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

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

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

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

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 θ'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 $\gamma_{y,x} = \gamma_{x,y}(1 - \bullet)$.
$\rightsquigarrow$ 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"

$v : X \to [0, \infty)$ ... "electric potential"

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

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

and a "covariant derivative" via

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

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 $\nabla_{\dot\gamma_{x,y}(0)}$ with $//^{\nabla}_{\gamma_{x,y}}(\delta)$ for some small $\delta > 0$.

Morally: Lie algebra $\to$ Lie group

We can define a **symmetric nonnegative and closable** sesquilinear form in $\ell^2(X, m)$ via

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

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

$$+ \sum_x v(x)\psi_1(x)\overline{\psi_2(x)} m(x), \qquad \psi_1, \psi_2 \in C_c(X).$$

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

$$H_{\theta,v}\psi(x) = \frac{1}{m(x)}\sum_y b(x,y)\big(\psi(x) - e^{i\theta(x,y)}\psi(y)\big) + v(x)\psi(x).$$

Example: Constant magnetic field $B(x) \equiv B \in \mathbb{R}$ on $\mathbb{R}^2$

$\rightsquigarrow$ induced by the 1-form $\tilde{\theta}_B(x) = Bx_2 dx^1 - Bx_2 dx^2$ on $\mathbb{R}^2$

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

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

$\rightsquigarrow$ 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 explicitely; 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 $e^{-itH_{\theta,v}}$...

$\Omega :=$ right-continuous paths $\gamma : [0, \infty) \to X$ having left limits,

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

the coordinate process and $\mathscr{F}$ the sigma-algebra on Ω generated by $\mathbb{X}$. **Important data:**

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

Strategy: For each x define a probability measure $\mathbb{P}^x$ on Ω with $\mathbb{P}^x\{\mathbb{X}_0 = x\} = 1$ from $H := H_{0,0}$, so that H becomes our $-\Delta$...

$H = H_{0,0}$ is self-adjoint and ≥ 0 in $\ell^2(X, m)$, so that

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

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

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

$$\mathbb{P}^x\{\mathbb{X}_{t_1} \in U_1, \ldots, \mathbb{X}_{t_l} \in U_l\}$$
$$= \sum_{x_1,\ldots,x_l \in X} e^{-\delta_0 H}(x_0, x_1) \cdots e^{-\delta_{l-1} H}(x_{l-1}, x_l) m(x_1) \cdots m(x_l).$$

Some path properties of $\mathbb{X}$ under $\mathbb{P}^x$:

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

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

(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**.

⇝ the **(Itô-) integral** of θ along $\mathbb{X}$:

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

⇝ $\mathbb{P}^x$-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

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

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

If $\deg$ *is bounded, then one has*

$$\begin{aligned} &e^{-itH_{\theta,v}}\psi(x) \\ &= \int i^{N_t} e^{i\int_0^t \theta(d\mathbb{X}_s) - i\int_0^t (v(\mathbb{X}_s) + \deg(\mathbb{X}_s))ds + \int_0^t \deg(\mathbb{X}_s)ds}\psi(\mathbb{X}_t)d\mathbb{P}^x. \end{aligned}$$

A sketch of proof of the Feynman formula:

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

$$e^{-itH^{(W_n)}_{v,\theta}}\psi(x) = P_t\psi(x)$$
$$:= \int_{\{t<\tau_{W_n}\}} i^{N_t} e^{i\int_0^t \theta(d\mathbb{X}_s) - i\int_0^t (v(\mathbb{X}_s)+\mathrm{deg}(\mathbb{X}_s))ds + \int_0^t \mathrm{deg}(\mathbb{X}_s)ds} \psi(\mathbb{X}_t) d\mathbb{P}^x.$$

Indeed, $P_t\psi(x)$ defines a continuous semigroup in the finite dimensional Hilbert space $\ell^2(W_n, m)$. It remains to show $P_t\dot{\psi}(x)|_{t=0} = -iH^{(W_n)}_{v,\theta}\psi(x)$...

Explanation of $P_t\dot{\psi}(x)|_{t=0} = -iH^{(W_n)}_{v,\theta}$**:** one has

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

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

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

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

The remainder $R(t)$ produces $-i$ times the θ-part as $t \to 0+$.

Second step (local to global): Take $n \to \infty$:

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

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

$$\left|1_{\{t<\tau_{W_n}\}} i^{N_t} e^{i\int_0^t \theta(d\mathbb{X}_s) - i\int_0^t (v(\mathbb{X}_s)+\deg(\mathbb{X}_s))ds + \int_0^t \deg(\mathbb{X}_s)ds}\psi(\mathbb{X}_t)\right|$$
$$\leq e^{\int_0^t \deg(\mathbb{X}_s)ds}\psi(\mathbb{X}_t),$$

which corresponds to the nonmagnetic operator $H_{0,-\deg}$ by the well-known Feynman-Kac formula (Trotter+Markov)

$$e^{-tH_{0,-\deg}}|\psi|(x) = \int e^{\int_0^t \deg(\mathbb{X}_s)ds}|\psi|(\mathbb{X}_t)d\mathbb{P}^x < \infty.$$

Remarks, applications and outlook:

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

ii) $|e^{-itH_{\theta,v}}\psi(x)| \leq e^{-tH_{0,-\mathrm{deg}}}|\psi|(x)$ ... seems completely new

iii) $|e^{-tH_{\theta,v}}\psi(x)| \leq |e^{-tH_{0,v}}|\psi|(x)$ ... as expected,

$$\rightsquigarrow \text{diamagnetism:} \quad \inf \mathrm{spec}(H_{\theta,v}) \geq \inf \mathrm{spec}(H_{0,v}).$$

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

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

v) Physical interpretation of i^{N_t} in the Feynman formula?

Thank you for listening!