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, $\{\alpha_i(t)\}_{i=1;0 < t < 1}^{\nu}$ 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 $\alpha(s) = b(s) - sb(1)$ is an explicit realization of the Brownian bridge.

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

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

Throughout this paper, let

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

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

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

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

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

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

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

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 $V(x) \geq -C_1 C_2 x^2$ 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 $H = -\Delta + \mathbf{F} \cdot \mathbf{x}$, 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

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

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 $Exp(X^2) =$ 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

$$|\theta x + (1 - \theta)y + \alpha|^2 \le 2|\theta x + (1 - \theta)y|^2 + 2|\alpha|^2$$

 $\le 2(x^2 + y^2 + |\alpha|^2).$

Thus, by (1.4),

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

By Jensen's inequality

(2.2)
$$E\left(\exp\left(2\int_0^1 \varepsilon t^2 \alpha(s)^2 ds\right)\right) \le \int_0^1 E(\exp(2\varepsilon t^2 \alpha(s)^2) ds).$$

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

RHS of
$$(2.2) \le E(\exp(2\varepsilon t^2 \alpha(\frac{1}{2})^2))$$

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

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

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 $A_n o A$ 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 $\lim_{|x|\to\infty}|F(x)|/x=\infty.$

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

$$f_m(x) = egin{cases} m & ext{if } f(x) \ge m \\ f(x) & ext{if } |f(x)| \le m \\ -m & ext{if } f(x) \le -m. \end{cases}$$

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

$$||f_m(A)\psi|| = \lim_n ||f_m(A_n)\psi||$$

$$\leq \sup_n ||f_m(A_n)\psi|| \leq \sup_n ||f(A_n)\psi||.$$

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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