

Mathematics of the Feynman path integral

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1 Introduction

The Feynman path integral is known to be a powerful tool in different domains of physics.¹ At the same time, the mathematical theory underlying lots of (often formal) physical calculations is far from being complete. Various known approaches to the rigorous construction of the Feynmann path integral representation to the solution of the Schrödinger equation

$$\frac{\partial \psi}{\partial t} = \left(\frac{i}{2m} \Delta - iV(x) \right) \psi \quad (1.1)$$

(and its generalisations that include magnetic fields) can be roughly divided into two classes. In the approaches of the first class that we shall not discuss here in detail the Feynman integral is not supposed to be a genuine integral, but is specified as some generalised functional on an appropriate space of functions, which can be defined, for example, as the limit of certain discrete approximations (see e.g. [16], [44] and more recent papers [24], [25], [34]), by means of analytical continuation (see e.g. [26], [23] and references therein), by extensions of Parceval's identity and by related axiomatic definitions (see [2], [5], [30], [11], [42] and references therein) or by means of the white noise analysis (see [22]), see also [46] for the discussion of path integral applied to the Dirac equation. These approaches still cover only a very restrictive class of potentials, for example, singular potentials were considered only by white noise analysis approach but only in one-dimensional case (see e.g. [6] and references therein).

In the approaches of the second class, one tries to define the infinite-dimensional Feynmann integral as a genuine integral over a bona fide σ -additive measure on an appropriate space of trajectories. The first attempt made in [19] to construct such a measure was erroneous and led to understanding that there is no direct generalisation of Wiener measure that can give an analog of Feynman-Kac formula for the case of Schrödinger operators. A correct construction of the Feynman integral in terms of the Wiener measure was proposed in [15] and was based on the idea of the rotation of the classical trajectories in complex

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domains. Namely, changing the variables x to $y = \sqrt{i}x$ in equation (1.1) leads to the equation

$$\frac{\partial \psi}{\partial t} = \left(-\frac{1}{2m}\Delta - iV(-\sqrt{i}y)\right)\psi, \quad (1.2)$$

which is of diffusion type (with possibly complex source) and can be treated by means of the Feynman-Kac formula and the Wiener measure. Clearly this works only under very restrictive analytic assumptions on V (see e.g. [20], [21], [5]). However, if one is interested only in semiclassical approximation to the solutions of the Schrödinger equation one can obtain along these lines an approximate path integral representation for even non-analytic potentials that yields all terms of semiclassical expansion (see [7]).

Another approach to the construction of the genuine path integral initiated in [37], [36] defines it as an expectation with respect to a certain compound Poisson process, or as an integral over a measure concentrated on piecewise constant paths, see e.g. [13], [23], [29], [39], and references therein. Though this method was successfully applied to different models (see e.g. [18] for many particle problems, [41] for simple quantum field models, [12] for computational aspects and tunneling problems, [17] and [27] for Dirac equations), the restriction on interaction forces were always very strong, for example, for a usual Schrödinger equation, this approach was used only in the case of potentials which are Fourier transforms of finite measures. However in [30], [31] following this trend, a construction was given that covered already essentially more general potentials. To achieve this, one uses a coordinate representation for the Schrödinger equation (and not the momentum representation as in [37]) and also uses an appropriate regularisation of the Schrödinger equation. As the simplest reasonable regularisation one can take the same one as is used to define standard finite-dimensional (but not absolutely convergent) integrals. A relevant finite-dimensional example is given by the integral

$$(U_0 f)(x) = (2\pi ti)^{-d/2} \int_{\mathcal{R}^d} \exp\left\{-\frac{|x - \xi|^2}{2ti}\right\} f(\xi) d\xi \quad (1.3)$$

defining the free propagator $e^{it\Delta/2}f$. This integral may be not well defined for a general $f \in L^2(\mathcal{R}^d)$. One of the way to define this integral is based on the observation that according to the spectral theorem $e^{it\Delta/2}f = \lim_{\epsilon \rightarrow 0+} e^{it(1-i\epsilon)\Delta/2}f$ in $L^2(\mathcal{R}^d)$ for all $t > 0$ (i.e. one can approximate real times t by complex times $t(1 - i\epsilon)$). Hence, for an arbitrary $f \in L^2(\mathcal{R}^d)$, one can define the integral in (1.3) as

$$(U_0 f)(x) = \lim_{\epsilon \rightarrow 0+} (2\pi t(i + \epsilon))^{-d/2} \int_{\mathcal{R}^d} \exp\left\{-\frac{|x - \xi|^2}{2t(i + \epsilon)}\right\} f(\xi) d\xi \quad (1.4)$$

(notice that for any $\epsilon > 0$ and $f \in L^2(\mathcal{R}^d)$, the integral in (1.4) is well defined). We shall use the same approach for Feynman's integral. Namely, if the operator

