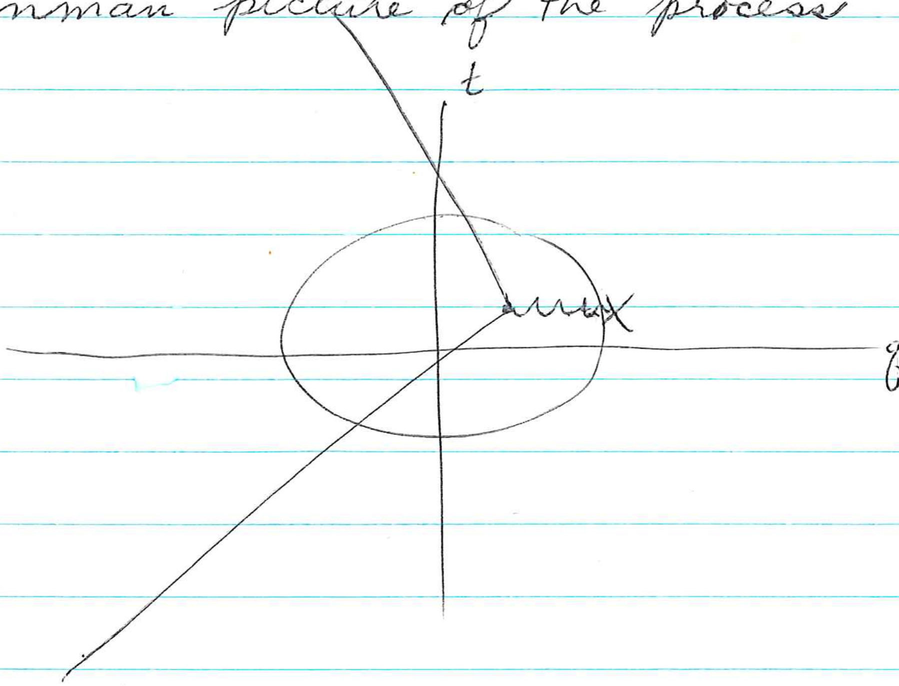
June 26, 1979 phonons 30
potential scattering p.35

To understand scattering by an external electro-magn. field of compact support in space-time. Notice that a closed compactly supported 2-form in $\mathbb{R}^n$ with $n > 2$ is the differential of a compactly supported 1-form. Hence it it reasonable to suppose, even for $n=2$, that A has compact support.

What I want to do now is to compute the scattering to various orders in A, or better, [redacted] as a power series in the charge e. I have this Feynman picture of the process



and the problem is how to describe it. Let's begin by listing the trajectories when $e = 0$. Each trajectory is described by (p, q) where p is its momentum and q is the position at $t=0$. The equations of motion are (non-relativistic case)

$$m\ddot{q} = +eE(t,q) \qquad\qquad E(t,q) = -\frac{\partial\varphi}{\partial q} - \frac{\partial A}{\partial t}$$

$$p = m\dot{q} + eA$$

$$\ddot{q}(t) = \ddot{q}_0(t) + e\ddot{q}_1(t) + e^2\ddot{q}_2(t) + \cdots$$
$$= eE(t, q_0 + eq_1 + \cdots)$$
$$= eE(t, q_0) + e^2\frac{\partial E}{\partial q} q_1 + \cdots$$

This gives
$$\ddot{q}_0 = 0$$
$$\ddot{q}_1 = E(t, q_0(t))$$
$$\ddot{q}_2 = \frac{\partial E}{\partial q}(t, q_0(t))\, q_1(t)$$
$$\cdots$$

So start with [redacted] a specific solution for q_0
$$q_0(t) = [redacted]\ \alpha t + \beta$$
Then we have to solve
$$\ddot{q}_1(t) = E(t, \alpha t + \beta)$$
with the boundary conditions that $q_1 \equiv 0$, $t \ll 0$. Hence one needs the forward Green's function for the operator $\frac{d^2}{dt^2}$ which is
$$G(t,t') = \begin{cases} 0 & t < t' \\ t - t' & t > t' \end{cases}$$

so
$$q_1(t) = \int G(t,t')\, E(t', \alpha t' + \beta)\, dt'$$
$$= \int_{-\infty}^{t} (t-t')\, E(t', \alpha t' + \beta)\, dt'$$

Therefore the first order scattering converts $q = \alpha t + \beta$ into
$$\alpha t + \beta + e\int_{-\infty}^{\infty} (t-t')\, E(t', \alpha t' + \beta)\, dt'$$
and here $m = 1$.

The 2nd order term is

$$q_2(t) = \int_{-\infty}^{t} (t-t') \frac{\partial E}{\partial q}(t', \alpha t' + \beta)\, q_1(t')\, dt'$$

$$= \int_{-\infty}^{t} dt_1 \int_{-\infty}^{t_1} dt_2 \;\; (t-t_1) \frac{\partial E}{\partial q}(t_1, \alpha t_1 + \beta)(t_1 - t_2)\, E(t_2, \alpha t_2 + \beta)$$

Next let's try the Hamilton-Jacobi approach. The Hamilton-Jac. equation in the non-rel. case is

$$-\frac{\partial S}{\partial t} = e\varphi + \frac{1}{2m}\left(\frac{\partial S}{\partial q} - eA\right)^2$$

Take $m=1$ and look for a perturbation expansion

$$S = S_0 + eS_1 + e^2 S_2 + \cdots$$

$$-\left(\frac{\partial S_0}{\partial t} + e\frac{\partial S_1}{\partial t} + e^2\frac{\partial S_2}{\partial t}\right) = e\varphi + \frac{1}{2}\left[\left(\frac{\partial S_0}{\partial q}\right)^2 - e\,2\frac{\partial S_0}{\partial q}A + e\,2\frac{\partial S_0}{\partial q}\frac{\partial S_1}{\partial q}\right]$$

$$= e\varphi + \frac{1}{2}\left[\frac{\partial S_0}{\partial q} + e\left(\frac{\partial S_1}{\partial q} - A\right) + e^2\frac{\partial S_2}{\partial q}\right]^2$$

$$= e\varphi + \frac{1}{2}\left[\left(\frac{\partial S_0}{\partial q}\right)^2 + e\,2\frac{\partial S_0}{\partial q}\left(\frac{\partial S_1}{\partial q} - A\right) + e^2\,2\frac{\partial S_0}{\partial q}\frac{\partial S_2}{\partial q} + e^2\left(\frac{\partial S_1}{\partial q} - A\right)^2\right]$$

This leads to the equations

$$-\frac{\partial S_0}{\partial t} = \frac{1}{2}\left(\frac{\partial S_0}{\partial q}\right)^2 \qquad -\frac{\partial S_1}{\partial t} = \varphi + \underbrace{\frac{\partial S_0}{\partial q}}_{p}\left(\frac{\partial S_1}{\partial q} - A\right)$$

$$-\frac{\partial S_2}{\partial t} = \frac{\partial S_0}{\partial q}\frac{\partial S_2}{\partial q} + \frac{1}{2}\left(\frac{\partial S_1}{\partial q} - A\right)^2$$

We start with a "plane wave" solution for S_0 namely

$$S_0 = -Et + pq$$

where $E = \frac{p^2}{2}$ and p is a given momentum. Then you get

$$\left(\frac{\partial}{\partial t} + p\frac{\partial}{\partial q}\right)S_1 = -\varphi + pA$$

$$\left(\frac{\partial}{\partial t} + p\frac{\partial}{\partial q}\right)S_2 = -\frac{1}{2}\left(\frac{\partial S_1}{\partial q} - A\right)^2$$

The first formula says that we obtain S_1 by integrating, over straight lines $q = pt + \text{const}$, the form $-\varphi dt + A dx$.

Let's do the relativistic version. The basic energy relation is

$$\left(\frac{E - e\varphi}{c}\right)^2 = (p - eA)^2 + m^2c^2$$

and the action function $S(t, q)$ satisfies

$$dS = p\,dq - E\,dt \qquad \text{so} \qquad p = \frac{\partial S}{\partial q} \qquad E = -\frac{\partial S}{\partial t}.$$

Thus the Hamilton-Jacobi equation is

$$\left(\frac{\partial S}{\partial t} + e\varphi\right)^2 = c^2\left(\frac{\partial S}{\partial q} - eA\right)^2 + m^2c^4$$

We want a solution S in the form

$$S = S_0 + e S_1 + e^2 S_2 + \cdots$$

where S_0 is linear

$$S_0 = -Et + pq \qquad E = \sqrt{m^2c^4 + c^2p^2}.$$

S_0 is a solution of the Hamilton-Jac equation when $e = 0$, and corresponds to free motion of momentum p and energy E. Recall

$$p = \frac{mv}{\sqrt{1 - v^2/c^2}} \qquad E = \frac{mc^2}{\sqrt{1 - \frac{v^2}{c^2}}}$$

so that

$$\frac{p}{E} = \frac{v}{c^2} \quad \text{or}$$

$$\boxed{v = \frac{pc^2}{E} \quad \text{for a free particle}}$$

To get an equation for S_1 differentiate HJ wrt e and ~~sot~~ set $e = 0$:

$$2\,\frac{\partial S_0}{\partial t}\left(\frac{\partial S_1}{\partial t} + \varphi\right) = 2c^2\,\frac{\partial S_0}{\partial q}\left(\frac{\partial S_1}{\partial q} - A\right)$$

$$-E\left(\frac{\partial S_1}{\partial t} + \varphi\right) = c^2 p\left(\frac{\partial S_1}{\partial q} - A\right)$$

or

$$\frac{\partial S_1}{\partial t} + \frac{c^2 p}{E}\frac{\partial S_1}{\partial q} = -\varphi + \frac{c^2 p}{E} A$$

$$\left(\frac{\partial}{\partial t} + \frac{c^2 p}{E}\frac{\partial}{\partial q}\right) S_1 = i\left(\frac{\partial}{\partial t} + \frac{c^2 p}{E}\frac{\partial}{\partial q}\right)\left(-\varphi\,dt + A\,dq\right)$$

This means that S_1 is obtained by integrating the basic 1-form $-\varphi\, dt + A\, dq$ backward along the trajectories associated to S_0.

