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FEYNMAN-KAC FUNCTIONAL AND THE SCHRÖDINGER EQUATION*

by

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The Feynman-Kac formula and its connections with classical analysis were initiated in [3]. Recently there has been a revival of interest in the associated probabilistic methods, particularly in applications to quantum physics as treated in [7]. Oddly enough the inherent potential theory has not been developed from this point of view. A search into the literature after this work was under way uncovered only one paper by Khas'minskii [4] which dealt with some relevant problems. But there the function q is assumed to be nonnegative and the methods used do not apparently apply to the general case; see the remarks after Corollary 2 to Theorem 2.2 below.** The case of q taking both signs is appealing as it involves oscillatory rather than absolute convergence problems. Intuitively, the Brownian motion must make intricate cancellations along its paths to yield up any determinable averages. In this respect Theorem 1.2 is a decisive result whose significance has yet to be explored. Next we solve the boundary value problem for the Schrödinger equation $(\Delta+2q)\varphi = 0$. In fact, for a

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**The case $q \le 0$ is "trivial" in the context of this paper. For this case in a more general setting see [9, Chapter 13].

positive continuous boundary function f, a solution is obtained in the explicit formula given in (2) of §1 below, provided that this quantity is finite (at least at one point x in D). Thus the Feynman-Kac formula supplies the natural Green's operator for the problem. For a domain with finite measure, the result is the best possible as it includes the already classical solution of the Dirichlet problem by probability methods. Other results are valid for an arbitrary domain and it seems that some of them are proved here under less stringent conditions than usually given in non-probabilistic treatments. For instance, *no condition on the smoothness of the boundary is assumed beyond that* of regularity in the sense of the Dirichlet problem, and the basic results hold without this regularity. Of course, the Schrödinger equation is a case of elliptic partial differential equations on which there exists a huge literature, but we make no recourse to the latter theory. Comparisons between the methods should prove worthwhile and will be discussed in a separate publication.

It is well known that the Schrödinger equation differs essentially from the Laplace equation in that a condition on the size of the domain is necessary to guarantee the uniqueness of solution. In our context it is evident at the outset that the key to this is the quantity $u_D(x) = E^x\{ \exp(\int_0^{\tau_D} q(x(t))\, dt) \}$, the finiteness of which lies at the base of the probabilistic considerations. As natural as it is from our point of view, this quantity does not lend itself easily to non-probabilistic analysis. The identification in the simplest case (see the remark after Lemma D) as a particular solution of the equation is one of those amusing twists not uncommon in other theories when dealing with an object which has really a simple probabilistic existence.

The one-dimensional case of this investigation has appeared in [1] though the orientation is somewhat different there. A summary of the present results has been announced in [2].

1. Harnack inequality; global bound; boundary limit

Let $\{ X(t), t \geq 0 \}$ be the Brownian motion process in R^d, $d \geq 1$; with all paths continuous. The transition semigroup is $\{ P_t, t \geq 0 \}$ and F_t is the σ-field generated by $\{ X_s, 0 \leq s \leq t \}$ and augmented in the usual way. The qualifying phrase "almost surely" (a.s.) will be omitted when readily understood. A "set" is always a Borel set and a "function" is always a Borel measurable function. The class of bounded functions will be denoted by $b\mathcal{B}$; if its domain is A this is indicated by $b\mathcal{B}(A)$. Similarly for other classes of functions to be used later. The sup-norm of $f \in b\mathcal{B}$ is denoted by $\|f\|$; restricted to A it is denoted by $\|f\|_A$. P^x and E^x denote the probability and expectation for the process starting at x.

For any set B we put

$$\tau(B) = \tau_B = \inf\{ t > 0 \mid X(t) \notin B \} \quad ;$$

namely the first exit time from B, with the usual convention that $\inf \phi = \infty$. Let $q \in b\mathcal{B}$; as an abbreviation we put

$$(1) \qquad e_q(t) = \exp\{ \int_0^t q(X(s))\, ds \} \quad ;$$

when q is fixed it will be omitted from the notation. A domain in R^d is an open connected set; its boundary is $\partial D = \bar{D} \cap \overline{D^c}$, where $\bar{D}$ is the closure and D^c the complement of D. For $f \geq 0$ on ∂D we put for $x \in \bar{D}$:

$$(2) \qquad u(q,f;x) = E^x\{ e_q(\tau_D)\, f(X(\tau_D));\ \tau_D < \infty \}.$$

The following result is a case of Harnack's inequality, on which there is a considerable literature for elliptic partial differential equations.

Theorem 1.1. Let D be a domain and K a compact subset of D. There exists a constant $A > 0$ which depends only on D, K and Q, such that for any q with $\|q\| \le Q$ and $f \ge 0$ such that $u(q,f;\cdot) \not\equiv \infty$ in D, we have for any two points x_1 and x_2 in K:

$$A^{-1}\, u(q,f;x_2) \le u(q,f;x_1) \le A\, u(q,f;x_2) \quad . \tag{3}$$

Proof. We write $u(x)$ for $u(q,f;x)$. By hypothesis there exists $x_0 \in D$ such that $u(x_0) < \infty$. We may suppose $x_0 \in K$ by enlarging K. For any $r > 0$ define

$$T(r) = \inf\{\, t > 0 \mid \rho(X(t), X(0)) \ge r \,\}$$

where ρ denotes the Euclidean distance. It is well known (cf. Lemma A below) that there exists $\delta > 0$ (which depends only on Q and the dimension d) such that for all $x \in R^d$:

$$\frac{1}{2} \le E^x\{\exp(-QT(2\delta))\}; \qquad E^x\{\exp(QT(2\delta))\} \le 2. \tag{4}$$

