Feynman (-Kac-Itô) path integrals on infinite weighted graphs

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For $H$ a magnetic Schrödinger operator on a Riemannian manifold, there are path integral formulae of the form

$$e^{-tH}\psi(x) \overset{\text{Itô integrals}}{=} \int_{\gamma(0)=x} e^{-S_t(\gamma)}\psi(\gamma(t))D\gamma \quad \ldots \text{Feynman-Kac-Itô}$$

$$e^{-itH}\psi(x) \overset{\text{heuristic}}{=} \int_{\gamma(0)=x} e^{-iS_t(\gamma)}\psi(\gamma(t))D\gamma \quad \ldots \text{Feynman}$$

Are there path integral formulae for $e^{-tH}$ and $e^{-itH}$ in case $H$ is a magnetic Schrödinger operator on an infinite weighted graph?

These $H$’s are self-adjoint in Hilbert spaces of square summable complex-valued functions on infinite countable sets, and arise naturally in approximations to solid state physics (Harper,...).
A **weighted graph** is a triple \((X, b, m)\), such that

- \(X\) is a countable set (discrete topology)
- \(b : X \times X \rightarrow [0, \infty)\) is a symmetric function with \(\sum_y b(x, y) < \infty\) for all \(x \in X\)
- \(m\) is an arbitrary function \(m : X \rightarrow (0, \infty)\).

**Interpretation:**

- \(X\): vertices of a graph
- \((x, y) \in X \times X\) with \(b(x, y) > 0\): weighted and directed edges of a graph
- \(m(x)\): weight of a vertex \(x \in X\).

**Example:** The “obvious” graph on the lattice \(X = \mathbb{Z}^d\) is given by \(b_{\mathbb{Z}^d}(x, y) = 1\) if \(|x - y|_{\mathbb{R}^d} = 1\) and \(b_{\mathbb{Z}^d}(x, y) = 0\) else. One can put weights in the obvious way.
Define the **1-forms** $\Omega^1(X)$ on $(X, b)$ to be the antisymmetric maps $\theta : \{b > 0\} \to \mathbb{C}$.

**Interpretation:** for each $x$, the only possible tangential directions are the edges emerging from $x$. Why antisymmetric $\theta$’s?

**Example:** Assume $X$ is embedded in a manifold $\tilde{X}$ and that for all $x \sim y$ there is a canonically given path $\gamma_{x,y} : [0, 1] \to \tilde{X}$ from $x$ to $y$ such that $\gamma_{y,x} = \gamma_{x,y}(1 - \bullet)$. 

$\sim$ every $\tilde{\theta} \in \Omega^1(\tilde{X})$ induces a $\theta \in \Omega^1(X)$ via

$$
\theta(x, y) := \int_0^1 \tilde{\theta}(d\gamma_{x,y}(s)).
$$
On arbitrary weighted graph \((X, b, m)\) arbitrary, we now fix...

\[ \theta \in \Omega^1_{\mathbb{R}}(X) \] ...

“magnetic potential”

\[ \nu : X \to [0, \infty) \] ...

“electric potential”
On $\Omega^1_c(X)$ we define a scalar product ("Riemannian metric") via

$$(\theta_1, \theta_2)(x) := \frac{1}{m(x)} \sum_y b(x, y) \theta_1(x, y) \theta_2(x, y),$$

and a "covariant derivative" via

$$\nabla^\theta : C_c(X) \rightarrow \Omega^1_c(X), \quad \nabla^\theta f(x, y) := e^{i\theta(x, y)} f(y) - f(x).$$

Why not $i\theta(x, y)f(y) - f(x)$ or so instead?

**Lattice gauge theory**: in the embedded case, we have to replace the infinitesimal $\nabla_{\gamma_x, y(0)}$ with $\nabla_{\gamma_x, y(\delta)}$ for some small $\delta > 0$.

**Morally**: Lie algebra $\rightarrow$ Lie group
We can define a symmetric nonnegative and closable sesquilinear form in $\ell^2(X, m)$ via

$$Q_{\theta, v}(\psi_1, \psi_2) := \frac{1}{2} \sum_x (\nabla^\theta \psi_1, \nabla^\theta \psi_2)(x)m(x) + \sum_x v(x)\psi_1(x)\psi_2(x)m(x)$$

$$= \frac{1}{2} \sum_x \sum_y b(x, y)(\psi(x) - e^{i\theta(x,y)}\psi(y))(\psi(x) - e^{i\theta(x,y)}\psi(y))$$

$$+ \sum_x v(x)\psi_1(x)\psi_2(x)m(x), \quad \psi_1, \psi_2 \in C_c(X).$$

$\Rightarrow$ $Q_{\theta, v}$ canonically induces a self-adjoint operator $H_{\theta, v} \geq 0$ in $\ell^2(X, m)$. Formally:

$$H_{\theta, v}\psi(x) = \frac{1}{m(x)} \sum_y b(x, y)(\psi(x) - e^{i\theta(x,y)}\psi(y)) + v(x)\psi(x).$$
Example: Constant magnetic field $B(x) \equiv B \in \mathbb{R}$ on $\mathbb{R}^2$

