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Scalar field with Robin boundary conditions in the worldline formalism

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Abstract

The worldline formalism has been widely used to compute physical quantities in quantum field theory. However, applications of this formalism to quantum fields in the presence of boundaries have been studied only recently. In this paper we show how to compute in the worldline approach the heat kernel expansion for a scalar field with boundary conditions of Robin type. In order to describe how this mechanism works, we compute the contributions due to the boundary conditions to the coefficients A_1 , $A_{3/2}$ and A_2 of the heat kernel expansion of a scalar field on the positive real line.

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1. Introduction

Many problems in quantum field theory can be studied in the worldline formalism. This approach provides an intuitive and, in many cases, more efficient method to carry out computations in the 1-loop approximation (see [2–4] and references therein).

This formalism makes use of the connection between some quantities in quantum field theory, like the effective action, and the operator e^{-TA} corresponding to some relevant differential operator A . The first important step in this approach is to identify a classical particle whose Hamiltonian, after first quantization, is this differential operator A . If this identification is found, then the heat kernel corresponds to the evolution operator of the particle in Euclidean time T . The kernel $\langle y|e^{-TA}|x\rangle$ of the operator e^{-TA} is a quantum-mechanical transition amplitude and therefore can also be computed in the path integral formulation of first quantization.

It is important to mention that many physical quantities of the quantum field theory are determined by the small- T asymptotic expansion of the heat kernel $\langle y|e^{-TA}|x\rangle$. In this

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sense, the path integral computation of this transition amplitude results particularly appropriate because the small- T expansion comes out in a natural way. By this procedure the worldline formalism has been proved useful in the study of quantum fields of different spins and their coupling to external gravity.

The purpose of the present paper is to describe how the worldline formalism can also be applied to quantum field theory on manifolds with boundaries. In order to do this, one has to deal with the path integral formulation of the quantum mechanics of a point particle on a manifold with boundaries. The main difficulty is to implement the boundary conditions imposed on the quantum fields, i.e. on the domain of the differential operator A , in the path integral calculation of the quantum-mechanical transition amplitude $\langle y | e^{-TA} | x \rangle$. This problem has been solved in [1] for Dirichlet and Neumann boundary conditions by the method of images. In this paper we show how to implement Robin boundary conditions in the path integral calculation and compute the contributions of the boundary conditions to the coefficients A_1 , $A_{3/2}$ and A_2 of the small- T asymptotic expansion of the heat kernel for a scalar field on the positive half-line. For this setting, Robin boundary conditions are the most general boundary conditions determined by the selfadjointness of the differential operator A .

The method of images is not straightforwardly applicable to Robin boundary conditions. However, as is shown in the appendix (see also [5]), one can implement Robin boundary conditions on the heat kernel by using the image construction for Neumann boundary conditions supplemented by a suitable delta-function potential at the boundary. This delta-function then constrains the paths which contribute to the path integral computation of the transition amplitude.

In the next section, we describe the worldline method by considering the heat kernel trace for a scalar field on a manifold without boundaries. In section 3, we apply the worldline approach to a scalar field on the positive half-line under Robin boundary conditions at the origin and compute the contributions of the boundary to the first coefficients of the heat kernel expansion. In section 4, we draw our conclusions and comment on possible generalizations of our technique.

2. Heat kernel expansion without boundaries

In order to describe the worldline approach to quantum field theories let us consider the 1-loop effective action of a scalar field $\phi(x)$ with a self-interaction $U(\phi(x))$ on a flat manifold \mathcal{M} . The classical action $I[\phi(x)]$ of the scalar field is given by

$$I[\phi(x)] = \int_{\mathcal{M}} dx \left\{ \frac{1}{2} (\partial\phi(x))^2 + U(\phi(x)) \right\} \tag{2.1}$$

and the 1-loop effective action can be represented as

$$\begin{aligned} \Gamma[\phi(x)] &= I[\phi(x)] - \hbar \log \text{Det}^{-1/2} \{-\Delta + U''(\phi(x))\} \\ &= I[\phi(x)] - \frac{\hbar}{2} \int_0^\infty \frac{dT}{T} \text{Tr}(e^{-T\{-\Delta + U''(\phi(x))\}}) \\ &= I[\phi(x)] - \frac{\hbar}{2} \int_0^\infty \frac{dT}{T} \int_{\mathcal{M}} dx \langle x | e^{-T\{-\Delta + U''(\phi(x))\}} | x \rangle. \end{aligned} \tag{2.2}$$

