

The rotating Morse potential model for diatomic molecules in the tridiagonal J -matrix representation: I. Bound states

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Abstract

This is the first in a series of articles in which we study the rotating Morse potential model for diatomic molecules in the tridiagonal J -matrix representation. Here, we compute the bound-state energy spectrum by diagonalizing the finite-dimensional Hamiltonian matrix of H_2 , LiH, HCl and CO molecules for arbitrary angular momentum. The calculation was performed using the J -matrix basis that supports a tridiagonal matrix representation for the reference Hamiltonian. Our results for these diatomic molecules have been compared with available numerical data satisfactorily. The proposed method is handy, very efficient, and it enhances accuracy by combining analytic power with a convergent and stable numerical technique.

1. Introduction

The Morse potential plays a dominant role in describing the interaction of atoms in diatomic and even polyatomic molecules [1–3]. An effective potential, which is the sum of the centrifugal potential term that depends on the angular momentum ℓ and the Morse potential, has been used as a model for such interactions. It is referred to as the rotating Morse potential. For $\ell = 0$, the radial Schrödinger equation with this potential has been solved exactly [1]. However, for $\ell > 0$ only numerical solutions are possible where several approximation techniques have been proposed and extensively used with varying degrees of accuracy and stability [4–19].

Numerical solutions, with and without the Pekeris approximation, have been used to calculate the energy spectrum [4–7]. The Pekeris approximation [4] is based on the expansion of the centrifugal part in exponential terms with exponents that depend on an inter-nuclear distance parameter. This is why the Pekeris approximation is valid only for very small spatial variations from the inter-nuclear separation (i.e. for low vibrational energy). Other methods that have also been used include the variational method with the Pekeris approximation [8], supersymmetry (SUSY) [9, 10], the hyper-virial (HV) perturbation method with the full