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Quasi-Feynman formulas – a method of obtaining the evolution operator for the Schrödinger equation

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ABSTRACT

For a densely defined self-adjoint operator $\mathcal{H}$ in Hilbert space $\mathcal{F}$ the operator $\exp(-it\mathcal{H})$ is the evolution operator for the Schrödinger equation $i\psi'_t = \mathcal{H}\psi$, i.e. if $\psi(0,x) = \psi_0(x)$ then $\psi(t,x) = (\exp(-it\mathcal{H})\psi_0)(x)$ for $x \in Q$. The space $\mathcal{F}$ here is the space of wave functions ψ defined on an abstract space Q, the configuration space of a quantum system, and $\mathcal{H}$ is the Hamiltonian of the system. In this paper the operator $\exp(-it\mathcal{H})$ for all real values of t is expressed in terms of the family of self-adjoint bounded operators $S(t)$, $t \geq 0$, which is Chernoff-tangent to the operator $-\mathcal{H}$. One can take $S(t) = \exp(-t\mathcal{H})$, or use other, simple families S that are listed in the paper. The main theorem is proven on the level of semigroups of bounded operators in $\mathcal{F}$ so it can be used in a wider context due to its generality. Two examples of application are provided.

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Contents

1. Introduction

A Feynman formula (in the sense of Smolyanov [38]) is a representation of a function as the limit of a multiple integral where the multiplicity tends to infinity. Usually this function is a solution to the Cauchy problem for a partial differential equation (PDE). In this paper we introduce a more general concept:

Definition 1.1. A quasi-Feynman formula is a representation of a function in a form which includes multiple integrals of an infinitely increasing multiplicity.

The difference with a Feynman formula is that in a quasi-Feynman formula summation and other functions/operations may be used while in a Feynman formula only the limit of a multiple integral where the multiplicity tends to infinity is allowed. Both Feynman formulas and quasi-Feynman formulas approximate Feynman path integrals.

Formula (2) and other formulas from Theorem 3.1 are examples of quasi-Feynman formulas for the case when the (later discussed) family $(S(t))_{t\geq 0}$ consists of integral operators; the obtained formulas give the exact solution to the Cauchy problem for the Schrödinger equation.

It is known that the solution to the Cauchy problem for the Schrödinger equation $i\psi_t'(t,x) = \mathcal{H}\psi(t,x)$, $\psi(0,x) = \psi_0(x)$ is given by the formula $\psi(t,x) = (\exp(-it\mathcal{H})\psi_0)(x)$; the evolution operator $\exp(-it\mathcal{H})$ is a one-dimensional (parametrized by $t \in \mathbb{R}$) group of unitary operators in Hilbert space. Because of the quantum mechanical significance, the properties of $\exp(-it\mathcal{H})$ have been extensively studied. Research topics include e.g. exact solutions to the Cauchy problem, asymptotic behavior, estimates, related spatio-temporal structures, wave traveling, boundary conditions and other. Some of the recent papers related to the Cauchy problem solution study are [22,28,26,41,14,15,23,25,1].

In this paper we propose a method of obtaining formulas that express $\exp(-it\mathcal{H})$ in terms of the coefficients of the operator $\mathcal{H}$. The solution is obtained in the form of a quasi-Feynman formula. Quasi-Feynman formulas are easier to obtain (compared with Feynman formulas) but they provide lengthier approximation expressions.

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