In fact, the two expectations in (4) do not depend on x by the spatial homogeneity of the process. Now put

$$2r = \rho(K, \partial D) \wedge 2\delta. \tag{5}$$

Then for any $s < 2r$ we have, by the strong Markov property, since $T(s) < \tau_D$ under P^{x_0}:

$$(6) \qquad \infty > u(x_0) = E^{x_0}\{ e(T(s))\, u(X(T(s))) \}$$

$$\geq E^{x_0}\{ \exp(-QT(s))\, u(X(T(s)) \} .$$

The isotropic property of the Brownian motion implies that the random variables $T(s)$ and $X(T(s))$ are stochastically independent for each s. *Hence we obtain from* (6) *and the first inequality in* (4):

$$(7) \qquad u(x_0) \geq \frac{1}{2} E^{x_0}\{ u(X(T(s))) \} .$$

The expectation on the right side above is the area average of the values of u on the boundary of $B(x_0,s)$. Hence we obtain by integrating with respect to the radius:

$$(8) \qquad a_d \int_0^{2r} E^{x_0}\{ u(X(T(s))) \}\, s^{d-1}\, ds = \int_{B(x_0,2r)} u(y)\, dy,$$

where $a_d\, s^{d-1}$ is the area of $\partial B(x_0,s)$. It follows from (7) and (8) that

$$(9) \qquad u(x_0) \geq \frac{1}{2V(2r)} \int_{B(x_0,2r)} u(y)\, dy,$$

where $V(2r)$ is the volume of $B(x_0,2r)$. [The terms "area" and "volume" used above have their obvious meanings in dimension $d = 1$ or 2.]

Next, let $x \in B(x_0,r)$ so that $\rho(x,\partial D) \geq r$ by (5). We have for $0 < s < r$:

$$(10) \qquad u(x) = E^{x}\{ e(T(s))\, u(X(T(s))) \} \leq E^{x}\{ \exp(QT(s))\, u(X(T(s))) \}$$

$$= E^{x}\{ e(QT(s))\}\, E^{x}\{ u(X(T(s))) \} \leq 2E^{x}\{ u(X(T(s))) \}$$

by independence and the second inequality in (4). Integrating as before we obtain

$$u(x) \le \frac{2}{V(r)} \int_{B(x,r)} u(y)\, dy \quad . \tag{11}$$

Since $B(x,r) \subset B(x_0,2r)$ and $u \ge 0$, (9) and (10) together yield

$$u(x) \le 2^{d+2}\, u(x_0) \; . \tag{12}$$

In particular we have proved that $u(x) < \infty$ if $\rho(x,x_0) < r$ and consequently we may interchange the roles of x_0 and x in the above. Since the number r is fixed independently of x, and K is compact, a familiar "chain argument" establishes the theorem. Indeed if N is the number of overlapping balls of fixed radius r which are needed to lead in a chain from any point to any other point in K, then the constant A in (3) may be taken to be $2^{(d+2)N}$. □

Corollary. If K is fixed and D is enlarged, the inequalities in (3) remain valid with the same constant A.

This is clear from the proof, and will be needed for the application in Theorem 3.1.

The following lemma plays a key role below. Its essential feature is that only the (Lebesgue) measure $m(E_n)$ of E_n, and not its shape or smoothness, is involved.

Lemma A. Let $\{E_n\}$ be sets with $m(E_n)$ decreasing to zero. Then we have for each $t > 0$:

$$\lim_{n\to\infty} \sup_{x\in \bar{E}_n} P^x\{\ \tau(E_n) > t\ \} = 0\ . \tag{13}$$

For any constant Q we have

$$\lim_{n\to\infty} \sup_{x\in \bar{E}_n} E^x\{\ \exp(Q\tau(E_n))\ \} = 1\ . \tag{14}$$

Proof. We have for any E and $t > 0$:

$$\sup_{x\in \bar{E}} P^x\{\ \tau(E) > t\ \} \le \sup_{x\in \bar{E}} P^x\{\ X(t) \in E\ \} \le \frac{m(E)}{(2\pi t)^{d/2}} \tag{15}$$

because the probability density of $X(t)$ is bounded by $(2\pi t)^{-d/2}$. This implies (13). Next we obtain from (15) followed by a Markovian iterative argument:

$$\sup_{x\in \bar{E}} P^x\{\ \tau(E) > nt\ \} \le \left(\frac{m(E)}{(2\pi t)^{d/2}}\right)^n .$$

Therefore we have

$$E^x\{\ \exp(Q(\tau(E)))\ \} \le \sum_{n=0}^{\infty} e^{Q(n+1)t}\, P^x\{\ \tau(E) > nt\ \}$$

$$\le e^{Qt} \sum_{n=0}^{\infty} [\ e^{Qt}\, m(E)\ (2\pi t)^{-d/2}\ ]^n\ .$$

Given Q, chose t so small that Qt is near zero. For this t, if $m(E)$ is small enough the infinite series above has a sum near 1. This proves (14). □

It follows from Theorem 1.1 that if $u \not\equiv \infty$ in D then $u < \infty$ in D. When $m(D) < \infty$, this result has a sharpening which is not valid in the usual analytical setting of Harnack inequalities, in which only local boundedness can be claimed. The situation will be clarified in later sections when we relate the function u to a positive solution of the Schrödinger equation.

Theorem 1.2. Let D be a domain with $m(D) < \infty$, and let q and f be as in Theorem 1.1, but f be bounded as well as nonnegative. If $u(q,f;\cdot) \not\equiv \infty$ in D, then it is bounded in $\bar{D}$.

