Path integral approach to the heat kernel

(Appunti per il corso di Fisica Teorica 2011/12)

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The heat kernel finds many applications in physics and mathematics (calculation of effective actions in quantum field theories, study of anomalies, proofs of index theorems). A method of computing the heat kernel makes use of path integrals, which bring physical intuition into the problem and are quite efficient calculationally. They allow to visualize quantum processes as arising from the contribution of all possible paths which satisfy given boundary conditions, and allow simple perturbative calculations in terms of Feynman diagrams.

1 Introduction

The Schrödinger equation is the fundamental equation describing quantum physics. Its solutions can be obtained by computing path integrals, introduced by Feynman who arrived at his proposal by extending previous ideas due to Dirac. The analytical continuation in the time variable $t \to -i\beta$ (the so-called Wick rotation) relates the Schrödinger equation

$$i\frac{\partial}{\partial t}\psi = \hat{H}\psi \tag{1}$$

to the heat equation

$$-\frac{\partial}{\partial \beta}\psi = \hat{H}\psi \tag{2}$$

where $\hat{H}$ is a second order differential operator. Similarly the quantum mechanical path integral can be Wick rotated to an euclidean path integral, which generates the solution of the heat equation. Euclidean path integrals had been previously considered by Wiener in the discussion of the brownian motion. Here we discuss the use of path integrals to obtain a particular solution of the heat equation, the so-called "heat kernel or "fundamental solution", and compute perturbatively its asymptotic expansion for small euclidean time in terms of Feynman diagrams.

2 Example

Let us consider the simple case of a differential operator given by

$$\hat{H} = -\frac{1}{2}\nabla^2 + V(x) \tag{3}$$

where ∇^2 is the laplacian in the cartesian coordinates of R^D, denoted by x^μ, and $V(x)$ is an arbitrary smooth potential. Using the "bra" and "ket" language of Dirac, the heat kernel can be represented by

$$\psi(x,y;\beta) = \langle y|e^{-\beta\hat{H}}|x\rangle \tag{4}$$

It satisfies eq. (2) and the boundary condition

$$\psi(x,y;0) = \delta^D(x-y) \ . \tag{5}$$

It is well-known that the solution in the free case (i.e. for $V = 0$) is given by

$$\psi(x,y;\beta) = \frac{1}{(2\pi\beta)^{\frac{D}{2}}}\, e^{-\frac{(x-y)^2}{2\beta}} \ . \tag{6}$$

The path integral which computes (4) can be written formally as

$$\psi(x,y;\beta) = \int_{q(0)=x}^{q(\beta)=y} \mathcal{D}q \ e^{-S[q]} \tag{7}$$

where the symbol $\int_{q(0)=x}^{q(\beta)=y} \mathcal{D}q$ indicates the sum over all functions $q^\mu(t)$ which satisfy the boundary conditions $q^\mu(0) = x^\mu$ and $q^\mu(\beta) = y^\mu$, whereas the euclidean action $S[q]$ is given by

$$S[q] = \int_0^\beta dt \left(\frac{1}{2}\delta_{\mu\nu}\dot{q}^\mu\dot{q}^\nu + V(q)\right) \ . \tag{8}$$

The precise definition of path integrals, as usually given by physicists, requires the introduction of a regularization scheme, which means a procedure that makes sense of the integration over paths (that usually implies a discretization), and the fixing of certain renormalization conditions, which make sure that different regularization schemes will produce the same final answer once the continuum limit is taken. This general picture comes the study of renormalization in quantum field theory. We describe here a specific regularization scheme, even though it is not necessary for performing explicit calculations in simple cases. One of the simplest methods is based on Fourier expansion of all possible paths, and it is called "mode regularization".

2.1 Mode regularization

To start with let us first rescale for commodity the euclidean time variable $t = \beta\tau$, so that the new variable $\tau \in [0,1]$. The action (8) can now be written as follows

$$S[q] = \frac{1}{\beta}\int_0^1 d\tau \left(\frac{1}{2}\delta_{\mu\nu}\dot{q}^\mu\dot{q}^\nu + \beta^2 V(q)\right) \tag{9}$$

where of course dots (as in $\dot{q}^\mu$) represent now derivatives with respect to τ. This rescaling is useful especially since we are going to compute the path integral in a perturbative expansion valid for small β.

