

Origins of Quantum Theory.

On classical theory, any accelerated charged particle radiates energy. So an electron going round a proton should always emit radiation, lose energy and fall into proton. Atoms would be unstable, emit radiation and disappear.

Study of spectra shows that any atom or molecule has certain "spectral terms" $\nu_1, \nu_2, \nu_3, \dots$ and the emitted frequencies are differences of these terms. $\nu_{mn} = \nu_m - \nu_n$. The "Ritz combination principle".

Black body radiation Energy between λ and $\lambda + d\lambda$ being $S_\lambda d\lambda$, Rayleigh-Jeans predicted $S_\lambda = 2\pi ck T / \lambda^4$. "The Rayleigh Jeans catastrophe" [Rayleigh (1900), Jeans (1905)]

Gives infinite total, and infinite energy for very short waves. It agrees with observation for long waves.

Actual curve 

Stefan Boltzmann Law. The total emissive power of any body $\propto T^4$ (T Temperature absolute.) Proved by thermodynamics: first conjectured experimentally.

Suggested formulas. Wien $e_\lambda = a \lambda^{-5} e^{-b/\lambda T}$
 $\int_0^\infty e_\lambda d\lambda = \int_0^\infty a x^3 e^{-bx/T} dx$ (by $x = \lambda/T$) $\int_0^\infty \left(\frac{T}{b}\right)^4 x^3 e^{-x} dx = \frac{3! T^4}{b^4}$
 in agreement with Stefan Boltzmann

Fits data well for λ large.

It can also be proved by thermodynamics that if e_1 is emissive power for monochromatic light of wave length λ_1 at temp. T_1 , then at temperature T_2 , for $\lambda_2 = \lambda_1 \frac{T_1}{T_2}$, $e_2 = e_1 \left(\frac{T_2}{T_1}\right)^5$.

This enables us to transform curve for distribution at one temperature to that for another temperature.

It follows that if the maximum emissive power at temperature T is e_m for λ_m , then $e_m = BT^5$, $\lambda_m T = A$.

Annalen d. Physik - 1926 - Vol. 79.

p 361. E. Schrödinger. Quantisierung als Eigenwertproblem (1st communication).

$H(q, \partial S / \partial q) = E$. Let $S = K \ln \psi$.
(Later he says K must have dimensions of action, and finds $K = h/2\pi$ for $-E = 2\pi^2 m e^4 / h^2 e^2$ as required.)

$$\text{Then } E = H(q, \frac{K}{\psi} \frac{\partial \psi}{\partial q})$$

For $V = -e^2/r$ this gives

$$\left(\frac{\partial \psi}{\partial x}\right)^2 + \left(\frac{\partial \psi}{\partial y}\right)^2 + \left(\frac{\partial \psi}{\partial z}\right)^2 - \frac{2m}{K^2} \left(E + \frac{e^2}{r}\right) \psi^2 = 0$$

$$r = \sqrt{x^2 + y^2 + z^2}. \quad \text{He minimizes } \int_0^a \int_0^a \int_0^a$$

and gets

$$\nabla^2 \psi + \frac{2m}{K^2} \left(E + \frac{e^2}{r}\right) \psi = 0.$$

p 489. Second communication.

H.P. = Hamilton's P.D.E. Previously he had used "incomprehensible" $S = K \ln \psi$ and the equally incomprehensible $\delta \iiint = 0$.

Nothing new in associating mechanics with wave propagation. Hamilton knew it. Hamilton's principle, minimize $\int L dt$ corresponds to Fermat's least time.

The general problem of classical mechanics.

$$(1) \quad \partial W / \partial t + T(q, \frac{\partial W}{\partial q}) + V(q) = 0$$

W is action function $\int (T - V) dt$ along an orbit, as function of time and final position. T is $K \cdot E$ as function of position and momenta, quadratic in momenta, which are replaced by $\partial W / \partial q_k$. To solve it we put $W = -Et + S(q)$ and it becomes

$$* 2T(q, \frac{\partial W}{\partial q}) = 2(E - V) \quad (1')$$

The statement (1') can be expressed very simply by an idea of Heinrich Hertz. Define a non-Euclidean metric in configuration space by

* Usually with S , instead of W . No difference.

Schrödinger $T = \frac{1}{2}(\dot{x}^2 + \dot{y}^2 + \dot{z}^2)$ Potential V .

$$\frac{\partial W}{\partial t} = T(q, \dot{q})$$

$$q_1 = \dot{x} \quad q_2 = \dot{y} \quad q_3 = \dot{z} \quad \text{momenta.}$$

$$\frac{\partial W}{\partial t} + \frac{1}{2}(q_1^2 + q_2^2 + q_3^2) + V(x, y, z) = E \quad 0$$

$$W = -Et + S(q)$$

$$\frac{1}{2}(q_1^2 + q_2^2 + q_3^2) = E - V.$$

$$ds^2 = dx^2 + dy^2 + dz^2 \text{ as usual.}$$

$$\text{grad } W = \left(\frac{\partial W}{\partial x}, \frac{\partial W}{\partial y}, \frac{\partial W}{\partial z} \right)$$

$$q_1 = \frac{\partial W}{\partial x} \quad q_2 = \frac{\partial W}{\partial y} \quad q_3 = \frac{\partial W}{\partial z}$$

$$(\text{grad } W)^2 = 2(E - V)$$

$$\text{grad } W = \sqrt{2(E - V)}.$$

Along normal to $dV = \text{const.}$ $dW = \sqrt{2(E - V)} ds$

So, to get to $W + dW$ surface we go

$$ds = \frac{dW}{\sqrt{2(E - V)}} \text{ along normal}$$

Try step fn.

W
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A particle moves in a plane under no force.

$$V=0 \therefore T=E.$$

$$\therefore S = \int_0^t 2T dt = 2Tt = 2Et.$$

$$\frac{1}{2}mv_0^2 = E \therefore v_0 = \sqrt{\frac{2E}{m}}$$

If it reaches distance r in time t

$$r = v_0 t \therefore t = \frac{r}{v_0}$$

$$\therefore S = \frac{2Er}{v_0} = 2Er \sqrt{\frac{m}{2E}} = r\sqrt{2mE}$$

If it is at (x, y) after time t

$$S = \sqrt{2mE} \sqrt{x^2 + y^2}$$

$$h_1 = \frac{\partial S}{\partial x} = \sqrt{2mE} \cdot \frac{x}{\sqrt{x^2 + y^2}}$$

$$= m \sqrt{\frac{2E}{m}} \cos \theta = mv_0 \cos \theta$$

x-mom.

$$h_2 = m \sqrt{\frac{2E}{m}} \sin \theta = \sqrt{2mE} \frac{y}{\sqrt{x^2 + y^2}}$$

$$W = S - Et = \sqrt{2mE} \sqrt{x^2 + y^2} - Et.$$

If we fix a value of W , surface having this value has equation

$$W_0 = \sqrt{2mE} \sqrt{x^2 + y^2} - Et.$$

$$\text{At time } t, \quad r = \frac{W_0 + Et}{\sqrt{2mE}}$$

$$\frac{dr}{dt} = \frac{E}{\sqrt{2mE}} = \sqrt{\frac{E}{2m}}$$

$$E = \frac{1}{2}mv_0^2$$

$$\frac{E}{2m} = \frac{v_0^2}{2}$$

$$\frac{dr}{dt} = \frac{1}{2}v_0.$$

P.T.O.

A unit mass moves in 2 dimensions, under a force numerically equal to the distance from the origin.