The equation for S_2 is computed to be

$$2\left(E\frac{\partial}{\partial t} + c^2 p\frac{\partial}{\partial q}\right)S_2 = \left(\frac{\partial S_1}{\partial t}+\varphi\right)^2 - c^2\left(\frac{\partial S_1}{\partial q} - A\right)^2$$

The next thing to do is to look at the quantum mechanics version. First find the non-relativistic Schroedinger equation:

$$H = e\varphi + \frac{1}{2m}(p - eA)^2$$

$$p \mapsto \frac{\hbar}{i}\frac{\partial}{\partial q}, \qquad E \mapsto -\frac{\hbar}{i}\frac{\partial}{\partial t}$$

Schroedinger equation:

$$-\frac{\hbar}{i}\frac{\partial \psi}{\partial t} = \left[e\varphi + \frac{1}{2m}\left(\frac{\hbar}{i}\frac{\partial}{\partial q} - eA\right)^2\right]\psi$$

The way to understand this is to think of ψ as approximately being

$$e^{\frac{i}{\hbar}S}$$

where S satisfies the Hamilton-Jacobi DE.

We should recall what the ordinary scattering looks like for such a Schroedinger equation, ~~[illegible]~~ which is a time-dependent perturbation of a free

Schroedinger equation

$$i\hbar \frac{\partial \psi}{\partial t} = H_0 \psi \qquad H_0 = \frac{1}{2m}\left(\frac{\hbar}{i}\frac{\partial}{\partial q}\right)^2$$

The first thing is to describe all the trajectories for the free equation; such a trajectory is in the form

$$\psi(t) = e^{-\frac{i}{\hbar}H_0 t}\,\psi(0)$$

where $\psi(0)$ is a L^2-function of q. Then the scattering is given by a unitary operator called the scattering matrix, defined as follows. Let $U(t,t')$ be the propagator for the given Schroedinger equation:

$$i\hbar\frac{\partial}{\partial t}U(t,t') = H(t)\,U(t,t')$$

$$U(t',t') = I$$

(whence $U_0(t,t') = \exp\left(-\frac{i}{\hbar}H_0(t-t')\right)$). The scattering operator is the unitary operator given by

$$S = e^{\frac{i}{\hbar}H_0 t_f}\,U(t_f, t_i)\,e^{-\frac{i}{\hbar}H_0 t_i}$$

where $t_f \gg 0 \gg t_i$.

To describe the scattering operator we have to give its matrix elements relative to a basis of states for the free equation. The most convenient basis is furnished by the momentum representation. This means that for each p we take the free wave function with momentum p:

$$\psi(q) = e^{i\frac{pq}{\hbar}}$$

The corresponding function on space-time is

$$\psi(t,q) = e^{\frac{i}{\hbar}(pq - Et)} \qquad E = \frac{p^2}{2m}$$

June 27, 1979

Continue to look at scattering of a charged particle of charge e mass m by an external electromagnetic field $-A_\mu dx^\mu =$ [redacted] $-\varphi$ [redacted] $dt + A\,dq$.

[redacted] Recall

$$-p_\mu dx^\mu = -E\,dt + p\,dq$$

so the energy relation is

$$(p_0 - eA_0)^2 - (p_1 - eA_1)^2 = m^2c^2$$

or

[redacted] $$(E - e\varphi)^2 = c^2(p - eA)^2 + m^2c^4$$

To obtain Hamilton-Jacobi put $E = -\frac{\partial S}{\partial t}$, $p = \frac{\partial S}{\partial q}$ whence

$$\boxed{\left(\frac{\partial S}{\partial t} + e\varphi\right)^2 = c^2\left(\frac{\partial S}{\partial q} - eA\right)^2 + m^2c^4}$$

We seek a solution in the form

$$S = S_0 + eS_1 + e^2S_2 + \cdots\cdots$$

where $S_0 = -Et + pq$ is a wavefront for a free particle with momentum p and energy $E = \sqrt{m^2c^4 + c^2p^2}$.

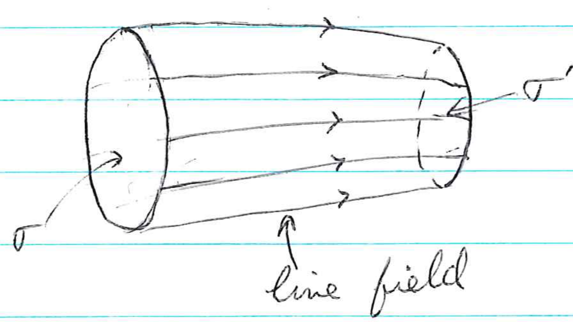
Yesterday we found

$$S_1(t,q) = \int^{(t,q)} -\varphi\,dt + A\,dq$$

trajectory going backwards from (t,q) with momentum p.

Question: How can we describe the scattering classically? We know what the free trajectories are, namely straight lines in space-time which are time-like. The trajectories form a symplectic manifold (this has to be checked in the relativistic case), so the scattering is going to be a symplectic automorphism of free trajectories.

Let's digress to review the symplectic structure in the relativistic case. Recall that in the relativistic description of a mechanical system we are given a hypersurface Y in the cotangent bundle of space-time and that the canonical 1-form $\eta = p\,dq$ gives us a contact structure on Y. In particular there is a canonical line field on Y and any hypersurface transversal to the line field inherits a symplectic form. What I want to see is that if I have two hypersurfaces transversal to the line field, so that the line field gives a correspondence between points on these surfaces, then the symplectic forms are compatible with the correspondence.



But take a piece σ of 2-surface in one hypersurface and let σ' be its image in the other hypersurface. Apply Stoke's thm to the closed form Ω whose kernel is the line field and you get

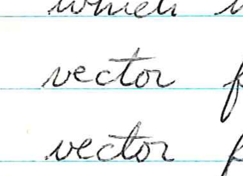
$$-\int_\sigma \Omega + \int_{\sigma'} \Omega + \underbrace{\int_{\text{sides}} \Omega}_{=0} = 0$$

so one sees the correspondence is indeed symplectic. (Compare Feb 19, p. 597).

Let us describe free trajectories by giving their position q at $t=0$ and their momentum p. Then $\Omega = dp\,dq$ is the canonical 2-forms of the space of free trajectories. The scattering to first order will be given by an infinitesimal symplectic automorphism, which is essentially the same as a symplectic vector field. Recall that symplectic vector fields are of the Poisson bracket form

$$\{f, \ \} = \frac{\partial f}{\partial p}\frac{\partial}{\partial q} - \frac{\partial f}{\partial q}\frac{\partial}{\partial p}$$

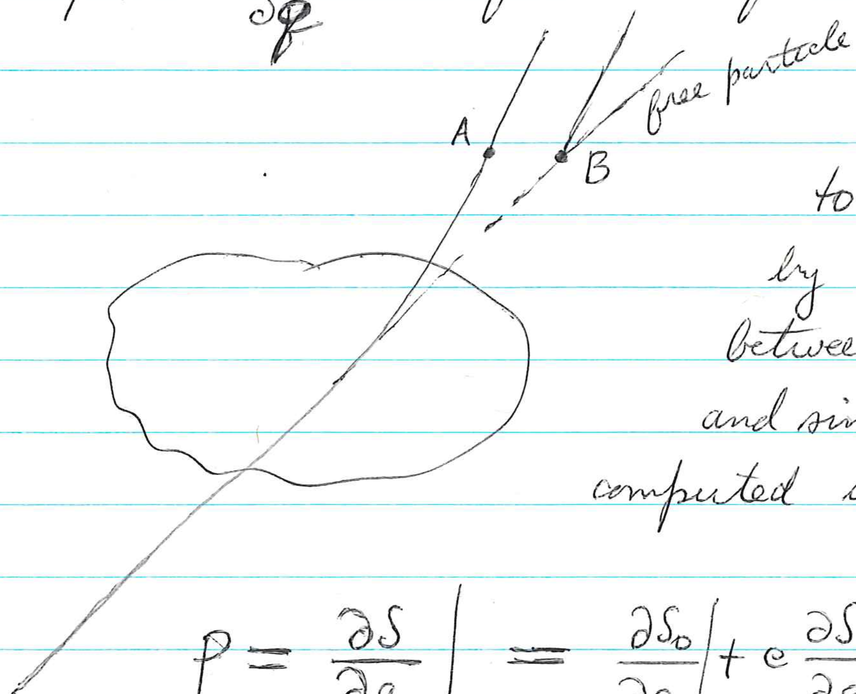
for some function f (at least locally). Thus if Q, P describe the final trajectory obtained from the initial trajector with parameters q, p, then we have



$$\boxed{(Q, P) = (q, p) + e\left(\frac{\partial f}{\partial p}, -\frac{\partial f}{\partial q}\right) + \cdots}$$

The problem now becomes to compute the function f. It should be something like the integral of $-\varphi dt + A dq$ over the free trajectory belonging to (q, p).

Suppose we want to compute P the momentum after the scattering corresponding the initial momentum p. Start with the wavefront $S_0 = -Et + pq$ describing momentum p. Then you follow the non-free trajectory through the scattering and after it emerges you compute $\frac{\partial S}{\partial q}$ to find the final momentum.



The idea will be to approximate A by B, since the difference between A, B is of order e and since the change being computed is of order e.

$$P = \frac{\partial S}{\partial q}\Big|_A = \frac{\partial S_0}{\partial q}\Big|_A + e\frac{\partial S_1}{\partial q}\Big|_A$$

$$= p + e\frac{\partial S_1}{\partial q}\Big|_B$$

So this shows that the desired function f is the negative of $S_1 = \int -\varphi dt + A dq$ over the trajectory.

Now let us consider quantum scattering, first the non-relativistic case. Consider

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

where $H = H_0 + H_{in}(t)$ and $H_{in}(t)$ has compact support.

$$e^{\frac{i}{\hbar}H_0 t}\left[\frac{\partial}{\partial t} + \frac{i}{\hbar}H_0\right]\psi = e^{\frac{i}{\hbar}H_0 t}\left(-\frac{i}{\hbar}\right) H_{in}(t)\psi(t)$$

$$\left[e^{\frac{i}{\hbar}H_0 t}\psi(t)\right]_{t'}^{t} = \int_{t'}^{t} dt_1\, e^{\frac{i}{\hbar}H_0 t_1}\left(-\frac{i}{\hbar}\right) H_{in}(t_1)\,\psi(t_1)$$

For $t' \ll 0$ $\quad \psi(t) = \psi_0(t)$ a free wave fn., so

$$\psi(t) = \psi_0(t) + \int_{-\infty}^{t} dt_1\, e^{-\frac{i}{\hbar}H_0(t-t_1)}\left(-\frac{i}{\hbar}\right) H_{in}(t_1)\,\psi(t_1)$$

is a basic integral equation. For the problem at hand

$$H = e\varphi + \frac{1}{2m}(p - eA)^2$$

$$= \underbrace{\frac{p^2}{2m}}_{H_0} + \underbrace{e\left(-\frac{pA + Ap}{2m} + \varphi\right) + e^2\frac{A^2}{2m}}_{H_{in}}$$

Working to first order in e, the last term can be dropped; and we get

$$\psi(t) = \psi_0(t) + \int_{-\infty}^{t} dt_1\, e^{-\frac{i}{\hbar}\frac{p^2}{2m}(t-t_1)}\left(-\frac{i}{\hbar}\right) e\left(-\frac{pA+Ap}{2m} + \varphi\right)\psi_0(t_1) + \cdots$$

Here p, A, φ are to be interpreted as operators. Let's take ψ_0 to be a free wave function with definite momentum

$$\psi_0(t) = e^{\frac{i}{\hbar}\left(pq - \frac{p^2}{2m}t\right)}$$

where here p denotes a number.

