -10.0$ electron-volts.

29. Use the phase-integral method to find the eigenvalues of the anharmonic oscillator problem,

$$\frac{d^2u}{dx^2} + (E - x^2 - ax^4)\, u = 0,$$

for small values of a, correct to and including terms in a^2. (To put the phase integral in suitable form for expansion in powers of a, introduce a new variable Ψ by setting $\sin \Psi = x/x_1$, where x_1 is the positive real turning point).

30. Use perturbation theory to find the eigenvalues of the above anharmonic oscillator problem, correct to and including terms in a^2. Compare with results of Problem 29. In what sorts of circumstances can one or the other result be presumed to be the more reliable? (Matrix elements of x^4 can be found by matrix multiplication from the known matrix x_{nm} for the unperturbed harmonic oscillator (natural units)

$$x_{mn} = \sqrt{\frac{m}{2}}\ \delta_{m,n+1} + \sqrt{\frac{n}{2}}\ \delta_{m+1,n} \quad .$$

The general matrix multiplication rule

$$(AB)_{mn} = \sum_k A_{mk} B_{kn}$$

is probably already familiar, though we haven't quite got around to bringing it into the lectures.

Assignment #1
Problem Set #1

Paul Grant
DEAP-AP-16
P251a
10-15-60

6

1. (1) We will take the following transformations between co-ordinate and momentum space:

$$\psi = h^{-1/2} \int e^{i p_x x/\hbar} \varphi \, dp_x$$

$$\varphi = h^{-1/2} \int e^{-i p_x x/\hbar} \psi \, dx$$

In co-ordinate space:

$x \to x$

$\underline{p_x} \to \frac{\hbar}{i} \frac{\partial}{\partial x}$

In momentum space:

$\underline{x} \to -\frac{\hbar}{i} \frac{\partial}{\partial p_x}$

$p_x \to p_x$

We will show that the operators in momentum space are true.

(2) $$\overline{x^n} = \int \psi^* x^n \psi \, dx = h^{-1/2} \int \psi^* dx \cdot \int x^n e^{i p_x x/\hbar} \varphi \, dp_x$$

We now recognize that: $x^n e^{i p_x x/\hbar} \equiv \left(\frac{\hbar}{i} \frac{\partial}{\partial p_x}\right)^n e^{i p_x x/\hbar}$

(3) $$\therefore \overline{x^n} = h^{-1/2} \int \psi^* dx \cdot \int \left(\frac{\hbar}{i} \frac{\partial}{\partial p_x}\right)^n e^{i p_x x/\hbar} \varphi \, dp_x$$

(4) Integrating n times by parts:

$$\overline{x^n} = \underbrace{h^{-1/2} \int \psi^* dx \cdot \int e^{i p_x x/\hbar}}_{\varphi^*} \left(-\frac{\hbar}{i} \frac{\partial}{\partial p_x}\right)^n \varphi \, dp_x$$

(5) $$\therefore \overline{x^n} = \int \varphi^* \left(-\frac{\hbar}{i} \frac{\partial}{\partial p_x}\right)^n \varphi \, dp_x$$

Thus we may define $\underline{x} \to -\frac{\hbar}{i} \frac{\partial}{\partial p_x}$

Proceeding to the evaluation of $\overline{x^n p_x^m}$: we shall start in co-ordinate space:

(6) $$\overline{x^n p_x^m} = \int \psi^* x^n \underline{p_x}^m \psi \, dx = \int \psi^* x^n \left(\frac{\hbar}{i} \frac{\partial}{\partial x}\right)^m \psi \, dx$$

We underline operators whose form is different from the variables themselves

Substituting for ψ from (1):

(7) $$\overline{x^n p_x^m} = \int \psi^* x^n \left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^m \left[h^{-1/2} \int e^{i p_x x/\hbar} \varphi \, dp_x \right] dx$$

$$= h^{-1/2} \int \psi^* x^n \left[\int \left(\frac{\hbar}{i} \cdot \frac{i}{\hbar} p_x \right)^m e^{i p_x x/\hbar} \varphi \, dp_x \right] dx$$

$$= h^{-1/2} \int \psi^* dx \cdot \int x^n e^{i p_x x/\hbar} p_x^m \varphi \, dp_x$$

$$= h^{-1/2} \int \psi^* dx \cdot \int \left(\frac{\hbar}{i} \frac{\partial}{\partial p_x} \right)^n e^{i p_x x/\hbar} p_x^m \varphi \, dp_x$$

Integrate the second integral n times by parts:

(8) $$\overline{x^n p_x^m} = \underbrace{h^{-1/2} \int \psi^* dx \cdot \int e^{i p_x x/\hbar}}_{\varphi^*} \underbrace{\left(-\frac{\hbar}{i} \frac{\partial}{\partial p_x} \right)^n}_{= \underline{x}^n} p_x^m \varphi \, dp_x$$

(9) $$\therefore \quad \overline{x^n p_x^m} = \int \psi^* x^n \underline{p}_x^m \psi \, dx = \int \varphi^* \underline{x}^n p_x^m \varphi \, dp_x$$

✓

For $\overline{p_x^n x^m}$, we will start with the momentum representation for convenience:

(10) $$\overline{p_x^n x^m} = \int \varphi^* p_x^n \underline{x}^m \varphi \, dp_x = \int \varphi^* p_x^n \left(\frac{\hbar}{-i} \frac{\partial}{\partial p_x} \right)^m \left[h^{-1/2} \int e^{-i p_x x/\hbar} \psi \, dx \right] dp_x$$

$$= h^{-1/2} \int \varphi^* dp_x \cdot p_x^n \int \left(-\frac{\hbar}{i} \cdot \frac{-i}{\hbar} x \right)^m e^{-i p_x x/\hbar} \psi \, dx$$

$$= h^{-1/2} \int \varphi^* dp_x \cdot \int p_x^n e^{-i p_x x/\hbar} x^m \psi \, dx$$

$$= h^{-1/2} \int \varphi^* dp_x \cdot \int \left(-\frac{\hbar}{i} \frac{\partial}{\partial x} \right)^n e^{-i p_x x/\hbar} x^m \psi \, dx$$

Integrating by parts n times:

(11) $$\overline{p_x^n x^m} = \underbrace{h^{-1/2} \int \varphi^* dp_x \cdot \int e^{-i p_x x/\hbar}}_{\psi^*} \underbrace{\left(\frac{\hbar}{i} \frac{\partial}{\partial x} \right)^n}_{= \underline{p}_x^n} x^m \psi \, dx$$

$$= \int \psi^* \underline{p}_x^n x_n \psi \, dx$$

✓

Assignment #1
Continued

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Problem 1
Continued

In General: $\overline{x^n p_x^m} \neq \overline{p_x^m x^n}$ Why should it be?

Proof:

(12) It can be shown that (see Prob. #5):

$$[x^n, p_x^m]\psi = -\left\{ \sum_{k=1}^{m} (-i\hbar)^k \binom{m}{k} \left[\prod_{l=1}^{k} (n-l+1) \right] x^{n-k} p_x^{m-k} \right\} \psi$$

(13) Multiply by ψ^* and integrate over all position space:

$$\overline{x^n p_x^m} - \overline{p_x^m x^n} = - \sum_{k=1}^{m} (-i\hbar)^k \binom{m}{k} \left[\prod_{l=1}^{k} (n-l+1) \right] \overline{x^{n-k} p_x^{m-k}}$$

Therefore, we may not, in general, arbitrarily arrange a product if that is what is meant by the question. If it is meant that: 10.

$$\int \psi^* (x^a p_x^b x^c p_x^d) \psi \, dx = \int \varphi^* (x^a p_x^b x^c p_x^d) \varphi \, dp_x$$

this is true as long as the last operator in the chain is a momentum operator. This can be seen from the fact that we can continue "pushing thru" each operator past the exponential by performing the differentiation or integration by parts as required by the operator and the space one is working in.

True in general!

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2\. (1) We assert that:

a. $\psi = h^{-1/2} \int e^{i p_x x/\hbar} \varphi \, dp_x$

b. $\varphi = h^{-1/2} \int e^{-i p_x x/\hbar} \psi \, dx$

$\psi(x,0) = \psi = \frac{1}{(2\pi\sigma^2)^{1/4}} e^{-x^2/4\sigma^2}$

$\sigma = \overline{(\Delta x)^2} = \overline{x^2} \; ; \; \overline{x} = 0$

We thus make use of the Fourier transform defined by (1b).

(2) $$\varphi = \frac{h^{-1/2}}{(2\pi\sigma^2)^{1/4}} \int_{-\infty}^{\infty} \exp\left[-\frac{x^2}{4\sigma^2} - i\frac{p_x x}{\hbar}\right] dx$$

$$= \frac{h^{-1/2}}{(2\pi\sigma^2)^{1/4}} \left[\int_{-\infty}^{\infty} e^{-x^2/4\sigma^2} \cos\frac{p_x}{\hbar}x \, dx - i \int_{-\infty}^{\infty} e^{-x^2/4\sigma^2} \sin\frac{p_x}{\hbar} x \, dx\right]$$

Since the integrand of the second integral is odd, the integral of course vanishes and we have

(3) $$\varphi = \frac{2h^{-1/2}}{(2\pi\sigma^2)^{1/4}} \int_0^{\infty} e^{-x^2/4\sigma^2} \cos\frac{p_x}{\hbar} x \, dx$$

$$= \frac{2h^{-1/2}\sigma\sqrt{\pi}}{(2\pi\sigma^2)^{1/4}} e^{-\frac{\sigma^2}{\hbar^2}p_x^2} \text{, by tables}$$ ✓

Checking for normalization:

(4) $$\int \varphi^* \varphi \, dp_x = \frac{4h^{-1}\sigma^2\pi}{(2\pi\sigma^2)^{1/2}} \cdot 2\int_0^{\infty} e^{-\frac{2\sigma^2}{\hbar^2}p_x^2} dp_x$$

$$= \frac{8h^{-1}\sigma^2\pi}{(2\pi\sigma^2)^{1/2}} \cdot \frac{\sqrt{\pi}}{2\cdot\sqrt{2}\sigma} \cdot \frac{h}{2\pi} = 1$$ ✓

(5) $$\overline{p_x^2} = \int \varphi^* p_x^2 \varphi \, dp_x = \frac{8h^{-1}\sigma^2\pi}{(2\pi\sigma^2)^{1/2}} \int_0^{\infty} p_x^2 e^{-\frac{2\sigma^2}{\hbar^2}p_x^2} dp_x$$

$$= \frac{8h^{-1}\sigma^2\pi}{(2\pi\sigma^2)^{1/2}} \cdot \frac{h^2\sqrt{\pi}}{4\cdot 4\pi^2 \cdot 2\sigma^2} \cdot \frac{h}{2\pi} \cdot \frac{1}{\sqrt{2}\sigma} = \frac{1}{4}\frac{\hbar^2}{\sigma^2}$$ ✓

which is the same result obtained using the wave function in position space.

Assignment #1
Continued

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3. (1) In choosing a suitable relation between the operators, we must satisfy the minimum of the Schwartz inequality. A simple proportionality will do this and we will choose the following which we hope will position our wave packet around a non-zero value:

$$p_x \psi = c(x+\mu)\psi$$, where μ is a real positive or negative number

This satisfies the equal sign in the Schwartz inequality and generalizes the proportionality between the operators. Choosing the position-space form for p_x:

(2) $$\frac{d\psi}{dx} = c(x+\mu)\psi$$ where $\frac{\hbar}{i}$ has been lumped into the constant c.

(3) $$\frac{d\psi}{\psi} = c(x+\mu)\,dx \quad ; \quad \ln c'\psi = c\left(\frac{x^2}{2}+\mu x\right)$$
$$= c\left(\frac{x^2}{2}+\mu x+\frac{\mu^2}{2}\right) - c\frac{\mu^2}{2} = \frac{c}{2}(x+\mu)^2 - \frac{c}{2}\mu^2$$

(4) $$\psi = K' e^{-K(x+\mu)^2} \quad ; \quad K' = c'^{-1} e^{-\frac{c\mu^2}{2}}, \quad K = -\frac{c}{2}$$

We demand normality:

(5) $$\int_{-\infty}^{\infty} \psi^*\psi\,dx = 2K'^2\int_0^{\infty} e^{-2K(x+\mu)^2}\,dx = 2K'^2\cdot\frac{1\sqrt{\pi}}{2\sqrt{2K}} = 1$$

$$K' = \sqrt[4]{\frac{2K}{\pi}}$$, using tables

(6) $$\therefore \quad \psi = \sqrt[4]{\frac{2K}{\pi}}\, e^{-K(x+\mu)^2}$$

We now find $\bar{x}$:

(7) $$\bar{x} = \sqrt{\frac{2K}{\pi}}\int_{-\infty}^{\infty} x\, e^{-2K(x+\mu)^2}\,dx = \sqrt{\frac{2K}{\pi}}\int_{-\infty}^{\infty}(v-\mu)\,e^{-2Kv^2}\,dv$$

Let $v = x+\mu$
$dv = dx$

$$= \sqrt{\frac{2K}{\pi}}\left[\underbrace{\int_{-\infty}^{\infty} v\,e^{-2Kv^2}\,dv}_{=\,0} - \mu\underbrace{\int_{-\infty}^{\infty} e^{-2Kv^2}\,dv}_{=\,\sqrt{\frac{\pi}{2K}}}\right] = -\mu$$

Thus we have $\bar{x} = -\mu$. If we change the sign of μ in the distribution we have $\bar{x} = \mu$ and:

(8) $$\psi = \sqrt[4]{\frac{2k}{\pi}}\, e^{-k(x-\mu)^2}$$

We now take $\sigma^2 = \overline{(\Delta x)^2} = \overline{(x-\mu)^2} = \overline{x^2} - \overline{2\mu x} + \mu^2$

$= \overline{x^2} - \mu^2$

(9) $$\overline{x^2} = \sqrt{\frac{2k}{\pi}} \int_{-\infty}^{\infty} x^2 e^{-2k(x-\mu)^2} dx = \sqrt{\frac{2k}{\pi}} \left[\int_{-\infty}^{\infty} v^2 e^{-2kv^2} dv + 2\mu \underbrace{\int_{-\infty}^{\infty} v e^{-2kv^2} dv}_{=0} + \mu^2 \underbrace{\int_{-\infty}^{\infty} e^{-2kv^2} dv}_{=\sqrt{\frac{\pi}{2k}}} \right]$$

Let $v = x - \mu$
$dv = dx$

(10) $$\sigma^2 = 2\sqrt{\frac{2k}{\pi}} \int_0^{\infty} v^2 e^{-2kv^2} dv = 2\sqrt{\frac{2k}{\pi}} \cdot \frac{1}{4} \cdot \frac{1}{2k} \cdot \frac{\sqrt{\pi}}{\sqrt{2k}} \;;\; k = \frac{1}{4\sigma^2}$$

(11) $$\therefore \psi = \frac{1}{(2\pi\sigma^2)^{1/4}}\, e^{-\frac{(x-\mu)^2}{4\sigma^2}}$$
, which is the square root of the general form of the normal distribution, as one would expect.

For simplicity, we have only considered the case of a non-zero value for the position. Since the addition of an abitrary constant, μ, to the operator x which had the same dimensions as x and satisfied the Schwartz inequality turned out to be the mean value of x, there is hope that the same procedure with the momentum operator p_x will yield the same result, that is, the mean value of momentum.

(12) $$(p_x + \alpha)\psi = c(x+\mu)\psi;$$
α being real, positive or negative constant with the dimensions of momentum

The operators on ψ must satisfy:

(13) $$c^2 \int |(x+\mu)\psi|^2 dx \cdot \int |(x+\mu)\psi|^2 dx = \left[\left| \int c^* (x+\mu)^* \psi^* \cdot (x+\mu)\psi \; dx \right| \right]^2$$

Since $x+\mu$ is real, it is immediate that the equal sign of the Schwartz inequality is satisfied.

Assignment #1
Continued

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Problem 3
Continued

Introducing operator notation in position space:

(14) $\left(\frac{\hbar}{i} \frac{\partial}{\partial x} + \alpha \right) \psi = c(x + \mu)\psi$

(15) $\frac{d\psi}{dx} = c(x+\mu)\psi - \frac{i\alpha}{\hbar}\psi$; where $\frac{\hbar}{i}$ is lumped into c.

Immediately we see that:

(16) $\psi = \frac{1}{(2\pi\sigma^2)^{1/4}} e^{-\frac{(x-\mu)^2}{4\sigma^2}} e^{-i\frac{\alpha}{\hbar}x}$

Now $\overline{(\Delta p_x)^2} = \overline{(p_x - \overline{p_x})^2} = \overline{p_x^2} - \overline{p_x}^2$

(17) $\overline{p_x} = \frac{\hbar}{i}\int_{-\infty}^{\infty} \psi^* \frac{d\psi}{dx}\, dx$

(18) $\frac{d\psi}{dx} = \psi \left[-\frac{(x-\mu)}{2\sigma^2} - i\frac{\alpha}{\hbar} \right]$

(19) $\overline{p_x} = \frac{\hbar}{i}\underbrace{\int_{-\infty}^{\infty} -\frac{(x-\mu)}{2\sigma^2}\psi\psi^*\, dx}_{=0} - \alpha \underbrace{\int_{-\infty}^{\infty}\psi^*\psi\, dx}_{=1} = -\alpha$

(20) $\therefore \quad \psi = \frac{1}{(2\pi\sigma^2)^{1/4}} e^{-\frac{(x-\mu)^2}{4\sigma^2}} e^{i\frac{\alpha}{\hbar}x}$ ✓ is the distribution that satisfies the Schwartz equality and yields non-vanishing values of $\bar{x}$ and $\overline{p_x}$. We now show that it gives the equal sign in the uncertainty relation.

(21) $\overline{p_x^2} = -\hbar^2 \int_{-\infty}^{\infty} \psi^* \frac{d^2\psi}{dx^2}\, dx$

(22) $$\frac{d^2\psi}{dx^2} = \left[-\frac{(x-\mu)}{2\sigma^2} + i\frac{\alpha}{\hbar}\right]\frac{d\psi}{dx} + \psi\left[-\frac{1}{2\sigma^2}\right]$$

$$= \left[\frac{(x-\mu)^2}{4\sigma^4} - 2\frac{i\alpha}{\hbar}\frac{(x-\mu)}{2\sigma^2} + \frac{\alpha^2}{\hbar^2}\right]\psi - \frac{\psi}{2\sigma^2}$$

It is apparent which term will vanish and which will give unity upon integration:

(23) $$\overline{p_x^2} = -\frac{\hbar^2}{4\sigma^4}\int_{-\infty}^{\infty}(x-\mu)^2\,\psi^*\psi\,dx + \alpha^2 + \frac{\hbar^2}{2\sigma^2} = \frac{\hbar^2}{4\sigma^2} + \alpha^2$$

(24) $$\overline{(\Delta x)^2}\;\overline{(\Delta p_x)^2} = \left(\overline{x^2} - \mu^2\right)\left(\overline{p_x^2} - \alpha^2\right) = \left(\sigma^2 + \mu^2 - \mu^2\right)\left(\frac{\hbar^2}{4\sigma^2} + \alpha^2 - \alpha^2\right)$$

$$= \frac{\hbar^2}{4}$$

(25) $\therefore$ $\sqrt{\overline{(\Delta x)^2}}\,\sqrt{\overline{(\Delta p_x)^2}} = \frac{\hbar}{2}$ which is the minimum of the uncertainty condition given by the wave function:

$$\psi = \frac{1}{(2\pi\sigma^2)^{1/4}}\,e^{-\frac{(x-\mu)^2}{4\sigma^2}}\,e^{i\frac{\alpha}{\hbar}x}$$

✓

I forgot the form ψ of prob 2

Assignment #1
Continued

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4. (1) Expanding the exponential:

$$\exp(ia p_x/\hbar) = 1 + \left(\frac{i a p_x}{\hbar}\right) + \frac{1}{2!}\left(\frac{i a p_x}{\hbar}\right)^2 + \frac{1}{3!}\left(\frac{i a p_x}{\hbar}\right)^3 + \cdots$$

(2) Introducing the operator $p_x \to \frac{\hbar}{i}\frac{\partial}{\partial x}$:

$$\exp\left(\frac{i a p_x}{\hbar}\right) \to 1 + a\frac{\partial}{\partial x} + \frac{a^2}{2!}\frac{\partial^2}{\partial x^2} + \frac{a^3}{3!}\frac{\partial^3}{\partial x^3} + \cdots$$

(3) If $\psi(x,y,z,t)$ is analytic, it has continuous derivatives of all orders and at all points if there are no singular points. Thus:

$$e^{\frac{i a p_x}{\hbar}}\psi(x,y,z,t) = \psi + a\psi' + \frac{a^2}{2!}\psi'' + \frac{a^3}{3!}\psi''' + \cdots$$

(4) The right hand side is recognized as the Taylor expansion of $\psi(x+a)$.

$$e^{\frac{i a p_x}{\hbar}}\psi(x,y,z,t) = \psi(x+a,y,z,t)$$

✓

The effect of the operator is to translate the wave function "a" units in the x direction. Equation (4) is sometimes known as Bloch's Theorem and is helpful in solving Schroedinger's Equation for particle motion in a periodic potential.

5. (1) We now demonstrate the equation used in Problem #1. We start by considering the following operation on ψ:

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$$p_x^m x^n \psi \rightarrow (-i\hbar)^m \frac{\partial^m}{\partial x^m}(x^n \psi)$$

Now the formula for the m th derivative of the product of two commuting functions is:

(2) $$\frac{\partial^m}{\partial x^m}(fg) = \sum_{k=0}^{m} \binom{m}{k} f^{(k)} g^{(m-k)}$$

in which $\binom{m}{k} = \dfrac{m(m-1)\cdots(m-k+1)}{k!}$

and $f \Rightarrow x^n$, $g \Rightarrow \psi$

(3) $$(x^n)^{(k)} = n(n-1)(n-2)\cdots(n-k+1)\, x^{n-k} = k!\binom{n}{k} x^{n-k}$$

(4) Thus $$p_x^m x^n \psi = (-i\hbar)^m \sum_{k=0}^{m} k! \binom{m}{k}\binom{n}{k} x^{n-k} \psi^{(m-k)}$$

Now $$(-i\hbar)^m \psi^{(m-k)} = (-i\hbar)^m \frac{\partial^{m-k}\psi}{\partial x^{m-k}}$$

$$= (-i\hbar)^k \left(-i\hbar \frac{\partial \psi}{\partial x}\right)^{m-k} = (-i\hbar)\, p_x^{m-k} \psi$$

(5) $$p_x^m x^n \psi = \sum_{k=0}^{m} (-i\hbar)^k k! \binom{m}{k}\binom{n}{k} x^{n-k} p_x^{m-k} \psi$$

$$= \sum_{k=1}^{m} (-i\hbar)^k k! \binom{m}{k}\binom{n}{k} x^{n-k} p_x^{m-k}\psi + x^n p_x^m \psi$$

(6) $$\therefore \; [x^n, p_x^m] = -\sum_{k=1}^{m \le n} (-i\hbar)^k k! \binom{m}{k}\binom{n}{k} x^{n-k} p_x^{m-k}$$

the condition $m \le n$ must be made to end the summation at n instead of m if $m > n$.

Although this equation is useful in generating a series from the commutator, another form will be more helpful for forming symmetérized products.