Thus $\ddot{r} = r$

$$\therefore r = Ae^t + Be^{-t}$$

Initially $r_0 = 0$ $\dot{r}_0 = v_0$

$$\therefore B = -A \quad r = A(e^t - e^{-t})$$

$$v_0 = A(e^t + e^{-t})_{t=0} = 2A$$

$$\therefore A = \frac{v_0}{2} \quad r = \frac{v_0}{2} \sinh t$$

$$T = \frac{1}{2} \dot{r}^2 = \frac{v_0^2}{8} \cosh^2 t$$

$$S = \int_0^t 2T dr = \frac{v_0^2}{4} \int_0^t \cosh^2 t \, dt$$

$$\int_0^t \cosh^2 t \, dt = \int_0^t \left(\frac{e^t + e^{-t}}{2} \right)^2 dt$$

$$= \frac{1}{4} \int_0^t e^{2t} + 2 + e^{-2t} dt$$

$$= \frac{1}{4} \left[\frac{1}{2} e^{2t} - \frac{1}{2} e^{-2t} + 2t \right]_0^t$$

$$= \frac{1}{4} \sinh 2t + \frac{1}{2} t \quad \text{replace } t \text{ by } \frac{1}{2} t$$

$$2 \sinh t \cosh t = 2 \left(\frac{e^t - e^{-t}}{2} \right) \left(\frac{e^t + e^{-t}}{2} \right) = \frac{1}{2} (e^{2t} - e^{-2t})$$

$$= \sinh 2t$$

$$\therefore \text{If } r \text{ is given, } t = \sinh^{-1} \frac{2r}{v_0}$$

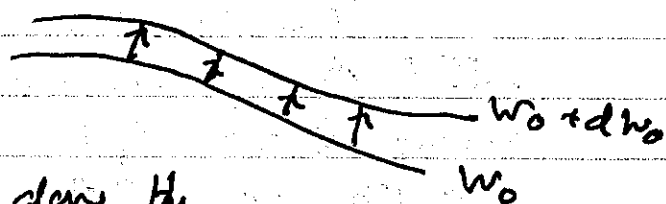
$$S = \frac{1}{2} \frac{2r}{v_0} \sqrt{\frac{4r^2}{v_0^2} - 1} + \frac{1}{2} \sinh^{-1} \frac{2r}{v_0}$$

It is easy to show the meaning of this requirement. Suppose we have a function $W = -Et + S(q)$ that satisfies this condition. We can represent this function at a definite time t by drawing the family $W = \text{constant}$, each surface being labelled with the value of W for it.

Given one surface and the value of W for it, we can successively construct the other surfaces with their values. Alternatively, we can choose any surface quite arbitrarily as the one from which the construction starts. The time is kept constant. This construction gives the total meaning of the P.D.E.

At each point of $W = W_0$ we go a distance

$$(4) \quad ds = \frac{dW_0}{\sqrt{2(E-V)}} \text{ along the}$$



normal. The point so reached from $W = W_0 + dW_0$.

The initial direction may be either way. We get the same set of surfaces whichever we choose. The values run in opposite directions.

Now consider the simple dependence on time. We get the same set of surfaces at t & t' as at t_0 , but with a value of W on each less by $E(t - t_0)$. So a fixed value moves from one surface to another in the direction of increasing t . We can equally well think of the surfaces moving, carrying their W values with them. The surface with W_0 at t moves, at time $t + dt$, to the surface that had $W = W_0 + E dt$ at time t . So

$$dW_0 = E dt \quad \text{and} \quad (5) \quad ds = \frac{E dt}{\sqrt{2(E-V)}} \quad \text{So surfaces}$$

$$\text{have normal velocity } (6) \quad \frac{ds}{dt} = \frac{E}{\sqrt{2(E-V)}} \quad \text{where } E \text{ is}$$

given this is purely a function of position.

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§2 "Geometrized" and "Wave" Mechanics.

We assume the waves given by sine functions. We emphasize the arbitrariness of this fundamental assumption but it is the simplest and most plausible (naheliegendste). So the wave function is to involve time only in the form $\sin(\dots)$, the brackets containing a linear function of W . As we can only find sine of a pure number, W must have coefficient with dimension reciprocal of action. We assume this coefficient is universal, independent of E and of the mechanical system. Let it be $2\pi/h$. Then time factor runs

$$(10) \quad \sin\left(2\pi W/h + \text{const.}\right) = \sin\left(-\frac{2\pi E t}{h} + \frac{2\pi S(q)}{h} + \text{const.}\right)$$

So frequency ν is given by

$$(11) \quad \nu = E/h.$$

In classical mechanics E involves an arbitrary additive constant: here E is absolute. Wavelength, by (6) and (11) is

$$(12) \quad \lambda = u/\nu = h/\sqrt{2(E-V)}.$$

(The classical added constant does not appear here, as $E - V = \text{kinetic energy}$.)

[He shows that this wavelength is of the order of magnitude at which classical mechanics fails.]

$$(6') \quad u = h\nu/\sqrt{2(h\nu - V)}$$

so we get dispersion: the velocity of phase propagation depends on the frequency. From (9), (11), (6') we find

$$(13) \quad v = d\nu/d(\nu/u)$$

where v is the velocity of the representative point in (9).

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W₁₅

The wave equation is not determined by what we know but it seems reasonable to consider a P.D.E. of second order $\nabla^2 \psi - \frac{1}{u^2} \frac{\partial^2 \psi}{\partial t^2} = 0$ (18)

valid for processes in which time factor is $e^{2\pi i \nu t}$.

In view of (6), (6'), (11)

$$(18') \quad \nabla^2 \psi + \frac{8\pi^2}{h^2} (\hbar \nu - V) \psi = 0$$

$$(18'') \quad \nabla^2 \psi + \frac{8\pi^2}{h^2} (E - V) \psi = 0.$$

(He uses divgrad instead of ∇^2 , in metric defined by (3).)

A reference to earlier paper in which

$$U'' + (\delta_0 + \frac{\delta_1}{r})U' + (\epsilon_0 + \frac{\epsilon_1}{r})U = 0$$

is solved by Laplace Transformation

$$U = \int_L e^{r\beta} (\beta - c_1)^{\alpha_1 - 1} (\beta - c_2)^{\alpha_2 - 1} d\beta$$

where path L in complex must make

$$\int_L d\beta [e^{r\beta} (\beta - c_1)^{\alpha_1} (\beta - c_2)^{\alpha_2}] = 0$$

c_1 and c_2 are roots of quadratic $\beta^2 + \delta_0 \beta + \epsilon_0 = 0$

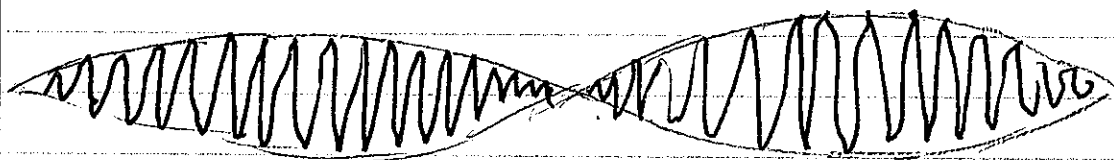
$$\text{and } \alpha_1 = \frac{\epsilon_1 + \delta_1 c_1}{c_1 - c_2} \quad \alpha_2 = \frac{\epsilon_1 + \delta_1 c_2}{c_2 - c_1}$$

Group velocity and phase velocity.

$$\text{def } y = \cos 2\pi(x-t) + \cos 2\pi(1.02x - 1.06t) \\ = 2 \cos 2\pi(1.01x - 1.03t) \cos 2\pi(.01x - .03t)$$

$\cos 2\pi(1.01x - 1.03t)$ repeats when x increases by $1/1.01$; $\cos 2\pi(.01x - .03t)$ when x increases by 100.

Thus the graph is much like a modulated radio signal, a slow variation of amplitude



The second factor essentially determines the appearance of the process. Its maximum occurs (for example) where $.01x - .03t = 0$ i.e. $x = 3t$, and so moves with velocity 3. (group velocity)

$\cos 2\pi(x-t)$ and $\cos 2\pi(1.02x - 1.06t)$ have peaks that move with velocity $\div 1$. (phase velocity)

It will be seen that we can arrange for phase velocity to remain 1, and have any group velocity we may fancy.

$$\text{Consider now } \cos 2\pi(\alpha x - \nu t) + \cos 2\pi((\alpha + \delta\alpha)x - (\nu + \delta\nu)t) \\ = 2 \cos \left[(\alpha + \frac{\delta\alpha}{2})x - (\nu + \frac{\delta\nu}{2})t \right] \cos \left[\frac{\delta\alpha}{2}x - \frac{\delta\nu}{2}t \right]$$

As before, the position of the group maximum depends on the behaviour of the second factor. It has a

maximum where $\frac{\delta\alpha}{2}x - \frac{\delta\nu}{2}t = 0$ i.e. $x = \frac{\delta\nu}{\delta\alpha} t$

so the group velocity is $\frac{d\nu}{d\alpha}$.