One can decompose all paths to be summed over as follows

$$q^\mu(\tau) = q^\mu_{bg}(\tau) + \phi^\mu(\tau) \tag{10}$$

where $q^\mu_{bg}(\tau)$ is a fixed path (sometimes called the background path, or the classical path) which can be taken to satisfy the boundary conditions and the classical equation of motion for $V = 0$. Thus

$$q^\mu_{bg}(\tau) = x^\mu + (y^\mu - x^\mu)\tau \ . \tag{11}$$

This is the classical solution for $V = 0$ as it satisfies the boundary conditions $q^\mu_{bg}(0) = x^\mu$ and $q^\mu_{bg}(1) = y^\mu$, as well as the equation of motion $\ddot{q}^\mu_{bg}(\tau) = 0$. The remaining arbitrary "quantum fluctuations" $\phi^\mu(\tau)$ must then have vanishing boundary conditions, $\phi^\mu(0) = \phi^\mu(1) = 0$. They can be expanded in a Fourier sum

$$\phi^\mu(\tau) = \sum_{m=1}^{\infty} \phi^\mu_m \sin(\pi m \tau) \ . \tag{12}$$

The path integral in (7) can now be concretely defined as the limit $M \to \infty$ of a big number M of usual Lebesgue integrations over the Fourier coefficients ϕ^μ_m suitably normalized, namely with a measure given by

$$\mathcal{D}q = \lim_{M\to\infty} A \prod_{m=1}^{M} \prod_{\mu=1}^{D} \sqrt{\frac{\pi m^2}{4\beta}}\, d\phi^\mu_m \tag{13}$$

where A is fixed by the consistency condition that the path integral should reproduce the correct solution to the heat equation. This requirement gives $A = (2\pi\beta)^{-D/2}$ (it may be considered as the renormalization condition mentioned above).

In fact, for $V = 0$ the action (which we denote by $S_2[q]$ to differentiate it from the full action with $V \neq 0$) can be written in terms of the paths parametrized as in (10), and reads

$$S_2[q] = \frac{(x-y)^2}{2\beta} + \sum_{m=1}^{\infty} \frac{\pi^2 m^2}{4\beta} \phi^\mu_m \phi^\nu_m \delta_{\mu\nu} \tag{14}$$

where the first term is due to the classical path $q^\mu_{bg}(\tau)$, and the rest from the quantum fluctuations $\phi^\mu(\tau)$. Of course, this action can also be presented in a discretized form by including in the sum only the first M modes. The free path integral is then defined by

$$\begin{aligned}
\int_{q(0)=x}^{q(\beta)=y} \mathcal{D}q\; e^{-S_2[q]} &\equiv \lim_{M\to\infty} \int A \prod_{m=1}^{M} \prod_{\mu=1}^{D} \sqrt{\frac{\pi m^2}{4\beta}}\, d\phi^\mu_m\, e^{-\frac{(x-y)^2}{2\beta}}\, e^{-\sum_{m=1}^{M} \frac{\pi^2 m^2}{4\beta}\phi^\mu_m \phi^\nu_m \delta_{\mu\nu}} \\
&= A\, e^{-\frac{(x-y)^2}{2\beta}} \lim_{M\to\infty} \prod_{m=1}^{M} \prod_{\mu=1}^{D} \int_{-\infty}^{\infty} d\phi^\mu_m \sqrt{\frac{\pi m^2}{4\beta}}\, e^{-\frac{\pi^2 m^2}{4\beta}\phi^\mu_m \phi^\mu_m} \\
&= \frac{1}{(2\pi\beta)^{\frac{D}{2}}}\, e^{-\frac{(x-y)^2}{2\beta}} \ .
\end{aligned} \tag{15}$$