$H = -\Delta/2 + V(x)$ is self-adjoint and bounded from below, by the spectral theorem we have

$$\exp\{-itH\} = \lim_{\epsilon \rightarrow 0} \exp\{-(i + \epsilon)tH\} \quad (1.5)$$

for all positive t . In other words, solutions to equation (1.1) (with $m = 1$ for brevity) can be approximated by the solutions to the regularised equation

$$\frac{\partial \psi}{\partial t} = \frac{1}{2}(i + \epsilon)\Delta\psi - (i + \epsilon)V(x)\psi, \quad (1.6)$$

i.e. to the Schrödinger equation in complex time. In Section 3 we shall define a measure on a path space (actually a measure on the Cameron-Martin space of paths having square integrable derivatives) such that for any $\epsilon > 0$ and for rather general class of potentials V , the solution $\exp\{it(1 - i\epsilon)(\Delta/2 - V(x))\}u_0$ to the Cauchy problem of equation (1.6) can be expressed as the Lebesgue (or even the Riemann) integral of some functional F_ϵ with respect to this measure, which would give a rigorous definition (analogous to (1.4)) of an improper Riemann integral corresponding to the case $\epsilon = 0$, i.e. to equation (1.1). Therefore, unlike the usual method of analytical continuation often used for defining Feynman's integral, where rigorous integral is defined only for purely imaginary Planck's constant \hbar and for real h the integral is defined as the analytical continuation by rotating h through the right angle, in our approach the (positive σ -finite) measure is rigorously defined and is the same for all complex h with a non-negative real part, and only on the boundary $\text{Im } h = 0$ the corresponding integral usually becomes an improper Riemann's integral.

Surely, the idea to use equation (1.6) as an appropriate regularisation for defining Feynman's integral is not new and goes back at least to the paper [19]. However, this was not carried out there, because, as we already noted, there exist no direct generalisations of the Wiener measure that could be used to define Feynman's integral for equation (1.6) for any real ϵ . As it turns out, one can carry out this regularization using measures of Poisson type.

A more physically motivated regularisation to (1.1) (but also technically more difficult to work with) can be obtained from the theory of continuous quantum measurement (see [30], [31] for the corresponding results).

In the original papers of Feynman the path integral was defined (heuristically) in such a way that the solutions to the Schrödinger equation were expressed as the integrals of the function $\exp\{iS\}$, where S is the classical action along the paths. It seems that rigorously the corresponding measure was not constructed even for the case of the heat equation with sources (notice that in the famous Feynman-Kac formula that gives rigorous path integral representation for the solutions to the heat equation a part of the action is actually "hidden" inside the Wiener measure). As shown in [30], the construction described below can be modified in a way to yield a representation of this kind.

As is also shown in [30], there is a natural Fock space representation of infinite dimensional path integrals of Poisson-type considered above that allows

to rewrite them in terms of the integrals over a usual Wiener measure.

It is worth noting also that in one-dimensional case, one obtains the path integral representation of Poisson type for very general Schrödinger equation without any regularisation (see [30], [31]).

The paper is organised as follows. In the next section we describe a general approach to the construction of measures on the space of all paths that give in a unified way both Wiener measure and Poisson type measures from [37]. In Section 3 we give new results on path integral representations for general (even singular) Schrödinger equations with magnetic fields using the regularisation by introducing complex times.

Sections 2 and 3 are written in a way that they can be read almost independently.

2 Infinitely divisible complex distributions and complex Markov processes

We present here (following essentially [29]) a general construction of the complex-valued measures (that can be considered as an appropriately generalised complex-valued version of Nelson's construction of the Wiener measure) on the path space that can be used for the path integral representation of various evolutionary equations, where the path integral representation can be obtained without any regularisation.

Let $\mathcal{B}(\Omega)$ denote the class of all Borel sets of a topological space (i.e. it is the σ -algebra of sets generated by all open sets). If Ω is locally compact we denote (as usual) by $C_0(\Omega)$ the space of all continuous complex-valued functions on Ω vanishing at infinity. Equipped with the uniform norm $\|f\| = \sup_x |f(x)|$ this space is known to be a Banach space. It is also well known (Riesz-Markov theorem) that if Ω is a locally compact space, then the set $\mathcal{M}(\Omega)$ of all finite complex regular Borel measures on Ω equipped with the norm $\|\mu\| = \sup | \int_{\Omega} f(x) \mu(dx) |$, where \sup is taken over all functions $f \in C_0(\Omega)$ with $\|f(x)\| \leq 1$, is a Banach space, which coincides with the set of all continuous linear functionals on $C_0(\Omega)$. Any complex σ -additive measure μ on \mathcal{R}^d has a representation of form

$$\mu(dy) = f(y)M(dy) \quad (2.1)$$

with a positive measure M and a bounded complex-valued function f . Moreover, the measure M in (2.1) is uniquely defined under additional assumption that $|f(y)| = 1$ for all y . If this condition holds, the positive measure M is called the total variation measure of the complex measure μ and is denoted by $|\mu|$. In general, if (2.1) holds, then $\|\mu\| = \int |f(y)|M(dy)$.

We say that a map ν from $\mathcal{R}^d \times \mathcal{B}(\mathcal{R}^d)$ into \mathcal{C} is a *complex transition kernel*, if for every x , the map $A \mapsto \nu(x, A)$ is a (finite complex) measure on \mathcal{R}^d , and for every $A \in \mathcal{B}(\mathcal{R}^d)$, the map $x \mapsto \nu(x, A)$ is \mathcal{B} -measurable. A (time

homogeneous) *complex transition function* (abbreviated CTF) on \mathcal{R}^d is a family ν_t , $t \geq 0$, of complex transition kernels such that $\nu_0(x, dy) = \delta(y - x)$ for all x , where $\delta_x(y) = \delta(y - x)$ is the Dirac measure in x , and such that for every non-negative s, t , the Chapman-Kolmogorov equation

$$\int \nu_s(x, dy) \nu_t(y, A) = \nu_{s+t}(x, A)$$

is satisfied. (We consider only time homogeneous CTF for simplicity, the generalisation to non-homogeneous case is straightforward).