The magnitude of this will depend on the way ν is related to α .

A wave group, restricted to a certain small region, goes a substitute for a particle in the classical theory. Such groups can be built up by the construction that Debye and Lense used in ordinary optics to obtain the exact analytic representation of a cone or bundle of rays. There is an interesting connection with the Jacobi-Hamilton theory by which the integral eqns of motion can be obtained by differentiating the constants in H-S eqn. We shall see that this agrees with the wave result, the moving point coincides with the place where a certain continuum of waves are in phase.

Debye's method is to superpose ^{plane} waves, each of which fills the whole space. In fact, superpose a continuum of such waves with the normals varying inside a certain cone. The waves cancel each other by interference almost completely outside a double cone.

It is possible to use an infinitesimal solid angle for the cone. I have used this in his celebrated paper (1916). tacitly we have supposed the waves monochromatic.

By varying frequencies suitably we can suitably within an infinitesimal range we can get a domain that is relatively small longitudinally. The portion of the energy packet is the place where all the superposed waves are exactly in phase.

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In q -space we choose a point P , a direction R and a prescribed mean frequency ω (energy E) at time t .

We take a sol W of H.P.(1')

$$\frac{\partial W}{\partial t} + T(q, \frac{\partial W}{\partial q}) + V(q) = 0$$

Let $W = W_0$ be the surface through P with normal R at time t .

$P = (q_1, \dots, q_n)$. We vary W so infinitesimally so as to give $(n-1)$ dimensional solid angle for normals, and an infinitesimal 1-dimensional domain for the frequency $E/\hbar$. We must make all of them have same phase at P . We then have to show where this coincidence of phases occurs at a later time.

The soln W must be of form $W(\alpha_1, \dots, \alpha_n)$. Take $\alpha_1 = E$. We suppose $\alpha_2, \dots, \alpha_n$ so chosen that normal at P has direction R . We suppose $\alpha_1, \dots, \alpha_n$ have these values throughout

$$(14) \quad W \neq \frac{\partial W}{\partial \alpha_1} d\alpha_1 + \dots + \frac{\partial W}{\partial \alpha_n} d\alpha_n = \text{constant}$$

is taken with fixed $d\alpha_1, \dots, d\alpha_n$ and constant varying gives a family of surfaces. The surface that goes through P at time t is given by

$$(15) \quad W + \frac{\partial W}{\partial \alpha_1} d\alpha_1 + \dots + \frac{\partial W}{\partial \alpha_n} d\alpha_n = W_0 + \left(\frac{\partial W}{\partial \alpha_1} \right) d\alpha_1 + \left(\frac{\partial W}{\partial \alpha_n} \right) d\alpha_n$$

The surfaces (15'), for all possible $d\alpha_i$ form a family. At time t they all go through P , their normals fill an infinitesimal solid angle and their E -value varies in a small domain. ~~Eq~~ (15') picks out one representative of each family (15), namely the one through P at time t . We suppose the phases of the wave functions in (15) agree with those of the representative (15').

At an arbitrary time, will there be a place where all the ~~phases~~ the surfaces (15') meet and to all wave fns in (15) agree in phase?

The answer: there is a point where phases agree, but it is not the common point of (15'), for such a point never exists again. Rather the point of agreeing phases comes about by the families (15) continuously change their representative in (15').

We see this as follows.

For the common point of intersection of all members of (15') at any time we must have simultaneously

$$(16) \quad \left\{ \begin{array}{l} W = W_0 \\ \partial W / \partial x_k = (\partial W / \partial x_k)_0 \dots \quad \frac{\partial W}{\partial a_n} = \left(\frac{\partial W}{\partial a_n} \right)_0 \end{array} \right.$$

as a_k are arbitrary within a small domain.

RHS are constants. LHS functions of $n+1$ quantities

$t, q_1, \dots, q_n$. The eqns are satisfied for the initial conditions, words of P and time t .

Proceed as follows. Leave $W = W_0$ aside and find $q_1, \dots, q_n$ as fns of time from n other eqns. Let this be Q . For it, naturally, the first eqn will not be satisfied, but RHS and LHS will differ by a certain amount. If we go back from (16) to its origin from (15') we see that RHS differ from LHS if (15') changes by a number that is the same for all families. Q is not a common point of (15'), but is for (15'') which arises by changing RHS of (15') by a fixed number, the same for all surfaces of the family. This comes by changing the constant in (15) by the same amount for all representatives. Thus the phase angle of all representatives is changed by the same amount. As the old representatives agreed in phase, the new must do the same. This means, the pair given by the n eqns. $\frac{\partial W}{\partial a_1} = \left(\frac{\partial W}{\partial a_1} \right)_0 \quad \frac{\partial W}{\partial a_n} = \left(\frac{\partial W}{\partial a_n} \right)_0 \quad (17)$

as a fn of time is always a point where phases agree.

Of the n surfaces, fixing Q as point of intersection for (17), only the first is movable.

(only the first eqn involves the time.) The other $n-1$ eqns determine the orbit of Q . It is easy to see that this orbit is orthogonal to the family

$W = \text{constant}$. By the assumption, W satisfies the H.P (1') $2T(q, \partial W / \partial q) = 2(E - V)$ identically in $x_1, \dots, x_n$. Differentiating H.P w.r.t x_k ($k=2, \dots, n$)

we get the result that the normal of a surface $\partial W / \partial x_k = \text{const}$ at each point of the surface is $\perp$ to the normal of the surface $W = \text{const}$ through this point. i.e. that each surface contains the normal to the other. Hence intersection is orthogonal. Proved. $\perp$ to surfaces $W = \text{const}$.

(17) is known to give the orbits for mechanical problems.

Remark & def.

Hamilton's Principle. $\delta \int L dt = 0$

$$S = \int 2T dt$$

$$2T = \sum p_k \dot{q}_k$$

$$S = \int p_k dq_k$$

$$p_k = \frac{\partial S}{\partial q_k}$$

$$W = -Et + S$$

$$= -\int E dt + \int 2T dt$$

$$= \int 2T - E dt$$

$$= \int T - (E - T) dt$$

$$= \int T - V dt = \int L dt$$

Hamilton's Principal Function.

W is a function of final position and time.

$W = \int L dt$ in terms of final position and time values.

Lagrange's Equations. $L = T - V$

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}} \right) = \frac{\partial L}{\partial q}$$

express that $\delta \int_{t_0}^{t_f} L dt = 0$.

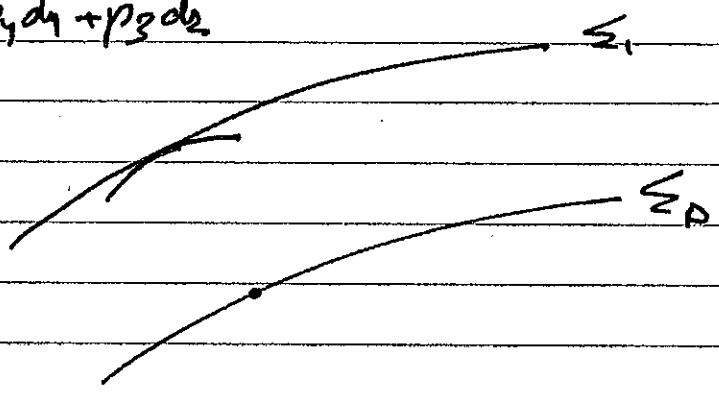
Thus, if $W = \int_{t_0}^{t_f} L dt$, the orbit goes from initial to final position by the path that makes W a minimum. Thus 'least W ' replaces Fermat's least Time.

