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Functional integrals for parabolic differential equations†

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Abstract. The proof of convergence of a discretisation procedure for path integrals associated with parabolic second-order differential equations is presented.

1. Introduction

The aim of this paper is to present a proof of convergence for a class of path integrals associated with parabolic second-order differential equations and defined as limits of finite-dimensional integrals. We consider the following differential equation

$$\frac{\partial f(x;t)}{\partial t} = \mathscr{L}(x, D) f(x;t) \tag{1.1}$$

where $x = (x^1, \ldots, x^\nu) \in \mathbb{R}^\nu$, $D = (\partial_1 \ldots \partial_\nu)$, $\partial_\alpha \equiv \partial/\partial x^\alpha$

$$\mathscr{L}(x, D) = a^{\alpha\beta}(x)\partial_\alpha\partial_\beta + b^\alpha(x)\partial_\alpha + c(x) \tag{1.2}$$

and the Einstein summation convention is used for Greek letters only. We assume that $\mathscr{L}(x, D)$ is strictly elliptic, i.e. there exists a constant $A > 0$ such that

$$A \sum_\alpha \xi_\alpha^2 \leqslant a^{\alpha\beta}(x)\xi_\alpha\xi_\beta \leqslant A^{-1} \sum_\alpha \xi_\alpha^2 \tag{1.3}$$

for all $x \in \mathbb{R}^\nu$ and all $\xi = (\xi_1, \ldots, \xi_\nu) \in \mathbb{R}^\nu$.

The following notation will be used. $a_{\alpha\beta}(x)$ is an inverse of $a^{\alpha\beta}(x)$, i.e.

$$a_{\alpha\beta}(x)a^{\beta\gamma}(x) = \delta_\alpha{}^\gamma$$

$$|a(x)| = \det(a^{\alpha\beta}(x)). \tag{1.4}$$

$a^{1/2}_{\alpha\beta}(x)(a^{\alpha\beta}_{1/2}(x))$ is the square root matrix of $a_{\alpha\beta}(x)$ $(a^{\alpha\beta}(x))$.

The formal path integral representation often used in physics literature may be written as follows:

(1) *Phase space form*

$$f(x_0; t) = \lim_{N\to\infty} \int_{\mathbb{R}^{2N\nu}} \prod_{k=1}^N \frac{\mathrm{d}x_k\,\mathrm{d}p^k}{2\pi} \times \exp\left[-\sum_{k=1}^N \Delta t\left(-\mathrm{i}p_\alpha^k \frac{\Delta x_k^\alpha}{\Delta t} + a^{\alpha\beta}(x_{k-1})p_\alpha^k p_\beta^k + \mathrm{i}b^\alpha(x_{k-1})p_\alpha^k + c(x_{k-1})\right)\right] \times f(x_N; 0). \tag{1.5}$$

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(2) *Configuration space form* (obtained by integration over p^k)

$$f(x_0;t)=\lim_{N\to\infty}\int_{\mathbb{R}^{N\nu}}\prod_{k=1}^{N}\mathrm{d}x_k\prod_{k=1}^{N}(4\pi\Delta t)^{-\nu/2}|a(x_{k-1})|^{-1/2}$$
$$\times\exp\left\{-\sum_{k=1}^{N}\Delta t\left[\tfrac{1}{4}a_{\alpha\beta}(x_{k-1})\left(\frac{\Delta x_k^\alpha}{\Delta t}+b^\alpha(x_{k-1})\right)\right.\right.$$
$$\left.\left.\times\left(\frac{\Delta x_k^\beta}{\Delta t}+b^\beta(x_{k-1})\right)+c(x_{k-1})\right]\right\}f(x_N;0) \tag{1.6}$$

where $\Delta t=t/N$, $\Delta x_k^\alpha=x_{k-1}^\alpha-x_k^\alpha$.

