One thing [redacted] I don't understand at all [redacted] is why multiple instantons contribute to the amplitude

$$\langle x | e^{-T\frac{H}{\hbar}} | x' \rangle$$

in the $T \to \infty$ limit. Recall that as $T \to \infty$

$$\langle x | e^{-T\frac{H}{\hbar}} | x' \rangle \approx e^{-T\frac{E_0}{\hbar}} \varphi_0(x) \overline{\varphi_0(x')}$$

with an error which is a faster decaying exponential. After we take the $T \to \infty$ limit, we tends to single out the ground state we then want to have an asymptotic expansion as $\hbar \to 0$.

A natural formulation of the problem it seems is to consider E_0 as a function of $\hbar$: $E_0 = E_0(\hbar)$ and to expand it as an asymptotic [redacted] series in powers of $\hbar$. For example, suppose we take the simple harmonic oscillator

$$H = \frac{p^2}{2} + \frac{1}{2}\omega^2 q^2 = -\hbar^2 \frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}\omega^2 x^2$$

The eigenvalues of H are $(n+\frac{1}{2})\hbar\omega$, $n = 0, 1, 2, \ldots\ldots$ and hence the eigenvalues of $H/\hbar$ are $(n+\frac{1}{2})\omega$. Thus

$$E_0(\hbar) = \frac{1}{2}\hbar\omega$$

In this case

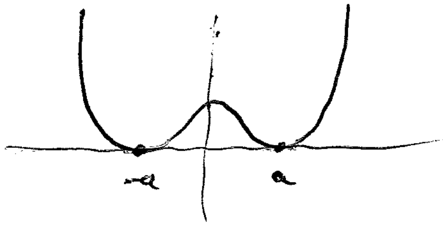
$$\varphi_0(x) = \left(\frac{\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{1}{2}\frac{\omega}{\hbar}x^2}$$

and we get

$$\langle x | e^{-T\frac{H}{\hbar}} | x' \rangle \approx e^{-\frac{1}{2}\omega T} \left(\frac{\omega}{\pi\hbar}\right)^{1/2} e^{-\frac{1}{2}\frac{\omega}{\hbar}(x^2 + x'^2)}$$

as $T \to \infty$ which is exact in $\hbar$.

So now let us consider the double well



The problem is to compute $E_0(\hbar)$ and $\varphi_0(x,\hbar)$ asymptotically in $\hbar$, i.e. I want to understand the formal behavior of these quantities as $\hbar \to 0$.

This is the sort of thing that can be done by standard WKB technique. Let's put $E = \lambda\hbar$ so that we want to solve

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

or

$$\left[\hbar^2 \frac{d^2}{dx^2} - 2V + 2\lambda\hbar\right]\psi = 0$$

Put $\psi = fu$. $\qquad \psi'' = fu'' + 2f'u' + f''u$

$$u'' + 2\frac{f'}{f}u' + \left(\frac{f''}{f} - \frac{2V}{\hbar^2} + \frac{2\lambda}{\hbar}\right)u = 0$$

Now WKB tells us to try $\psi = V^{-1/4}e^{-\frac{1}{\hbar}\int^x \sqrt{2V}}$ so we take this to be f whence

$$\frac{f'}{f} = -\frac{1}{4}\frac{V'}{V} - \frac{1}{\hbar}\sqrt{2V}$$

$$\frac{f''}{f} - \left(\frac{f'}{f}\right)^2 = -\frac{1}{4}\left(\frac{V'}{V}\right)' - \frac{1}{\hbar}(\sqrt{2V})'$$

$$\frac{f''}{f} = -\frac{1}{4}\left(\frac{V'}{V}\right)' - \frac{1}{\hbar}(\sqrt{2V})' + \underbrace{\left(\frac{\sqrt{2V}}{\hbar} + \frac{1}{4}\frac{V'}{V}\right)^2}_{\frac{2V}{\hbar^2} + \frac{\sqrt{2}}{2\hbar}\frac{V'}{\sqrt{V}} + \left(\frac{1}{4}\frac{V'}{V}\right)^2}$$

So
$$\frac{f''}{f} - \frac{2V}{h} = -\frac{1}{4}\left(\frac{V'}{V}\right)' + \left(\frac{1}{4}\frac{V'}{V}\right)^2$$

You're missing the point which is to choose f so that a formal power series in h becomes possible. Hence if we choose
$$f = e^{-\frac{1}{h}\int^x \sqrt{2V}} \qquad \frac{f'}{f} = -\frac{1}{h}\sqrt{2V}$$

we have
$$\frac{f''}{f} - \left(\frac{f'}{f}\right)^2 = -\frac{1}{h}\left(\sqrt{2V}\right)'$$

or
$$\frac{f''}{f} = \frac{1}{h^2}2V - \frac{1}{h}\left(\sqrt{2V}\right)'$$

Then
$$\frac{f''}{f} - \frac{2V}{h^2} = -\frac{1}{h}\left(\sqrt{2V}\right)'$$

and the DE becomes
$$u'' + 2\left(-\frac{1}{h}\sqrt{2V}\right)u' + \left[-\frac{1}{h}\left(\sqrt{2V}\right)' + \frac{2\lambda}{h}\right]u = 0$$

or
$$\left(2\sqrt{2V}\right)u' + \left(\left(\sqrt{2V}\right)' - 2\lambda\right)u = hu''$$

This can be solved formally at least by starting with the solution for $h=0$:
$$u' + \left(\frac{1}{4}\frac{V'}{V} - \frac{\lambda}{\sqrt{2V}}\right)u = 0$$

$$u = V^{-1/4} e^{\lambda\int^x \frac{dx}{\sqrt{2V}}}$$

Hence
$$\boxed{\psi = V^{-1/4} e^{-\frac{1}{h}\int^x \sqrt{2V}\,dx + \lambda\int^x \frac{dx}{\sqrt{2V}}}\left(1 + a_1(x)h + \cdots\right)}$$

October 20, 1979

It seems that when you do WKB for scalar functions one should try to put the asymptotic series in the exponential.

$$\psi = e^{\frac{1}{h}(u_0 + hu_1 + h^2 u_2 + \cdots)}$$

The computations seem to be easier.

$$\psi'' = \left(e^{\frac{u}{h}}\right)'' = \left(e^{\frac{u}{h}}\frac{u'}{h}\right)' = e^{\frac{u}{h}}\frac{u''}{h} + e^{\frac{u}{h}}\left(\frac{u'}{h}\right)^2$$

$$\psi'' + \frac{2E-2V}{h^2}\psi = 0 \quad \text{becomes} \quad \frac{u''}{h} + \frac{(u')^2}{h^2} + \frac{2E-2V}{h^2} = 0$$

or

$$hu'' + (u')^2 + 2E - 2V = 0$$

We want the approximation with $E = h\lambda$. Notice that this is a Riccati equation for u', i.e. a first order non-linear DE. Set $u = u_0 + u_1 h + \cdots$

$$(u_0' + u_1' h + \cdots)^2 + h(u_0'' + hu_1'' + \cdots) + 2\lambda h - 2V = 0$$

$$(u_0'^2 - 2V) + h(2u_0'u_1' + u_0'' + 2\lambda) + h^2(u_1'^2 + 2u_0'u_2' + u_1'') + \cdots = 0$$

so

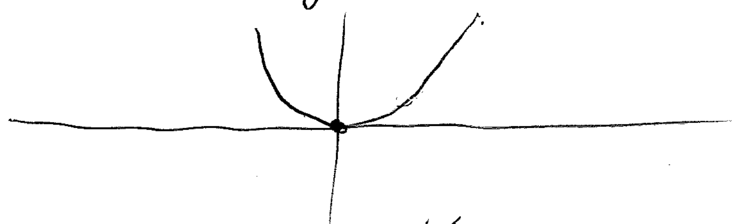
$$u_0' = \pm\sqrt{2V} \qquad\qquad u_0 =$$

$$u_1' = -\frac{u_0''}{2u_0'} - \frac{\lambda}{u_0'} \qquad\qquad u_1 = -\frac{1}{4}\log V \mp \int^x \frac{\lambda}{\sqrt{2V}}$$

$$u_2' = \left(-(u_1')^2 - u_1''\right)/2u_0' \qquad\qquad \text{etc.}$$

Problem: We are told that we can obtain the WKB answers by instanton methods. We want to understand this. One idea I have is to make the WKB method precise as an asymptotic method. It really should be possible to grind out formal series solutions.