A CTF is said to be (spatially) homogeneous, if $\nu_t(x, A)$ depends on x, A only through the difference $A - x$. If a CTF is homogeneous it is natural to denote $\nu_t(0, A)$ by $\nu_t(A)$ and to write the Chapman-Kolmogorov equation in the form

$$\int \nu_t(dy) \nu_s(A - y) = \nu_{t+s}(A).$$

A CTF will be called *regular*, if there exists a positive constant K such that for all x and $t > 0$, the norm $\|\nu_t(x, \cdot)\|$ of the measure $A \mapsto \nu_t(x, A)$ does not exceed $\exp\{Kt\}$.

CTFs appear naturally in the theory of evolutionary equations: if T_t is a strongly continuous semigroup of bounded linear operators in $C_0(\mathcal{R}^d)$, then there exists a time-homogeneous CTF ν such that

$$T_t f(x) = \int \nu_t(x, dy) f(y). \quad (2.2)$$

In fact, the existence of a measure $\nu_t(x, \cdot)$ such that (2.2) is satisfied follows from the Riesz- Markov theorem, and the semigroup identity $T_s T_t = T_{s+t}$ is equivalent to the Chapman-Kolmogorov equation. Since $\int \nu_t(x, dy) f(y)$ is continuous for all $f \in C_0(\mathcal{R}^d)$, it follows by the monotone convergence theorem (and the fact that each complex measure is a linear combination of four positive measures) that $\nu_t(x, A)$ is a Borel function of x .

We say that the semigroup T_t is *regular*, if the corresponding CTF is regular. Clearly, this is equivalent to the assumption that $\|T_t\| \leq e^{Kt}$ for all $t > 0$ and some constant K .

Now we construct a measure on the path space corresponding to each regular CTF, introducing first some (rather standard) notations. Let $\dot{\mathcal{R}}_d$ denote the one point compactification of the Euclidean space \mathcal{R}^d (i.e. $\dot{\mathcal{R}}_d = \mathcal{R}^d \cup \{\infty\}$ and is homeomorphic to the sphere S^d). Let $\dot{\mathcal{R}}_d^{[s,t]}$ denote the infinite product of $[s, t]$ copies of $\dot{\mathcal{R}}_d$, i.e. it is the set of all functions from $[s, t]$ to $\dot{\mathcal{R}}_d$, the path space. As usual, we equip this set with the product topology, in which it is a compact space (Tikhonov's theorem). Let $Cyl_{[s,t]}^k$ denote the set of functions on $\dot{\mathcal{R}}_d^{[s,t]}$ having the form

$$\phi_{t_0, t_1, \dots, t_{k+1}}^f(y(\cdot)) = f(y(t_0), \dots, y(t_{k+1}))$$

for some bounded complex Borel function f on $(\dot{\mathcal{R}}^d)^{k+2}$ and some points t_j , $j = 0, \dots, k+1$, such that $s = t_0 < t_1 < t_2 < \dots < t_k < t_{k+1} = t$. The union $Cyl_{[s,t]} = \cup_{k \in \mathcal{N}} Cyl_{[s,t]}^k$ is called the set of cylindrical functions (or functionals) on $\dot{\mathcal{R}}_d^{[s,t]}$. It follows from the Stone-Weierstrasse theorem that the linear span of all continuous cylindrical functions is dense in the space $C(\dot{\mathcal{R}}_d^{[s,t]})$ of all complex continuous functions on $\dot{\mathcal{R}}_d^{[s,t]}$. Any CTF ν defines a family of linear functionals $\nu_{s,t}^x$, $x \in \mathcal{R}^d$, on $Cyl_{[s,t]}$ by the formula

$$\begin{aligned} & \nu_{s,t}^x(\phi_{t_0 \dots t_{k+1}}^f) \\ &= \int f(x, y_1, \dots, y_{k+1}) \nu_{t_1-t_0}(x, dy_1) \nu_{t_2-t_1}(y_1, dy_2) \dots \nu_{t_{k+1}-t_k}(y_k, dy_{k+1}). \end{aligned} \quad (2.3)$$

Due to the Chapman-Kolmogorov equation, this definition is correct, i.e. if one considers an element from $Cyl_{[s,t]}^k$ as an element from $Cyl_{[s,t]}^{k+1}$ (any function of l variables y_1, \dots, y_l can be considered as a function of $l+1$ variables y_1, \dots, y_{l+1} , which does not depend on y_{l+1}), then the two corresponding formulae (2.3) will be consistent.