The integrand in the last expression is the heat kernel

$$\langle y | e^{-T\{-\Delta + U''(\phi(x))\}} | x \rangle \tag{2.3}$$

of the Schrödinger operator

$$-\Delta + U''(\phi(x)) \tag{2.4}$$

evaluated at the diagonal $x = y$. Inspection of expression (2.2) shows that the small- T asymptotic expansion of this heat kernel contains information about the ultraviolet divergences of the theory.

In the worldline approach, the kernel (2.3) is regarded as the quantum-mechanical transition amplitude in Euclidean time T between x and y of a point particle whose Hamiltonian is given by (2.4). In fact, the Schrödinger operator (2.4) can be regarded as the Hamiltonian, after first quantization, of a point particle whose Euclidean classical action is

$$S[x(t)] = \int_0^T dt \left\{ \frac{1}{4} \dot{x}^2(t) + V(x(t)) \right\} \tag{2.5}$$

where

$$V(x) := U''(\phi(x)). \tag{2.6}$$

Therefore, we can represent the transition amplitude (2.3) in the path integral approach

$$\langle y | e^{-T\{-\Delta+V(x)\}} | x \rangle = \int_{x(0)=x}^{x(T)=y} \mathcal{D}x(t) e^{-\int_0^T dt \left\{ \frac{1}{4} \dot{x}^2 + V(x(t)) \right\}}. \tag{2.7}$$

With this procedure we can compute some quantities in quantum field theory in terms of quantum-mechanical path integrals. An essential step in this description is the identification of the differential operator appearing in the first line of expression (2.2) with the quantized Hamiltonian of a point particle.

Next, we show how the path integral in expression (2.7) turns out to be convenient for the computation of the small- T asymptotic expansion of the transition amplitude. In order to do that, we rescale the Euclidean time variable t by introducing $\tau := t/T$ and we replace the integration over trajectories $x(t)$ by an integration over the ‘quantum fluctuations’ $y(\tau) := x(T\tau) - (y-x)\tau - x$

$$\begin{aligned} \langle y | e^{-T\{-\Delta+V(x)\}} | x \rangle &= e^{-\frac{(y-x)^2}{4T}} \int_{y(0)=0}^{y(1)=0} \mathcal{D}y(\tau) e^{-\frac{1}{4T} \int_0^1 d\tau \dot{y}^2(\tau)} e^{-T \int_0^1 d\tau V((y-x)\tau + x + y(\tau))} \\ &=: e^{-\frac{(y-x)^2}{4T}} \langle e^{-T \int_0^1 d\tau V((y-x)\tau + x + y(\tau))} \rangle = e^{-\frac{(y-x)^2}{4T}} \sum_{n=0}^{\infty} \frac{(-T)^n}{n!} \int_0^1 d\tau_1 \dots \int_0^1 d\tau_n \\ &\quad \times \left\langle \prod_{k=1}^n V((y-x)\tau_k + x + y(\tau_k)) \right\rangle. \end{aligned} \tag{2.8}$$

Note that we end up with a perturbative calculation in $(0+1)$ -field theory where the number of loops is related to the power of T and the propagator is proportional to T .