To avoid confusion let's use the Schroedinger coordinate representation and the notation

$$|p\rangle = e^{\frac{i}{\hbar}pq}.$$

for the eigenfunctions for the momentum operator $\hat{p}$. The normalization for these eigenfunctions is

$$\langle p'|p\rangle = \int e^{\frac{i}{\hbar}(p-p')q}\,dq = 2\pi\hbar\,\delta(p-p')$$

What we want to do is to compute the scattering matrix element

$$\langle p'|S|p\rangle = \langle p'|e^{\frac{i}{\hbar}H_0 t_f}\underbrace{U(t_f,t_i)\underbrace{e^{-\frac{i}{\hbar}H_0 t_i}|p\rangle}_{\psi_0(t_i)}}_{\psi(t_f)}$$

where $t_f \gg 0 \gg t_i$. (preceding page)

Hence

$$\psi(t_f) = e^{-\frac{i}{\hbar}H_0 t_f}|p\rangle + \left(\frac{-i}{\hbar}e\right)\int dt_1\, e^{-\frac{i}{\hbar}H_0(t_f-t_1)}\left(-\frac{\hat{p}A+A\hat{p}}{2m}+\varphi\right)e^{-\frac{i}{\hbar}H_0 t_1}|p\rangle$$

so

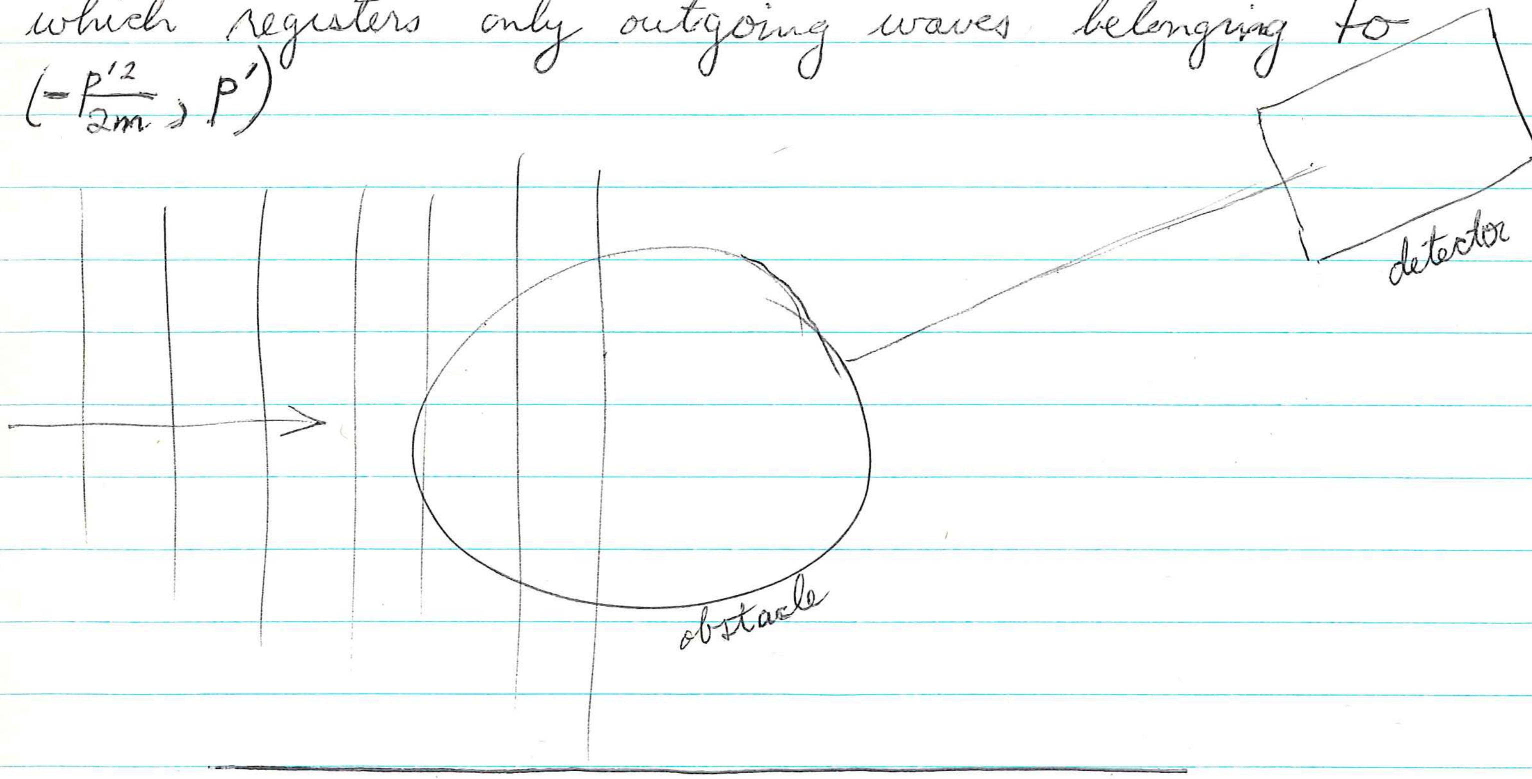
$$\boxed{\langle p'|S|p\rangle = \underbrace{\langle p'|p\rangle}_{2\pi\hbar\,\delta(p'-p)} + \left(-\frac{ie}{\hbar}\right)\int_{-\infty}^{\infty} dt_1\,\langle p'|-\frac{\hat{p}A+A\hat{p}}{2m}+\varphi|p\rangle\, e^{\frac{i}{\hbar}\frac{p'^2-p^2}{2m}t_1}}$$

The term

$$\int dt_1\,\langle p'|\varphi|p\rangle\, e^{\frac{i}{\hbar}\frac{p'^2-p^2}{2m}t_1} = \int dq\,dt\,\varphi(q,t)\,e^{\frac{i}{\hbar}\left(\frac{p'^2-p^2}{2m}t+(p-p')q\right)}$$

is the Fourier transform of φ as a function on space time evaluated at the difference of the energy-momentum vectors for p and p'. If φ were time independent it gives a δ-function contribution $\delta\left(\frac{p'^2}{2m}-\frac{p^2}{2m}\right)$.

Question: What does the above expression mean? Is there some way of thinking of the second term as an interference effect. Somehow one would like to visualize the second term using an incoming wave belonging to $(-\frac{p^2}{2m}, p)$ and a detector which registers only outgoing waves belonging to $(-\frac{p'^2}{2m}, p')$



Our next project is to do the above calculation relativistically. Instead of the Schroedinger equation we use the Klein-Gordon equation, but restricted to positive energy solutions, so that a wave function $\psi(q)$ extends to a $\psi(t,q)$ in a unique way. Free eigenfunctions of definite energy-momentum are

$$(*) \qquad \psi_0(t,q) = e^{\frac{i}{\hbar}(pq - Et)} \qquad E = \sqrt{c^2p^2 + m^2c^4}$$

Let's refer all functions to $t = 0$; then we get the wave function

$$|p\rangle = e^{\frac{i}{\hbar}pq}$$

and $$H_0|p\rangle = \sqrt{c^2p^2 + m^2c^4}\,|p\rangle.$$

Here's how to obtain the S-matrix. Start with

ψ_0 as in $(*)$ for $t \ll 0$ and let $\psi(t,q)$ be the solution of the Klein-Gordon equation

$$\left(-\frac{\hbar}{i}\frac{\partial}{\partial t} - e\varphi\right)^2 \psi = c^2\left(\frac{\hbar}{i}\frac{\partial}{\partial q} - eA\right)^2 \psi + m^2c^4\psi$$

which agrees with ψ_0 for $t \ll 0$.

June 28, 1979

Review:

$$-p_\mu dx^\mu = -E\,dt + p\,dq \qquad \left(\frac{E}{c}\right)^2 - p^2 = m^2c^2$$

$$-A_\mu dx^\mu = -\varphi\,dt + A\,dq \qquad (E - e\varphi)^2 = c^2(p - eA)^2 + m^2c^4$$

For non-rel. approx. replace E by $E + mc^2$ and let $c \to \infty$

$$\cancel{m^2c^4} + 2mc^2(E - e\varphi) + (E - e\varphi)^2 = c^2(p - eA)^2 + \cancel{m^2c^4}$$

or

$$E = e\varphi + \frac{(p - eA)^2}{2m} = \frac{p^2}{2m} + e\underbrace{\left(\frac{-pA + Ap}{2m} + \varphi\right)}_{\tilde{\varphi}} + O(e^2)$$

To compute scattering for Schroedinger eqn:

$$i\hbar\frac{\partial\psi}{\partial t} = \left[\frac{p^2}{2m} + e\left(-\frac{pA + Ap}{2m} + \varphi\right) + e^2\frac{A^2}{2m}\right]\psi$$

[redacted] put $\psi = \psi_0 + e\psi_1 + \cdots$ where ψ_0 satisfies free equation. Take ψ_0 to be

$$\psi_0(t) = e^{-\frac{i}{\hbar}H_0 t}|p\rangle \qquad \text{where } |p\rangle = e^{\frac{i}{\hbar}pq}$$