Paul Grant
DEAP-AP-1G
P251a
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Problem 5
Continued

(7) Consider the following commutator:

$$[A^n, B^m] \; ;$$

Using the two identities:

$$[X, YZ] = [X, Y]Z + Y[X, Z]$$

$$[YZ, X] = [Y, X]Z + Y[Z, X]$$

we may expand as follows:

(8) $$[A^n, B^m] = [A^n, BB^{m-1}] = [A^n, B]B^{m-1} + B[A^n, B]B^{m-2} + B^2[A^n, B]B^{m-3} + \dots + B^{m-1}[A^n, B] = \sum_{k=1}^{m} B^{k-1}[A^n, B]B^{m-k}$$

(9) Similarly: $$[A^n, B] = \sum_{l=1}^{n} A^{l-1}[A, B]A^{n-l}$$

(10) $$[A^n, B^m] = \sum_{k=1}^{m}\sum_{l=1}^{n} B^{k-1}A^{l-1}[A, B]A^{n-l}B^{m-k}$$

(11) Suppose $A \to x$, $B \to p_x$

then $$[x^n, p_x^m] = i\hbar n \sum_{k=1}^{m} p_x^{k-1} x^{n-1} p_x^{m-k}$$

(12) $$[x^2, p_x^2] = i\hbar 2 \sum_{k=1}^{2} p_x^{k-1} x \, p_x^{2-k}$$

$$= i\hbar 2 (x p_x + p_x x)$$

$$= i\hbar 4 \cdot \tfrac{1}{2}\{x, p_x\}$$ ✓

(13) $$[x^5, p_x^3] = i\hbar 5 \sum_{k=1}^{3} p_x^{k-1} x^4 p_x^{3-k}$$

$$= i\hbar 5 \left(x^4 p_x^2 + p_x x^4 p_x + p_x^2 x^4 \right)$$

(14) We now recognize:

$$\{AB, C\} = ABC + CAB$$

$$\{A, BC\} = ABC + BCA$$

or $$\{p_x x^4, p_x\} = p_x x^4 p_x + p_x^2 x^4$$

$$\{p_x, x^4 p_x\} = p_x x^4 p_x + x^4 p_x^2$$

Equation (13) can be written:

(15) $$[x^5, p_x^3] = i\hbar 5 \left(\frac{x^4 p_x^2}{2} + \frac{p_x^2 x^4}{2} + \frac{x^4 p_x^2}{2} + \frac{p_x x^4 p_x}{2} + \frac{p_x^2 x^4}{2} + \frac{p_x x^4 p_x}{2} \right)$$

or $$[x^5, p_x^3] = i\hbar 5 \left(\frac{1}{2}\{x^4, p_x^2\} + \frac{1}{2}\{p_x x^4, p_x\} + \frac{1}{2}\{p_x, x^4 p_x\} \right)$$

✓

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Assignment #2
Probs. 6-11

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6. a. (1) Consider $w_1 = 1$, $w_2 = x$, $w_3 = x^2$, on the interval $0 < x < 1$. We form the following linear combinations orthogonormal to each other:

$$u_1 = \frac{w_1}{[(w_1, w_1)]^{1/2}} \quad ; \quad (w_1, w_1) = \int_0^1 \rho w_1^2 \, dx$$

$$u_2 = \frac{v_2}{[(v_2, v_2)]^{1/2}} \quad ; \quad v_2 = w_2 - (u_1, w_2) u_1$$

$$u_3 = \frac{v_3}{[(v_3, v_3)]^{1/2}} \quad ; \quad v_3 = w_3 - (u_1, w_3) u_1 - (u_2, w_3) u_2$$

(2) $(w_1, w_1) = \int_0^1 dx = 1$, $\therefore u_1 = 1$ ✓

(3) $(u_1, w_2) = \int_0^1 x \, dx = 1/2$, $\therefore v_2 = x - 1/2$

(4) $(v_2, v_2) = \int_0^1 (x^2 - x + 1/4) dx = \frac{x^3}{3} - \frac{x^2}{2} + \frac{x}{4} \Big]_0^1 = \frac{1}{12}$

(5) $\therefore u_2 = 2\sqrt{3} \, (x - 1/2)$ ✓

(6) $(u_1, w_3) = \int_0^1 x^2 dx = \frac{1}{3}$; $(u_2, w_3) = 2\sqrt{3} \int_0^1 (x^2 - \frac{x}{2}) dx$

$= 2\sqrt{3} \left[\frac{x^3}{3} - \frac{x^2}{4} \right]_0^1 = 2\sqrt{3} \cdot \frac{1}{12} = \sqrt{3}/6$

(7) $v_3 = x^2 - \frac{1}{3} - \frac{\sqrt{3}}{6} \left(2\sqrt{3} \{ x - \frac{1}{2} \} \right) = x^2 - \frac{1}{3} - x + \frac{1}{2} = x^2 - x + \frac{1}{6}$

(8) $(v_3, v_3) = \int_0^1 (x^4 - 2x^3 + \frac{4}{3}x^2 - \frac{1}{3}x + \frac{1}{36}) dx$

$= \frac{x^5}{5} - \frac{x^4}{2} + \frac{4}{9}x^3 - \frac{1}{6}x^2 + \frac{x}{36} \Big]_0^1 = \frac{1}{5} - \frac{1}{2} + \frac{4}{9} - \frac{1}{6} + \frac{1}{36} = \frac{1}{5(36)}$

(9) $u_3 = 6\sqrt{5} \, (x^2 - x + \frac{1}{6})$ ✓

$u_2 = 2\sqrt{3} \, (x - 1/2)$

$u_1 = 1$ ✓

b. (1) We now require orthonormality with the weight factor $\rho(x) = x$:

(2) $(w_1, w_0) = \int_0^1 \rho(x)\,dx = \int_0^1 x\,dx = \frac{1}{2}$

(3) $\therefore \quad u_1 = \sqrt{2}$ ✓

(4) $(u_1, w_2) = \sqrt{2} \int_0^1 x^2 dx = \frac{\sqrt{2}}{3}$

(5) $v_2 = x - \frac{2}{3}$

(6) $(v_2, v_2) = \int_0^1 \left(x^3 - \frac{4}{3}x^2 + \frac{4}{9}x \right) dx = \frac{1}{4} - \frac{4}{9} + \frac{2}{9} = \frac{1}{4} - \frac{2}{9} = \frac{1}{36}$

(7) $\therefore \quad u_2 = 6\left(x - \frac{2}{3} \right)$ ✓

(8) $(u_1, w_3) = \sqrt{2} \int_0^1 x^3\,dx = \sqrt{2}/4$

(9) $(u_2, w_3) = 6 \int_0^1 \left(x^4 - \frac{2}{3}x^3 \right) dx = 6\left[\frac{1}{5} - \frac{1}{6} \right] = \frac{1}{5}$

(10) $v_3 = x^2 - \frac{1}{2} - \frac{6}{5}\left(x - \frac{2}{3} \right) = x^2 - \frac{6}{5}x + \frac{3}{10}$

(11) $(v_3, v_3) = \int_0^1 \left(x^4 - \frac{12}{5}x^3 + \frac{204}{100}x^2 - \frac{18}{25}x + \frac{9}{100} \right) dx$

$= \frac{1}{5} - \frac{3}{5} + \frac{204}{300} - \frac{9}{25} + \frac{9}{100} = \frac{81}{100}$

(12) $u_3 = \frac{10}{9} \left(x^2 - \frac{6}{5}x + \frac{3}{10} \right)$ ✓ [corrected in red: $\frac{10}{9}$ struck out, $10\sqrt{6}$]

$u_2 = 6\left(x - \frac{2}{3} \right)$

$u_1 = \sqrt{2}$ ✓

Assignment #2
Continued

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7. (1) We write the wave equation for the free particle in general as:

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$$\nabla^2 u + k^2 u = 0$$

(2) Now, in cylindrical co-ordinates;

$$\rho = [x^2+y^2]^{1/2}, \quad \varphi = \tan^{-1} y/x, \quad z = z$$

and $\nabla^2 = \frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right) + \frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2} + \frac{\partial^2}{\partial z^2}$

and we have for the wave equation.

$$\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial u}{\partial\rho}\right) + \frac{1}{\rho^2}\frac{\partial^2 u}{\partial\varphi^2} + \frac{\partial^2 u}{\partial z^2} + k^2 u = 0$$

(3) We now argue that $u = P(\rho)\,\Phi(\varphi)\,Z(z)$. Substituting in the equation and dividing by u:

$$\frac{1}{P\rho}\frac{d}{d\rho}\left(\rho\frac{dP}{d\rho}\right) + \frac{1}{\rho^2\Phi}\frac{d^2\Phi}{d\varphi^2} + \frac{1}{Z}\frac{d^2 Z}{dz^2} + k^2 = 0$$

We now make all the time honored arguments about equations in this form and state that since it is split into two parts, one dependent on ρ and φ and the other on z, and their sum a constant, then the z part is equal to a constant and the ρ, φ part is equal to a constant whose sum is k^2. Let the constants be such that:

$$k^2 = \underset{\rho,\varphi}{\underset{\uparrow}{\alpha^2}} + \underset{z}{\underset{\uparrow}{K^2}}$$

Then:

(4) $$\frac{d^2 Z}{dz^2} + K^2 Z = 0, \quad \text{or} \quad Z(z) = \exp(\pm i K z)$$ ✓

$$\frac{1}{P\rho}\frac{d}{d\rho}\left(\rho\frac{dP}{d\rho}\right) + \frac{1}{\rho^2\Phi}\frac{d^2\Phi}{d\varphi^2} + \alpha^2 = 0$$

or $$\frac{\rho}{P}\frac{d}{d\rho}\left(\rho\frac{dP}{d\rho}\right) + \frac{1}{\Phi}\frac{d^2\Phi}{d\varphi^2} + \alpha^2\rho^2 = 0$$

(5) We now have the same situation between φ and ρ as we had between φ, ρ and z. Making the φ part equal to $-m^2$:

$$\frac{d^2\Phi}{d\varphi^2} + m^2\Phi = 0 \quad , \quad \Phi = e^{\pm i m \varphi}$$

Since we demand nice things of wave functions, one of them being that they be single-valued, we see that m must be a $\pm$ integer because $\varphi = 0$, $\varphi = 2\pi$ are the same points in space and Φ must have the same value there which it would not have if m were not an integer. This need not be demanded of K in the solution for Z as the points $z = 0$, $z = 2\pi$ are not the same points in space. φ is called an ignorable co-ordinate.

(6) Finally:
$$\rho \frac{d}{d\rho}\left(\rho \frac{dP}{d\rho}\right) + (\alpha^2\rho^2 - m^2)P = 0$$

Let us make the substitution $x = \alpha\rho$; $P(\rho) = F(x)$, then

(7)
$$x \frac{d}{dx}\left(x \frac{dF}{dx}\right) + (x^2 - m^2)F = 0$$

or
$$x^2 \frac{d^2F}{dx^2} + x\frac{dF}{dx} + (x^2 - m^2)F = 0$$

which is the standard form of Bessel's equation which has as the solution for integral values of m:

$$F(x) = c_1 J_{|m|}(x) + c_2 J_{-|m|}(x)$$

where $|m|$ is used to avoid ambiguity since m is a $\pm$ integer. $J_{|m|}(x)$ is a Bessel function of the first kind and $J_{-|m|}(x)$ is a Bessel function of the second kind or a Neumann function:

$$J_{|m|}(x) = \sum_{n=0}^{\infty} \frac{(-1)^n \left(\frac{x}{2}\right)^{|m|+2n}}{n!\,(|m|+n)!}$$

$$J_{-|m|}(x) = N_{|m|}(x) = \sum_{n=0}^{\infty} \frac{(-1)^n \left(\frac{x}{2}\right)^{2n-|m|}}{n!\,(n-|m|)!}$$

We now examine the behaviour of $J_{|m|}(x)$:
For $x \ll 1$

$$J_{|m|}(x) \simeq \frac{x^{|m|}}{|m|!\, 2^{|m|}}$$

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7. continued

For $x >> 1$, $x >> |m|$:

$$J_{|m|}(x) \simeq \sqrt{\frac{2}{\pi x}} \cos\left(x - \frac{2|m|+1}{4}\pi\right) = 0 \quad \text{for } x = \infty$$

For the behaviour of $N_{|m|}(x)$ at the boundaries:
For $x << 1$; $|m| \geq 1$

$$N_{|m|}(x) \cong -\frac{(|m|-1)!}{\pi}\left(\frac{2}{x}\right)^{|m|} = -\infty \quad \text{for } x = 0$$

$$N_0(x) \simeq -\frac{2}{\pi} \ln \frac{2}{1.78\,x} = -\infty \quad \text{for } x = 0$$

For $x >> 1$, $x >> |m|$:

$$N_{|m|}(x) \simeq \sqrt{\frac{2}{\pi x}} \sin\left(x - \frac{2|m|+1}{4}\pi\right) = 0 \quad \text{for } x = \infty$$

Since we demand that the wave functions be bounded every where, the Neumann functions are clearly not admissable since $N_{|m|}(x) = -\infty$ at $x = 0$. Therefore

(8) $F(x) = P(\rho) = J_{|m|}(x)$ with a normalization constant to be determined later.

We begin the normalization procedure by setting up the following condition:

(9) $$N^2 \int_{\text{all space}} |P \Phi Z|^2 \rho \, d\rho \, d\varphi \, dz = N^2 \int_{\text{all space}} |F \Phi Z|^2 \frac{x\,dx}{\alpha^2} \, d\varphi \, dz = \delta_{mm'} \delta(k-k') \delta(\alpha-\alpha')$$

We know that the wave functions are orthogonal since they are solutions of a Sturm-Liouville equation and this was shown in lecture.

We begin with the normalization of Φ:

(10) $$N_\varphi^2 \int_0^{2\pi} \Phi \Phi^* \, d\varphi = N_\varphi^2 \int_0^{2\pi} d\varphi = N_\varphi^2 \, 2\pi = 1$$

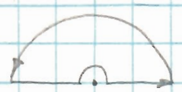
(11) $$\therefore \quad \Phi = \frac{1}{\sqrt{2\pi}} e^{im\varphi}, \quad m = 0, \pm 1, \pm 2, \ldots$$

We now wish to normalize $Z(z) = Ce^{iKz}$ in the scale of K. Set up the function:

(12) $$Z(z;K,\Delta K) = \int_{K-\Delta K/2}^{K+\Delta K/2} Z(z)\,dK = c\int_{K-\Delta K/2}^{K+\Delta K/2} e^{iKz}\,dK$$

$$= \frac{c}{iz}\left[e^{i(K+\Delta K)z} - e^{i(K-\Delta K)z}\right]$$

(13) $$\int_{-\infty}^{\infty} Z^*_{K'}\, Z(z;K,\Delta K)\,dz = \frac{c^2}{i}\int_{-\infty}^{\infty}\left[e^{i(K+\frac{\Delta K}{2}-K')z} - e^{i(K-\frac{\Delta K}{2}-K')z}\right]\frac{dz}{z}$$

Region	Contour	Result
$K' > K + \Delta K/2$		0
$K' < K - \Delta K/2$		0
$K - \frac{\Delta K}{2} < K' < K + \frac{\Delta K}{2}$	 1st term; second term 	$\frac{c^2 2\pi i}{i}$ (residue of 1st term)

(14) The residue at $z=0$ of the first term is clearly 1.

$$\therefore \int_{-\infty}^{\infty} Z^*_{K'}\, Z(z;K,\Delta K)\,dz = c^2\, 2\pi = 1, \quad K - \frac{\Delta K}{2} < K' < K + \frac{\Delta K}{2}$$

$$\therefore \quad Z(z) = \frac{1}{\sqrt{2\pi}}\, e^{iKz}$$

We now proceed to normalize the Bessel functions $J_{|m|}(\alpha\rho)$ in the α scale:

(15) $$P(\rho) = C\, J_{|m|}(\alpha\rho), \quad P(\rho;\alpha,\Delta\alpha) = C\int_{\alpha-\frac{\Delta\alpha}{2}}^{\alpha+\frac{\Delta\alpha}{2}} J_{|m|}(\alpha\rho)\,\alpha\, d\alpha$$

We demand that:

(16) $$C^2\int_0^{\infty} J_{|m|}(\alpha'\rho)\,\rho\,d\rho \int_{\alpha-\Delta}^{\alpha+\Delta} J_{|m|}(\alpha\rho)\,\alpha\,d\alpha = \begin{cases} 1, & \alpha - \frac{\Delta\alpha}{2} < \alpha' < \alpha + \frac{\Delta\alpha}{2} \\ 0, & \text{otherwise} \end{cases}$$

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Problem 7 Continued

(17) We will find it convenient to rearrange the integration as follows:

$$C^2 \int_{\alpha-\Delta}^{\alpha+\Delta} \alpha \, d\alpha \int_0^\infty J_{|m|}(\alpha'\rho)\, J_{|m|}(\alpha\rho)\, \rho \, d\rho$$

Now, the Bessel functions are not quadratically integrable even though they vanish in the limit $\rho = \infty$ which is a necessary though not sufficient condition for a function to be quadratically integrable. Since the Bessel function is well bounded for small ρ, it must be for large ρ that the function begins to take off. Therefore it seems reasonable to replace the Bessel function above with its asymptotic value at large ρ as this will, in the limit of the sum, amount to neglecting a finite quantity in the face of an infinite one. The asymptotic value is well known and is:

$$J_{|m|}(\alpha\rho)\Big|_{\rho\to\infty} = \sqrt{\frac{2}{\pi\alpha\rho}} \cos\left(\alpha\rho - \frac{2|m|+1}{4}\pi\right)$$

$$= \sqrt{\frac{2}{\pi\alpha\rho}} \cos(\alpha\rho + \varphi)$$

(18) Concentrating on the second integral in (17):

$$\int_0^\infty J_{|m|}(\alpha'\rho)\, J_{|m|}(\alpha\rho)\, \rho\, d\rho = \frac{2}{\pi\sqrt{\alpha\alpha'}} \int_0^\infty \cos(\alpha'\rho+\varphi)\cos(\alpha\rho+\varphi)\, d\rho$$

(19) We not that: $\cos\left[(\alpha'+\alpha)\rho + 2\varphi\right] = \cos(\alpha'\rho+\varphi)\cos(\alpha\rho+\varphi) - \sin(\alpha'\rho+\varphi)\sin(\alpha\rho+\varphi)$

$\cos(\alpha'-\alpha)\rho = \cos(\alpha'\rho+\varphi)\cos(\alpha\rho+\varphi) + \sin(\alpha'\rho+\varphi)\sin(\alpha\rho+\varphi)$

Then $\cos(\alpha'\rho+\varphi)\cos(\alpha\rho+\varphi) = \frac{1}{2}\cos\left[(\alpha'+\alpha)\rho+2\varphi\right] + \frac{1}{2}\cos(\alpha'-\alpha)\rho$

(20) $$\frac{1}{2}\int_0^\infty \cos\left[(\alpha'+\alpha)\rho+2\varphi\right] d\rho = \frac{1}{4}\int_0^\infty \left\{\exp i\left[(\alpha'+\alpha)\rho+2\varphi\right] + \exp -i\left[(\alpha'+\alpha)\rho+2\varphi\right]\right\} d\rho$$

$$= \frac{1}{4}\int_{-\infty}^\infty \exp i\left[(\alpha'+\alpha)\rho+2\varphi\right] d\rho = 0$$ by Cauchy's Theorem since the exponential is an analytic function and the path of integration encloses no singularities.

(21) $\frac{1}{2}\int_0^\infty \cos(\alpha'-\alpha)\rho \; d\rho = \frac{1}{4}\int_{-\infty}^{\infty} e^{i(\alpha'-\alpha)\rho} d\rho$

This integral is well known to give the Dirac Delta function, viz., $\delta(\alpha'-\alpha)$.

$$\int_{-\infty}^{\infty} e^{i(\alpha'-\alpha)\rho} d\rho = \delta(\alpha'-\alpha) = 0, \quad \alpha' \neq \alpha$$
$$= \infty, \quad \alpha' = \alpha$$

(22) Hence, (17) becomes:

$$\frac{C^2}{2\pi}\int_{\alpha-\Delta}^{\alpha+\Delta} \frac{\alpha}{\sqrt{\alpha'\alpha}} \delta(\alpha'-\alpha)\, d\alpha = \frac{C^2}{2\pi}, \quad \alpha - \frac{\Delta\alpha}{2} < \alpha' < \alpha + \frac{\Delta\alpha}{2}$$
$$= 0, \quad \text{otherwise}$$

However, we demand normality, therefore $C = \sqrt{2\pi}$ ~~X~~ $C = \sqrt{\alpha}$

The complete solution for the wave functions of the cylindrical free particle is then:

(23) $\psi(\rho, \varphi, z) = \frac{\sqrt{\alpha}}{2\pi} \sout{\frac{1}{\sqrt{2\pi}}} e^{\pm i k z} e^{i m \varphi} J_{|m|}(\alpha\rho)$

with $\int_{-\infty}^{\infty} |\psi(\rho,\varphi,z)|^2 \rho\, d\rho\, d\varphi\, dz = \delta_{mm'}\delta_{kk'}\delta_{\alpha\alpha'}$

where $\delta_{kk'}$, $\delta_{\alpha\alpha'}$, mean in the scale of $k \pm \Delta$, $\alpha \pm \Delta$ respectively.

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8. (1) $$\lim_{\beta\to 0}\int_{-\infty}^{\infty} e^{-\beta|x|}\, u_{k_2}^*(x)\, u_{k_1}(x)\, dx = 0 \quad , \quad k_1 \neq k_2$$

(2) For free particles, $u_{k_2} = \frac{1}{\sqrt{2\pi}} e^{ik_2x}$, $u_{k_1} = \frac{1}{\sqrt{2\pi}} e^{ik_1x}$,

we have: This should be β|x|

$$\lim_{\beta\to 0}\frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-\beta^2x^2 + i(k_1-k_2)x}\, dx = \lim_{\beta\to 0} I(\beta)$$

(3) $$-\beta^2x^2 + i(k_1-k_2)x = -\beta^2\left[x^2 - \frac{i(k_1-k_2)x}{\beta^2}\right]$$

$$= -\beta^2\left[x^2 - \frac{i(k_1-k_2)x}{\beta^2} - \frac{(k_1-k_2)^2}{4\beta^4} + \frac{(k_1-k_2)^2}{4\beta^4}\right]$$

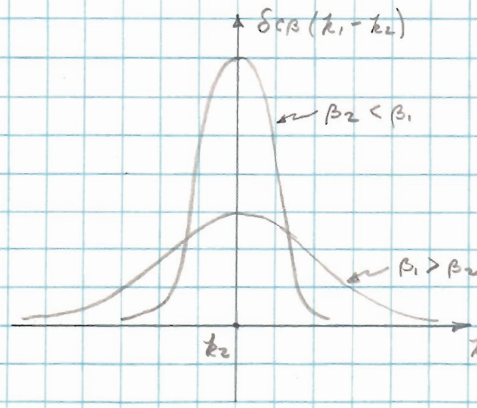
$$= -\beta^2\left[x - \frac{i(k_1-k_2)}{\beta^2}\right]^2 - \frac{(k_1-k_2)^2}{4\beta^2}$$

(4) Letting $y = x - \frac{i(k_1-k_2)}{\beta^2}$; $dy = dx$, we have:

$$I(\beta) = \frac{1}{2\pi} e^{-\frac{(k_1-k_2)^2}{4\beta^2}}\int_{-\infty}^{\infty} e^{-\beta^2y^2}\, dy = \frac{1}{2\sqrt{\pi}\,\beta} e^{-\frac{(k_1-k_2)^2}{4\beta^2}}$$

(5) We now define $\delta_{c\beta}(k_1-k_2) = \frac{1}{2\sqrt{\pi}\,\beta} e^{-\frac{(k_1-k_2)^2}{4\beta^2}}$

We note that $\delta_{c\beta}(k_1-k_2)$ has the form of a gaussian probability density in k_1 with mean k_2 and variance $2\beta^2$ and it will be convenient to consider it in this sense:



For a gaussian probability density:

$$\int_{-\infty}^{\infty}\delta_{c\beta}(k_1-k_2)\, dk_1 = 1$$

Regardless of the values of the parameters

As the variance $2\beta^2$ becomes smaller and smaller, the gaussian distribution becomes more concentrated about the mean value k_2 which is expected. At the mean, $k_1 = k_2$;

$\delta_{c\beta}(0) = \frac{1}{2\sqrt{\pi}\,\beta}$, so that one sees that the value of

$\delta_{c\beta}(k_1 - k_2)$ becomes large here as $\beta \to 0$. However, since the distribution narrows, the value of $\delta_{c\beta}(k_1 - k_2)$ is very small even for values of k_1 slightly different from k_2 because of $1/\beta^2$ in the exponent of the exponential.

It is clear now that in the limiting case as $\beta \to 0$, $\delta_{c\beta}(k_1 - k_2)$ will become unbounded for $k_1 = k_2$ and zero for $k_1 \neq k_2$ or we will have the gaussian of a random variable with no variance, that is:

$$\text{For } \beta \to 0: \quad \delta(k_1 - k_2) = 0, \quad k_1 \neq k_2$$
$$= \infty, \quad k_1 = k_2$$

✓

However, as it is the limit of a gaussian and since the integral;

$$\int_{-\infty}^{\infty} \delta_{c\beta}(k_1 - k_2)\, dk_1 = 1$$

did not depend on the parameters, we have every reason to expect:

$$\int_{-\infty}^{\infty} \delta(k_1 - k_2)\, dk_1 = 1$$

should hold in the limit $\beta \to 0$.

Now $\delta(k_1 - k_2)$ can be seen to have precisely the same meaning as the Dirac delta function. If the limits of the above integral did not include k_2, it would vanish, which is another property of the delta function. That is, the above function has the same properties as:

$$\int_a^b \delta(x)\, dx = 1 \quad a < 0 < b$$
$$= 0 \quad \text{otherwise}$$

Fine, but this wasn't the problem as stated.

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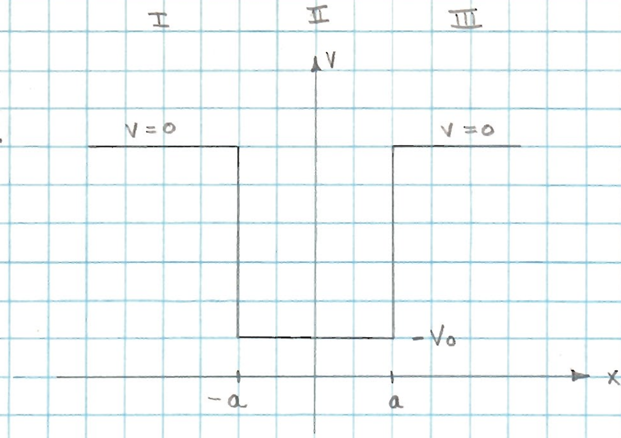
9.



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

We are interested only in those states with $E<0$, that is, the bound states. We demand also that the wave functions vanish at $+\infty$ and $-\infty$ and that wave propagation is only in the direction away from the well.

(2) Our complete Schroedinger equation is now:

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(V_0 - E)\psi = 0$$

(3) Define: $\kappa = \left[\frac{2m}{\hbar^2}(V_0-E)\right]^{1/2}$; $k = \left[\frac{2mE}{\hbar^2}\right]^{1/2}$

with $\kappa^2 + k^2 = \frac{2mV_0}{\hbar^2}$

(4) I, III : $\frac{d^2\psi}{dx^2} - k^2\psi = 0$

II : $\frac{d^2\psi}{dx^2} + \kappa^2\psi = 0$

(5) I : $\psi = c_1 e^{kx}$; III : $\psi = c_2 e^{-kx}$

III : $\psi = c_3 e^{i\kappa x} + c_4 e^{-i\kappa x} = c_5 \sin \kappa x + c_6 \cos \kappa x$

(6) From the continuity of ψ and $\frac{d\psi}{dx}$ at the boundaries:

$$c_5 \sin \kappa a + c_6 \cos \kappa a = c_2 e^{-ka}$$

$$\kappa c_5 \cos \kappa a - \kappa c_6 \sin \kappa a = -k c_2 e^{-ka}$$

$$-c_5 \sin \kappa a + c_6 \cos \kappa a = c_1 e^{-ka}$$

$$\kappa c_5 \cos \kappa a + \kappa c_6 \sin \kappa a = k c_1 e^{-ka}$$

(7) $$2 c_6 \cos \kappa a = (c_1 + c_2) e^{-ka}$$
$$2 c_5 \sin \kappa a = (c_2 - c_1) e^{-ka}$$

$$2\kappa c_5 \cos \kappa a = (c_1 - c_2) k e^{-ka}$$
$$2\kappa c_6 \sin \kappa a = (c_1 + c_2) k e^{-ka}$$

(8) If $c_6 \neq 0$, $c_1 \neq -c_2$: $\varkappa \tan \varkappa a = k$

If $c_5 \neq 0$, $c_1 \neq c_2$: $\varkappa \cot \varkappa a = -k$

We see that there are two independent solutions, which one could expect from the fact that the wave functions should approximate standing waves in the well with one set with equal ψ at $\pm a$, but with $\psi'(-a) = -\psi'(a)$ and the other with $\psi(-a) = -\psi(a)$ and $\psi'(-a) = \psi'(a)$. The lowest state should be the latter.

These two transcendental equations cannot be solved explicilty, but a graphical solution will be of help.

(9) Let $\xi = \varkappa a$, $\eta = ka$:

$$\eta = \xi \tan \xi$$
$$\eta = -\xi \cot \xi$$

with $$\xi^2 + \eta^2 = \frac{2mV_0 a^2}{\hbar^2}$$

The graph demonstrates the behaviour of the roots of equations (8) with a and V_0. The lowest level is encountered on the $\eta = \xi \tan \xi$ curve which means that $c_6 \neq 0$, $c_1 \neq -c_2$ and from equation (7) one can see that even symmetry is implied. Conversely, if $c_5 \neq 0$, $c_1 \neq c_2$, equations (7) imply odd symmetry of the wave function.