Proof. Let us remark that if $m(D) < \infty$, then $P^x\{ \tau_D < \infty \} = 1$ for all $x \in R^d$, so that we may omit "$\tau_D < \infty$" in the definition (2). Write u as before and let $\|q\| = Q$. Let K be a compact subset of D such that $m(E) < \delta$ where $E = D-K$, and where δ is so small that

$$\sup_{x\in E} E^x\{ \exp(Q\tau(E)) \} \le 1+\varepsilon . \tag{16}$$

This is possible by Lemma A. Note that E is open and $\tau_E \le \tau_D$. For $x \in \bar{E}$ let us put

$$(17)\qquad \begin{aligned} u_1(x) &= E^x\{ e(\tau_D)\ f(X(\tau_D));\ \tau_E < \tau_D \}, \\ u_2(x) &= E^x\{ e(\tau_D)\ f(X(\tau_D));\ \tau_E = \tau_D \}. \end{aligned}$$

We have by the strong Markov property:

$$(18)\qquad \begin{aligned} u_1(x) &= E^x\{ \tau_E < \tau_D;\ e(\tau_E)\ E^{X(\tau_E)}[e(\tau_D)\ f(X(\tau_D))] \} \\ &= E^x\{ \tau_E < \tau_D;\ e(\tau_E)\ u(X(\tau_E)) \}. \end{aligned}$$

On the set $\{ \tau_E < \tau_D \}$, we have $X(\tau_E) \in K$, and u is bounded on K by Theorem 1.1. Hence we have by (16) and (18):

(19) $$u_1(x) \le E^x\{\exp(Q\tau_E)\}\,\|u\|_K \le (1+\varepsilon)\,\|u\|_K\,.$$

On the other hand, we have for $x \in \bar{E}$:

(20) $$u_2(x) \le E^x\{e(\tau_E)\,f(X(\tau_E))\}$$
$$\le E^x\{e(\tau_E)\}\,\|f\| \le (1+\varepsilon)\,\|f\|\,.$$

Combining the last two inequalities we have

(21) $$u(x) \le (1+\varepsilon)(\,\|u\|_K + \|f\|\,).$$

Since $\bar{D}-\bar{E} \subset K$, (21) holds trivially for $x \in \bar{D}-\bar{E}$. Thus (21) holds for all $x \in \bar{D}$. □

It is clear how we can make more precise the dependence of ε in (21) on K, thereby giving an estimate of the global bound $\|u\|_{\bar{D}}$ in terms of a local bound $\|u\|_K$ and $\|f\|$. Theorem 1.2 is true without any condition on the smoothness of ∂D. In the probabilistic treatment of the Dirichlet problem a point z is said to be a regular boundary point iff $z \in \partial D$ and $P^z\{\tau_D = 0\} = 1$, namely iff z is regular for D^c. The equivalence of this definition of regularity with the classical definition based on the solvability of the boundary value problem is well known. The next result is an extension of the probabilistic solution to the Dirichlet problem (D,f) to the present setting when the Feynman-Kac functional e_q is attached to the Brownian motion process. It will be seen in §2 that this extension is tantamount to replacing the Laplacian operator Δ by the Schrödinger operator $\Delta+2q$. When $q \equiv 0$ the theorem below reduces to Dirichlet's first boundary value problem.

Theorem 1.3. Let D and q be as in Theorem 1.2, but $f \in b\mathcal{B}(\partial D)$. If z is a regular point of ∂D and f is continuous at z, then we have

$$\lim_{x \to z} u(x) = f(z). \tag{22}$$

Remark. Since u is defined in $\bar{D}$ it is natural that the variable x in (22) should vary in $\bar{D}$, and not just in D. This minor but nontrivial point is sometimes overlooked.

Proof. Without loss of generality we may suppose $f \geq 0$. Given $\varepsilon > 0$, there exists $\delta > 0$ such that

$$\sup_{x \in R^d} E^x\{ e^{2QT_r} \} \leq 1 + \varepsilon \qquad \text{for } r \leq \delta; \tag{23}$$

$$\sup_{y \in B(z,2\delta) \cap (\partial D)} |f(y)-f(z)| \leq \varepsilon. \tag{24}$$

Let $x \in B(z,\delta)$, and $0 < r < \delta$. Write τ for τ_D and put

$$u_1(x) = E^x\{ T_r < \tau;\ e(\tau)\ f(X(\tau)) \},$$

$$u_2(x) = E^x\{ \tau \leq T_r;\ e(\tau)\ f(X(\tau)) \}.$$

It is well known that for each $t > 0$, $P^x\{ \tau > t \}$ is upper semi-continuous in $x \in R^d$. Since $P^z\{ \tau > t \} = 0$, it follows easily that

$$\lim_{x \to z} P^x\{ \tau > T_r \} = 0 \tag{25}$$

where $x \in \bar{D}$. We have by the strong Markov property:

$$u_1(x) = E^x\{ T_r < \tau;\ e(T_r)u(X(T_r)) \}.$$

Hence by Theorem 1.2 followed by Schwarz's inequality:

$$u_1(x) \le E^x\{ T_r < \tau;\ e^{QT_r} \}\ \|u\|_D$$

$$\le P^x\{ T_r < \tau \}^{\frac{1}{2}}\ E^x(e^{2QT_r})^{\frac{1}{2}}\ \|u\|_D .$$

Therefore $\lim_{x\to z} u_1(x) = 0$ by (23) and (25). Next we have by (24), since $X(\tau) \in B(z,2\delta)$ on $\{ \tau \le T_r \}$ under P^x:

$$|u_2(x)-E^x\{ \tau \le T_r;\ e(\tau)f(z) \}| \le E^x\{ \tau \le T_r;\ e^{QT_r} \}\varepsilon \le (1+\varepsilon)\varepsilon ;$$

and by (23):

$$|1-E^x\{ \tau \le T_r;\ e(\tau) \}| \le P^x\{ T_r < \tau \} + E^x\{ \tau \le T_r;\ e(\tau)-1 \}$$

$$\le P^x\{ T_r < \tau \} + E^x\{ e^{QT_r} \} - 1$$

$$\le P^x\{ T_r < \tau \} + \varepsilon.$$

Since ε is arbitrary, it follows from the above inequalities and (25) that $\lim_{x\to z} u_2(x) = f(z)$. Thus (22) is true. □

The intuitive content of Theorems 1.2 and 1.3 is this: the motion of the Brownian path in a domain is such that large positive values cancel large negative values of $q(X(t))$ so neatly that no after-effect is felt as it approaches the boundary, provided that cancellation is possible in an average sense, measured exponentially. Moreover the latter possibility is irrespective of the starting point of the path.