Then

$$i\hbar\frac{\partial\psi_1}{\partial t} = \frac{p^2}{2m}\psi_1 + \tilde{\varphi}\psi_0$$

or

$$\psi_1(t) = \frac{1}{i\hbar}\int_{-\infty}^{t} e^{-\frac{i}{\hbar}H_0(t - t_1)}\tilde{\varphi}\psi_0(t_1)\,dt_1$$

assuming $\psi_1 = 0$ for $t \ll 0$. The [redacted] scattering matrix is given by

$$\langle p'|S|p\rangle = \langle p'|p\rangle + e\left\langle e^{-\frac{i}{\hbar}H_0 t}|p\rangle, \psi_1(t)\right\rangle + \cdots \quad \text{for } t \gg 0$$

so the first order part of S is

$$\langle p'|S_1|p\rangle = \frac{e}{i\hbar}\int_{-\infty}^{\infty} \langle p'|\, e^{\frac{i}{\hbar}H_0 t_1}\,\tilde{\varphi}\, e^{-\frac{i}{\hbar}H_0 t_1}|p\rangle \, dt_1$$

$$= \frac{e}{i\hbar}\int_{-\infty}^{\infty} \langle p'|\tilde{\varphi}|p\rangle\, e^{\frac{i}{\hbar}(E_{p'}-E_p)t_1} \, dt_1$$

Now I want to do the analogous thing in the relativistic case. There are two possibilities – using either the Klein-Gordon or the Dirac equation. First try the former:

$$\left(i\hbar\frac{\partial}{\partial t} - e\varphi\right)^2\psi = \left[c^2\left(p - eA\right)^2 + m^2c^4\right]\psi$$

Again let the solution be $\psi = \psi_0 + e\psi_1 + \cdots$ where ψ_0 is a free wave function

$$\psi_0(t) = e^{\frac{i}{\hbar}(pq - E_p t)} \qquad E_p = \sqrt{c^2p^2 + m^2c^4}$$

Differentiate wrt e and set $e=0$ to find an equation for ψ_1:

$$\left(i\hbar\frac{\partial}{\partial t}\right)^2\psi_1 + \left[-\varphi\left(i\hbar\frac{\partial}{\partial t}\right) - \left(i\hbar\frac{\partial}{\partial t}\right)\varphi\right]\psi_0 = \left[c^2p^2 + m^2c^4\right]\psi_1 + c^2(-pA - Ap)\psi_0$$

or

$$\left[\frac{\partial^2}{\partial t^2} + \frac{c^2p^2 + m^2c^4}{\hbar^2}\right]\psi_1 = \underbrace{\frac{1}{\hbar^2}\left[-\varphi\left(i\hbar\frac{\partial}{\partial t}\right) - \left(i\hbar\frac{\partial}{\partial t}\right)\varphi + c^2(pA + Ap)\right]}_{K}\psi_0$$

We need the Green's function for $\frac{\partial^2}{\partial t^2} + \omega^2$ which is

$$\begin{cases} \dfrac{\sin\omega t}{\omega} & t > 0 \\ 0 & t < 0 \end{cases}$$

if we want the solution of $\left(\frac{\partial^2}{\partial t^2}+\omega^2\right)\psi_1 = f$ to vanish for $t \ll 0$. Let's introduce the free Hamiltonian

$$H_0 = \sqrt{c^2p^2+m^2c^4}\,.$$

This makes sense on the Fourier transform level:

$$H_0\,|p\rangle = E_p\,|p\rangle \qquad \text{where } E_p = \sqrt{c^2p^2+m^2c^4}\,.$$

So the formula for ψ_1 is

$$\psi_1(t) = \int_{-\infty}^{t} \frac{\sin \frac{H_0}{\hbar}(t-t_1)}{\frac{H_0}{\hbar}}\, K\psi_0(t_1)\,dt_1$$

The problem with this is that for $t \gg 0$ the sine contributes negative energy solutions.

In order to remedy this problem one goes to second quantization to allow for the creation and annihilation of particles, which has to happen when the energy for pair creation is finite. Mathematically it seems to make sense to ask why one can't produce a good single particle quantum theory.

The philosophy should be as follows. We look in the cotangent bundle of the manifold of space-time at the hypersurface:

$$E = e\varphi + \text{[redacted]} \sqrt{c^2(p-eA)^2+m^2c^4} \qquad \text{call this } Y$$

which carries a natural contact structure given by the energy-momentum 1-form $-p_\mu dx^\mu = p\,dq - E\,dt$. Any space-like hypersurface in space-time has an inverse image in the energy hypersurface which is a hypersurface in Y transversal to the time evolution line field, so this smaller hypersurface has a canonical symplectic structure, in fact it is clearly isomorphic to the cotangent bundle of the space-like hypersurface. **Notation:** σ for space-like hypersurface and T^*_σ for its lift in Y. Time evolution gives a symplectic isomorphism of T^*_σ and $T^*_{\sigma'}$ for any 2 space-like hypersurfaces σ, σ' in space-time. Put another way, the set of classical trajectories is a symplectic manifold $\mathcal{S}$ and for each σ we have an isomorphism

$$\mathcal{S} \xrightarrow{\sim} T^*_\sigma$$

giving the position and energy-momentum of the trajectory where it intersects σ.

The philosophy is that quantization associates to T^*_σ a Hilbert space. Better: To the symplectic manifold $\mathcal{S}$ belongs a Hilbert space $\mathcal{H}$ which is its quantization, and corresponding to the above isom. is an isomorphism of $\mathcal{H}$ with the Hilbert space of L^2 functions on σ.

<u>Question</u>: Is it possible to carry over the non-relativistic formulas

$$\langle p' | S_1 | p \rangle = \int \langle p' | \Psi | p \rangle e^{\frac{i}{\hbar}(E_{p'} - E_p)t} \, dt$$

with $E_p = \sqrt{c^2p^2 + m^2c^4}$ at least in some formal way, so as to be both unitary and Lorentz-invariant?

June 30, 1979

Let's review some of the mathematics involved in the $\bar\partial$ problem. Work over $\mathbb{R}^n$, specifically in $L^2(\mathbb{R}^n)$ with the operators $q_i =$ mult. by x_i, $p_i = \frac{1}{i}\frac{\partial}{\partial x_i}$. These operators generate a complex vector space V with symplectic structure and conjugation. Now let us consider an isotropic subspace of V, call it W, and let us pick a basis $A_1, \dots, A_k$ for W. These operators commute and so one can form the Koszul complex of them "acting" on $L^2(\mathbb{R}^n)$.

Examples.

1) $n = 1$. Take $A = \frac{\partial}{\partial x} + \omega x$, so that the Koszul complex is

$$L^2(\mathbb{R}) \xrightarrow{\frac{\partial}{\partial x} + \omega x} L^2(\mathbb{R})$$

If

$$\left(\frac{\partial}{\partial x} + \omega x\right) u = 0$$

then $\quad u = \text{const.}\ e^{-\frac{1}{2}\omega x^2}$ which will be in L^2 exactly when $\mathrm{Re}(\omega) > 0$. If we conjugate the operator A by the unitary transformation $e^{-\frac{1}{2}i\alpha x^2}$ with α real we get

$$e^{+\frac{1}{2}i\alpha x^2}\left(\frac{\partial}{\partial x} + \omega x\right) e^{-\frac{1}{2}i\alpha x^2} = \frac{\partial}{\partial x} + (\omega - i\alpha)x$$

so we might as well suppose ω is real.

The adjoint of $\frac{\partial}{\partial x} + \omega x$ is $-\frac{\partial}{\partial x} + \bar\omega x$ or $\frac{\partial}{\partial x} - \bar\omega x$ up to sign. The situation concerning the cohomology of the Koszul complex is as follows:

If $\omega > 0$, then H^0 spanned by $e^{-\frac{1}{2}\omega x^2}$, $H^1 = 0$

If $\omega < 0$, then H^1 is 1-dimensional, $H^0 = 0$.

2) Using the fact that we have available arbitrary symplectic automorphisms of $V_{\mathbb{R}}$ realizable as unitary transformations of $L^2(\mathbb{R}^n)$, we can transform the problem to a simpler form. The situation is that we have an isotropic subspace W of $V_{\mathbb{C}}$.

First case to consider is $W \cap \overline{W} = 0$, $W + \overline{W} = V$. In this case W defines a complex structure on $V_{\mathbb{R}}$ via the isomorphism $V_{\mathbb{R}} \subset V \longrightarrow V/\overline{W} \cong W$.

Given $\omega_1, \omega_2 \in W$ form

$$f(\omega_1, \omega_2) = [\omega_1, \omega_2^*]$$

Then $f(\omega_1, \omega_2)^* = [\omega_2^*, \omega_1^*] = f(\omega_2, \omega_1)$ so that f is a sesqui-linear form on W. What's more it is a non-degenerate Hermitian form, because we know that the pairing $W \otimes \overline{W} \to \mathbb{C}$ given by $[\ ,\ \bar{}\ ]$ is non-degenerate, since W is isotropic. The hermitian form f has a signature which we can find by choosing an inner product on W and then taking the eigenvalues of the hermitian operator belonging to f.

Example: $V = \mathbb{C}q + \mathbb{C}p$ with q, p self-adj and $[p, q] = \frac{1}{i}$. Suppose W spanned by $ip + \omega q$. Then

$$f(ip+\omega q, ip+\omega q) = [ip+\omega q, -ip+\bar{\omega} q] = \bar{\omega}+\omega$$

In general choose a basis $w_1, \ldots, w_n$ for W which is orthogonal for f. If $f(w_j, w_j) = [w_j, w_j^*] = 1$, then let $\sqrt{2}\, w_j = ip_j + q_j$ with p_j, q_j real, and you find

$$[ip_j, q_j] = \left[\frac{w_j - w_j^*}{\sqrt{2}}, \frac{w_j + w_j^*}{\sqrt{2}}\right] = 1$$

On the other hand if we have $f(w_j, w_j) = -1$ then put $\sqrt{2}\, w_j = ip_j - q_j$ and the same commutation relation holds.

So what happens is that the Koszul complex is expressed as a tensor product of 1-dimensional ones. So we see that in the case where $W \oplus \bar{W} = V$ that the cohomology (which is 1-dimensional) will occur in dimension r where r = number of negative eigenvalues for the form $f(w_1, w_2) = [w_1, w_2^*]$.

3) If $W \cap \bar{W} \neq 0$, then the cohomology will be zero because because we are going to have as factor, the 1-dimensional situation

$$L^2(\mathbb{R}) \xrightarrow{\ q\ } L^2(\mathbb{R})$$

If $W + \bar{W} < V$, then we have as factor the situation

$$L^2(\mathbb{R}) \xrightarrow{\ 0\ } L^2(\mathbb{R})$$

so the cohomology will be infinite-dimensional (assuming $W \cap \bar{W} = 0$), and not in any single degree.

One of the reasons for looking at the above is my feeling that harmonic motion:

$$\ddot{q} = -Qq$$

where Q is a quadratic form, say non-degenerate but not necessarily positive definite, might lead to a refined Hilbert space where the ground state is in some higher-cohomology. Something like this occurs with group representations.