It is absolutely clear from the graph that no matter how small we make a or V_0, we will always have an intersection with the first curve of $\eta = \xi \tan \xi$. Therefore, the criteria that only one energy exist in the well in terms of a and V_0 is:

(10) $$0 < V_0 a^2 \leq \frac{\pi^2}{4}\left(\frac{\hbar}{2m}\right)$$

The criteria for only n levels to exist is:

(11) $$\frac{(n-1)^2}{4}\pi^2\left(\frac{\hbar}{2m}\right) < V_0 a^2 \leq n^2 \frac{\pi^2}{4}\left(\frac{\hbar}{2m}\right)$$

For n odd, there is even symmetry of wave functions. For n even, there is odd symmetry of wave functions.

Also, since $\eta \propto \sqrt{E}$, the η components of the intersections provides some what of an energy level diagram. This shows that the highest $|E|$ is always even, and that at high V_0, the levels approach those of the potential box since the asymptotes of the tan and cot are approached.

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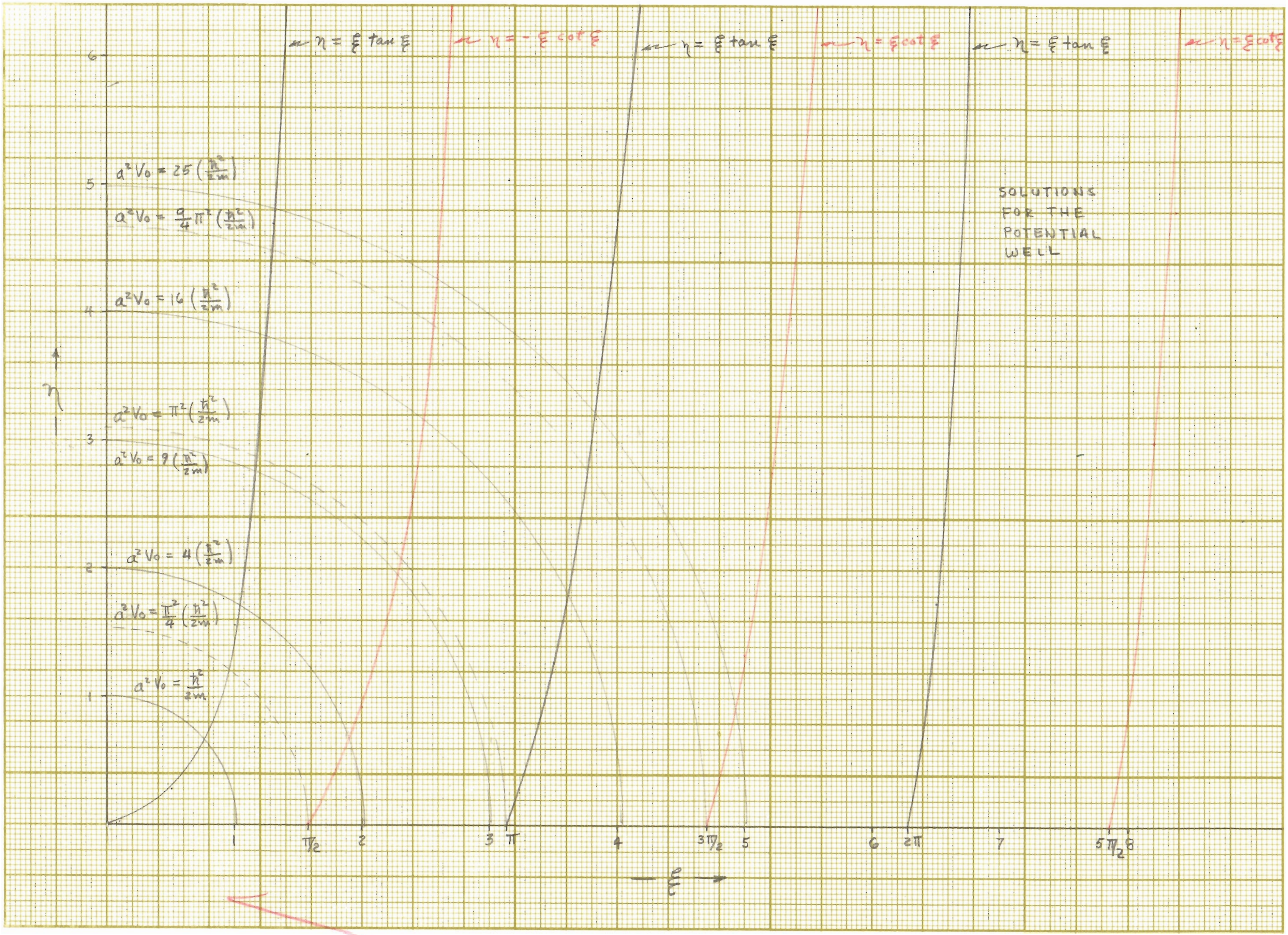
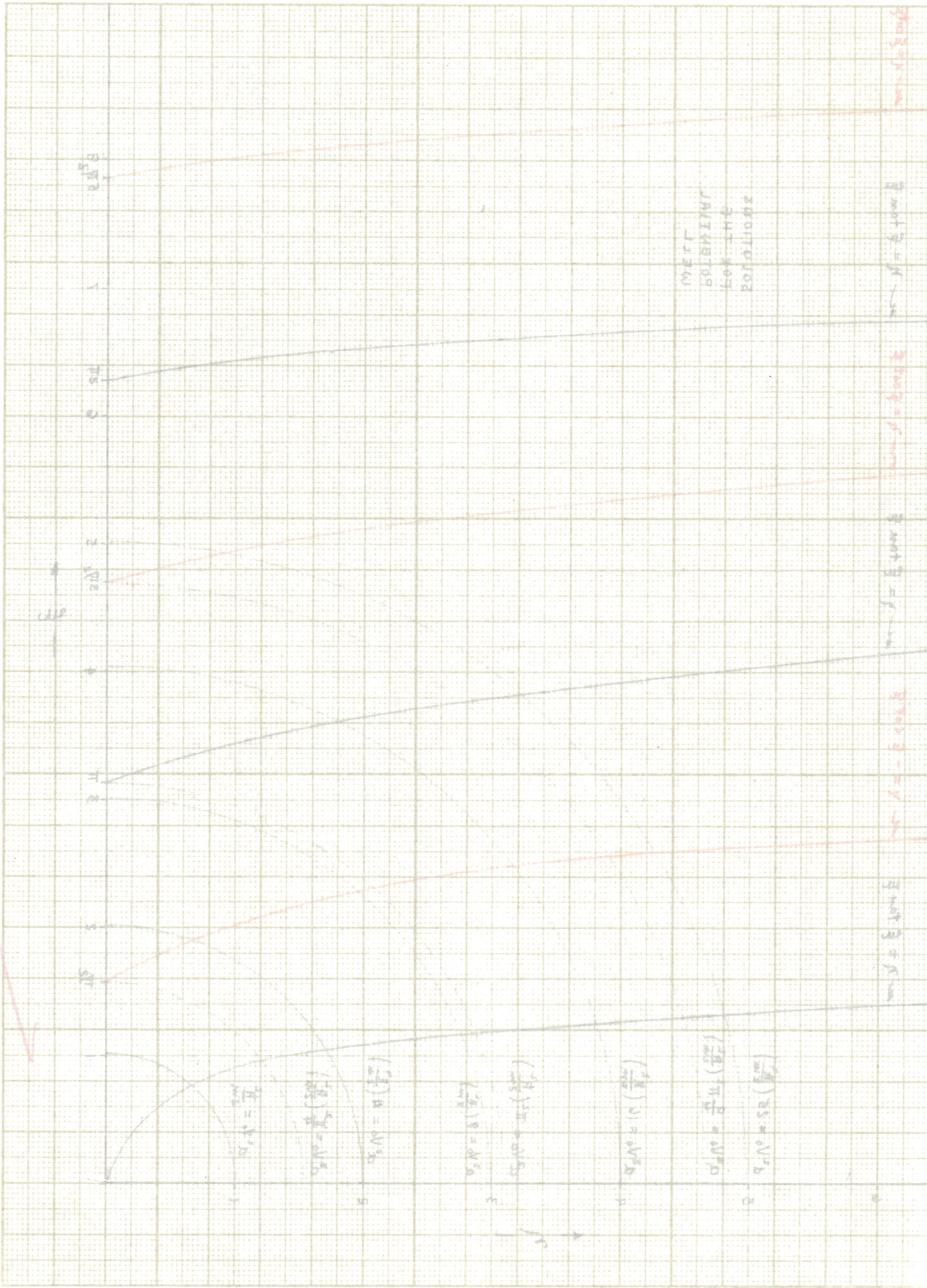

$\eta = \xi \tan \xi$
$\eta = -\xi \cot \xi$
$\eta = \xi \tan \xi$
$\eta = \xi \cot \xi$
$\eta = \xi \tan \xi$
$\eta = \xi \cot \xi$
SOLUTIONS FOR THE POTENTIAL WELL
$a^2 V_0 = 25\left(\frac{\hbar^2}{2m}\right)$
$a^2 V_0 = \frac{9}{4}\pi^2\left(\frac{\hbar^2}{2m}\right)$
$a^2 V_0 = 16\left(\frac{\hbar^2}{2m}\right)$
$a^2 V_0 = \pi^2\left(\frac{\hbar^2}{2m}\right)$
$a^2 V_0 = 9\left(\frac{\hbar^2}{2m}\right)$
$a^2 V_0 = 4\left(\frac{\hbar^2}{2m}\right)$
$a^2 V_0 = \frac{\pi^2}{4}\left(\frac{\hbar^2}{2m}\right)$
$a^2 V_0 = \frac{\hbar^2}{2m}$
η
ξ
1 2 3 4 5 6
1 $\pi/2$ 2 3 π 4 $3\pi/2$ 5 6 2π 7 $5\pi/2$ 8



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Paul Grant
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10. (1) It is clear from Problem (9) and the graph that for at least one more state to exist, the following criteria must hold:

$$a^2 V_0 > \frac{\pi^2}{4}\left(\frac{\hbar^2}{2m}\right)$$

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(2) For just one more state, the criteria is, from equation (11) of Problem (9):

$$\frac{\pi^2}{4}\left(\frac{\hbar^2}{2m}\right) < a^2 V_0 \leq \pi^2\left(\frac{\hbar^2}{2m}\right)$$

✓

11. (1) the largest value of the product $a^2 V_0$ for which there is still only one bound state is clearly, from the graph:

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$$a^2 V_0 = \frac{\pi^2}{4}\left(\frac{\hbar^2}{2m}\right)$$

(2) The value of $\eta = ka$ for this state can be found graphically and is approximately:

$$ka = 1.2 = \sqrt{\frac{2mE}{\hbar^2}}\, a$$

(3) We fix V_0 and have for a:

$$a = \frac{\pi}{2}\sqrt{\frac{\hbar^2}{2mV_0}}$$

(4) $\therefore \quad \frac{\pi}{2}\sqrt{\frac{E}{-V_0}} = 1.2 \quad , \quad E = -1.44\left(\frac{4}{\pi^2}\right)V_0 = -.582\ V_0$

$$= -(.582)(15) = -8.75 \approx -9\ \text{Mev}$$

(5) The problem may also be approached analytically by trial and error:

$$\eta = \xi \tan \xi = \left[\frac{2mV_0a^2}{\hbar^2} - \eta^2\right]^{1/2} \tan\left[\frac{2mV_0a^2}{\hbar^2} - \eta^2\right]^{1/2}$$

For our problem: $\eta = \left[\frac{\pi^2}{4} - \eta^2\right]^{1/2} \tan\left[\frac{\pi^2}{4} - \eta^2\right]^{1/2}$

or $\eta^2 \left\{1 + \tan^2\left[\frac{\pi^2}{4} - \eta^2\right]^{1/2}\right\} = \frac{\pi^2}{4} \tan^2\left[\frac{\pi^2}{4} - \eta^2\right]^{1/2}$

We wish to solve for η^2 and plug it in:

$$E = \eta^2 \left[\frac{4}{\pi^2}\right] V_0$$

Choose $\eta = 1.2$, $\eta^2 = 1.44$:

(6) $\eta^2 \sec^2\left[\frac{\pi^2}{4} - \eta^2\right]^{1/2} = \frac{\pi^2}{4} \tan^2\left[\frac{\pi^2}{4} - \eta^2\right]^{1/2}$

$\eta \sec\left[2.46 - \eta^2\right]^{1/2} = 1.57 \tan\left[2.46 - \eta^2\right]^{1/2}$

$1.2 \sec(1.01) = \frac{1.2}{\cos(1.01)} = \frac{1.2}{.532} = 2.25$

$1.57 \tan(1.01) = (1.57)(1.59) = 2.49$, about 11% error

(7) Choose $\eta = 1.25$, $\eta^2 = 1.56$

$\frac{1.25}{\cos .90} = \frac{1.25}{.622} = 2.01$

$1.57 \tan .90 = (1.57)(1.26) = 1.99$, about 1% error

(8) $E = -(1.56)(.406)(15) = -9.5$ Mev ≈ -10 Mev., so our graphical result was off by about 1 Mev, not too bad.

This, of course, is the magnitude of E, the relative position of the level with respect to the model is −10 Mev or 5 Mev above the bottom of the well.

Signs!

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Assignment #3
Problems 12-15

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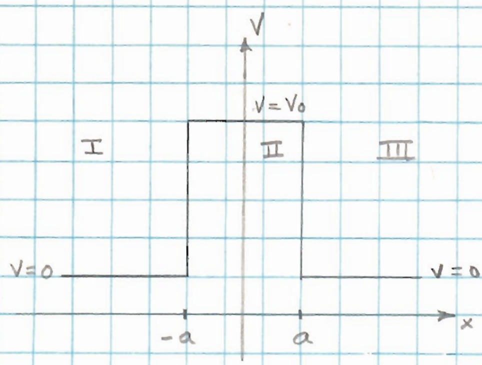
12.



a. (1) $E > V_0$

(2) we take Schroedingers equation:

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

as the guide to the type of solutions required.

(3) We assume a wave traveling from left to right from I to III. Thus our boundary condition is that in III:

$$\psi = e^{i\sqrt{\frac{2mE}{\hbar^2}}x} = e^{ikx} \quad \text{where } k = \left[\frac{2mE}{\hbar^2}\right]^{1/2}$$

(4) In region I: $\psi = Ae^{ikx} + Be^{-ikx}$ clearly holds for the incident and transmitted portions of the wave.

(5) In region II, for $E > V_0$, defining $\beta = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$

we have $\psi = Ce^{i\beta x} + De^{-i\beta x}$

(6) Imposing the usual BC on ψ and ψ', we obtain:

$$Ae^{-ika} + Be^{ika} = Ce^{-i\beta a} + De^{i\beta a}$$
$$kAe^{-ika} - ke^{ika} = \beta Ce^{-i\beta a} - \beta De^{i\beta a}$$

$$Ce^{i\beta a} + De^{-i\beta a} = e^{ika}$$
$$\beta Ce^{i\beta a} - \beta De^{-i\beta a} = ke^{ika}$$

(7) Solving for C and D:

$$C = \frac{\beta+k}{2\beta}e^{i(k-\beta)a}$$
$$D = \frac{\beta-k}{2\beta}e^{i(k+\beta)a}$$

$$Ae^{-ika} + Be^{ika} = \frac{\beta+k}{2\beta}e^{i(k-2\beta)a} + \frac{\beta-k}{2\beta}e^{i(k+2\beta)a}$$
$$kAe^{-ika} - kBe^{ika} = \frac{\beta+k}{2}e^{i(k-2\beta)a} - \frac{\beta-k}{2}e^{i(k+2\beta)a}$$

(8) We now solve for A and B in the same way as for C and D and obtain, after tedious but trivial simplification:

$$A = \frac{e^{i2ka}}{4\beta k}\left[(\beta+k)^2 e^{-i2\beta a} - (\beta-k)^2 e^{i2\beta a}\right]$$

$$B = \frac{-i}{2\beta k}(k^2-\beta^2)\sin 2\beta a$$

(9) Now $|A|^2 = AA^*$, $|B|^2 = BB^*$

$$|A|^2 = \frac{1}{16\beta^2 k^2}\left[(\beta-k)^4 + (\beta+k)^4 - 2(\beta-k)^2(\beta+k)^2 \cos 4\beta a\right]$$

$$= \frac{1}{8\beta^2 k^2}\left[\beta^4 + 6\beta^2 k^2 + k^4 - (\beta^2-k^2)^2 + 2(\beta^2-k^2)^2 \sin^2 2\beta a\right]$$

$$= \frac{1}{8\beta^2 k^2}\left[8\beta^2 k^2 + 2(\beta^2-k^2)^2 \sin^2 2\beta a\right]$$

(10) $$|A|^2 = \left[1 + \frac{(\beta^2-k^2)^2 \sin^2 2\beta a}{4\beta^2 k^2}\right]$$

(11) $$|B|^2 = \frac{(\beta^2-k^2)^2}{4\beta^2 k^2} \sin^2 2\beta a$$

We now take our transmission and reflection coefficients for plane waves to be those given in the lecture, viz.

$$T = \frac{v_r}{v_l}\frac{1}{|A|^2} \; ; \quad R = \frac{|B|^2}{|A|^2} \; ; \quad v_r = \frac{\hbar k_r}{m}, \quad v_l = \frac{\hbar k_l}{m}$$

Our notation throughout has been consistent with that used in lecture so we may substitute directly.

It is to be noticed that $k_r = k_l = k$, $\therefore \frac{v_r}{v_l} = 1$

(12) $$T = \left[1 + \frac{(\beta^2-k^2)^2 \sin^2 2\beta a}{4\beta^2 k^2}\right]^{-1} = \left[1 + \frac{V_0^2 \sin^2 2\left[\frac{2m(E-V_0)}{\hbar^2}\right]^{1/2} a}{4E(E-V_0)}\right]^{-1}$$

(13) $$R = \frac{\frac{(\beta^2-k^2)^2}{4\beta^2 k^2}\sin^2 2\beta a}{\left[1 + \frac{(\beta^2-k^2)^2 \sin^2 2\beta a}{4\beta^2 k^2}\right]}$$

This is of the form: $\frac{x}{1+x} = \left[\frac{1+x}{x}\right]^{-1} = \left[1 + \frac{1}{x}\right]^{-1}$

(14) $$\therefore R = \left[1 + \frac{4\beta^2 k^2}{(\beta^2-k^2)^2 \sin^2 2\beta a}\right]^{-1} = \left[1 + \frac{4E(E-V_0)}{V_0^2 \sin^2 2\left[\frac{2m(E-V_0)}{\hbar^2}\right]^{1/2} a}\right]^{-1}$$

Assignment #3
Continued

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Problem 12
Continued

12. b. (1) For $E < V_0$, we define $\gamma = \sqrt{\frac{2m(V_0-E)}{\hbar^2}} = i\beta$. All we do is merely substitute this into a(12) and a(14), that is, $\beta = i\gamma$; realizing that:

$$\sin i2\gamma a = i \sinh 2\gamma a \quad , \quad \sin^2 i2\gamma a = -\sinh^2 2\gamma a$$

(2) $$T = \left[1 + \frac{(\gamma^2+k^2)^2 \sinh^2 2\gamma a}{4\gamma^2 k^2}\right]^{-1} = \left[1 + \frac{V_0^2 \sinh^2\left\{\frac{2m(V_0-E)}{\hbar^2}\right\}^{1/2} 2a}{4E(V_0-E)}\right]^{-1}$$

(3) $$R = \left[1 + \frac{4\gamma^2 k^2}{(\gamma^2+k^2)^2 \sinh^2 2\gamma a}\right]^{-1} = \left[1 + \frac{4E(V_0-E)}{V_0^2 \sinh^2\left\{\frac{2m(V_0-E)}{\hbar^2}\right\}^{1/2} 2a}\right]^{-1}$$

(4) We have given $ka = \left[\frac{2mE}{\hbar^2}\right]^{1/2} a = \pi$; $a = \frac{\pi}{\left[\frac{2mE}{\hbar^2}\right]^{1/2}}$

$$\left[\frac{2mE}{\hbar^2} - \frac{2mV_0}{\hbar^2}\right]^{1/2} \cdot \frac{\pi}{\left[\frac{2mE}{\hbar^2}\right]^{1/2}} = \left[1 - \frac{V_0}{E}\right]^{1/2} \pi$$

(5) $$\therefore T = \left[1 + \left(\frac{V_0}{E}\right)^2 \frac{\sin^2\left[1-\frac{V_0}{E}\right]^{1/2} \cdot 2\pi}{4\left(1-\frac{V_0}{E}\right)}\right]^{-1}$$

$$= \left[1 + \frac{n^2 \sin^2[1-n]^{1/2} \cdot 2\pi}{4(1-n)}\right]^{-1}, \quad n \equiv \frac{V_0}{E}, \quad n \le 1$$

$$= \left[1 + \frac{n^2 \sinh^2[n-1]^{1/2} \cdot 2\pi}{4(n-1)}\right]^{-1}, \quad n > 1$$

We wish to plot T versus n for n from -4 to $+2$

n	$\{1-n\}^{1/2} \cdot 2\pi$	$\sin^2[1-n]^{1/2} \cdot 2\pi$	$[\ ]^{-1}$	T
-4	85°	.99	1.79	.56
-3	0°	0	1	1
-2	265°	.99	1.32	.76
-1	150°	.25	1.031	.97
0	0°	0	1	1
1	0°	0	10.9	.092
	$[n-1]^{1/2} \cdot 2\pi$	$\sinh^2[n-1]^{1/2} \cdot 2\pi$	$[\ ]^{-1}$	
2	6.28	~ 40000	~ ∞	~ 0

Not easy.

(6) There arises some difficulty when $n \to 1$. Either of equations (5) may be used. We choose the following procedure:

$$\frac{1}{4} \lim_{n\to 1} \frac{n^2 \sin^2 [1-n]^{1/2} \cdot 2\pi}{(1-n)} = \frac{1}{4} \lim_{n\to 1} \frac{\sin^2 [1-n]^{1/2} \, 2\pi}{(1-n)}$$

$$= \left\{ \begin{matrix} \text{Let } x = 1-n \\ a = 2\pi \end{matrix} \right\} \left[\lim_{x\to 0} \right] \frac{\sin^2 a x^{1/2}}{4x} = \frac{a \sin a x^{1/2} \cos a x^{1/2}}{4 x^{1/2}}$$

$$= \frac{a^2}{4} \left(\cos^2 a x^{1/2} - \sin^2 a x^{1/2} \right) = \frac{a^2}{4} = \pi^2 \text{, leading to } T = .092.$$

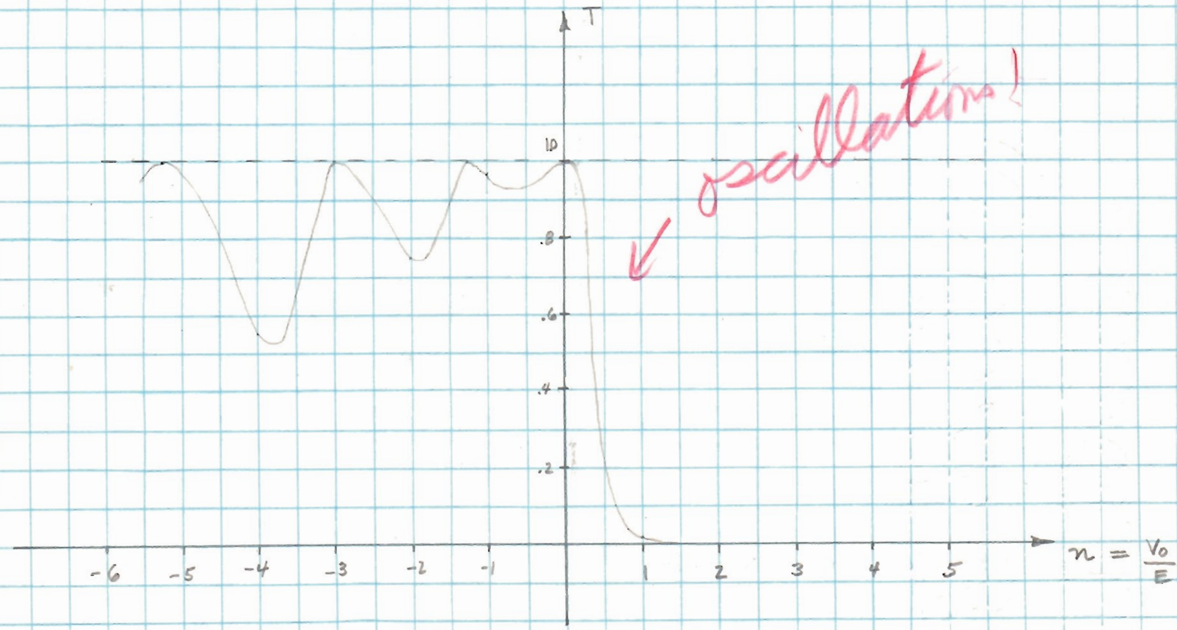
(7) Clearly, in the range $n < 1$, maxima appear in T at

$\sin [1-n]^{1/2} \cdot 2\pi = 0$; $2\pi [1-n]^{1/2} = m\pi$; $n = 1 - \frac{m^2}{4}$, $m = 2, 3, 4, \ldots$

with $n = 0, -1\frac{1}{4}, -3, -5\frac{1}{4}, -8, \ldots$ where $T = 1$

(8) As n becomes negatively large, $T \to \left[1 + \frac{|n|}{4} \sin n^{1/2} \cdot 2\pi \right]^{-1}$

and each minima approaches zero.



— Graph of T vs. $n = \frac{V_0}{E}$ for $ka = \pi$ —

It is interesting to note the parallel between this model of potential barrier for plane Schroedinger waves and the model of films of material whose index of refraction is not equal to one for plane Maxwell waves. As V_0 increase from below E to above E one has essentially the same effect as that given by the Schelkunoff equation as the material changes from a dielectric to a conductor or its index of refraction goes from real to imaginary. Even the "quarter wave plate" effect occurs for $V_0 < E$.

ASSIGNMENT #3
Continued

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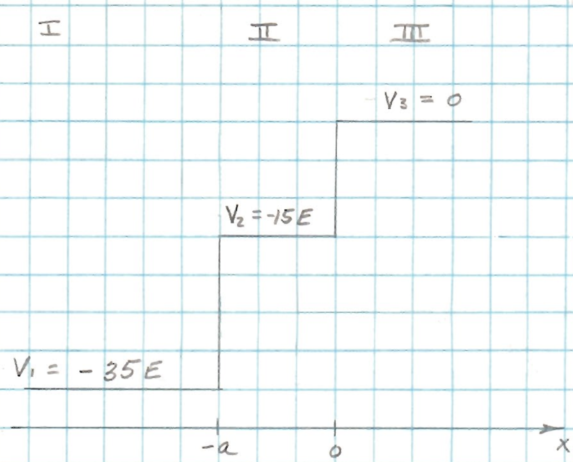
13.