$\leadsto$ induced by the 1-form $\tilde{\theta}_B(x) = Bx_2dx^1 - Bx_2dx^2$ on $\mathbb{R}^2$

$\leadsto$ with $\gamma_{x,y} : [0, 1] \to \mathbb{R}^2$ the straight line from $x$ to $y$, define $\theta_B$ on the standard graph $(\mathbb{Z}^2, b_{\mathbb{Z}^2})$ by

$$\theta_B \psi(x, x \pm e_j) := \int_0^1 \tilde{\theta}_B(d\gamma_{x,x\pm e_j}(s)).$$

$\leadsto$ For $v : \mathbb{Z}^2 \to \mathbb{R}$ bounded, $H_{\theta_B, v}$ is bounded in $\ell^2(\mathbb{Z}^2)$ and can be calculated explicitly; this is the famous Harper operator (perturbed by $v$). The spectral theory of $H_{\theta_B, v}|_{v=0}$ is very exotic (ten martini problem...
Let us now collect the probabilistic ingredients of our path integral formulae for $e^{-tH_{\theta,v}}$ and $e^{-itH_{\theta,v}}$ ...
\[ \Omega := \text{right-continuous paths } \gamma : [0, \infty) \to X \text{ having left limits,} \]

\[ \text{with } X : [0, \infty) \times \Omega \to X, \quad X_t(\gamma) := \gamma(t) \]

the coordinate process and \( \mathcal{F} \) the sigma-algebra on \( \Omega \) generated by \( X \). \textbf{Important data:}

\[ \tau_W : \Omega \to [0, \infty] \quad \text{... first exit time of } X \text{ from } W \subset X, \]
\[ N : [0, \infty) \times \Omega \to [0, \infty] \quad \text{... } N_t := \text{number of jumps of } X \text{ until } t \geq 0, \]
\[ \tau_j : \Omega \to [0, \infty) \quad \text{... } j\text{-th jump time of } X, \quad j \in \mathbb{N}. \]

\textbf{Strategy:} For each \( x \) define a probability measure \( \mathbb{P}^x \) on \( \Omega \) with
\[ \mathbb{P}^x \{ X_0 = x \} = 1 \text{ from } H := H_{0,0}, \text{ so that } H \text{ becomes our } -\Delta \ldots \]
Introduction
Foundations of magnetic Schrödinger operators on graphs
Stochastic processes for magnetic Schrödinger operators on graphs
Feynman-Kac-Itô (FKI) formula and Feynman formula on graphs

\[ H = H_{0,0} \text{ is self-adjoint and } \geq 0 \text{ in } \ell^2(X, m), \text{ so that} \]

\[
\sum_{y \in X} e^{-tH}(x, y)m(y) \leq 1 \quad \text{for all } t > 0, \ x \in X. \quad (1)
\]

For simplicity we assume equality in (1) \( \rightsquigarrow (X, b, m) \) stochastically complete.

For every \( x \in X \) there exists a unique probability measure \( P^x \) on \( (\Omega, \mathcal{F}) \) s.t. for all \( 0 = t_0 < t_1 < \cdots < t_l, \ U_j \subset X \), with \( \delta_j := t_{j+1} - t_j, \)

\[
P^x \{ \mathbf{X}_{t_1} \in U_1, \ldots, \mathbf{X}_{t_l} \in U_l \} = \sum_{x_1, \ldots, x_l \in X} e^{-\delta_0 H(x_0, x_1)} \cdots e^{-\delta_{l-1} H(x_{l-1}, x_l)} m(x_1) \cdots m(x_l).
\]
Some path properties of $X$ under $\mathbb{P}^x$:

(i) Markov ("memoryless") property w.r.t. $\mathcal{F}_*$

(ii) $\mathbb{P}^x \{ b(X_{\tau_j}, X_{\tau_{j+1}}) > 0 \text{ for all } j \in \mathbb{N} \} = 1$

(iii) $\mathbb{P}^x \{ N_t < \infty \} = 1$, $\mathbb{P}^x \{ N_t = 0 \} = e^{-t \deg(x)}$,

with $\deg(x) := \frac{1}{m(x)} \sum_{y \in X} b(x, y)$ weighted degree function.

$\Rightarrow$ the (Itô-) integral of $\theta$ along $X$:

$$\int_0^t \theta(dX_s) : [0, \infty) \times \Omega \to \mathbb{R}, \quad \int_0^t \theta(dX_s) := \sum_{j=1}^{N_t} \theta(X_{\tau_{j-1}}, X_{\tau_j}).$$

$\Rightarrow$ $\mathbb{P}^x$-almost surely well-defined by (ii) and (iii).
Main results: let $t \geq 0$, $\psi \in \ell^2(X, m)$, $x \in X$ be arbitrary.