We see that the free solution is reproduced, and the exponent is due to the action evaluated on the classical (or background) trajectory. Note that we have used repeatedly the standard gaussian integrals

$$\int_{-\infty}^{\infty} dx\, e^{-ax^2} = \sqrt{\frac{\pi}{a}} \ . \tag{16}$$

The same path integral formula is then extended to the more general actions of the type given in (9). The inclusion of an arbitrary potential V makes the problem quite difficult to solve in full generality. However it can be treated in perturbation theory, and the emerging solution will be of the form

$$\psi(x,y;\beta) = \frac{1}{(2\pi\beta)^{\frac{D}{2}}}\, e^{-\frac{(x-y)^2}{2\beta}} \Big(a_0(x,y) + a_1(x,y)\beta + a_2(x,y)\beta^2 + \dots \Big) \tag{17}$$

where the so-called Seeley-DeWitt coefficients a_n depend on the points x^μ and y^μ and on the potential V. It is also useful to use as a variable the difference

$$\xi^\mu = (y^\mu - x^\mu) \tag{18}$$

whose length (i.e. the distance between the two points) may be considered of order $\sqrt{\beta}$ for the brownian motion, and thus β controls the perturbative expansion. Of course $a_0(x,y) = 1$.

2.2 Perturbative expansion

The perturbative expansion is based on the gaussian averages of the path integral with the free quadratic action S_2 (i.e. the one with $V = 0$), namely

$$\begin{aligned}
A &= \int \mathcal{D}\phi\, e^{-S_2[\phi]} = \frac{1}{(2\pi\beta)^{\frac{D}{2}}} \\
\langle \phi^\mu(\tau) \rangle &= \frac{1}{A} \int \mathcal{D}\phi\, \phi(\tau)\, e^{-S_2[\phi]} = 0 \\
\langle \phi^\mu(\tau)\phi^\nu(\sigma) \rangle &= \frac{1}{A} \int \mathcal{D}\phi\, \phi^\mu(\tau)\phi^\nu(\sigma)\, e^{-S_2[\phi]} = -\beta\delta^{\mu\nu}\Delta(\tau,\sigma) \\
\dots
\end{aligned} \tag{19}$$

where $\Delta(\tau,\sigma)$ is the Green function of the operator $\frac{\partial^2}{\partial\tau^2}$ on the space of functions $f(\tau)$ with vanishing boundary conditions at $\tau = 0$ and $\tau = 1$,

$$\frac{\partial^2}{\partial\tau^2}\Delta(\tau,\sigma) = \delta(\tau-\sigma)\ . \tag{20}$$

It reads (for τ and σ in $[0,1]$)

$$\begin{aligned}
\Delta(\tau,\sigma) &= \sum_{m=1}^{\infty} \Big[-\frac{2}{\pi^2 m^2} \sin(\pi m\tau)\sin(\pi m\sigma) \Big] = (\tau-1)\sigma\,\theta(\tau-\sigma) + (\sigma-1)\tau\,\theta(\sigma-\tau) \\
\delta(\tau-\sigma) &= \sum_{m=1}^{\infty} 2\,\sin(\pi m\tau)\sin(\pi m\sigma)
\end{aligned} \tag{21}$$

where $\theta(x)$ is the standard step function ($\theta(x) = 1$ for $x > 0$, $\theta(0) = 1/2$ for $x = 0$, and $\theta(x) = 0$ for $x < 0$). Note that in general one may define the average of an arbitrary functional $F[\phi]$ as

$$\langle F[\phi] \rangle = \frac{1}{A} \int \mathcal{D}\phi\, F[\phi]\, e^{-S_2[\phi]}\ . \tag{22}$$

Now the perturbative expansion is computed as follows. The action is written as

$$S[q] = S_2[q] + S_{int}[q] \tag{23}$$

where

$$S_2[q] = \frac{1}{\beta}\int_0^1 d\tau\, \frac{1}{2}\delta_{\mu\nu}\dot{q}^\mu \dot{q}^\nu \tag{24}$$