For a special case $\mathscr{L}(x,D)=\Delta+V(x)$ with a large class of potentials $V(\ )$ the rigorous meaning to (1.3) and (4) may be given using the Trotter product formula. Indeed, in this case (1.5) and (1.6) are manifest representations of the Trotter formula

$$\exp[t(\Delta+V)]f=\lim_{N\to\infty}\{\exp[(t/N)\Delta]\exp[(t/N)V]\}^N f \tag{1.7}$$

and the limit $N\to\infty$ is a strong limit on Banach spaces $L^p(\mathbb{R}^\nu)$.

The application of the formal expressions (1.5), (1.6) are presented in a book by Langouche *et al* (1982). We should also mention the approach of Truman (1976, 1977) and Elworthy and Truman (1984) who applied the discretisation method for operators $\mathscr{L}(x,D)=z(\Delta+V(x))$ where $z=1$ or $\pm\mathrm{i}$ and used the different meaning of limit $N\to\infty$. Some efforts to prove the convergence of (1.5) and (1.6) for a very general class of parabolic equations were presented by Alimov (1972). However, the published proofs are incomplete.

2. The convergence theorem

We consiaer the class of operators $\mathscr{L}(x,D)$ which satisfy the following conditions.

(i) $\mathscr{L}(x,D)$ given by (1.2) and (1.3) is fulfilled. Moreover the real functions $a^{\alpha\beta}(x)$ and $b^\alpha(x)$ are continuously differentiable up to the third order and $c(x)$ is continuous.

(ii) The functions $a^{\alpha\beta}(x)$, $\partial_\gamma a^{\alpha\beta}(x)$, $\partial_\gamma\partial_\sigma a^{\alpha\beta}(x)$, $b^\alpha(x)$, $\partial_\beta b^\alpha(x)$, $c(x)$ are bounded on $\mathbb{R}^\nu$ by a number $Q<\infty$.

(iii) Let $\mathscr{L}(x,D)$ be treated as an operator defined on the domain $C_0^\infty(\mathbb{R}^\nu)$ which is dense in $\mathscr{F}(\mathbb{R}^\nu)$ where $\mathscr{F}(\mathbb{R}^\nu)$ denotes one of the following Banach spaces: $L^p(\mathbb{R}^\nu)$, $1\leqslant p<\infty$, $C_\infty(\mathbb{R}^\nu)=\{f;f\in C(\mathbb{R}^\nu)\lim_{|x|\to\infty}f(x)=0\}$. The closure L of $\mathscr{L}(x,D)$ generates a strongly continuous one-parameter semigroup of contractions on the Banach space $\mathscr{F}(\mathbb{R}^\nu)$ denoted by $\{\exp(tL);t\geqslant 0\}$.

The following remarks may be made.

(1) The only difficult condition to check is condition (iii). However, we show in § 4 that there exists a large class of operators $\mathscr{L}(x,D)$ satisfying (iii) on different spaces $\mathscr{F}(\mathbb{R}^\nu)$.

(2) The contraction property may be always replaced by the exponential bound $\|\exp(tL)\|\leqslant\exp(\lambda t)$, $t\geqslant 0$.

We now formulate the main result.

Theorem 2.1. Suppose that $\mathscr{L}(x,D)$ satisfies the condiions (i), (ii) and (iii). Then for an arbitrary element $g(\cdot)\in\mathscr{F}(\mathbb{R}^\nu)$ the function

$$f(\cdot,t)=\exp(tL)g(\cdot),\qquad t\geqslant 0 \tag{2.1}$$

is given by (1.5) or (1.6) where the limit $N\to\infty$ is taken in the norm on $\mathscr{F}(\mathbb{R}^\nu)$ and $f(x;0)=g(x)$.

In order to prove the above theorem we need the following lemmas. First we formulate a certain generalisation of the Trotter product formula proved by Chernoff (1968) (see books by Davies 1980, and Bratteli and Robinson 1979).

