PATH INTEGRATION and WKB APPROXIMATION

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December 29, 2010

Abstract

In evaluating path integral for quantum mechanics, there is an efficient technic called saddle point approximation It is, in essence,the classical approximation of a path integral and in quantum field theory it corresponds to evaluating the generating functional with all tree diagrams, and it is the leading contribution from a small Planck constant. We also know that in the Schodinger equation discription of quantum mechanics we can use WKB approximation to get the wave functions of energy eigenstates, it also involves leading contributions from small Planck constant. A natural expect is that, these two approaches are equivalent, a proof, however, is needed. Further, we can demonstrate that, path integral approach, besides getting propagators, can also solve stationary state problems, including barrier penetration, yielding the same results with WKB. The extension of this method to quantum field theory leads directly the way that Coleman used to treat vacuum decay process. We also mention the connection between semi-classical approximation and mean-field theory in statistical mechanics.

1 Saddle point approximation in field theory, quantum particle mechanics, and statistical mechanics

After we define a quantum theory with path integration, the only calculation we do, is to solve a non-linear oscillator of general form:

$$\int [d\phi] e^{iS[\phi]} = \int [d\phi] e^{\int dx \mathscr{L}} \tag{1}$$

With $\mathscr{L}$ a general function of the field ϕ. If $\mathscr{L}$ is a quadratic function, it is easy to see the integration is a functional determinant:

$$\int [d\phi] e^{iS[\phi]} = det[\hat{O}]^{-\frac{1}{2}} \tag{2}$$

$\hat{O}$ is an operator in functional space:

$$S = \int dx \phi \hat{O} \phi \tag{3}$$

However, for a general function $\mathscr{L}$, lacking of an exact solution, the common approximation is perturbation theory based on a dimensionless, and small parameter. There is another way, in essence non-perturbative,to approximate the integral, called stationary phase method or saddle point method, the idea is simple: fields near the lowest point of the action functional contributes most to the path integration, extracting this lowest point gives zeroth approximation of the integral.

The stationary point $\phi_c$is defined by:

$$\frac{\delta S}{\delta \phi}|_{\phi_c} = 0 \tag{4}$$

Decompose field ϕ as the stationary point and the fluctuation around it: $\phi = \phi_c + \delta\phi$ the path integral decomposed as:

$$Z = e^{iS[\phi_c]} \int [d\delta\phi] \exp i\frac{1}{2}\delta\phi \frac{\delta^2 S}{\delta\phi\delta\phi}|_{\phi_c}\delta\phi \tag{5}$$

It is the multiplication of a phase and a functional determinant. We see that the phase is given by the classical action evaluated at classical solution of the field theory,while the functional determinant gives the variation of the amplitude.This decomposition is equivalent to recovering the $\hbar$ in the path integral below the classical action and expand the integral with respect to $\hbar$, and if we denote the expansion with diagrams, we see it is also an expansion with respect to the number of loops: zero loop approximation,i.e. tree diagrams give a phase which equals to the classical action, the next leading order of the expansion gives the variation of the amplitude. It is worth noting that, the method is different from a perturbation theory because the expansion parameter is not dimensionless.

We see the same thing happens in particle quantum mechanics, which is a one-dimensional field theory:

$$Z = < x_f | e^{-\frac{iHT}{\hbar}} | x_i > = \int [d\phi] e^{iS[x(t)]} \simeq e^{iS[x_c(t)]} \int [d\delta x(t)] \exp i\frac{1}{2}\delta x \frac{\delta^2 S}{\delta x \delta x}|_{x_c}\delta x \tag{6}$$

Therefore we see the classical equation of motion gives a pure phase while the next leading order of $\hbar$ gives a variation of amplitude. This is in complete parallel with the WKB method of evaluating the Schrodinger equation, which we will briefly review below.