is the free action, and

$$S_{int}[q] = \beta \int_0^1 d\tau\, V(q) \tag{25}$$

is the interaction part. The path integral can now be manipulated as follows

$$\begin{aligned}
\int_{q(0)=x}^{q(\beta)=y} \mathcal{D}q\; e^{-S[q]} &= \int_{q(0)=x}^{q(\beta)=y} \mathcal{D}q\; e^{-(S_2[q]+S_{int}[q])} \\
&= e^{-S_2[q_{bg}]}\int_{\phi(0)=0}^{\phi(\beta)=0} \mathcal{D}\phi\, \left(e^{-S_{int}[q_{bg}+\phi]}\right) e^{-S_2[\phi]} \\
&= A\, e^{-S_2[q_{bg}]}\left\langle e^{-S_{int}[q_{bg}+\phi]}\right\rangle \\
&= \frac{1}{(2\pi\beta)^{\frac{D}{2}}}\, e^{-\frac{(x-y)^2}{2\beta}}\left\langle \left(1 - S_{int}[q_{bg}+\phi] + \frac{1}{2}S_{int}^2[q_{bg}+\phi] + \cdots\right)\right\rangle .
\end{aligned} \tag{26}$$

Usually one describe the transition from the first to the second line by saying that one has used the translation invariance of the path integral measure. In fact here we have just used the definition of the measure (13), which could be named by $\mathcal{D}\phi$ as well. Then we have used the notation introduced in (22) to indicate averages with the free path integral. Finally, the expansion of the exponential of the interaction part in the last line generates the perturbative expansion.

Let us compute systematically the various terms appearing in the last line of eq. (26). The first one is trivial

$$\langle 1 \rangle = 1 \ . \tag{27}$$

Next we have to consider $\langle S_{int}[q_{bg}+\phi]\rangle$. We can Taylor expand the potential around the initial point x^μ

$$\begin{aligned}
S_{int}[q_{bg}+\phi] &= \beta\int_0^1 d\tau\, V(q_{bg}+\phi) \\
&= \beta\int_0^1 d\tau\, \Big(V(x) + [(y^\mu - x^\mu)\tau + \phi^\mu(\tau)]\partial_\mu V(x) \\
&+ \frac{1}{2}[(y^\mu - x^\mu)\tau + \phi^\mu(\tau)]\,[(y^\nu - x^\nu)\tau + \phi^\nu(\tau)]\,\partial_\mu\partial_\nu V(x) + \cdots\Big)
\end{aligned} \tag{28}$$

from which one obtains

$$\begin{aligned}
\langle(-S_{int}[q_{bg}+\phi])\rangle &= -\beta V(x) - \frac{\beta}{2}\xi^\mu\partial_\mu V(x) - \frac{\beta}{6}\xi^\mu\xi^\nu\partial_\mu\partial_\nu V(x) \\
&- \frac{\beta}{2}\partial_\mu\partial_\nu V(x)\int_0^1 d\tau\, \langle\phi^\mu(\tau)\phi^\nu(\tau)\rangle + \cdots \ .
\end{aligned} \tag{29}$$

The last term is easily computed using (19) and (21)

$$\int_0^1 d\tau\, \langle \phi^\mu(\tau)\phi^\nu(\tau)\rangle = \int_0^1 d\tau\, (-\beta\delta^{\mu\nu}\Delta(\tau,\tau)) = -\beta\delta^{\mu\nu}\int_0^1 d\tau\, \tau(\tau-1) = \frac{\beta}{6}\delta^{\mu\nu} \quad (30)$$

so that

$$\begin{aligned}\langle(-S_{int}[q_{bg}+\phi])\rangle &= -\beta V(x) - \frac{\beta}{2}\xi^\mu\partial_\mu V(x) - \frac{\beta}{6}\xi^\mu\xi^\nu\partial_\mu\partial_\nu V(x)\\ &- \frac{\beta}{12}\nabla^2 V(x) + \cdots \ . \end{aligned} \quad (31)$$

Similarly, at lowest order one finds for the next term in (26)

$$\Big\langle \frac{1}{2}S^2_{int}[q_{bg}+\phi]\Big\rangle = \frac{\beta^2}{2}V^2(x) + \cdots \ . \quad (32)$$