2. Schrödinger equation

Let D be a domain in R^d. We introduce the notation

(1) $$Q_t f(x) = E^x\{ t < \tau_D ;\ f(X_t) \}$$

for $f \in b\mathcal{B}$. Then $\{ Q_t,\ t \geq 0 \}$ is the transition semigroup of the Brownian motion killed upon the exit from D. Let

(2) $$G_D f(x) = E^x\{ \int_0^{\tau_D} f(X_t)\, dt \}$$

where the right member is defined first for $f \geq 0$, then through $f = f^+ - f^-$ in the usual way, provided either $G_D f^+$ or $G_D f^-$ is finite. We shall be concerned only with the case where $G_D|f| < \infty$. Let $C^{(0)}(D)$ and $C^{(k)}(D)$, $k \geq 1$, denote respectively the classes of continuous and k times continuously differentiable functions on D. We write $f \in H(D)$ and say that f is Hölder continuous in D, iff for any compact subset C of D there exist two constants $\alpha > 0$ and M such that $|f(x)-f(y)| \leq M|x-y|^\alpha$ for x and y in C. For a proof of the following lemma see e.g. [6; Chapter 4, §§5-6].

Lemma B. If f is locally bounded in D and $G_D|f| < \infty$ then $G_D f \in C^{(1)}(D)$. If in addition $f \in H(D)$ then $G_D f \in C^{(2)}(D)$, and

(3) $$\Delta(G_D f) = -2f .$$

On the other hand if $f \in C^{(2)}(D)$ then

$$G_D(\Delta f) = -2f + h,$$

where h is harmonic in D.

Let $q \in b\mathcal{B}$ as in §1. The Feynman-Kac semigroup $\{ K_t, t \geq 0 \}$ is defined as follows:

$$K_t f(x) = E^x\{ e_q(t) f(X_t) \} \tag{4}$$

for $f \in b\mathcal{B}$. Actually Feynman considered a purely imaginary q and Kac a nonpositive q. For our q the semigroup need not be submarkovian. It is known that its infinitesimal generator is $\frac{\Delta}{2} + q$ (see [3]). When $q \equiv 0$, of course $\{K_t\}$ reduces to the Brownian semigroup $\{P_t\}$. In this case the function u in (2) of §1 is harmonic in D, namely it satisfies the Laplace equation $\Delta u = 0$ there. Theorem 1.1 becomes a classical Harnack theorem for harmonic functions and Theorem 1.3 becomes Dirichlet's first boundary value problem. We are now going to show that for a general bounded q the function u satisfies the Schrödinger equation (5) below.

Theorem 2.1. Let D, q and f be as in the definition (2) of §1 except that f need not be nonnegative. If $u(q, |f|; \cdot) \not\equiv \infty$ in D, then $u(q,f;\cdot) \in C^{(1)}(D)$. If in addition $q \in H(D)$, then $u(q,f;\cdot)$ satisfies the equation

$$(\Delta+2q)u = 0 \quad \text{in } D . \tag{5}$$

Proof. Since the conclusions are local properties let us begin by localization. Writing u as before we see that it is locally bounded by Theorem 1.1. Let B be a small ball such that $\bar{B} \subset D$, and

$$\sup_{x\in\bar{B}} E^x\{ \exp(Q\tau_B) \} < \infty . \tag{6}$$

We have for $x \in B$:

$$(7)\qquad u(x) = E^x\{\ e(\tau_B)\ u(X(\tau_B))\ \}\ .$$

Comparing this with the definition of u we see that we have replaced (D,f) by (B,u), where B is bounded and satisfies (6), and u is bounded in $\bar{B}$. We need only prove the conclusions of the theorem for x in B. Reverting to the original notation we may therefore suppose that the domain D has the properties of B above, in particular $\tau_D < \infty$ and $E^x\{\ e(\tau_D)\ \}$ is bounded in $\bar{D}$; and f is bounded. These conditions will be needed in the use of Fubini's theorem in the calculations which follow. [Warning: one must check the finiteness of the quantities below when q and f are replaced by $|q|$ and $|f|$; the former replacement is *not* trivial.] We write τ for τ_D and put for $0 \le s < t$:

$$e(s,t) = \exp\left(\int_s^t q(X(r))\, dr \right),$$

thus $e(\tau) = e(0,\tau)$. We have by the Markov property:

$$(8)\qquad E^x\{\ 1_{\{s<\tau\}}\ e(s,\tau)\ f(X_\tau) \mid F_s\ \} = 1_{\{s<\tau\}}\ u(X_s).$$

This relation is used in the first and last equations below:

$$(9)\qquad E^x\left\{ \int_0^t 1_{\{s<\tau\}}\ q(X_s)\ u(X_s)\ ds \right\}$$
$$= E^x\left\{ \int_0^{t\wedge\tau} q(X_s)\ e(s,\tau)\ f(X_\tau)\ ds \right\}$$
$$= E^x\{\ [e(\tau) - e(t\wedge\tau,\ \tau)]\ f(X_\tau)\ \}$$

$$= E^x\{\ t < \tau;\ [e(\tau)-e(t,\tau)]\ f(X_\tau)\} + E^x\{\ t \ge \tau;\ [e(\tau)-1]\ f(X_\tau)\}$$

$$= E^x\{\ e(\tau)\ f(X_\tau)\ \} - E^x\{\ t < \tau;\ u(X_t)\ \} - E^x\{\ t \ge \tau;\ f(X_\tau)\ \}.$$