(1) We take $E > 0$ and write the general Schroedinger equation for guidance:

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

(2) We define:

$$k = \sqrt{\frac{2mE}{\hbar^2}}$$

$$\kappa_1 = \left[\frac{2m}{\hbar^2}(E - V_1)\right]^{1/2}$$

$$\kappa_2 = \left[\frac{2m}{\hbar^2}(E - V_2)\right]^{1/2}$$

and as the BC in III: $\psi = e^{ikx}$

(3) Clearly: in I: $\psi = Ae^{i\kappa_1 x} + Be^{-i\kappa_1 x}$
II: $\psi = Ce^{i\kappa_2 x} + De^{-i\kappa_2 x}$
III: $\psi = e^{ikx}$

(4) Imposing the usual BC at $x = -a$ and $x = 0$:

$$Ae^{-i\kappa_1 a} + Be^{i\kappa_1 a} = Ce^{-i\kappa_2 a} + De^{i\kappa_2 a}$$

$$\kappa_1 A e^{-i\kappa_1 a} - \kappa_1 B e^{i\kappa_1 a} = \kappa_2 C e^{-i\kappa_2 a} - \kappa_2 D e^{i\kappa_2 a}$$

$$\left.\begin{array}{l} C + D = 1 \\ \kappa_2 C - \kappa_2 D = k \end{array}\right\} \rightarrow \quad C = \frac{\kappa_2 + k}{2\kappa_2}, \quad D = \frac{\kappa_2 - k}{2\kappa_2}$$

(5)

$$\kappa_1 A e^{-i\kappa_1 a} + \kappa_1 B e^{i\kappa_1 a} = \kappa_1\left(\frac{\kappa_2 + k}{2\kappa_2}\right)e^{-i\kappa_2 a} + \kappa_1\left(\frac{\kappa_2 - k}{2\kappa_2}\right)e^{i\kappa_2 a}$$

$$\kappa_1 A e^{-i\kappa_1 a} - \kappa_1 B e^{i\kappa_1 a} = \kappa_2\left(\frac{\kappa_2 + k}{2\kappa_2}\right)e^{-i\kappa_2 a} - \kappa_2\left(\frac{\kappa_2 - k}{2\kappa_2}\right)e^{i\kappa_2 a}$$

(6)

$$A = \frac{e^{i\kappa_1 a}}{4\kappa_1\kappa_2}\left\{\left[\kappa_1(\kappa_2 + k) + \kappa_2(\kappa_2 + k)\right]e^{-i\kappa_2 a} + \left[\kappa_1(\kappa_2 - k) - \kappa_2(\kappa_2 - k)\right]e^{i\kappa_2 a}\right\}$$

$$= \frac{e^{i\kappa_1 a}}{4\kappa_1\kappa_2}\left[(\kappa_1 + \kappa_2)(\kappa_2 + k)e^{-i\kappa_2 a} + (\kappa_1 - \kappa_2)(\kappa_2 - k)e^{i\kappa_2 a}\right]$$

$$B = \frac{e^{-i\kappa_1 a}}{4\kappa_1\kappa_2}\left[(\kappa_1 - \kappa_2)(\kappa_2 + k)e^{-i\kappa_2 a} + (\kappa_1 + \kappa_2)(\kappa_2 - k)e^{i\kappa_2 a}\right]$$

(7) We form $R = \frac{|B|^2}{|A|^2} = \frac{BB^*}{AA^*}$ since our notation is consistent with that used in lecture and after some tribulation obtain:

$$R = \frac{\kappa_2^2(\kappa_1 - k)^2 - (\kappa_1^2 - \kappa_2^2)(\kappa_2^2 - k^2)\sin^2\kappa_2 a}{\kappa_2^2(\kappa_1 + k)^2 - (\kappa_1^2 - \kappa_2^2)(\kappa_2^2 - k^2)\sin^2\kappa_2 a}$$

(8) Using the definitions of κ_1, κ_2, k and making the definition:

$$\theta = 4ka, \quad a = \frac{\theta \hbar}{4\sqrt{2mE}}$$

we have:

$$R = \frac{(E - V_2)(\sqrt{E - V_1} - \sqrt{E})^2 + V_2(V_2 - V_1)\sin^2\left[1 - \frac{V_2}{E}\right]^{1/2}\frac{\theta}{4}}{(E - V_2)(\sqrt{E - V_1} + \sqrt{E})^2 + V_2(V_2 - V_1)\sin^2\left[1 - \frac{V_2}{E}\right]^{1/2}\frac{\theta}{4}}$$

(9) Substituting the values of V_1 and V_2 we arrive at

$$R = \frac{100 - 75\sin^2\theta}{196 - 75\sin^2\theta}$$ ✓

(10) For the single jump from $-35E$ to 0, that is, $\theta = 0$,

$$R = \frac{100}{196} = .51$$ ✓

(11) To test for extrema; take $\frac{dR}{d\theta} = 0$

$$\frac{dR}{d\theta} = \frac{(196 - 75\sin^2\theta)\cdot -75\cdot 2\cos\theta\sin\theta - (100 - 75\sin^2\theta)\cdot -75\cdot 2\cos\theta\sin\theta}{(196 - 75\sin\theta)^2} = 0$$

Clearly the roots are: $\sin\theta = 0$, $\theta = n\pi$, $n = 0, 1, 2, 3, \ldots$
$\cos\theta = 0$, $\theta = (2n+1)\pi/2$, $n = 0, 1, 2, 3, \ldots$

with the minima at $\theta = (2n+1)\pi/2$ by inspection:

(12) $\therefore$ $R_{min} = \frac{25}{121} = .206$ ✓

(13) $\frac{R_0}{R_{min}} = 2.48$ ✓

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14. a. (1) We first derive a few properties of the one dimensional time independent Schroedinger equation, viz:

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}\left[E - V(x)\right]\psi = 0, \quad \frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2}\left[V(x) - E\right]\psi$$

where $V(x)$ is non-singular and single valued such that well-behaved solutions exist.

(2) We consider E to be constant and now hypothesize two solutions ψ_1, ψ_2 to exist. Clearly:

$$\frac{\psi_1''}{\psi_1} = \frac{\psi_2''}{\psi_2} = \frac{2m}{\hbar^2}\left[V(x) - E\right]$$

$$\psi_2\psi_1'' - \psi_1\psi_2'' = 0$$

(3) Integrating, $\psi_2\psi_1' - \psi_1\psi_2' = \text{constant}$

or $$\begin{vmatrix} \psi_1 & \psi_2 \\ \psi_1' & \psi_2' \end{vmatrix} = \text{constant}$$

If ψ_1 and ψ_2 are not independent ($\psi_1 = c\,\psi_2$), the determinant will vanish. If ψ_1 and ψ_2 are independent for the same energy (degenerate) the determinant will be a finite constant. Note that no mention is made of the continuous or discrete nature of the energy.

(4) We take the complex conjugate of (1) knowing that the energy and potential are real:

$$\psi''^* = \frac{2m}{\hbar^2}\left[V(x) - E\right]\psi^*$$

considering this time the same solution for the same state.

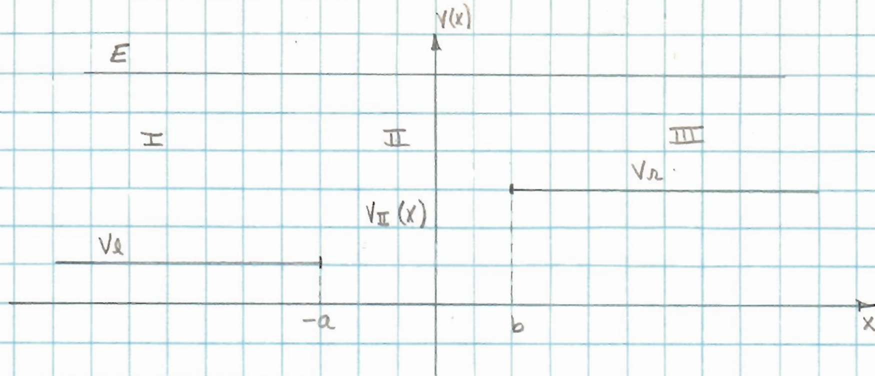
(5) Proceeding as before:

$$\psi'\psi^* - \psi'^*\psi = \text{constant}, \text{ or, } \begin{vmatrix} \psi^* & \psi \\ \psi'^* & \psi' \end{vmatrix} = \text{constant}$$

(6) Also, it is clear that $\begin{vmatrix} \psi_1^* & \psi_2 \\ \psi_1'^* & \psi_2' \end{vmatrix} = \text{constant}$

All our conditions hold under the same energy state.

Consider the following collision problem:



$V_{II}(x)$ is an arbitrary potential satisfying the conditions set forth in (1)

Definitions: $k_r = \frac{2m}{\hbar^2}\left[E - V_r\right]^{1/2}$; $k_l = \frac{2m}{\hbar^2}\left[E - V_l\right]^{1/2}$

Case 1. Particle incident from the left:

(7)

$$\text{I}: \quad \psi_1 = A e^{i k_l x} + B e^{-i k_l x} \qquad T \equiv \frac{k_r}{k_l}\frac{1}{|A|^2}$$

$$\text{III}: \quad \psi_1 = e^{i k_r x} \qquad R \equiv \frac{|B|^2}{|A|^2}$$

Case 2. Particle incident from the right:

(8)

$$\text{I}: \quad \psi_2 = e^{-i k_l x} \qquad T' \equiv \frac{k_l}{k_r}\frac{1}{|A'|^2}$$

$$\text{III}: \quad \psi_2 = A' e^{-i k_r x} + B' e^{i k_r x} \qquad R' \equiv |B'|^2/|A'|^2$$

We now see that ψ_1 and ψ_2 are independent solutions of the same Schroedinger equation for the same energy and thus the energy possesses a two-fold degeneracy characteristic of this part of the spectrum. Since our Wronskian is independent of position (that is, constant), the Wronskians at any two points should be equal.

(9)

$$\begin{vmatrix} {}_{I}\psi_1 & {}_{I}\psi_2 \\ {}_{I}\psi_1' & {}_{I}\psi_2' \end{vmatrix} = \begin{vmatrix} {}_{III}\psi_1 & {}_{III}\psi_2 \\ {}_{III}\psi_1' & {}_{III}\psi_2' \end{vmatrix}$$

Plugging in and solving, we find

(10) $k_r A' = k_l A$; $k_r |A'|^2 = k_l A A^{*\prime} = k_l \left(\frac{k_l}{k_r} |A|^2 \right)$

(11) $\therefore \quad \frac{k_l}{k_r}\frac{1}{|A'|^2} = \frac{k_r}{k_l}\frac{1}{|A|^2}$ or $T = T'$

and the transmission coefficient is the same for incidence from the left or right.

Assignment #3
Continued

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Problem 14
Continued

(12) We now set up the same two Wronskians as in equation (9) except now between the conjugates as in equation (6):

$$\begin{vmatrix} {}_{I}\psi_1^* & {}_{I}\psi_2 \\ {}_{I}\psi_1^{*\prime} & {}_{I}\psi_2' \end{vmatrix} = \begin{vmatrix} {}_{III}\psi_1^* & {}_{III}\psi_2 \\ {}_{III}\psi_1^{*\prime} & {}_{III}\psi_2' \end{vmatrix}$$

Plugging in and solving:

(13) $k_r B' = -k_l B$, or, $k_r |B'|^2 = -k_l \left(-\frac{k_l}{k_r} B^*\right) B$, $\frac{k_r}{k_l} |B'|^2 = \frac{k_l}{k_r} |B|^2$

(14) Multiplying by equation (11) : $\frac{|B'|^2}{|A'|^2} = \frac{|B|^2}{|A|^2}$, or, $R' = R$

These relations could also have been derived using conservation of probability current density as this quantity is proportional to the Wronskian.

b. (1) We now use the principle of conservation of probability to show that $T + R = 1$. The probability current density (pcd) of the incident wave must equal the pcd of the reflected wave plus the pcd of the transmitted wave. We hold that regardless of the nature of the potential V_{II} (as long as it is well-behaved) it will approach V_l and V_r if a and b are taken large enough. Clearly there are two cases: If $E > V_l, V_r$, some part of the wave will be transmitted and some reflected. If $V_l < E < V_r$ there will be no transmission and $R = 1$. We take this case to be trivial and concentrate on the former.

(2) $J = \frac{\hbar}{2m i}\left(\psi^* \psi' - \psi \psi^{*\prime}\right)$

(4) Incident current: $\psi_l = A e^{i k_l x}$, considering the wave to be incident from the left.

$$J_i = \frac{\hbar}{2m i}\left(i k_l |A|^2 + i k_l |A|^2\right) = \frac{\hbar}{m} k_l |A|^2$$

(5) Reflected : $\psi_r = B e^{-i k_\ell x}$

$$J_r = \frac{\hbar}{2mi}\left(-ik_\ell |B|^2 - i k_\ell |B|^2\right) = -\frac{\hbar}{m} k_\ell |B|^2$$

(6) Transmitted : $\psi_t = e^{i k_r x}$

$$J_t = \frac{\hbar}{2mi}\left(i k_r + i k_r\right) = \frac{\hbar}{m} k_r$$

As probability current density is a vector and we are working in only one dimension, we may take the magnitudes as J_r flows in the opposite direction of J_i, J_t. This is the reason for the minus sign in (5).

(7) $|J_i| = |J_r| + |J_t|$; $\frac{\hbar}{m} k_\ell |A|^2 = \frac{\hbar}{m} k_\ell |B|^2 + \frac{\hbar}{m} k_r$

(8) $\frac{|B|^2}{|A|^2} + \frac{k_r}{k_\ell}\frac{1}{|A|^2} = 1$, or, $R + T = 1$, QED. ✓

It is obvious by now that the same result would be obtained by considering a wave incident from the right since $R = R'$, $T = T'$

Assignment # 3
Continued

Paul Grant
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15. (1) We refer to the diagram of Problem 14:

In I: $u = C_\ell \left[A e^{i k_\ell x} + B e^{-i k_\ell x} \right]$

$v = C_\ell' \, e^{-i k_\ell x}$

In III: $u = C_r e^{i k_r x}$

$v = C_r' \left[A' e^{-i k_r x} + B' e^{i k_r x} \right] = C_r' \frac{k_\ell}{k_r} \left[A e^{-i k_r x} - B e^{i k_r x} \right]$

(2) We wish to form $v^*(x, k') \, u(x, k)$; valid in each of the regions I and III:

In I: $v^*(x, k') \, u(x, k) = C_\ell C_\ell'^* \left[A e^{i(k_\ell + k_\ell')x} + B e^{-i(k_\ell - k_\ell')x} \right]$

In III: $v^*(x, k') \, u(x, k) = C_r C_r'^* \frac{k_\ell}{k_r'} \left[A^* e^{i(k_r + k_r')x} - B^* e^{i(k_r - k_r')x} \right]$

(3) We integrate region I from $-\infty$ to 0 and region III from 0 to ∞ noticing that the first term in each expression vanishes. Integrating over the entire range of x is justified because equations (1) are the asymptotic waves regardless of the nature of V_{II}. We have:

Not too clean.

$$C_\ell C_\ell'^* B \int_{-\infty}^{0} e^{-i(k_\ell - k_\ell')x} \, dx - C_r C_r'^* \frac{k_\ell}{k_r'} B^* \int_{0}^{\infty} e^{i(k_r - k_r')x} \, dx$$

We note the following identifications: $\int_{-\infty}^{0} e^{-ax} dx = \int_{0}^{\infty} e^{ax} dx$

From the lecture: $k_\ell (k_\ell - k_\ell') \simeq k_r (k_r - k_r')$

Only near $k_1 \approx k_1'$

$x \rightarrow \frac{k_r}{k_\ell} x \; ; \quad dx \rightarrow \frac{k_r}{k_\ell} dx$

(4) Thus: $\left[C_\ell C_\ell'^* B - C_r C_\ell'^* B^* \frac{k_r}{k_r'} \right] \int_0^\infty e^{i(k_\ell - k_\ell')x} dx$

$$= \left[C_\ell C_\ell'^* B - C_r C_r'^* B^* \frac{k_r}{k_r'} \right] \cdot 2\pi \, \delta(k_\ell - k_\ell')$$

Not true.

$\int_{-\infty}^{\infty} = 2\pi \, \delta(\;)$
↑

(5) It was shown in lecture that: $C_r = \sqrt{\frac{I}{2\pi}}$, $C_r' = \sqrt{\frac{I}{2\pi}}$

Similarly, it may be shown that: $C_l = \sqrt{\frac{k_l}{k_r}}\sqrt{\frac{I}{2\pi}} = C_l'$ Show this.

and these constants may now be factored out leaving,

$$CC' \left[B - \frac{k_r}{k_r'} B^* \right] \cdot 2\pi\, \delta(k_l - k_l')$$

(6) Considering the real part and using $k_l(k_l - k_l') = k_r(k_r - k_r')$:

$$- CC' \cdot \frac{k_l}{k_r k_r'} \operatorname{Re} B \left[k_l - k_l' \right] \cdot 2\pi\, \delta(k_l - k_l')$$

such that when $k_l = k_l'$ the coefficient of the δ function vanishes.

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Assignment #4
Problems 16-20

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16. (1) We evaluate the products $A_l^+ A_l$ and $A_l A_l^+$.

Let A_l operate on u, then

$$A_l^+ A_l u = \left(\frac{l}{r} - \frac{1}{l} - \frac{d}{dr}\right)\left(\frac{l}{r}u - \frac{u}{l} + \frac{du}{dr}\right)$$

$$= \frac{l^2}{r^2}u - \frac{u}{r} + \frac{l}{r}\frac{du}{dr} - \frac{u}{r} + \frac{u}{l^2} - \frac{1}{l}\frac{du}{dr}$$
$$- \frac{l}{r}\frac{du}{dr} + \frac{l}{r^2}u + \frac{1}{l}\frac{du}{dr} - \frac{d^2u}{dr^2}$$

$$= \left[\frac{l(l+1)}{r^2} - \frac{2}{r} + \frac{1}{l^2} - \frac{d^2}{dr^2}\right]u$$

$$A_l^+ A_l = H_l + \frac{1}{l^2}$$ ✓

(2) Let A_l^+ operate on u:

$$A_l A_l^+ u = \left(\frac{l}{r} - \frac{1}{l} + \frac{d}{dr}\right)\left(\frac{l}{r}u - \frac{1}{l}u - \frac{du}{dr}\right)$$

$$= \frac{l^2}{r^2}u - \frac{u}{r} - \frac{l}{r}\frac{du}{dr} - \frac{u}{r} + \frac{u}{l^2} + \frac{1}{l}\frac{du}{dr}$$
$$+ \frac{l}{r}\frac{du}{dr} - \frac{l}{r^2}u - \frac{1}{l}\frac{du}{dr} - \frac{d^2u}{dr^2}$$

$$= \left[\frac{l(l-1)}{r^2} - \frac{2}{r} + \frac{1}{l^2} - \frac{d^2}{dr^2}\right]u$$

$$A_l A_l^+ = H_{l-1} + \frac{1}{l^2}$$ ✓

(3) $$[A_l^+, A_l] = \frac{2l}{r^2} = H_l - H_{l-1}$$ ✓

(4) We now notice that from the results of (1) and (2), upon letting $l \to l+1$:

$$A_{l+1}^+ A_{l+1} = H_{l+1} + \frac{1}{(l+1)^2}$$

$$A_{l+1} A_{l+1}^+ = H_l + \frac{1}{(l+1)^2}$$

(5) We can now write: Using equation (1):

$$H_\ell u_{n\ell} = \left[A_\ell^+ A_\ell - \frac{1}{\ell^2} \right] u_{n\ell} = E_n u_{n\ell}$$

or $$A_\ell^+ A_\ell u_{n\ell} = \left(E_n + \frac{1}{\ell^2}\right) u_{n\ell}$$

Operating with A_ℓ:

$$A_\ell A_\ell^+ A_\ell u_{n\ell} = \left(E_n + \frac{1}{\ell^2}\right) A_\ell u_{n\ell} \qquad (\text{as } E_n, \tfrac{1}{\ell^2} \text{ are constants})$$

$$\left(H_{\ell-1} + \frac{1}{\ell^2}\right) A_\ell u_{n\ell} = \left(E_n + \frac{1}{\ell^2}\right) A_\ell u_{n\ell}$$

or $$H_{\ell-1} \left[A_\ell u_{n\ell}\right] = E_n \left[A_\ell u_{n\ell}\right] \quad ✓$$

so $A_\ell u_{n\ell}$ is a function satisfying the above differential equation.

(6) Using the second of equations (4), we write:

$$H_\ell u_{n,\ell} = \left[A_{\ell+1} A_{\ell+1}^+ - \frac{1}{(\ell+1)^2} \right] u_{n\ell} = E_n u_{n\ell}$$

or $$A_{\ell+1} A_{\ell+1}^+ u_{n\ell} = \left(E_n + \frac{1}{(\ell+1)^2} \right) u_{n\ell}$$

Operating with $A_{\ell+1}^+$:

$$A_{\ell+1}^+ A_{\ell+1} A_{\ell+1}^+ u_{n\ell} = \left(E_n + \frac{1}{(\ell+1)^2}\right) A_{\ell+1}^+ u_{n\ell}$$

$$\left(H_{\ell+1} + \frac{1}{(\ell+1)^2}\right) A_{\ell+1}^+ u_{n\ell} = \left(E_n + \frac{1}{(\ell+1)^2}\right) A_{\ell+1}^+ u_{n\ell}$$

or $$H_{\ell+1} \left[A_{\ell+1}^+ u_{n\ell}\right] = E_n \left[A_{\ell+1}^+ u_{n\ell}\right] \quad ✓$$

so that $A_{\ell+1}^+ u_{n\ell}$ is the second desired function.

(7) We now define $\varphi \equiv A_\ell u_{n\ell}$; $\varphi^+ \equiv A_{\ell+1}^+ u_{n\ell}$; we then write for the two differential equations:

$$0 = E_n\left[A_\ell u_{n\ell}\right] - H_{\ell-1}\left[A_\ell u_{n\ell}\right] : \quad \frac{d^2}{dr^2}\varphi + \left[E_n + \frac{2}{r} - \frac{\ell(\ell-1)}{r^2} \right] \varphi = 0$$

$$0 = E_n\left[A_{\ell+1}^+ u_{n\ell}\right] - H_{\ell+1}\left[A_{\ell+1}^+ u_{n\ell}\right] : \quad \frac{d^2}{dr^2}\varphi^+ + \left[E_n + \frac{2}{r} - \frac{(\ell+1)(\ell+2)}{r^2} \right] \varphi^+ = 0$$

We can now, for convenience, lump these two equations into one by the following identifications: $(n-1), (n+1) \to \lambda$; $\varphi, \varphi^+ \to \xi$:

$$\therefore \frac{d^2}{dr^2}\xi + \left\{ E_n + \frac{2}{r} - \frac{\lambda(\lambda+1)}{r^2} \right] \xi = 0$$

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16 Continued:

(8) We note that this is exactly the form of the usual radial differential equation for the hydrogenic case. Instead of laboriously copying the method of solution which was given in lecture, we will merely transfer the appropriate results: For $E<0$, $\frac{1}{\sqrt{-E'}} \equiv n$.

$$\xi = \left[\frac{(n+\lambda)!}{(n-\lambda-1)!}\right]^{1/2} \cdot \frac{1}{2\left(\frac{n}{2}\right)^{\lambda+2}(2\lambda+1)!} \cdot r^{\lambda+1} e^{-r/n} {}_1F_1\left\{\lambda+1-n;\, 2\lambda+2;\, \frac{2r}{n}\right\}$$

with $_1F_1(a;b;x) = 1 + \frac{a}{1\cdot b}x + \frac{a(a+1)}{1\cdot 2\, b(b+1)}x^2 + \frac{a(a+1)(a+2)}{1\cdot 2\cdot 3\, b(b+1)(b+2)}x^3 + \cdots$

where: $a = \lambda+1-n$
$b = 2\lambda+2$
$x = \frac{2r}{n}$

with the recursion relation: $C_{k+1} = \frac{k+a}{(k+1)(k+b)} C_k$

(9) The following properties are now clearly apparent:

$\lambda \to l: \quad \xi \to u_{nl}$

$\lambda \to l-1: \quad \xi \to \varphi = u_{n,l-1}$, with $\varphi = A_l u_{nl}$ $\quad \therefore \quad A_l u_{nl} = u_{n,l-1}$

$\lambda \to l+1: \quad \xi \to \varphi^+ = u_{n,l+1}$, with $\varphi^+ = A^+_{l+1} u_{nl}$ $\quad \therefore \quad A^+_{l+1} u_{nl} = u_{n,l+1}$

Thus we see that the operators A_l, A^+_{l+1} acting on the eigenfunction u_{nl} perform the function of lowering and raising operators, respectively, on the angular momentum quantum number l.

(10) The boundary conditions on u_{nl} are $u(0)=0$, $u_{nl}\to 0$ as $r\to\infty$. In lecture, it was shown that unless $_1F_1$ was terminated, u would become unbounded as $e^{r/n}$. If the series was terminated at some term n', u would vanish in large r as $e^{-r/n}$. This cutoff condition on the recursion equation led to the following equation:

$$\frac{1}{\sqrt{-E_n}} = l + 1 + n' \equiv n \quad , \quad n = l+1,\ l+2,\ \ldots \quad \text{as } n' = 0, 1, 2, 3, \ldots$$

All this was shown in detail in lecture so it is senseless to repeat it now. We see that l follows the rule:

$$l = n-1,\ n-2,\ n-3,\ \ldots\ 0,$$

so that the maximum value of l is $n-1$.

(11) Now, if the above is defined as giving the required boundary condition on u_{nl}, then for $u_{n,l+1}$ we have, letting $l \to l+1$:

$$\frac{1}{\sqrt{-E_n}} = l + 2 + n'' = n \quad , \quad \text{since we are still considering the same state } n.$$

For this expression to be equal to the above, the series is cut off one term earlier. Obviously, for $l \to l-1$, the series must cut off one term later to still remain in the same state n. The point is that for $0 < l < n$, the series cuts off and will approach zero exponentially, as shown in lecture, as $r \to \infty$, independently of l.

