A Feynman-Kac Formula for Unbounded Semigroups

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Abstract. We prove a Feynman-Kac formula for Schrödinger operators with potentials $V(x)$ that obey (for all $\varepsilon > 0$)

$$V(x) \geq -\varepsilon |x|^2 - C_\varepsilon.$$

Even though e^{-tH} is an unbounded operator, any $\varphi, \psi \in L^2$ with compact support lie in $D(e^{-tH})$ and $\langle \varphi, e^{-tH}\psi \rangle$ is given by a Feynman-Kac formula.

1. Introduction

One of the most useful tools in the study of Schrödinger operators, both conceptually and analytically, is the Feynman-Kac formula. All the standard proofs, (see, e.g., [**7**]) assume the Schrödinger operator H is bounded below, so the Schrödinger semigroup e^{-tH} is bounded. This means, for example, that Stark Hamiltonians are not included.

But the restriction to semibounded H is psychological, not real. We deal with unbounded H's all the time, so why not unbounded e^{-tH}? Once one considers the possibility, the technical problems are mild, and it is the purpose of this note to show that.

The form of the Feynman-Kac formula we will discuss is in terms of the Brownian bridge (Theorem 6.6 of [**7**]). Once one has this, it is easy to extend to the various alternate forms of the Feynman-Kac formula.

The ν-dimensional Brownian bridge consists of ν jointly Gaussian processes, $\{\alpha_i(t)\}_{i=1;0\leq t\leq 1}^{\nu}$ with covariance

$$E(\alpha_i(t)\alpha_j(s)) = \delta_{ij}\min(t,s)[1-\max(t,s)]$$
$$E(\alpha_i(t)) = 0.$$

If b is Brownian motion, then $\boldsymbol{\alpha}(s) = \boldsymbol{b}(s) - s\boldsymbol{b}(1)$ is an explicit realization of the Brownian bridge.

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For any real function V on $\mathbb{R}^\nu$ and $t > 0$, define (the expectation may be infinite):

$$Q(x,y;V,t) = E\left(\exp\left(-\int_0^t V\left(\left(1-\frac{s}{t}\right)x + \frac{s}{t}\,y + \sqrt{t}\,\alpha\left(\frac{s}{t}\right)\right)\,ds\right)\right). \tag{1.1}$$

Throughout this paper, let

$$H_0 = -\tfrac{1}{2}\Delta$$

on $L^2(\mathbb{R}^\nu)$, so

$$e^{-tH_0}(x,y) = (2\pi t)^{-\nu/2}\exp\left(-\frac{|x-y|^2}{2t}\right). \tag{1.2}$$

The Feynman-Kac formula I'll start with — one of many in [**7**] — is

Theorem 1.1. *Suppose V is a continuous function on $\mathbb{R}^\nu$ which is bounded from below. Let $H = H_0 + V$. Then for any $t > 0$ and $\varphi, \psi \in L^2(\mathbb{R}^\nu)$:*

$$\langle \varphi, e^{-tH}\psi\rangle = \int \overline{\varphi(x)}\,\psi(y)\,e^{-tH_0}(x,y)Q(x,y;V,t). \tag{1.3}$$

In this paper, we will consider potentials $V(x)$ for which for any $\varepsilon > 0$, there is C_ε so that

$$V(x) \geq -\varepsilon|x|^2 - C_\varepsilon. \tag{1.4}$$

It is known (see [**5**], Theorem X.38) that for such V, $H = H_0 + V$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^\nu)$, so we can use the functional calculus to define e^{-tH} which might be unbounded. Our main goal here is to prove:

Theorem 1.2. *Suppose V is a continuous function which obeys* (1.4). *Then for all $x, y \in \mathbb{R}^\nu$, $t > 0$,* (1.1) *is finite. Let $\varphi, \psi \in L^2(\mathbb{R}^\nu)$ have compact support. Then for all $t > 0$, $\varphi, \psi \in D(e^{-tH})$ and* (1.3) *holds.*

Remarks. 1. It isn't necessary to suppose that φ, ψ have compact support. Our proof shows that it suffices that $e^{\varepsilon x^2}\psi, e^{\varepsilon x^2}\varphi \in L^2$ for some $\varepsilon > 0$. In particular, φ, ψ can be Gaussian.