Lemma 2.2. Let X be a Banach space. The function

$$F\colon (0,\delta)\to \mathscr{B}(X), \qquad \delta>0$$

into bounded linear operators on X satisfies the following conditions:
(a) $\|F(t)\|\leqslant \exp(\alpha t)$, $\quad t\in(0,\delta) \quad \alpha\in\mathbb{R}$,
(b) $\lim_{t\to 0} t^{-1}(F(t)f-f)=Lf$
where L is a generator of a strongly continuous one-parameter semigroup of contractions on X denoted by $\{\exp(tL);\, t\geqslant 0\}$ and f is an arbitrary element from the core $\mathscr{D}$ of L.

Then

$$\exp(tL)g=\lim_{N\to\infty}[F(t/N)]^N g \tag{2.2}$$

for all $g\in X$.

We define now a family of integral kernels

$$0\leqslant t\to G_t(x\,|\,y) \qquad x,y\in\mathbb{R}^\nu$$

$$G_t(x\,|\,y)=\int_{\mathbb{R}^\nu}\frac{\mathrm{d}p}{(2\pi)^\nu}\exp[\mathrm{i}p_\alpha(x^\alpha-y^\alpha)]\exp[-t(a^{\alpha\beta}(x)p_\alpha p_\beta+\mathrm{i}b^\alpha(x)p_\alpha)] \tag{2.3}$$

$$=(4\pi t)^{-\nu/2}|a(x)|^{-1/2}$$
$$\times\exp\{-\tfrac{1}{4}t^{-1}(a_{\alpha\beta}(x)(x^\alpha-y^\alpha+tb^\alpha(x))(x^\beta-y^\beta+tb^\beta(x))\}. \tag{2.4}$$

Lemma 2.3. There exists $\delta>0$ such that for $t\in(0,\delta)$ the integral kernel (2.3) and (2.4) defines a bounded operator G_t on $\mathscr{F}(\mathbb{R}^\nu)$ satisfying condition (a) of lemma 2.2 with certain $\alpha>0$.

Proof. Let $g\in\mathscr{F}(\mathbb{R}^\nu)$. We use the following estimation (Kato 1966):

$$\|G_t g\|\leqslant \max(M',M'')\|g\| \tag{2.5}$$

where using $G_t(x\,|\,y)\geqslant 0$ we have

$$M'=\sup_{x\in\mathbb{R}^\nu}\int_{\mathbb{R}^\nu}G_t(x\,|\,y)\,\mathrm{d}y \tag{2.6}$$

$$M''=\sup_{y\in\mathbb{R}^\nu}\int_{\mathbb{R}^\nu}G_t(x\,|\,y)\,\mathrm{d}x. \tag{2.7}$$

By direct calculation we obtain

$$M'=1.$$

Now for a fixed $y \in \mathbb{R}^\nu$ and $t \geq 0$ let

$$I(y, t) = \int_{\mathbf{R}^\nu} G_t(x|y)\,dx = \int_{|x-y|\leq r} G_t(x|y)\,dx + \int_{|x-y|>r} G_t(x|y)\,dx \equiv I_r(y, t) + I'_r(y, t). \tag{2.8}$$

Here $|x| = (\Sigma_\alpha x^\alpha x^\alpha)^{1/2}$.

For a suitable small $r>0$ and $\delta'>0$ the conditions (i) and (ii) allow a change of variables to be carried out in the integral $I_r(y, t)$, $t\in[0, \delta')$:

$$x_\beta \to z_\beta = a^{1/2}_{\beta\alpha}(x)(x^\alpha - y^\alpha + tb^\alpha(x)) \tag{2.9}$$

such that

$$0 \leq I_r(y, t) \leq \frac{1}{(4\pi t)^{\nu/2}} \int_{|z|\leq 2r} dz\,\Phi(z)\exp(-|z|^2/4t) \tag{2.10}$$

where $\Phi(z)$ is a Jacobian of the inverse transformation to (2.9).