Now put

$$v(x) = E^x\{\ f(X(\tau_D))\ \}$$

for $x \in D$. Then v is the probabilistic solution of the Dirichlet problem (D,f) reviewed above; hence $\Delta v = 0$ in D. The last member of (9) may be written as

$$u(x) - Q_t u(x) - v(x) + Q_t v(x).$$

Since both u and v are bounded, and $\lim_{t\to\infty} Q_t 1 = 0$ because D is bounded, we have $\lim_{t\to\infty} Q_t(u-v) = 0$. We may therefore let $t \to \infty$ in the first member of (9) to obtain, with the notation of (2):

$$(10) \qquad G_D(qu) = u-v \qquad \text{in } D\ .$$

Since u as well as q is bounded, and $G_D 1 < \infty$ because D is bounded, we have $G_D(|qu|) < \infty$. Since v is harmonic it follows from (10) and Lemma B that $u \in C^{(1)}(D)$; if $q \in H(D)$ then $u \in C^{(2)}(D)$ and

$$\Delta u = \Delta v + \Delta G_D(qu) = -2qu$$

which is (5). □

Before going further let us recapitulate the essential part of Theorems 1.3 and 2.1, leaving aside the generalizations. Let D be a bounded domain, $q \in b\mathcal{B}(D) \cap H(D)$, $f \in C^{(0)}(\partial D)$. Suppose that for some x_0 in D we have $u(q,1;x_0) < \infty$, then writing $u(x)$ for $u(q,f;x)$, we have $u \in C^{(2)}(D)$ and u is a solution of the Schrödinger equation $(\Delta+2q)u = 0$ in D. Furthermore $u(x)$ converges to $f(z)$ as x approaches each regular point z of ∂D. In particular if ∂D is regular then $u \in C^{(0)}(\bar{D})$. For $q \equiv 0$, u is the well known solution to the Dirichlet problem (D,f). Now in the latter case there is a converse as follows. Let $\varphi \in C^{(2)}(D) \cap C^{(0)}(\bar{D})$ and $\Delta\varphi = 0$ in D, then we have for all x in D:

$$\varphi(x) = E^x\{ \varphi(X(\tau_D)) \} .$$

This provides an extension of Gauss's average theorem for harmonic functions and implies the uniqueness of the solution to the Dirichlet problem. We proceed to establish corresponding results in the present setting.

The following lemma is stated for the sake of explicitness.

Lemma C. Let D, q, f be as in the definition of (2) of §1, except that f need not be nonnegative. If $u(q,|f|;\cdot) \not\equiv \infty$ in D, then we have for all $x \in D$ and $t \geq 0$:

$$E^x\{ e(\tau_D)\, f(X(\tau_D)) | F_t \} = e(t \wedge \tau_D)\, u(X(t \wedge \tau_D)) \quad . \tag{11}$$

Proof. We have

$$E^x\{1_{\{t<\tau_D\}} e(\tau_D) f(X(\tau_D)) | F_t\} = 1_{\{t<\tau_D\}} e(t)\, E^x\{e(t,\tau_D) f(X(\tau_D)) | F_t\}$$

$$= 1_{\{t<\tau_D\}}\, e(t)\, u(X_t)$$

by (8) (with s replaced by t). *On the other hand,*

$$E^x\{ 1_{\{t\geq\tau_D\}} e(\tau_D)\ f(X(\tau_D)) | F_t \} = 1_{\{t\geq\tau_D\}} e(\tau_D)\ f(X(\tau_D))$$

because the trace of F_t on $\{ t \geq \tau_D \}$ contains the trace of F_{τ_D} on $\{ t \geq \tau_D \}$. Now by Kellogg's theorem (see e.g. [6]) irregular points of ∂D form a polar set, hence $X(\tau_D)$ is a regular point of ∂D almost surely under P^x, $x \in D$; and consequently $u(X(\tau_D)) = f(X(\tau_D))$ by (2) of §1. Using this in the second relation above and adding it to the first relation we obtain (11). □

Theorem 2.2. Let D be an arbitrary domain and $q \in bC^{(0)}(D)$. Suppose that the function φ has the following properties:

$$\varphi \in C^{(2)}(D); \quad \varphi > 0 \quad \text{and} \quad (\Delta+2q)\varphi = 0 \quad \text{in} \quad D. \tag{12}$$

Then for any bounded subdomain E such that $\bar{E} \subset D$, we have

$$\forall \ x \in D: \ \varphi(x) = E^x\{ e(\tau_E)\ \varphi(X(\tau_E)) \} . \tag{13}$$

Proof. Although we can prove this result without stochastic integration, it is expedient to use Ito's formula. We have then in the customary notation:

$$d(e(t)\ \varphi(X_t)) = e(t)\{ \nabla\varphi(X_t)\ dX_t + (2^{-1}\Delta\varphi + q\varphi)(X_t)\ dt \} \tag{14}$$

where ∇ denotes the gradient and dX_t the stochastic differential (see e.g., [8]). The second term on the right side of (14) vanishes for $t < \tau_D$ by (12), and the first term is a local martingale. Since

$\bar{E}$ is compact and $\varphi \in C^{(2)}$ in a neighborhood of $\bar{E}$, we have

(15) $$\sup_{0 \le s \le t\wedge\tau_E} \| e(s)\, \nabla\varphi(X_s) \| \le e^{\|q\| t}\, \|\nabla\varphi\|_{\bar{E}} < \infty.$$

Hence (14) has the formal expression:

(16) $$e(t\wedge\tau_E)\,\varphi(X(t\wedge\tau_E)) - e(0)\varphi(X(0)) = \int_0^{t\wedge\tau_E} e(s)\, \nabla\varphi(X_s)\, dX_s = M_t,$$

say, where $\{ M_t, F_t, t \ge 0 \}$ is a martingale, under P^x for each $x \in D$, with $E^x(M_t) = 0$ for $t \ge 0$. Taking E^x in (16) we obtain

(17) $$\varphi(x) = E^x\{ e(t\wedge\tau_E)\, \varphi(X(t\wedge\tau_E)) \} .$$

By enlarging E if necessary, we may assume that all boundary points of E are regular. By Theorem 1.3, the function v defined by

(18) $$v(x) = E^x\{ e(\tau_E)\, \varphi(X(\tau_E)) \}$$

is continuous on $\bar{E}$ and equals φ on ∂E. We can apply Lemma C with D and f replaced by E and φ to obtain