Therefore, if $u_{n,l-1}$ and $u_{n,l+1}$ satisfy the boundary conditions $u(0) = 0$, $u(\infty) = 0$; then obviously, $A_l u_{nl}$ and $A_{l+1}^{+} u_{nl}$ satisfy them.

The condition $u(0) = 0$ is obvious from equation (8).

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Identification $A_l u_l$ with u_{l-1} & $A_{l+1} u_l$ " u_{l+1} is possible after showing $A_l u_l$ & $A_{l+1}^{+} u_l$ have the same b.c. as u's

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17. (1) It was shown in problem 16 from results in lecture that for a given fixed value of n, l has an upper limit of $n-1$. That l cannot be indefinitely large is easily seen from:

$$u_{nl} \sim r^{l+1} e^{-r/n} \, {}_1F_1 \left\{ l+1-n ; \; 2l+2 ; \; \frac{2r}{n} \right\}$$

Simpler reason can be given.

with ${}_1F_1$ defined as in (8) of problem 16. As $l \to \infty$ ${}_1F_1$ clearly approaches a constant as the numerator and denominator of each term contains equal powers of l. However the term r^{l+1} will make the function unbounded. At any rate, the selection rule for l states that $l < n$ and this conclusively shows that for fixed n, l cannot be indefinetely large.

(2) From equations (11) and (10) of problem 16, it is obvious that; for $E < 0$:

$$E = \frac{1}{n^2}$$

✓

and our selection rule gives the possible values of l for each n, viz.,

$$l = n-1, n-2, n-3, \ldots, 0.$$

(3) In attempting to construct various eigenfunctions with the relations (9) of problem 16, we run into the paradox of eventually violating our selection rule on l by repeated application of A_{l+1}^+.

Therefore, in analogy with the harmonic oscillator case, we stipulate that the result of trying to raise the function $u_{n,n-1}$ one more step in angular momentum must be necessarily zero. That is:

$$A_n^+ u_{n,n-1} = 0$$

(4) This yields a simple differential equation, when the proper substitutions are made in A_l^+:

$$\left(\frac{d}{dr} + \frac{1}{n} - \frac{n}{r} \right) u_{n,n-1} = 0$$

✓

(5) $$\frac{d\,u_{n,n-1}}{u_{n,n-1}} = \left(\frac{n}{r} - \frac{1}{n} \right) dr$$

$$\ln u_{n,n-1} = n \ln r - \frac{r}{n} + \ln c$$

$$= \ln r^n + \ln e^{-r/n} + \ln c$$

$$\therefore \quad u_{n,n-1} = c\, r^n e^{-r/n}$$

(6) We normalize:

$$\int_0^\infty |u_{n,n-1}|^2 dr = c^2 \int_0^\infty r^{2n} e^{-2r/n} dr = c^2 \frac{(2n)!}{\left(\frac{2}{n}\right)^{2n+1}} = 1$$

by tables.

(7) $$\therefore \quad u_{n,n-1} = \frac{\left(\frac{2}{n}\right)^{n+\frac{1}{2}}}{\left[(2n)!\right]^{1/2}} r^n e^{-r/n} \quad \checkmark$$

(8) $$u_{n,n-2} = A_{n-1} u_{n,n-1} = c \left[\frac{n-1}{r} - \frac{1}{n-1} + \frac{d}{dr} \right] r^n e^{-r/n}$$

$$= c \left\{ (n-1) r^{n-1} e^{-r/n} - \frac{r^n e^{-r/n}}{n-1} + n r^{n-1} e^{-r/n} - \frac{r^n e^{-r/n}}{n} \right\}$$

$$= c \left\{ \frac{n-1}{r} - \frac{1}{n-1} + \frac{n}{r} - \frac{1}{n} \right\} r^n e^{-r/n}$$

$$= c \cdot (2n-1) \left\{ \frac{1}{r} - \frac{1}{n(n-1)} \right\} r^n e^{-r/n}$$

(9) $$\int_0^\infty |u_{n,n-2}|^2 dr = c^2 \cdot (2n-1)^2 \int_0^\infty \left\{ r^{2n-2} e^{-2r/n} - \frac{2 r^{2n-1} e^{-2r/n}}{n(n-1)} + \frac{r^{2n} e^{-2r/n}}{n^2 (n-1)^2} \right\} dr$$

$$= c^2 \cdot (2n-1)^2 \left\{ \frac{(2n-2)!}{\left(\frac{2}{n}\right)^{2n-1}} - \frac{2(2n-1)!}{n(n-1)\left(\frac{2}{n}\right)^{2n}} + \frac{(2n)!}{n^2(n-1)^2 \left(\frac{2}{n}\right)^{2n+1}} \right\}$$

$$= \frac{c^2 \cdot (2n-1)^2 \cdot (2n)!}{n \left(\frac{2}{n}\right)^{2n+1}} \left\{ \frac{2\left(\frac{1}{n}\right)^2}{(2n-1)} - \frac{\left(\frac{2}{n}\right)}{n(n-1)} + \frac{1}{n(n-1)^2} \right\}$$

$$= c^2 \cdot \frac{(2n-1) \cdot (2n)!}{\left(\frac{2}{n}\right)^{2n+1} \cdot n^2 (n-1)^2}$$

(10) $$u_{n,n-2} = \frac{n(n-1) \left(\frac{2}{n}\right)^{n+1/2} (2n-1)^{1/2}}{\left[(2n)!\right]^{1/2}} \left\{ \frac{1}{r} - \frac{1}{n(n-1)} \right\} r^n e^{-r/n}$$

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Problem 17
Continued

(11) Now: $u_{n,n-3} = A_{n-2}\, u_{n,n-2}$

$$u_{n,n-3} = C\left[\frac{n-2}{r} - \frac{1}{n-2} + \frac{d}{dr}\right]\left\{r^{n-1} - \frac{r^n}{n(n-1)}\right\} e^{-r/n}$$

$$= C\left\{(n-2)r^{n-2} - \frac{(n-2)r^{n-1}}{n(n-1)} - \frac{r^{n-1}}{n-2} + \frac{r^n}{n(n-1)(n-2)} - \frac{r^{n-1}}{n} + \frac{r^n}{n^2(n-1)}\right.$$

$$\left. + (n-1)r^{n-2} - \frac{r^{n-1}}{n-1}\right\} e^{-r/n}$$

$$= C\left\{(2n-3)r^{n-2} - \frac{2(2n-3)}{n(n-2)} r^{n-1} + \frac{2r^n}{n^2(n-2)}\right\} e^{-r/n}$$

(12) $$\int_0^\infty |u_{n,n-3}|^2 dr = C^2 \int_0^\infty \left\{(2n-3)^2 r^{2n-4} - \frac{4(2n-3)^2}{n(n-2)} r^{2n-3} + \frac{4(2n-3)}{n^2(n-2)} r^{2n-2}\right.$$

$$\left. + \frac{4(2n-3)^2}{n^2(n-2)^2} r^{2n-2} - \frac{8(2n-3)}{n^3(n-2)^2} r^{2n-1} + \frac{4r^{2n}}{n^4(n-2)^2}\right\} e^{-2r/n} dr$$

$$= \left\{\frac{(2n-3)^2(2n-4)!}{\left(\frac{2}{n}\right)^{2n-3}} - \frac{4(2n-3)^2(2n-3)!}{n(n-2)\left(\frac{2}{n}\right)^{2n-2}} + \frac{4(2n-3)(2n-2)!}{n^2(n-2)\left(\frac{2}{n}\right)^{2n-1}}\right.$$

$$\left. \frac{4(2n-3)^2(2n-2)!}{n^2(n-2)^2\left(\frac{2}{n}\right)^{2n-1}} - \frac{8(2n-3)(2n-1)!}{n^3(n-2)^2\left(\frac{2}{n}\right)^{2n}} + \frac{4(2n)!}{n^4(n-2)^2\left(\frac{2}{n}\right)^{2n+1}}\right\} C^2$$

$$= \frac{(2n)!\, C^2}{\left(\frac{2}{n}\right)^{2n+1}}\left\{\frac{(2n-3)^2\left(\frac{2}{n}\right)^4}{(2n)(2n-1)(2n-2)(2n-3)} - \frac{4(2n-3)^2\left(\frac{2}{n}\right)^3}{n(n-2)(2n)(2n-1)(2n-2)} + \frac{4(2n-3)\left(\frac{2}{n}\right)^2}{n^2(n-2)(2n)(2n-1)}\right.$$

$$\left. + \frac{4(2n-3)^2\left(\frac{2}{n}\right)^2}{n^2(n-2)^2(2n)(2n-1)} - \frac{8(2n-3)\left(\frac{2}{n}\right)}{n^3(n-2)^2(2n)} + \frac{4}{n^4(n-2)^2}\right\}$$

$$= C^2 \cdot \frac{(2n-3)(2n)!\,4}{(2n-1)(n-2)^2 n^5 \left(\frac{2}{n}\right)^{2n+1}}\left\{\frac{(n-2)^2 - 2(2n-3)(n-2)}{n-1} + 2(n-2) + 2(2n-3) - 2(2n-1) + \frac{n(2n-1)}{2n-3}\right\}$$

(13) $(12) = \dfrac{c^2 \cdot 4(2n)!}{(n-1)(2n-1)(n-2)^2 \; n^5 \left(\frac{2}{n}\right)^{2n+1}} \Big\{ -6n^3 + 20n^2 - 16n + 9n^2 - 30n + 24 + 4n^3 - 10n^2$

$+ 6n - 16n^2 + 40n - 24 + 2n^3 - 3n^2 + n \Big\}$

$$= \frac{c^2 \cdot 4(2n)!}{(n-1)(2n-1)(n-2)^2 \, n^4 \left(\frac{2}{n}\right)^{2n+1}} = 1$$

(14) $$\mathcal{U}_{n,n-3} = \frac{(n-1)^{1/2}(2n-1)^{1/2}(n-2)\, n^2 \left(\frac{2}{n}\right)^{n+1/2}(2n-3)}{2\left[(2n)!\right]^{1/2}} \left\{ 1 - \frac{2}{n(n-2)} r + \frac{2r^2}{n^2(n-2)(2n-3)} \right\} r^{n-2} e^{-r/n}$$

Verification of results using equations (8) of problem 16 which was given in lecture, letting $\xi \to \mathcal{U}_{nl}$, $\lambda \to l$:

(15) $$\mathcal{U}_{n,n-1} = \underbrace{\left[(2n-1)!\right]^{1/2} \frac{1}{2\left(\frac{n}{2}\right)^{n+1}(2n-1)!}} \, r^n e^{-r/n} \underbrace{{}_1F_1\left\{0;\, 2n;\, \frac{2r}{n}\right\}}_{=1}$$

$$= \frac{1}{2} \cdot \frac{\left(\frac{2}{n}\right)^{n+1}}{\left[(2n-1)!\right]^{1/2}}$$

$$= \frac{\frac{1}{2} \cdot \left(\frac{2}{n}\right)^{n+1} (2n)^{1/2}}{\left[(2n)!\right]^{1/2}} = \frac{\left(\frac{2}{n}\right)^{n+1/2}}{\left[(2n)!\right]^{1/2}}$$

(16) $$\therefore \quad \mathcal{U}_{n,n-1} = \frac{\left(\frac{2}{n}\right)^{n+1/2}}{\left[(2n)!\right]^{1/2}} r^n e^{-r/n}$$; which checks with equation (7).

(17) $$\mathcal{U}_{n,n-2} = \underbrace{\left[(2n-2)!\right]^{1/2} \cdot \frac{1}{2\left(\frac{n}{2}\right)^n (2n-3)!}} \, r^{n-1} e^{-r/n} \underbrace{{}_1F_1\left\{-1;\, 2n-2;\, \frac{2r}{n}\right\}}_{=\left\{1 - \frac{r}{(n-1)n}\right\} r^{n-1} e^{-r/n}}$$

$$= \frac{\left[(2n)!\right]^{1/2} (2n)(2n-1)(2n-2)}{(2n)^{1/2}(2n-1)^{1/2} \cdot 2\left(\frac{n}{2}\right)^n \left[(2n)!\right]^{1/2}}$$

$$= \frac{n(n-1)(2n-1)^{1/2}\left(\frac{2}{n}\right)^{n+1/2}}{\left[(2n)!\right]^{1/2}}$$

(18) $$\therefore \quad \mathcal{U}_{n,n-2} = \frac{n(n-1)(2n-1)^{1/2}\left(\frac{2}{n}\right)^{n+1/2}}{\left[(2n)!\right]^{1/2}} \left\{1 - \frac{r}{n(n-1)}\right\} r^{n-1} e^{-r/n}$$

which is identical to equation (10).

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Problem 17
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(19) $$U_{n,n-3} = \underbrace{\left[\frac{(2n-3)!}{2}\right]^{1/2} \frac{1}{2\left(\frac{n}{2}\right)^{n-1}(2n-5)!}}\, r^{n-2} e^{-r/n}\, \underbrace{{}_1F_1\left\{-2;\, 2n-4;\, \frac{2r}{n}\right\}}$$

$$= \frac{[(2n)!]^{1/2} \cdot 8n(2n-1)(n-1)(2n-3)(n-2)}{2(2n-1)^{1/2}(n-1)^{1/2} \cdot \underbrace{\underbrace{2\left(\frac{n}{2}\right)^{n-1}(2n)^{1/2}}_{4\left(\frac{n}{2}\right)^{n-1/2}}}_{\frac{8}{n}\left(\frac{n}{2}\right)^{n+1/2}} (2n)!}$$

$$= 1 - \frac{2r}{n(n-2)} + \frac{4r^2}{n^2(2n-4)(2n-3)}$$

$$= \left\{1 - \frac{2r}{n(n-2)} + \frac{2r^2}{n^2(n-2)(2n-3)}\right\}$$

$$= \frac{n^2(2n-1)^{1/2}(n-1)^{1/2}(2n-3)(n-2)\left(\frac{2}{n}\right)^{n+1/2}}{2\{(2n)!\}^{1/2}}$$

(20) $$\therefore\ U_{n,n-3} = \frac{n^2(2n-1)^{1/2}(n-1)^{1/2}(2n-3)(n-2)\left(\frac{2}{n}\right)^{n+1/2}}{2\{(2n)!\}^{1/2}} \left\{1 - \frac{2r}{n(n-2)} + \frac{2r^2}{n^2(n-2)(2n-3)}\right\} r^{n-2} e^{-r/n}$$

which is identical to equation (14).

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18. (1) In this problem, we wish to find essentially:

$$R_{0k}(0) = \lim_{\substack{l \to 0 \\ r \to 0}} R_{lk}(r)$$

where $$R_{lk}(r) = \frac{(2k)^{l+1} e^{-\pi\nu/2} |\Gamma(l+1+i\nu)|}{(2\pi)^{1/2}(2l+1)!} r^l e^{-ikr} F(l+1-i\nu; 2l+2; 2ikr)$$

(2) It is clear that because of r^l, it is very important that the limit be taken on l first and then r. Physically, this means we first choose our state ($l=0$) and then let the coordinate of the wave function vanish. Taking the limit in this way, we obtain:

$$R_{0k}(0) = \frac{2k\, e^{-\pi\nu/2} |\Gamma(1+i\nu)|}{(2\pi)^{1/2}} F(1-i\nu; 2, 0)$$

$$= \frac{2k\, e^{-\pi\nu/2} |\Gamma(1+i\nu)|}{(2\pi)^{1/2}}.$$

since $F(1-i\nu; 2; 0) = 1$

(3) We now consider the well-known relations between Γ functions derived from Euler's limit Theorem (see Copson, ¶ 9.22):

$$z\Gamma(z) = \Gamma(z+1) \quad ; \quad \Gamma(z)\Gamma(1-z) = \frac{\pi}{\sin \pi z}$$

Let $z \to i\nu$: $$i\nu\,\Gamma(i\nu) = \Gamma(i\nu+1)$$

$$\Gamma(i\nu)\Gamma(1-i\nu) = \frac{\pi}{i \sinh \pi\nu}$$

(4) Dividing: $$\frac{\Gamma(1-i\nu)}{i\nu} = \frac{\pi}{i \sinh \pi\nu\, \Gamma(i\nu+1)}$$

$$\Gamma(1-i\nu)\Gamma(1+i\nu) = |\Gamma(1+i\nu)|^2 = \frac{\pi\nu}{\sinh \pi\nu}$$

(5) $$|\Gamma(1+i\nu)| = \left[\frac{\pi\nu}{\sinh \pi\nu}\right]^{1/2}$$

(6) $$R_{0k}(0) = \frac{2k}{(2\pi)^{1/2}} e^{-\pi\nu/2} \left[\frac{\pi\nu}{\sinh \pi\nu} \right]^{1/2}$$

$$|R_{0k}(0)|^2 = 2k \frac{\nu e^{-\pi\nu}}{\sinh \pi\nu}$$

(7) $$\lim_{\nu \to 0} |R_{0k}(0)|^2 = 2k \lim_{\nu \to 0} \frac{\nu}{\sinh \pi\nu} = 2k \lim_{\nu \to 0} \frac{1}{\pi \cosh \pi\nu}$$

$$= \frac{2k}{\pi}$$

(8) $\therefore$ $$\frac{|R_{0k}(0)|^2}{|R_{0k}(0)|^2_{\nu=0}} = c = \frac{\pi\nu e^{-\pi\nu}}{\sinh \pi\nu}$$

$$= \frac{2\pi\nu e^{-\pi\nu}}{e^{\pi\nu} - e^{-\pi\nu}} = \frac{2\pi\nu}{e^{2\pi\nu} - 1}$$

✓ (10)

This is the probability of a particle to be at the center of force with respect to the probability of a free particle at this point, all in a repulsive field. This is useful in the theory of elastic collisions (Landau-Lifshitz; ¶ 113).

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19. (1) We carry over the following equations that were given and derived in lecture:

$$Q = \sqrt{\frac{m\omega}{2\hbar}}\, q \quad ; \quad P = \frac{p}{\sqrt{2m\hbar\omega}}$$

$$a = Q + iP \quad ; \quad a^{+} = Q - iP \quad ; \quad Q = \frac{a + a^{+}}{2} \quad ; \quad P = \frac{a - a^{+}}{2i}$$

$$q = \sqrt{\frac{2\hbar}{m\omega}} \left\{ \frac{a + a^{+}}{2} \right\} \quad ; \quad p = \sqrt{2m\hbar\omega} \left\{ \frac{a - a^{+}}{2i} \right\}$$

$$a\, u_n = \sqrt{n}\, u_{n-1} \quad ; \quad a^{+} u_n = \sqrt{n+1}\, u_{n+1}$$

(2) We now form q^2 and p^2:

$$q^2 = \frac{\hbar}{2m\omega} \left\{ a^2 + aa^{+} + a^{+}a + a^{+2} \right\}$$

$$p^2 = -\frac{m\hbar\omega}{2} \left\{ a^2 - aa^{+} - a^{+}a + a^{+2} \right\}$$

(3) Let q^2, p^2 operate on u_n, evaluating each operator product apart:

$$a^2 u_n = a \cdot a\, u_n = \sqrt{n}\, a\, u_{n-1} = \sqrt{n}\sqrt{n-1}\, u_{n-2}$$

$$a^{+2} u_n = a^{+} \cdot a^{+} u_n = \sqrt{n+1}\, a^{+} u_{n+1} = \sqrt{n+1}\sqrt{n+2}\, u_{n+2}$$

$$aa^{+} u_n = \sqrt{n+1}\, a\, u_{n+1} = (n+1)\, u_n$$

$$a^{+}a\, u_n = \sqrt{n}\, a^{+} u_{n-1} = n\, u_n$$

(4) $\therefore$

$$q^2 u_n = \frac{\hbar}{2m\omega} \left\{ \sqrt{(n)(n-1)}\, u_{n-2} + (2n+1)\, u_n + \sqrt{(n+1)(n+2)}\, u_{n+2} \right\}$$

$$p^2 u_n = -\frac{m\hbar\omega}{2} \left\{ \sqrt{(n)(n-1)}\, u_{n-2} - (2n+1)\, u_n + \sqrt{(n+1)(n+2)}\, u_{n+2} \right\}$$

(5) We now multiply by $\int u_n^* \, dq$ to find $\overline{q^2}$ and $\overline{p^2}$.

However, it was shown in lecture that the u_n's are orthonormal and we hold that the wave functions used here have been normalized. Therefore, the only terms that remain in the integration are the $(2n+1)\,u_n$ terms.

(6) $\therefore \quad \overline{q^2} = \langle n|q^2|n\rangle = \frac{\hbar}{m\omega}(n+\frac{1}{2})$ ✓

$\overline{p^2} = \langle n|p^2|n\rangle = m\hbar\omega\,(n+\frac{1}{2})$ ✓

(7) It is well known (See any Freshman Physics Text) that for the classical harmonic oscillator the mean kinetic energy is equal to the mean potential energy is equal to one-half the total energy which is a constant of the motion once the system is vibrating in its steady state. That is,

$$\overline{T} = \overline{V} = \tfrac{1}{2}E$$

(8) If $E = (n+\frac{1}{2})\hbar\omega$ for this oscillator, we have:

$$\overline{T} = \frac{\overline{p^2}}{2m} = \tfrac{1}{2}E = \tfrac{1}{2}(n+\tfrac{1}{2})\hbar\omega$$

or $\overline{p^2} = m\hbar\omega\,(n+\frac{1}{2})$, the same result as above. ✓

(9) Now $\overline{V} = \frac{1}{2}s\,\overline{q^2}$, $s = m\omega^2$ (from the lecture notes: this relation is well-known also)

$$\therefore \quad \overline{V} = \tfrac{1}{2}m\omega^2\,\overline{q^2} = \tfrac{1}{2}E = \tfrac{1}{2}(n+\tfrac{1}{2})\hbar\omega$$

or $\overline{q^2} = \frac{\hbar}{m\omega}(n+\frac{1}{2})$, the same result as above.

(10) An easier way may be to recall: $\overline{K} = (n+\frac{1}{2})$

or $\overline{H} = E = \hbar\omega\overline{K} = \hbar\omega(n+\frac{1}{2})$ ✓

Now $\overline{H} = \frac{\overline{p^2}}{2m} + \frac{1}{2}m\omega^2\,\overline{q^2} = \hbar\omega(n+\frac{1}{2})$

Knowing that the averge value of a quantum mechanical operator gives the classical result tells us that, for the harmonic oscillator:

$$\frac{\overline{p^2}}{2m} = \tfrac{1}{2}m\omega^2\,\overline{q^2} = \tfrac{1}{2}\hbar\omega(n+\tfrac{1}{2})$$

or $\overline{p^2} = m\hbar\omega\,(n+\frac{1}{2})$; $\overline{q^2} = \frac{\hbar}{m\omega}(n+\frac{1}{2})$

(10)

Assignment # 4
Continued

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20. (1) $$S(t,y) = e^{-t^2+2ty} = e^{y^2-(t-y)^2} = \sum_{n=0}^{\infty} H_n(y)\frac{t^n}{n!}$$

(2) $$\frac{\partial S}{\partial t} = (-2t+2y)e^{-t^2+2ty} = (-2t+2y)\sum_{n=0}^{\infty} H_n(y)\frac{t^n}{n!}$$

$$= \sum_{n=0}^{\infty} \frac{H_n(y)\, t^{n-1}}{(n-1)!} = \sum_{n=0}^{\infty} -2H_n(y)\frac{t^{n+1}}{n!} + \sum_{n=0}^{\infty} 2y\, H_n(y)\frac{t^n}{n!}$$

(3) Equating coefficients of t^n:

$$\frac{H_{n+1}(y)}{n!} = \frac{-2H_{n-1}(y)}{(n-1)!} + \frac{2y\,H_n(y)}{n!}$$

or $$H_{n+1}(y) = -2n\,H_{n-1}(y) + 2y\,H_n(y)$$

(4) $$\frac{\partial S}{\partial y} = 2t\,e^{-t^2+2ty} = 2t\sum_{n=0}^{\infty} H_n(y)\frac{t^n}{n!} = \sum_{n=0}^{\infty} H_n'(y)\frac{t^n}{n!}$$

$$= \sum_{n=0}^{\infty} 2\,H_n(y)\frac{t^{n+1}}{n!}$$

(5) Equating coefficients: $\dfrac{H_n'(y)}{n!} = \dfrac{2H_{n-1}(y)}{(n-1)!}$

or $H_n'(y) = 2n\,H_{n-1}(y)$

(6) $$H_n''(y) = 2n\,H_{n-1}'(y) = 2n\left[2(n-1)H_{n-2}(y)\right] = 4n(n-1)H_{n-2}(y)$$

(7) Let $n \to n-1$ in (3):

$$H_n(y) = -2(n-1)H_{n-2}(y) + 2y\,H_{n-1}(y)$$

(8) Substituting from (5) and (6):

$$H_n(y) = -\frac{1}{2n}H_n''(y) + \frac{y}{n}H_n'(y)$$

or $$H_n''(y) - 2y\,H_n'(y) + 2n\,H_n(y) = 0$$

which is identical with $v'' - 2yv' + (\epsilon-1)v = 0$, with $\epsilon = 2n+1$

so that the identification $v \to H_n(y)$ is made and $H_n(y)$ satisfies the differential equation.

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Assignment # 5
Problems 21-25

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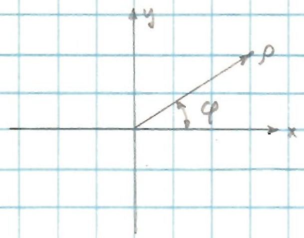
21. (1) We use as the Schroedinger equation:

$$\nabla^2 u + \frac{2m}{\hbar^2}\left[E - V(\rho)\right] u = 0$$

where $V(\rho) = \frac{1}{2} m \omega^2 \rho^2$ for the isotropic harmonic oscillator in two-demensional polar form.



(2) The Laplacian is:

$$\nabla^2 = \frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right) + \frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2}$$

(2) $\therefore$ $\nabla^2 u + \frac{2m}{\hbar^2}\left[E - \frac{1}{2} m \omega^2 \rho^2\right] u = 0$

we now choose appropriate units:

$\hbar = 1$, $2m = 1$, $\omega^2 = 4$

unit of energy: $\frac{\hbar\omega}{2}$; unit of $(\text{length})^2 = \frac{\hbar}{m\omega}$

$\therefore$ $\nabla^2 u + (E - \rho^2) u = 0$

(3) $$\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial u}{\partial\rho}\right) + \frac{1}{\rho^2}\frac{\partial^2 u}{\partial\varphi^2} + (E - \rho^2) u = 0$$

Separate variables: choose $u = P(\rho)\,\Phi(\varphi)$

$$\frac{1}{P\rho}\frac{d}{d\rho}\left(\rho\frac{dP}{d\rho}\right) + \frac{1}{\rho^2\Phi}\frac{d^2\Phi}{d\varphi^2} + (E - \rho^2) = 0$$

or $$\frac{\rho}{P}\frac{d}{d\rho}\left(\rho\frac{dP}{d\rho}\right) + \frac{1}{\Phi}\frac{d^2\Phi}{d\varphi^2} + (E - \rho^2)\rho^2 = 0$$

(4) Now that the equation is separated, we choose:

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

based on traditional arguments.