The first thing to make precise is the case when V has a single minimum at $x=0$.



Then I should obtain the ground energy of $\frac{1}{2}\omega\hbar$ approximately where $V''(0)=\omega^2$. The real question is whether [redacted] there is a formal power series [redacted] expansion

$$E_0(\hbar) = \frac{1}{2}\omega\hbar + a_1\hbar^2 + \cdots$$

October 21, 1979

DHN papers (Dashen, Hasslacher, Neveu Phys. Rev D11 (1975) 3424. This begins as follows: One has a Hamiltonian with discrete levels E_n and wants to understand

$$tr \frac{1}{E-H} = \sum_n \frac{1}{E-E_n}$$

so as to find E_0. One uses Fourier transform

$$tr \frac{1}{H-E} = i \int_0^\infty e^{itE} tr\left(e^{-itH}\right) dt$$

and the path integral formula

$$tr\left(e^{-iTH}\right) = \int_{\substack{x \text{ periodic} \\ \text{of period } T}} \mathcal{D}x \; e^{iS}$$

Then one "calculates" the latter by stationary phase, i.e. looking at classical periodic trajectories.

Let's look at the simpler problem of finding the amplitude $\langle x | e^{-iTH} | x' \rangle$ by stationary phase. Assume there is one classical path [redacted] $\bar{x}$ with $\bar{x}(0) = x'$, $\bar{x}(T) = x$ and let's use the stationary phase approximation

$$\int_{\substack{q(0)=x' \\ q(T)=x}} \mathcal{D}q \; e^{iS(q)} \approx e^{iS(\bar{x})} \underbrace{\int_{\substack{y(0)=0 \\ y(T)=0}} \mathcal{D}y \; e^{i\int_0^T \frac{1}{2}(\dot{y}^2 - V''(\bar{x})y^2)dt}}_{\left(\frac{\det\left(-\partial_t^2 - V''(\bar{x})\right)}{\det\left(-\partial_t^2\right)}\right)^{-1/2} \int \mathcal{D}y \; e^{-\int_0^T \frac{1}{2}\dot{y}^2 dt}}$$

The free propagator is $\langle x | e^{-it\frac{p^2}{2}} | x' \rangle$

$$= \int \frac{dp}{2\pi} e^{-ip(x-x') - it\frac{p^2}{2}} = \frac{1}{\sqrt{2\pi i t}} e^{-\frac{1}{2}\frac{(x-x')^2}{it}}$$

so [redacted]

$$\int \mathcal{D}y \, e^{-\int_0^T \frac{1}{2}\dot{y}^2 dt} = \frac{1}{\sqrt{2\pi i T}}$$

Next we want to evaluate the determinant factor. Recall my old formula

$$\frac{\det(-\partial_t^2 + g)}{\det(-\partial_t^2)} = \frac{W(\phi, \psi)}{W(\phi^\circ, \psi^\circ)}$$

where ϕ satisfies the bdry condition at 0 and ψ at T. Choose ϕ so that

$$(-\partial_t^2 + g)\phi = 0 \qquad \phi(0) = 0 \quad \phi'(0) = 1$$

$$(-\partial_t^2 + g)\psi = 0 \qquad \psi(T) = 0 \quad \psi'(T) = 1$$

Then $\phi^\circ = t$, $\psi^\circ = t - T$ and

$$W(\phi, \psi) = \begin{vmatrix} \phi & 0 \\ \phi' & 1 \end{vmatrix}(T) = \phi(T)$$

$$W(\phi^\circ, \psi^\circ) = t(T) = T$$

hence

$$\frac{\det(-\partial_t^2 + g)}{\det(-\partial_t^2)} = \frac{\phi(T)}{T}$$

e.g. if $g = -\omega^2$, then $\phi(T) = \frac{\sin \omega T}{\omega}$ and so we get

$$\int \mathcal{D}y \, e^{i\int_0^T \frac{1}{2}(\dot{y}^2 - \omega^2 y^2)\, dt} = \frac{1}{\sqrt{2\pi i T}} \left(\frac{\omega T}{\sin \omega T} \right)^{1/2} = \left(\frac{\omega}{\pi}\right)^{1/2} \left(\frac{1}{e^{i\omega T} - e^{-i\omega T}} \right)^{1/2}$$

Gelfand + Yaglom have a better way to obtain the determinant, based on the idea that there is a Volterra operator which connects the operators $-\partial_t^2$ and $-\partial_t^2 + q$. This probably gives a nice isomorphism between the desired path integral and a free path integral where the T endpoint of the paths is displaced from 0.

October 26, 1979

Let us consider a path integral

$$\langle x | e^{-iTH} | x' \rangle = \int \mathcal{D}x(t)\, e^{iS}$$

where
$$S = \int_0^T \left[\tfrac{1}{2}\dot{x}^2 - V(x)\right] dt$$

and make Gaussian expansion around the classical motion: $x = \bar{x} + y$. What this effectively does is to replace the Schroedinger equation

$$i\frac{\partial \psi}{\partial t} = \left[\frac{p^2}{2} + V(q)\right]\psi$$

by a time-dependent oscillator problem:

$$i\frac{\partial \tilde{\psi}}{\partial t} = \left[\frac{p^2}{2} + V''(\bar{x}(t))\frac{q^2}{2}\right]\tilde{\psi}$$

so we should carefully look at this sort of problem.

So we are given $V(t)$ on $\mathbb{R}$ and

$$i\frac{\partial \psi}{\partial t} = \left(\frac{p^2}{2} + V(t)\frac{q^2}{2}\right)\psi$$

and we want to compute the propagator

$$\langle x | U(T,0) | x' \rangle = \int \mathcal{D}x(t)\, e^{i\int_0^T \frac{1}{2}[\dot{x}^2 - Vx^2]dt}$$

The integrand e^{iS} on the left is Gaussian, or rather S is a quadratic function on the space of paths on $[0,T]$ [redacted] starting at x' and ending at x. This example should be understood carefully.

The Lagrangian is

[redacted]. $L(t,x,\dot{x}) = \frac{1}{2}(\dot{x}^2 - V(t)x^2)$

and the Euler-Lagrange equations of motion are

$$\frac{\partial L}{\partial \dot{x}} = \dot{x} \qquad \ddot{x} = \frac{\partial L}{\partial x} = -V(t)\, x$$

i.e.
$$\left[\partial_t^2 + V(t)\right] x = 0$$

Thus there is a unique classical trajectory going from x' to x when $\partial_t^2 + V(t)$ has no null eigenfunction on $[0,T]$. The index of the form $\int L\,dt$ on [redacted] fns. with 0 eigenvalues, i.e. number of negative eigenvalues is the number of critical points encountered on $(0,T]$, i.e. the number of zeroes the ϕ solution has.