It might be interesting to consider in 1-dimension an oscillator with the wrong sign. Classically

$$\ddot{q} = \omega q \qquad \omega > 0$$

has the solution $q = c_1 e^{\sqrt{\omega}t} + c_2 e^{-\sqrt{\omega}t}$ which is defined for all time. We could look at the Schroedinger equation

$$\left(-\frac{1}{2}\frac{d^2}{dx^2} - \frac{1}{2}\omega x^2\right)\psi = E\psi$$

and ask whether this is well-posed in the sense that the differential operator is self-adjoint, i.e. one has the limit point case as $x \to \pm\infty$.

Recall facts about Hermite DE:

$$\left(-\frac{d}{dx}+x\right)\left(\frac{d}{dx}+x\right)y = \left(-\frac{d^2}{dx^2}+x^2-1\right)y = -2sy$$

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

basic symmetries: $\quad (x,s) \mapsto (-x,s)$

$$(x,s) \longmapsto (ix, 1-s)$$

Set $\quad y = e^{-x^2/2} u$

$$e^{x^2/2}\left(-\frac{d}{dx}+x\right)\left(\frac{d}{dx}+x\right)e^{-x^2/2} = \left(-\frac{d}{dx}+2x\right)\frac{d}{dx}$$

so
$$\left(\frac{d^2}{dx^2} - 2x\frac{d}{dx} + 2s\right)u = 0$$

Solve by contour integral (Laplace method

$$u = \int e^{xt}\varphi(t)\,\frac{dt}{t}$$

$$x\frac{d}{dx}u = \int \underbrace{x e^{xt}}_{\frac{d}{dt}(e^{xt})}\varphi\, dt \underset{\substack{\uparrow \\ \text{assume bdry term vanishes}}}{=} -\int e^{xt}\varphi'\,dt$$

$$t\varphi + 2\varphi' - 2s\frac{\varphi}{t} = 0$$

$$\frac{t}{2} + \frac{\varphi'}{\varphi} + \frac{\cancel{2}s}{t} = 0$$

$$\frac{t^2}{4} + \log\varphi - s\log t = 0$$

$$\varphi = e^{-t^2/4}t^s \qquad \text{works}$$

So
$$u = \int e^{2xt-t^2}\, t^s\,\frac{dt}{t}$$

So
$$\left[\frac{d^2}{dx^2} - x^2 + (1-2s)\right]y = 0 \qquad \text{has solution}$$

$$y_s(x) = e^{-x^2/2}\int e^{-2xt-t^2}\, t^s\,\frac{dt}{t}$$

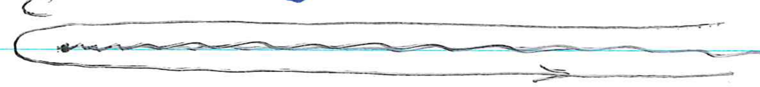
where the contour is chosen so the integral converges and so as to avoid cut along $\mathbb{R}_{\geq 0}$.

Set $\alpha = e^{i\pi/4}$ and change x to αx. Then

$$\left[\frac{d^2}{dx^2} + x^2 + (1-2s)i\right]\psi = 0$$

has solution $\quad \psi(x) = y_s(\alpha x) = e^{-\frac{ix^2}{2}} \int e^{-2\alpha x t - t^2}\, t^s \frac{dt}{t}$

Suppose $x > 0$ and $x \to \infty$, and take the contour to be



Then

$$\psi(x) = e^{-\frac{ix^2}{2}} \int_C e^{-2\alpha u - \frac{u^2}{x^2}} \left(\frac{u}{x}\right)^s \frac{du}{u}$$

$$\sim \frac{e^{-\frac{ix^2}{2}}}{x^s} \underbrace{\int_C e^{-2\alpha u}\, u^s \frac{du}{u}}$$

nice number expressible in terms of $\Gamma(s)$

Therefore if $Re(s) > \frac{1}{2}$, then $\psi(x)$ is in L^2 but if $Re(s) < \frac{1}{2}$ and you avoid integer values of s, then ψ will not be in L^2 as $x \to +\infty$. This means that one has the limit point case as $x \to +\infty$. (Limit circle occurs when all solns. are L^2).

Earlier work on Hermite DE occurs June 26, 1977 - two years ago!

July 2, 1979

Let's review the harmonic oscillator with perturbation

$$H = \tfrac{1}{2}p^2 + \tfrac{1}{2}q\cdot(\omega^2+\varepsilon)q.$$

Assuming ε is time-independent, we compute the shift in ground state energy by building ε up using infinitesimal $\delta\varepsilon$. (The answer is $\tfrac{1}{2}\,\mathrm{tr}\left(\sqrt{\omega^2+\varepsilon}-\omega\right)$.)

From

$$(H-E_G)\psi_G = 0 \qquad \text{we get}$$

$$(\delta H-\delta E_G)\psi_G + (H-E_G)\psi_G = 0 \qquad \text{or}$$

$$\langle \psi_G | (\delta H - \delta E_G)\psi_G\rangle = 0 \qquad \text{or}$$

$$\delta E_G = \langle \psi_G | \delta H\, \psi_G\rangle$$

$$= \frac{\delta\varepsilon}{2}\langle \psi_G | q^2 | \psi_G\rangle$$

Introduce the Green's function

$$G(t-t') = i\langle T\,\tilde q(t)\,\tilde q(t')\rangle$$

where $\langle A\rangle = \langle \psi_G | A | \psi_G\rangle$, T denotes time ordering, and $\tilde q(t)$ is the Heisenberg operator

$$\tilde q(t) = e^{iHt}\,q\,e^{-iHt}. \qquad \text{so} \quad \frac{d}{dt}\tilde q(t) = i[H,\tilde q]$$

Then $(H=\tilde H)$

$$\frac{d}{dt}\tilde q = i[H,\tilde q] = i\left[\frac{\tilde p^2}{2},\tilde q\right] = \tilde p$$

$$\frac{d}{dt}\tilde p = i[\tilde H,\tilde p] = -(\omega^2+\varepsilon)\tilde q$$

so

$$\frac{d}{dt}G(t-t')\Big]_{t'-}^{t'+} = i\langle T\,\tilde p(t)\,\tilde q(t')\rangle\Big]_{t'-}^{t'+} = i\langle pq-qp\rangle = 1$$

and $$\left(\frac{d^2}{dt^2} + \omega^2 + \varepsilon\right) G(t-t') = \delta(t-t')$$

Also we know that ψ_G is killed by $ip + \sqrt{\omega^2+\varepsilon}\, q$ which means that for $t < t'$ one has

$$\left(i\frac{d}{dt} + \sqrt{\quad}\right) G(t-t') = 0$$

and similarly at the other end so that

$$G(t-t') = \frac{e^{-i\sqrt{\omega^2+\varepsilon}\,|t-t'|}}{-2i\sqrt{\omega^2+\varepsilon}}$$

Thus $$G(0) = i\langle q^2\rangle = \frac{1}{-2i\sqrt{\omega^2+\varepsilon}} \quad \text{or} \quad \langle q^2\rangle = \frac{1}{2\sqrt{\omega^2+\varepsilon}}$$

which is a result we could [redacted] have obtained directly. So

$$\delta E_G = \frac{1}{4}\frac{\delta\varepsilon}{\sqrt{\omega^2+\varepsilon}} = \frac{1}{2}\delta\sqrt{\omega^2+\varepsilon}$$

and integrating one finds $\Delta E_G = \frac{1}{2}(\sqrt{\omega^2+\varepsilon} - \omega)$; this is a one-dimensional calculation which can easily be extended to the case where ω, ε are matrices.

Next we want to consider the change in free energy of the oscillator [redacted] due to the perturbation. Recall F is defined by

$$e^{-\beta F} = \mathrm{tr}(e^{-\beta H})$$

where $\beta = \frac{1}{kT}$. As $T \to 0$, $\beta \to \infty$ and $F \to E_G$. For [redacted] a simple harmonic oscillator of frequency ω one has

$$\mathrm{tr}(e^{-\beta H}) = \sum_{n\geq 0} e^{-\beta(n+\frac{1}{2})\omega} = \frac{e^{-\frac{1}{2}\beta\omega}}{1-e^{-\beta\omega}} = \frac{1}{e^{\frac{1}{2}\beta\omega} - e^{-\frac{1}{2}\beta\omega}}$$

so that

$$F = \frac{1}{\beta}\log\left(e^{\frac{1}{2}\beta\omega} - e^{-\frac{1}{2}\beta\omega}\right)$$

The idea now will be to derive the resulting formula for ΔF by perturbation methods.

$$F = -\frac{1}{\beta}\log\big(\underbrace{\mathrm{tr}\, e^{-\beta H}}_{Z}\big)$$

$$\delta F = -\frac{1}{\beta}\frac{1}{Z}\mathrm{tr}\left(\delta e^{-\beta H}\right)$$

$$\frac{d}{d\beta}e^{-\beta H} = -He^{-\beta H}$$

$$\frac{d}{d\beta}\delta e^{-\beta H} = -H\delta e^{-\beta H} - \delta H\cdot e^{-\beta H}$$

$$\left(\frac{d}{d\beta} + H\right)\delta e^{-\beta H} = -\delta H\, e^{-\beta H}$$

$$\delta e^{-\beta H} = -\int_0^\beta e^{-(\beta-\sigma)H}\,\delta H\, e^{-\sigma H}\, d\sigma$$

$$\frac{1}{Z}\mathrm{tr}\left(\delta e^{-\beta H}\right) = -\int_0^\beta \left\langle e^{\sigma H}\delta H e^{-\sigma H}\right\rangle d\sigma$$

where now $\langle A\rangle = \frac{1}{Z}\mathrm{tr}\left(e^{-\beta H}A\right)$.

