Introduction to mathematical physics: Quantum dynamics Exam Project

Project 8: Trotter product formula and "Feynman path integrals"

Suggestion for an outline

As a first step, prove the following result given in Theorem VIII.30 of the book "M. Reed, B. Simon, *Methods of Modern Mathematical Physics I: Functional Analysis*":

Let $\mathcal{H}$ be a complex Hilbert space and assume A and B are self-adjoint operators on $\mathcal{H}$ such that $A+B$ is self-adjoint on $D_0 := D(A) \cap D(B)$. Show that then for any $t \in \mathbb{R}$ and $\psi \in \mathcal{H}$

$$\lim_{n\to\infty} \left(\mathrm{e}^{-\mathrm{i}\frac{t}{n}A}\mathrm{e}^{-\mathrm{i}\frac{t}{n}B}\right)^n \psi = \mathrm{e}^{-\mathrm{i}t(A+B)}\psi\,.$$

Apply this result to find a class of potentials $V : \mathbb{R}^d \to \mathbb{R}$ for which the "Feynman path integral approximation works". More precisely, set $\mathcal{H} := L^2(\mathbb{R}^d)$ and define $H := H_0 + V$ as an operator sum, with V "nice enough". Choose initial data $\psi_0 \in \mathcal{H}$ and set $\psi_t := \mathrm{e}^{-\mathrm{i}tH}\psi_0$ for $t \in \mathbb{R}$. Show that then for all testfunctions $f \in \mathcal{S}_d$ and any $t \neq 0$ one has

$$(f, \psi_t) = \lim_{n\to\infty} \int_{(\mathbb{R}^d)^{n+1}} \left(\prod_{k=0}^{n} \mathrm{d}^d\mathbf{x}_k\right) \left(\frac{n}{\mathrm{i}2\pi t}\right)^{\frac{nd}{2}} f(\mathbf{x}_0)^*\psi_0(\mathbf{x}_n)\mathrm{e}^{\mathrm{i}tS_n(t,x)}\,,$$

where the notation refers to an iterated integral, performed in the order dictated by k, i.e., $\mathrm{d}^d\mathbf{x}_k$ with $k = 0$ first, then $k = 1$, etc., and S_n reads

$$S_n(t,x) := \frac{1}{n}\sum_{k=1}^{n} \frac{1}{2}\frac{n^2}{t^2}(\mathbf{x}_k - \mathbf{x}_{k-1})^2 - \frac{1}{n}\sum_{k=1}^{n} V(\mathbf{x}_k)\,.$$

(S_n corresponds to an approximation to an action functional over a path which is stepwise constant. Hint: Homework set 7.)

If you wish, you can try to add suitable regularizations to find a formula which does not require any specific order of integration, or is valid, for instance, for molecular Hamiltonians.