[redacted]

The path integral formula shows that
$$\langle x | U(T,0) | x' \rangle = e^{iS(x,x')} \langle x{=}0 | U(T,0) | x'{=}0 \rangle$$

where S is the action of the classical path joining x' to x. Since the equation of motion is linear we can express $\bar{x}$ in terms of the ϕ and ψ solutions on $[0,T]$

$$\bar{x}(t) = x' \frac{\psi(t)}{\psi(0)} + x \frac{\phi(t)}{\phi(T)}$$

Now
$$S(\bar{x}) = \frac{1}{2}\int_0^T \left[(\partial_t \bar{x})^2 - V(t)\,\bar{x}^2\right] dt$$

$$= \frac{1}{2}\left[\bar{x}\,\partial_t \bar{x}\right]_0^T - \frac{1}{2}\int_0^T \bar{x}\,\underbrace{\left[\partial_t^2 \bar{x} + V(t)\bar{x}\right]}_{=0} dt$$

$$= \frac{1}{2}\, x \left(x' \frac{\psi'(T)}{\psi(0)} + x \frac{\phi'(T)}{\phi(T)} \right) - \frac{1}{2}\, x' \left(x' \frac{\psi'(0)}{\psi(0)} + x \frac{\phi'(0)}{\phi(T)} \right)$$

$$= \frac{1}{2}\left[x^2 \frac{\phi'(T)}{\phi(T)} + x x' \left(\frac{\psi'(T)}{\psi(0)} - \frac{\phi'(0)}{\phi(T)} \right) - x'^2 \frac{\psi'(0)}{\psi(0)} \right]$$

As a check take $V = \omega^2$, whence $\phi = \sin \omega t$, $\psi = \sin \omega(T-t)$. Then you get

$$S(\bar{x}) = \frac{1}{2}\left[x^2 \frac{\omega \cos \omega T}{\sin \omega T} + x x'\left(\frac{-\omega \cos 0}{\sin \omega T} - \frac{\omega \cos 0}{\sin \omega T}\right) + x'^2 \frac{\omega \cos \omega T}{\sin \omega T}\right)$$

$$= \frac{1}{2}\frac{\omega}{\sin \omega T}\left[x^2 \cos \omega T - 2 x x' + x'^2 \cos \omega T\right]$$

which agrees with p. 333.

Let's look next at the Gelfand-Yaglom idea which is to reduce the quadratic form $\int \frac{1}{2}(\dot{x}^2 - V x^2)$ to $\int \frac{1}{2}\dot{x}$ via a Volterra operator. Choose a solution N of

$$N'' + VN = 0$$

on $[0,T]$ which doesn't vanish. This is possible provided ϕ doesn't vanish on $(0,T]$. Then one has the factorization

$$-\partial_t^2 - V = (+\partial_t + p)(-\partial_t + p) \qquad p = \frac{N'}{N}$$

or

$$\partial_t^2 + V = (\partial_t + p)\partial_t^{-1}\partial_t^2\,\partial_t^{-1}(\partial_t - p)$$

$$= K^* \partial_t^2 K$$

where K is the Volterra operator

$$Kx = \partial_t^{-1}(\partial_t - p)x = (1 - \partial_t^{-1}p)x = x(t) - \int_0^t p(t')x(t')dt'$$

Then

$$\partial_t K = \partial_t - p$$

hence

$$\int_0^T (\partial_t K x)^2\, dt = \int_0^T (\partial_t x)^2 \underbrace{- p x \partial_t x - p \partial_t x \cdot x}_{p\,\partial_t(x^2)} + p^2 x^2\, dt$$

$$= \left[-p x^2\right]_0^T + \int_0^T \left[(\partial_t x)^2 - V x^2\right] dt \qquad \text{as } -V = p^2 + p'$$

Suppose we want to evaluate the path integral with 0 endpoint. Then we can change variables by putting

$$y = Kx \qquad \text{or} \qquad y(t) = x(t) - \int_0^t p(t')x(t')\,dt'$$

and we get

$$\int_{x(0)=x(T)=0} \mathcal{D}x(t)\, e^{i\int_0^T \frac{1}{2}(\dot{x}^2 - Vx^2)\,dt} = \int \mathcal{D}y(t) \underbrace{\left|\frac{\mathcal{D}x(t)}{\mathcal{D}y(t)}\right|}_{\text{Jacobian factor which should be } \underline{1}.} e^{i\int_0^T \frac{1}{2}\dot{y}^2\,dt}$$

at least formally. The only problem is what happens to the condition that $x(0) = x(T) = 0$. Let's work out the inverse of K. One has a linear DE

$$\partial_t y = \partial_t x - p x$$

with integrating factor $e^{-\int p} = e^{-\int \frac{N'}{N}} = \frac{1}{N}$ so

$$\partial_t \left(\frac{x}{N}\right) = \frac{x}{N} - \frac{N'}{N^2}x = \frac{1}{N}\partial_t y = \partial_t\left(\frac{1}{N}y\right) + \frac{1}{N}N'\frac{1}{N}y$$

so

$$\frac{x}{N} = \frac{y}{N} + \int_0^t \frac{N'}{N^2} y$$

or

$$x(t) = y(t) + N(t)\int_0^t \frac{N'}{N^2}(t')\,y(t')\,dt'$$

Therefore the condition $x(T) = 0$ becomes

$$y(T) + N(T)\int_0^T \frac{N'}{N^2}(t)\,y(t)\,dt = 0.$$

Idea: [redacted]

Look at the quadratic form $\frac{1}{2}\int_0^T \dot{y}^2\,dt$ on the space of $y(t)$ with $y(0)=0$. Then its positive-definite because if $\dot{y}=0$ and $y(0)=0$, then $y=0$.

Next question: Does

$$\int_{y(0)=0} \mathcal{D}y \; e^{i\int_0^T \frac{1}{2}\dot{y}^2\,dt}$$

make sense? We know that

$$\int_{\substack{y(0)=0\\ y(T)=y}} \mathcal{D}y(t)\, e^{i\int_0^T \frac{1}{2}\dot{y}^2\,dt} = \frac{1}{\sqrt{2\pi i T}}\, e^{\frac{i y^2}{2T}}$$

from the calculations of the free propagator, so the integral we want is

$$\int \frac{1}{\sqrt{2\pi i T}}\, e^{-\frac{y^2}{2iT}}\,dy = \frac{\sqrt{2\pi i T}}{\sqrt{2\pi i T}} = 1.$$

Now one goes back to

$$\frac{1}{2}\int_0^T (\dot{x}^2 - Vx^2)\,dt - \frac{1}{2}p x^2\Big]_0^T = \frac{1}{2}\int_0^T (\dot{Kx})^2\,dt$$

so

$$\int_{x(0)=0} \mathcal{D}x(t)\, e^{i\frac{1}{2}\int_0^T (\dot{x}^2 - Vx^2)\,dt - \frac{i}{2}p(T)\,x(T)^2} = \int_{y(0)=0} \mathcal{D}y(t)\, e^{i\int_0^T \frac{\dot{y}^2}{2}\,dt} = 1$$

assuming the Jacobian factor $\left|\frac{\mathcal{D}x}{\mathcal{D}y}\right|$ is 1. This assumption can't be correct because the left side depends on $p(T)$. We can evaluate the left side by first integrating over $x(T)$ which gives the Gaussian factor

$$\frac{1}{\sqrt{2\pi i\, p(T)}}$$

October 27, 1979

The problem is to understand the Volterra transform methods of Gelfand-Yaglom for evaluating Feynman path integrals. The transform is

$$y(t) = (Kx)(t) = x(t) - \int_0^t p(t')x(t')dt'$$

on functions defined on $[0,T]$ and vanishing for $t=0$. The first question is whether the Jacobian

$$\left|\frac{\mathcal{D}y(t)}{\mathcal{D}x(t)}\right|$$

should be different from 1. (How (maybe) to think of this Jacobian: $\mathcal{D}x(t)$ and $\mathcal{D}y(t)$ weight curves evenly but the transformation $x \longmapsto Kx = y$ might tend to bunch them up somewhere, hence giving a Jacobian factor)

This Jacobian factor is something like the determinant of the linear transformation K whose kernel is $\delta(t-t') -$

$$\tilde{K}(t,t') = \begin{cases} 0 & t<t' \\ p(t') & t>t' \end{cases}$$

It should be possible to reconstruct $\det K$ by varying p, and hence we probably need only define $\operatorname{tr}(\tilde{K})$. This is problematic because $\tilde{K}$ is not continuous on the diagonal.

