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STOPPED FEYNMAN–KAC FUNCTIONALS AND THE SCHRÖDINGER EQUATION

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In the late 1970s, Kai Lai Chung began investigating connections between probability and the (reduced) Schrödinger equation:

$$\tfrac{1}{2}\Delta u(x) + q(x)u(x) = 0 \quad \text{for } x \in \mathbb{R}^d, \tag{1}$$

where q is a real-valued Borel-measurable function on $\mathbb{R}^d$, and Δ is the d-dimensional Laplacian. His work in this area extended over the next 15 years or so. It included collaborations with several colleagues and students, and inspired the work of others. His book, *From Brownian Motion to Schrödinger's Equation* [1995], written with Zhongxin Zhao, is a compilation and refinement of much of the research conducted in this area up through 1994.

In the following, I will describe some of the background and early advances in this research involving connections with Brownian motion. A complementary article written by Michael Cranston, which also appears in this volume, focuses on related developments involving connections with conditioned Brownian motion. My account is not meant to be exhaustive, but rather to provide a sample of some of the intriguing aspects of the topic and to illustrate the pivotal role that Kai Lai Chung played in some of the developments. My description is necessarily influenced by my own personal recollections.

Background

Stimulated by Feynman's [1948] proposed "path integral" solution of the complex time-dependent Schrödinger equation, Kac [1949; 1951] considered, for a Borel-measurable function $q : \mathbb{R} \to \mathbb{R}$ satisfying $q \le 0$, the following multiplicative functional of one-dimensional Brownian motion B:

$$e_q(t) = \exp\Big(\int_0^t q(B_s)\, ds\Big) \quad \text{for } t \ge 0,$$

This functional can also be defined for suitable Borel-measurable functions $q : \mathbb{R}^d \to \mathbb{R}$, and for B a d-dimensional Brownian motion or even a d-dimensional diffusion process. Such functionals are now called *Feynman–Kac functionals*.

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Consider a continuous bounded function $q : \mathbb{R}^d \to \mathbb{R}$, and a continuous bounded function $g : \mathbb{R}^d \to \mathbb{R}$. If $\psi : [0, \infty) \times \mathbb{R}^d \to \mathbb{R}$ is a continuous bounded function, with continuous partial derivatives $\partial\psi/\partial t$, $\partial\psi/\partial x_i$, and $\partial^2\psi/\partial x_i \partial x_j$ for $i, j = 1, \ldots, d$, defined on $(0, \infty) \times \mathbb{R}^d$, and such that the following time-dependent Schrödinger equation holds:

$$\frac{\partial\psi(t,x)}{\partial t} = \frac{1}{2}\Delta\psi(t,x) + q(x)\psi(t,x) \quad \text{for } t > 0, x \in \mathbb{R}^d, \tag{2}$$

with initial condition $\psi(0, x) = g(x)$ for $x \in \mathbb{R}^d$, and where

$$\Delta\psi(t,x) = \sum_{i=1}^{d} \frac{\partial^2\psi}{\partial x_i^2}(t,x), \tag{3}$$

then it can be shown (for example, by using Itô's formula), that

$$\psi(t,x) = E^x\big[e_q(t)g(B_t)\big] \quad \text{for } t \geq 0, x \in \mathbb{R}^d. \tag{4}$$

Here, E^x denotes the expectation operator under which B is a d-dimensional Brownian motion starting from x.

Kac [1949; 1951] was interested in (2) when $d = 1$ and $q \leq 0$. However, rather than considering this equation directly, he worked with a reduced Schrödinger equation similar to (1) (with $q - s$ in place of q, and $d = 1$) obtained by formally taking the Laplace transform (with parameter s) in equation (2) to eliminate the time variable t. Under mild conditions, for example when q is bounded and continuous in addition to being non-positive, Kac [1951] showed that the Laplace transform of the right member of (4) with $g = 1$ satisfies this reduced Schrödinger equation.