For our purposes it suffices to consider the trace of the heat kernel

$$\begin{aligned} \text{Tr} e^{-T\{-\Delta+V(x)\}} &= \int_{\mathcal{M}} dx \langle e^{-T \int_0^1 d\tau V(x+y(\tau))} \rangle \\ &= \sum_{n=0}^{\infty} \frac{(-T)^n}{n!} \int_{\mathcal{M}} dx \int_0^1 d\tau_1 \dots \int_0^1 d\tau_n \left\langle \prod_{k=1}^n V(x + y(\tau_k)) \right\rangle. \end{aligned} \tag{2.9}$$

If the potential is an analytic function, we can make a Taylor expansion and write the integrand in the previous expression as a sum whose terms consist, in general, of a product between the potential and its derivatives evaluated at x and many-point functions, which, due to Wick’s theorem, can be written in terms of two-point functions $\langle y(\tau_{k_1})y(\tau_{k_2}) \rangle$. Since these propagators are proportional to T we obtain an asymptotic expansion in integer powers of T whose coefficients are integrals on \mathcal{M} of products of the potential and its derivatives.

Finally, we normalize the expectation value $\langle 1 \rangle$ such that for the case $V(x) \equiv 0$ we obtain:

$$\langle y | e^{-T\{-\Delta\}} | x \rangle = e^{-\frac{(y-x)^2}{4T}} \cdot \langle 1 \rangle = \frac{e^{-\frac{(y-x)^2}{4T}}}{\sqrt{4\pi T}} \tag{2.10}$$

which is the known value for the transition amplitude for a free particle. Note that the numerator in the last expression corresponds to the contribution of the classical trajectory whereas the denominator corresponds to the contributions of the quantum fluctuations.

We end this section by recalling that for a Schrödinger differential operator on a manifold with boundaries the trace of the heat kernel admits the following small- T asymptotic expansion⁴,

$$\text{Tr} e^{-T\{-\Delta+V(x)\}} = \frac{1}{(4\pi T)^{m/2}} \sum_{n=0}^{\infty} A_{n/2} \cdot T^{n/2} \tag{2.11}$$

where m is the dimension of the base manifold \mathcal{M} . The coefficients $A_{n/2}$ for odd n vanish for manifolds without boundary (see the discussion after equation (2.9)). In the following section, it will become clear how these half-integer powers of T appear due to the presence of boundaries.

3. Heat kernel expansion under Robin boundary conditions

In this section, we consider the small- T asymptotic expansion of the trace of the heat kernel corresponding to a Schrödinger operator on the positive half-line $\mathcal{M} = \mathbb{R}^+$. We impose Robin boundary conditions on the functions $\psi(x)$ in the domain of the Schrödinger operator

$$\partial_x \psi(x) + \gamma \cdot \psi(x)|_{x=0} = 0 \tag{3.1}$$

where $\gamma \in \mathbb{R}$.

This type of boundary conditions can be implemented in the path integral by computing the contributions of all paths that correspond to Neumann boundary conditions and, at the same time, introducing a Dirac delta-function in the potential (see the appendix.) The computation of the contribution of all paths that correspond to Neumann boundary conditions can be performed by the method of images, according to which

$$\langle x | e^{-T\{-\Delta+V(x)\}} | x \rangle_N = \langle x | e^{-T\{-\Delta+V_{\mathbb{R}}(x)\}} | x \rangle_{\mathbb{R}} + \langle -x | e^{-T\{-\Delta+V_{\mathbb{R}}(x)\}} | x \rangle_{\mathbb{R}}, \tag{3.2}$$

where the subscript N stands for ‘Neumann’ and the subscript \mathbb{R} indicates that the corresponding transition amplitudes are computed in the whole real line. Accordingly, $V_{\mathbb{R}}(x)$ is the extension to the whole real line of the potential $V(x)$, which is defined only on \mathbb{R}^+ , by a reflection about the origin. As just mentioned, in order to obtain the transition amplitude for Robin boundary conditions we still have to include in the potential a Dirac delta-function. Finally, using equation (2.8) to compute the transition amplitudes in the whole real line, the trace of the heat kernel for Robin boundary conditions can be written as,

$$\begin{aligned} \text{Tr}_{\gamma} e^{-T\{-\Delta+V(x)\}} &= \int_0^{\infty} dx \langle x | e^{-T\{-\Delta+V_{\mathbb{R}}(x)\}} | x \rangle_{\mathbb{R}} + \int_0^{\infty} dx \langle -x | e^{-T\{-\Delta+V_{\mathbb{R}}(x)\}} | x \rangle_{\mathbb{R}} \\ &= \sum_{n=0}^{\infty} \frac{(-T)^n}{n!} \int_0^{\infty} dx \int_0^1 d\tau_1 \dots \int_0^1 d\tau_n \\ &\quad \times \left\{ \left\langle \prod_{k=1}^n V_{\mathbb{R}}^{\gamma}(x + y(\tau_k)) \right\rangle + e^{-\frac{x^2}{T}} \left\langle \prod_{k=1}^n V_{\mathbb{R}}^{\gamma}((1 - 2\tau_k)x + y(\tau_k)) \right\rangle \right\}, \tag{3.3} \end{aligned}$$

