Recent progress with the Mapped Fourier Grid Method

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February 25, 2002

The Fourier grid method is known as an efficient numerical tool to solve the radial Schrödinger equation [1]. For an accurate determination of the energies and wavefunctions of vibrational levels of cold molecules it is convenient to use an adaptive coordinate scaled on the local de Broglie wave length [2]. The transformed Schrödinger equation is expanded in orthogonal basis functions [3, 4, 5]. Problems may arise with unphysical solutions, reducing the accuracy of wave packet propagation in time-dependent problems. In order to solve this problem, we have examined various sets of basis functions.

We shall discuss two basis sets:

- Plane waves obeying periodic boundary conditions. The kinetic energy operator is evaluated by discrete Fourier transforms. Spurious levels may be partly suppressed through use of a periodic mapping function.

- Sine functions obeying strict boundary conditions. The kinetic energy operator is evaluated by discrete sine / cosine transforms. No spurious levels were found.

Examples of the accuracy of the method will be given. Vibrational levels of alkali dimers such as Rb$_2$, RbCs, Cs$_2$ with binding energies as small as 10$^{-10}$ cm$^{-1}$ and with wavefunctions extending up to 10$^6$ a.u. have been computed.

References