Proposition 2.1 *If the semigroup T_t in $C_0(\mathcal{R}^d)$ is regular and ν is its corresponding CTF, then the functional (2.3) is bounded. Hence, it can be extended by continuity to a unique bounded linear functional ν^x on $C(\dot{\mathcal{R}}_d^{[s,t]})$, and consequently there exists a (regular) complex Borel measure $D_x^{s,t}$ on the path space $\dot{\mathcal{R}}_d^{[s,t]}$ such that*

$$\nu_{s,t}^x(F) = \int F(y(\cdot)) D_x^{s,t}(dy(\cdot)) \quad (2.4)$$

for all $F \in C(\dot{\mathcal{R}}_d^{[s,t]})$. In particular,

$$(T_t f)(x) = \int f(y(t)) D_x^{s,t}(dy(\cdot)).$$

Proof. It is a direct consequence of the Riesz-Markov theorem, because the regularity of CTF implies that the norm of the functional $\nu_{s,t}^x$ does not exceed $\exp\{K(t-s)\}$. ■

Formula (2.3) defines the family of finite complex distributions on the path space, which gives rise to a finite complex measure on this path space (under the regularity assumptions). Therefore, this family of measures can be called a complex Markov process. Unlike the case of the standard Markov processes, the generator, say A , of the corresponding semigroup T_t and the corresponding bilinear "Dirichlet form" (Av, v) are complex.

The following simple fact can be used in proving the regularity of a semigroup.

Proposition 2.2 *Let B and A be linear operators in $C_0(\mathcal{R}^d)$ such that A is bounded and B is the generator of a strongly continuous regular semigroup T_t . Then $A + B$ is also the generator of a regular semigroup, which we denote by \tilde{T}_t .*

Proof. It follows directly from the fact that \tilde{T}_t can be presented as the convergent (in the sense of the norm) series of standard perturbation theory

$$\tilde{T}_t = T_t + \int_0^t T_{t-s} A T_s ds + \int_0^t ds \int_0^s d\tau T_{t-s} A T_{s-\tau} A T_\tau + \dots \quad (2.5)$$

■

Of major importance for our purposes are the spatially homogeneous CTFs. Let us discuss them in greater detail, in particular, their connection with infinitely divisible characteristic functions.

Let $\mathcal{F}(\mathcal{R}^d)$ denote the Banach space of Fourier transforms of elements of $\mathcal{M}(\mathcal{R}^d)$, i.e. the space of (automatically continuous) functions on \mathcal{R}^d of form

$$V(x) = V_\mu(x) = \int_{\mathcal{R}^d} e^{ipx} \mu(dp) \quad (2.6)$$

for some $\mu \in \mathcal{M}(\mathcal{R}^d)$, with the induced norm $\|V_\mu\| = \|\mu\|$. Since $\mathcal{M}(\mathcal{R}^d)$ is a Banach algebra with convolution as the multiplication, it follows that $\mathcal{F}(\mathcal{R}^d)$ is also a Banach algebra with respect to the standard (pointwise) multiplication. We say that an element $f \in \mathcal{F}(\mathcal{R}^d)$ is *infinitely divisible* if there exists a family $(f_t, t \geq 0)$ of elements of $\mathcal{F}(\mathcal{R}^d)$ such that $f_0 = 1$, $f_1 = f$, and $f_{t+s} = f_t f_s$ for all positive s, t . Clearly if f is infinitely divisible, then it has no zeros and a continuous function $g = \log f$ is well defined (and is unique up to an imaginary shift). Moreover, the family f_t has the form $f_t = \exp\{tg\}$ and is defined uniquely up to a multiplier of the form $e^{2\pi i k t}$, $k \in \mathcal{N}$. Let us say that a continuous function g on \mathcal{R}^d is a *complex characteristic exponent* (abbreviated CCE), if e^g is an infinitely divisible element of $\mathcal{F}(\mathcal{R}^d)$, or equivalently, if e^{tg} belongs to $\mathcal{F}(\mathcal{R}^d)$ for all $t > 0$.

Remark. The problem of the characterisation of the whole class of infinitely divisible functions (or of the corresponding complex CCEs) seems to be quite nontrivial. When dealing with this problem, it is reasonable to describe first some natural subclasses. For example, it is easy to show that if $f_1 \in \mathcal{F}(\mathcal{R})$ is infinite divisible and such that the measures corresponding to all functions f_t , $t > 0$, are concentrated on the half line \mathcal{R}_+ (complex generalisation of subordinators) and have densities from $L_2(\mathcal{R}_+)$, then f_1 belongs to the Hardy space H_2 of analytic functions on the upper half plane, which have no Blaschke product in its canonical decomposition.

It follows from the definitions that the set of spatially homogeneous CTFs $\nu_t(dx)$ is in one-to-one correspondence with CCE g , in such a way that for any

positive t the function e^{tg} is the Fourier transform of the transition measure $\nu_t(dx)$.

Proposition 2.3 *If V is a CCE, then the solution to the Cauchy problem*

$$\frac{\partial u}{\partial t} = V\left(\frac{1}{i} \frac{\partial}{\partial y}\right)u \quad (2.7)$$

defines a strongly continuous and spatially homogeneous semigroup T_t of bounded linear operators in $C_0(\mathcal{R}^d)$ (i.e. $(T_t u_0)(y)$ is the solution to equation (2.7) with the initial function u_0). Conversely, each such semigroup is the solution to the Cauchy problem of an equation of type (2.7) with some CCE g .

