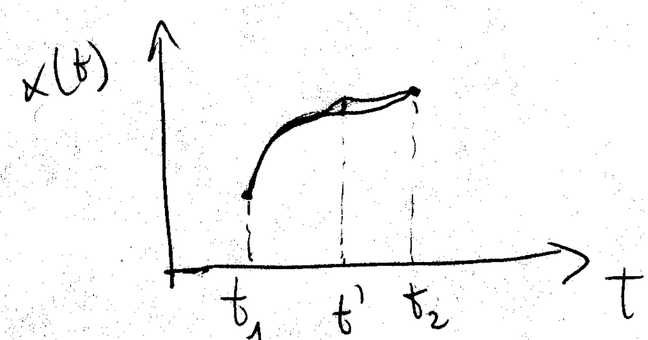
Notes from the discussion of Friday, 2/4/2005

the functional derivative is defined as

$$\frac{\delta S[x(t)]}{\delta x(t')} = \lim_{\epsilon \to 0} \left[S\left[x(t) + \epsilon\,\delta(t-t')\right] - S[x(t)] \right]$$

for a functional $S[x(t)]$.

The physical meaning of the variation $\epsilon\,\delta(t-t')$ is that the trajectory $x(t)$ is slightly perturbed only at one (<u>arbitrary</u>) time t' between t_1 and t_2.



the previous definition can be rewritten by replacing

$$\delta(t-t') = \lim_{\Delta t \to 0} \frac{1}{\Delta t}\,\delta_{ij}$$

so that
$$\frac{\delta S_N}{\delta x(t)} = \lim_{\Delta t \to 0} \frac{\partial S_N}{\partial x_i}$$

In other words, the trajectory has been discretized, so that

$$S_N = \Delta t \sum_{i=0}^{N-1} \left[\frac{m}{2} \left(\frac{x_{i+1} - x_i}{\Delta t} \right)^2 - V(x_i) \right]$$

for a system whose classical Lagrangian does not depend on time explicitly nor has terms of the type $x\dot{x}$.

Now

$$\frac{\partial S_N}{\partial x_i} = \Delta t \left[m \left(\frac{x_i - x_{i-1}}{\Delta t^2} - \frac{x_{i+1} - x_i}{\Delta t^2} \right) - \frac{\partial V}{\partial x_i} \right]$$

$$= \frac{2m \left(x_i - x_{i+1} \right)}{\Delta t} - \frac{\partial V}{\partial x_i} = \frac{\partial L}{\partial \dot{x}_i} + \frac{\partial L}{\partial x_i}$$

in the limit of $\Delta t \to 0$

this can be useful, since the first variation of the action

$$\delta S[x(t)] = \lim_{\Delta t \to 0} d S_N = \lim_{\Delta t \to 0} \sum_{i=0}^{N-1} \frac{\partial S_N}{\partial x_i} dx_i$$

is, in the limit $\Delta t \to 0$

$$\int_{t_1}^{t_2} dt \left(\frac{\partial L}{\partial \dot{x}_i} \delta \dot{x}_i + \frac{\partial L}{\partial x_i} \delta x_i \right)$$

In general, it turns out that

$$\delta^n S = \int_{t_1}^{t_2} dt \left[\frac{\partial^n L}{\partial \dot{x}^n} \delta \dot{x}^n + \frac{\partial^n L}{\partial \dot{x}^{n-1} \partial x^n} \delta \dot{x}^n \delta x + \dots + \frac{\partial^n L}{\partial x^n} \delta x^n \right]$$

this comes in hand everytime we want to expand the action about one of its stationary points:

$$S\left[\bar{x}(t) + \delta x(t)\right] = S\left[\bar{x}(t)\right] + \delta S + \frac{1}{2} \delta^2 S + \dots$$

Path integral formulation for the one-dimensional ~~to~~ simple harmonic oscillator: (From Itzykson-Zuber, QFT, McGraw-Hill 1980)