Example: Consider a convolution operator on $S^1 = \mathbb{R}/2\pi\mathbb{Z}$.

$$(Tf)(x) = \int T(x-y)f(y)dy = \int T(y)f(x-y)dy$$

Then

$$Te^{inx} = e^{inx}\underbrace{\int T(y)e^{-iny}dy}_{\hat{T}(n)}$$

so the trace of T is

$$2\pi T(0) = \int T(x-x)\,dx = \sum_{n\in\mathbb{Z}} \hat{T}(n)$$

It's clear that T is of trace class when the above series is absolutely convergent, which implies that $T(x)$ is continuous, and hence $T(0)$ is unambiguous.

Now a jump discontinuity of $T(x)$ produces a behavior $\hat{T}(n) = O(\frac{1}{n})$, so the series doesn't converge absolutely. However the obvious choice is to use Eisenstein summation for the series, which amounts to averaging $T(0^+)$ and $T(0^-)$.

When this averaging is done for $\tilde{K}$ we get

$$\mathrm{tr}(\tilde{K}) = \frac{1}{2}\int_0^T p(t)\,dt$$

$$\det(K) = e^{-\frac{1}{2}\int_0^T p(t)\,dt}$$

Notice that because the transformation K is linear, the determinantal factor should be a constant function of the path, and hence should depend only on T. Let's return to

$$1 = \int_{y(0)=0} \mathcal{D}y\, e^{i\int_0^T \frac{1}{2}\dot{y}^2 dt} = \int_{x(0)=0} \mathcal{D}x \left|\frac{\mathcal{D}y}{\mathcal{D}x}\right| e^{i\int_0^T \frac{1}{2}(\dot{x}^2 - Vx^2)dt - i\frac{1}{2}p(T)x(T)^2}$$

$$= \int dx(T) \left|\frac{\mathcal{D}y}{\mathcal{D}x}\right| e^{-i\frac{1}{2}p(T)x(T)^2} \underbrace{\int_{\substack{x(0)=0 \\ x(T)=x(T)}} \mathcal{D}x(t)\, e^{i\int_0^T \frac{1}{2}(\dot{x}^2 - Vx^2)dt}}$$

We know the amplitude $\longrightarrow$ $\langle x(T) \,|\, U(T,0)\,|\, 0\rangle$ is proportional to $e^{i\frac{1}{2}\frac{\phi'(T)}{\phi(T)}x(T)^2}$ by p. 366

Consequently we get

$$1 = \left|\frac{\mathcal{D}y}{\mathcal{D}x}\right| \cdot \begin{pmatrix}\text{prop. const} \\ \text{dep. on } V \\ \text{alone}\end{pmatrix} \underbrace{\int e^{-\frac{i}{2}\left(p(T) - \frac{\phi'(T)}{\phi(T)}\right) x(T)^2} dx(T)}_{\frac{2\pi}{\sqrt{2\pi i \left(p(T) - \frac{\phi'(T)}{\phi(T)}\right)}}}$$

Now $p = \dfrac{X'}{X}$ where X is a non-vanishing soln of $X'' + VX = 0$. Also

$$p(T) - \frac{\phi'(T)}{\phi(T)} = \frac{1}{X(T)\phi(T)} W(\phi, X)$$

and the Wronskian doesn't change if a multiple of ϕ is added to X. So therefore if we multiply:

$$\frac{X(T)}{X(0)}\left(p(T) - \frac{\phi'(T)}{\phi(T)}\right) = \frac{1}{X(0)\phi(T)} W(\phi, X)$$

we get something independent of the change $X \mapsto aX + b\phi$ (recall $\phi(0) = 0$). So we expect

$$\left|\frac{\mathcal{D}y}{\mathcal{D}x}\right| = \text{const} \cdot \sqrt{\frac{X(0)}{X(T)}}$$

But $$e^{-\frac{1}{2}\int p} = e^{-\frac{1}{2}\int_0^T X'/X} = e^{\left[-\frac{1}{2}\log X\right]_0^T} = \left(\frac{X(0)}{X(T)}\right)^{1/2}$$

so it checks.

Furthermore

$$\frac{X(T)}{X(0)}\left(p(T) - \frac{\phi'(T)}{\phi(T)}\right) = \frac{1}{X(0)\phi(T)} \begin{vmatrix}\phi & X \\ \phi' & X'\end{vmatrix}(0) = -\frac{\phi'(0)}{\phi(T)}$$

so the constant depending on V is $1\Big/\sqrt{2\pi i \dfrac{\phi(T)}{\phi'(0)}}$

and we get the formula:

$$\langle x | U(T,0) | x' \rangle = \int_{\substack{x(0)=x' \\ x(T)=x}} \mathcal{D}x \; e^{i\int_0^T \frac{1}{2}(\dot{x}^2 - Vx^2)\,dt}$$

$$= e^{iS(x,x')} \Big/ \sqrt{2\pi i \frac{\phi(T)}{\phi'(0)}}$$

where S is given at the bottom of 366. Note this agrees with

$$\int_{\substack{x(0)=0 \\ x(T)=0}} \mathcal{D}x \; e^{i\int_0^T \frac{1}{2}(\dot{x}^2 - Vx^2)\,dt} = \underbrace{\left(\frac{\det(-\partial_t^2 - V)}{\det(-\partial_t^2)}\right)^{-1/2}}_{} \frac{1}{\sqrt{2\pi i T}}$$

$$\frac{W(\phi,\psi)}{W(\phi^0,\psi^0)} = \frac{\begin{vmatrix} \phi(T) & 0 \\ \phi'(T) & 1 \end{vmatrix}}{\begin{vmatrix} T\phi'(0) & 0 \\ \phi'(0) & 1 \end{vmatrix}} = \frac{\phi(T)}{T\phi'(0)}$$

$$\| $$

$$\frac{1}{\sqrt{2\pi i \frac{\phi(T)}{\phi'(0)}}}$$

Notice also that

$$\frac{\partial^2 S}{\partial x \partial x'} = \frac{1}{2}\left(\frac{\psi'(T)}{\psi(0)} - \frac{\phi'(0)}{\phi(T)}\right) = -\frac{\phi'(0)}{\phi(T)}$$

because

$$W(\phi,\psi) = \begin{vmatrix} \phi & \psi \\ \phi' & \psi' \end{vmatrix} = -\phi'(0)\psi(0) = \phi(T)\psi'(T)$$

so

$$-\frac{\phi'(0)}{\phi(T)} = \frac{\psi'(T)}{\psi(0)} = \frac{\partial^2 S}{\partial x \partial x'}$$

October 28, 1979

Given $\quad i\hbar \frac{\partial \psi}{\partial t} = \left(-\frac{p^2}{2} + V(t,q)\right)\psi \quad$ we have two ways of constructing a semi-classical approximation to the amplitude

$$\langle x | U(T,0) | x' \rangle = \int_{\substack{x(0)=x' \\ x(T)=x}} \mathcal{D}x(t)\, e^{\frac{i}{\hbar}\int_0^T \left(\frac{1}{2}\dot{x}^2 - V\right)dt} .$$

One method uses stationary phase on the path integral, the other is to find a formal solution of the Schroedinger equation of the form

$$\psi = e^{\frac{i}{\hbar}u} \qquad\qquad u = u_0 + \hbar u_1 + \hbar^2 u_2 + \cdots\cdots$$

Substituting this in gives

$$i\hbar \frac{i}{\hbar}\partial_t u = -\frac{\hbar^2}{2}\left(\left(\frac{i}{\hbar}\partial_x u\right)^2 + \frac{i}{\hbar}\partial_x^2 u\right) + V$$

or

$$\partial_t u + \frac{1}{2}(\partial_x u)^2 + V - \hbar\frac{i}{2}\partial_x^2 u = 0$$

$$\begin{cases} \partial_t u_0 + \frac{1}{2}(\nabla u_0)^2 + V = 0 & \qquad \nabla = \partial_x \\ (\partial_t + \nabla u_0 \cdot \nabla)\, u_1 = \frac{i}{2}\nabla^2 u_0 & \end{cases}$$

The first equation is the Hamilton-Jacobi equation which is satisfied by the action $S(t,x)$ going from $(0,x')$ to (t,x).

