**Title：**

**Computing resonant states of a quantum mechanical three-body problem on supercomputers**

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Abstract：

This project focuses on solving large nonlinear eigenvalue equations in quantum mechanics. Some efficient numerical methods are introduced to compute resonant states of a quantum mechanical three-body problem in low dimensions which gives rise to large quadratic eigenvalue problems (QEP).

Computing resonant states of a quantum system is essentially equivalent to solving the stationary Schrödinger equation with some specific boundary conditions. Through pseudo-spectral methods, we can convert the original continuous equation into a matrix-represented quadratic eigenvalue problem. The main goal of the project is to find an efficient way to solve the large QEP.

Linearization is a conventional approach to solve QEPs, transforming a quadratic eigenvalue problem to a generalized (or standard) eigenvalue problem. Besides, to avoid reducing the original problem like linearization, one can also make use of some iterative methods directly. The Jacobi Davidson method is a good choice. Applying different variants of JD algorithm to find several eigenvalues of standard or generalized eigenvalue problems has been discussed a lot so far. However, searching several eigenvalues of a QEP based on JD algorithm can still be seen as a challenge. This project will exploit both linearization method and variants of JD algorithm to solve large quadratic eigenvalue problems. At last, this project will try to parallelize the algorithm on supercomputers.