The solution is: $\Phi = c\, e^{-im\varphi}$

Normalizing: $c^2\int_0^{2\pi} d\varphi = 1$: $\Phi = \frac{1}{\sqrt{2\pi}} e^{\pm im\varphi}$

(6) $G'' - 2r G' + \frac{2}{r} G' + \left(E - 3 - \frac{l(l+1)}{r^2} \right) G = 0$

(7) The indicial equation is:

$$\beta(\beta-1) + 2\beta - l(l+1) = 0 ; \quad \beta^2 + \beta - l(l+1) = 0$$

$$\beta = l, -(l+1)$$

We of course choose $\beta = l$ such that $G \neq \infty$ when $r = 0$.

(8) $\therefore \quad R = r^l e^{-r^2/2} w$ which gives:

$$w'' - 2r w' + \frac{2l}{r} w' + \frac{l(l-1)}{r^2} w - l w - (l+1) w$$

$$+ r^2 w + \frac{2w'}{r} + \frac{2l}{r^2} w - 2w + Ew - r^2 w$$

$$- \frac{l(l+1)}{r^2} w = 0$$

(9) $w'' + \left[\frac{2(l+1)}{r} - 2r \right] w' + \left[E - 3 - 2l \right] w = 0$

(10) Make the substitution $x = r^2$ and proceed as before:

$$4x w'' + \left[2(l+1) + 2 - 4x \right] w' + (E - 3 - 2l) w = 0$$

or $\quad w'' + \left[\frac{l+2}{2x} - 1 \right] w' - \frac{(2l+3-E)}{4x} w = 0$

with $\quad w = {}_1F_1 \left(\frac{2l+3-E}{4} = -n' ; \frac{l+2}{2} ; r^2 \right)$

(11) $\therefore \quad u_{nlm} = N_{lm} P_l^{|m|}(\cos\vartheta) e^{im\varphi} r^l e^{-r^2/2} {}_1F_1 \left(\frac{2l+3-E}{4} ; \frac{l+2}{2} ; r^2 \right)$

(13) $E = 4n' + 2l + 3 \quad ; \quad n' = 0, 1, 2, 3, \ldots$

Define: $\quad n = 2n' + l$

$\therefore \quad l = n, n-2, n-4, n-6, \ldots, 1$ or 0 for n odd or even.

Then $\quad E = 2n + 3 \quad ; \quad E = (n + \frac{3}{2}) \hbar\omega, \quad n = 0, 1, 2, 3, \ldots$

Assignment # 5
Continued

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21. Continued.

(10) Substituting:

$$\sum_{n=0}^{\infty} \Big\{ C_n (\beta+n)(\beta+n-1)\rho^{\beta+n-2} - 2C_n(n+\beta)\rho^{(n+\beta)} + C_n(\beta+n)\rho^{\beta+n-2}$$
$$+ (E-2)C_n \rho^{\beta+n} - m^2 C_n \rho^{\beta+n-2} \Big\} = 0$$

Setting $n=0$:

$$C_0(\beta)(\beta-1)\rho^{\beta-2} - 2C_0\beta\rho^{\beta} + C_0\beta\rho^{\beta-2} + (E-2)C_0\rho^{\beta} - m^2 C_0 \rho^{\beta-2} = 0$$

As this is an identity in ρ, the coefficients of each power must vanish. The indicial equation is formed from the coefficients of $\rho^{\beta-2}$:

$$\beta(\beta-1) + \beta - m^2 = 0 \quad ; \quad \beta^2 = m^2, \quad \beta = \pm m$$

We choose $\beta = |m|$ as the wave functions must be bounded at $\rho = 0$

(11) $$\therefore \quad P = \rho^{|m|} e^{-\rho^2/2} \sum_{n=0}^{\infty} C_n \rho^n$$

call $\sum_{n=0}^{\infty} C_n \cdot \rho^n = v$, then $P = \rho^{|m|} e^{-\rho^2/2} v$

(12) Substituting in (6):

$$\frac{dP}{d\rho} = \rho^{|m|} e^{-\rho^2/2} v' + |m|\rho^{|m|-1} e^{-\rho^2/2} v - \rho^{|m|+1} e^{-\rho^2/2} v$$

$$\frac{d^2P}{d\rho^2} = \rho^{|m|} e^{-\rho^2/2} v'' - 2\rho^{|m|+1} e^{-\rho^2/2} v' + 2|m|\rho^{|m|-1} e^{-\rho^2/2} v'$$
$$+ |m|(|m|-1)\rho^{|m|-2} e^{-\rho^2/2} v - |m|\rho^{|m|} e^{-\rho^2/2} v$$
$$- (|m|+1)\rho^{|m|} e^{-\rho^2/2} v + \rho^{|m|+2} e^{-\rho^2/2} v$$

(13) $$v'' + \frac{v'}{\rho} + \frac{|m|}{\rho^2} v - v - 2\rho v' + \frac{2|m|}{\rho} v' - (|m|+1) v + \rho^2 v$$
$$+ |m|(|m|-1)\frac{v}{\rho^2} - |m| v + E v - \rho^2 v - \frac{m^2}{\rho^2} v = 0$$

(14) $$v'' + \left(\frac{2|m|+1}{\rho} - 2\rho\right) v' + \left(E - 2 - 2|m|\right) v = 0$$ ✓

(15) Make the substitution $x = \rho^2$

$$\therefore \quad \frac{dv}{d\rho} = \frac{dx}{d\rho}\frac{dv}{dx} = 2\rho\frac{dv}{dx} = 2\sqrt{x}\,\frac{dv}{dx}$$

$$\frac{d^2v}{d\rho^2} = \frac{d^2x}{d\rho^2}\frac{dv}{dx} + \left(\frac{dx}{d\rho}\right)^2\frac{d^2v}{dx^2} = 2\frac{dv}{dx} + 4x\frac{d^2v}{dx^2}$$

(16) Putting in (14):

$$4x\frac{d^2v}{dx^2} + (2 + 2|m| + 1 - 4x)\frac{dv}{dx} + (E - 2 - 2|m|)\,v = 0$$

or $$\frac{d^2v}{dx^2} + \left[\frac{2|m|+3}{4x} - 1\right]\frac{dv}{dx} - \frac{\left(\frac{1}{2} + \frac{1}{2}|m| - \frac{E}{4}\right)}{x}\,v = 0$$

(17) Now it was shown in lecture that the differential equation:

$$\frac{d^2v}{dx^2} + \left(\frac{b}{x} - 1\right)\frac{dv}{dx} - \frac{a}{x}\,v = 0$$

has the confluent hypergeometric function as a solution, viz:

$$v = {}_1F_1(a; b; x) = 1 + \frac{a}{1\cdot b}x + \frac{a(a+1)}{1\cdot 2\, b(b+1)}x^2 + \cdots$$

It was also shown in lecture that this function becomes unbounded as $x \to \infty$ so that it must be cut off at some term, say the nth, by putting $a = -n'$ such that $a(a+1)\cdots(a+n') = 0$ when $a = -n'$. There fore:

$$v = {}_1F_1(a = -n'; b; x) \quad \text{where } a = \tfrac{1}{2} + \tfrac{1}{2}|m| - \tfrac{E}{4};\ b = \frac{2|m|+3}{4};$$
$$x = \rho^2$$

(18) $$\therefore \quad P = C\rho^{|m|}e^{-\rho^2/2}\,{}_1F_1\left(\tfrac{1}{2} + \tfrac{1}{2}|m| - \tfrac{E}{4} = -n';\ \frac{2|m|+3}{4};\ \rho^2\right)$$

Now: $E = 4n' + 2 + 2|m| = 2(2n' + |m|) + 2$, $\quad n' = 0, 1, 2, 3, \ldots$
$|m| = 0, 1, 2, 3, \ldots$

Let $n = 2n' + |m|$

then $n = |m|,\ |m| + 2,\ |m| + 4,\ |m| + 6,\ \ldots$

or $|m| = n,\ n-2,\ n-4,\ n-6,\ \ldots,\ 1$ or 0 depending on whether n is odd or even.

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21. Continued:

(19) $\therefore \quad E = 2n+2 = 2(n+1) = (n+1)\hbar\omega$ upon introducing the energy unit.

(20) $$u_{n|m|} = N e^{im\varphi} \rho^{|m|} e^{-\rho^2/2} {}_1F_1\left\{\tfrac{1}{2}(|m|-n);\ \frac{2|m|+3}{4};\ \rho^2\right\}$$

We now calculate the degree of degeneracy associated with each level n. Define the degeneracy as D

n	0	1	2	3	4	5	6	7	8	9
$\|m\|$	0	1	2 0	3 1	4 2 0	5 3 1	6 4 2 0	7 5 3 1	8 6 4 2 0	9 7 5 3 1
$\pm m$	0	x2	+1	x2	+2	x2	+3	x2	+4	x2
D	1	2	3	4	5	6	7	8	9	10

Clearly: $D = n+1$

(21) In the two dimensional rectangular representation, we have from the lecture:

$$u_{n_x n_y} = u_{n_x} v_{n_y} \quad \text{with} \quad n = n_x + n_y\ ; \quad E = (n+1)\hbar\omega$$

n	0	1	2	3	4	5	6	7	8	9
n_x, n_y	00	10	20 11	30 12	40 31 22	50 41 32	60 51 42 33	70 52 61 43	80 71 62 53 44	90 81 72 54 63
double factor	0	x2	+1	x2	+2	x2	+3	x2	+4	x2
D	1	2	3	4	5	6	7	8	9	10

Clearly, $D = n+1$, so the degeneracy is the same in each representation as it physically should be.

Assignment #5
Continued

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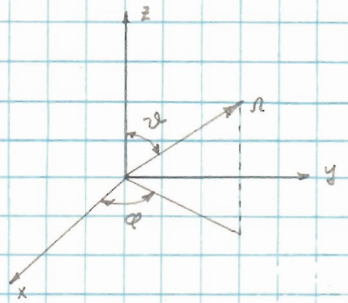
22. (1) We use as the Schroedinger equation:

$$\nabla^2 u + \frac{2m}{\hbar^2}\left[E - V(r)\right] u = 0$$

where $V(r) = \frac{1}{2} m\omega^2 r^2$



(2) The Laplacian is:

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) + \frac{1}{r^2 \sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta \frac{\partial}{\partial\vartheta}\right)$$

$$+ \frac{1}{r^2 \sin^2\vartheta}\frac{\partial}{\partial\varphi^2}$$

(3) We define the same units as in example 21, so:

$$\nabla^2 u + (E - r^2) u = 0$$

or $$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial u}{\partial r}\right) + \frac{1}{r^2 \sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta \frac{\partial u}{\partial\vartheta}\right) + \frac{1}{r^2\sin^2\vartheta}\frac{\partial u}{\partial\varphi^2} + (E - r^2) u = 0$$

(4) We take the solution to be of the form

$u = R(r)\, Y_l^m(\vartheta, \varphi)$ as per lecture and obtain

after separation of variables, as per lecture, the following radial equation:

$$\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} + \left(E - r^2 - \frac{l[l+1]}{r^2}\right) R = 0$$

with $Y_l^m(\vartheta, \varphi) = C_{ml}\, P_l^{|m|}(\cos\vartheta)\, e^{im\varphi}$

$l = 0, 1, 2, 3, \dots$
$m = -l, -l+1, \dots, l-1, l$

These are the well-known spherical harmonics.

(5) At this point, we note that the radial equation above is identical to the radial equation in 21, letting $m^2 \to l(l+1)$, except for the factor 2 on $\frac{dR}{dr}$. We thus carry over results as much as possible:

we have $R = e^{-r^2/2}\, G(r)$, $G(r) = \sum_{n=0}^{\infty} C_n \rho^{\beta+n}$

(5) Since we require our wave functions to be single valued, m must be an integer, for clearly, if it is not, Φ will take on the same value at least twice in the interval $0 \le \varphi \le 2\pi$.

Thus: $m = 0, \pm 1, \pm 2, \pm 3, \ldots$

(6) The P equation is now:

$$\frac{1}{\rho}\frac{d}{d\rho}\left(\rho \frac{dP}{d\rho}\right) + \left(E - \rho^2 - \frac{m^2}{\rho^2}\right)P = 0$$

or $$\frac{d^2P}{d\rho^2} + \frac{1}{\rho}\frac{dP}{d\rho} + \left(E - \rho^2 - \frac{m^2}{\rho^2}\right)P = 0 \quad ; \quad 0 \le \rho < \infty$$

(7) Take the asymptotic solution for large ρ:

$$\frac{d^2P}{d\rho^2} - \rho^2 P = 0$$

Try $P = e^{\pm \rho^2/2}$, $\dfrac{d^2 e^{\pm\rho^2/2}}{d\rho^2} = \dfrac{d}{d\rho}\left[\pm \rho e^{\pm \rho^2/2}\right]$

$= \rho^2 e^{\pm\rho^2/2} \pm e^{\pm\rho^2/2} \rightarrow \rho^2 e^{\pm\rho^2/2}$ for even larger ρ
so it looks good for an asymptotic solution.
We choose $e^{-\rho^2/2}$ as the other $\to \infty$ as $\rho \to \infty$ as is not allowed.

(8) Resubstituting in (6); setting $P = e^{-\rho^2/2} L(\rho)$

$$\frac{dP}{d\rho} = e^{-\rho^2/2} L'(\rho) - \rho e^{-\rho^2/2} L(\rho)$$

$$\frac{d^2P}{d\rho} = e^{-\rho^2/2} L''(\rho) - 2\rho e^{-\rho^2/2} L'(\rho) - e^{-\rho^2/2} L(\rho) + \rho^2 e^{-\rho^2/2} L(\rho)$$

$$\therefore \quad L''(\rho) - 2\rho L'(\rho) + \frac{1}{\rho} L'(\rho) + \left(E - 2 - \frac{m^2}{\rho}\right) L(\rho) = 0$$

(9) We note that the coefficients of L' and L which are the worst singularities are $\frac{1}{\rho}$ and $\frac{1}{\rho^2}$ respectively. Thus we can apply the Frobenius method of series solution and write for the solution:

$$L(\rho) = \sum_{n=0}^{\infty} C_n \rho^{s+n}$$

Assignment #5
Continued

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22 Continued:

(14) Now: $l = 0, 1, 2, 3, \ldots$

with $m = -l, -l+1, \ldots, 0, \ldots l-1, l$

Thus for every l, there are $2l+1$ values of m.

We now can sum over the possible values of l and thus get the total number of independent wave functions ~~them~~ for each n and thus the degree of degeneracy

(15) For n even; we have:

$$D = \sum_{\substack{l=0\\ \text{even}}}^{n} (2l+1) = 1 + 5 + 9 + 13 + 17 + 21 + \cdots$$

$$= \sum_{p=0}^{n/2} (4p+1) = 4\sum_{p=0}^{n/2} p + \frac{n}{2} + 1$$

Using the idendity: $\sum n = \frac{n(n+1)}{2}$

$$\therefore \quad D = \frac{4 \cdot \frac{n}{2}\left(\frac{n}{2}+1\right)}{2} + \frac{n}{2} + 1 = \frac{n^2 + 3n + 2}{2}$$

$$= \frac{(n+1)(n+2)}{2}$$ ✓ which is equal to that found in lecture using rectangular co-ordinates

(16) For n odd, we have

$$D = \sum_{\substack{l=1\\ \text{odd}}}^{n} (2l+1) = 3 + 7 + 11 + 15 + 19 + 23 + \cdots$$

$$= \sum_{p=1}^{\frac{n+1}{2}} (4p-1) = 4\sum_{p=1}^{\frac{n+1}{2}} - \left(\frac{n+1}{2}\right)$$

$$= \frac{4\left(\frac{n+1}{2}\right)\left(\frac{n+1}{2}+1\right)}{2} - \left(\frac{n+1}{2}\right) = \left(\frac{n+1}{2}\right)\left(2\left[\frac{n+1}{2}+1\right] - 1\right)$$

$$= \frac{(n+1)(n+2)}{2}$$ ✓, which is equal to that found in lecture using rectangular co-ordinates.

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Continued

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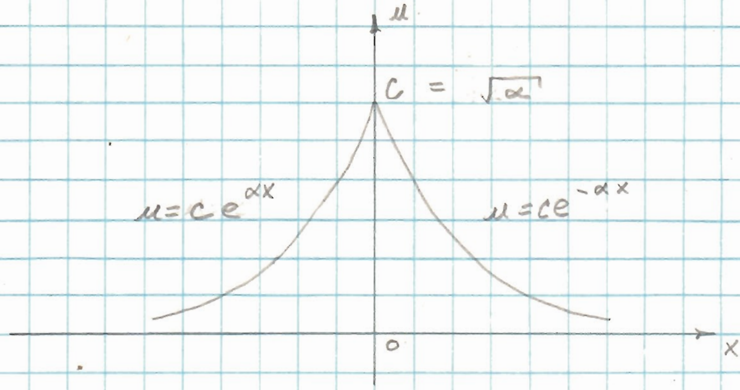
23. Trial Function: $u = Ce^{-\alpha|x|}$

a.



b. (1) $\int_{-\infty}^{\infty} u^2 dx = C^2 \int_{-\infty}^{\infty} e^{-2\alpha|x|} dx = 2C^2 \int_0^{\infty} e^{-2\alpha x} dx$ (since $e^{-2\alpha|x|}$ even)

$= C^2 \cdot -\frac{1}{\alpha} e^{-2\alpha x}\Big]_0^{\infty} = C^2 \cdot \frac{1}{\alpha} = 1$

(2) $\therefore \quad C = \sqrt{\alpha}\,; \quad u = \sqrt{\alpha}\, e^{-\alpha|x|}$

c. (1) Now $H = T + V\,; \quad Tu = \frac{-\hbar^2}{2m}\frac{d^2u}{dx^2}\,; \quad V = \frac{1}{2} m \omega^2 x^2$

It was show in lecture that the second derivative of a function with a discontinuous first derivative is:

$$\frac{d^2u}{dx^2} = u'' + \delta(x - x_0)\left[u'(x_0^+) - u'(x_0^-)\right]$$

(2) $u' = -\alpha\sqrt{\alpha}\, e^{-\alpha|x|}\,; \quad u'' = \alpha^2\sqrt{\alpha}\, e^{-\alpha|x|}$

$u'(0^+) = -\alpha\sqrt{\alpha}\,; \quad u'(0^-) = \alpha\sqrt{\alpha}$

(3) $Tu = -\frac{\hbar^2}{2m}\alpha^2\sqrt{\alpha}\, e^{-\alpha|x|} + \frac{\hbar^2}{m}\alpha\sqrt{\alpha}\,\delta(x)$

d. (1) $\int_{-\infty}^{\infty} u\,Tu\,dx = -\frac{\hbar^2\alpha^3}{2m}\int_{-\infty}^{\infty} e^{-2\alpha|x|}dx + \frac{\hbar^2\alpha^2}{m}\int_{-\infty}^{\infty} e^{-\alpha|x|}\delta(x)\,dx$

$= \frac{-\hbar^2\alpha^3}{m}\int_0^{\infty} e^{-2\alpha x} dx + \frac{\hbar^2\alpha^2}{m}$

d. (2) $\int_{-\infty}^{\infty} u T u \, dx = -\frac{\hbar^2 \alpha^2}{2m} + \frac{\hbar^2 \alpha^2}{m} = \frac{\hbar^2 \alpha^2}{2m}$

(3) $\int_{-\infty}^{\infty} u V u \, dx = \frac{1}{2} m \omega^2 \cdot 2\alpha \int_{-\infty}^{\infty} x^2 e^{-2\alpha|x|} dx$

$= 2 m \omega^2 \alpha \int_0^{\infty} x^2 e^{-2\alpha x} dx = 2 m \omega^2 \alpha \cdot \frac{2}{(2\alpha)^3}$ (by tables)

$= \frac{m \omega^2}{4 \alpha^2}$

(4) $\therefore \int_{-\infty}^{\infty} u H u \, dx = \bar{H} = \frac{m \omega^2}{4 \alpha^2} + \frac{\hbar^2 \alpha^2}{2m}$ ✓

e. (1) $\frac{d \bar{H}}{d\alpha} = -\frac{m \omega^2}{2 \alpha^3} + \frac{\hbar^2 \alpha}{m} = 0$

$\frac{m \omega^2}{2 \alpha^3} = \frac{\hbar^2 \alpha}{m}$; $\alpha^4 = \frac{m^2 \omega^2}{2 \hbar^2}$

$\therefore \alpha = \sqrt{\frac{m \omega}{\sqrt{2} \hbar}}$

(2) $\bar{H}_{min} = \frac{\sqrt{2} \hbar}{m\omega} \cdot \frac{m \omega^2}{4} + \frac{\hbar^2}{2m} \cdot \frac{m\omega}{\sqrt{2} \hbar} = \frac{\sqrt{2}}{2} \hbar \omega = .707 \hbar \omega$ ✓

(3) $E_{0\,est} = \bar{H}_{min} = .707 \hbar \omega$, which is about 42% greater than the true value $\frac{1}{2} \hbar\omega$. Not a very good choice.

f. (1) Consider $\bar{H} = \int u H u \, dx$, with $u = \sum_{n=0}^{\infty} a_n u_n$ where u_n are the true normalized eigenfunctions and $\sum_{n=0}^{\infty} |a_n|^2 = 1$

(2) Then $\bar{H} = \sum_n \sum_{n'} a_n a_{n'} \underbrace{\int u_{n'} H u_n \, dx}_{E_n \delta_{nn'}} = \sum_n a_n^2 E_n$

(3) However: $\bar{H} - E_0 = \sum_n a_n^2 (E_n - E_0) \geq \sum_{n=1}^{\infty} a_n^2 (E_1 - E_0)$

(4) $\therefore \sum_{n=1}^{\infty} a_n^2 \leq \frac{\bar{H} - E_0}{E_1 - E_0}$. In this case E_1 must be taken as E_2 because the eigenvalue E_1 corresponds to the eigenfunction u_1 which is odd unlike the variation function which is even. Also $a_1 = 0$ for the same reason, and so are all all odd numbered coefficients.

(5) $\sum_{n=1}^{\infty} a_n^2 \leq \frac{.707 \hbar \omega - \frac{1}{2} \hbar \omega}{\frac{5}{2} \hbar \omega - \frac{1}{2} \hbar \omega}$

$= .1035$ ✓

Assignment #5
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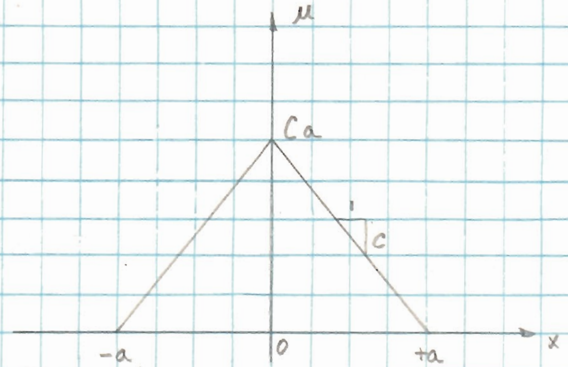
23. Continued

Trial Function: $u = c(a - |x|),\ |x| < a\ ;\ u = 0,\ |x| > a$

a.



b. (1) $\int_{-\infty}^{\infty} u^2\,dx = c^2 \int_{-a}^{a} (a^2 - 2a|x| + x^2)\,dx = 2c^2 \int_0^a (a^2 - 2ax + x^2)\,dx$

$= 2c^2 \int_0^a (a-x)^2\,dx = -\frac{2c^2}{3}\,(a-x)^3\Big]_0^a = \frac{2c^2a^3}{3} = 1$

(2) $\therefore\quad c = \sqrt{\frac{3}{2a^3}}\ ;\quad u = \sqrt{\frac{3}{2a^3}}\,(a - |x|),\ |x| < a;\ 0$ otherwise

c. (1) $Tu = -\frac{\hbar^2}{2m}\,\delta(x) \cdot \sqrt{\frac{3}{2a^3}} \cdot [-1-1] = \frac{\hbar^2}{m}\sqrt{\frac{3}{2a^3}}\,\delta(x)$

X Discontinuities also at $x = \pm a$!

d. (1) $\int_{-\infty}^{\infty} u\,T u\,dx = \frac{\hbar^2}{m}\sqrt{\frac{3}{2a^3}} \int_{-a}^{a} \delta(x) \cdot \sqrt{\frac{3}{2a^3}}\,(a - |x|)\,dx$

$= \frac{3\hbar^2}{2ma^2}$

(2) $\int_{-\infty}^{\infty} u\,V\,u\,dx = \frac{1}{2}m\omega^2 \cdot \frac{3}{2a^3} \cdot 2\int_0^a x^2 (a-x)^2\,dx$

(3) $\int_0^a (a^2x^2 - 2ax^3 + x^4)\,dx = \frac{a^2x^3}{3} - \frac{ax^4}{2} + \frac{x^5}{5}\Big]_0^a$

$= \frac{a^5}{3} - \frac{a^5}{2} + \frac{a^5}{5} = \frac{10a^5 - 15a^5 + 6a^5}{30} = \frac{a^5}{30}$

d. (4) $\overline{V} = m\omega^2 \cdot \frac{3}{2a^3} \cdot \frac{a^5}{30} = \frac{m\omega^2 a^2}{20}$

(5) $\therefore \quad \overline{H} = \frac{3\hbar^2}{2ma^2} + \frac{m\omega^2 a^2}{20}$

e. (1) $\frac{d\overline{H}}{da} = \frac{-6\hbar^2}{2ma^3} + \frac{m\omega^2 a}{10} = 0 \quad ; \quad \frac{3\hbar^2}{ma^3} = \frac{m\omega^2 a}{10}$

(2) $a^4 = \frac{30\hbar^2}{m^2\omega^2} \quad ; \quad a^2 = \frac{\sqrt{30}\,\hbar}{m\omega}$

(3) $\overline{H}_{min} = \frac{3\hbar^2}{2m} \cdot \frac{m\omega}{\sqrt{30}\,\hbar} + \frac{m\omega^2}{20} \cdot \frac{\sqrt{30}\,\hbar}{m\omega}$

$$= \left[\frac{3}{2\sqrt{30}} + \frac{\sqrt{30}}{20} \right] \hbar\omega = \left[\frac{120}{40\sqrt{30}} \right] \hbar\omega = \frac{3}{\sqrt{30}} \hbar\omega$$

(4) $\therefore \quad E_{0_{est}} = \overline{H}_{min} = \frac{\sqrt{30}}{10} \hbar\omega = .548\,\hbar\omega$

(5) $E_{0_{est}} = \frac{\sqrt{30}}{5} E_0 = 1.096\,E_0 \quad ; \quad \frac{E_{0_{est}} - E_0}{E_0} \cong 10\%$

f. (1) $\sum_{n=1}^{\infty} a_n^2 \leq \frac{\overline{H} - E_0}{E_1 - E_0}$. Again E_2 must used as u_1 is odd and $a_1 = 0$ along with other odd numbered coefficients.