Proof. This is straightforward. Since (2.7) is a pseudo-differential equation, it follows that the Fourier transform $\tilde{u}(t, x)$ of the function $u(t, y)$ satisfies the ordinary differential equation

$$\frac{\partial \tilde{u}}{\partial t}(t, x) = V(x)\tilde{u}(t, x),$$

whose solution is $\tilde{u}_0(x) \exp\{tV(x)\}$. Since e^{tV} is the Fourier transform of the complex transition measure $\nu_t(dy)$, it follows that the solution to the Cauchy problem of equation (2.7) is given by the formula $(T_t u_0)(y) = \int u_0(z) \nu_t(dz - y)$, which is as required. ■

We say that a CCE is *regular*, if equation (2.7) defines a regular semigroup.

It would be very interesting to describe explicitly all regular CCE. We only give here two classes of examples. First of all, if a CCE is given by the Lévy-Khintchine formula (i.e. it defines a transition function consisting of probability measures), then this CCE is regular, because all CTF consisting of probability measures are regular. Another class is given by the following result.

Proposition 2.4 *Let $V \in \mathcal{F}(\mathcal{R}^d)$, i.e. it is given by (2.6) with $\mu \in \mathcal{M}(\mathcal{R}^d)$. Then V is a regular CCE. Moreover, if the positive measure M in the representation (2.1) for μ has no atom at the origin, i.e. $M(\{0\}) = 0$, then the corresponding measure $D_x^{0,t}$ on the path space from Proposition 2.1 is concentrated on the set of piecewise-constant paths in $\dot{\mathcal{R}}_d^{[0,t]}$ with a finite number of jumps. In other words, $D_x^{0,t}$ is the measure of a jump-process.*

Proof. Let $W = W_M$ be defined as

$$W(x) = \int_{\mathcal{R}^d} e^{ipx} M(dp). \quad (2.8)$$

The function $\exp\{tV\}$ is the Fourier transform of the measure $\delta_0 + t\mu + \frac{t^2}{2}\mu \star \mu + \dots$ which can be denoted by $\exp^*(t\mu)$ (it is equal to the sum of the standard

exponential series, but with the convolution of measures instead of the standard multiplication). Clearly $\|\exp^*(t\mu)\| \leq \|\exp^*(t\bar{f}M)\|$, where we denoted by \bar{f} the supremum of the function f , and both these series are convergent series in the Banach algebra $\mathcal{M}(\mathcal{R}^d)$. Therefore $\|e^{Vt}\| \leq \|e^{Wt}\| \leq \exp\{t\bar{f}\|\mu\|\}$, and consequently V is a regular CCE. Moreover, the same estimate shows that the measure on the path space corresponding to the CCE V is absolutely continuous with respect to the measure on the path space corresponding to the CCE W . But the latter coincides up to a positive constant multiplier with the probability measure of the compound Poisson process with the Lévy measure M defined by the equation

$$\frac{\partial u}{\partial t} = (W(\frac{1}{i} \frac{\partial}{\partial y}) - \lambda_M)u, \quad (2.9)$$

where $\lambda_M = M(\mathcal{R}^d)$, or equivalently

$$\frac{\partial u}{\partial t} = \int (u(y + \xi) - u(y)) M(d\xi). \quad (2.10)$$

It remains to note that as is well known the measures of compound Poisson processes are concentrated on piecewise-constant paths.

Therefore, we have two different classes (essentially different, because they obviously are not disjoint) of regular CCE: those given by the Lévy-Khintchine formula, and those given by Proposition 2.4. It is easy to prove that one can combine these regular CCEs, more precisely that the class of regular CCE is a convex cone, see [29].

Let us apply the simple results obtained sofar to the case of the pseudo-differential equation of the Schrödinger type

$$\frac{\partial \tilde{u}}{\partial t} = -G(-\Delta)^\alpha \tilde{u} + (A, \frac{\partial}{\partial x})\tilde{u} + V(x)\tilde{u}, \quad (2.11)$$

where G is a complex constant with a non-negative real part, α is any positive constant, A is a real-valued vector (if $\operatorname{Re} G > 0$, then A can be also complex-valued), and V is a complex-valued function of form (2.6). The standard Schrödinger equation corresponds to the case $\alpha = 1$, $G = i$, $A = 0$ and V being purely imaginary. We consider a more general equation to include the Schrödinger equation, the heat equation with drifts and sources, and also their stable (when $\alpha \in (0, 1)$) and complex generalisations in one formula. This general consideration also shows directly how the functional integral corresponding to the Schrödinger equation can be obtained by the analytic continuation from the functional integral corresponding to the heat equation, which gives a connection with other approaches to the path integration. The equation on the inverse Fourier transform

$$u(y) = (2\pi)^{-d} \int_{\mathcal{R}^d} e^{-iyx} \tilde{u}(x) dx$$

of \tilde{u} (or equation (2.11) in momentum representation) clearly has the form

$$\frac{\partial u}{\partial t} = -G(y^2)^\alpha u + i(A, y)u + V\left(\frac{1}{i}\frac{\partial}{\partial y}\right)u. \quad (2.12)$$

One easily sees that already in the trivial case $V = 0$, $A = 0$, $\alpha = 1$, equation (2.11) defines a regular semigroup only in the case of real positive G , i.e. only in the case of the heat equation. It turns out however that for equation (2.12) the situation is completely different. The following simple result (obtained from Proposition 2.3 and the Trotter formula, see [29] for details) generalises the corresponding result from [36], [37] on the standard Schrödinger equation to equation (2.11). ■

Proposition 2.5 *The solution to the Cauchy problem of equation (2.12) can be written in the form of a complex Feynman-Kac formula*

$$u(t, y) = \int \exp\left\{-\int_0^t [G(q(\tau)^2)^\alpha - (A, q(\tau))] d\tau\right\} u_0(q(t)) D_y^{0,t}(dq(.)), \quad (2.13)$$

where D_y is the measure of the jump process corresponding to equation (2.7).

