An efficient method to approximate wave packets on the whole real line

Arieh Iserles, Karen Luong
University of Cambridge (United Kingdom)

Marcus Webb
University of Manchester (United Kingdom)

k.luong@damtp.cam.ac.uk

Abstract

Highly oscillatory wave packets play an important role in quantum mechanics especially in the semi-classically scaled time dependent Schrödinger equation. We compare three different orthogonal system in $L_2(\mathbb{R})$ which can be used to build a spectral method for solving such problems. These systems all have banded skew-Hermitian differentiation matrices, which implies that they will respect the Born interpretation of quantum mechanics, and the linear algebra of the spectral method is simplified. We show in the high-frequency regime, that the Malmquist–Takenaka basis is superior, in a practical sense, to the more commonly used Hermite functions and Stretched Fourier expansions for approximating wave packets. We also show that Malmquist–Takenaka expansions converge exponentially fast to wave packets, which goes against the established theory on this basis. The main body of the talk will look at our proof which uses the method of steepest descent in the complex plane. This is joint work with Arieh Iserles (Cambridge) and Marcus Webb (Manchester).