In the late 1950s and early 1960s, in developing a potential theory for Markov processes, Dynkin (see [1965], Chapter XIII, §4, Theorem 13.16) and others, considered expressions of the form

$$E^x\Big[\exp\Big(\int_0^\tau q(X_s)\,ds\Big) f(X_\tau)\Big] \quad \text{for } x \in \overline{D}, \tag{5}$$

where X is a diffusion process in $\mathbb{R}^d$, $\tau = \inf\{s > 0 : X_s \notin D\}$ is the first exit time of X from a bounded domain D in $\mathbb{R}^d$, $\overline{D}$ is the closure of D, f is a continuous function defined on the boundary of D, and $q \leq 0$ is Hölder-continuous and bounded on D. Here, P^x and E^x denote respectively probability and expectation operators for X starting from $x \in \overline{D}$. The domain D is *regular* if

$$P^x(\tau = 0) = 1 \quad \text{for each } x \in \partial D.$$

Under suitable assumptions on X and assuming that D is regular, Dynkin showed that expressions of the form (5) yield continuous functions on $\overline{D}$ that satisfy the equation

$$\mathcal{L}u(x) + q(x)u(x) = 0 \quad \text{for } x \in D, \tag{6}$$

with continuous boundary values given by f, where $\mathcal{L}$ is the infinitesimal generator of the diffusion process X. The assumption that $q \leq 0$ implies that the action of the stopped Feynman–Kac functional,

$$e_q(\tau) = \exp\Big(\int_0^\tau q(X_s)\,ds\Big), \tag{7}$$

is to "kill" the diffusion process at a state dependent exponential rate given by $-q$ up until the stopping time τ. The assumption that q is non-positive ensures that the mean value of the stopped Feynman–Kac functional is always finite; in fact, it is bounded by one. In contrast, Khasminskii [Has′minskiĭ 1959] considered the case where q is *non-negative*. In this case, the action of the stopped Feynman–Kac functional can be interpreted as "creating mass" at a state-dependent exponential rate given by q up until the stopping time τ. Accordingly, the expression in (5) can fail to be finite if the domain is sufficiently large. Indeed, the results of Khasminskii [1959] imply that (under similar conditions to those imposed by Dynkin except that $q \geq 0$) the expression in (5) is finite for all $x \in \overline{D}$ if and only if there is a continuous function u that is strictly positive on $\overline{D}$ and satisfies (6).

It was not until the work of Chung [1980] that probabilistic solutions of (1) for general (signed) q became an object of considerable interest. The question of how the oscillations of such a q affect the behavior of the stopped Feynman–Kac functional (7) is an intriguing one; in particular, killing of mass in some locations may cancel creation of mass in others. The next section describes some of K. L. Chung's investigations on stopped Feynman–Kac functionals with general q.

Feynman–Kac gauge and positive solutions of the Schrödinger equation

One-dimensional diffusions. Kai Lai Chung initiated his research on stopped Feynman–Kac functionals in [Chung 1980] by considering a one-dimensional diffusion process (i.e., continuous strong Markov process) X, and the functional (7) with bounded Borel-measurable $q : \mathbb{R} \to \mathbb{R}$, and

$$\tau = \tau_b \equiv \inf\{t > 0 : X_t = b\} \quad \text{for } b \in \mathbb{R}.$$

Assume that $P^x(\tau_b < \infty) = 1$ for each $x \in \mathbb{R}$ and $b \in \mathbb{R}$, and define

$$v(x, b) = E^x\left[\exp\left(\int_0^{\tau_b} q(X_s)\, ds\right)\right] \quad \text{for } x \in \mathbb{R}, b \in \mathbb{R}.$$

Two fundamental properties of v are that $0 < v(x, b) \leq \infty$ for all $x, b \in \mathbb{R}$, and that

$$v(a, b)v(b, c) = v(a, c)$$

for any $a < b < c$ or $c < b < a$ in $\mathbb{R}$. The latter follows from the strong Markov property. These properties lead to the following:

Lemma 1. *For fixed* $b \in \mathbb{R}$,

(a) *if* $v(x, b) < \infty$ *for some* $x < b$, *then* $v(x, b) < \infty$ *for all* $x < b$,

(b) *if* $v(x, b) < \infty$ *for some* $x > b$, *then* $v(x, b) < \infty$ *for all* $x > b$.