(2) $\sum_{n=1}^{\infty} a_n^2 \leq \frac{.048}{2} = .024$

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24. (1) $$\frac{d^2 v}{dx^2} + \left[E^{(0)} - x^2 \right] v = 0$$

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with eigenvalues $E_n^{(0)} = 2n+1$

and matrix elements:

$$\langle m|x|n\rangle = \sqrt{\frac{m}{2}}\, \delta_{m,n+1} + \sqrt{\frac{n}{2}}\, \delta_{m+1,n}$$

(2) Consider:

$$\frac{d^2 u}{dx^2} + (E - x^2 - \alpha x)\, u = 0$$

As this is a one dimensional stationary state problem, the energy levels are non-degenerate as to every eigenvalue there is only eigenfunction.

(3) We consider the Hamiltonian as: $H = -\frac{d^2}{dx^2} + x^2 + \alpha x$

we $V = \alpha x$ as the perturbing potential. Taking the perturbed wave functions expanded as a series of the unperturbed wave functions, we have:

$$u = \sum_n c_n v_n$$

It was shown in lecture that the first and second order corrections in non-degenerate perturbation theory are given by:

$$E_n^{(1)} = \langle n|V|n\rangle$$

$$E_n^{(2)} = \sum_{m \neq n} \frac{\langle n|V|m\rangle\langle m|V|n\rangle}{E_n^{(0)} - E_m^{(0)}}$$

(4) Applying these equations to our problem:

$$E_n^{(1)} = \alpha \langle n|x|n\rangle = 0$$

(5) $$E_n^{(2)} = \alpha^2 \sum_{m \neq n} \frac{\langle n|x|m\rangle\langle m|x|n\rangle}{E_n^{(0)} - E_m^{(0)}}$$

$$= \alpha^2 \sum_{m\neq n} \frac{\left[\sqrt{\frac{n}{2}}\,\delta_{n,m+1} + \sqrt{\frac{m}{2}}\,\delta_{n+1,m}\right]^2}{E_n^{(0)} - E_m^{(0)}}$$

$$= \alpha^2 \left\{ \frac{\frac{n}{2}}{E_n^{(0)} - E_{n-1}^{(0)}} + \frac{\frac{n+1}{2}}{E_n^{(0)} - E_{n+1}^{(0)}} \right\}$$

$$= \frac{\alpha^2}{2}\left\{ \frac{n}{2n+1-2n+1} + \frac{n+1}{2n+1-2n-3} \right\} = -\frac{\alpha^2}{4}$$

(6) $\therefore \quad E_n = 2n+1 - \frac{\alpha^2}{4}$

(7) $\frac{d^2u}{dx^2} + (E - x^2 - \alpha x)u = 0$:

Consider the substitution $\xi = x + \frac{\alpha}{2}$:

$$x^2 + \alpha x = x(x+\alpha) = \left(\xi - \frac{\alpha}{2}\right)\left(\xi + \frac{\alpha}{2}\right) = \xi^2 - \frac{\alpha^2}{4}$$

(8) $$\frac{du}{dx} = \frac{d\xi}{dx}\frac{du}{d\xi} \; ; \quad \frac{d^2u}{dx^2} = \frac{d^2\xi}{dx^2}\frac{du}{d\xi} + \frac{d\xi}{dx}\frac{d}{dx}\left(\frac{du}{d\xi}\right)$$

$$= \frac{d^2\xi}{dx^2}\frac{du}{d\xi} + \left(\frac{d\xi}{dx}\right)^2 \frac{d^2u}{d\xi^2}$$

Since $\frac{d\xi}{dx} = 1$, $\frac{d^2\xi}{dx^2} = 0$; $\quad \frac{d^2u}{dx^2} = \frac{d^2u}{d\xi^2}$

(9) $\therefore \quad \frac{d^2u}{d\xi^2} + \left(E - \xi^2 + \frac{\alpha^2}{4}\right)u = 0$

(10) Define: $\lambda = E_n + \frac{\alpha^2}{4}$: $\quad \frac{d^2u}{d\xi^2} + (\lambda - \xi^2)u = 0$

However, this is the idendical eigenvalue problem as the harmonic oscillator in equation (1) and thus has eigenvalues, transferring results:

$$\lambda_n = 2n+1 = E_n + \frac{\alpha^2}{4}$$

or $E_n = 2n+1 - \frac{\alpha^2}{4}$

Therefore, the second order perturbation treatment gives precisely the correct result.

The eigenfunctions are the Hermite polynomials $H(\xi)$ times $e^{-\xi^2/2}$ and normalized.

Assignment #5
Continued

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25. (1) $$v_n = \frac{H_n(x)\, e^{-x^2/2}}{\sqrt{2^n n! \sqrt{\pi}}}$$

Now, it was shown in class that the eigenfunctions of the perturbed problem can be expanded in terms of the eigenfunctions of the unperturbed problem along the lines of the usual expansion of a function in a series of orthonormal functions.

$$u_k = \sum_n v_n S_{nk}$$

where the S_{nk} can be considered expanded in terms of the perturbation tag λ:

$$S_{nk} = \delta_{nk} + \lambda C_{nk}^{(1)} + \lambda^2 C_{nk}^{(2)} + \cdots$$

and it was shown that the first order term in the coefficient is given by:

$$C_{nk}^{(1)} = \frac{\langle n | V | k \rangle}{E_k^{(0)} - E_n^{(0)}}$$

(2) We now use these results here:

$$C_{nk}^{(1)} = \frac{\alpha \langle n | x | k \rangle}{E_k^{(0)} - E_n^{(0)}} = \frac{\alpha \left[\sqrt{\frac{n}{2}}\, \delta_{n,k+1} + \sqrt{\frac{k}{2}}\, \delta_{n+1,k} \right]}{E_k^{(0)} - E_n^{(0)}}$$

(3) Letting $\lambda \to 1$ above:

$$u_k = \sum_n \left\{ \delta_{nk} + \alpha \frac{\left[\sqrt{\frac{n}{2}}\, \delta_{n,k+1} + \sqrt{\frac{k}{2}}\, \delta_{n+1,k} \right]}{E_k^{(0)} - E_n^{(0)}} \right\} v_n$$

$$= v_k + \alpha \left\{ \frac{\sqrt{\frac{k+1}{2}}}{E_k^{(0)} - E_{k+1}^{(0)}} \right\} v_{k+1} + \alpha \left\{ \frac{\sqrt{\frac{k}{2}}}{E_k^{(0)} - E_{k-1}^{(0)}} \right\} v_{k-1}$$

$$= v_k - \frac{\alpha}{2} \sqrt{\frac{k+1}{2}}\, v_{k+1} + \frac{\alpha}{2} \sqrt{\frac{k}{2}}\, v_{k-1}$$

(4) $$u_n = v_n - \frac{\alpha}{2} \sqrt{\frac{n+1}{2}}\, v_{n+1} + \frac{\alpha}{2} \sqrt{\frac{n}{2}}\, v_{n-1} + \cdots$$

(5) Now the exact eigenfunctions as shown in problem 24 are

$$u_n(\xi) = u_n\left(x + \frac{\alpha}{2}\right) = \frac{H_n\left(x + \frac{\alpha}{2}\right) e^{-\left(x + \frac{\alpha}{2}\right)^2/2}}{\sqrt{2^n\, n!\, \sqrt{\pi}}}$$

(6) Now, expanding in a Taylor series in $\frac{\alpha}{2}$:

$$u_n(\xi) = u_n\left(x + \frac{\alpha}{2}\right) = u_n(x) + \frac{\alpha}{2} u_n'(x) + \cdots$$

(7) Now: $$u_n'(\xi) = \frac{H_n'(\xi)\, e^{-\xi^2/2}}{\sqrt{2^n\, n!\, \sqrt{\pi}}} - \frac{\xi\, H_n(\xi)\, e^{-\xi^2/2}}{\sqrt{2^n\, n!\, \sqrt{\pi}}}$$

$$\therefore u_n(\xi) = \frac{e^{-x^2/2}}{\sqrt{2^n\, n!\, \sqrt{\pi}}} \left[H_n(x) + H_n'(x)\frac{\alpha}{2} - x\, H_n(x)\frac{\alpha}{2} + \cdots \right]$$

(8) Now $u_n(\xi) = u_n(x)$. We compare and equate terms in powers of $\frac{\alpha}{2}$ in (7) and (4):

This $u_n(x)$ that appears in equation (4) is not the same function form as $u_n\left(x + \frac{\alpha}{2}\right)$. The choice of notation was duplicated unfortunately. However, the eigenfunctions themselves are identical.

(9) $$\frac{e^{-x^2/2}}{\sqrt{2^n\, n!\, \sqrt{\pi}}} \left[H_n'(x) - x\, H_n(x) \right] = e^{-x^2/2} \left[-\sqrt{\frac{n+1}{2}} \cdot \frac{H_{n+1}(x)}{\sqrt{2^{n+1}(n+1)!\, \sqrt{\pi}}} + \sqrt{\frac{n}{2}} \cdot \frac{H_{n-1}}{\sqrt{2^{n-1}(n-1)!\, \sqrt{\pi}}} \right]$$

or $$H_n'(x) - x\, H_n(x) = n\, H_{n-1}(x) - \frac{1}{2} H_{n+1}(x)$$

which is a recursion relation, although not the simplest. It is essentially composed of two other recursion relations which are

$$H_{n+1}(x) - 2x\, H_n(x) + 2n\, H_{n-1}(x) = 0$$

$$H_n'(x) = 2n\, H_{n-1}(x)$$

✓

It is not in the scope of the problem to derive these two from the above equation (9).

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Assignment #6
Problems 26 - 30

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26. (1) We carry over the following equations for the 2-D harmonic oscillator from lecture:

$$\left[-\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} + x^2 + y^2 \right] u = E u$$

$$\langle n|x|m\rangle = \langle n|y|m\rangle = \sqrt{\frac{n}{2}}\,\delta_{m,n-1} + \sqrt{\frac{n+1}{2}}\,\delta_{m,n+1}$$

The unperturbed wave functions are:

$$v_{nm} = v_n(x)\, v_m(y)$$

with $E^{(0)} = 2(n+m+1)$

$E^{(0)}$	:	2	4	6
v_{nm}	:	v_{00}	v_{10}	v_{20}
			v_{01}	v_{02}
				v_{11}

(2) Now consider the oscillator to be perturbed by: $V = axy$. The lecture notes give for first order degenerate perturbation theory:

$$\sum_{\beta=1}^{g_k} \left\{ \langle \alpha k|V|k\beta\rangle - E^{(1)}_{k,\gamma}\,\delta_{\alpha\beta} \right\} S_{\beta\gamma}(k) = 0 \quad ; \quad \alpha = 1, 2, 3, \ldots$$

in which $k = m+n$ denotes the state under consideration.

Now $\langle \alpha k|V|k\beta\rangle = a\,\langle \alpha k|xy|k\beta\rangle$

Define: $|k\beta\rangle = |nm\rangle$ subject to $n+m=k$

$\langle \alpha k| = \langle pq|$ subject to $p+q=k$

Then: $\langle \alpha k|V|k\beta\rangle = a\,\langle pq|xy|nm\rangle$

$$= a\iint v_p^*(x)\, v_q^*(y)\; x\, y\; v_n(x)\, v_m(y)\, dx\, dy$$

$$= a\int v_p^*(x)\, x\, v_n(x)\, dx \cdot \int v_q^*(y)\, y\, v_m(y)\, dy$$

$$= a\,\langle p|x|n\rangle\langle q|y|m\rangle = a\,\langle p|x|n\rangle\langle q|x|m\rangle$$

(3) For our problem, $k = 2$, $g_k = 3$, $E^{(0)} = 6$

and the secular equation becomes:

$$\begin{vmatrix} \langle 1|V|1\rangle - E^{(1)} & \langle 1|V|2\rangle & \langle 1|V|3\rangle \\ \langle 2|V|1\rangle & \langle 2|V|2\rangle - E^{(1)} & \langle 2|V|3\rangle \\ \langle 3|V|1\rangle & \langle 3|V|2\rangle & \langle 3|V|3\rangle - E^{(1)} \end{vmatrix} \begin{vmatrix} S_1 \\ S_2 \\ S_3 \end{vmatrix} = 0$$

Now, we make the following assignments in accordance with the defined notation:

$|\beta\rangle = |nm\rangle$

$\langle\alpha| = \langle pq|$

$$\left.\begin{array}{l} 1 \rightarrow 02 \\ 2 \rightarrow 20 \\ 3 \rightarrow 11 \end{array}\right\} \text{ all satisfying } n+m = p+q = k$$

$\langle 1|V|1\rangle = \langle 2|V|2\rangle = \langle 3|V|3\rangle = a\langle 0|x|0\rangle\langle 2|x|2\rangle = 0$

$\langle 1|V|2\rangle = \langle 2|V|1\rangle = a\langle 0|x|2\rangle\langle 2|x|0\rangle = 0$

$\langle 1|V|3\rangle = \langle 3|V|1\rangle = a\langle 0|x|1\rangle\langle 2|x|1\rangle = \frac{a}{2}\sqrt{2}$

$\langle 2|V|3\rangle = \langle 3|V|2\rangle = a\langle 2|x|1\rangle\langle 0|x|1\rangle = \frac{a}{2}\sqrt{2}$

Thus:

(4) $$\begin{vmatrix} -E^{(1)} & 0 & \frac{a}{2}\sqrt{2} \\ 0 & -E^{(1)} & \frac{a}{2}\sqrt{2} \\ \frac{a}{2}\sqrt{2} & \frac{a}{2}\sqrt{2} & -E^{(1)} \end{vmatrix} = 0$$

$$-E^{(1)} \begin{vmatrix} -E^{(1)} & \frac{a}{2}\sqrt{2} \\ \frac{a}{2}\sqrt{2} & -E^{(1)} \end{vmatrix} + \frac{a}{2}\sqrt{2} \begin{vmatrix} 0 & \frac{a}{2}\sqrt{2} \\ -E^{(1)} & \frac{a}{2}\sqrt{2} \end{vmatrix}$$

$$= -E^{(1)}\left(E^{(1)2} - \frac{a^2}{2}\right) + \frac{a^2}{2}E^{(1)} = 0$$

or $-E^{(1)2} + a^2 = 0$, $E^{(1)} = +a, -a$

or $E^{(1)} = 0, +a, -a$

Thus the first order perturbation has completely removed the degeneracy and we can treat the perturbation in the second order by non-degenerate methods after forming the correct wave functions.

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Problem 26
Continued

(5) The secular equation gives the following homogeneous equations:

$$-E^{(1)} S_1 + \frac{a}{2}\sqrt{2}\, S_3 = 0$$

$$-E^{(1)} S_2 + \frac{a}{2}\sqrt{2}\, S_3 = 0$$

$$\frac{a}{2}\sqrt{2}\, S_1 + \frac{a}{2}\sqrt{2}\, S_2 - E^{(1)} S_3 = 0$$

(6) From the lecture, the right linear combination of wave functions that will assign only one wave function to each of the new energy levels is given by:

$$w_{k\gamma} = \sum_{\beta} v_{k,\beta}\, S_{\beta\gamma}$$

Now $k = m + n = 2$ which denotes the unperturbed level we are working with and will now be omitted. γ indexes the roots of the secular determinant and has the values 1, 2, 3 which we now define:

$$E^{(1)}_{2,1} = 0 = E^{(1)}_1$$

$$E^{(1)}_{2,2} = +a = E^{(1)}_2$$

$$E^{(1)}_{2,3} = -a = E^{(1)}_3$$

(7) $E^{(1)}_1 = 0$:

$$\frac{a}{2}\sqrt{2}\, S_{3,1} = 0$$

$$\frac{a}{2}\sqrt{2}\, S_{1,1} + \frac{a}{2}\sqrt{2}\, S_{2,1} = 0$$

$$S_{3,1} = 0 \qquad S_{1,1} = -S_{2,1}$$

$$w_1 = \eta\,(v_1 - v_2) = \frac{1}{\sqrt{2}}(v_1 - v_2)$$

(8) $E^{(1)}_2 = +a$:

$$-a\, S_{1,2} + \frac{a}{2}\sqrt{2}\, S_{3,2} = 0$$

$$-a\, S_{2,2} + \frac{a}{2}\sqrt{2}\, S_{3,2} = 0$$

$$\frac{a}{2}\sqrt{2}\, S_{1,2} + \frac{a}{2}\sqrt{2}\, S_{2,2} - a\, S_{3,2} = 0$$

$$S_{1,2} = S_{2,2} \qquad S_{3,2} = \sqrt{2}\, S_{1,2}$$

$$w_2 = \eta\,(v_1 + v_2 + \sqrt{2}\, v_3) = \frac{1}{2}(v_1 + v_2 + \sqrt{2}\, v_3)$$

(9) $E_3^{(1)} = -a$: $S_{1,3} = S_{2,3}$, $S_{3,3} = -\sqrt{2}\, S_{1,3}$

$$w_3 = \frac{1}{2}\left(v_1 + v_2 - \sqrt{2}\, v_3\right)$$

(10) We now take from the lecture, the equation for the non-degenerate second order perturbation correction:

$$E_\gamma^{(2)} = \sum_{\xi \neq \gamma} \frac{\langle \gamma | V | \xi \rangle \langle \xi | V | \gamma \rangle}{E_\gamma^{(0)} - E_\xi^{(0)}} \quad ; \quad \gamma = 1, 2, 3$$

γ indexes the split levels; ξ indexes all other eigenfunctions whose eigenvalues do not equal $E_{n,\gamma}^{(0)}$.

As we have properly chosen the correct wave functions, and as the degeneracy has been completely removed in the first order, we can use ordinary second order perturbation methods and find first the correction to $E_1^{(2)}$.

(11) $$\therefore \quad E_1^{(2)} = \sum_{\xi \neq 1} \frac{\left| \langle 1 | V | \xi \rangle \right|^2}{6 - E_\xi^{(0)}}$$

(12) $$\langle 1 | V | \xi \rangle = a \iint w_1^* \, xy \, v_\xi \, dx\, dy$$

$$= \frac{a}{\sqrt{2}} \iint v_1^* \, xy \, v_\xi \, dx\, dy - \frac{a}{\sqrt{2}} \iint v_2^* \, xy \, v_\xi \, dx\, dy$$

$$= \frac{a}{\sqrt{2}} \iint v_0^*(x)\, v_2^*(y)\; xy\; v_r(x)\, v_s(y)\, dx\, dy$$

$$- \frac{a}{\sqrt{2}} \iint v_2^*(x)\, v_0^*(y)\; xy\; v_r(x)\, v_s(y)\, dx\, dy$$

$$= \frac{a}{\sqrt{2}} \int v_0^*(x)\, x\, v_r(x)\, dx \cdot \int v_2^*(y)\, y\, v_s(y)\, dy$$

$$- \frac{a}{\sqrt{2}} \int v_2^*(x)\, x\, v_r(x)\, dx \cdot \int v_0^*(y)\, y\, v_s(y)\, dy$$

$$= \frac{a}{\sqrt{2}} \left[\langle 0 | x | r \rangle \langle 2 | x | s \rangle - \langle 2 | x | r \rangle \langle 0 | x | s \rangle \right]$$

Now, for non-vanishing matrix elements for the harmonic oscillator, the indices must differ by unity. Also, $r + s \neq 2$. The following choice is satisfactory:

$$r, s = 1, 3 \; ; \; 3, 1 \quad : \quad r + s = 4 = \xi \quad , \quad E_4^{(0)} = 10$$

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Problem 26
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(13) $\therefore \quad E_1^{(2)} = \frac{|\langle 0|x|1\rangle\langle 2|x|3\rangle|^2 a^2}{6 - 10}$

$= \frac{|\sqrt{\frac{1}{2}}\sqrt{\frac{3}{2}}|^2 a^2}{-4} = -\frac{3a^2}{16}$

(14) We now proceed to calculate $E_2^{(2)}$:

$$E_2^{(2)} = \sum_{\xi \neq 2} \frac{|\langle 2|V|\xi\rangle|^2}{6 - E_\xi^{(0)}}$$

(15) $\langle 2|V|\xi\rangle = a \iint w_2^* \, x y \, v_\xi \, dx\, dy$

$= \frac{a}{2}\iint v_1^* \, xy \, v_\xi \, dx\, dy + \frac{a}{2}\iint v_2^* \, xy \, v_\xi \, dx\, dy$

$+ \frac{a\sqrt{2}}{2}\iint v_3^* \, xy \, v_\xi \, dx\, dy$

$= \frac{a}{2}\left[\langle 0|x|r\rangle\langle 2|x|s\rangle + \langle 2|x|r\rangle\langle 0|x|s\rangle\right]$

$+ \frac{a\sqrt{2}}{2}\langle 1|x|r\rangle\langle 1|x|s\rangle$

(16) The matrix elements of the harmonic oscillator will click with:

$r, s = 1,3;\ 3,1;\ 0,0;\ 2,2$

(17) Then: $E_2^{(2)} = \frac{|\langle 0|x|1\rangle\langle 2|x|3\rangle|^2}{6 - 10} \cdot \frac{a^2}{2}$

$+ \frac{\frac{a^2}{2}|\langle 1|x|0\rangle\langle 1|x|0\rangle|^2}{6 - 2} + \frac{\frac{a^2}{2}|\langle 1|x|2\rangle\langle 1|x|2\rangle|^2}{6 - 10}$

$= -\frac{3a^2}{32} + \frac{a^2}{2}\cdot\frac{1}{4}\cdot\frac{1}{4} - \frac{a^2}{2}\cdot\frac{1}{4}\cdot 1$

$= -\frac{3a^2}{32} + \frac{a^2}{32} - \frac{4a^2}{32} = -\frac{3a^2}{16}$

(18) For $E_3^{(2)}$, we have $\omega_3 = \frac{1}{2}(v_1 + v_2 - \sqrt{2}\, v_3)$

so that only the sign of $\sqrt{2}$ has changed which becomes squared giving the same result as $E_2^{(2)}$.

$$\therefore \quad E_3^{(2)} = -\frac{3a^2}{16}$$

(19) Thus we have for the third energy level ($k = 2$) in the second order correction:

$$E = 6 - \frac{3a^2}{16}$$

$$E = 6 + a - \frac{3a^2}{16}$$

$$E = 6 - a - \frac{3a^2}{16}$$

(20) It was shown in lecture that the precise solution was of the form:

$$E = \sqrt{1 + \frac{a}{2}}\,(2n_\xi + 1) + \sqrt{1 - \frac{a}{2}}\,(2n_\eta + 1)$$

with
$$\sqrt{1 + \frac{a}{2}} = 1 + \frac{a}{4} - \frac{a^2}{32} + \cdots$$
$$\sqrt{1 - \frac{a}{2}} = 1 - \frac{a}{4} - \frac{a^2}{32} - \cdots$$

(21) Then, to the degree of a^2:

$n_\xi = 2$, $n_\eta = 0$: $\quad E = 6 + a - \frac{3a^2}{16}$

$n_\xi = 0$, $n_\eta = 2$: $\quad E = 6 - a - \frac{3a^2}{16}$

$n_\xi = 1$, $n_\eta = 1$: $\quad E = 6 - \frac{3a^2}{16}$

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Thus the perturbation treatment to the second order checks with the precise result to this same degree.

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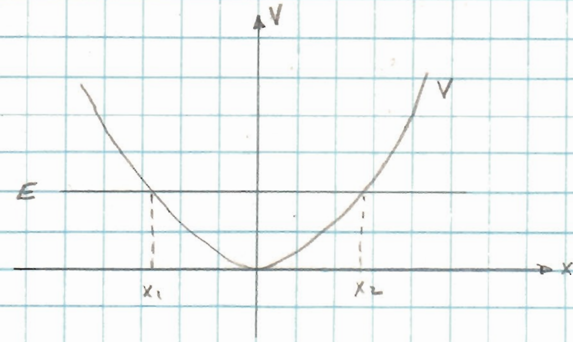
27. (1) We investigate the case of the WKB method applied to a potential with a well-defined minimum:



$$p = \sqrt{2m(E-V)}$$

(2) We will use the first connection formula:

$$\sqrt{\frac{m}{|p|}}\, e^{-\frac{1}{\hbar}\int_x^{x_0} |p|\,dx} \rightarrow 2\sqrt{\frac{m}{p}} \cos\left[\frac{1}{\hbar}\int_{x_0}^{x} p\,dx - \frac{\pi}{4}\right]$$

(3) Then:

$$\underbrace{\sqrt{\frac{m}{|p|}}\, e^{-\frac{1}{\hbar}\int_x^{x_1} |p|\,dx}}_{x < x_1} \rightarrow \underbrace{2\sqrt{\frac{m}{p}} \cos\left[\frac{1}{\hbar}\int_{x_1}^{x} p\,dx - \frac{\pi}{4}\right]}_{x_1 < x < x_2}$$

$$\underbrace{A\sqrt{\frac{m}{|p|}}\, e^{-\frac{1}{\hbar}\int_{x_2}^{x} |p|\,dx}}_{x > x_2} \rightarrow \underbrace{2A\sqrt{\frac{m}{p}} \cos\left[\frac{1}{\hbar}\int_{x}^{x_2} p\,dx - \pi/4\right]}_{x_1 < x < x_2}$$

(4) We demand that the two waves in $x_1 < x < x_2$ be equal:

$$\cos\left[\frac{1}{\hbar}\int_{x_1}^{x} p\,dx - \pi/4\right] = A\cos\left[\frac{1}{\hbar}\int_{x}^{x_2} p\,dx - \pi/4\right]$$

$$= A\cos\left[\frac{1}{\hbar}\int_{x_1}^{x} - \pi/4 - \varphi\right]$$

where $\varphi = \frac{1}{\hbar}\int_{x_1}^{x_2} p\,dx - \frac{\pi}{2}$

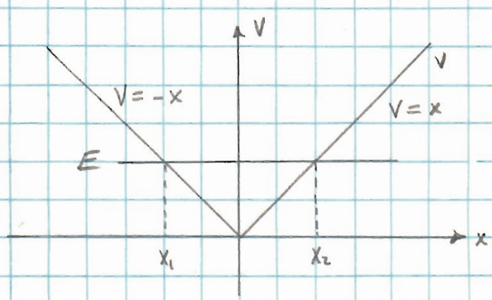
Since the two waves must fit together, $A = 1$ and

$\varphi = n\pi$, $n = 0, 1, 2, \ldots$

(5) $\therefore \quad \int_{x_1}^{x_2} p\,dx = (n+\frac{1}{2})\hbar\pi \quad , \quad p = \sqrt{2m(E-V)}$

(6) Consider: $\frac{d^2 u}{dx^2} + (E - |x|)\,u = 0$

Evidently $\frac{2m}{\hbar^2} = 1$, then $2m = \hbar^2$, $V = |x|$



$p = \hbar\sqrt{E - |x|}$

$x_1 = -E \quad , \quad x_2 = E$

(7) $\int_{-E}^{E} \sqrt{E-|x|}\,dx = (n+\frac{1}{2})\pi$

(8) $\int_{-E}^{E} \sqrt{E-|x|}\,dx = 2\int_0^E \sqrt{E-x}\,dx = -\frac{4}{3}(E-x)^{3/2}\Big]_0^E$

$= \frac{4}{3}E^{3/2} = (n+\frac{1}{2})\pi$

(9) $E = \left\{\frac{3\pi}{4}(n+1/2)\right\}^{2/3}$

$n = 0: \quad E = \left(\frac{3\pi}{8}\right)^{2/3} = 1.116$, True $E = 1.019$, error $\sim$ 10%

$n = 1: \quad E = \left(\frac{9\pi}{8}\right)^{2/3} = 2.320$, True $E = 2.338$, error $\sim$ .8%

(10) Kemble has shown that connection formulae leading to the phase integral can be found by considering the path around both turning points in the complex plane. As the approximation becomes better the further the path is from the turning points, any potential which does not create branch points (singularities) in other parts of the complex plane can be expected to yield good results for low quantum numbers. The discontinuity in the potential at the origin perhaps accounts for the slight discrepancy that exists.