Using the Taylor expansion of $\Phi(z)$ at $z=0$ up to the third order and properties of Gaussian integrals we may finally estimate the t dependence of $I_r(y; t)$ for $t\in[0, \delta')$ by

$$I_r(y, t) \leq (1+\kappa_1 t + \kappa_2 t^{3/2}). \tag{2.11}$$

Here the constants κ_1, κ_2 are independent of y and t because of condition (ii).

$I'_r(y, t)$ may be estimated as follows:

$$I'_r(y, t) \leq (4\pi t)^{\nu/2} \sup_{x\in\mathbf{R}^\nu}(|a(x)|^{-1/2}) \int_{|x-y|\geq r} dx\,\exp\left(-\frac{1}{4At}|x-y+tb(x)|^2\right).$$

Due to the well known fact that for all $\varepsilon>0$

$$\lim_{t\to 0} t^\mu \int_{|z|\geq\varepsilon} dz\,\exp(-|z|^2/t) = 0 \tag{2.12}$$

for all $\mu\in\mathbb{R}$, we may estimate for $t\in(0, \delta'')$, $\delta''>0$

$$I'_r(y, t) \leq \kappa_3 t. \tag{2.13}$$

Hence using (2.11) and (2.13) we prove the lemma choosing suitable $\alpha>0$ and $\delta = \min\{\delta', \delta''\}$.

We define now a short-time propagator for $\mathscr{L}(x, D)$ by the following formula

$$F_t(x|y) = \exp(tc(x))G_t(x|y). \tag{2.14}$$

Obviously $F_t(x|y)$ also satisfies condition (a) of lemma 2.2 with $\alpha' = \alpha + Q$.

Lemma 2.4. Let $g\in C_0^\infty(\mathbb{R}^\nu)$ and F_t be an operator on $\mathscr{F}(\mathbb{R}^\nu)$ defined by the integral kernel (2.14) and $t>0$. Hence

$$\lim_{t\to 0} t^{-1}(F_t g - g)(x) = \mathscr{L}(x, D)g(x) \tag{2.15}$$

in the sense of norm on $\mathscr{F}(\mathbb{R}^\nu)$.

Proof. The proof is based on the method of Nelson (1964). Let for $\varepsilon > 0$ and $g \in C_0^\infty(\mathbb{R}^\nu)$

$$N_\varepsilon = \left\{ x \in \mathbb{R}^\nu ; \underset{y \in \operatorname{supp} g}{\exists} |x - y| < \varepsilon \right\}.$$

For $x \in N_\varepsilon$ and $t > 0$ we define a function

$$\mathcal{K}_t(x) = t^{-1}\left(\int_{\mathbf{R}^\nu} \mathrm{d}y\, F_t(x \mid y) g(y) - g(x) - t\mathcal{L}(x, D) g(x) \right). \tag{2.16}$$

For a fixed x we transform y

$$y^\alpha \to z_\alpha = a_{\alpha\beta}^{1/2}(x)(y^\beta - x^\beta - tb^\beta(x))$$

and obtain

$$\mathcal{K}_t(x) = t^{-1}\left((4\pi t)^{-\nu/2} \exp(tc(x)) \int_{\mathbf{R}^\nu} \mathrm{d}z\, g(\xi(z)) \exp(-\tfrac{1}{4}t^{-1}|z|^2) - g(x) - t\mathcal{L}(x, D) g(x) \right) \tag{2.17}$$

where $\xi(z) = x^\alpha + tb^\alpha(x) + a_{1/2}^{\alpha\beta}(x) z_\beta$.

Using the expansion of $g(\xi)$ around $x + tb$ up to the third order and properties of Gaussians we see that for all $x \in N_\varepsilon$

$$\lim_{t \to 0} \mathcal{K}_t(x) = 0. \tag{2.18}$$

Because N_ε is a compact set then $\mathcal{K}_t(\ )$ tends to 0 in the $L^p(N_\varepsilon)$ or $C(N_\varepsilon)$ sense also.

