Feyman path integral via jump-type Markov processes for singular potentials, many particle systems and curvilinear state spaces

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Jump-type path integrals: abstract formulations

Let us start with abstract formulations that form the basis for the path integral representation of regularized Schrödinger equations in momentum, position, or energy representations.

Consider the linear equation

$$\dot{\psi} = A\psi + V\psi, \tag{1}$$

where A and V are operators in the complex Hilbert space $\mathcal{H}$. If A generates a strongly continuous semigroup e^{tA} in $\mathcal{H}$, the mild form of (1) is

$$\psi_t = e^{tA}\psi_0 + \int_0^t e^{(t-s)A} V \psi_s \, ds, \tag{2}$$

leading to the perturbation series solutions:

$$\psi_t = e^{tA}\psi_0 + \int_0^t e^{(t-s)A} V e^{sA} \psi_0 \, ds + \cdots$$

$$+ \int_{0 \le s_1 \le \cdots \le s_n \le t} e^{(t-s_n)A} V e^{(s_n - s_{n-1})A} V$$

$$+ \cdots + V e^{s_1 A} \psi_0 \, ds_1 ... ds_n + ... \tag{3}$$

Theorem 1. *Let* $(\Omega, \mathcal{F}, M)$ *be a Borel measure space such that in* $L_2(\Omega)$ *the operator* A *is represented as the multiplication operator on the function* $A(x)$, *and* V *be an integral operator of the form* $Vf(x) = \int f(y)V(x, dy)$ *with certain (possibly unbounded) transition kernel* $V(x, dy)$. *Suppose* $Re\, A(x) \leq c$ *and*

$$\|Ve^{tA}\|_{C_b(\Omega)} \leq ct^{-\beta}, \qquad (4)$$

with $c > 0$ *and* $\beta < 1$. *Then series (3) converges in* $C_b(\Omega)$ *for any* $\psi_0 \in C_b(\Omega)$ *and all finite* $t > 0$. *Its sum* ψ_t *solves equation (2) and is represented as the path integral (where* $y = y_n$*)*

$$\psi_t(y) = \int_{PC_y(t)} \mathcal{V}^{PC}(dY(.))F(Y(.))\psi_0(Y(t)),$$

$$= \sum_{n=0}^{\infty} \int_{PC_y^n(t)} \mathcal{V}_n^{PC}(dY(.))F(Y(.))\psi_0(Y(t)),$$

$$= \sum_{n=0}^{\infty} \int_{Sim_t^n} ds_1...ds_n \int_{\Omega^n} \prod_{j=1}^{n} V(y_{j+1}, dy_j)\psi_0(y_1)$$

$$\exp\{(t-s_n)A(y)+(s_n-s_{n-1})A(y_n)+\cdots+s_1A(y_1)\}. \qquad (5)$$

Proof. Condition (4) ensures that the terms of this series are estimated as

$$\int_{0\le s_1\le\cdots\le s_n\le t} e^{c(t-s_n)} c^n (s_n - s_{n-1})^{-\beta} s_1^{-\beta},$$

which implies the required convergence. □

Aiming at the Schrödinger equation in position representation, denote by CPL the set of continuous piecewise linear paths in $\mathbf{R}^d$. Let $CPL^{x,y}(0,t)$ denote the class of paths joining x and y in time t. $CPL_n^{x,y}(0,t) \subset CPL^{x,y}(0,t)$ have exactly n jumps of their derivative.

$$CPL^{x,y}(0,t) = \cup_{n=0}^{\infty} CPL_n^{x,y}(0,t).$$

Notice also that the set $CPL^{x,y}(0,t)$ belongs to the Cameron-Martin space of curves that have derivatives in $L^2([0,t])$.