We first compute the increment in action of the oscillator in going from (q_1, t) to $(q_2, t+\Delta t)$.
On this infinitesimal time-interval $(t, t+\Delta t)$ we approximate an arbitrary path by a linear one in such a way that the increment in action is —

$$\Delta I(2,1) = \frac{1}{2} m \left[\frac{(q_2-q_1)^2}{\Delta t} - \omega^2 \Delta t \, \frac{q_2^2 + q_1 q_2 + q_1^2}{3} \right]$$

Set $t = t_f - t_i$

So, now —

$$\langle f | i \rangle = \lim_{n \to \infty} \int \prod_{p=1}^{n-1} dq_p \left(\frac{nm \, e^{-i\pi/2}}{2\pi t} \right)^{n/2} \exp\left\{ \frac{im}{2} \sum_{p=1}^{n} \left[\frac{n}{t} (q_p - q_{p-1})^2 - \frac{\omega^2 t}{3n} (q_p^2 + q_p q_{p-1} + q_{p-1}^2) \right] \right\}$$

The argument of the exponential function ~~&~~ can be cast in the form of ~~the~~ a positive-definite form:

$$\exp\left(\frac{im}{2} [q^T M q] \right)$$

where $q = (q_0 = q_i, q_1, \ldots, q_n = q_f)$ and M is a $n \times n$ matrix such that —

$$M_{00} = M_{nn} = \frac{n}{t} - \frac{\omega^2}{3n} t$$

$$M_{kk} = 2\left(\frac{n}{t} - \frac{\omega^2 t}{3n} \right) \qquad 1 \le k \le n-1$$

$$M_{k,k+1} = M_{k-1,k} = -\left(\frac{n}{t} + \frac{\omega^2 t}{6n} \right)$$

all other matrix elements being zero.

If N is the matrix obtained from M by deleting the rows and columns with indices 0 and n, then we can write —

$$q^T M q = M_{00}\,(q_0^2 + q_n^2) + 2M_{01}\,(q_0 q_1 + q_{n-1} q_n) + \sum_{j,l=1}^{n-1} q_j N_{jl} q_l$$

So the N-integral is evaluated as —

$$\int d^{n-1}q \; e^{\frac{im}{2} q^T N q} = \left(\frac{2\pi}{m} e^{i\pi/2}\right)^{\frac{n-1}{2}} (\det N)^{-1/2}$$

Since the problem has translational invariance, that takes ~~to~~ care of the linear terms in the exponential, so we are left with —

$$\langle f|i\rangle = \lim_{n\to\infty} \left(\frac{nm\, e^{-i\pi/2}}{2\pi t}\right)^{n/2} \left(\frac{2\pi e^{i\pi/2}}{m}\right)^{(n-1)/2} (\det N)^{-1/2} \times$$
$$\exp\left\{\frac{im}{2}\left[M_0(q_0^2 + q_n^2) - M_{01}^2\,(N_{11}^{-1} q_0^2 + N_{n-1,n-1}^{-1} q_n^2 + 2N_{1,n-1}^{-1} q_0 q_n)\right]\right\}$$

Let us now define

$$a = \frac{1}{2}\left(\frac{1 + \omega^2 t^2/6n^2}{1 - \omega^2 t^2/3n^2}\right)$$

Now,

$$\det N = 2^{n-1}\left(\frac{n}{t} - \frac{\omega^2 t}{3n}\right)^{n-1} \det_{n-1} \begin{vmatrix} 1 & -a & 0 & \cdots & \\ -a & 1 & -a & \cdots & \\ 0 & -a & 1 & -a & \\ \vdots & \vdots & \vdots & \vdots & \end{vmatrix}$$

Let us call the $(n-1)\times(n-1)$ determinant $I_{n-1}(a)$. Then for fixed 'a' we have the recursion relation —

$$I_p(a) = I_{p-1}(a) - a^2 I_{p-2}(a) \qquad I_0(a) = I_1(a) = 1$$

or, in matrix form —

$$\begin{pmatrix} I_p(a) \\ I_{p-1}(a) \end{pmatrix} = \begin{pmatrix} 1 & -a^2 \\ 1 & 0 \end{pmatrix}^{p-1} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

