

The rotating Morse potential model for diatomic molecules in the J -matrix representation: II. The S -matrix approach

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Received 6 July 2008, in final form 21 September 2008

Published 13 October 2008

Online at stacks.iop.org/JPhysB/41/215001

Abstract

This is the second article in which we study the rotating Morse potential model for diatomic molecules using the tridiagonal J -matrix approach. Here, we further improve the accuracy of computing the bound states and resonance energies for this potential model from the poles of the S -matrix for arbitrary angular momentum. The calculation is performed using an infinite square integrable basis that supports a tridiagonal matrix representation for the reference Hamiltonian, which is included in the computations analytically without truncation. Our method has been applied to both the regular and inverted Morse potential with favourable results in comparison with available numerical data. We have also shown that the present method adds a few significant digits to the accuracy obtained from the finite dimensional approach (e.g. the complex rotation method). Moreover, it allows us to easily handle both analytic and non-analytic potentials as well as $1/r$ singular potentials.

It is well known that the Morse potential model describes very well the vibrations of diatomic molecules [1]. This is because such systems can be modelled by two positive charges (the two atomic nuclei) that produce the Coulomb potential in which the electronic cloud moves. A similar type of modelling was also applied to nuclear molecules [2]. However, in this case there are no well-defined centres and the potential in which the nucleons move arises from the sum of interaction between all nucleons. In the language of energy scales, the electronic excitation energy, the vibration energy and the rotational molecular energy for diatomic molecules are widely separated energy scales, hence making the three degrees of freedom completely uncoupled. For a nuclear molecule, on the other hand, the single nucleon excitation and rotational energies are comparable for even the lowest angular momentum. Thus, it is expected that the energy associated with vibrations of the inter-nuclear coordinates will also be of the same order of magnitude. This will lead to a more complex energy spectrum reflecting the much stronger coupling among the intrinsic, vibrational and rotational degrees of freedom of nuclear molecules.

The Morse potential is an element in the class of potentials for which an analytic solution of the Schrödinger equation exists for zero angular momentum [3]. It is written as

$$V_M(r) = V_0[e^{-2\alpha(x-r_0)} - 2e^{-\alpha(x-r_0)}], \quad x = r/r_0, \quad (1)$$

where V_0 is the strength of the potential (or the dissociation energy in the context of diatomic molecules), r_0 is the equilibrium intermolecular distance and α is a positive number controlling the decay length of the potential. For $V_0 > 0$, this potential has a minimum of $-V_0$ at $r = r_0$ and it is called the regular Morse potential. For $V_0 < 0$, it has a maximum of $-V_0$ there and it is called the inverted Morse potential. Asymptotically (as r becomes very large), it goes to zero. The rotating Morse potential is the sum of the repulsive centrifugal potential barrier, $\frac{\hbar^2 \ell(\ell+1)}{2m r^2}$, and the Morse potentials (1). Generally, this effective potential shows a valley followed by a potential barrier which will then have two major effects. For the inverted Morse potentials where $V_0 < 0$, some resonances will be developed and the number of bound states will be reduced as ℓ increases. There will also be a critical angular momentum value, ℓ_c , beyond which no bound states