Chung [1980] introduced the following measures of finiteness of v:

$$\alpha = \inf\{b \in \mathbb{R} : v(x, b) < \infty \;\text{ for all } x > b\},$$
$$\beta = \sup\{b \in \mathbb{R} : v(x, b) < \infty \;\text{ for all } x < b\},$$

and showed the next two results.

Lemma 2.

$$\alpha = \sup\{b \in \mathbb{R} : v(x,b) = \infty \ \textit{for all } x > b\},$$
$$\beta = \inf\{b \in \mathbb{R} : v(x,b) = \infty \ \textit{for all } x < b\}.$$

Furthermore, if $\beta \in \mathbb{R}$, then $v(x,\beta) = \infty$ for all $x < \beta$, and, if $\alpha \in \mathbb{R}$, then $v(x,\alpha) = \infty$ for all $x > \alpha$.

Theorem 3. *The following conditions* (*a*)–(*c*) *are equivalent.*

(a) $\beta = +\infty$.
(b) $\alpha = -\infty$.
(c) *For all $a, b \in \mathbb{R}$, $v(a,b)\, v(b,a) \le 1$.*

Following on from this, Chung and Varadhan [1980] proved the next two theorems for $q : \mathbb{R} \to \mathbb{R}$ bounded and continuous, and X a one-dimensional Brownian motion.

Theorem 4. *Fix $b \in \mathbb{R}$. Suppose that $v(x,b) < \infty$ for some* (*and hence all*) *$x < b$. Then, $u(x) = v(x,b)$ is twice continuously differentiable for $x \in (-\infty, b)$, continuous for $x \in (-\infty, b]$, and u satisfies the reduced Schrödinger equation*:

$$\tfrac{1}{2}u''(x) + qu(x) = 0 \quad \textit{for } x \in (-\infty, b), \tag{8}$$

with the boundary condition $u(b) = 1$.

Theorem 5. *The following conditions are equivalent.*

(a) *There is a twice continuously differentiable, strictly positive function u satisfying (8) with $b = +\infty$.*
(b) $\beta = +\infty$.
(c) $\alpha = -\infty$.
(d) *For all $a, b \in \mathbb{R}$,*
$$v(a,b)v(b,a) \le 1. \tag{9}$$
(e) *There is some pair of distinct real numbers a, b such that (9) holds.*

The equivalence of (a), (b) and (c) is an analogue of Khasminskii's [Has′minskiĭ 1959] results, but with $d = 1$, $D = (-\infty, \infty)$ and q allowed to change sign. Further discussion of this one-dimensional case for Brownian motion can be found in Chapter 9 of the book by Chung and Zhao [1995].

Multidimensional Brownian motion. Chung soon moved on to consider multidimensional Brownian motions and domains of finite Lebesgue measure in the work [1981] with K. Murali Rao. This paper appeared in the proceedings of the first "Seminar on Stochastic Processes", held at Northwestern University in 1981. This series of annual conferences was initiated by K. L. Chung, E. Çinlar and R. K. Getoor. The "Seminars" have grown in size over the years, but the novel format of a few invited talks, with ample time reserved for less formal presentations and discussions, has persisted and is one of the attractions of these annual meetings held over two and a half days.

The paper [Chung and Rao 1981] was a significant advance. In particular, it contained the first “gauge theorem.” It is stated in its original form below, and then some generalizations are mentioned.

For this, assume that B is a d-dimensional Brownian motion ($d \geq 1$), P^x and E^x are respectively probability and expectation operators for B starting from $x \in \mathbb{R}^d$, $q : \mathbb{R}^d \to \mathbb{R}$ is a bounded Borel-measurable function, D is a domain in $\mathbb{R}^d$ with closure $\overline{D}$ and boundary ∂D, m is d-dimensional Lebesgue measure, and $f : \partial D \to \mathbb{R}$ is a bounded Borel-measurable function with $f \geq 0$. Let

$$\tau_D = \inf\{t > 0 : B_t \notin D\},$$

be the first exit time of B from D. Define

$$u(D, q, f; x) = E^x\Big[\exp\Big(\int_0^{\tau_D} q(B_s)\, ds\Big) f(B_{\tau_D}); \tau_D < \infty\Big] \quad \text{for } x \in \overline{D}. \tag{10}$$

When $m(D) < \infty$, $P^x(\tau_D < \infty) = 1$ for all $x \in \overline{D}$ (see [Chung and Zhao 1995], Theorem 1.17) and the qualifier $\tau_D < \infty$ in (10) may be omitted. The following is Theorem 1.2 in Chung and Rao [1981].