(19) $$E^x\{ e(\tau_E)\, \varphi(X(\tau_E)) \mid F_t \} = e(t\wedge\tau_E)\, v(X(t\wedge\tau_E)).$$

Since $\varphi > 0$, v cannot vanish; and since v is continuous, it is bounded below on $\bar{E}$. We conclude from (19) that

(20) $$e(t\wedge\tau_E) \le (\inf_{\bar{E}} v)^{-1}\, E^x\{ e(\tau_E)\, \varphi(X(\tau_E)) \mid F_t \} .$$

A simple consequence of (2) is that the family $e(t\wedge\tau_E)$, $t \ge 0$, of random variables is uniformly integrable. We can thus let t tend to infinity in (17) to obtain

$$\varphi(x) = E^x\{ e(\tau_E)\, \varphi(X(\tau_E)) \}, \tag{21}$$

which shows (13) for $x \in \bar{E}$. Note that (13) is trivial for $x \in D-\bar{E}$.

Let us introduce the notation, for any $E \subset D$:

$$u_E(x) = E^x\{ e(\tau_E) \} ; \tag{22}$$

in particular u_D is $u(q,1;\cdot)$ in our previous notation. Parts of Theorem 2.2 are important enough to be stated as corollaries.

Corollary 1. For each bounded domain (or open set) E such that $\bar{E} \subset D$, we have u_E bounded in D.

Corollary 2. If there exists a function φ satisfying the conditions in (12) and is furthermore bounded above and bounded away from zero, then u_D is bounded in $\bar{D}$. In particular, this is the case if D is bounded and $\varphi \in C^{(0)}(\bar{D})$.

Proof. For then we have from (13), for all $x \in D$:

$$(\inf_{\bar{D}} \varphi)\, u_E(x) \leq \varphi(x) \leq \sup_{\bar{D}} \varphi$$

and consequently u_E is uniformly bounded with respect to E. There exists a sequence of such subdomains E_n increasing to D so that

$\tau(E_n)$ increases to $\tau(D)$. Hence it follows by Fatou's lemma that

$$E^x\{\, e(\tau_D)\,\} \le \varliminf_n E^x\{\, e(\tau(E_n))\,\}$$

is also bounded in D. Now it is easily shown that u_D is indeed bounded in $\bar{D}$. □

When $q \ge 0$, $\bar{D}$ is compact and ∂D is regular, the second assertion in Corollary 2 was proved by Khas'minskii [4] for strong Markov processes with strong Feller property and continuous paths. His method uses the Taylor series for $e(\tau_D)$, an iterative argument à la Picard, and a maximum principle. These depend essentially on the non-negativeness of q. The methods used in this paper can also be partially generalized to the class of processes considered by him, but the more difficult theorems such as Theorem 1.2 elude us at the moment.

Without the further assumption in Corollary 2 we cannot conclude that $u_D \not\equiv \infty$ in D; nor that (13) holds when E is replaced by D. The simplest example is in R^1 when $D = (0,\pi)$, $q = 1/2$, $\varphi(x) = \sin x$. The fact that $u_D \equiv \infty$ in this example will follow by contraposition from the results below. We need an easy but important lemma.

Lemma D. Let D be a domain with $m(D) < \infty$, and $u_D \not\equiv \infty$ in D. There exists a constant $c_0 > 0$ such that for all $x \in \bar{D}$:

$$u_D(x) \ge c_0(1 \vee u_E(x)) \tag{23}$$

where E is any set with $\bar{E} \subset D$. For all D and q such that $m(D) \le M < \infty$ and $\|q\| \le Q < \infty$, the constant c_0 depends only on M and Q.

Proof. It follows from (15) of §1 that for some t_0 depending only on M we have $P^x\{\tau_D \le t_0\} \ge 1/2$ for all $x \in \bar{D}$. We have then

$$u_D(x) \ge E^x\{ e(\tau_D);\ \tau_D \le t_0 \} \ge E^x\{ e^{-Qt_0};\ \tau_D \le t_0 \} \ge c_0,$$

where $c_0 = e^{-Qt_0}/2$. If $\bar{E} \subset D$ we have $\tau_E < \tau_D$ and so by the strong Markov property

$$u_D(x) = E^x\{ e(\tau_E)\, u_D(X(\tau_E)) \} \ge E^x\{ e(\tau_E) \}\, c_0 = u_E(x)\, c_0. \qquad \square$$

A simple consequence of Lemma D is the following converse to Corollary 2 above. If $m(D) < \infty$, and $u_D = \varphi$, then this φ satisfies (12); it is bounded above by Theorem 1.2 and bounded away from zero by Lemma D. In particular if D is bounded and ∂D is regular then $u_D \in C^{(0)}(\bar{D})$ by Theorem 1.3. The importance of this particular solution of the Schrödinger equation will become apparent in what follows.

Theorem 2.3. Let D be a domain with $m(D) < \infty$ and $u_D \not\equiv \infty$. Suppose that the function φ has the following properties:

(24) $$\varphi \in C^{(2)}(D) \cap bC^{(0)}(\bar{D});\quad (\Delta+2q)\varphi = 0 \text{ in } D.$$

Then we have

(25) $$\forall\ x \in D:\quad \varphi(x) = E^x\{ e(\tau_D)\, \varphi(X(\tau_D)) \}.$$

Proof. Although φ is no longer positive, the proof of Theorem 2.2 needs no change up to (17) there. Now by (23), $u_E \le c_0^{-1} u_D < \infty$ in D; hence $e(\tau_E)$ is integrable under P^x, $x \in \bar{E}$. We may therefore apply Lemma C to E with $f \equiv 1$ to obtain

(26) $E^x\{ e(\tau_E)|F_t \} = e(t \wedge \tau_E)\, u_E(X(t \wedge \tau_E)) \geq e(t \wedge \tau_E)\, c_0$

since $\inf_{\bar{E}} u_E \geq c_0$ by Lemma D. It follows that the family of random variables $\{ e(t \wedge \tau_E),\ t \geq 0 \}$ is uniformly integrable. Since φ is bounded continuous in $\bar{D}$ we may let $t \to \infty$ under E^x in (17) to deduce