As another example, let us consider the case of complex anharmonic oscillator. i.e. the equation

$$\frac{\partial \tilde{\psi}}{\partial t} = \frac{1}{2} (G\Delta - x^2 - iV(x)) \tilde{\psi}, \quad (2.14)$$

where $V = V_\mu$ is an element of $\mathcal{F}(\mathcal{R}^d)$. The Fourier transform of this equation has the form

$$\frac{\partial \psi}{\partial t} = \frac{1}{2} \left(\Delta - Gp^2 - iV\left(\frac{1}{i}\frac{\partial}{\partial p}\right) \right) \psi. \quad (2.16)$$

Proposition 2.6 *If $\operatorname{Re} G \geq 0$, the Cauchy problem of equation (2.15) defines a regular semigroup of operators in $C_0(\mathcal{R}^d)$, and thus can be presented as the path integral from Proposition 2.1.*

Proof. If $V = 0$, the Green function for equation (2.16) can be calculated explicitly, and from this formula one easily deduces that in case $V = 0$ the semigroup defined by equation (2.16) is regular. For general V the statement follows from Proposition 2.2.

The statement of the Proposition can be generalised easily to the following situation, which includes all Schrödinger equations, namely to the case of the equation

$$\frac{\partial \phi}{\partial t} = i(A - B)\phi,$$

where A is selfadjoint operator, for which therefore exists (according to spectral theory) a unitary transformation U such that UAU^{-1} is the multiplication operator in some $L^2(X, d\mu)$, where X is locally compact, and B is such that UBU^{-1} is a bounded operator in $C_0(X)$.

Since any complex measure has a density with respect to its total variation measure, it is easy to rewrite the integral in (2.13) as an integral over a positive measure. In the next section such a positive measure is constructed directly in a much more general situation. ■

3 Singular Schrödinger equations with magnetic fields

To include the case of singular Schrödinger equations, we shall consider here a formal Schrödinger operator with a magnetic field, namely the operator

$$H = \left(-i \frac{\partial}{\partial x} + A(x) \right)^2 + V(x), \quad (3.1)$$

where $\frac{\partial}{\partial x} = (\frac{\partial}{\partial x_1}, \dots, \frac{\partial}{\partial x_n})$ is the gradient operator in \mathbf{R}^d , under the following conditions (possible generalisations of these conditions are discussed in [28]):

C1) the magnetic vector-potential $A = (A^1, \dots, A^d)$ is a bounded measurable \mathbf{R}^d -valued function on \mathbf{R}^d ,

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

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

$$|\operatorname{div} A|(B_r(x)) \leq Cr^\alpha, \quad |V|(B_r(x)) \leq Cr^\alpha, \quad (3.2)$$

where $|V|, |\operatorname{div} A|$ denote the total variations of the (possibly non-positive) measures V and $\operatorname{div} A$ respectively, and $B_r(x)$ denotes the ball in \mathbf{R}^d of the radius r centered at x ; if $d = 1$, then the same holds for $\alpha = 0$.

The most popular examples of such Schrödinger operators are given by systems with δ -interaction, i.e. with potentials supported by points or smooth submanifolds (see [4], [32] and references therein), because such potentials appear in different physical models. However other generalised potentials are studied as well. In [8], the generalised Kato class of potentials (which consists of Radon measures with certain conditions) was introduced and local heat kernel estimates were obtained for the corresponding Schrödinger semigroups (without magnetic fields) using a generalisation of the probabilistic technique developed in [40]. In [9], one can find several results on the spectral analysis of singular Schrödinger equations and an extensive review of different approaches to the analysis of singular Schrödinger equations, which include non-standard analysis, the theory of Dirichlet forms, the theory of quadratic form and others. Useful

methods for studying operators (3.1) with vanishing A are developed in [3], and [43]. These methods are applied even in cases when the corresponding bilinear form is not closable. In particular, the Schrödinger operators on Riemannian manifolds (with a bounded below Ricci curvature) with potentials being almost general measures is given in [43]. The measures in [43] have neither to be regular nor to be σ -finite, the only requirement is that they do not charge polar sets. Usually, quite essential simplifications occur when applying general techniques to one-dimensional situations.

In [14], the study of the Schrödinger equations with potentials supported by a smooth surface in the presence of magnetic fields was initiated. However, no general results seem to be obtained up to now on Schrödinger equation with a magnetic field and with a potential V being a distribution. The case of magnetic fields and potentials from the Kato class (not distributions) were considered in [10], where the self-adjointness was proved by probabilistic technique of [40]. Concerning heat kernel estimates for these operators we refer to [35], [33] and references therein.