⁴ This expansion holds under certain regularity assumptions on the manifold, the potential and the (local) boundary conditions.

where

$$V_{\mathbb{R}}^{\gamma}(x) = V(x) + \theta(-x)(V(-x) - V(x)) - 2\gamma \cdot \delta(x). \tag{3.4}$$

The term with the Heaviside function $\theta(x)$ represents the extension of the potential to the negative half-line whereas the term with the Dirac delta-function is needed in order to obtain the transition function for the boundary conditions given by (3.1). Note that the factor $e^{-x^2/T}$ in the second term of equation (3.3) is responsible for the appearance of half-integer powers of T .

Next, we compute the contributions to the first coefficients $A_{n/2}$ of the heat kernel expansion (2.11) due to Robin boundary conditions. Since $\gamma = 0$ corresponds to Neumann boundary conditions these contributions, which are proportional to positive powers of γ , must be added to the coefficients $A_{n/2}$ corresponding to Neumann boundary conditions. The coefficients $A_{n/2}$ for Neumann boundary conditions have been already computed in the worldline formalism in [1].

It is interesting to note that the inclusion of the Dirac delta-function leads to Dirichlet boundary conditions for $\gamma \rightarrow -\infty$. Indeed, by the method of images, the transition function for these boundary conditions is given by the difference of the terms on the RHS of (3.2). This subtraction amounts to omitting from the computation the contribution of all those paths that hit the origin at least once. In accordance, as can be seen from the first line of equation (2.9), the Dirac delta-function in (3.4) cancels the contributions of the paths that hit the origin.

To compute the contributions of the boundary condition (3.1) to the coefficients $A_{n/2}$ (with respect to Neumann boundary conditions) we do not use the procedure described in the previous section. Due to the singularities introduced in the potential by the Dirac delta-function and also by making the reflection with respect to the origin, one cannot make a Taylor expansion of $V_{\mathbb{R}}^{\gamma}$ in expression (3.3) (see the discussion after (2.9)). Nevertheless, one can deal with the Heaviside and the delta-function introduced in (3.4) by appropriately constraining the paths in the functional integration. We describe this mechanism by computing the contributions to the coefficients $A_1, A_{3/2}$ and A_2 .

The first non-vanishing contribution due to Robin boundary conditions comes from the term corresponding to $n = 1$ in equation (3.3),

$$-T \int_0^{\infty} dx \int_0^1 d\tau_1 \left\{ -2\gamma \cdot \delta(x + y(\tau_1)) + e^{-\frac{x^2}{T}} \left\langle -2\gamma \cdot \delta((1 - 2\tau_1)x + y(\tau_1)) \right\rangle \right\}. \tag{3.5}$$

Let us consider the delta-function in the expectation value. For the first term, this means that one should consider the contributions of only those paths $y(\tau)$ beginning and ending at the origin in Euclidean time T such that at $\tau = \tau_1$ reach the point $-x$. This restriction can be implemented by computing the product of the (free) transition amplitude (see equation (2.10)) from the origin to $-x$ in time $T\tau_1$ times the (free) transition amplitude from $-x$ back again to the origin in time $T(1 - \tau_1)$. The same calculation can be implemented for the second term in (3.5) but considering the intermediate point $-(1 - 2\tau_1)x$ instead of $-x$. The result can be written as