Let now $x \in \mathbb{R}^\nu - N_\varepsilon$ then

$$t^{-1}((F_t g)(x) - g(x) - t\mathcal{L}(x, D) g(x)) = t^{-1}(F_t g)(x)$$

and the following estimation holds

$$|t^{-1}(F_t g)(x)| \leq \int_{\mathbf{R}^\nu} |g(y)|\, \mathrm{d}y \sup_y (|a(y)|^{-1/2})(4\pi)^{-\nu/2} t^{-(\nu/2+1)} \exp(tQ)$$
$$\times \exp\left(-\frac{1}{4At} |x - \xi + tb(x)|^2 \right)$$

where $\xi \in \operatorname{supp} g$ according to the generalised mean-value theorem of integral calculus. Hence $|x - \xi| > \varepsilon$.

For suitable small $0 \leq t \leq \delta$ $|x - \xi + tb(x)| > \varepsilon/2$ and then by monotonic convergence theorem and (2.12)

$$\lim_{t \to 0} t^{-1} F_t g = 0 \tag{2.19}$$

in the sense of the strong limit on $L^p(\mathbb{R}^\nu - N_\varepsilon)$ $1 \leq p < \infty$ or $C_\infty(\mathbb{R}^\nu - N_\varepsilon)$. Combining (2.18) and (2.19) we obtain (2.15).

Using now the statements of lemmas 2.3 and 2.4 we conclude that the short-time propagator F_t satisfies the assumptions (a), (b) of lemma 2.2. Therefore the formula (2.2) is valid. Obviously the path integrals (1.5) and (1.6) are manifest expressions of (2.2) and hence the theorem 2.1 is proved.

3. The ordering problem

The representation (1.2) of the differential operator $\mathscr{L}(x, D)$ is not unique. For example we may write it in the following equivalent form

$$\mathscr{L}(x, D) = \partial_\alpha \partial_\beta A^{\alpha\beta}(x) + \partial_\alpha B^\alpha(x) + C(x) \tag{3.1}$$

where

$$\begin{aligned} A^{\alpha\beta}(x) &\equiv a^{\alpha\beta}(x) \\ B^\alpha(x) &= b^\alpha(x) - 2\partial_\beta a^{\alpha\beta}(x) \\ C(x) &= c(x) - \partial_\alpha(b^\alpha(x) - \partial_\beta a^{\alpha\beta}(x)). \end{aligned} \tag{3.2}$$

According to the usual prescription we now define the short-time propagator as follows

$$\begin{aligned} \bar{F}_t(x|y) = {} & (4\pi t)^{\nu/2}|A(y)|^{-1/2} \\ & \times \exp[-\tfrac{1}{4}t^{-1}A_{\alpha\beta}(y)(x^\alpha - y^\alpha + tB^\alpha(y))(x^\beta - y^\beta + tB^\beta(y))] \exp(tC(y)) \end{aligned} \tag{3.3}$$

and the path integrals (1.5) and (1.6) are appropriately modified.

The question arises whether $\bar{F}_t$ fulfils the conditions (a) and (b) of lemma 2.2 and therefore the discretisation limit exists. Obviously the estimation (a) may be proved as before, but the proof of (2.5) is now more difficult. The reason is that in the integral over z in the expression (2.17) the Jacobian $\Phi(z)$ appears. However, we may prove (2.5) for any function $g_r \in C_0^\infty(\mathbb{R}^\nu)$ with a support in a ball with a small enough radius $r > 0$, using the Taylor expansion of $\Phi(z)$ up to the third order. Then due to the differentiable partition of unity we may extend the proof for all $g \in C_0^\infty(R^\nu)$.