(27) $$\varphi(x) = E^x\{ e(\tau_E)\varphi(X(\tau_E)) \}, \qquad x \in D.$$

Next we have, since $u_D < \infty$:

(28) $$E^x\{ e(\tau_D)|F(\tau_E) \} = e(\tau_E)\, u_D(X(\tau_E)) \geq e(\tau_E)\, c_0 \quad ,$$

by Lemma D. Hence the family $\{e(\tau_E)\}$ is uniformly integrable as E ranges over all sets with closures contained in D. Let E_n be open bounded, $\bar{E}_n \subset E_{n+1} \subset D$ and $\bigcup_n E_n = D$. We obtain (25) by putting $E = E_n$ in (27) and passing to the limit as before.

Let us remark that under the assumptions of Theorem 2.3 it is possible to apply Ito's formula directly to D instead of E as we did, provided that we can deduce the boundedness of $\nabla\varphi$ in (14) from that of φ (and hence of $\Delta\varphi$). This would require some kind of global estimate of Schauder's type which might require stronger smoothness conditions.

If $q \equiv 0$ and D is bounded, the preceding theorem reduces to the classical result of the representation of a harmonic function by its boundary values. We are now ready to solve a similar problem for the Schrödinger equation.

Theorem 2.4. Let D be as in Theorem 2.3, ∂D be regular, and $q \in H(D)$. For any $f \in bC^0(\bar{D})$ there is a unique φ satisfying (24) such that $\varphi \equiv f$ on ∂D. Indeed this φ is given by

$$\varphi(x) = E^x\{ e(\tau_D) f(X(\tau_D)) \}, \quad x \in D. \tag{29}$$

Proof. That this φ satisfies (24) is proved by Theorem 2.1 and Theorem 1.3. The uniqueness follows from Theorem 2.3. □

The relationship between the preceding results and those obtainable by the usual methods of partial differential equations will be discussed in a separate publication.

3. Further results

As a by-product of the methods used above which can be stated without mentioning probability, we give the following theorem about positive solutions of the Schrödinger equation. This will be needed in the next theorem.

Theorem 3.1. Let D be a domain and D_n be bounded domains such that $\bar{D}_n \subset D_{n+1}$ and $\bigcup_n D_n = D$. Let $q_n \in H(D_n)$ and $q_n \to q$ boundedly where $q \in H(D)$. Suppose that for each $n \geq 1$, there exists φ_n such that

$$\varphi_n > 0, \qquad (\Delta + 2q_n)\varphi_n = 0 \quad \text{in } D_n. \tag{1}$$

Then there exists φ such that

(2) $$\varphi > 0, \qquad (\Delta+2q)\varphi = 0 \quad \text{in } D.$$

Proof. Let Q be a common bound of all $\|q_n\|$ (and $\|q\|$). By Corollary 1 to Theorem 2.2, the existence of φ_n implies that for each $n \geq 2$ the function u_n defined by

(3) $$u_n(x) = E^x\{ e_{q_{n+1}}(\tau_{D_n}) \}$$

is bounded in $\bar{D}_n$. Choose any $x_0 \in D_1$ and put

(4) $$v_n(x) = u_n(x)/u_n(x_0) \quad .$$

According to the Corollary to Theorem 1.1, applied for $k > n$ to v_k on $\bar{D}_n$ and with $f \equiv 1$, there exists a constant $A_n > 0$ (depending only on D_{n+1}, D_n and Q) such that we have for all $k > n$:

(5) $$A_n^{-1} \leq \inf_{\bar{D}_n} v_k \leq \sup_{\bar{D}_n} v_k \leq A_n.$$

Define the measures below:

(6) $$\mu_k^{\pm}(dx) = q_{k+1}^{\pm}(x)v_k(x)dx, \quad \mu_k(dx) = \mu_k^{+}(dx)-\mu_k^{-}(dx) = q_{k+1}(x)v_k(x)dx$$

where $q_k = q_k^+ - q_k^-$ is the usual decomposition. The two sequences of measures $\{ \mu_k^{\pm}, k > n \}$ on D_n are vaguely bounded because

(7) $$\mu_k^{\pm}(D_n) \leq QA_n\, m(D_n), \qquad k > n.$$

We have by Theorem 2.1: $v_k \in C^{(2)}(D_k)$ and

(8) $$(\Delta+2q_{k+1})v_k = 0, \quad \text{in } D_k .$$

Hence it follows from Lemma B that for $k > n$:

(9) $$v_k = G_{D_n}(q_{k+1} v_k) + h_k$$

where h_k is harmonic in D_n. We have by (9) and (5):

(10) $$\| h_n \|_{D_n} \leq A_n + QA_n \, G_{D_n} 1 < \infty .$$

Hence by Harnack's theorem on harmonic functions, followed by a diagonal argument, there exists a sequence $\{k_j\}$ such that $\{h_{k_j}\}$ converges uniformly on each D_n, $n \geq 1$; and the limit is a harmonic function h in D. By (7), the sequence $\{k_j\}$ may be chosen so that both $\mu^+_{k_j}$ and $\mu^-_{k_j}$ converge vaguely on each D_n, $n \geq 1$. The bounds in (5) then imply that for every $f \in L^1(D)$ (not only for $f \in bC(D_n)$), $\int_{D_n} f d\mu_{k_j}$ converges as $j \to \infty$. Since D_n is bounded, we know that $G_{D_n}(x,dy) = g_{D_n}(x,y)\,dy$ where $g_{D_n}(x,\cdot) \in L^1(D_n)$. Here the function g_{D_n} is the Green's function for D_n. Therefore if we substitute k_j for k in (9), the first term on the right side converges as $j \to \infty$. Thus $\lim_j v_{k_j} = v$ exists on D_n for each $n \geq 1$, and we obtain from (9):