To any σ-finite measure M on $\mathbf{R}^d$ there corresponds a unique σ-finite measure M^{CPL} on $CPL^{x,y}(0,t)$ such that if

$$q(s) = q^{s_1 \dots s_n}_{\eta_1 \dots \eta_n}(s)$$

$$= \eta_j + (s - s_j)\frac{\eta_{j+1} - \eta_j}{s_{j+1} - s_j}, \quad s \in [s_j, s_{j+1}] \quad (6)$$

(where $s_0 = 0, s_{n+1} = t, \eta_0 = y, \eta_{n+1} = x$) is a typical path in $CPL^{x,y}_n(0,t)$ and Φ is a functional on $CPL^{x,y}(0,t)$, then

$$\int_{CPL^{x,y}(0,t)} \Phi(q(.)) M^{CPL}(dq(.))$$

$$= \sum_{n=0}^{\infty} \int_{CPL^{x,y}_n(0,t)} \Phi(q(.)) M^{CPL}_n(dq(.))$$

$$= \sum_{n=0}^{\infty} \int_{Sim^n_t} ds_1 \dots ds_n \int_{\mathbf{R}^{dn}} M(d\eta_1) \dots M(d\eta_n) \Phi(q(.)). \quad (7)$$

Theorem 2. *Let the operator V in (1) is the multiplication operator by a function V on $\mathbf{R}^d$ or, more generally, by a measure V on $\mathbf{R}^d$, and the operator e^{tA} in $L_2(\mathbf{R}^d)$ be an integral operator of the form $e^{tA}f(x) = \int A_t(x,y)f(y)dy$ with certain measurable function $A_t(x,y)$. Suppose $\|e^{tA}\|_{C_b(\Omega)} \leq c$ and*

$$\|e^{tA}V\|_{C_b(\Omega)} \leq ct^{-\beta} \tag{8}$$

with $c > 0$ and $\beta < 1$. Then series (3) converges in $C_b(\Omega)$ for any $\psi_0 \in C_b(\Omega)$ and all finite $t > 0$. Its sum ψ_t solves equation (2) and is represented as a path integral on the space CPL:

$$\psi_t(x) = \int_{CPL^{x,y}(0,t)} \int_{\mathbf{R}^d} \psi_0(y)\Phi^A(q(.))V^{CPL}(dq(.)), \tag{9}$$

where $\Phi^A(q(.))$ equals

$$A_{t-s_n}(x,\eta_n)A_{s_n-s_{n-1}}(\eta_n,\eta_{n-1})\cdots A_{s_1}(\eta_1,y). \tag{10}$$

Proof. Similar estimates to the previous case.

□

For applications to the Schödinger equation with magnetic fields one needs to handle the case when V is the composition of a multiplication and the derivation operator, which is the subject of the next result.

Theorem 3. *As in Theorem 3, assume that* e^{tA} *is an integral operator of the form* $e^{tA}f(x) = \int A_t(x,y)f(y)dy$ *with certain measurable function* $A_t(x,y)$ *such that* $\|e^{tA}\|_{C_b(\Omega)} \le c$. *But suppose now that* $V = (\nabla, F)$ *with a bounded measurable vector-function* F *on* $\mathbf{R}^d$, *i.e.*

$$V(f) = \sum_{j=1}^{d} \nabla^j (F_j f)(x).$$

Assume that $A_t(x,y)$ *is differentiable with respect to the second variable for* $t > 0$ *and* $A_t(x,y) \to 0$ *as* $y \to \infty$ *for any* x. *Denote by* $\nabla_2 e^{tA}$ *the integral operator with the kernel being the derivative of* A *with respect to the second variable, i.e.*

$$[(\nabla_2 e^{tA})f(x)]^j = \int [\frac{\partial}{\partial y_j} A_t(x,y)] f(y)\, dy.$$

Finally, assume

$$\|(\nabla_2 e^{tA}, F)\|_{C_b(\Omega)} \le ct^{-\beta} \qquad (11)$$

with $c > 0$ and $\beta < 1$. Then series (3) converges in $C_b(\Omega)$ for any $\psi_0 \in C_b(\Omega)$ and all finite $t > 0$. Its sum ψ_t solves equation (2) and is represented as a path integral on the space CPL:

$$\psi_t(x) = \int_{CPL^{x,y}(0,t)} \int_{\mathbf{R}^d} \psi_0(y) \tilde{\Phi}^A(q(.)) F^{CPL}(dq(.)), \tag{12}$$

where $\tilde{\Phi}^A(q(.))$ equals

$$\frac{\partial}{\partial \eta_n} A_{t-s_n}(x, \eta_n) \cdots \frac{\partial}{\partial \eta_1} A_{s_2 - s_1}(\eta_2, \eta_1) A_{s_1}(\eta_1, y). \tag{13}$$