Interestingly, in statistical mechanics we have the same approximation method, which is disguised with the name "mean field approximation", we know that the partition function of a many-body system is a path integral:

$$Z = Tr[e^{-\beta H}] = \int [d\phi] e^{-\int_0^\beta \mathscr{H}(\phi(\tau), \partial\phi(\tau))d\tau} \tag{7}$$

Mean field approximation is that: extract the phase given by the field configuration that extremizes the action on the exponential, and we know that the free energy is given by the logarithm of the partition function, therefore we see that, mean field approximation is to approximate the free energy of the system as the classical action, corresponding to the QFT case, which is an expansion with respect to Planck constant $\hbar$, mean field theory is to expand the partition function with respect to Boltzman constant k_B, the quantum fluctuation in the QFT path integral corresponds to statistical fluctuation in path integral—-they are beyond the leading order of LOOP EXPANSION.

2 Brief notes on WKB approximation

Given the Schrodinger equation:

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar}{2m}\nabla^2\psi + V(x)\psi \tag{8}$$

The wave function can always be decomposed as an amplitude and a phase:

$$\psi = \sqrt{\rho}e^{\frac{iS}{\hbar}} \tag{9}$$

Bringing this decomposition into the equation we see: The leading order of $\hbar$ terms give:

$$\frac{\partial S}{\partial t} + \frac{1}{2m}|\nabla S|^2 + V = 0 \tag{10}$$

Which is the classical Hamilton-Jacobi equation, with S being the principal Hamilton function, deferring from the classical action only by a constant.

The next leading order terms give:

$$\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\frac{\nabla S}{m}) = 0 \tag{11}$$

which is the conservation of probability current, by substituting the classical Hamilton principal function into the conservation equation we get a nontrivial variation of the amplitude, one can see the path integration.

The approximated wave function is:

$$\psi_{WKB} \sim k^{-\frac{1}{2}}\exp[\pm\frac{i}{\hbar}\int^x k(x') - \frac{iEt}{\hbar}] \tag{12}$$

Where k is the classical momentum of the particle:

$$k(x) = \sqrt{2m[E - V(x)]} \tag{13}$$

Although the $\hbar$ expansion of the Schrodinger equation is general, we have to assume we are solving for a stationary state function in order to get equation (12), where the time variable in the Hamilton principal function can be separated. We get an impression that WKB approximation here is efficient for treating stationary states while path integration is efficient in treating propagation, we will see below the two methods are actually equivalent in the semi classical sense.

3 Equivalence in the small $\hbar$ limit

Below we will show that, with WKB approximated energy eigenfunctions, we can construct the approximate propagator, which is the same as one obtained by expanding the path integral with respect to $\hbar$. Since WKB approximation is for stationary state problems and the propagator method is time-dependent, we need a bridge to connect the two, the bridge is:

$$G(x,t;x,t') =< x|e^{-\frac{iH(t-t')}{\hbar}}|x' >= \sum_n < x|n >< n|x' > e^{-\frac{iE_n(t-t')}{\hbar}} \tag{14}$$

Where

$$< x|n >= \psi_n(x) \tag{15}$$

is the energy eigenstate wave function, if we use WKB wave functions in the expansion, we will get the semi-classical approximation of the propagator.

With equation (11), we get:

$$G(x,t;x',t') = \sum_n \frac{1}{\sqrt{k_n(x)k_n(x')}} e^{\frac{-iE_n(t-t')}{\hbar}} [\exp{(i\int_{x'}^{x} k(z)dz)} + \exp{(-i\int_{x'}^{x} k(z)dz)}] \tag{16}$$

Here we consider the degeneracy by simply adding the degenerate wave functions by the same weight. We have to take the continuum limit:

$$G(x,t;x',t') = \int \frac{f(E)dE}{\sqrt{k(x)k(x')}} e^{\frac{-iE\Delta}{\hbar}} [\exp{(i\int_{x'}^{x} k(z)dz)} - \exp{(i\int_{x'}^{x} k(z)dz)}] \tag{17}$$