Let's use the stationary phase method:

$$\langle x | U(T,0) | x' \rangle \approx e^{\frac{i}{\hbar}S(T,x)} \int_{\substack{y(0)=0 \\ y(T)=0}} \mathcal{D}y(t)\, e^{\frac{i}{\hbar}\int_0^T \frac{1}{2}\left(\dot{y}^2 - V''(\bar{x})y^2\right)dt}$$

The second path integral is

$$\left(\frac{\det\left(-\partial_t^2 - V''(\bar{x})\right)}{\det\left(-\partial_t^2\right)}\right)^{-1/2} \frac{1}{\sqrt{2\pi i h T}} = \frac{1}{\sqrt{2\pi i h\, \phi(T)}}$$

where ϕ satisfies $\quad \left(\partial_t^2 + V''(\bar{x})\right)\phi = 0, \quad \phi(0) = 0, \quad \phi'(0) = 1.$

Hence it should be possible to show that

$$e^{i u_1} = \text{const.}\ \phi^{-1/2}$$

Recall how we construct a solution to the Hamilton-Jacobi equation

$$\partial_t S + \tfrac{1}{2}(\nabla S)^2 + V = 0.$$

It is convenient to remember that a Lagrangian submanifold of T^* (q, p space) which projects non-singularity on q-space is a section dS, i.e. $p = \nabla S$ for some $S = S(q)$. One starts with $S(0,q)$ being given and let's the Hamilton flow in (t,q,p) space sweep out the section $p = \nabla S(0,q)$ over $t=0$ to get $S(t,q)$. However one could also start with the submanifold of $(0,q,p)$-space given by $q = x'$ and arbitrary p and this gives the solution $S(t,x)$ we are interested in.

Thus to find S we first let $x(t,\alpha)$ denote the solution of the classical motion

$$\ddot{x}(t,\alpha) = -\nabla V(t, x(t,\alpha))$$

with $\qquad x(0,\alpha) = x', \qquad \dot{x}(0,\alpha) = \alpha.$

Then differentiating with respect to α we get

$$\ddot{\partial_\alpha x}(t,\alpha) = -\nabla^2 V(t, x(t,\alpha))\, \partial_\alpha x(t,\alpha)$$

$$\partial_\alpha x(0,\alpha) = 0 \qquad \partial_\alpha \dot{x}(0,\alpha) = 1$$

In other words $\partial x(t,\alpha) = \phi_\alpha(t)$ is the solution of the linearized equations with the good boundary conditions at $t=0$. Now

$$\dot{x}(t,\alpha) = p(t,\alpha) = \partial_x S(t, x(t,\alpha))$$

so

$$\partial_\alpha \dot{x}(t,\alpha) = \partial_x^2 S(t, x(t,\alpha))\, \partial_\alpha x(t,\alpha)$$

or

$$\dot{\phi}_\alpha(t) = \partial_x^2 S(t, x(t,\alpha))\, \phi_\alpha(t).$$

This last equation shows what I want namely that along a trajectory $x = \bar{x}(t) = x(t,\alpha_0)$ one has

$$\nabla^2 S = \frac{\phi'(t)}{\phi(t)}$$

so that

$$\frac{d}{dt} i u_1 = -\frac{1}{2}\frac{d}{dt}\log\phi$$

or

$$e^{iu_1} = \text{const.}\ \phi^{-1/2}.$$

The above shows that we can get the stationary phase approximation to the path integral by elementary WKB arguments. Recall that for fixed energy one has WKB, but the path integral isn't so clear, so maybe it would be worthwhile to investigate this case in more detail. The Schroedinger equation is

$$\left(-\frac{h^2}{2}\nabla^2 + V\right)\psi = E\psi$$

and if we set $\psi = e^{\frac{i}{h} u}$ we get

$$-\frac{h^2}{2}\left(\left(\frac{i}{h}\nabla u\right)^2 + \frac{i}{h}\nabla^2 u\right) + V = E$$

or

$$\frac{1}{2}(\nabla u)^2 + V - E = h\frac{i}{2}\nabla^2 u$$

leading to

$$\begin{cases} (\nabla u_0)^2 = 2(E-V) \\ (\nabla u_0 \cdot \nabla) u_1 = \frac{i}{2}\nabla^2 u_0 \end{cases}$$

In this situation we can use the Hamilton-Jacobi DE to give us the appropriate action. We want to solve

$$(\nabla W)^2 = 2(E-V)$$

or better $\frac{1}{2}(\nabla W)^2 + V = E$. So we are given a hypersurface in T^* or (q,p) space. From the symplectic structure we get a field of one-dimensional tangent spaces. In fact since we have represented the hypersurface by $H(q,p) = \frac{1}{2}p^2 + V(q) = E$, we have the Hamiltonian flow on this hypersurface. To get dW we choose a transversal to this flow and a Lagrangian subspace inside the transversal and then let the Lagrangian subspace be swept out. A suitable Lagrangian subspace is furnished by $q = x'$ and all the p with $\frac{1}{2}p^2 + V(q) = E$. Hamilton's equations

$$\dot{q} = p, \quad \dot{p} = -\nabla V$$

then give all trajectories issuing from x' with the energy E. The action function then is

$$W(x,x') = \int dW = \int \sqrt{2(E-V)}\, ds$$

where the integral is taken over the trajectory going from x' to x. Notice that if we a curve $x(t)$ of energy E, then

$$|\dot{x}| = \sqrt{2(E-V)} \qquad \frac{ds}{dt} = \sqrt{2(E-V)}$$

so the action along this curve is

$$\int p\dot{x}\,dt = \int \dot{x}^2\,dt = \int (2(E-V))\frac{ds}{\sqrt{2(E-V)}} = \int \sqrt{2(E-V)}\,ds.$$

[redacted] This checks with the principle of least action, namely, that the action is stationary for trajectory curves. Another interpretation is that the trajectories are geodesics for the arclength $dW = \sqrt{2(E-V)}\,ds$. Note the time is not necessarily stationary for

$$dt = \frac{ds}{\sqrt{2(E-V)}}.$$

At this stage we have the action $W(x,x')$ so I can try to construct a path integral

$$\int_{\substack{x(0)=x' \\ x(T)=x}} \mathcal{D}x(t)\, e^{i\int dW}$$

except that the parameterization of the path shouldn't matter, which means you have to divide out by different parametrizations, say by means of projection on a "time" axis.

Another question is what amplitude or "kernel" $K(x,x')$ this path integral should represent. It's "obviously" a solution of the Schroedinger equation for $x \neq x'$.