Proof. It is a consequence of Theorem 3, if one notices that

$$e^{tA} V = e^{tA}(\nabla, F) = (\nabla_2 e^{tA}, F)$$

by the integration by parts. $\square$

Finally, when working with Schrödinger equation, the most natural convergence is mean square. The following statement is a mean square version of the above results. Its proof is straightforward.

Proposition 1. *Under the assumptions of Theorems 1 or 2 suppose instead of* (4) *and* (8) *one has the estimates*

$$\|Ve^{tA}\|_{L_2(\Omega)} \leq ct^{-\beta} \tag{14}$$

or respectively

$$\|e^{tA}V\|_{L_2(\mathbf{R}^d)} \leq ct^{-\beta}. \tag{15}$$

Then the statements of the theorems remain true, but for $\psi_0 \in L_2(\Omega)$*, and with the convergence of the series understood in the mean square sense (meaning that the corresponding path integral should be considered as an improper Riemann integral).*

Regularization by complex time or mass, or continuous observation

To apply the path integral construction (as well as their extensions) to the Schrödinger equations beyond the case of potentials representing Fourier transform of finite measures, one often needs certain regularization. For instance, one can use the same regularization as is used to define the finite- dimensional integral

$$(2\pi t i)^{-d/2} \int_{\mathbf{R}^d} \exp\{-\frac{|x-\xi|^2}{2ti}\} f(\xi)\, d\xi \tag{16}$$

giving the free propagator $e^{it\Delta/2}f$. Namely, this integral is not well defined for general $f \in L^2(\mathbf{R}^d)$. The most natural way to define it is based on the observation that, according to the spectral theorem, for all $t > 0$

$$e^{it\Delta/2}f = \lim_{\epsilon \to 0_+} e^{it(1-i\epsilon)\Delta/2} f \tag{17}$$

in $L^2(\mathbf{R}^d)$. Hence the integral (16) can be defined as

$$\lim_{\epsilon \to 0_+} (2\pi t(i+\epsilon))^{-d/2} \int_{\mathbf{R}^d} \exp\{-\frac{|x-\xi|^2}{2t(i+\epsilon)}\} f(\xi)\, d\xi, \tag{18}$$

where convergence holds in $L^2(\mathbf{R}^d)$.

More generally, if the operator $-\Delta/2 + V(x)$ is self-adjoint and bounded from below, by the spectral theorem,

$$\exp\{it(\Delta/2 - V(x))\}f$$

$$= \lim_{\epsilon \to 0_+} \exp\{it(1 - i\epsilon)(\Delta/2 - V(x))\}f. \quad (19)$$

In other words, solutions to the Schrödinger equation

$$\frac{\partial \psi_t(x)}{\partial t} = \frac{i}{2}\Delta \psi_t(x) - iV(x)\psi_t(x) \qquad (20)$$

can be approximated by the solutions to the equation

$$\frac{\partial \psi_t(x)}{\partial t} = \frac{1}{2}(i + \epsilon)\Delta \psi_t(x) - (i + \epsilon)V(x)\psi_t(x), \qquad (21)$$

which describes the Schrödinger evolution in complex time. The corresponding equation on the Fourier transform u is

$$\frac{\partial u}{\partial t} = -\frac{1}{2}(i + \epsilon)y^2 u - (i + \epsilon)V(i\frac{\partial}{\partial y})u. \quad (22)$$

As we shall see, the results of the previous section are often applicable to regularized equations (21) with arbitrary $\epsilon > 0$, so that (19) yields an improper Riemann integral representation for $\epsilon = 0$, i.e. to the Schrödinger equation per se. Thus, unlike the usual method of analytical continuation often used for defining Feynman integrals, where the rigorous integral is defined only for purely imaginary Planck's constant h, and for real h the integral is defined as the analytical continuation by rotating h through a right angle, in our approach, the measure is defined rigorously and is the same for all complex h with non-negative real part. Only on the boundary $Im\, h = 0$ the corresponding integral does usually become an improper Riemann integral.