Where $f(E)$ is a chosen state density to ensure that:

$$\lim_{t\to t'} G(x,t;x',t') = \delta(x-x') \tag{18}$$

By doing the limit is free particle case we see that

$$f(E) = \frac{m}{2\pi\hbar^2} \tag{19}$$

It is general since it is irrelevant of specific dynamics, i.e. independent of potentials. In the integration (16), we have integration of a function in the exponential, this invoke the stationary phase method:

$$I = \int dx g(x) e^{ih(x)} \simeq g(x_0)e^{ih(x_0)} \int dx e^{\frac{ih''(x_0)(x-x_0)^2}{2}} \tag{20}$$

This yields:

$$I = g(x_0)e^{ih(x_0)} \sqrt{\frac{2\pi i}{h''(x_0)}} \tag{21}$$

x_0 is the stationary point of the exponential, i.e. the region near this point contributes the largest part to the exact integral.

$$h'(x_0) = 0 \tag{22}$$

In the problem we care,

$$h(E) = \pm\frac{1}{\hbar}\int_{x'}^{x} dx\sqrt{2m[E - V(x)]} - \frac{E\Delta t}{\hbar} \tag{23}$$

Note that the integral we care is not about x, it is about E.

Therefore the classical equation we seek is:

$$h'(E) = -\frac{\Delta t}{\hbar} \pm \frac{1}{\hbar}\int dx\sqrt{\frac{m}{2[E - V(x)]}} \tag{24}$$

For region $E > V(x)$ only plus sign gives sensible solution.

Since

$$\frac{d^2h}{dE^2} = -\frac{m^2}{\hbar}\int_{x'}^{x}\frac{dx}{[2m[E - V(x)]]^{\frac{3}{2}}} = -\frac{m^2}{\hbar^4}\int_{x'}^{x}\frac{dx}{k(x)^3} \tag{25}$$

We see

$$G(x,t;x',t') = \frac{m}{2\pi\hbar^2}\frac{1}{\sqrt{k(x)k(x')}}\sqrt{\frac{2\pi i}{-\frac{m^2}{\hbar^4}\int_{x'}^{x}\frac{dx}{k(x)^3}}}\exp\left(-iE_{classical}\frac{\Delta t}{\hbar} + i\int_{x'}^{x}k(x)dx\right) \tag{26}$$

This gives the propagator under WKB approximation. To prove the equivalence, we have to obtain the same thing with directly evaluating the path integral, we have seen in equation (6) that the semi-classical approximation to the next leading order of $\hbar$ is a classical action phase and a functional determinant. The contribution of the classical action phase is easily seen to be identical to the phase in equation (25), the non-trivial thing is to obtain the functional determinant:

$$\det\left[-m\partial_t^2 - V''(x_c)\right] \tag{27}$$

Where $x_c(t)$ is fixed to be the classical path, which satisfies Hamilton-Jacobi equation. Actually the path integral is approximated as:

$$Z \simeq e^{\frac{iS_{classical}}{\hbar}}\left[\det\left[-m\partial_t^2 - V''(x_c)\right]\right]^{-\frac{1}{2}} \tag{28}$$

We follow the method given by Sidney Coleman in "Aspects of Symmetry" to compute the determinant(just a brief sketch).

Step One:

Specify BOUNDARY CONDITION problem:

$$-m\partial_t^2\psi - W(t)\psi = \lambda\psi, \psi(-\frac{T}{2}) = \psi(\frac{T}{2}) = 0 \tag{29}$$

Where W(t) is a given function of time, here $W(t) = V''(x_c(t))$

Then $\det\left[-m\partial_t^2 - W(t)\right] = \prod_n \lambda_n$

Step one is defining the problem, but we will see only steps 2 and 3 are important in the evaluation of the determinant.

Step Two:

Define auxiliary INITIAL CONDITION problem:

$$-m\partial_t^2\phi_\lambda - W(t)\phi_\lambda = \lambda\phi_\lambda, \phi_\lambda(-\frac{T}{2}) = 0, \phi'_\lambda(-\frac{T}{2} = 1) \tag{30}$$

Pay attention that as an initial condition problem, the spectrum of λ here can be different from the original boundary condition problem.

