Numerical solution of the Schrödinger equation on the whole real line

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Abstract

A common approach to approximating the solution to the Schrödinger equation is Fourier spectral methods, because special properties of the Fourier basis allow fast algorithms to compute them. However, this forces the solution to live in the periodic domain of the Fourier basis, which conflicts with the Schrödinger equation's natural setting in Euclidean space. This actually poses a time limit on the accuracy of the approximation, because any waves which encounter the edge of the periodic domain experience a non-physical wrap-around effect. In this talk, we discuss whether the success of Fourier spectral methods can be translated to the whole real line.

This is joint work with Katharina Schratz (Sorbonne), Arieh Iserles (Cambridge), Karen Luong (Cambridge), and Karolina Kropielnicka (IM PAN).