Action $S = \int_{t_0}^{t_f} 2T dt$.

$$\begin{aligned} W &= \int_{t_0}^{t_f} (T - V) dt = \int_{t_0}^{t_f} T - (E - T) dt \\ &= \int_{t_0}^{t_f} 2T - E \cdot dt = \int_{t_0}^{t_f} 2T dt - Et \\ &= S - Et. \end{aligned}$$

$$\text{Action} = \int 2T dt = \int m\dot{x}^2 + m\dot{y}^2 + m\dot{z}^2 dt = \int m\dot{x} dx + m\dot{y} dy + m\dot{z} dz \\ = \int p_x dx + p_y dy + p_z dz$$

(x_0, y_0, z_0) on surface Σ_0
 $S(x, y, z, x_0, y_0, z_0) = k$
 is equation of constant
 action, bounding Σ_1 at x, y, z



Let l, m, n be normal

to Σ_1 at x, y, z . As surfaces coincide there

$$\frac{\partial S}{\partial x_1} = kl, \quad \frac{\partial S}{\partial y_1} = km, \quad \frac{\partial S}{\partial z_1} = kn, \quad \text{for some } k.$$

Now suppose we consider path of moving object from
 (x, y, z_1) to $(x_1 + \delta x_1, y_1 + \delta y_1, z_1 + \delta z_1)$. This is
 along normal at (x, y, z_1) so $\delta x_1 = l ds, \delta y_1 = m ds,$
 $\delta z_1 = n ds$. The change in action is

$$\oint p_x l ds + p_y m ds + p_z n ds \\ \text{This must equal } \delta S = \frac{\partial S}{\partial x_1} \delta x_1 + \frac{\partial S}{\partial y_1} \delta y_1 + \frac{\partial S}{\partial z_1} \delta z_1 \\ = kl^2 ds + km^2 ds + kn^2 ds \\ = k ds.$$

$$\therefore k = p_x l + p_y m + p_z n.$$

Now $p_x = pl, p_y = pm, p_z = pn$ where $p = \sqrt{p_x^2 + p_y^2 + p_z^2}$

$$\therefore k = p(l^2 + m^2 + n^2) = p.$$

$$\therefore \frac{\partial S}{\partial x_1} = pl = p_x, \text{ similarly } \frac{\partial S}{\partial y_1} = p_y, \frac{\partial S}{\partial z_1} = p_z.$$

We can show in the same way $\frac{\partial S}{\partial x_0} = -p_{x0}$ etc.

The minus sign is due to the fact that path of
 integration is reduced when its starting point moves forward.

Whittaker. Analytical Dynamics. Chap XI.

Fermat's principle $\int \mu(x, y, z) ds$ stationary

Principle of least Action asserts $\int \{E - \phi(x, y, z)\}^{1/2} ds$ stationary

$\phi(x, y, z)$ potential energy, E energy.

The trajectories of the particle in the dynamical problem coincide with the rays in the optical problem.

Huygens (1690). $V(x, y, z, x', y', z')$ the time taken by light to travel from (x, y, z) to (x', y', z')
Secondary waves.

Disturbance occurs at (x, y, z) at time t , at t' will extend over surface with eqn Σ in co-ords x', y', z'
is $V(x, y, z, x', y', z') = t' - t$.

Wave front σ at time t' , Σ at t .
Normal to σ at (x', y', z') (l', m', n')
to Σ at (x, y, z) (l, m, n)

σ is envelope of surfaces V corresponding to point on σ
 $\frac{\partial V}{\partial x} dx + \frac{\partial V}{\partial y} dy + \frac{\partial V}{\partial z} dz = 0$

must be satisfied by all these values of dx, dy, dz that correspond to directed in tangent plane to σ
ie for which $l dx + m dy + n dz = 0$

$$\therefore \frac{l}{l} \frac{\partial V}{\partial x} = \frac{m}{m} \frac{\partial V}{\partial y} = \frac{n}{n} \frac{\partial V}{\partial z} \quad (2)$$

(l', m', n') being normal to surface V at (x', y', z') we have

$$\frac{l'}{l'} \frac{\partial V}{\partial x'} = \frac{m'}{m'} \frac{\partial V}{\partial y'} = \frac{n'}{n'} \frac{\partial V}{\partial z'} \quad (3)$$

A ray of light passing through (x, y, z) in direction (l, m, n) at t will pass through (x', y', z') in direction (l', m', n') at time t'

$$l'^2 + m'^2 + n'^2 = 1 \quad (4)$$

Eqs (1), (2), (3), (4) are 6 eqns, suff to determine x', y', z', l', m', n' in terms of x, y, z, l, m, n . So the single function $V(x, y, z, x', y', z')$ completely determines the behavior of light (further division from geometrical optics)

Whitaker 2 W
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These are not differential eqs. They explicitly
give the quantities in question.

$V(x, y, z, x', y', z')$ defines a contact transformation

Action function $S = \int_{t_0}^{t_1} 2T dt$.

Hamilton's Principal function $W = -Et + S$

$$\begin{aligned} W &= \int 2T dt - \int E dt \\ &= \int 2T - E \cdot dt = \int 2T - (T + V) \cdot dt \\ &= \int T - V dt = \int L dt. \end{aligned}$$

Hamilton's Principle. $\int L dt$ is stationary for actual orbit when small deviations considered

Schrödinger emphasizes that S is to be expressed in terms of the co-ordinates.

Simplest example Particle in plane. $V = 0$. Then $T = E$
 If particle starts at origin at time $t=0$, at time t_1

$$S = \int_0^{t_1} 2T dt = 2Et_1.$$

To reach (x, y) at time t_1 , particle must have $v_0 t_1 = \sqrt{x^2 + y^2}$ $E = \frac{1}{2} m v_0^2 \therefore v_0 = \sqrt{\frac{2E}{m}}$
 $\therefore t_1 = \sqrt{\frac{m}{2E}} \sqrt{x^2 + y^2} \therefore S = 2Et_1 = \sqrt{2mE} \sqrt{x^2 + y^2}$

$$W = -Et + \sqrt{2mE} \sqrt{x^2 + y^2}$$

The surface $W=0$ at time t has

$$\sqrt{2mE} \sqrt{x^2 + y^2} = Et$$

$$\therefore \sqrt{x^2 + y^2} = \sqrt{\frac{E}{2m}} t$$

$$S = \sqrt{2mE} \sqrt{x^2 + y^2} = m v_0 \sqrt{x^2 + y^2}$$

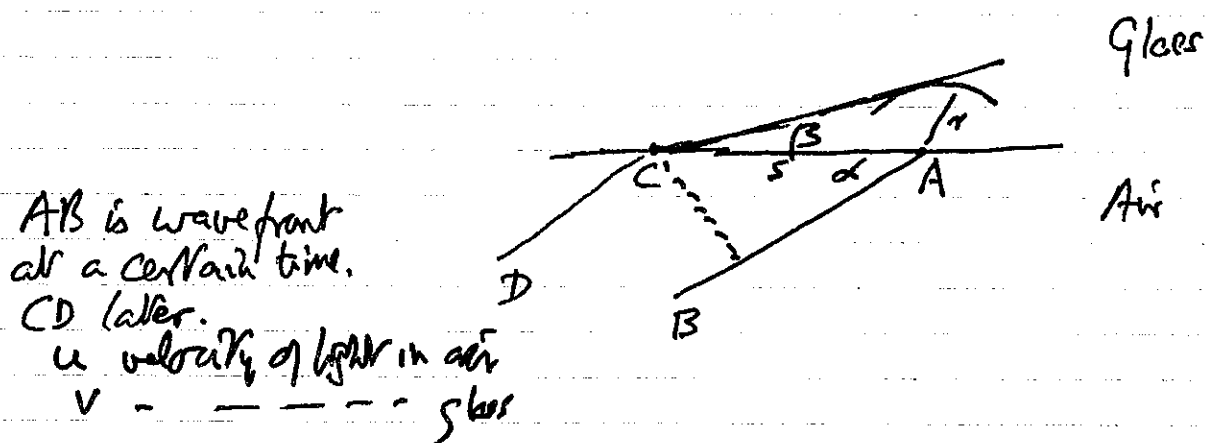
$$\frac{\partial S}{\partial x} = \frac{m v_0 x}{\sqrt{x^2 + y^2}} \quad \frac{\partial S}{\partial y} = \frac{m v_0 y}{\sqrt{x^2 + y^2}}$$

These are the components of the momentum parallel to the axes.

1.

W
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Optics: refraction.



If $AC = s$, the wave has moved through a distance $s \sin \alpha$ as it goes from AB to CD.

$$\text{Time} = \frac{s \sin \alpha}{u}$$

When it has just reached C, the disturbance has had this time to spread out from A.