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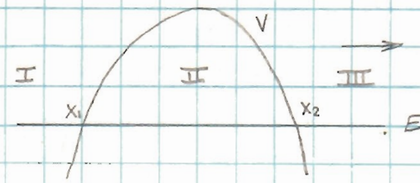
28. 

$$\longrightarrow \sqrt{\frac{m}{p}}\, e^{\frac{i}{\hbar}\int_{x_2}^{x} p\,dx + i\varphi} \quad , \quad p = \sqrt{2m(E-V)}$$

(1) We begin with the general case of transmission through a potential barrier.

(2) The BC is a wave traveling to the right in III of the form, choosing the phase to be $-\pi/4$ for convenience in using the connection formulae:

$$\psi_{III} \sim \sqrt{\frac{m}{p}}\left\{\cos\left(\frac{1}{\hbar}\int_{x_2}^{x} p\,dx - \frac{\pi}{4}\right) + i \underbrace{\sin\left(\frac{1}{\hbar}\int_{x_2}^{x} p\,dx - \pi/4\right)}_{\cos\left(\frac{1}{\hbar}\int_{x_2}^{x} p\,dx + \pi/4\right)}\right\}$$

(3) The connection formulae are:

$$\sqrt{\frac{m}{|p|}}\, e^{-\frac{1}{\hbar}\int_{x}^{x_0}|p|\,dx} \longrightarrow 2\sqrt{\frac{m}{p}}\cos\left[\frac{1}{\hbar}\int_{x_0}^{x} p\,dx - \frac{\pi}{4}\right]$$

$$\sqrt{\frac{m}{|p|}}\, e^{\frac{1}{\hbar}\int_{x}^{x_0}|p|\,dx} \longleftarrow \sqrt{\frac{m}{p}}\cos\left[\frac{1}{\hbar}\int_{x_0}^{x} p\,dx + \pi/4\right]$$

(4) Then:

$$\psi_{II} \sim \frac{1}{2}\sqrt{\frac{m}{|p|}}\exp\left\{-\frac{1}{\hbar}\int_{x}^{x_2}|p|\,dx\right\} + i\sqrt{\frac{m}{|p|}}\exp\left\{\frac{1}{\hbar}\int_{x}^{x_2}|p|\,dx\right\}$$

$$= \frac{1}{2}\sqrt{\frac{m}{|p|}}\exp\left\{-\frac{1}{\hbar}\int_{x_1}^{x_2}|p|\,dx + \frac{1}{\hbar}\int_{x_1}^{x}|p|\,dx\right\}$$

$$+ i\sqrt{\frac{m}{|p|}}\exp\left\{\frac{1}{\hbar}\int_{x_1}^{x_2}|p|\,dx - \frac{1}{\hbar}\int_{x_1}^{x}|p|\,dx\right\}$$

(5)
$$\psi_{I} \sim \frac{1}{2}\sqrt{\frac{m}{p}}\exp\left\{-\frac{1}{\hbar}\int_{x_1}^{x_2}|p|\,dx\right\}\cos\left[\frac{1}{\hbar}\int_{x}^{x_1} p\,dx - \pi/4\right]$$

$$+ 2i\sqrt{\frac{m}{p}}\exp\left\{\frac{1}{\hbar}\int_{x_1}^{x_2}|p|\,dx\right\}\cos\left[\frac{1}{\hbar}\int_{x}^{x_1} p\,dx + \pi/4\right]$$

(6) or $\psi_I \sim \sqrt{\frac{m}{p}} \left\{ \frac{1}{4} \exp\left[-\frac{1}{\hbar}\int_{x_1}^{x_2} |p|\,dx\right] + \exp\left[\frac{1}{\hbar}\int_{x_1}^{x_2}|p|\,dx\right] \right\} \exp\left[i\left(\frac{1}{\hbar}\int_x^{x_1} p\,dx - \pi/4\right)\right]$

Incident

$+ \sqrt{\frac{m}{p}} \left\{ \frac{1}{4} \exp\left[-\frac{1}{\hbar}\int_{x_1}^{x_2} |p|\,dx\right] - \exp\left[\frac{1}{\hbar}\int_{x_1}^{x_2}|p|\,dx\right] \right\} \exp\left[-i\left(\frac{1}{\hbar}\int_x^{x_1} p\,dx - \pi/4\right)\right]$

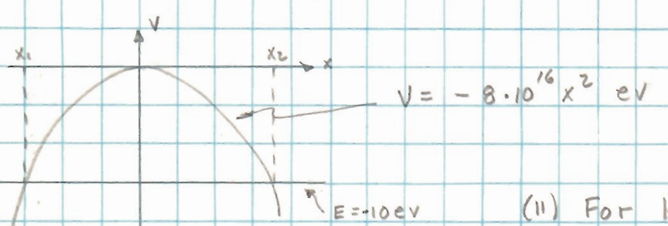
Reflected

(7) $$T = \frac{p_{III}\,|\psi_{III}|^2}{p_I\,|\psi_{I\,i}|^2} = \left[\exp\left(\frac{1}{\hbar}\int_{x_1}^{x_2}|p|\,dx\right) + \frac{1}{4}\exp\left(-\frac{1}{\hbar}\int_{x_1}^{x_2}|p|\,dx\right)\right]^{-2}$$

(8) We hold that under the WKB approximation, $\frac{1}{\hbar}\int_{x_1}^{x_2}|p|\,dx \gg 1$, so that we can drop the negative exponential in favor of the positive.

(9) $$\therefore \quad T = \exp\left[-2\left(\frac{1}{\hbar}\int_{x_1}^{x_2}|p|\,dx\right)\right]$$

(10) The model for this problem consists of:



The turning points occur when $V=E$:

$8\cdot10^{16}x^2 = 10$; $x = \pm\frac{\sqrt{5}}{2}\cdot10^{-8}$ cm

(11) For $|p|$: $\sqrt{2m(V-E)} = \sqrt{10-8\cdot10^{16}x^2}\cdot\sqrt{2m}$

(12) $$\frac{1}{\sqrt{2m}}\int_{x_1}^{x_2}|p|\,dx = 2\int_0^{\frac{\sqrt{5}}{2}\cdot10^{-8}}\sqrt{10-8\cdot10^{16}x^2}\,dx = 4\sqrt{2}\cdot10^{8}\cdot\int_0^{\frac{\sqrt{5}}{2}\cdot10^{-8}}\sqrt{\frac{5}{4}\cdot10^{-16}-x^2}\,dx$$

$$= 4\sqrt{2}\cdot10^{8}\cdot\frac{1}{2}\cdot\frac{5}{4}\cdot10^{-16}\sin^{-1}1 = \frac{20\cdot\sqrt{2}\,\pi}{16}\cdot10^{-8} = \frac{5}{4}\sqrt{2}\,\pi\cdot10^{-8}\sqrt{ev}\cdot cm$$

(13) $$\sqrt{\frac{2m}{\hbar^2}} = 5.12\cdot10^{7}\,/\sqrt{ev}\cdot cm$$

(14) $$T = \exp\left\{-2(5.12\cdot10^{7})\cdot\frac{5}{4}\sqrt{2}\,\pi\cdot10^{-8}\right\}$$

$$= \exp\{-5.68\} = \frac{1}{290} = .00345$$

Note that $e^{2.84} \gg \frac{1}{4}e^{-2.84}$ so the approximation is valid

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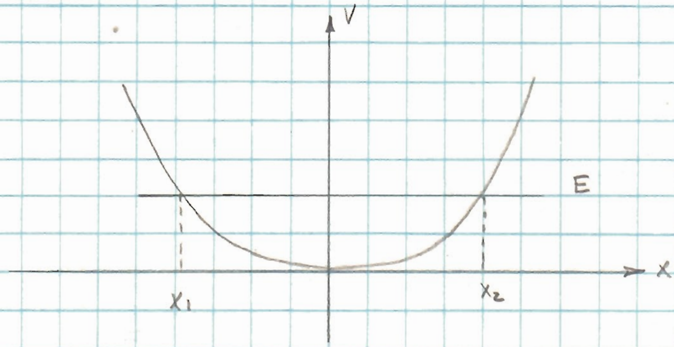
29. (1) $\frac{d^2 u}{dx^2} + (E - x^2 - a x^4) u = 0$

Evidently we are using natural units such that $\frac{2m}{\hbar^2} = 1$, $\frac{1}{2} m\omega^2 = 1$ The potential is then: $V = x^2 + ax^4$ in these units.



(2) Since we have a potential with a well-defined minimum, this problem is suitable for the application of the phase-integral method.

$$\int_{x_1}^{x_2} \sqrt{2m(E-V)}\, dx = (n+\tfrac{1}{2})\hbar\pi$$

or, in our units, $\int_{x_1}^{x_2} \sqrt{(E-V)}\, dx = (n+\frac{1}{2})\pi$

where the unit of energy is $\frac{1}{2}\hbar\omega$.

(3) The turning points are found when $V = E$ or by the roots of:

$$ax^4 + x^2 - E = 0, \quad \text{or} \quad x^4 + \frac{x^2}{a} - \frac{E}{a} = 0$$

$$x^2 = \frac{-1 \pm [1 + 4aE]^{1/2}}{2a}$$

The negative solution is disregarded as it will give imaginary distances. Thus:

$$x_1 = -\left\{ \frac{[1+4aE]^{1/2} - 1}{2a} \right\}^{1/2}; \quad x_2 = -x_1$$

(4) $\therefore \int_0^{x_2} [E - x^2 - ax^4]^{1/2} dx = (n+\frac{1}{2})\frac{\pi}{2}$

We now choose the Trig substitution $\sin\psi = \frac{x}{x_2}$ with $dx = x_2 \cos\psi\, d\psi$, and $\psi = \sin^{-1}\frac{x}{x_2}$.

(5) Now $x^2 = x_2^2 \sin^2\psi = \left\{ \frac{[1+4aE]^{1/2} - 1}{2a} \right\} \sin^2\psi$

$$x^4 = x_2^4 \sin^4\psi = \left\{ \frac{E}{a} - \frac{x_2^2}{a} \right\} \sin^4\psi$$

$$E - x^2 - ax^4 = E - x_2^2 \sin^2\psi - E\sin^4\psi + x_2^2 \sin^4\psi$$

(6) $E - x_2^2 - a x_2^4 = 0$;

Then $E - x^2 - ax^4 = x_2^2 + a x_2^4 - x_2^2 \sin^2\psi - x_2^2 \sin^4\psi$

$$- a x_2^4 \sin^4\psi + x_2^2 \sin^4\psi \quad .$$

$$= x_2^2 + a x_2^2 - x_2^2 \sin^2\psi - a x_2^4 \sin^4\psi$$

$$= x_2^2 (1 - \sin^2\psi) + a x_2^4 (1 + \sin^2\psi)(1 - \sin^2\psi)$$

$$= x_2^2 \cos^2\psi \left[1 + a x_2^2 (1 + \sin^2\psi) \right]$$

(7) $\therefore \int_0^{x_2} [E - x^2 - ax^4]^{1/2} \, dx = x_2^2 \int_0^{\pi/2} \cos^2\psi \left[1 + a x_2^2 (1 + \sin^2\psi) \right]^{1/2} d\psi$

We now argue that if a is very small,

$a x_2^2 (1 + \sin^2\psi) \ll 1$ as $1 + \sin^2\psi \sim 2$

and x_2, although it involves a, is a constant because it contains E which can be adjusted to keep x_2 constant whatever the value of a. We then expand the radical to the 3rd order in a:

$$[\;]^{1/2} = 1 + \frac{1}{2} a x_2^2 (1 + \sin^2\psi) - \frac{1}{8} a^2 x_2^4 (1 + \sin^2\psi)^2$$

$$+ \frac{1}{16} a^3 x_2^6 (1 + \sin^2\psi)^3$$

$$(1 + \sin^2\psi)^2 = 1 + 2\sin^2\psi + \sin^4\psi$$

$$(1 + \sin^2\psi)^3 = 1 + 3\sin^2\psi + 3\sin^4\psi + \sin^6\psi$$

(8) $\int_0^{\pi/2} \sin^n x \, dx = \frac{1 \cdot 3 \cdot 5 \cdots (n-1)}{2 \cdot 4 \cdot 6 \cdots n} \frac{\pi}{2}$

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Problem 29
Continued:

(9) $n = 2$: $\pi/4 = \frac{1}{2} \cdot \pi/2$

$n = 4$: $\frac{1 \cdot 3}{8} \cdot \pi/2 = 3\pi/16 = 3/8 \cdot \pi/2$

$n = 6$: $\frac{15}{48} \cdot \pi/2 = \frac{5}{16} \cdot \pi/2$

$n = 8$: $\frac{90}{364} \cdot \pi/2 = \frac{45}{182} \cdot \pi/2$

$n = 10$: $\frac{63}{256} \cdot \pi/2$

(10) $\int_0^{\pi/2} (1 - \sin^2\phi)\, d\phi = \frac{1}{2}\, \pi/2$

$\int_0^{\pi/2} (1 - \sin^4\phi)\, d\phi = \frac{5}{8}\, \pi/2$

$\int_0^{\pi/2} (1 - \sin^4\phi)(1 + \sin^2\phi)\, d\phi = \int_0^{\pi/2} (1 + \sin^2\phi - \sin^4\phi - \sin^6\phi)\, d\phi$

$= (1 + \frac{1}{2} - 3/8 - 5/16)\, \pi/2 = \frac{13}{16} \cdot \pi/2$

$\int_0^{\pi/2} (1 - \sin^4\phi)(1 + \sin^2\phi)^2\, d\phi = \frac{5}{16} \cdot \pi/2 - \int_0^{\pi/2} (\sin^4\phi + \sin^6\phi$
$- \sin^8\phi - \sin^{10}\phi)\, d\phi$

$= \left(\frac{5}{16} - \frac{6}{16} - \frac{5}{16} + \frac{45}{182} + \frac{63}{256}\right) \cdot \pi/2$

(11) We keep only terms in a^2:

$\frac{1}{2} \cdot \frac{\pi}{2} \cdot x_2^2 + \frac{1}{2} \cdot a \cdot x_2^4 \cdot \frac{5}{8} \cdot \frac{\pi}{2} - \frac{1}{8} \cdot a^2 \cdot x_2^6 \cdot \frac{13}{16} \cdot \frac{\pi}{2}$

$= (n + \frac{1}{2})\, \frac{\pi}{2}$

(12) $\frac{1}{2} x_2^2 + \frac{5}{16} a x_2^4 - \frac{13}{128} a^2 x_2^6 = (n + \frac{1}{2})$

or $x_2^2 + \frac{5}{8} a x_2^4 - \frac{13}{64} a^2 x_2^6 = 2n+1$

(13) Now: $x_2^2 = \dfrac{[1+4aE]^{1/2}-1}{2a} \cong E - \dfrac{1}{8}\cdot\dfrac{16a^2E^2}{2a}$

$+ \dfrac{1}{16}\cdot\dfrac{64a^3E^3}{2a} = E - aE^2 + 2a^2E^3$

(14) Substituting in (12), keeping terms to a^2:

$E - aE^2 + 2a^2E^3 + \frac{5}{8}\left(aE^2 - 2a^2E^3\right)$

$- \frac{13}{64}a^2E^3 = E - \frac{3}{8}aE^2 + \frac{35}{64}a^2E^3 = 2n+1$

(15) By reversion of series:

$y = a_1x + a_2x^2 + a_3x^3 + \ldots$

$x = A_1y + A_2y^2 + A_3y^3 + \ldots$

$A_1 = \dfrac{1}{a_1}, \quad A_2 = -\dfrac{a_2}{a_1^3}, \quad A_3 = \dfrac{1}{a_1^5}(2a_2^2 - a_1a_3)$

$E = x, \quad y = (2n+1)$

$A_1 = 1, \quad A_2 = +\dfrac{3/8\,a}{1}$

$A_3 = \left(\dfrac{18}{64} - \dfrac{35}{64}\right)a^2 = -\dfrac{17}{64}a^2$

(16) $\therefore \quad E = (2n+1) + \frac{3}{8}a(2n+1)^2 - \frac{17}{64}(2n+1)^3a^2 + O(a^{n>2})$

or $E = \Big\{(2n+1) + \frac{3}{4}a\left(2n^2+2n+\frac{1}{2}\right) - \frac{a^2}{16}\big(34n^3 + 51n^2$

$+ 25\tfrac{1}{2}n + 4\tfrac{1}{4}\big)\Big\}\dfrac{\hbar\omega}{2}$

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30. (1) Anharmonic oscillator: $\frac{d^2 u}{dx^2} + (E - x^2 - ax^4) u = 0$

where $\frac{2m}{\hbar^2} = 1$, $\frac{1}{2} m\omega^2 = 1$

unit of energy $= \frac{1}{2}\hbar\omega$; unit of (length)$^2 = \frac{\hbar}{m\omega}$

(2) Consider $V = ax^4$ as the perturbation to harmonic oscillator whose equation is

$$\frac{d^2 u}{dx^2} + (E - x^2) u = 0, \qquad E_n^{(0)} = 2n+1$$

and the matrix elements of the co-ordinate are:

$$\langle m|x|n\rangle = \sqrt{\frac{m}{2}}\,\delta_{m,n+1} + \sqrt{\frac{n}{2}}\,\delta_{m+1,n}$$

$$= \sqrt{\frac{n+1}{2}}\,\delta_{n,m-1} + \sqrt{\frac{n}{2}}\,\delta_{n,m+1}$$

(3) In the calculations to follow, we will wish to know the matrix elements of x^4; we then proceed:

$$\langle m|x^2|n\rangle = \langle m|x\cdot x|n\rangle = \sum_k \langle m|x|k\rangle\langle k|x|n\rangle$$

$$= \sum_k \left\{\sqrt{\frac{k+1}{2}}\,\delta_{k,m-1} + \sqrt{\frac{k}{2}}\,\delta_{k,m+1}\right\}\left\{\sqrt{\frac{n+1}{2}}\,\delta_{n,k-1} + \sqrt{\frac{n}{2}}\,\delta_{n,k+1}\right\}$$

$$= \frac{1}{2}\sum_k \Big\{ \sqrt{(k+1)(n+1)}\,\delta_{k,m-1}\,\delta_{n,k-1} + \sqrt{(k+1)n}\,\delta_{k,m-1}\,\delta_{n,k+1}$$

$$+ \sqrt{k(n+1)}\,\delta_{k,m+1}\,\delta_{n,k-1} + \sqrt{kn}\,\delta_{k,m+1}\,\delta_{n,k+1}\Big\}$$

$$= \frac{1}{2}\Big\{ \sqrt{(n+2)(n+1)}\,\delta_{m,n+2} + n\,\delta_{m,n} + (n+1)\,\delta_{m,n}$$

$$+ \sqrt{n(n-1)}\,\delta_{m,n-2}\Big\}$$

(4) $\therefore$ $\langle m|x^2|n\rangle = \frac{1}{2}\Big\{ \sqrt{(n+2)(n+1)}\,\delta_{m,n+2} + (2n+1)\,\delta_{m,n}$

$$+ \sqrt{n(n-1)}\,\delta_{m,n-2}\Big\}$$

(5) $\langle m|x^4|n\rangle = \sum_k \langle m|x^2|k\rangle\langle k|x^2|n\rangle$

$$= \frac{1}{4}\sum_k \left\{ \sqrt{(k+1)(k+2)}\,\delta_{m,k+2} + (2k+1)\,\delta_{m,k} + \sqrt{k(k-1)}\,\delta_{m,k-2} \right\}$$

$$\left\{ \sqrt{(n+2)(n+1)}\,\delta_{k,n+2} + (2n+1)\,\delta_{k,n} + \sqrt{n(n-1)}\,\delta_{k,n-2} \right\}$$

$$= \frac{1}{4}\sum_k \Big\{ \sqrt{(k+1)(k+2)(n+2)(n+1)}\,\delta_{m,k+2}\,\delta_{k,n+2} + (2n+1)\sqrt{(k+1)(k+2)}\,\delta_{m,k+2}\,\delta_{k,n}$$

$$+ \sqrt{n(n-1)(k+1)(k+2)}\,\delta_{m,k+2}\,\delta_{k,n-2} + (2k+1)\sqrt{(n+2)(n+1)}\,\delta_{m,k}\,\delta_{k,n+2}$$

$$+ (2k+1)(2n+1)\,\delta_{k,n}\,\delta_{m,k} + (2k+1)\sqrt{n(n-1)}\,\delta_{m,k}\,\delta_{k,n-2}$$

$$+ \sqrt{k(k-1)(n+2)(n+1)}\,\delta_{m,k-2}\,\delta_{k,n+2} + (2n+1)\sqrt{k(k-1)}\,\delta_{m,k-2}\,\delta_{k,n}$$

$$+ \sqrt{k(k-1)\,n(n-1)}\,\delta_{m,k-2}\,\delta_{k,n-2} \Big\}$$

$$= \frac{1}{4}\Big\{ \sqrt{(n+4)(n+3)(n+2)(n+1)}\,\delta_{m,n+4} + (2n+1)\sqrt{(n+1)(n+2)}\,\delta_{m,n+2}$$

$$+ \overbrace{n(n-1)}^{n^2-n}\,\delta_{m,n} + (2n+5)\sqrt{(n+1)(n+2)}\,\delta_{m,n+2}$$

$$+ (4n^2+4n+1)\,\delta_{m,n} + (2n-3)\sqrt{n(n-1)}\,\delta_{m,n-2}$$

$$+ (n^2+3n+2)\,\delta_{m,n} + (2n+1)\sqrt{n(n-1)}\,\delta_{m,n-2}$$

$$+ \sqrt{(n-3)(n-2)(n-1)n}\,\delta_{m,n-4} \Big\}$$

(6) $\therefore$ $\langle m|x^4|n\rangle = \frac{1}{4}\Big\{ \sqrt{(n+4)(n+3)(n+2)(n+1)}\,\delta_{m,n+4}$

$$+ 2(2n+3)\sqrt{(n+1)(n+2)}\,\delta_{m,n+2} + 3(2n^2+2n+1)\,\delta_{m,n} + 2(2n-1)\sqrt{n(n-1)}\,\delta_{m,n-2}$$

$$+ \sqrt{(n-3)(n-2)(n-1)n}\,\delta_{m,n-4} \Big\}$$

(7) The first order correction is:

$$E_n^{(1)} = \langle n|V|n\rangle = a\,\langle n|x^4|n\rangle$$

$$= \frac{3}{4}\,a\,(2n^2+2n+1)$$

Assignment # 6
Continued

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Problem 30
Continued

(8) The second order correction is:

$$E_n^{(2)} = \sum_{k \neq n} \frac{|\langle k|V|n\rangle|^2}{E_n^{(0)} - E_k^{(0)}} = a^2 \sum_k \frac{|\langle k|x^4|n\rangle|^2}{E_n^{(0)} - E_k^{(0)}}$$

$$= \frac{a^2}{16} \left\{ \frac{(n+4)(n+3)(n+2)(n+1)}{-8} + \frac{4(2n+3)^2(n+1)(n+2)}{-4} \right.$$

$$\left. + \frac{4(2n-1)^2\, n(n-1)}{4} + \frac{(n-3)(n-2)(n-1)n}{8} \right\}$$

$$= \frac{a^2}{16 \cdot 8} \left\{ -\left[n^2 + 3n + 2\right]\left[n^2 + 7n + 12 + 32n^2 + 96n + 72\right] \right.$$

$$\left. + \left[n^2 - n\right]\left[32n^2 - 32n + 8 + n^2 - 5n + 6\right] \right\}$$

$$= -\frac{a^2}{8 \cdot 16} \left\{ 272n^3 + 408n^2 + 472n + 168 \right\}$$

$$= -\frac{a^2}{16} \left\{ 34n^3 + 51n^2 + 59n + 21 \right\}$$

(9) $$\therefore \quad E = \left\{ (2n+1) + \frac{3a}{4}(2n^2+2n+1) - \frac{a^2}{16}\left(34n^3 + 51n^2 + 59n + 21\right) \right\} \frac{\hbar\omega}{2}$$

(10) In comparing this result with the phase integral method, we see that they approach each other for high quantum numbers. This is expected as the phase integral method is a good approximation for high n. For low a, the perturbation theory gives good results. In this problem, $a \ll 1$ was taken in computing the phase integral, thus highlighting the fact that the two approach

each other for high n. For low n, in this problem, the perturbation theory gives better results.

In choosing the method to use, one must decide whether or not low quantum numbers will be important. Also, in using the perturbation method, a must be small which may not be the case thus causing one to have to use the phase integral method.

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