We shall formulate now a result from [28] on self-adjointness and asymptotics for the heat kernel of operator (1.1) under conditions C1)–C3). In order to give meaning to operator (3.1) we construct the corresponding semigroup e^{-tH} . Moreover, for our purposes, it will be useful to consider the following more general formal Cauchy problem

$$\frac{\partial u}{\partial t} = -DHu, \quad u|_{t=0} = u_0, \quad (3.3)$$

where the (generalised) diffusion coefficient D is an arbitrary complex number such that $\epsilon = \operatorname{Re} D \geq 0$, $|D| > 0$. In the interaction representation, equation (3.3) takes the form

$$u(t) = e^{-Dt\Delta/2}u_0 - D \int_0^t e^{-D(t-s)\Delta/2}(W - 2i(A, \nabla))u(s) ds, \quad (3.4)$$

where

$$W(x) = V(x) + |A(x)|^2 - i \operatorname{div} A(x). \quad (3.5)$$

More precisely, W is the measure, which is the sum of the measure $V - i \operatorname{div} A$ and the measure having the density $|A|^2$ with respect to Lebesgue measure. The letter W in (3.4) stands for the operator of multiplication by W .

Equation (3.4) can be solved by iterations. In the case of the Green function $G^D(t, x, y)$ (or fundamental solution) of equation (3.4), i.e. its solution with the Dirac initial condition $u_0(x) = \delta(x - y)$, the iteration procedure leads to the following representation:

$$G^D(t, x, y) = \sum_{k=0}^{\infty} I_k^D(t, x, y) \quad (3.6)$$

with $I_0^D(t, x, y) = G_{free}^D(t, x, y)$ and with other I_k^D , $k > 1$, being defined inductively by the formula

$$I_k^D(t, x, y) = -D \int_0^t \int_{\mathbf{R}^d} I_{k-1}^D(t-s, x, \xi) (W(d\xi) + 2i \frac{(A, \xi - y)}{Ds} d\xi) G_{free}^D(s, \xi - y) ds, \quad (3.7)$$

where G_{free}^D is the Green function of the "free" equation (1.1) (i.e. with $V = 0$):

$$G_{free}^D(t, x - y) = (2\pi t D)^{-d/2} \exp\left\{-\frac{(x - y)^2}{2Dt}\right\}.$$

The following theorem is proved in [28].

Theorem 3.1 (i) *If $\epsilon = \operatorname{Re} D > 0$, then all terms of series (3.6) are well defined as absolutely convergent integrals, the series itself is absolutely convergent and its sum $G^D(t, x, y)$ is continuous in $x, y \in \mathbf{R}^d$, $t > 0$ (and D) and satisfies the following estimate*

$$|G^D(t, x, y)| \leq K G_{free}^{|D|^2/\epsilon}(t, x, y) \exp\{B|x - y|\} \quad (3.8)$$

uniformly for $t \leq t_0$ with any fixed t_0 , where B, K are constants.

(ii) *The integral operators*

$$(U^D(t)u_0)(t, x) = \int u_G^D(t, x, y) u_0(y) dy \quad (3.9)$$

defining the solutions to equation (3.4) for $t \in [0, t_0]$ form a uniformly bounded family of operators $L_2(\mathbf{R}^d) \mapsto L_2(\mathbf{R}^d)$.

(iii) *If D is real, i.e. $D = \epsilon > 0$, then there exists a constant $\omega > 0$ such that the Green function G^ϵ has the asymptotic representation*

$$G^\epsilon(t, x, y) = G_{free}^\epsilon(t, x, y)(1 + O(t^\omega) + O(|x - y|)) \quad (3.10)$$

for small t and $x - y$. In case of vanishing A , the multiplier $\exp\{B|x - y|\}$ in (3.8) can be omitted, and the term $O(|x - y|)$ in (3.10) can be dropped. In this case, formula (3.10) gives global (uniform for all x, y) small time asymptotics for G^ϵ .

(iv) *One can give rigorous meaning to formal expression (3.1) as a bounded below self-adjoint operator in such a way that the family (3.9) of operators $U^D(t)$ (giving solutions to equation (3.4), which is formally equivalent to the evolutionary equation (3.3) with the formal generator DH) coincides with the semigroup $\exp\{-tDH\}$ defined by means of the functional calculus. Hence for the integral kernel of the operators $\exp\{-tDH\}$ the estimates (3.8) and (3.10) hold.*

To construct a path integral representation for the solution $U^D(t)u_0$ of equation (1.1), we shall construct a measure on a path space that is supported on the set of continuous piecewise linear paths. Denote this set by CPL . Let $CPL^{x,y}(0,t)$ denote the class of paths $q : [0, t] \mapsto \mathcal{R}^d$ from CPL joining x and y in time t , i.e. such that $q(0) = x$, $q(t) = y$. By $CPL_n^{x,y}(0,t)$ we denote its subclass consisting of all paths from $CPL^{x,y}(0,t)$ that have exactly n jumps of their derivative. Clearly, each $CPL_n^{x,y}(0,t)$ is parametrised by the simplex

$$Sim_t^n = \{s_1, \dots, s_n : 0 < s_1 < s_2 < \dots < s_n \leq t\}$$

of the times of jumps s_1, \dots, s_n of the derivatives of a path and by n positions $q(s_j)$, $j = 1, \dots, n$, of this path at these points. In other words, an arbitrary path in $CPL_n^{x,y}(0,t)$ has the form

$$q(s) = q_{\eta_1 \dots \eta_n}^{s_1 \dots s_n}(s) = \eta_j + (s - s_j) \frac{\eta_{j+1} - \eta_j}{s_{j+1} - s_j}, \quad s \in [s_j, s_{j+1}] \quad (3.11)$$