October 29, 1979

Recall that we trying to solve

$$\left(-\tfrac{1}{2}\Delta + V\right)\psi = E\psi$$

by a WKB method. We put $\psi = e^{\frac{i}{h}(u_0 + hu_1 + \cdots)}$ and derived the equations

$$\begin{cases} \frac{1}{2}(\nabla u_0)^2 + V = E \\ \nabla u_0 \cdot \nabla u_1 = \frac{i}{2}\nabla^2 u_0 \end{cases}$$

To solve these we consider the solution of the [redacted] classical motion starting from a fixed point x' with the energy E. Let $x = q(t,\alpha)$ denote the solution of

$$\ddot{x} = -\nabla V(x)$$

[redacted]

$$q(0,\alpha) = x' \qquad \dot{q}(0,\alpha) = \alpha$$

where α runs over all vectors with $\frac{1}{2}\alpha^2 + V(x') = E$. Fix α_0 and consider small variations around the α_0-trajectory. Denote by ∂_α taking the derivative in a direction $\alpha \perp \alpha_0$. Then from

$$\partial_t^2 q = -\nabla V(q)$$

we get

$$\partial_t^2 \partial_\alpha q = -\partial_\alpha \nabla V(q) = -\nabla^2 V(q)\, \partial_\alpha q.$$

Now we know already that

$$\partial_t q = \nabla W(q)$$

hence $\partial_t \partial_\alpha q = \nabla^2 W(q)\, \partial_\alpha q$. More precisely putting $q = (q_i)$ we have

$$\partial_t q_i = \nabla_i W(q)$$
$$\partial_t \partial_\alpha q_i = \sum_j \nabla^2_{ij} W(q)\, \partial_\alpha q_j$$

In other words for each $\alpha \perp \alpha_0$ we get a vector field $\partial_\alpha q$ along the α_0-trajectory, which is a normal vector field (because $\partial_\alpha W(q) = \nabla W(q)\cdot \partial_\alpha q = 0$). These Jacobi fields $\partial_\alpha q$ are solutions of the first order DE

$$\partial_t \partial_\alpha q = \nabla^2 W(q)\cdot \partial_\alpha q$$

~~taking place in the normal bundle to the α_0-trajectory. (Notice that because W is the distance in a metric differing from the Euclidean metric only conformally perpendicular directions are the same. It's also clear that the symmetric matrix $\nabla^2_{ij} W$ is trivial in the direction of ∇W~~

Simpler: Start with

$$\partial_t q_i = \nabla_i W(q)$$

and differentiate with respect to α and t to get

$$\partial_t \partial_\alpha q_i = \sum_j \nabla^2_{ij} W(q)\, \partial_\alpha q_j$$
$$\partial_t \partial_t q_i = \sum_j \nabla^2_{ij} W(q)\, \partial_t q_j$$

By Abel's thm one has

$$\partial_t \log \det\{\partial_\alpha q_i, \partial_t q_i\} = \sum_i \nabla^2_i W = \nabla^2 W$$

hence the solution to $\partial_t(iu_1) = \nabla W \cdot \nabla(iu_1) = -\frac{1}{2}\nabla^2 W$ is

$$e^{iu_1} = \text{const}\, \det\{\partial_\alpha q_i, \partial_t q_i\}^{-1/2}$$

Notice that $\partial_\alpha q$, $\partial_t q$ are independent solutions of the 2nd variation equations

$$\partial_t^2 \begin{cases} \partial_\alpha q \\ \partial_t q \end{cases} = -\nabla^2 V(q) \begin{cases} \partial_\alpha q \\ \partial_t q \end{cases}$$

Example: Suppose V is constant and take $x' = 0$. We have

$$\frac{1}{2}(\nabla W)^2 + V = E$$

or

$$|\nabla W| = \sqrt{2(E-V)} \quad , \quad \text{call this } k.$$

Then it's more or less clear that $W(x) = k|x|$. The second variation equations require $\partial_\alpha q$, $\partial_t q$ to be linear in t, hence

$$\det\{\partial_\alpha q, \partial_t q\} = \text{const } t^{n-1} = \text{const } |x|^{n-1}$$

because the fields $\partial_\alpha q$ which are transverse vanish at $t=0$, but $\partial_t q$ which is tangential is, in fact, constant. Thus WKB gives the solution

$$\text{Const } \frac{e^{\frac{i}{\hbar}k|x|}}{|x|^{\frac{n-1}{2}}} \qquad \frac{k^2}{2} = E - V$$

which is exact for $n = 1, 3$

<u>October 31, 1979</u>

We've been looking at the WKB approximation method for solving $\left(-\frac{h^2}{2}\Delta + V\right)\psi = E\psi$. We have been thinking of the case $E \gg V$ where classical motion is allowed, and it is governed by the Hamiltonian

$$H = \frac{p^2}{2} + V(q)$$

However Victor's lectures on Titchmarsh together with barrier penetration show that one should also look at the case $E \ll V$. In this case you put

$$\psi = e^{\frac{1}{h}u} \qquad u = u_0 + hu_1 + \cdots$$

and you get the equations

$$-\frac{h^2}{2}\left(\left(\frac{1}{h}\nabla u\right)^2 + \frac{1}{h}\nabla^2 u\right) + V = E$$

$$-\frac{1}{2}(\nabla u)^2 + V - \frac{h}{2}\nabla^2 u = E$$

or

$$\begin{cases} (\nabla u_0)^2 = 2(V-E) \\ \nabla u_0 \cdot \nabla u_1 = -\frac{1}{2}\nabla^2 u_0 \end{cases}$$

The former equation is the Hamilton-Jacobi equation for motion in the potential $-V$ with energy $-E$.

Now we have seen that u_0 is Hamilton's W function:

$$|\nabla W| = \sqrt{2(E-V)}$$

which measures arclength relative to the infinitesimal arclength

$$\sqrt{2(E-V)}\,|dx|$$

In particular $W(x,x') = \int \sqrt{2(E-V)}\,|dx|$ along the trajectory joining x' to x. So in our approximate solution to the Schroedinger equation we have

$$\psi = e^{\frac{i}{h} W(x,x') + iu_1 + \cdots}$$

The natural question is whether this approximate solution can also be obtained by pseudo-differential operator methods.

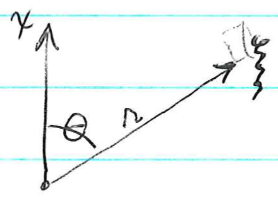
So let's begin with the constant coefficient case. Suppose $E - V = \frac{k^2}{2}$. We want to solve

$$\left[-h^2 \Delta^2 - k^2\right]\psi = 2\delta(x)$$

The Fourier transform solution is

$$\psi(x) = 2\,(2\pi)^{-n} \int \frac{e^{ix\xi}}{h^2\xi^2 - k^2}\, d\xi = 2 \int \frac{e^{ix\frac{\xi}{h}}}{\xi^2 - k^2} \frac{d\xi}{(2\pi h)^n}$$

There are problems with this integral — even if $k^2 < 0$, it $\frac{1}{\xi^2 + k^2}$ is not integrable for $n \geq 2$. So pass to spherical coordinates.



$$d^n\xi = dr\, r\, d\theta\, (r\sin\theta)^{n-2} \underbrace{d\Omega}_{\text{volume elt in } S^{n-2}}$$

$$\therefore\ \psi(x) = 2\,(2\pi h)^{-n}\, \mathrm{vol}(S^{n-2}) \int_0^\infty \frac{r^{n-1}\,dr}{r^2 - k^2} \int_0^\pi e^{i|x|\frac{r\cos\theta}{h}} (\sin\theta)^{n-2}\, d\theta$$

Very complicated!