Actually things are simpler here because

$$\mathrm{tr}\left(e^{-\beta H}e^{\sigma H}\delta H e^{-\sigma H}\right) = \mathrm{tr}\left(e^{-\beta H}\delta H\right)$$

so the good formula is

$$\delta F = \frac{\delta\varepsilon}{2}\langle q^2\rangle.$$

In order to compute $\langle q^2 \rangle$ we use the Green's function

$$G(\sigma-\sigma') = -\langle T\, \tilde{q}(\sigma)\, \tilde{q}(\sigma') \rangle$$

$$= \frac{-1}{Z} \operatorname{tr}\left(e^{-\beta H} e^{\sigma H} q\, e^{-\sigma H} e^{\sigma' H} q\, e^{-\sigma' H} \right) \qquad \sigma \geq \sigma'$$

$$= -\frac{1}{Z} \operatorname{tr}\left(e^{-\beta H} \cdot e^{(\sigma-\sigma')H} q\, e^{-(\sigma-\sigma')H} q \right) \qquad ''$$

This is defined for $\sigma, \sigma' \in [0, \beta]$ so that the various operators have traces. In addition

$$G(\beta-\sigma') = -\frac{1}{Z} \operatorname{tr}\left(q e^{-\beta H} e^{\sigma' H} q\, e^{-\sigma' H} \right)$$

$$G(0-\sigma') = -\frac{1}{Z} \operatorname{tr}\left(e^{-\beta H} e^{\sigma' H} q\, e^{-\sigma' H} q \right)$$

are equal, so G is periodic with period β. Also

$$\frac{d}{d\sigma} G(\sigma-\sigma') = -\langle T\, [H, \tilde{q}(\sigma)]\, \tilde{q}(\sigma') \rangle$$

$$= i \langle T\, \tilde{p}(\sigma)\, \tilde{q}(\sigma') \rangle$$

$$\frac{d}{d\sigma} G(\sigma, \sigma') \Big]_{\sigma'-}^{\sigma'+} = i \langle (\tilde{p}\tilde{q} - \tilde{q}\tilde{p})(\sigma') \rangle = 1$$

$$\frac{d^2}{d\sigma^2} G(\sigma-\sigma') = i \langle T\, [H, \tilde{p}](\sigma)\, \tilde{q}(\sigma') \rangle$$

$$= \langle T (-)(\omega^2+\varepsilon)\, \tilde{q}(\sigma)\, \tilde{q}(\sigma') \rangle = (\omega^2+\varepsilon) G(\sigma-\sigma')$$

or

$$\left(\frac{d^2}{d\sigma^2} - \omega^2 - \varepsilon \right) G(\sigma-\sigma') = \delta(\sigma-\sigma')$$

Let's compute $G(\sigma)$. We have (replace $\omega^2+\varepsilon$ by ω^2)

$$G(\sigma) = A e^{\omega\sigma} + B e^{-\omega\sigma}$$

and the periodicity condition $G(0) = G(\beta)$ can be achieved by $\quad G(\sigma) = \text{const} \cdot \cosh \omega(\sigma - \tfrac{1}{2}\beta)$

We want the derivative jump $\quad G'(0^+) - G'(0^-) = 1$ or by symmetry $\quad G'(0^+) = 1/2$. Thus

$$G(\sigma) = \frac{\cosh \omega(\sigma - \frac{1}{2}\beta)}{2\omega \sinh\left(\omega(-\frac{1}{2}\beta)\right)} = \frac{\cosh \omega(\sigma - \frac{1}{2}\beta)}{-2\omega \sinh\left(\frac{\omega\beta}{2}\right)}$$

Then we have $\quad -\langle q^2 \rangle = G(0^+) = \dfrac{\cosh \frac{1}{2}\omega\beta}{-2\omega \sinh(\frac{1}{2}\omega\beta)}$

or

$$\langle q^2 \rangle = \frac{1}{2\omega} \frac{\cosh(\frac{1}{2}\omega\beta)}{\sinh(\frac{1}{2}\omega\beta)}$$

Put back in $\sqrt{\omega^2+\varepsilon}$ for ω and you get

$$\delta F = \frac{\delta\varepsilon}{\frac{1}{2}\beta 2} \underbrace{\frac{\frac{1}{2}\beta}{2\sqrt{\omega^2+\varepsilon}} \frac{\cosh(\frac{1}{2}\sqrt{\omega^2+\varepsilon}\,\beta)}{\sinh(\frac{1}{2}\sqrt{\omega^2+\varepsilon}\,\beta)}}$$

$$\frac{\delta\varepsilon}{\beta} \frac{\partial}{\partial\varepsilon} \log 2\left(\sinh \tfrac{1}{2}\sqrt{\omega^2+\varepsilon}\,\beta\right)$$

which is consistent with $\quad F = \frac{1}{\beta} \log\left(2\sinh\left(\frac{1}{2}\sqrt{\omega^2+\varepsilon}\,\beta\right)\right)$.

Up to now for the simple harmonic oscillator, and more generally for any harmonic oscillator, we have determined the 0-temperature Green's fn.

$$G(t,t') = \langle \psi_G | T\, \tilde{q}(t)\, \tilde{q}(t') | \psi_G \rangle \qquad \tilde{q}(t) = e^{iHt} q e^{-iHt}$$

and the temperature Green's function

$$G(\sigma,\sigma') = \operatorname{tr}\left(e^{-\beta H}\, T\left(e^{H\sigma} q e^{-H\sigma}\right)\left(e^{H\sigma'} q e^{-H\sigma'}\right)\right) \Big/ \operatorname{tr} e^{-\beta H}.$$

It remains to discuss the real-time temperature Green's function, which is the thermal average of $T\tilde{q}(t)\tilde{q}(t')$.

This is

$$G(t) = \frac{\mathrm{tr}(e^{-\beta H}\, e^{iHt} q e^{-iHt} q)}{\mathrm{tr}(e^{-\beta H})} \qquad t \geq 0.$$

Since we know $\displaystyle \frac{\mathrm{tr}(e^{-\beta H}\, e^{\sigma H} q e^{-\sigma H} q)}{\mathrm{tr}(e^{-\beta H})} = \frac{\cosh \omega(\sigma - \frac{1}{2}\beta)}{2\omega \sinh(\frac{1}{2}\beta\omega)}$

for $0 \leq \sigma \leq \beta$ we can use analytic continuation to conclude that

$$\frac{\mathrm{tr}(e^{-\beta H}\, e^{iHt} q e^{-iHt} q)}{\mathrm{tr}(e^{-\beta H})} = \frac{\cosh \omega(it - \frac{1}{2}\beta)}{2\omega \sinh(\frac{1}{2}\beta\omega)}$$

$$= \frac{1}{2\omega} \frac{e^{-\frac{1}{2}\omega\beta} e^{i\omega t} + e^{\frac{1}{2}\omega\beta} e^{-i\omega t}}{e^{\frac{1}{2}\beta\omega} - e^{-\frac{1}{2}\beta\omega}}$$

$$= \frac{1}{2\omega}\left\{ \frac{e^{\beta\omega}}{e^{\beta\omega}-1} e^{-i\omega t} + \frac{1}{e^{\beta\omega}-1} e^{i\omega t} \right\}$$

Alternative derivation:

$$a = \frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{\omega}} \frac{\partial}{\partial q} + \sqrt{\omega}\, q\right)$$

$$a^* = \frac{1}{\sqrt{2}}\left(-\frac{1}{\sqrt{\omega}} \frac{\partial}{\partial q} + \sqrt{\omega}\, q\right)$$

$$q = \frac{a + a^*}{\sqrt{2\omega}}$$

$$e^{iHt} q e^{-iHt} = \frac{e^{-i\omega t} a + e^{i\omega t} a^*}{\sqrt{2\omega}}$$

$$\frac{1}{2}\mathrm{tr}(e^{-\beta H} e^{iHt} q e^{-iHt} q) = \frac{1}{2\omega}\frac{1}{2}\mathrm{tr}\left(e^{-\beta H}(e^{-i\omega t} a + e^{i\omega t} a^*)(a + a^*)\right)$$

Because H is diagonal in the number representation only the terms in $a^*a = N$ and $aa^* = a^*a+1 = N+1$ matter so we get

$$\langle e^{iHt} q e^{-iHt} q \rangle = \frac{1}{2\omega}\left(\langle N\rangle e^{+i\omega t} + (\langle N\rangle + 1)e^{-i\omega t}\right)$$

where

$$\langle N \rangle = \sum_{n\geq 0} n e^{-\beta(n+\frac{1}{2})\omega} \Big/ \sum_{n \geq 0} e^{-\beta(n+\frac{1}{2})\omega}$$

$$= -\frac{1}{\beta}\frac{d}{d\omega}\left(\sum e^{-(\beta\omega)n}\right) \Big/ \sum e^{-(\beta\omega)n}$$

$$= -\frac{1}{\beta}\frac{d}{d\omega}\log\left(\frac{1}{1-e^{-\beta\omega}}\right) = +\frac{1}{\beta}\frac{+\beta e^{-\beta\omega}}{1-e^{-\beta\omega}}$$

$$= \frac{1}{e^{\beta\omega}-1} \qquad \text{(Plank law)}$$

It's clear from this derivation that because $e^{iHt} q e^{-iHt}$ is a linear combination of a, a^*, it follows that $\langle \tilde{q}(t)\tilde{q}\rangle$ is entire in t for any $\beta > 0$. There is no problem with the operator having a trace.

Next project will be to understand phonons in a crystal. Picture: We are given a lattice Γ in $\mathbb{R}^3$, i.e. a discrete subgroup with compact quotient. At each point γ of Γ lives an atom which is allowed to move slightly. Denote the displacement of the γ-th atom by $\vec{u}_\gamma$ and its momentum by $\vec{p}_\gamma$. We suppose the lattice vibrations are governed by a Hamiltonian of the form

$$H = \frac{p_\gamma^2}{2M} + \frac{1}{2}\sum_{\gamma\neq\gamma'} V(X_\gamma - X_{\gamma'}) \qquad \vec{X}_\gamma = \vec{\gamma} + \vec{u}_\gamma$$

so that the interaction between two sites depends only on their relative position. Notice that

$$\frac{1}{2}\sum_{\gamma\neq\gamma'} V(X_\gamma - X_{\gamma'}) = \sum_{\substack{\text{pairs}\\ \gamma,\gamma'}} \frac{1}{2}\left\{V(X_\gamma - X_{\gamma'}) + V(X_{\gamma'} - X_\gamma)\right\}$$

so one may suppose $V(X) = V(-X)$.