(11) $$v = G_{D_n}(qv) + h \quad \text{in } D_n .$$

Since $v \geq A_n^{-1}$ in D_n by (5), $v > 0$ in D. Using Lemma C, we see first that $v \in C^{(1)}(D)$ since qv is bounded by (5), and then $v \in C^{(2)}(D)$ since $qv \in H(D)$; finally by (11):

(12) $$\Delta v = \Delta G_{D_n}(qv) + \Delta h = -2qv.$$

This is true in D_n for $n \geq 1$, hence also in D. We have proved the existence of φ in (2) since v is such a function. □

Several experts in partial differential equations were consulted about Theorem 3.1. Hans Weinberger said it could be proved by classical eigenvalue methods of solving the Dirichlet problem for strongly elliptic equations. S.T. Yau said it could be proved (and the bounded convergence of q_n generalized) by variational methods. N. Trudinger said he would prove it by using Harnack's inequalities as we did above. A related result is given in [5].

From our point of view, the interest of Theorem 3.1 lies in the observation that its probabilistic analogue is false. Namely, if D_n increases to D, the finiteness of u_{D_n} for all n does not imply the finiteness of u_D. Yet u_{D_n} satisfies (1) (with $q_n \equiv q$) for each n, and if $u < \infty$ it will satisfy (2). A counterexample is furnished by the example in R^1 given above.

Let

$$L_t f(x) = E^x\{\, t < \tau_D;\ e(t)f(X_t)\,\}$$

in analogy with (4) of §2. In the next theorem we relate the finiteness of u_D to several conditions on the semigroup $\{L_t\}$ just defined. The results hold for the u in (2) of §1 with bounded f, but we put $f \equiv 1$ for simplicity. Since D and q are fixed below we will write u for u_D, τ for τ_D and $e(t)$ for $e_q(t)$. Consider then the following statements:

(a) $u \not\equiv \infty$ in D;

(b) for every $x \in D$, we have

(13) $$\int_0^\infty L_t 1(x)dt < \infty ;$$

(c) there is at least one x_0 in D having the property that for every $\delta > 0$, there exist $A(\delta)$ and $N(\delta)$ such that

(14) $$L_t\, 1(x_0) \le A(\delta)\, e^{\delta t} \quad \text{for} \quad t \ge N(\delta) \quad ;$$

(d) there exists φ satisfying (12) of §2 above;

(e) for any bounded open set E such that $\bar{E} \subset D$, u_E is bounded in $\bar{E}$.

Theorem 3.2. For any domain D, (a) and (b) are equivalent; and (b) implies (c). If $q \in bC^{(0)}(D)$, then (d) implies (e). If $q \in H(D)$, then (c) implies (d).

Proof. By Theorem 1.1, (a) implies that $u(x) < \infty$ for all $x \in D$. For any $s > 0$ and $n \ge 1$ we have by the Markov property:

(15) $$E^x\{e(\tau);\ ns < \tau \le (n+1)s\} = E^x\{e(ns);\ ns < \tau;\ E^{X(ns)}[e(\tau);\ 0<\tau\le s]\}.$$

Using (15) of §1, we can choose s so that $C = \inf_{x\in R^d} P^x\{\tau \le s\} > 0$. Then it is trivial that for every $y \in D$, we have

(16) $$Ce^{-Qs} \le E^y\{\ e(\tau);\ 0 < \tau \le s\ \} \le e^{Qs}$$

where $Q = \|q\|$. It follows from (15) and (16) that (a) is equivalent to:

(17) $$\sum_{n=0}^{\infty} E^x\{\ e(ns);\ ns < \tau\ \} < \infty.$$

For $ns < t < (n+1)s$, we have $e^{-Qs}e(ns) \le e(t) \le e^{Qs}e(ns)$. Hence (17) is equivalent to (13) by an easy comparison. This proves that (a) and (b) are equivalent. Of course, (c) is a much weakened form of (b) via (17).

Next, for a fixed $\varepsilon > 0$, we have by (15) and the second inequality in (16) applied to the functional $e_{q-\varepsilon}$ instead of e_q:

$$E^x\{ e_{q-\varepsilon}(\tau);\ n < \tau \le n+1 \} \le e^{Q+\varepsilon}\ E^x\{ e_{q-\varepsilon}(n);\ n < \tau \}$$

$$= e^{Q+\varepsilon-n\varepsilon}\ E^x\{ e_q(n);\ n < \tau \} \quad .$$

If (c) is true, the last member above is bounded by $e^{Q+\varepsilon+n(\delta-\varepsilon)}\ A(\delta)$ for $n \ge N(\delta)$. We may choose $0 < \delta < \varepsilon$; then

$$\text{(18)} \qquad E^x\{e_{q-\varepsilon}(\tau)\} = \sum_{n=0}^{\infty} E^x\{e_{q-\varepsilon}(\tau);\ n<\tau\le n+1\} \le A(\delta)\ e^{Q+\varepsilon} \sum_{n=0}^{\infty} e^{n(\delta-\varepsilon)} < \infty.$$

Now assume $q \in H(D)$. We can then apply Theorem 2.1 to obtain $u_{q-\varepsilon} \in C^{(2)}(D)$ and

$$\text{(19)} \qquad (\Delta+2(q-\varepsilon))\ u_{q-\varepsilon} = 0.$$

Since this is true for every $\varepsilon > 0$, and $q-\varepsilon$ converges to q boundedly as $\varepsilon \to 0$, we can apply Theorem 3.1 to conclude that (d) is true. Finally, if $q \in bC^{(0)}(D)$, then (d) implies (e) by Corollary 1 to Theorem 2.2.

The conditions in (b) and (c) are meaningful in the spectral theory of the semigroup $\{L_t\}$, or its infinitesimal generator the Schrödinger operator. At least when (14) holds for all x in D, this interpretation should yield (d) in some sense as a result on the point spectrum of the operator. It is not clear under what precise conditions the classical approach will confirm the results above obtained by probabilistic methods.

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