After diagonalization of the 2x2 matrix the solution is obtained as —

$$I_{n-1}(a) = \frac{\lambda_+^n(a) - \lambda_-^n(a)}{\lambda_+(a) - \lambda_-(a)} \qquad \lambda_\pm(a) = \frac{1 \pm i\sqrt{4a^2-1}}{2} \underset{n\to\infty}{\sim} \frac{1}{2} e^{\pm \frac{i\omega t}{n}}$$

so for large n,

$$I_{n-1}(a) \sim \frac{n}{2^{n-1}} \frac{\sin\omega t}{\omega t}$$

Thus,

$$\langle f|i\rangle = \left(\frac{m\omega e^{-i\pi/2}}{2\pi\sin\omega t}\right)^{1/2} \lim_{n\to\infty} \exp\left\{\frac{im}{2}\left[(q_i^2+q_f^2)(M_{00} - M_{01}^2 N_{11}^{-1}) - 2q_i q_f M_{01}^2 N_{1,n-1}^{-1}\right]\right\}$$

We assume $0 < \omega t < \pi$ and then evaluate —

$$N_{11}^{-1} = \frac{t}{2n(1-\omega^2t^2/3n^2)} \frac{I_{n-2}(a)}{I_{n-1}(a)} \sim \frac{t}{n}\left(1 - \frac{\omega t}{n}\cot\omega t\right) + O\left(\frac{1}{n^3}\right)$$

similarly, $N_{1\,n-1}^{-1} \sim \dfrac{\omega t^2}{n^2 \sin\omega t} + O\left(\dfrac{1}{n^3}\right)$

So finally —

$$\langle f|i\rangle = \left(\frac{m\omega e^{-i\pi/2}}{2\pi\sin\omega t}\right)^{1/2} \exp\left\{\frac{im\omega}{2}\left[(q_f^2+q_i^2)\cot\omega t - \frac{2q_f q_i}{\sin\omega t}\right]\right\}$$

Now, how to get to the energy spectrum?

In general, the propagator (or Green's function)

$$K(x', x', t) = \sum_j \langle x' | \psi_j \rangle \langle \psi_j | x \rangle e^{-\frac{i E_j t}{\hbar}}$$

assuming that the system has a discrete spectrum of eigenenergies.

Now

$$K(x, x, t) = \sum_j |\langle x | \psi_j \rangle|^2 e^{-\frac{i E_j t}{\hbar}}$$

is the propagator for a periodic orbit, and

$$G(t) = \int d^{\bullet}x \, K(x, x, t) = \int dx \sum_j |\langle x | \psi_j \rangle|^2 e^{-\frac{i E_j t}{\hbar}}$$

$$= \sum_j e^{-\frac{i E_j t}{\hbar}} \int dx \, |\langle \psi_j | x \rangle|^2 = \sum_j e^{-\frac{i E_j t}{\hbar}}$$

~~[illegible]~~ which is nothing but the trace of the time-evolution operator $K(x', x, t)$

~~Let's~~ Let's now take a Laplace-Fourier transform of $G(t)$:

$$\hat{G}(\mathcal{E}) = -i \int_0^\infty dt\, G(t)\, e^{\frac{i\mathcal{E}t}{\hbar}} =$$

$$= -i \int_0^\infty dt \sum_j e^{\frac{i(\mathcal{E}-\mathcal{E}_j)t}{\hbar}}$$ which does not

exist, but if we add a small imaginary part to the energy, i.e. $\mathcal{E} \to \mathcal{E} + i\epsilon$, then

$$\hat{G}(\mathcal{E}) = \lim_{\epsilon \to 0} (-i) \int_0^\infty dt \sum_j e^{i(\mathcal{E}-\mathcal{E}_j)\frac{t}{\hbar} - \epsilon \frac{t}{\hbar}} =$$

$$= \lim_{\epsilon \to 0} \sum_j \frac{\hbar}{\mathcal{E} - \mathcal{E}_j - \epsilon} = \sum_j \frac{\hbar}{\mathcal{E} - \mathcal{E}_j}$$ [cf. Sakurai]

So that, given the propagator, the recipe is to study the analytical properties (i.e. to find the poles) of the function $\hat{G}(\mathcal{E}) = \int_0^\infty (-i)\, dt\, e^{\frac{i\mathcal{E}t}{\hbar}} \int dx\, K(x,x,t)$