Step Three:

It can be proved that

$$\frac{\det[-\partial_t^2 - W(t) - \lambda]}{\phi_\lambda(\frac{T}{2})} \tag{31}$$

Is independent of the potential W(t), we define a normalization factor by:

$$\frac{\det[-\partial_t^2 - W(t)]}{\phi_0(\frac{T}{2})} = N \tag{32}$$

Therefore the auxiliary initial condition problem tells us that, by solving equation:

$$\partial_t^2\phi_0 + W(t)\phi 0 = 0, \phi_0(-\frac{T}{2}) = 0, \phi'_0(-\frac{T}{2}) = 1 \tag{33}$$

and take value at the later boundary we get the functional determinant.

It is not hard to solve:

$$\phi_0(\frac{T}{2}) = v(\frac{T}{2})v(-\frac{T}{2})\int_{-\frac{T}{2}}^{\frac{T}{2}} \frac{dx}{v(t)^2} \tag{34}$$

Where $v(t)$ is $\frac{dx_{classical}}{dt} = \frac{\hbar k}{m}$ Now we see this reproduces the result of WKB method, in small $\hbar$ limit, the path integration and WKB approximation yield the same propagator.

4 Barrier penetration with path integration

In the discussion above, when we try to obtain the propagator $G(x,t;x',t')$, we assume there is a classical path from x to x', this is always true if the energy is not given: for any given x,t and x',t', there is one and only one classical path that connecting the two "starting" and "ending" points, and then the energy associated with the path is also determined, this is why in path integration we usually don't care about the problem of "classical forbidden region", because it is the starting and ending point given instead of energy. One may then think that, maybe path integral loses its power when treating stationary state problems. However, this is not the case. In the last section we saw that the classical approximation of propagator can be obtained by WKB energy eigenfunctions, below we will see that reciprocally we can use semi-classical propagator to get approximated energy eigenfunction.

First, by the definition of propagator:

$$\psi(x,t) = \int G(x,t;x',t')\psi(x',t') \tag{35}$$

We claim that,

$$\psi_{WKB}(x,t) = \int G_{classical}(x,t;x',t')\psi_{WKB}(x',t') \tag{36}$$

This can be seen by directly evaluating the integral:

$$\psi(x,t) = \int dx'[2\pi i k(x)k(x')\int_{x'}^{x}\frac{dz}{k(z)^3}]^{-\frac{1}{2}} \times e^{-\frac{iE(t-t')}{\hbar}} \exp{(i\int_{x'}^{x}k(z)dz)}\psi_{WKB}^{E_0}(x',t') \tag{37}$$

Where

$$\psi_{WKB}^{E_0}(x',t') = \frac{1}{\sqrt{k_0(x')}} \times \exp{(i\int^{x'}k_0(z)dz - \frac{iE_0t'}{\hbar})} \tag{38}$$

Here we should make clear that, E not necessarily equals E_0, $E0$ is the energy of the wave function, E is the energy of the classical path around which the propagator is approximated, one may think if E and E_0 do not match, there will be a problem, but it is not a problem—since we integrate x', one expects that there must be a special x', making the two energies match, that point dominates the integral—it is also the stationary point of the integral.

Actually if we evaluate the integral on x' with stationary phase method: We demand that

$$\frac{\partial(phase)}{\partial x'} = 0 \tag{39}$$

One can check that this implies the stationary x'_0 is given by $E = E_0$, and further following the steps as before we can prove our claim: a WKB function, propagated by a WKB propagator, is still a WKB function.

We see that if we use WKB propagator to propagate a WKB energy eigenfunction, the energy of the two must, at least approximately, match. Then the problem comes: What if the energy of the wave function, at some points lower than the potential? Then we cannot find a classical path which matches that energy, therefore, we should in this sense, analytical continuate the path integral to "classically forbidden region".