$$\begin{aligned} 2T\gamma \int_0^{\infty} dx \int_0^1 d\tau \left\{ \frac{e^{-\frac{x^2}{4T\tau_1}}}{\sqrt{4\pi T\tau_1}} \cdot \frac{e^{-\frac{x^2}{4T(1-\tau_1)}}}{\sqrt{4\pi T(1-\tau_1)}} + e^{-\frac{x^2}{T}} \frac{e^{-\frac{(1-2\tau_1)^2 x^2}{4T\tau_1}}}{\sqrt{4\pi T\tau_1}} \cdot \frac{e^{-\frac{(1-2\tau_1)^2 x^2}{4T(1-\tau_1)}}}{\sqrt{4\pi T(1-\tau_1)}} \right\} \\ = \frac{T}{\sqrt{4\pi T}} \cdot 2\gamma, \end{aligned} \tag{3.6}$$

where the result can be easily obtained by interchanging the order of integration. We conclude that the contribution of the boundary conditions to A_1 is given by 2γ .

Next, we proceed with the term corresponding to $n = 2$ in equation (3.3). There are two contributions to be considered: one is proportional to γ and the other one is proportional to γ^2 . The contribution proportional to γ^2 is given by

$$\begin{aligned} & \frac{T^2}{2} 4\gamma^2 \int_0^\infty dx \int_0^1 d\tau_1 \int_0^1 d\tau_2 \{ \langle \delta(x + y(\tau_1)) \cdot \delta(x + y(\tau_2)) \rangle \\ & \quad + e^{-\frac{x^2}{T}} \langle \delta((1 - 2\tau_1)x + y(\tau_1)) \cdot \delta((1 - 2\tau_2)x + y(\tau_2)) \rangle \} \\ & = 4T^2\gamma^2 \int_0^\infty dx \int_0^1 d\tau_1 \int_0^1 d\tau_2 \left\{ \frac{e^{-\frac{x^2}{4T\tau_1}}}{\sqrt{4\pi T\tau_1}} \frac{1}{\sqrt{4\pi T(\tau_2 - \tau_1)}} \frac{e^{-\frac{x^2}{4T(1-\tau_2)}}}{\sqrt{4\pi T(1-\tau_2)}} \right. \\ & \quad \left. + e^{-\frac{x^2}{T}} \frac{e^{-\frac{(1-2\tau_1)^2 x^2}{4T\tau_1}}}{\sqrt{4\pi T\tau_1}} \frac{e^{-\frac{(\tau_2-\tau_1)x^2}{T}}}{\sqrt{4\pi T(\tau_2 - \tau_1)}} \frac{e^{-\frac{(1-2\tau_2)^2 x^2}{4T(1-\tau_2)}}}{\sqrt{4\pi T(1-\tau_2)}} \right\} = \frac{T^{3/2}}{\sqrt{4\pi T}} \cdot \sqrt{\pi} \gamma^2. \quad (3.7) \end{aligned}$$

Therefore, the contribution of the boundary conditions to $A_{3/2}$ is given by $\sqrt{\pi} \gamma^2$.

The leading order in T of the contribution proportional to γ in the $n = 2$ term of equation (3.3) contributes to the coefficient A_2 and is given by

$$\begin{aligned} & \frac{T^2}{2} (-2\gamma) \int_0^\infty dx \int_0^1 d\tau_1 \int_0^1 d\tau_2 \{ \langle 2V(x + y(\tau_1)) \delta(x + y(\tau_2)) \rangle \\ & \quad + e^{-\frac{x^2}{T}} \langle 2V((1 - 2\tau_1)x + y(\tau_1)) \delta((1 - 2\tau_2)x + y(\tau_2)) \rangle \}. \quad (3.8) \end{aligned}$$