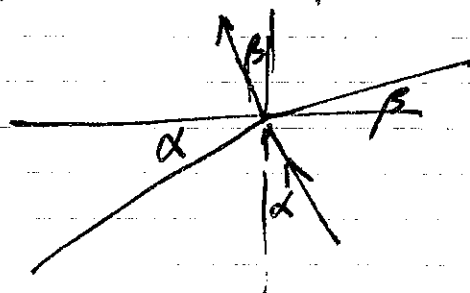
Moving with velocity v it can go $\frac{s \sin \alpha}{u} v = r$

$$\therefore \frac{r}{s} = \frac{v}{u} \sin \alpha \text{ which is constant}$$

$$\text{Thus } \sin \beta = \frac{r}{s} = \frac{v}{u} \sin \alpha$$

$$\text{So } \frac{\sin \beta}{\sin \alpha} = \frac{v}{u}$$

Rays are perpendicular to plane wave fronts

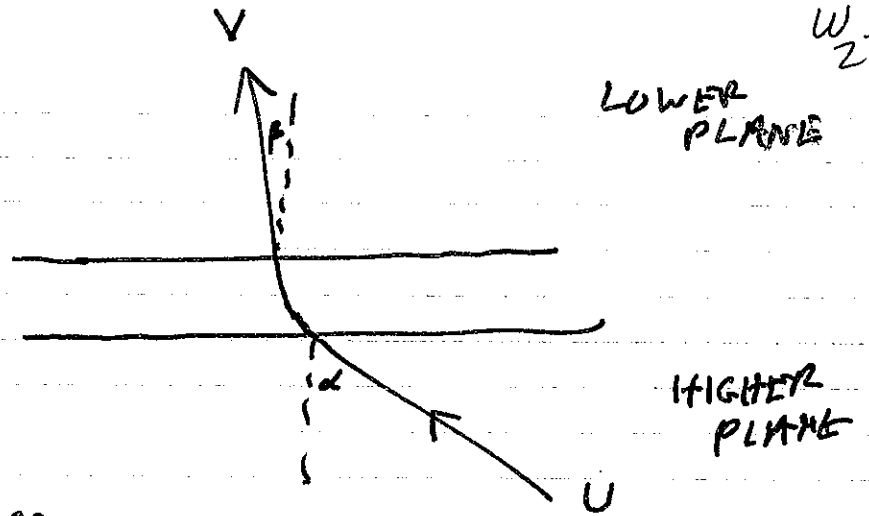


Thus α, β are angles between original ray, and

refracted ray and the normal to interface.

Note that, on wave theory, light travels more slowly in glass.

(2)
W
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Particle Theory

Imagine a green on a golf course that has two level parts with a slope between.

We suppose the slope has the same cross section everywhere, so that it has no tendency to divert the ball to left or right.

Let h be the difference in height of the parts.

Momentum is conserved in x -direction.

$$U \sin \alpha = V \sin \beta$$

From energy $\frac{1}{2} m V^2 = \frac{1}{2} m U^2 + mgh$

$$\therefore V^2 = U^2 + 2gh.$$

$$\frac{\sin \beta}{\sin \alpha} = \frac{U}{V}$$

Now $\frac{V^2}{U^2} = 1 + \frac{2gh}{U^2}$ so $\frac{V}{U}$ will

differ from a constant unless U is constant. If U is constant, V will be. To get the known law, we have to assume that all rays of light travel at a rate, which is characteristic of the medium.

The velocity in glass would have to be higher than in air.

Problem das 48

Wie weit 34 $I = 2-2$

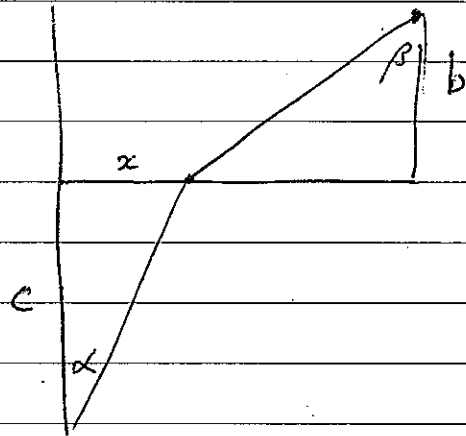
③

W

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$$\text{Time} = \frac{\sqrt{c^2 + x^2}}{u} + \frac{\sqrt{(a-x)^2 + b^2}}{v}$$

$$0 = \frac{dx}{dx}$$



$$0 = \frac{x}{u\sqrt{c^2 + x^2}} - \frac{a-x}{v\sqrt{(a-x)^2 + b^2}}$$

$$\frac{x}{\sqrt{c^2 + x^2}} = \sin \alpha \quad \frac{a-x}{\sqrt{(a-x)^2 + b^2}} = \sin \beta$$

$$0 = \frac{\sin \alpha}{u} - \frac{\sin \beta}{v} \text{ so } \frac{\sin \beta}{\sin \alpha} = \frac{v}{u} \text{ as required!}$$

Least Action $\int T dt$ is a minimum

$$\int \frac{1}{2} U^2 dt = \int \frac{1}{2} U ds$$

so $\int U ds + \int V ds$ is

to be a minimum

i.e. $U \cdot PQ + V \cdot QR$ a minimum

$$U \sqrt{x^2 + c^2} + V \sqrt{(a-x)^2 + b^2}$$

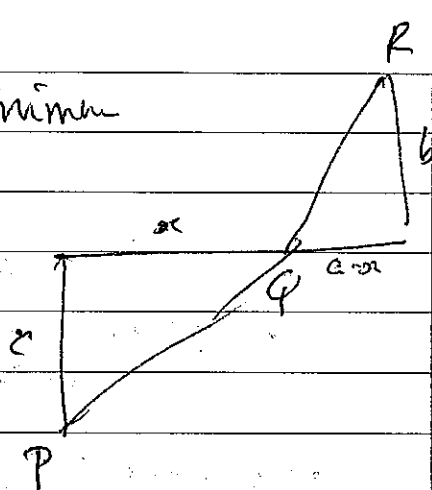
This is the same as before, but with

U for $\frac{1}{a}$, V for $\frac{1}{v}$.

$$\text{so gives } \frac{\sin \beta}{\sin \alpha} = \frac{1/V}{1/U} = \frac{U}{V}$$

⑥

W
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Hamilton. page A3 in SaNardau file.

The role of phase is played by W

$$W = \int_0^t (T - V) dt = \int_0^t T - (E - T) dt = \int_0^t 2T - E dt$$

$$= \int_0^t 2T dt - Et = S - Et.$$

$$\int_{t_0}^t L(q, \dot{q}, t) dt$$

$$= \int_{t_0}^t \left(\frac{\partial L}{\partial q} \delta q + \frac{\partial L}{\partial \dot{q}} \delta \dot{q} + \frac{\partial L}{\partial t} \delta t \right) dt$$

$$= \left[\frac{\partial L}{\partial \dot{q}} \delta q \right]_{t_0}^t$$

$$\frac{\partial L}{\partial \dot{q}} \delta q_{s1} - \frac{\partial L}{\partial \dot{q}} \delta q_{s0}$$

$$\frac{\partial S}{\partial q_s} = \frac{\partial L}{\partial \dot{q}} = p_s$$

Early quantum theory.

1900 Planck Radiation of frequency ν associated with packets of energy, $h\nu$.

1905 Einstein shows this in agreement with observed facts for photoelectric effect.

Classically an accelerated electron radiates and thus loses energy. Electrons would spiral down into nucleus and disappear. Impossible on this basis to explain discrete lines in the spectrum.

Bohr 1913 made revolutionary proposal.

- (i) most of the time electrons do not radiate energy, but remain in stable orbits. (ii) Radiation occurs when an electron suddenly passes from one such orbit to another. (iii) If the orbits have energies E_n and E_m , the frequency of the radiation is given by $\nu = \frac{E_n - E_m}{h}$.

Conjugate quantities.

A theory known as general dynamics gives results that are not confined to a particular problem, but apply (with certain restrictions) to all dynamical systems.

The uncertainty principle relates two quantities known as conjugate: the more precisely one is measured, the less information there can be about the other. The most familiar example is position, x , and momentum mx .

Unfamiliar examples constitute an immense family: the conjugate quantities are a generalized coordinate and its generalized momentum.

