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**An efficient Multigrid calculation of the Far Field Map for
Schrödinger Equations**

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Predicting the outcome of collisions between small atomic and molecular systems is of fundamental importance for many areas of science. Understanding their dynamics is crucial for example for plasma physics, combustion and electron driven chemistry, amongst other examples. However, it is computationally very challenging to predict from first principles the outcome of these collisions since it requires the solution of high-dimensional Schrödinger equation. These are known to be hard to solve even with the best current iterative methods. To calculate, for example, the breakup reaction rates of the hydrogen molecule requires the solution of a 7-dimensional scattering problem. The reaction rates, also known as the cross sections, are the far field amplitudes of solution. The development of efficient solvers for this problem remains important challenge. In this talk we discuss the development of solvers for these scattering based on multigrid.

The Schrödinger equation in d -dimensions is

$$(-\frac{1}{2}\Delta + V(\mathbf{x}) - E)\psi(\mathbf{x}) = \phi(\mathbf{x}), \quad \text{for } \mathbf{x} \in \mathbb{R}^d \quad (1)$$

where $V(\mathbf{x})$ is the potential, ψ is the wave function and ϕ is the right hand side that is related to the initial state of the system.

Scattering problems are described by solutions of (1) with a positive energy E and for these energies the equation is equivalent to a Helmholtz equation

$$(-\Delta - k^2(\mathbf{x}))u = f \quad (2)$$

with a wave number $k^2(\mathbf{x}) = 2(E - V(\mathbf{x}))$ solved with absorbing boundary conditions.

In this talk we discuss the current practices in solving the Schrödinger equation [1, 2] and relate them to the challenges of solving the Helmholtz equation. We also illustrate how advances such as Complex Shifted Laplacian [3] and complex contour multigrid [4] are applied to solve the Schrödinger equation.

Bibliography

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