Collecting all the terms, we find that at this order the heat kernel computed from the path integral is given by

$$\begin{aligned}\psi(x,y;\beta) &= \frac{1}{(2\pi\beta)^{\frac{D}{2}}}\, e^{-\frac{(x-y)^2}{2\beta}}\Big[1 - \beta V(x) - \frac{\beta}{2}\xi^\mu\partial_\mu V(x) - \frac{\beta}{6}\xi^\mu\xi^\nu\partial_\mu\partial_\nu V(x)\\ &- \frac{\beta^2}{12}\nabla^2 V(x) + \frac{\beta^2}{2}V^2(x) + \cdots\Big]\end{aligned} \quad (33)$$

from which one reads off the Seeley-DeWitt coefficients a_0, a_1 and a_2

$$\begin{aligned}a_0(x,y) &= 1\\ a_1(x,y) &= -V(x) - \frac{1}{2}\xi^\mu\partial_\mu V(x) - \frac{1}{6}\xi^\mu\xi^\nu\partial_\mu\partial_\nu V(x) + \cdots\\ a_2(x,y) &= \frac{1}{2}V^2(x) - \frac{1}{12}\nabla^2 V(x) + \cdots \ .\end{aligned} \quad (34)$$

In particular, their values at coinciding points $y^\mu = x^\mu$ (i.e. for $\xi^\mu = 0$) are given by

$$\begin{aligned}a_0(x,x) &= 1\\ a_1(x,x) &= -V(x)\\ a_2(x,x) &= \frac{1}{2}V^2(x) - \frac{1}{12}\nabla^2 V(x) \ .\end{aligned} \quad (35)$$

This calculation exemplifies the use of the path integral to compute the heat kernel.

To be completely self contained, we should perhaps address a bit more in detail how the averages (also named correlation functions) in (19) are computed. Let us use a hypercondensed notation $\phi(\tau) \to \phi^i$, where the dependence on τ is indicated by the index i, and generalize the Einstein summation convention to imply an integration for repeated indices, as for example in $\phi^i\chi_i = \int_0^1 d\tau\, \phi(\tau)\chi(\tau)$. Then the required formulas arise from the following gaussian integrals

$$\begin{aligned}Z &\equiv \int \frac{d^n\phi}{(2\pi)^{\frac{n}{2}}}\, e^{-\frac{1}{2}\phi^i K_{ij}\phi^j} = (\det K_{ij})^{-\frac{1}{2}}\\ Z[J] &\equiv \int \frac{d^n\phi}{(2\pi)^{\frac{n}{2}}}\, e^{-\frac{1}{2}\phi^i K_{ij}\phi^j + J_i\phi^i} = (\det K_{ij})^{-\frac{1}{2}}\, e^{\frac{1}{2}J_i G^{ij} J_j}\end{aligned} \quad (36)$$

where G^{ij} is the inverse of K_{ij} (i.e. $K_{ij}G^{jk} = \delta_i^k$). It corresponds to a Green function when K_{ij} is a differential operator. The second integral is obtained by simply "completing the square" and shifting integration variables. The required averages then follow from differentiating $Z[J]$

$$
\begin{aligned}
\langle \phi^{i_1}\phi^{i_2}\cdots\phi^{i_n}\rangle &= \frac{1}{Z}\int D\phi\; \phi^{i_1}\phi^{i_2}\cdots\phi^{i_n} e^{-\frac{1}{2}\phi^i K_{ij}\phi^j} \\
&= \frac{1}{Z}\frac{\delta^n}{\delta J_{i_1}J_{i_2}\cdots J_{i_n}} Z[J]\Big|_{J=0} \\
&= \frac{\delta^n}{\delta J_{i_1}J_{i_2}\cdots J_{i_n}} e^{\frac{1}{2}J_i G^{ij} J_j}\Big|_{J=0}
\end{aligned} \tag{37}
$$

obtaining in particular

$$
\begin{aligned}
&\langle 1\rangle = 1 \\
&\langle \phi^i\rangle = 0 \\
&\langle \phi^i\phi^j\rangle = G^{ij} \\
&\langle \phi^i\phi^j\phi^k\rangle = 0 \\
&\langle \phi^i\phi^j\phi^k\phi^l\rangle = G^{ij}G^{kl} + G^{ik}G^{jl} + G^{il}G^{jk}
\end{aligned} \tag{38}
$$

and so on. In particular correlation functions of an odd number of fields vanish, while those with an even number of fields are given by sums of products of two-point functions (a fact sometimes known as Wick theorem). The two-point function is also known as the Feynman propagator.