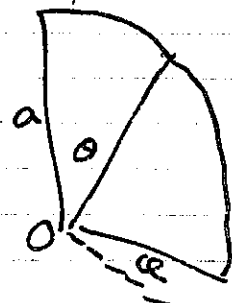
Examples of generalized coordinates:

r, θ in polar coordinates

θ, ϕ for double pendulum

Latitude and longitude for particle moving on a sphere.

For a particle constrained to move on a sphere (say by a thread joining it to point O), it is often convenient to use the longitude, ϕ , and θ , the latitude subtracted from a right angle, so $\theta = 0$ gives North Pole, $\theta = \frac{\pi}{2}$ the equator.



Q2

W
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The kinetic energy is given by T ,

$$T = \frac{1}{2} m (a^2 \dot{\theta}^2 + a^2 \sin^2 \theta \dot{\phi}^2)$$

The momentum conjugate to θ is given by

$$\frac{\partial T}{\partial \dot{\theta}} = m a^2 \dot{\theta}$$

The momentum conjugate to ϕ is

$$\frac{\partial T}{\partial \dot{\phi}} = m a^2 \sin^2 \theta \dot{\phi}$$

which we can recognize as the angular momentum about ON , where N is the North pole.

The simplest example is for a single mass.

$$T = \frac{1}{2} m (\dot{x}^2 + \dot{y}^2 + \dot{z}^2)$$

$$\frac{\partial T}{\partial \dot{x}} = m\dot{x}, \quad \frac{\partial T}{\partial \dot{y}} = m\dot{y}, \quad \frac{\partial T}{\partial \dot{z}} = m\dot{z}$$

the three components of momentum.

For a rotating flywheel, $T = \frac{1}{2} I \dot{\theta}^2$ and the angular momentum is $\frac{\partial T}{\partial \dot{\theta}} = I \dot{\theta}$.

There is a perfect analogy here with a mass moving in 1 dimension. $T = \frac{1}{2} m \dot{x}^2$, $\partial T / \partial \dot{x} = m \dot{x}$.

In 1788 Lagrange showed that what happened in a system was completely determined by the form of the expression for T , the kinetic energy and V , the potential energy.

If, for example, the position of a system is determined by 3 generalized co-ordinates, q_1, q_2, q_3 , the equations of motion for the system are, with $L = T - V$,

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_1} \right) = \frac{\partial L}{\partial q_1}, \quad \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_2} \right) = \frac{\partial L}{\partial q_2}, \quad \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_3} \right) = \frac{\partial L}{\partial q_3}$$

There is an unbroken chain from Lagrange's work in 1788, through Hamilton's (around 1835) work, showing a method equally applicable to optics and mechanics, to

23.4.94

Schrödinger's wave mechanics, 1926

In Hamilton's work it was found convenient to work with p & q , rather than with $\dot{q}$ & q .

The energy equation for a mass in 3-D is

$$\frac{1}{2} m \dot{x}^2 + \frac{1}{2} m \dot{y}^2 + \frac{1}{2} m \dot{z}^2 + V(x, y, z) = E$$

As $p_1 = m\dot{x}$ $p_2 = m\dot{y}$ $p_3 = m\dot{z}$, the energy equation takes the form

$$\frac{p_1^2}{2m} + \frac{p_2^2}{2m} + \frac{p_3^2}{2m} + V = E.$$

Schrödinger's rule for writing the wave equation is to replace p_1 by $+\frac{\hbar}{i} \frac{\partial}{\partial x}$ etc.

Then we have

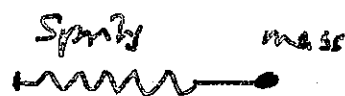
$$-\frac{\hbar^2}{2m} \left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} \right) + V\psi = E\psi.$$

[There is a more general method, depending on the Hamilton-Jacobi equation, that can be used when kinetic energy is not simply a sum of squares. See Remark & Exer. p 578.]

SHM 1. W

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For simple harmonic oscillator



$$T = \frac{1}{2} m \dot{x}^2 \quad V = \frac{1}{2} k x^2$$

This leads to $\frac{p^2}{2m} + \frac{1}{2} k x^2 = E$

and so to $-\frac{\hbar^2}{2m} \psi'' + \frac{1}{2} k x^2 = E$

so $\psi'' + \frac{2m}{\hbar^2} (E - \frac{1}{2} k x^2) \psi = 0$.

Let $x = a v$ and choose a so that eqn. takes form $\psi_{vv}'' + (1 - v^2) \psi = 0$.

With $x = a v$, $\psi'' = \frac{1}{a^2} \psi_{vv}''$

Coeff of ψ is $-\frac{2m}{\hbar^2} \cdot \frac{1}{2} k a^2$

So we want $\frac{1}{a^2} = \frac{mk}{\hbar^2} a^2$

$$a^4 = \frac{\hbar^2}{mk}$$

The equation becomes

$$\psi_{vv}'' + \left(\frac{2m a^2 E}{\hbar^2} - v^2 \right) \psi = 0$$

i.e. $\psi_{vv}'' + \left(\frac{2E}{\hbar} \sqrt{\frac{m}{k}} - v^2 \right) \psi = 0$.

Now, for SHM, $x = \sin \omega t$ and so, from $m\ddot{x} + kx = 0$ $\omega^2 = k/m$

Thus the constant in the bracket is $\frac{4\pi E}{\hbar \omega}$

$\sin \omega t$ has the period frequency $\omega/2\pi$

so $\omega = 2\pi \nu_0$ where ν_0 is the frequency associated with the system.

Thus the equation takes the form

$$\psi_{vv}'' + \left(\frac{2E}{\hbar \nu_0} - v^2 \right) \psi = 0$$

We consider the equation $\psi'' + (A - x^2)\psi = 0$.

For large x , this resembles $\psi'' - x^2\psi = 0$.

If ~~$\psi = e^{\alpha x^2} u$~~ we get

Let $\psi = e^{\alpha x^2} u$. Then $\psi' = e^{\alpha x^2} u' + 2\alpha x e^{\alpha x^2} u$

$$\psi'' = e^{\alpha x^2} u'' + 4\alpha x e^{\alpha x^2} u' + u(2\alpha e^{\alpha x^2} + 4\alpha^2 x^2 e^{\alpha x^2})$$

So, removing the factor $e^{\alpha x^2}$ we have

$$0 = u'' + 4\alpha x u' + u(A + 2\alpha + (4\alpha^2 - 1)x^2)$$

So we take $4\alpha^2 = 1$, $\alpha = \pm \frac{1}{2}$.

We require ψ to be bounded for all values of x , which will not be the case if it involves $e^{\pm \frac{1}{2}x^2}$. So we take $\alpha = -\frac{1}{2}$.

Then
$$0 = u'' - 2xu' + u(A - 1)$$

If $u \sim cx^p$ for small x , we find

$2ct \sim cx^{p-2} [p(p-1)]$. There is no other term to cancel this, so $c p(p-1) = 0$

If $c \neq 0$ we must have $p=0$ or $p=1$.

Let
$$u = \sum_{n=0}^{\infty} a_n x^n \quad (a_0 \neq 0 \text{ is allowed})$$

Substitute in the differential eqn.

$$0 = \sum_{n=0}^{\infty} n(n-1) a_n x^{n-2} - \sum_{n=0}^{\infty} 2n a_n x^n + (A-1) \sum_{n=0}^{\infty} a_n x^n$$

From the coefficient of x^n

$$0 = (n+2)(n+1) a_{n+2} + a_n (A-1-2n)$$

$$\therefore a_{n+2} = \frac{2n - A + 1}{(n+1)(n+2)} a_n$$

If $a_0 = 1$, only even terms will occur,

so $n = 2r$ and $a_{2r+2} x^{2r+2}$ is $(r+1)^{\text{th}}$ term, c_{r+1}

$$\text{So } c_{r+1} = \frac{4r - A + 1}{(2r+1)(2r+2)} c_r x^2$$

STAT 3.

