Numerical solutions of the Schrödinger equation for the ground lithium by the finite element method

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Abstract

In the present paper, the authors transfers the nine-dimensional Schrödinger equation of the ground lithium into a six-dimensional partial differential equation. A six-dimensional variational formulation is also derived from the weak energy equation. A kind of six-dimensional finite element methods are constructed to solve the transferred energy equation. With very coarse mesh, the authors get highly precise approximate eigenvalue. The relative error of approximate eigenvalue is order of 10^{-5} in atomic unit.

Keywords: Finite element method; Eigenvalue problem; Schrödinger equation

1. Introduction

Multi-body Coulomb problems are traditional challenging problems. The failure of theory to describe precisely the system stimulated many mathematicians and physicists to devote themselves in using various methods to obtain the energies and other expectation values. Few-electron systems like helium and lithium are typical models. Furthermore, helium and lithium atomic systems have their physical importance.

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