A more physically motivated regularization can be obtained from the quantum theory of continuous measurement describing spontaneous collapse of quantum states, which regularizes the divergences of Feynman's integral for large position or momentum. The work with this regularization is technically more difficult. Not going into detail here, note only that for regularization the momentum measurement is most handy, given by the equation

$$d\psi = \left(\frac{1}{2}(i + \frac{\lambda}{2})\Delta\psi - iV(x)\psi\right) dt + \frac{1}{i}\sqrt{\frac{\lambda}{2}}\frac{\partial}{\partial x}\psi \, dW. \tag{23}$$

As $\lambda \to 0$, equation (23) approaches the standard Schrödinger equation.

Singular potentials and magnetic fields

Using regularization we can apply the abstract results given at the beginning to the Schrödinger equation with various kinds of potentials and with a possibly curvilinear state space.

Proposition 2. *Let* $V(x) = \int e^{-ixp} f(p)dp$ *(in the sense of distributions) and* $f \in L^1 + L^q$, *i.e.* $f = f_1 + f_2$ *with* $f_1 \in L^1(\mathbf{R}^d)$, $f_2 \in L^q(\mathbf{R}^d)$, *with* q *in the interval* $(1, d/(d-2))$, $d > 2$. *Then for any* $\epsilon > 0$ *the regularized Schrödinger equation in momentum representation* (22) *satisfies the conditions of Theorem 1 yielding a representation for its solutions in terms of the path integral. Moreover, the operator* $-\Delta/2 + V$ *is self-adjoint so that* (19) *yields an improper Riemann integral representation for* $\epsilon = 0$, *i.e. to the Schrödinger equation per se.*

Proof. One sees that the conditions of Theorem 1 are satisfied using the Hölder inequality. Self-adjointness of the Schrödinger operators for this class of potentials is well known. □

Remark 1. *The class of potentials from Proposition 2 includes the Coulomb case* $V(x) = |x|^{-1}$ *in* $\mathbf{R}^3$*. For this case* $f(y) = |y|^{-2}$*.*

We shall turn now to the Schrödinger equation in the position representation, aiming at the application of Theorem 2. Of course, if V is a bounded function, the conditions of this theorem for regularized Schrödinger equation (21) are trivially satisfied (with $\beta = 0$). Let us discuss singular potentials. The most important class of these potentials represent Radon measures supported by null sets such as discrete sets (point interaction), smooth surfaces (surface delta interactions), Brownian paths and more general fractals. Less exotic examples of potentials satisfying the assumptions of Proposition 4 below are given by measures with a density $V(x)$ having a bounded support and such that $V \in L^p(\mathbf{R}^d)$ with $p > d/2$.

The one-dimensional situation turns out to be particularly simple in our approach, because in this case no regularization is needed to express the solutions to the corresponding Schrödinger equation and its propagator in terms of path integral.

Proposition 3. *Let V be a bounded (complex) measure on $\mathbf{R}$. Then the solution ψ_G to equation* (21) *with $\epsilon \geq 0$ (i.e. including equation* (20)*) and the initial function $\psi_0(x) = \delta(x - x_0)$ (i.e. the propagator or the Green function of* (21)*) exists and is a continuous function of the form*

$$\psi_G(t,x) = (2\pi(i+\epsilon)t)^{-1/2} \exp\{-\frac{|x-x_0|^2}{2t(i+\epsilon)}\} + O(1)$$

uniformly for finite times. Moreover, the path integral representation for ψ_G is given by Theorem 2.

Proof. The condition of Theorem 2 are satisfied with $\beta = 1/2$ (one-dimensional effect).