November 2, 1979

The goal is to understand the approximation to a quantum problem obtained by expanding around a classical solution. Let's begin with motion in one-dim:

$$H = \frac{p^2}{2} + V(t,q)$$

The state vector $\psi(t)$ satisfies

$$i\,\partial_t \psi = \frac{1}{\hbar} H \psi .$$

Let $U(t,0)$ be the propagator, so that

$$\psi(t) = U(t,0)\psi_0 .$$

Consider the average momentum in the state $\psi(t)$:

$$\langle p\rangle(t) = \langle \psi(t)|p|\psi(t)\rangle = \langle \psi_0 | \underbrace{U(0,t)\,p\,U(t,0)}_{p_H(t)} | \psi_0 \rangle$$

Since

$$\frac{d}{dt} p_H(t) = \frac{i}{\hbar} U(0,t)\left[\frac{p^2}{2}+V, p\right] U(t,0)$$

$$= -\partial_q V(t, q_H(t)) \qquad \left(\text{note } [p,q] = \frac{\hbar}{i}\right)$$

we get

$$\frac{d}{dt}\langle p\rangle = -\langle (\partial_q V)(t,q)\rangle$$

Now if $\psi(t)$ is a wave packet peaked around $\langle q\rangle(t)$, then we get the approximation

$$\langle \partial_q V(t,q)\rangle \approx (\partial_q V)(t,\langle q\rangle)$$

and so we get the classical equations of motion

$$\frac{d}{dt}\langle q\rangle = \langle p\rangle \qquad \frac{d}{dt}\langle p\rangle \approx -\partial_q V(t,\langle q\rangle) .$$

Now suppose V is time-independent and that ψ_0 is an eigenfunction for H:

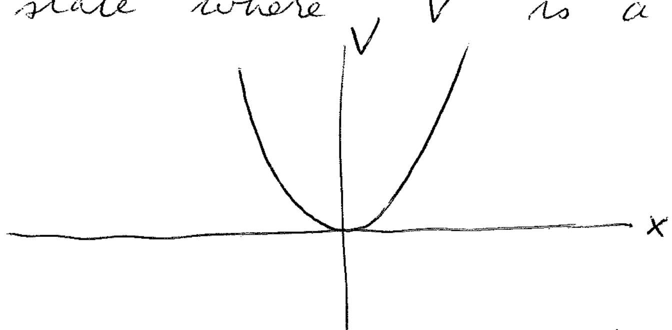
$$H\psi_0 = E_0\psi_0 .$$

Then $\langle A \rangle = \langle \psi(t) | A | \psi(t) \rangle = \langle \psi_0 | A | \psi_0 \rangle$ is independent of t, hence

$$\langle p \rangle = \frac{d}{dt}\langle q \rangle = 0$$

$$\langle \partial_q V(q) \rangle = -\frac{d}{dt}\langle p \rangle = 0$$

We want to concentrate on understanding the ground state where V is a potential of the form



so that $V(x) = \frac{1}{2}\omega^2 x^2 +$ higher terms. We expect there to be a good approximation by the harmonic oscillator $H_0 = \frac{1}{2}p^2 + \frac{1}{2}\omega^2 x^2$, hence there should be a unique ground ~~state~~ of energy approximately $\frac{1}{2}\omega h$ and the next energy levels are approximately $(n+\frac{1}{2})\omega h$.

What we are doing here is field theory with 0 space dimensions. The idea is the coordinate x is the unique value for the field ϕ. A generalization of the above to 1-space dimension is to consider a field ϕ with the Lagrangian density

$$\mathcal{L}(\phi) = \frac{1}{2}(\partial_t \phi)^2 - \frac{1}{2}(\partial_x \phi)^2 - U(\phi)$$

i.e. kinetic energy $\frac{1}{2}\int (\partial_t \phi)^2 dx$ and potential energy $V = \int \left[\frac{1}{2} (\partial_x \phi)^2 + U(\phi) \right] dx$

The quadratic approximation to V around $\phi = 0$ is

$$\int \frac{1}{2}(\partial_x \phi)^2 + \frac{1}{2}\omega^2 \phi^2) \, dx$$

and the corresponding approximate Lagrangian density is

$$\mathcal{L}_0(\phi) = \frac{1}{2}(\partial_t \phi)^2 - \frac{1}{2}(\partial_x \phi)^2 - \frac{1}{2}\omega^2 \phi^2$$

which describes a Klein-Gordon field of mass ω. Therefore the good situation occurs when this quadratic approx. is good: There's a unique ground state, a family of one-particle states of different momenta but with mass close to ω, then 2-particle states whose "total" mass is close to 2ω. Unfortunately, perhaps the effect of the perturbation is always large, so that ω is the bare mass and one still has to renormalize it. This means that one doesn't use the ω occurring in V in $\mathcal{L}_0$.

Let's go back to 0 space-dimensions.

November 3, 1979

Legendre transformation:

Recall derivation of Maxwell-Bolzman distribution.

Suppose one has a system with energy levels $E_0 \leq E_1 \leq \cdots$. given by H on $\mathcal{H}$. Then consider $H_N = H \otimes 1 \otimes \cdots + 1 \otimes H \otimes 1 \otimes \cdots + \cdots + 1 \otimes \cdots \otimes H$ on $\mathcal{H}^{\otimes N}$. If we take an operator A on $\mathcal{H}$ extend it to $A_N = A \otimes 1 \otimes 1 \otimes \cdots + \cdots + 1 \otimes \cdots \otimes A$ on $\mathcal{H}^{\otimes N}$ and compute the expected value of $\frac{1}{N} A_N$ when $\mathcal{H}^{\otimes N}$ is in energy E^N we get

$$\frac{1}{N} \sum_{\substack{n_1, \ldots, n_N \ni \\ E_{n_1} + \cdots + E_{n_N} = E^N}} \langle n_1, \ldots, n_N | A_N | n_1, \ldots, n_N \rangle \Big/ \sum_{\substack{n_1, \ldots, n_N \ni \\ E_{n_1} + \cdots + E_{n_N} = E^N}} 1$$

$$= \sum_n \langle n | A | n \rangle \left(\sum_{\substack{n_2, \ldots, n_N \\ E_{n_2} + \cdots + E_{n_N} = E^N - E_n}} 1 \Big/ \quad '' \quad \right)$$

Hence we want to calculate approximately when N is large the number of energy levels in $\mathcal{H}^{\otimes N}$ of energy E^N. Form

$$\sum_{n_1, \ldots, n_N} e^{-s(E_{n_1} + \cdots + E_{n_N})} = Q(s)^N$$

$$Q(s) = \sum e^{-sE_n} \qquad \text{partition fn.}$$

Then

$$\sum \delta(E^N - E_{n_1} - \cdots - E_{n_N}) = \frac{1}{2\pi i} \int_{a - i\infty}^{a + i\infty} Q(s)^N e^{sE^N} ds$$

by Laplace inversion. Put $E^N = N \cdot E$ where E is the energy per particle in $\mathcal{H}^{\otimes N}$. Use stationary phase to estimate the integral; the integrand is

$$e^{N(\log Q(s) + sE)}$$

and the function $\log Q(s) + sE$ has a unique critical point on the real axis. Why?

$$\frac{d}{ds} \log Q(s) + E = \frac{Q'(s)}{Q(s)} + E = -\frac{\sum E_n e^{-sE_n}}{\sum e^{-sE_n}} + E = 0$$

Now
$$-\frac{Q'(s)}{Q(s)} \longrightarrow +\infty \quad \text{as} \quad s \to 0$$
$$\longrightarrow E_0 \quad \text{as} \quad s \to +\infty$$

Furthermore

$$\frac{d}{ds}\frac{Q'(s)}{Q(s)} = \frac{QQ'' - (Q')^2}{Q^2} = \frac{1}{Q^2}\left(\sum e^{-sE_n} \sum E_n^2 e^{-sE_n} - \left(\sum E_n e^{-sE_n}\right)^2\right)$$

$$= \frac{1}{Q^2} \sum_{n,m} e^{-s(E_n+E_m)} (E_n^2 - E_n E_m)$$

$$= \frac{1}{Q^2} \sum_{n,m} e^{-s(E_n+E_m)} \frac{1}{2} \underbrace{(E_n^2 - 2E_nE_m + E_m^2)}_{(E_n-E_m)^2} > 0$$

Hence as long as $E_0 < E < \infty$, there is a unique critical point $s = \beta$ for the expenent; it occurs when

$$\frac{\operatorname{tr}(He^{-\beta H})}{\operatorname{tr}(e^{-\beta H})} = \frac{\sum E_n e^{-\beta E_n}}{\sum e^{-\beta E_n}} = E$$

that is, where the average energy wrt Maxwell-Bolzman in E.