The leading order in T of this expression is obtained by making a Taylor expansion of the potential about the origin

$$\begin{aligned} & -2T^2\gamma V(0) \int_0^\infty dx \int_0^1 d\tau_1 \int_0^1 d\tau_2 \left\{ \frac{e^{-\frac{x^2}{4T\tau_2}}}{\sqrt{4\pi T\tau_2}} \frac{e^{-\frac{x^2}{4T(1-\tau_2)}}}{\sqrt{4\pi T(1-\tau_2)}} \right. \\ & \quad \left. + e^{-\frac{x^2}{T}} \frac{e^{-\frac{(1-2\tau_2)^2 x^2}{4T\tau_2}}}{\sqrt{4\pi T\tau_2}} \frac{e^{-\frac{(1-2\tau_2)^2 x^2}{4T(1-\tau_2)}}}{\sqrt{4\pi T(1-\tau_2)}} \right\} = -\frac{T^2}{\sqrt{4\pi T}} \cdot 2\gamma V(0). \quad (3.9) \end{aligned}$$

This is a contribution to the coefficient A_2 proportional to γ . There is another contribution to this coefficient due to the boundary conditions which is proportional to γ^3 . We end this section by computing this contribution, which comes from the $n = 3$ term in equation (3.3) and is given by

$$\begin{aligned} & -\frac{T^3}{3!} (-8\gamma^3) \int_0^\infty dx \int_0^1 d\tau_1 \int_0^1 d\tau_2 \int_0^1 d\tau_3 \{ \langle \delta(x + y(\tau_1)) \delta(x + y(\tau_2)) \delta(x + y(\tau_3)) \rangle \\ & \quad + e^{-\frac{x^2}{T}} \langle \delta((1 - 2\tau_1)x + y(\tau_1)) \delta((1 - 2\tau_2)x + y(\tau_2)) \delta((1 - 2\tau_3)x + y(\tau_3)) \rangle \} \\ & = \frac{T^2}{\sqrt{4\pi T}} \cdot \frac{4}{3} \gamma^3. \quad (3.10) \end{aligned}$$

Taking into account this last result together with that given in equation (3.9), we conclude that the total contribution to A_2 due to the boundary conditions is given by $2\gamma V_0 + 4/3\gamma^3$. All these contributions are the expected ones (see, e.g., [6].)

4. Conclusions

Worldline approaches can be successfully used to study QFTs on manifolds with boundaries. After recalling the methods employed in [1], we have considered the inclusion of Robin

boundary conditions. These conditions can be enforced by adding a delta-function potential to the setup for Neumann boundary conditions described in [1]. In this way we have been able to recover the expected corrections to the heat kernel coefficients up to, and including, A_2 . We plan to further simplify and extend the methods reviewed in the present paper [7]. In addition, it would be interesting to extend them to include curved boundaries, curved spaces and fields with nontrivial spins.

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Appendix

Consider the following kernel, defined on the half-line

$$\psi(y, x; \beta) := \langle y | e^{-\beta H_\gamma} | x \rangle_{\mathbb{R}} + \langle -y | e^{-\beta H_\gamma} | x \rangle_{\mathbb{R}} \quad (\text{A.1})$$

with

$$H_\gamma = -\partial_y^2 - 2\gamma\delta(y). \quad (\text{A.2})$$

By construction, (A.1) is even under $y \rightarrow -y$. In other words $\psi(y, x; \beta)$ can be extended to the whole line such that it is continuous as a function of y . On the other hand, its first derivative is odd,

$$\partial_y \psi(y, x; \beta) = -\partial_y \psi(-y, x; \beta), \quad (\text{A.3})$$

and is not defined at $y = 0$ because of the presence of the delta function. In fact, (A.1) satisfies the heat equation

$$(\partial_\beta - \partial_y^2 - 2\gamma\delta(y)) \psi(y, x; \beta) = 0, \quad (\text{A.4})$$

which is equivalent to the heat equation for a free particle away from the boundary whose wavefunction satisfies the jump condition

$$-\partial_y \psi(0^+, x; \beta) + \partial_y \psi(0^-, x; \beta) - 2\gamma \psi(0, x; \beta) = 0. \quad (\text{A.5})$$

Using equations (A.3) and (A.5) we obtain

$$\partial_y \psi(0^+, x; \beta) + \gamma \cdot \psi(0, x; \beta) = 0. \quad (\text{A.6})$$

Therefore, (A.1) is the heat kernel for a free particle on the half-line subject to Robin boundary conditions. Note that taking $\gamma \rightarrow 0$ one correctly achieves Neumann boundary conditions.

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