2. Using standard techniques [**1**],[**3**],[**7**], one can extend the proof to handle $V = V_1 + V_2$ where V_1 obeys (1.4) but is otherwise in L^1_{loc} and V_2 is in the Kato class, K_ν.

3. If one only has $V(x) \geq -C_1 - C_2x^2$ for a fixed C_2, our proof shows that the Feynman-Kac formula holds for t sufficiently small. It may not hold if t is large since it will happen if $V(x) = -x^2$ that $E(\exp(-\int_0^t V(\alpha(s))\,ds))$ will diverge if t is large.

As for applications of Theorem 1.2, one should be able to obtain various regularity theorems as in [**6**]. Moreover, for $H = -\Delta + \boldsymbol{F}\cdot\boldsymbol{x}$, one can compute $e^{-tH}(x,y)$ explicitly and so obtain another proof of the explicit formula of Avron and Herbst [**2**].

Dedication. Sergio Albeverio has been a master of using and extending the notion of path integrals. It is a pleasure to dedicate this to him on the occasion of his 60th birthday.

2. A Priori Bounds on Path Integrals

Our goal in this section is to prove

THEOREM 2.1. *Let V obey* (1.4) *and let Q be given by* (1.1). *Then, for each $t > 0$ and $\delta > 0$, we have that*

$$Q(x, y; V, t) \leq D \exp(\delta x^2 + \delta y^2),$$

where D depends only on t, δ and the constants $\{C_\varepsilon\}$.

LEMMA 2.2. *Let X be a Gaussian random variable. Suppose $\varepsilon \operatorname{Exp}(X^2) < \frac{1}{2}$. Then $E(\exp(\varepsilon X^2)) < \infty$* (and is bounded by a function of $\varepsilon \operatorname{Exp}(X^2)$ alone).

PROOF. A direct calculation. Alternately, we can normalize X so $\operatorname{Exp}(X^2) = 1$. Then $E(\exp(\varepsilon X^2)) = (2\pi)^{-1/2} \int \exp((\varepsilon - \frac{1}{2})x^2)\, dx < \infty$. □

PROOF OF THEOREM 2.1. Note that if $0 < \theta < 1$, and $x, y, \alpha \in \mathbb{R}^\nu$, then

$$\begin{aligned} |\theta x + (1-\theta)y + \alpha|^2 &\leq 2|\theta x + (1-\theta)y|^2 + 2|\alpha|^2 \\ &\leq 2(x^2 + y^2 + |\alpha|^2). \end{aligned}$$

Thus, by (1.4),

$$Q(x, y; V, t) \leq E\left(\exp\left(C_\varepsilon t + 2\varepsilon t(x^2 + y^2) + 2\varepsilon \int_0^1 t^2 \alpha(s)^2\, ds\right)\right). \tag{2.1}$$

By Jensen's inequality,

$$E\left(\exp\left(2\int_0^1 \varepsilon t^2 \alpha(s)^2\, ds\right)\right) \leq \int_0^1 E(\exp(2\varepsilon t^2 \alpha(s)^2)\, ds). \tag{2.2}$$

Since $E(\alpha(s)^2)$ is maximized at $s = \frac{1}{2}$ when it is $\frac{1}{4}$, we see that

$$\text{RHS of (2.2)} \leq E(\exp(2\varepsilon t^2 \alpha(\tfrac{1}{2})^2))$$

is finite if $\varepsilon t^2 < 1$, so we can pick $\varepsilon = \delta_0/t^2$ with $\delta_0 < 1$ and find (using the explicit value of $E(\exp(X^2))$ in that case

$$Q(x, y; V, t) \leq \sqrt{2}\, (1 - \delta_0)^{-1/2} \exp(C_\varepsilon t + 2\delta_0(x^2 + y^2)/t),$$

which proves Theorem 2.1. □

3. A Convergence Lemma

In this section, we will prove:

THEOREM 3.1. *Let A_n, A be self-adjoint operators on a Hilbert space $\mathcal{H}$ so that $A_n \to A$ in strong resolvent sense. Let f be a continuous function on $\mathbb{R}$ and $\psi \in \mathcal{H}$ with $\psi \in D(f(A_n))$ for all n. Then*

(i) *If $\sup_n \|f(A_n)\psi\| < \infty$, then $\psi \in D(f(A))$.*
(ii) *If $\sup_n \|f(A_n)^2\psi\| < \infty$, then $f(A_n)\psi \to f(A)\psi$.*

REMARK. Let $\mathcal{H} = L^2(0,1)$, $\psi(x) \equiv 1$, $A_n =$ multiplication by $n^{1/2}$ times the characteristic function $[0, 1/n]$, and $A \equiv 0$. Then $A_n \to A$ in strong resolvent sense and $\sup_n \|A_n\psi\| < \infty$, but $A_n\psi$ does not converge to $A\psi$ so one needs more than $\sup_n \|f(A_n)\psi\| < \infty$ to conclude that $f(A_n)\psi \to f(A)\psi$. The square is overkill. We need only $\sup_n \|F(f(A_n))\psi\| < \infty$ for some function $F : \mathbb{R} \to \mathbb{R}$ with $\lim_{|x|\to\infty} |F(x)|/x = \infty$.

Proof. Suppose that $\sup_n \|f(A_n)\psi\| < \infty$. Let

$$f_m(x) = \begin{cases} m & \text{if } f(x) \geq m \\ f(x) & \text{if } |f(x)| \leq m \\ -m & \text{if } f(x) \leq -m. \end{cases}$$

Then ([**4**], Theorem VIII.20) for each fixed m, $f_m(A_n) \to f_m(A)$ strongly. It follows that

$$\begin{aligned} \|f_m(A)\psi\| &= \lim_n \|f_m(A_n)\psi\| \\ &\leq \sup_n \|f_m(A_n)\psi\| \leq \sup_n \|f(A_n)\psi\|. \end{aligned}$$

Thus, $\sup_m \|f_m(A)\psi\| < \infty$, which implies that $\psi \in D(f(A))$.

Now suppose $\sup_n \|f(A_n)^2\psi\| < \infty$. Then

$$\|(f(A_n) - f_m(A_n))\psi\| \leq \frac{1}{m} \|f(A_n)^2\psi\|.$$

Thus $f_m(A_n)\psi \to f(A_n)\psi$ uniformly in n which, given that $f_m(A_n)\psi \to f_m(A)\psi$, implies that $f(A_n)\psi \to f(A)\psi$. □

4. Putting It Together

We are now ready to prove Theorem 1.2. Let V be continuous and obey (1.4). Let $V_n(x) = \max(V(x), -n)$. Then V_n is bounded from below, so Theorem 1.1 applies, and so (1.3) holds. Let $\varphi \in L^2$ with compact support. By Theorem 2.1, we have

$$\sup_n \| \exp(-tH_n)\varphi\| < \infty$$

for each t positive.

By the essential self-adjointness of H on $C_0^\infty(\mathbb{R}^\nu)$ and $(V_n - V)\eta \to 0$ for any $\eta \in C_0^\infty$, we see that H_n converges to H in strong resolvent sense. Hence setting $A_n = H_n$, $A = H$, $f(x) = e^{-tx}$, and $\psi = \varphi$, we can use Theorem 3.1 to see that $\varphi \in D(\exp(-tH))$ and $\|[\exp(-tH_n) - \exp(-tH)]\varphi\| \to 0$. Thus as $n \to \infty$, the left-hand side of the Feynman-Kac formula converges. By the a priori bound in Theorem 2.1 and the dominated convergence theorem, the right-hand side converges. So Theorem 1.2 is proven.

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