The way out is to introduce imaginary time, the reason for an imaginary time is that, for the path of a given energy and given starting and ending points, the time period for the path can be derived:

$$\Delta T = \int_{x'}^{x} dy[\frac{m}{2[E-V(y)]}]^{\frac{1}{2}} \tag{40}$$

We see in the case of barrier penetration, this time cannot be real, therefore we extend it to be imaginary in the classically forbidden region.

Suppose we have a classically forbidden region with boundaries a and b, a and b are between x and x'.

We solve the classical equation:

$$m\frac{d^2x_{cl}}{dt^2} = -\frac{dV(x)}{dx}|_{x_{cl}} \tag{41}$$

In classically allowed region, time t is real while in classical forbidden region, time t is imaginary.

Then we have the total time:

$$T^{(n)} = \int_{x'}^{a} dy[\frac{m}{2[E-V(y)]}]^{\frac{1}{2}} + \int_{b}^{x} dy[\frac{m}{2[E-V(y)]}]^{\frac{1}{2}} - i(2n+1)\int_{a}^{b} dy[\frac{m}{2[V(y)-E]}] \tag{42}$$

Where n could be any natural number, n specifies different $T^{(n)}$, the real part of $T^{(n)}$ is easy to understand: it is the total real time of traveling in the classically allowed region. The imaginary part is the extended time of traveling in the barrier, it is a real number defined by:

$$t = i\tau \tag{43}$$

Therefore we see in the equation (42), $\tau_n = (2n+1)\int_a^b dy[\frac{m}{2[V(y)-E]}]$, it is the time of a particle with energy -E, moving in a potential -V(x), and the meaning of n is that, for a particle with energy $-E > -V(x)$, from a point to b point, there can be infinitely many different classical paths with different times. The particle can go straightly from a to b, also, it can go back after arriving b, and then go to b again after arriving a, etc. such motions are called "bounces". We will see that in the problem of barrier penetration, all the bounce paths should be included in the path integral.

The key point is: how to get a propagator with real time variable with a classical path with imaginary time variable? We do it by Fourier transformation:

$$G(x,t;x',t') = \int dE e^{-\frac{iE(t-t')}{\hbar}} G(x,x';E) \tag{44}$$

and

$$G(x,x';E) = \int \frac{dT}{2\pi\hbar} e^{\frac{iET}{\hbar}} G(x,T;x',0) \tag{45}$$

The integral on T is extended to complex plane and the integration contour passes all $T^{(n)}$ that are classical paths for a particular E, then after getting G(x,x';E), we integrate on E and transform back to get the real time propagator. It can be shown that:

$$G(x,x';E) = \sum_n G^{(n)} = \sum_n \frac{m}{2\pi}\frac{1}{[k(x)k(x')]^{\frac{1}{2}}} \times \exp[i(\int_{x'}^{a} + \int_{b}^{x})dyk(y) - (2n+1)\int_a^b \kappa(y)dy] \times (i\lambda)^{2n} \tag{46}$$

Where $\kappa = \sqrt{2[V-E]}$, and λ is a phase to be fixed by probability conservation.

Then the transmission amplitude can be determined by summing over all transmission amplitudes of the propagators.For the example of a single barrier:

$$t(E) = \sum_{n=0}^{\infty} e^{-\int_a^b \kappa(y)dy} (i\lambda e^{-\int_a^b \kappa(y)dy})^{2n} \tag{47}$$

We have seen that it is possible to solve for transmission amplitude with path integral approach, but we have to perform non-trivial extension just as in the treatment in the wave function language. However, the path integral approach has a great advantage that it can be generalized directly to field theory, where the problem of barrier penetration becomes the decay of false vacuum, in the next note we will summarize the works done by Coleman and Callan and see some basic ideas of vacuum decay.

This note is brief, with many calculational details omitted, on can find them in the references.

References

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[4] Sidney Coleman ⟨Aspect of Symmetry⟩