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$$\frac{c_{t+1}}{c_t} = \frac{4t - A + 1}{(2t+1)(2t+2)} x^2 \sim \frac{x^2}{t}$$

Now e^{x^2} has $c_t = \frac{x^{2t}}{t!}$ $c_{t+1} = \frac{x^{2t+2}}{(t+1)!}$

so $\frac{c_{t+1}}{c_t} = \frac{x^2}{t+1} \sim \frac{x^2}{t}$

This suggests that $u \sim e^{x^2}$, so $\psi = e^{-\frac{1}{2}x^2} u$ behaves like $e^{-\frac{1}{2}x^2} e^{x^2} = e^{\frac{1}{2}x^2}$, which $\rightarrow \infty$ as $x \rightarrow +\infty$ or $x \rightarrow -\infty$, so is not acceptable.

The only way out of this is if the series for u is a polynomial, not an infinite series.

If $a_{n+2} = 0$ but $a_n \neq 0$ we have $2n - A + 1 = 0$ i.e. $A = 2n + 1$.

Now $A = \frac{2E}{h\nu_0}$. $\frac{2E}{h\nu_0} = 2n + 1$

means $E = (n + \frac{1}{2}) h\nu_0$.

Thus particular discrete energies are picked out as being possible.

Note that $E = 0$ is not possible.

This is a departure from early quantum theory. The changes in E are still multiples of $h\nu_0$.

Schrodinger's Equation in One Dimension *

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V(x) \Psi.$$

Let $\Psi = X(x)T(t)$ $X(x)$ function of x
 $T(t)$ function of t (not KE).

$$\text{Then } i\hbar XT' = -\frac{\hbar^2}{2m} X''T + VXT$$

Divide by XT

$$i\hbar \frac{T'}{T} = -\frac{\hbar^2}{2m} \frac{X''}{X} + V$$

We take $T = e^{+Et/\hbar}$

$$\text{Then } i\hbar \frac{T'}{T} = i\hbar \frac{d}{dt} \ln T = i\hbar \frac{d}{dt} \left(+\frac{Et}{\hbar} \right) = +E$$

$$\text{Then } E = -\frac{\hbar^2}{2m} \frac{X''}{X} + V$$

$$\text{and } \frac{\hbar^2}{2m} X'' + (E - V)X = 0$$

We usually take ψ for X

$$\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + (E - V)\psi = 0.$$

* Schrodinger used $\frac{\partial^2 \Psi}{\partial t^2}$, not $\frac{\partial \Psi}{\partial t}$. But accounts lead to $T = e^{Et/\hbar}$.

Force free field. $V=0$. $E = K.E.$ positive.

$$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2} \psi = 0$$

Let $\frac{2mE}{\hbar^2} = k^2$

Then $\frac{d^2\psi}{dx^2} + k^2\psi = 0.$

Solutions e^{ikx} and $e^{-ikx}.$

Then $\psi_1 = e^{ikx - iEt/\hbar}$ or $\psi_2 = e^{-ikx - iEt/\hbar}$

ψ_1 takes a constant value if $ikx - iEt/\hbar$ is constant. If the value is zero $x = \frac{E}{\hbar k} t$

i.e. the wave front moves to the right

and we think of this as representing an electron moving to the right. $|\psi_1|^2 = 1$

So the electron is equally likely to be anywhere.

In the same way, ψ_2 represents an electron moving to the left, equally likely to be anywhere.

The momentum operator is $p = \frac{\hbar}{i} \frac{\partial}{\partial x}$

For ψ_1 , $\frac{\hbar}{i} \frac{\partial \psi_1}{\partial x} = \frac{\hbar}{i} ik e^{ikx - iEt/\hbar}$
 $= \hbar k \psi_1$

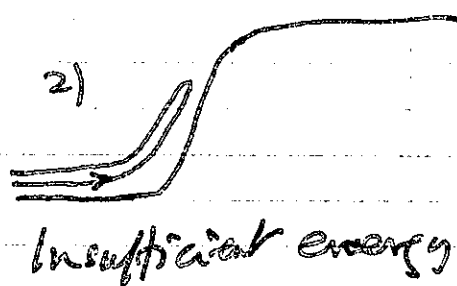
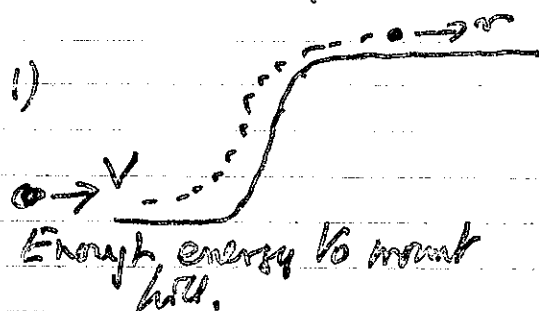
ψ_1 is an eigenvalue for $\frac{\hbar}{i} \frac{\partial}{\partial x}.$

This is interpreted to mean that the momentum has a definite value.

Thus for ψ_1 the momentum is exactly known, the position absolutely unknown.

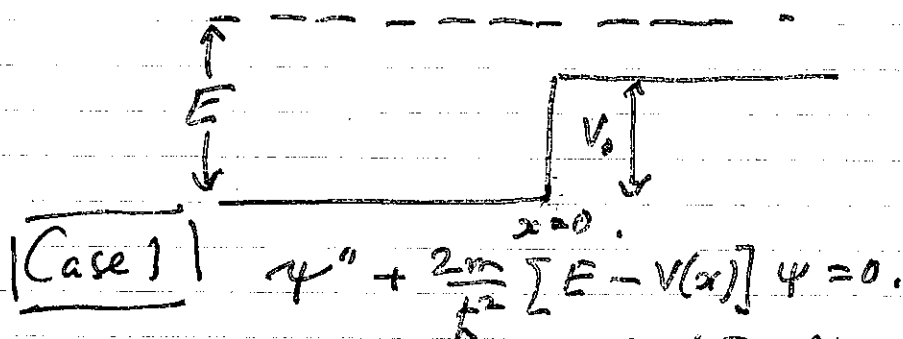
The same is true for $\psi_2.$

Potential Step.



What happens with wave mechanics differs in both cases.

We are going to neglect the transition period, so our energy diagram, in case (1) will be



$$\psi'' + \frac{2m}{\hbar^2} [E - V(x)] \psi = 0.$$

Write $\frac{2mE}{\hbar^2} = k^2$ $\frac{2m(E - V_0)}{\hbar^2} = q^2.$

For $x < 0$, $V(x) = 0$, eqn is $\psi'' + k^2 \psi = 0$

with general solution $\psi(x) = P e^{ikx} + R e^{-ikx}$

If V_0 were zero, R would be zero, and $\psi = e^{ikx}$

would represent a wave proceeding unhindered.

The wave does in fact proceed unhindered in the region $x > 0$. Here $\psi'' + q^2 \psi = 0$.

e^{-iqx} would represent a wave moving left. As there is no source of electron to the right, we do not use this solution. Thus for $x > 0$

$$\psi = A e^{iqx}.$$

We require ψ and ψ' to be continuous.

$$x < 0$$

$$\psi = P e^{ikx} + R e^{-ikx}$$

$$\psi' = ik(P e^{ikx} - R e^{-ikx})$$

$$x > 0$$

$$A e^{iqx}$$

$$iq A e^{iqx}$$

For $x > 0$ we have

$$P + R = A$$

$$P - R = \frac{q}{k} A$$

$$\therefore P = A \left(\frac{q+k}{2k} \right) \quad R = A \frac{k-q}{2k}$$

As $q < k$ in case (1) it is impossible for $R=0$.
There is bound to be a reflected wave.

The incoming wave is $P e^{ikx}$. If we assume $P=1$, so e^{ikx} coming in, $A = \frac{2k}{q+k}$ and

accordingly $R = \frac{k-q}{k+q}$. The transmitted wave is given by $\psi = \frac{2k}{q+k} e^{iqx}$

Case 2 Insufficient energy to reach top of hill.

$E - V_0$ is negative

$$\text{Let } \frac{2m(E-V_0)}{\hbar^2} = -b^2. \quad (b > 0)$$

$$\text{Then, for } x=0, \quad \psi'' - b^2 \psi = 0.$$

Solution, e^{bx} and e^{-bx} . $e^{bx} \rightarrow +\infty$, no good.

$$\text{So } \psi = C e^{-bx} \text{ for } x > 0.$$

$$x < 0$$

$$\psi: P e^{ikx} + Q e^{-ikx}$$

$$C e^{-bx}$$

$$\psi' = ik(P e^{ikx} - Q e^{-ikx})$$

$$-b C e^{-bx}$$

For $x > 0$, continuity of ψ, ψ' .

$$P + Q = C$$

$$ik(P - Q) = -bC$$

$$\text{So } P - Q = i \frac{b}{k} C.$$

$$\therefore P = \frac{1}{2} \left(1 + i \frac{b}{k} \right) C$$

$$Q = \frac{1}{2} \left(1 - i \frac{b}{k} \right) C$$

If we want $P=1$, then $Q = \frac{1 - ib/k}{1 + ib/k}$ Note $|Q|=1$ When $P=1$.