Summarising if the conditions (i), (ii) and (iii) are satisfied then the discretisation procedures lead to the convergent expressions of type (1.5) and (1.6) for arbitrary 'ordering of operators x^α and D' as expected from formal perturbation calculations (see Langouche *et al* 1982).

4. Examples

We present two examples of operators $\mathscr{L}(x, D)$ which satisfy conditions (i), (ii) and (iii).

(1) Let $\mathscr{F}(R^\nu)$ and define an operator on $C^\infty(\mathbb{R}^\nu)$

$$\mathscr{L}(x, D) = \Delta + \mathscr{L}'(x, D)$$

where

$$\begin{aligned} &\mathscr{L}'(x, D) = a'^{\alpha\beta}(x)\partial_\alpha\partial_\beta + b^\alpha(x)\partial_\alpha + c(x), \\ &a^{\alpha\beta}(x) = \delta^\alpha_\beta + a'^{\alpha\beta}(x),\ b^\alpha(x),\ c(x) \end{aligned}$$

fulfil the conditions (i) and (ii). Moreover we assume that $\mathscr{L}'(x, D)$ is symmetric on the domain $C_0^\infty(R^\nu)$ and

$$\|a'\|^2 = \sup_{x \in \mathbf{R}^\nu} \sum_{\alpha\beta} |a'^{\alpha\beta}(x)|^2 < 1.$$

It follows that for $f\in C_0^\infty(\mathbb{R}^\nu)$, $\mathscr{L}''=a'^{\alpha\beta}(x)\partial_\alpha\partial_\beta$

$$\|\mathscr{L}''f\|^2=\int \mathrm{d}x\, a'^{\alpha\beta}\partial_\alpha\partial_\beta\bar{f}a'^{\gamma\lambda}\partial_\gamma\partial_\lambda f\leqslant \|a'\|^2\sum_{\alpha\beta}\int \mathrm{d}x|\partial_\alpha\partial_\beta f|^2$$

$$=\|a'\|^2\sum_{\alpha\beta}\int \mathrm{d}p\, p_\alpha^2 p_\beta^2|\hat{f}(p)|^2=\|a'\|^2\|\Delta f\|^2.$$

Then $\mathscr{L}'(x, D)$ is relatively bounded with respect to the closure of Δ in $L^2(\mathbb{R}^\nu)$ with relative bound one. By standard theorems (Kato 1966, Davies 1980) a closure of $\mathscr{L}(x, D)$ is a self-adjoint semi-bounded operator and hence generates an exponentially bounded strongly continuous semigroup on $L^2(\mathbb{R}^\nu)$.

(2) Let $\mathscr{F}(\mathbb{R}^\nu)=C_\infty(\mathbb{R}^\nu)$ and let

$$\tilde{C}^\infty(\mathbb{R}^\nu)=\{f; f\in C^\infty(\mathbb{R}^\nu), |D^\alpha f(x)| \underset{|x|\to\infty}{\to} 0\}$$

where D^α is a derivative of an arbitrary order. We consider an operator on $C_0^\infty(\mathbb{R}^\nu)$

$$\mathscr{L}(x, D)=a^{\alpha\beta}(x)\partial_\alpha\partial_\beta+b^\alpha(x)\partial_\alpha$$

where $a^{\alpha\beta}(x)$ fulfils (1.3) and moreover

$$a^{\alpha\beta}(x)=a_0^{\alpha\beta}+a_1^{\alpha\beta}(x) \qquad [a_0^{\alpha\beta}]>0$$

$$b^\alpha(x)=b_0^\alpha+b_1^\alpha(x)$$

with $a_1^{\alpha\beta}(\cdot)$, $b_1^\alpha(\cdot)\in\tilde{C}^\infty(\mathbb{R}^\nu)$. Repeating now with slight modifications the arguments of Yosida (1974) we may prove that the closure of $\mathscr{L}(x, D)$ generates a contraction semigroup on $C_\infty(\mathbb{R}^\nu)$.

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