(where it is assumed that $s_0 = 0, s_{n+1} = t, \eta_0 = x, \eta_{n+1} = y$). Obviously,

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

To any \mathbf{R}^{d+1} -valued Borel measure $M = (\mu, \nu) = (\mu, \nu^1, \dots, \nu^d)$ on \mathbf{R}^d there corresponds a $(\sigma$ -finite) complex measure M^{CPL} on $CPL^{x,y}(0,t)$, which is defined as the sum of the measures M_n^{CPL} on the finite-dimensional spaces $CPL_n^{x,y}(0,t)$ such that M_0^{CPL} is just the unit measure on the one-point set $CPL_0^{x,y}(0,t)$ and each M_n^{CPL} , $n > 0$, is defined in the following way: if Φ is a functional on $CPL^{x,y}(0,t)$, then

$$\begin{aligned} \int_{CPL_n^{x,y}(0,t)} \Phi(q(\cdot)) M_n^{CPL}(dq(\cdot)) &= \int_{Sim_t^n} ds_1 \dots ds_n \\ &\times \int_{\mathcal{R}^d} \dots \int_{\mathcal{R}^d} \left(\mu + 2i \frac{(\eta_2 - \eta_1, \nu)}{s_2 - s_1} \right) (d\eta_1) \dots \left(\mu + 2i \frac{(y - \eta_n, \nu)}{t - s_n} \right) (d\eta_n) \Phi(q(\cdot)). \end{aligned} \quad (3.12)$$

Now, let $M = (W, D^{-1}A dx)$.

Theorem 3.2 *For any D with $\epsilon = \text{Re}D > 0$, the Green function G^D of equation (3.3) has the following path integral representation:*

$$G^D(t, x, y) = \int_{CPL^{x,y}(0,t)} \Phi_D(q(\cdot)) \exp\left\{-\int_0^t \dot{q}^2(s) ds / 2D\right\} M^{CPL}(dq(\cdot)), \quad (3.13)$$

with $q(s)$ given by (3.11) and

$$\Phi_D(q(\cdot)) = D^n \prod_{j=1}^{n+1} (2\pi(s_j - s_{j-1})D)^{-d/2}. \quad (3.14)$$

For any $u_0 \in L^2(\mathcal{R}^d)$ the solution $u(t, s)$ of the Cauchy problem (2.1) with $D = i$ has the form

$$u(t, x) = \lim_{\epsilon \rightarrow 0+} \int_{CPL^{x,y}(0,t)} \int_{\mathcal{R}^d} u_0(y) \Phi_{i+\epsilon}(q(\cdot)) \exp\left\{-\int_0^t \dot{q}^2(s) ds / 2(i+\epsilon)\right\} M^{CPL}(dq(\cdot)) dy, \quad (3.15)$$

where the limit is understood in L^2 -sense.

Due to the definition of M^{CPL} , the integral (3.13), if it exists, is the convergent sum of finite-dimensional integrals, which are all absolutely convergent. But one sees directly that these integrals are exactly the same as the integrals $I_k(t, x, y)$ from (3.6). This implies the validity of (3.13), because due to Theorem 3.1, series (3.6), (3.7) is absolutely convergent and all its terms are absolutely convergent integrals. Formula (3.15) follows immediately from (3.13) and (1.5).

As shown in [30], in case $A = 0$ and $d = 1$, formula (3.13) still holds for $D = i$ (i.e. for vanishing ϵ), so that in this case the Green function of the Schrödinger equation itself exists and is represented by a convergent path integral (without any regularisation). This is one of the performances of the fact mentioned in the introduction that in one-dimensional situation essential simplifications usually occur. In general, the question of existence of a pointwise limit for G^D as $D \rightarrow i$ is very subtle and is not considered here. It is reasonable to suggest (as a conjecture) that it exists if the fundamental solution (or the Green function) G^i of the Schrödinger semigroup exists as a continuous function. This latter question is quite non-trivial and only recently some results were obtained that include rather general potentials, see e.g. [45] for the case of smooth magnetic fields.

In case $A = 0$, integral (3.13) has a simple probabilistic interpretation in terms of an expectation with respect to a compound Poisson process. The following statement is a direct consequence of Theorem 3.2 and the standard properties of Poisson processes.

Theorem 3.3 *Suppose the vector potential A vanishes and V satisfies assumption C3). Suppose additionally that V has no atom at the origin and is a finite positive measure so that $\lambda_V = V(\mathcal{R}^d) > 0$. Let the paths of CPL be parametrised by (3.11). Let E_t denote the expectation with respect to the process of jumps η_j which are identically independently distributed according to the probability measure V/λ_V , and which occur at times s_j from $[0, t]$ distributed according to Poisson process of intensity λ_V . Then the integral (3.13) can be written in the form*

$$G^D(t, x, y) = e^{t\lambda_V} E_t \left(\Phi_D(q(\cdot)) \exp\left\{-\int_0^t \dot{q}^2(s) ds / 2D\right\} \right). \quad (3.16)$$

Similar representation surely holds for formula (3.15).

Let us note also that the restriction on V being finite (used in Theorem 3.3) is not essential, because clearly an arbitrary V has a density with respect to a certain finite (positive) measure \tilde{V} . Hence, one can include this density in the integrand and work with the Poisson process defined by the Lévy measure \tilde{V} .

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