Change notation: Use i to index a site in Γ and let $\vec{R}_i$ be its position, so that the position of the i-th atom is $X_i = R_i + u_i$. Assume $u_i = 0$ for all i is a minimum for the potential energy, say $V = 0$ in this case; assume small vibrations and make the quadratic approximation.

$$V(X_i - X_j) = V(R_i - R_j) + \frac{\partial V}{\partial x^\alpha}(R_i - R_j)(u_i^\alpha - u_j^\alpha)$$
$$+ \frac{1}{2}\sum_{\alpha,\beta} \frac{\partial^2 V}{\partial x^\alpha \partial x^\beta}(R_i - R_j)\underbrace{(u_i^\alpha - u_j^\alpha)(u_i^\beta - u_j^\beta)}_{u_i^\alpha u_i^\beta + u_j^\alpha u_j^\beta - u_i^\alpha u_j^\beta - u_j^\alpha u_i^\beta}$$

Because $u_i = 0$ is an equilibrium the linear terms added up cancel and we get

$$\text{Pot. En.} = \frac{1}{2}\sum_{i\neq j}' \frac{1}{2}\sum_{\alpha,\beta} \underbrace{\frac{\partial^2 V}{\partial x^\alpha \partial x^\beta}(R_i - R_j)}_{\text{symmetric under } i \leftrightarrow j}\left(u_i^\alpha u_i^\beta + u_j^\alpha u_j^\beta - u_i^\alpha u_j^\beta - u_j^\alpha u_i^\beta\right)$$

$$= \frac{1}{2}\sum_{\alpha,\beta} \sum_{\substack{\text{pairs}\\ (i,j)}} \frac{\partial^2 V}{\partial x^\alpha \partial x^\beta}(R_i - R_j)(u_i^\alpha u_i^\beta - u_i^\alpha u_j^\beta)$$

The term $\frac{1}{2}\sum_{\alpha,\beta}' \sum_i' u_i^\alpha u_i^\beta \sum_{j\neq i} \frac{\partial^2 V}{\partial x^\alpha \partial x^\beta}(R_i - R_j)$ represents the potential energy where each atom is acted on by the others assumed at their equilibrium positions. By translation invariance this term is the same for each atom[redacted], [redacted] The Einstein approximation consists in neglecting the $u_i^\alpha u_j^\beta$ term, which tends to correlate the atoms. In the Einstein approximation one has that each atom is a 3-diml oscillator with the same characteristics.

Notice that the mathematics is the same if the displacements take place in some transversal field direction, in the same sense that one looks at transversal displacements of a [redacted] string. So the point is that u_i is a vector function on Γ and that one has a quadratic Hamiltonian

$$\sum_i \frac{1}{2} p_i^2 + \frac{1}{2} \sum D_{ij} u_i u_j$$

invariant under translation on Γ. (For simplicity suppose u_i 1-dimensional, otherwise you have $D_{ij}^{\alpha\beta} u_i^\alpha u_j^\beta$ with no real difference.) The continuum analogue of the above Hamiltonian is

$$[redacted] \int \frac{1}{2} \left| \frac{\partial \phi}{\partial t}(x) \right|^2 dx + \frac{1}{2} \iint D(x,x') \phi(x) \phi(x') \, dx dx'$$

and translation invariance means that

$$D(x+a, x'+a) = D(x,x') \qquad \text{for all } a$$

so $D(x,x') = D(x-x', 0)$ is a function of the difference $x-x'$.

July 4, 1979

Scattering of a slow neutron by a crystal. The crystal is described by a lattice Γ in $\mathbb{R}^3$ with an atom vibrating near each lattice point. Let $x_\gamma = \gamma + q_\gamma$ be the position of the atom near γ and p_γ be its momentum. Assume small vibrations about the equilibrium $q_\gamma = 0$, so that the potential energy is a positive-definite quadratic form in the displacements q_γ. Assuming translation invariance over Γ this means the Hamiltonian for the crystal is

$$\frac{1}{2m}\sum_\gamma p_\gamma \cdot p_\gamma + \frac{1}{2}\sum_{\gamma,\gamma'} q_\gamma \cdot D(\gamma-\gamma') q_{\gamma'}$$

where $D(\gamma)$ is a positive-definite matrix function on Γ.

The equations of motion are

$$\ddot{q}_\gamma = -\sum_{\gamma'} D(\gamma-\gamma')\, q_{\gamma'} .$$

Normal modes of vibration are in the form

$$q_\gamma = e^{i(k\cdot\gamma - \omega t)}\, v ,$$

where v is a fixed vector in $\mathbb{R}^3$, satisfying

$$-\omega^2 e^{i(k\cdot\gamma-\omega t)} v = -\sum_{\gamma'} D(\gamma-\gamma') e^{i(k\cdot\gamma'-\omega t)} v$$

$$= -\sum_{\gamma'} D(\gamma-(\gamma-\gamma')) e^{i(k\gamma - k\gamma' - \omega t)} v$$

or

$$\omega^2 v = \hat{D}_k v$$

where

$$\hat{D}_k = \sum_{\gamma} D(\gamma) e^{-ik\cdot\gamma)}$$

Since $D_{[redacted]}$ is a positive-definite function on Γ, one knows $\hat{D}_k$ is a positive-definite 3×3 matrix, hence all the <u>frequencies</u> of vibration [redacted] are real.

Useful generalizations: It's better to think of the vibrations taking place in some equivariant [redacted] vector bundle over Γ. (The above case is when the vibrations take place in the normal bundle to the embedding $\Gamma \subset \mathbb{R}^3$.) Question: When can one talk about transversal and longitudinal modes of vibration?

Notice that $\hat{D}_k$ is a function periodic with respect to the dual lattice $\Gamma^* \subset \mathbb{R}^3$, which consists of all k such that $k \cdot \Gamma \subset 2\pi\mathbb{Z}$. It is customary to choose a fundamental domain for Γ^*, called the <u>Brillouin zone</u>, which consists of all k of minimal norm in the Γ^* coset, $k+\Gamma^*$.

Now the Hamiltonian for the free neutron is $\frac{P^2}{2M}$. The interaction will be given by a potential connecting the neutron with any of the atoms in the lattice:

$$\sum_{\gamma}{}' V(X-(R_\gamma + q_\gamma))$$

where X is the position of the neutron. Thus total Hamiltonian is

$$\frac{P^2}{2M} + \frac{1}{2m}\sum_{\gamma}{}' P_\gamma^2 + \frac{1}{2}\sum_{\gamma\gamma'} q_\gamma D(\gamma-\gamma') q_{\gamma'} + \sum_{\gamma}{}' V(X-R_\gamma-q_\gamma).$$

Notice the same Hamiltonian arises for a single electron moving through the crystal. The point is that the neutron nature hasn't been used as far as I can see.

An interesting special case occurs when the atoms are heavy so that we can assume $q_\gamma = 0$. Then we have the motion of a particle through a periodic potential. In the one-dimensional case I [redacted] know[redacted] the spectrum consists of bands. Maybe this also works in higher dimensions.

Notice that once an electron gets in the (lowest) conduction band it propagates indefinitely, so you don't see any resistance. Resistance has to come from interaction with the lattice.

It will [redacted] now be desirable to review potential scattering, the S-matrix, Lipmann-Schwinger, etc. The Schroedinger equation is

$$\left(\frac{-1}{2m}\Delta + V\right)\psi = E\psi \qquad \hbar = 1$$

where say V has compact support. The free wave function of momentum $\vec{k}$ is

$$\varphi_k = e^{ik\cdot x}$$

and the corresponding energy is $E = \frac{k^2}{2m}$. Take $m = \frac{1}{2}$ to simplify, so that we want to solve

$$(-\Delta + V)\psi = k^2\psi .$$

$$(*) \qquad (k^2+\Delta)\psi = V\psi$$

If $k^2 \notin \mathbb{R}_{\geq 0}$, then $k^2+\Delta$ is invertible on L^2; the inverse is given by convolution with the Green's function

$$G_{k+} = -\frac{1}{4\pi}\frac{e^{ikr}}{r}$$

where k is chosen in the UHP. From $(*)$ we see that $\psi - G_{k+}V\psi \in \mathrm{Ker}(k^2+\Delta)$.

Conversely if $\varphi \in \mathrm{Ker}(k^2+\Delta)$ is a free wave function, then any solution of the integral equation

$$\psi - G_{k+}V\psi = \varphi$$

gives a solution of $(*)$ with $\psi-\varphi \in L^2$. Let us denote by $\psi_{\mathbb{k}}^+$ the solution corresponding to $\varphi_{\mathbb{k}}$, so that

$$\psi_{\mathbb{k}}^+ = e^{i\mathbb{k}\cdot x} + \int -\frac{1}{4\pi}\frac{e^{ik|x-x'|}}{|x-x'|}V(x')\psi_{\mathbb{k}}^+(x')\,d^3x'$$

Since for large $r=|x|$ one has

$$|\vec{x}-\vec{x}'| - \underbrace{|\vec{x}|}_{r} = \sqrt{r^2+|x'|^2-2x\cdot x'} - r$$

$$= r\left(\left(1+\frac{|x'|^2-2x\cdot x'}{r^2}\right)^{1/2}-1\right) = -\frac{x\cdot x'}{r} + O\left(\frac{1}{r}\right)$$

one has

$$\frac{e^{ik|\vec{x}-\vec{x}'|}}{|\vec{x}-\vec{x}'|} = \frac{e^{ikr-ik\frac{x\cdot x'}{r}}}{r} + O\left(\frac{1}{r^2}\right)$$

as $r\to\infty$ and this is uniform for x' bounded. Consequently

$$\psi^{+}_{\underline{k}}(\underline{x}) = e^{i\underline{k}\cdot\underline{x}} - \frac{1}{4\pi}\frac{e^{ikr}}{r}\int e^{-ik\frac{x\cdot x'}{r}} V(x') e^{i\underline{k}\cdot\underline{x}'} d^3\underline{x}' + O\left(\frac{1}{r^2}\right)$$

as $\underline{x} = r \to \infty$. The second term represents outgoing spherical waves.

Similarly $(k^2+\Delta)^{-1}$ is given for k in the lower half plane by

$$G_{k-} = -\frac{1}{4\pi}\frac{e^{-ikr}}{r}$$

and so we can define ψ^{-}_{k} by the integral equation

$$\psi^{-}_{k} = e^{ik\cdot x} + G_{k-} V \psi^{-}_{k} .$$

By analytically continuing these functions which are nicely defined in the upper and lower half planes, we get them defined on the real axis.

We use these functions to derive the scattering operator. Let us begin with a square-integrable wave function which represents beam of free particles with momentum concentrated near p

$$\psi_0(x,t) = \int e^{i(k\cdot x - \frac{k^2}{2m}t)} \underbrace{\chi(k)}_{C^\infty \text{ with support near } p.} d^3k$$

For x, t large the method of stationary phase shows that $\psi_0(x,t)$ is small unless the solution of

$$\nabla_k\left(k\cdot x - \frac{k^2}{2m}t\right) = x - \frac{k}{m}t = 0$$

lies near p.