Theorem 6. *Suppose the domain D satisfies $m(D) < \infty$. If $u(D, q, f; \cdot) \not\equiv \infty$ in D, then it is bounded in $\overline{D}$.*

While visiting Chung at Stanford University in the early 1980s, Zhongxin Zhao [1983] (see also [Chung and Zhao 1995], Theorems 5.19 and 5.20) extended this result by relaxing the assumptions on q and D. In particular, he showed that the conclusion of Theorem 6 continues to hold if the boundedness condition on q is relaxed to simply require that $q : \mathbb{R}^d \to \overline{\mathbb{R}}$ is a Borel-measurable function satisfying

$$\lim_{\alpha \downarrow 0}\Big[\sup_{x \in \mathbb{R}^d} \int_{|y-x| \leq \alpha} \big|G(x-y)q(y)\big|\, dy\Big] = 0, \tag{11}$$

where $\overline{\mathbb{R}} = [-\infty, \infty]$ is the extended real line and, for $x \in \mathbb{R}^d$,

$$G(x) = \begin{cases} |x|^{2-d} & \text{if } d \geq 3, \\ \ln \dfrac{1}{|x|} & \text{if } d = 2, \\ |x| & \text{if } d = 1. \end{cases}$$

The set of Borel-measurable functions $q : \mathbb{R}^d \to \overline{\mathbb{R}}$ satisfying (11) is called the *Kato class* (on $\mathbb{R}^d$), and is usually denoted by K_d or J. Various properties of these functions, as well as analytic properties of associated weak solutions of the reduced Schrödinger equation (12), are described in an extensive paper of Aizenman and Simon [1982] which appeared shortly after the work [1981] of Chung and Rao. The paper [Aizenman and Simon 1982] also describes connections between the stopped Feynman–Kac functional and weak solutions of (12) under a spectral condition (see Theorem 8 below).

Neil Falkner also visited Chung at Stanford in the early 1980s. During this time, Falkner [1983] proved a gauge theorem, when conditioned Brownian motion is used in place of Brownian motion, for bounded Borel-measurable q and sufficiently smooth bounded domains D. (Zhao subsequently used conditioned Brownian motion in his work [1983].) For more details on the work in [Falkner 1983] and a discussion of subsequent generalizations, see the article by Michael Cranston in this volume, and Chapter 7 of the book by Chung and Zhao [1995].

The function $u(D,q,1;\,\cdot)$ obtained by setting $f \equiv 1$ is called the *gauge* (function) for (D,q), and we say that (D,q) is *gaugeable* if this function is bounded on D.

Under the assumptions of Theorem 6 and assuming (D,q) is gaugeable, a second key result in the paper of Chung and Rao [1981] provides sufficient conditions for $u(D,q,f;\,\cdot)$ to be a twice continuously differentiable solution of the reduced Schrödinger equation in D,

$$\tfrac{1}{2}\Delta u(x) + q(x)u(x) = 0 \quad \text{for } x \in D, \tag{12}$$

with continuous boundary values given by f. As is usual in the theory of elliptic partial differential equations, to ensure two continuous derivatives for u, in dimensions two and higher, one imposes a stronger condition on q than simple continuity. For example, locally Hölder-continuous functions are often used. For $d = 1$, let $\mathscr{C}_1(D)$ denote the set of bounded continuous functions $h : D \to \mathbb{R}$ and, for $d \geq 2$, let $\mathscr{C}_d(D)$ denote the set of bounded continuous functions $h : D \to \mathbb{R}$ such that, for each compact set $K \subset D$, there are strictly positive, finite constants α, M such that

$$|h(x) - h(y)| \leq M|x-y|^{\alpha} \quad \text{for all } x, y \in K.$$

The following theorem is proved in Chung and Rao [1981] for $d \geq 2$. For $d = 1$, they impose local Hölder continuity on q to obtain the result, but this condition can be relaxed by invoking a suitable analytic lemma for a Green potential, as was shown in Chung's book *Lectures from Markov Processes to Brownian Motion* [1982] (see Proposition 4 of Section 4.7). Note for this that, for $d = 1$, $m(D) < \infty$ implies that D is a bounded interval.

