COMPUTING SEMCLASSICAL QUANTUM DYNAMICS WITH THE HERMAN-KLUK PROPAGATOR

DAVID SATTLEGGER

Abstract.
Let us consider the Schrödinger equation on $L^2(\mathbb{R}^d)$ in semiclassical scaling, i.e.

$$i\varepsilon\frac{d}{dt}\psi_t = H^\varepsilon\psi_t \tag{0.1}$$

with a small parameter $\varepsilon > 0$ and a self-adjoint operator H^ε.

The Herman-Kluk propagator is introduced. It is a special case of a global Fourier Integral Operator with complex valued phase. It approximates the unitary propagator associated to (0.1) up to an error of order one in the semiclassical parameter ε in the operator norm.

The main goal of my work is to transform the Herman-Kluk propagator to a practical, numerically stable tool for the solution of for the Schrödinger equation.

The talk will be organized as follow. First, the Herman-Kluk propagator and its properties will be introduced. Then, some preliminary considerations of how to solve the underlying ordinary differential equations are made. After that I will present the actual algorithm I propose for the computation of the propagator. Finally, the results are illustrated by numerical experiments.