Hence ψ_0 represents a free wave packet with velocity $\frac{p}{m}$. Now what we want is the actual wave function $\psi(x,t)$ which is asymptotic to $\psi_0(x,t)$ as $t \to -\infty$. I claim this is given by

$$\psi^+(x,t) = \int e^{-i\frac{k^2}{2m}t} \psi^+_{\mathbb{k}}(x)\, \chi(\mathbb{k})\, d^3\mathbb{k}$$

The reason is that the outgoing spherical wave part e^{ikr}/r when multiplied by the time-dependence $e^{-i\frac{k^2}{2m}t}$ as $t \to -\infty$, gives rise to a rapidly varying phase

$$e^{i(kr - \frac{k^2}{2m}t)}$$

and so $\psi^+ - \psi_0$ decays as $t \to -\infty$.

Similarly

$$\psi^-(x,t) = \int e^{-i\frac{k^2}{2m}t} \psi^-_{\mathbb{k}}(x)\, \chi(\mathbb{k})\, d^3\mathbb{k}$$

is such that $\psi^- - \psi_0$ decays as $t \to +\infty$.

So the scattering matrix can be described as follows using the basis

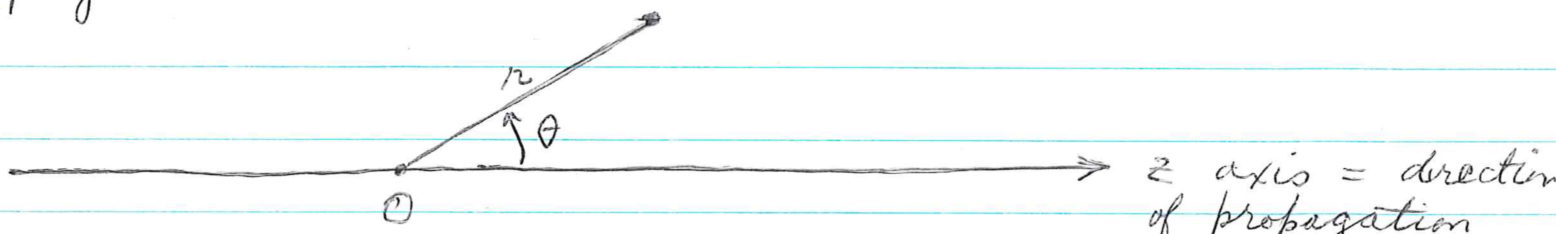
$$\varphi_{\mathbb{k}} = |\mathbb{k}\rangle = e^{i\mathbb{k}\cdot x}$$

for the free states. You start with the free state $\varphi_{\mathbb{k}}$ and form the state $\psi^+_{\mathbb{k}}$ which you think of as a beam of incoming particles of momentum $\mathbb{k}$. You then want to express $\psi^+_{\mathbb{k}}$ in terms of the states $\psi^-_{\mathbb{k}'}$, which you can think of as outgoing beams with momentum $\mathbb{k}'$. The scattering matrix gives the amplitude for the incoming state $\psi^+_{\mathbb{k}}$ to end in the outgoing state $\psi^-_{\mathbb{k}'}$, i.e.

$$\langle \mathbb{k}' | S | \mathbb{k} \rangle = \langle \psi^-_{\mathbb{k}'} | \psi^+_{\mathbb{k}} \rangle$$

July 5, 1979

To understand the scattering matrix when the potential V is spherically symmetric $V = V(r)$ (see Dec 12, 1978). Suppose the incoming wave is a plane wave coming along the z-axis. Use physics notation



where θ is the angle from positive z-axis. The plane wave is

$$\varphi = e^{ikr\cos\theta}$$

and the Laplacian in spherical coordinates is

$$\Delta = \frac{1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}$$

We expand φ, as well as our real wave function ψ, which are φ independent by axial symmetry, in a Legendre series in θ:

$$e^{ikr\cos\theta} = \sum_{\ell=0}^{\infty} \varphi_\ell(kr) P_\ell(\cos\theta)$$

$$\psi(r,\theta) = \sum_{\ell=0}^{\infty} \psi_\ell(r) P_\ell(\cos\theta)$$

The basic facts about Legendre polys. are:

$$(1 + r^2 - 2r\cos\theta)^{-1/2} = \sum_{\ell=0}^{\infty} r^\ell P_\ell(\cos\theta)$$

$$\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \ell(\ell+1)\right] P_\ell(\cos\theta) = 0$$

$$P_\ell(x) = \frac{1}{2^\ell \ell!}\frac{d^\ell}{dx^\ell}(x^2-1)^\ell \qquad = \frac{(2\ell)!}{2^\ell(\ell!)^2}x^\ell + \text{lower}$$

$$\int_{-1}^{1} P_\ell(x)P_{\ell'}(x)\,dx = \left(\frac{2}{2\ell+1}\right)\delta_{\ell\ell'}$$

One has

$$\left[\frac{d}{dr}r^2\frac{d}{dr} - \ell(\ell+1) + (kr)^2\right]\varphi_\ell(kr) = 0$$

from which one can deduce that $r^{1/2}\varphi_\ell$ satisfies Bessel's equation of order $\ell+\frac{1}{2}$, hence must be a multiple of $J_{\ell+\frac{1}{2}}$ since its regular at $r=0$. (The two exponents are $s=\ell, -(\ell+1)$.) To get the behavior at φ_ℓ at zero, use

$$e^{irx} = \sum_\ell \underbrace{\varphi_\ell(r)}_{\text{involves } r^\ell,\, r^{\ell+1},\ldots}\ \underbrace{P_\ell(x)}_{\text{involves } \frac{(2\ell)!}{2^\ell(\ell!)^2}x^\ell + \text{lower}}$$

$$\| \qquad \sum_\ell \frac{1}{\ell!}(irx)^\ell$$

so there's lots of cancelling on the right. If $\varphi_\ell = c_\ell r^\ell + \ldots$

$$\frac{1}{\ell!}i^\ell = c_\ell\frac{(2\ell)!}{2^\ell(\ell!)^2}$$

$$c_\ell = i^\ell\frac{2^\ell\ell!}{(2\ell)!} = \frac{i^\ell}{(2\ell-1)!!}$$

means $1.3\cdots(2\ell-1)$

hence

$$\boxed{\varphi_\ell(r) \sim \frac{i^\ell}{(2\ell-1)!!}r^\ell \qquad \text{as } r\to 0}$$

Next we want behavior as $r\to\infty$. By orthog.,

$$\varphi_\ell(r) = \left(\frac{2\ell+1}{2}\right)\int_{-1}^{1} e^{irx}P_\ell(x)\,dx$$

$$= \frac{2l+1}{2}\left[\frac{e^{irx}}{ir}P_l(x)\right]_{-1}^{1} - \underbrace{\frac{2l+1}{2}\int_{-1}^{1}\frac{e^{irx}}{ir}P_l'(x)\,dx}_{O(\frac{1}{r^2})}$$

$$\sum r^l P_l(1) = (1+r^2-2r)^{-1/2} = \frac{1}{1-r}$$

$\Longrightarrow \quad P_l(1) = 1$. Similarly $P_l(-1) = (-1)^l$. So

$$\boxed{\varphi_l(r) \sim \left(l+\tfrac{1}{2}\right)\frac{e^{ir} - (-1)^l e^{-ir}}{ir} \qquad \text{as } r \to \infty}$$

So now we consider the Schroedinger equation with potential:

$$(\ast) \qquad (\Delta - V + k^2)\psi = 0$$

and take a solution

$$\psi(r,\theta) = \sum_{l=0}^{\infty} \psi_l(r)\, P_l(\cos\theta)$$

so that each ψ_l satisfies

$$\left[\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr} - \frac{l(l+1)}{r^2} - V(r) + k^2\right]\psi_l = 0$$

Assuming $V(r)$ decays fast as $r \to \infty$ we know that any solution has the asymptotic form

$$\psi_l(r) \sim A\,\frac{e^{ikr}}{ikr} + B\,\frac{e^{-ikr}}{ikr}$$

Starting with $\varphi = e^{ikr\cos\theta}$ we want the solution ψ^+ of $(\ast)$ which differs from φ by outgoing spherical waves. We have

$$\varphi_l(kr) \sim \left(l+\tfrac{1}{2}\right)\frac{e^{ikr} - (-1)^l e^{-ikr}}{ikr}$$

Assuming $V(r) = O(\frac{1}{r})$ as $r \to 0$ we know the exponents for ψ_ℓ as $r \to 0$ are ℓ, $-(\ell+1)$ so that upon requiring ψ_ℓ to be reasonable as $r \to 0$ we get a boundary condition

$$\psi_\ell(r) \sim \text{const}\ r^\ell \qquad \text{as } r \to 0$$

and this pins down the ratio of the coefficients A, B. To get ψ_ℓ^+ we choose $B = (\ell+\frac{1}{2})(-1)^{\ell+1}$ in which case we get a unique solution of the ℓ-th radial equation satisfying the required boundary condition at $r \to 0$ with

$$\psi_\ell^+(r) \sim (\ell+\tfrac{1}{2}) \frac{S_\ell(k) e^{ikr} - (-1)^\ell e^{-ikr}}{ikr}$$

similarly

$$\psi_\ell^-(r) \sim (\ell+\tfrac{1}{2}) \frac{e^{ikr} - (-1)^\ell S_\ell^{-1}(k) e^{-ikr}}{ikr}$$

for a suitable constant $S_\ell(k)$. The scattering operator expresses the incoming state via the outgoing states so it is given by multiplication by $S_\ell^+(k)$:

$$\boxed{\psi_\ell^+ = S_\ell \psi_\ell^-}$$

Notice that if $V(r)$ has support in $r \leq a$, then the above asymptotic formulas would be exact for $r > a$ provided one replaces $\frac{e^{ikr}}{ikr}$ by the appropriate spherical Hankel functions. Also $S_\ell(k)$ is of absolute value 1 for k real, since ψ_ℓ^+ can be made real-valued by a constant factor. Also conjugating and changing k to $-k$ leaves ψ^+ unchanged so

$$\overline{S_\ell(k)} = S_\ell(-k)$$

Our next project will be to compute the scattering matrix $\langle \mathbb{k}'|S|\mathbb{k}\rangle$ in terms of the natural basis formed by the free eigenfunctions. We know this vanishes when the energies are different $k' \neq k$. For a fixed energy it is a function of 2 points of S^2 given by the directions of $\mathbb{k}'$ and $\mathbb{k}$. In the spherically symmetric case it depends only on the angle θ between $\mathbb{k}$ and $\mathbb{k}'$.