Theorem (FKI formula, B. G., M. Keller, M. Schmidt)

One has

$$e^{-tH_{\theta, v}} \psi(x) = \int e^{i \int_0^t \theta(dX_s) - \int_0^t v(X_s) ds} \psi(X_t) d\mathbb{P}^x.$$ 

Theorem (Feynman formula; B. G., M. Keller)

If deg is bounded, then one has

$$e^{-itH_{\theta, v}} \psi(x) = \int i^{N_t} e^{i \int_0^t \theta(dX_s) - i \int_0^t (v(X_s) + \text{deg}(X_s)) ds + \int_0^t \text{deg}(X_s) ds} \psi(X_t) d\mathbb{P}^x.$$
A sketch of proof of the Feynman formula:

First step (local formula): Pick exhaustion \( X = \bigcup_n W_n \) with finite subsets \( W_n \subset X \). Then:

\[
e^{-itH_{v,\theta}^{(W_n)}} \psi(x) = P_t \psi(x)
\]

\[
:= \int_{\{t < \tau_{W_n}\}} i N_t e^{i \int_0^t \theta (dX_s) - i \int_0^t (v(X_s) + \text{deg}(X_s)) ds + \int_0^t \text{deg}(X_s) ds} \psi(X_t) dP^X_x.
\]

Indeed, \( P_t \psi(x) \) defines a continuous semigroup in the finite dimensional Hilbert space \( \ell^2(W_n, m) \). It remains to show

\[
P_t \dot{\psi}(x)|_{t=0} = -iH_{v,\theta}^{(W_n)} \psi(x)...
\]
Explanation of $P_t\dot{\psi}(x)|_{t=0} = -iH_{\nu,\theta}^{(W_n)}$: one has

$$H_{\nu,\theta}^{(W_n)}\psi(x) = \text{deg}(x)\psi(x) + \nu(x)\psi(x) + \theta\text{-part}, \quad x \in W_n.$$ 

Using $1\{t<\tau_{W_n}\} = 1\{N_t=0\} + 1\{t<\tau_{W_n}, N_t\geq 1\}$ $\mathbb{P}^x$-a.s., we find

$$\frac{1}{t}P_t\psi(x) - \frac{1}{t}\psi(x)(x)$$
$$\frac{1}{t} \int_{\{N_t=0\}} e^{-it\nu(x)-it\text{deg}(x)+t\text{deg}(x)}\psi(x) d\mathbb{P}^x - \frac{1}{t}\psi(x) + R(t).$$

For $t \to 0+$, the difference produces the $-i(\text{deg}(x) + \nu(x))$ part of $-iH_{\nu,\theta}^{(W_n)}\psi(x)$, using $\mathbb{P}^x\{N_t = 0\} = e^{-t\text{deg}(x)}$.

The remainder $R(t)$ produces $-i$ times the $\theta$-part as $t \to 0+$. 
Second step (local to global): Take $n \to \infty$:

LHS $\ e^{-itH_{v,\theta}} \psi(x) \to e^{-itH_{v,\theta}^{(W_n)}} \psi(x)$ by Mosco convergence.

RHS: using $1\{t<\tau_{W_n}\} \to 1$ and dominated convergence. Integrable majorant:

$$\left| 1\{t<\tau_{W_n}\} i^{N_t} e^{i \int_0^t \theta (dX_s)} - i \int_0^t (\nu(X_s) + \deg(X_s)) ds + \int_0^t \deg(X_s) ds \psi(X_t) \right|$$

$$\leq e^{\int_0^t \deg(X_s) ds} \psi(X_t),$$

which corresponds to the nonmagnetic operator $H_0, -\deg$ by the well-known Feynman-Kac formula (Trotter + Markov)

$$e^{-tH_0, -\deg} |\psi|(x) = \int e^{\int_0^t \deg(X_s) ds} |\psi|(X_t) dP^x < \infty.$$
Remarks, applications and outlook:

i) stochastic completeness and $\nu \geq 0$ can be removed

ii) $|e^{-itH_\theta,\nu}\psi(x)| \leq e^{-tH_0,-\deg}|\psi|(x)$ ... seems completely new

iii) $|e^{-tH_\theta,\nu}\psi(x)| \leq |e^{-tH_0,\nu}|\psi|(x)$ ... as expected,

$\implies$ diamagnetism: $\inf\text{spec}(H\_\theta,\nu) \geq \inf\text{spec}(H_0,\nu)$.

Good for the existence of the world that we chose $e^{i\theta}$ and not $i\theta$!

iv) path integral formula for the composition $e^{itH_\theta,\nu}e^{-itH_{\theta'},\nu'}$. Scattering?

v) Physical interpretation of $i^N t$ in the Feynman formula?
Thank you for listening!