Theorem 7. *Let D be a regular domain in $\mathbb{R}^d$ satisfying $m(D) < \infty$. Suppose that $q \in \mathscr{C}_d(D)$ and $f : \partial D \to \mathbb{R}$ is bounded and continuous. Assume that (D,q) is gaugeable, that is, $u(D,q,1;\,\cdot) \not\equiv \infty$ in D. Then, $u = u(D,q,f;\,\cdot)$ defined by (10) on $\overline{D}$ is twice continuously differentiable in D, continuous and bounded on $\overline{D}$, satisfies (12) in D, and has $u = f$ on ∂D. Furthermore, u is the unique twice continuously differentiable solution of (12) that is continuous and bounded on $\overline{D}$ and agrees with f on the boundary ∂D.*

This theorem has been generalized to situations where q is a Kato-class function, and (12) is interpreted in the weak sense of partial differential equation theory (see [Chung and Zhao 1995], Section 4.4)

Note that under the assumptions of the theorem above, if $f \geq 0$, then $u(D,q,f;\,\cdot)$ is a non-negative solution of (12) and, if $f > 0$ on ∂D, then $u(D,q,f;\,\cdot) > 0$ on $\overline{D}$. One naturally expects there to be some relation between the existence of such positive solutions of (12) and the sign of

$$\lambda(D,q) = \sup_{\varphi}\Big[\int_D \big\{-\tfrac{1}{2}|\nabla\varphi(x)|^2 + q(x)\varphi(x)^2\big\}\,dx\Big],$$

where the supremum is over all $\varphi : D \to \mathbb{R}$ such that φ is infinitely continuously differentiable in D, has compact support in D, and satisfies $\int_D \varphi(x)^2 dx = 1$. The quantity $\lambda(D,q)$ is the supremum of the spectrum of the operator $\frac{1}{2}\Delta + q$ on $L^2(D)$ (see [Chung and Zhao 1995], Proposition 3.29). Indeed, there is a sharp relationship provided by the following theorem (see Theorem 4.19 of [Chung and Zhao 1995] for a proof).

Theorem 8. *Let D be a domain in $\mathbb{R}^d$ satisfying $m(D) < \infty$ and q be a Kato-class function. Then, (D, q) is gaugeable if and only if $\lambda(D, q) < 0$.*

For bounded domains D, Aizenman and Simon proved in Theorem A.4.1 of [1982] the "if" part of this theorem when $\lambda(D, q) < 0$, $u(D, q, f; \cdot)$ is a weak solution of (12), its boundary values are given by f, and they are assumed continuous if f is continuous and D is regular.

The work of Chung and Rao [1981] was the seed for much subsequent work on connections between the probabilistically defined quantity (10), gauges, and solutions of the reduced Schrödinger equation (12). Besides continuing his own work in this area, in the 1980s Chung had two students, Elton P. Hsu [Chung and Hsu 1986; Hsu 1985; 1987] and Vassilus Papanicolaou [1990], who worked on probabilistic representations for other boundary-value problems associated with the reduced Schrödinger equation. A conjecture of Chung on equivalent conditions for finiteness of the gauge in terms of finiteness of $u(D, q, f; \cdot)$, when f is a non-negative function that is positive only on a suitable subset of the boundary, stimulated my work [Williams 1985] (as a student of Chung) and then Neil Falkner's [1983] (as a visitor at Stanford). Falkner's work used conditioned Brownian motion, which became an object of intense interest, in its own right and for its connections with gauge theorems. For more on this fascinating subject, see the accompanying article by Michael Cranston. Other generalizations have also occurred, especially ones involving more general Markov processes than Brownian motion. The works related to this are too numerous to mention here.

Finally, on a personal note, I would like to thank Kai Lai Chung for the pleasure of our collaborations and for the many lively discussions I have enjoyed with him over the years.

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