Around the critical point

$$\log Q(s) + sE = (\log Q(\beta) + \beta E) + \frac{1}{2} \underbrace{\frac{QQ'' - (Q')^2}{Q^2}(\beta)}_{\text{call this } \gamma} (s-\beta)^2 + \cdots$$

Then stationary phase gives the approximation

$$\sum_{n_1, \ldots, n_N} \delta(NE - E_{n_1} - \cdots - E_{n_N}) = \frac{1}{2\pi i} \int e^{N(\log Q(s) + sE)} \, ds$$

$$\simeq e^{N(\log Q(\beta) + \beta E)} \frac{1}{\sqrt{2\pi N \gamma}}$$

Now return to computing the average value of A extended to $\mathcal{H}^{\otimes N}$ when H has the average value E. At this point I find it easier to argue classically where one integrates over phase space with measure dy.

$$Q(s)^N = \left(\int_M e^{-sH} dy\right)^N = \int_{M^N} e^{-sH_N} dy^N$$

$$= \int_0^\infty e^{-sE} dE \underbrace{\int_{H_N^{-1}(E)} \frac{dy^N}{dH_N}}_{\text{volume of } M^N \text{ in } H_N^{-1}[E,E+dE]}$$

$$\langle A \rangle = \underbrace{\int_{H_N^{-1}[E_N, E_N+dE]} A(y_1)\, dy^N}_{\int_M A(y_1)\, dy_1 \int_{H_{N-1}^{-1}[E_N - H(y_1),\, E_N - H(y_1)+dE]} dy^{N-1}} \Bigg/ \int_{H_N^{-1}[E_N, E_N+dE]} dy^N$$

both of these involve dE factors which cancel

Not much clearer, but the point is that the ratio

$$\sum_{\substack{n_2,\dots,n_N \\ E_{n_2}+\dots+E_{n_N} = E^N - E_{n_1}}} 1 \Bigg/ \sum_{\substack{n_1,\dots,n_N \\ E_{n_1}+\dots+E_{n_N} = E^N}} 1$$

should be approximable by

$$\frac{\frac{1}{2\pi i}\int Q(s)^{N-1} e^{s(E^N - E_{n_1})} ds}{\frac{1}{2\pi i}\int Q^N(s)\, e^{sE^N} ds} \approx \frac{e^{(N-1)(\log Q(\beta)+\beta E)} \frac{1}{\sqrt{2\pi(N-1)\gamma}}\, e^{\beta(E-E_n)}}{e^{N(\log Q(\beta)+\beta E)} \frac{1}{\sqrt{2\pi N\gamma}}}$$

There should be some more direct way of getting the answer which is
$$\frac{1}{Q(\beta)} e^{-\beta E_{n_1}} .$$

Thus in the $N \to \infty$ limit
$$\langle A \rangle = \frac{tr\left(Ae^{-\beta H}\right)}{tr\left(e^{-\beta H}\right)} .$$

~~Here's a first attempt at understanding Legendre's transformation. We are given the function~~
$$\cancel{L = -\log(Q(\beta))}$$
~~but we are interested~~

Legendre transformation: The partition function is given in terms of the variable β, however the natural independent variable is E which is related to β by
$$-\frac{Q'(\beta)}{Q(\beta)} = E \qquad \text{or} \qquad \frac{d}{d\beta}\left(-\log Q(\beta)\right) = E$$

Thus if we treat $-\log Q(\beta)$ as a Lagrangian with β as $\dot{q}$, then E is the conjugate momentum, and the Hamiltonian is
$$H = \beta E + \log Q(\beta)$$
Then one has, upon regarding H as a function of E:
$$\frac{dH}{dE} = \beta + E\frac{d\beta}{dE} + \frac{Q'(\beta)}{Q(\beta)}\frac{d\beta}{dE} = \beta$$
It is still not really clear what this all means.

Next thing is that this H function is the entropy.

(Recall that the entropy of a density matrix

$$\rho = \sum p_j |\psi_j\rangle\langle\psi_j| \qquad p_j \geq 0 \ , \ \sum p_j = 1 ,$$

is defined to be

$$S = -\operatorname{tr}(\rho \ln \rho)$$

If we do variations of S subject to the conditions $\operatorname{tr}(\rho) = 1$ $\operatorname{tr}(\rho H) = E$, we look at

$$F = -\operatorname{tr}(\rho \ln \rho) + \lambda(\operatorname{tr}(\rho H) - E) + \mu(\operatorname{tr}(\rho) - 1)$$

where λ, μ are Lagrange parameters.

$$\delta F = -\operatorname{tr}\left(\delta\rho \ln\rho + \rho \frac{1}{\rho}\delta\rho\right) + \lambda(\operatorname{tr}(\delta\rho\, H)) + \mu(\operatorname{tr}(\delta\rho)) = 0$$

$$\operatorname{tr}(\delta\rho\,(-\ln\rho - 1 + \lambda H + \mu)) = 0$$

so

$$\rho = C e^{\lambda H}$$

Then C is determined by $\operatorname{tr}\rho = 1$, and λ by $\operatorname{tr}(\rho H) = E$.)

Thus if we compute S for the Maxwell-Bolzman density matrix $\rho = e^{-\beta H}/Q(\beta)$, we get

$$S = -\operatorname{tr}(\rho(-\beta H - \log Q)) = \beta \operatorname{tr}(\rho H) + (\operatorname{tr}\rho)\log Q$$

$$= \beta E + \log Q$$

Coleman's version: Suppose you wish to minimize $\langle a|H|a\rangle$ subject to constraints $\langle a|a\rangle = 1$ and $\langle a|A|a\rangle = A_c$. Then introducing Lagrange multipliers E, J you vary a arbitrarily in

$$\langle a|H|a\rangle - E(\langle a|a\rangle - 1) - J(\langle a|A|a\rangle - A_c)$$

or more simply in $\langle a|H - E - JA|a\rangle$ so as to get

$$(H - E - JA)|a\rangle = 0$$

Thus $|a\rangle$ is an eigenvector of $H - JA$ and E is its energy. This makes E into a function of J (think of $|a\rangle$ as the ground state of $H - JA$), but really one is interested in the ground energy E as a function of the constraint constant A_c. Now from first order perturbation theory one has

$$\frac{dE}{dJ} = -\langle a|A|a\rangle = -A_c$$

so the original quantity to be minimized is

$$\langle a|H|a\rangle = E + JA_c = E - J\frac{dE}{dJ} = JA_c - (-E).$$

Hence if I call this quantity S, I have

$$\frac{dS}{dA_c} = J + A_c\frac{dJ}{dA_c} + \frac{dE}{dJ}\frac{dJ}{dA_c} = J$$

It's still not clear what this means, and perhaps the ultimate way of understanding it involves using diagrams.