In a sense, no loss.

Tunnel Effect.

W41

In 1 dimension the wave eqn is $\frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2} (E - V) \psi = 0$

Classically, $E - V$ represents kinetic energy, which must be positive or zero. It is impossible for the mass to reach (or pass through) any region in which $E - V$ is negative.

Suppose quantities are chosen that $\frac{2m}{\hbar^2} (E - V)$ is $+1$ for $-k < x < k$ and -1 for $|x| > k$.

The potential energy diagram is shown here. The particle has just half the energy needed (classically) to escape from the interval $(-k, k)$.



For $x > k$ we have $\frac{d^2 \psi}{dx^2} - \psi = 0$

$$\therefore \psi = A e^x + B e^{-x}$$

We must take $A = 0$ for ψ to remain finite and bounded everywhere, so $\psi = B e^{-x}$.

In the same way, for $x < -k$, $\psi = C e^x$.
Between $-k$ and k , $\frac{d^2 \psi}{dx^2} + \psi = 0$.

$$\text{So } \psi = P e^{ix} + Q e^{-ix}.$$

We require ψ and $\frac{d\psi}{dx}$ continuous.

$$\text{In } x < -k \quad \psi = C e^x \quad \frac{d\psi}{dx} = C e^x$$

$$\text{In } -k < x < k \quad \psi = P e^{ix} + Q e^{-ix}, \quad \frac{d\psi}{dx} = i P e^{ix} - i Q e^{-ix}$$

$$\text{For } x > k \quad \psi = B e^{-x} \quad \frac{d\psi}{dx} = -B e^{-x}$$

Hence

$$(1) \quad C e^{-k} = P e^{-ik} + Q e^{ik} \quad C e^{-k} = i P e^{-ik} - i Q e^{ik} \quad (2)$$

$$(3) \quad B e^{-k} = P e^{ik} + Q e^{-ik} \quad -B e^{-k} = i P e^{ik} - i Q e^{-ik} \quad (4)$$

$$\text{From (1) \& (2)} \quad P e^{-ik} + Q e^{ik} = i P e^{-ik} - i Q e^{-ik}$$

$$\text{So } P(1-i) e^{-ik} + Q(1+i) e^{ik} = 0 \quad (5)$$

$$\text{From (2) \& (4)} \quad P(1+i) e^{ik} + Q(1-i) e^{-ik} = 0 \quad (6)$$

A solution other than $P=0, Q=0$ is only possible if determinant $= 0$.

$$0 = \begin{vmatrix} (1-i) e^{-ik} & (1+i) e^{ik} \\ (1+i) e^{ik} & (1-i) e^{-ik} \end{vmatrix}$$

That is $(1-i)^2 e^{-2ik} = (1+i)^2 e^{2ik}$

i.e. $-2ie^{-2ik} = 2ie^{2ik}$

i.e. $e^{4ik} = -1$

$e^{i\theta}$ is the point on unit circle at angle θ . -1 is at π .

$\therefore 4ik = \pi + 2n\pi$

$k = \frac{\pi}{4} + n\frac{\pi}{2}$

Only such values of k allow a non-zero solution.

In practice, the situation would be reversed: k would be given, and only discrete values of E would be possible.

Consider the value $k = \pi/4$.

$P + Q \frac{1+i}{1-i} e^{2ik} = 0$

$1+i = i(1-i)$ so $P + ie^{2ik} Q = 0$

$e^{2ik} = e^{i\pi/2} = i \therefore P - Q = 0$

Take $P = Q = 1$.

Then $C e^{-\pi/4} = e^{-ik} + e^{ik} = 2 \cos k$ $e^{ix} + e^{-ix} = 2 \cos x$
 $= 2 \cos \frac{\pi}{4} = \sqrt{2}$

$C = \sqrt{2} e^{\pi/4}$

$B e^{-k} = e^{ik} + e^{-ik} = 2 \cos k = \sqrt{2}$

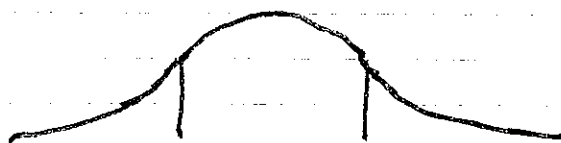
$B = \sqrt{2} e^{\pi/4}$

Thus

$x < -\frac{\pi}{4} \quad \psi = \sqrt{2} e^{\pi/4} e^{+x}$

$-\frac{\pi}{4} < x < \frac{\pi}{4} \quad \psi = 2 \cos x$

$x > \pi/4 \quad \psi = \sqrt{2} e^{\pi/4} e^{-x}$



More interesting, potential well for negative E .

$$\text{Let } \frac{2mE}{\hbar^2} = -k^2$$

The solutions outside well that are acceptable are

$$\psi(x) = C_1 e^{kx} \text{ for } x < -a$$

$$\psi(x) = C_2 e^{-kx} \text{ for } x > a.$$

These are real, and it is convenient to write solutions inside well as

$$u(x) = A \cos qx + B \sin qx$$

$$q^2 = \frac{2m}{\hbar^2} (E + V_0). \text{ We suppose } V_0 > 0$$

and E negative but $E > -V_0$.

At $x = -a$

$$\psi = C_1 e^{-ka}$$

$$\text{and } A \cos qa - B \sin qa \quad (1)$$

$x = +a$

$$\psi = C_2 e^{-ka}$$

$$A \cos qa + B \sin qa. \quad (2)$$

To left

~~At $x = -a$~~

$$\psi' = k C_1 e^{kx}$$

$$\text{and } -q A \sin qx + q B \cos qx.$$

So at $x = -a$

$$k C_1 e^{-ka}$$

$$= q (A \sin qa + B \cos qa) \quad (3)$$

To right

$$\psi' = -k C_2 e^{-ka}$$

$$\text{and } -q A \sin qa + q B \cos qa$$

$\therefore$

$$-k C_2 e^{-ka} = -q A \sin qa + q B \cos qa \quad (4)$$

Substitute in (3) from (1)

$$k (A \cos qa - B \sin qa) = q (A \sin qa + B \cos qa) \quad (5)$$

In (4) & (2),

$$-k (A \cos qa + B \sin qa) = q (A \sin qa - B \cos qa)$$

Potential well.

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

$$\psi'' + \frac{2m}{\hbar^2}(E - V(x))\psi = 0.$$

$$\text{Let } k^2 = \frac{2mE}{\hbar^2} \quad q^2 = \frac{2m}{\hbar^2}(E + V_0)$$

$$\text{In } x < -a, \quad \psi'' + k^2\psi = 0. \quad (1)$$

$$\psi = e^{ikx} + Re^{-ikx} \quad R \text{ because reflection can occur.}$$

$$\text{In } -a < x < a \quad \psi'' + q^2\psi = 0 \quad (2)$$

$$\psi = Ae^{iqx} + Be^{-iqx}$$

For $x > a$ eq (1) again, but nothing coming from right

$$\psi = Ce^{ikx}$$

$$\text{Continuity of } \psi \text{ at } x = -a \quad e^{-ika} + Re^{ika} = Ae^{-iga} + Be^{iga} \quad (i)$$

$$\text{of } \psi \text{ at } x = +a \quad Ce^{ika} = Ae^{iga} + Be^{-iga} \quad (ii)$$

$$\text{of } \psi' \text{ at } x = -a \quad ik(e^{-ika} - Re^{ika}) = iq(Ae^{-iga} - Be^{iga}) \quad (iii)$$

$$\text{at } x = +a \quad ikCe^{ika} = iq(Ae^{iga} - Be^{-iga}) \quad (iv)$$

These can be solved to give R , for the amount of reflected wave, and C , the amount of transmitted.