□

For the Schrödinger equation in finite-dimensional case one needs a regularization.

A number $dim(V)$ is called the *dimensionality* of a measure V if it is the least upper bound of all $\alpha \geq 0$ such that there exists a constant $C = C(\alpha)$ such that

$$|V(B_r(x))| \leq Cr^\alpha$$

for all $x \in \mathbf{R}^d$ and all $r > 0$.

Proposition 4. *Let V be a finite complex Borel measure on $\mathbf{R}^d$ with $dim(V) > d - 2$. Then (i) for any $\epsilon > 0$ the regularized Schrödinger equation* (21) *satisfies the conditions of Theorem 2 yielding a representation for its solutions in terms of the path integral; (ii) one can give rigorous meaning to the formal expression $H = -\Delta/2 + V$ as a bounded below self-adjoint operator in such a way that the operators* $\exp\{-t(i+\epsilon)H\}$ *defined by means of functional operator calculus are given by the path integral of Theorem 2; (iii) formula* (19) *yields an improper Riemann integral representation for $\epsilon = 0$.*

Proof. To check the conditions of Theorem 2 for the regularized Schrödinger equation (21) we need to show that for any $\epsilon > 0$

$$\int_{\mathbf{R}^d} [2\pi t(i+\epsilon)]^{-d/2} \exp\left\{-\frac{|x-\xi|^2}{2t(i+\epsilon)}\right\} V(d\xi) \leq c(\epsilon) t^{-\beta}$$

with $\beta < 1$ uniformly for all x. To this end, let us decompose this integral into the sum of two integrals $I_1 + I_2$ by decomposing the domain of integration into two parts:

$$D_1 = \{\xi : |x-\xi| \geq t^{-\delta+1/2}\}, \quad D_2 = \mathbf{R}^d \setminus D_1.$$

Then I_1 is exponentially small for small t and

$$I_2 \leq [2\pi t\sqrt{1+\epsilon^2}]^{-d/2} \int_{D_2} V(d\xi)$$

$$\leq c(\alpha, \epsilon) t^{-d/2} (t^{-\delta+1/2})^{\alpha}$$

with $\alpha > d-2$. This expression is of order $t^{-\beta}$ with $\beta = \delta\alpha + (d-\alpha)/2 < 1$ whenever $\delta < (\alpha - d + 2)/(2\alpha)$. It remains to prove self-adjointness. This can be obtained from the properties of the corresponding semigroup. □

Let us extend this result to the case of a formal Schrödinger operator with magnetic fields in $L^2(\mathbf{R}^d)$ of the form

$$H = \frac{1}{2}\left(\frac{1}{i}\frac{\partial}{\partial x} + A(x)\right)^2 + V(x) \qquad (24)$$

under the following conditions:

C1) the magnetic vector-potential A is a bounded measurable mapping $\mathbf{R}^d \to \mathbf{R}^d$,

C2) the potential V and the divergence $div\,A = \sum_{j=1}^{d} \frac{\partial A^j}{\partial x^j}$ (defined in hte sense of distributions) are both (signed) Borel measures,

C3) if $d > 1$ there exist $\alpha > d-2$ and $C > 0$ such that for all $x \in \mathbf{R}^d$ and $r \in (0, 1]$

$$|div\,A|(B_r(x)) \leq Cr^{\alpha}, \quad |V|(B_r(x)) \leq Cr^{\alpha},$$

if $d = 1$the same holds for $\alpha = 0$.

The corresponding regularized Schrödinger equation can be written in the form

$$\frac{\partial \psi}{\partial t} = -DH\psi,$$

where D is a complex number with $Re\, D = \epsilon \geq 0$, $|D| > 0$, and the corresponding integral (mild) equation is

$$\psi_t = e^{Dt\Delta/2}\psi_0 - D\int_0^t e^{D(t-s)\Delta/2}(W + i(\nabla, A))\psi_s\, ds, \tag{25}$$

where

$$W(x) = V(x) + \frac{1}{2}|A(x)|^2 + \frac{i}{2}\, div\, A(x).$$

More precisely, W is a measure, which is the sum of the measure $V(x) + i\, div\, A(x)/2$ and the measure having the density $|A(x)|^2/2$ with respect to Lebesgue measure.

Theorem 4. *Suppose C1)-C3) hold for operator* (24). *Then all the statements of Proposition 4 are valid for the operator H.*

Proof. It is the same as for Proposition 4 above, but one needs to use Theorem 3 instead of Theorem 2. □

Precise estimates for the *hear kernel* of e^{-tDH} are also available.

Growing potentials and curvilinear state spaces

Let us consider the Schrödinger equation

$$\frac{\partial \psi_t(x)}{\partial t} = -iH\psi_t(x) - iV(x)\psi_t(x), \qquad (26)$$

where V is the operator of multiplication by a function V and H is a selfadjoint operator in $L^2(\Omega)$ with discrete spectrum.

Basic examples:

(i) H is the Laplace operator (or more generally an elliptic operator) on a compact Riemann manifold (curvilinear state space),

(ii) $H = -\Delta + W(x)$ in $L^2(\mathbf{R}^d)$, where W is bounded below and $W(x) \to \infty$ for $x \to \infty$,

(iii) many particle versions of the situations from (i)-(ii).

In this case the most natural representation for the Schrödinger equation is the energy representation. In other words, if $\lambda_1 \leq \lambda_2 \leq$ ... are eigenvalues of H and $\psi_1, \psi_2, \cdots$ are the corresponding normalized eigenfunctions, then any $\psi \in L^2(\Omega)$ can be represented by its Fourier coefficients $\{c_n\}$, where $\psi = \sum_{n=1}^{\infty} c_n \psi_n$ is the expansion of ψ with respect to the orthonormal basis $\{\psi_j\}$. In terms of $\{c_n\}$ the operator e^{-itH} acts as the multiplication $c_n \mapsto$ $\exp\{-it\lambda_n\}c_n$, and V is represented by the infinite-dimensional symmetric matrix $V_{nm} =$ $\int \psi_n(x) V(x) \psi_m(x)\, dx$ (i.e. it is a discrete integral operator). If V is a bounded function, condition (14) of Proposition 1 is trivially satisfied (with $\beta = 0$) yielding a path integral representation for the solutions of equation (26) in the spectral representation of the operator H. It is not difficult to find examples when the conditions of Theorem 1 hold, but these examples do not seem to be generic.

Connection with infinite-dimensional oscillatory integrals

Proposition 5. *If V is the Fourier transform of a finite measure, suppose $X(s)$ be any continuous curve. Then*

$$\exp\{-i\int_0^t V(X(s))\,ds\}$$

$$= \int_{PC_0(t)} \exp\{-i\int_0^t X_s\,dY_s\}(-i\mu)^{PC}(dY(.)). \tag{27}$$

The r.h.s. of (27) is sometimes called the *Fourier-Feynman transform* of the complex measure $(-i\mu)^{PC}$.

The approach of infinite-dimensional oscillatory integrals of Albeverio-Hoegh-Krohn and Elworthy-Truman is based on the possibility to represent the function $\exp\{-i\int_0^t V(X(s))\,ds\}$ as the Fourier transform of a finite measure $\mathcal{M}_V$ on the Cameron-Martin space of curves with square integrable derivatives. Formula (27) yields a precise description of this measure.

Namely, as on the classical paths of the free dynamics the position and its velocity are connected via the trivial ODE $\dot{x} = p$, the set PC of piecewise constant paths in the velocity space corresponds to the set CPL of continuous piecewise linear paths in the position space. One can thus naturally transform a measure on the set PC to the measure on CPL. Formula (27) shows that the function $\exp\{-i \int_0^t V(X(s))\, ds\}$ can be represented as the Fourier transform of the measure on CPL (which is a subspace of the Cameron-Martin space) that is obtained by transforming the measure $(-i\mu)^{PC}$ from PC to CPC via the transformation aove.

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