The rotating Morse potential energy eigenvalues solved by using the analytical transfer matrix method*

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We study the eigenvalues of the rotating Morse potential by using the quantization condition from the analytical transfer matrix (ATM) method. A hierarchy of supersymmetric partner potentials is obtained with Pekeris approximation, which can be used to calculate the energies of higher rotational states from the energies of lower states. The energies of rotational states of the hydrogen molecule are calculated by the ATM condition, and comparison of the results with those from the hypervirial perturbation method reveals that the accuracy of the approximate expression of Pekeris for the eigenvalues of the rotating Morse potential can be improved substantially in the framework of supersymmetric quantum mechanics.

Keywords: rotating Morse potential, analytical transfer matrix (ATM), Pekeris approximation, supersymmetry quantum mechanics (SUSY QM)

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1. Introduction

The Schrödinger equation is an old and classical problem with a more than 80-year history. It describes the particle behaviour in nonrelativistic quantum mechanics and relates to many branches of physics. It can be used to compute the tunneling process involved in alpha emission and proton fusion. In a general condensed matter system, electronic properties of material are commonly described by nonrelativistic electrons, each of which has a finite mass and obeys the Schrödinger equation.

The Schrödinger equation can be solved exactly for several potentials. One of them is the Morse potential when the angular momentum quantum number is equal to zero. It plays an important role in describing the interaction between atoms in a diatomic molecule and those in a polyatomic molecule and has attracted much attention.[1−10] When rotation is included, the angular momentum quantum number is not equal to zero and an effective potential is used to describe the interactions between atoms in the Schrödinger equation. The effective potential is the sum of the centrifugal potential term that depends on the angular momentum and the Morse potential. It is known as the rotating Morse potential.

When the rotating Morse potential is used as a model to obtain the vibrational energy spectrum of diatomic molecules, many approximate methods are used to solve the Schrödinger equation analytically or semi-analytically.[4−10] Pekeris approximation is one of the widely used methods and it is based on the expansion of the centrifugal part in exponential terms with exponents that depend on an inter-nuclear distance parameter.[4] The Pekeris approximation is valid only for low vibrational energy. Other methods that have also been widely used include supersymmetry,[5,9] the shifted $1/N$ expansion,[6] the variational method with the Pekeris approximation,[8] and the hypervirial perturbation method with the full potential without the Pekeris approximation.[10]

Our approach to the study of the rotating Morse potential model is inspired by the analytical transfer matrix (ATM) method combined with supersymmetric quantum mechanics.[11] Taking into account the correct phase losses at the turning points and the phase contribution of the scattered subwaves, the ATM quantization condition was applied to an arbitrary one-dimensional potential successfully.[11−15] Supersymmetry (SUSY) is a symmetry that relates elementary particles of one spin to other particles that differ by half a unit of spin and are known as super-

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partners. We use SUSY quantum mechanics (QM) to improve the accuracy of the original Pekeris expression for the energy eigenvalues of the rotating Morse potential. With the developed approximation method, we can apply the ATM condition to the rotating Morse potential and obtain the solutions for all the partner potentials.

The rest of the present paper is organized as follows: in Section 2, we summarize the theoretical formalism of our approach. In Section 3, we apply our approach to the calculation of the energy eigenvalues for the rotating Morse potential and compare our results with those obtained by other methods. Finally, some conclusions are drawn from the present study in Section 4.

2. Theory

2.1. Basic equations of SUSY QM

In a theory with unbroken supersymmetry, for each type of boson there exists a corresponding type of fermion with the same mass and internal quantum numbers, and *vice versa*. A SUSY QM system is described by the Hamiltonians acting on the wave function[16]

$$\begin{aligned} H_{1,2}\psi_0^{(1)} &= \left(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + W^2(x) \mp \frac{\hbar}{\sqrt{2m}}W'(x)\right)\psi_0^{(1)} \\ &= \left(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V_{1,2}(x)\right)\psi_0^{(1)}, \end{aligned} \tag{1}$$

where Hamiltonian H_1 has a known ground state wave function $\psi_0^{(1)}$ and ground state energy adjusted to zero, i.e., $E_0^{(1)} = 0$. A basic idea of SUSY QM is to link the ground-state eigenfunction $\psi_0^{(1)}$ to the superpotential[17]

$$W(x) = -\frac{\hbar}{\sqrt{2m}}\frac{\psi_0^{(1)\prime}}{\psi_0^{(1)}}. \tag{2}$$

The superpotential $W(x)$ can be related to $V_{1,2}(x)$ through

$$\begin{aligned} V_1(x) &= W^2(x) - \frac{\hbar}{\sqrt{2m}}W'(x), \\ V_2(x) &= W^2(x) + \frac{\hbar}{\sqrt{2m}}W'(x). \end{aligned} \tag{3}$$

The potentials $V_1(x)$ and $V_2(x)$ are SUSY partner potentials according to the superpotential. In this case, Hamiltonians H_1 and H_2 have identical bound-state spectra, except for the ground state of H_1 which is missing from the spectrum of H_2, and their energy eigenvalues satisfy the following relation

$$E_n^{(2)} = E_{n+1}^{(1)}, \quad n = 0, 1, 2, \ldots, \quad E_0^{(1)} = 0. \tag{4}$$

With the operators

$$\begin{aligned} A &= \frac{\hbar}{\sqrt{2m}}\frac{\mathrm{d}}{\mathrm{d}x} + W(x), \\ A^\dagger &= -\frac{\hbar}{\sqrt{2m}}\frac{\mathrm{d}}{\mathrm{d}x} + W(x), \end{aligned} \tag{5}$$

we can factorize the Hamiltonian $H_{1,2}$ as

$$H_1 = A^\dagger A, \quad H_2 = AA^\dagger. \tag{6}$$

A hierarchy of SUSY partner Hamiltonians can be constructed by using the operators

$$H_n = A_n^\dagger A_n + E_{n-1}^{(1)} = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V_n(x), \tag{7}$$

where

$$A_n = \frac{\hbar}{\sqrt{2m}}\frac{\mathrm{d}}{\mathrm{d}x} + W_n(x), \tag{8}$$

$$W_n(x) = -\frac{\hbar}{\sqrt{2m}}\frac{\mathrm{d}\ln\psi_0^{(n)}(x)}{\mathrm{d}x}, \tag{9}$$

$$\begin{aligned} V_n(x) &= V_{n-1}(x) - \frac{\hbar^2}{m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\ln\psi_0^{(n-1)}(x) \\ &= V_1(x) - \frac{\hbar^2}{m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} \\ &\quad \times \ln\left(\psi_0^{(1)}(x)\ldots\psi_0^{(n-1)}(x)\right), \end{aligned} \tag{10}$$

$n = 2, 3, \ldots, N$, and whose spectra satisfy the conditions

$$\begin{aligned} &E_m^{(n)} = E_{m+1}^{(n-1)} = \cdots = E_{m+n-1}^{(1)}, \\ &m = 0, 1, 2, \ldots, N-n; \quad n = 2, 3, \ldots, N, \end{aligned} \tag{11}$$

with N being the number of bound states supported by the potential $V_1(x)$. If we have a known Hamiltonian H_1 which has N bound states with eigenvalues $E_m^{(1)}$ and eigenfunctions $\psi_m^{(1)}$ with $0 \le m \le N-1$, we can generate a hierarchy of $N-1$ Hamiltonians $H_2, H_3, \ldots, H_n$ with the property that the n-th member of the hierarchy H_n has the same spectrum as that of H_1 except H_n in which the first $n-1$ eigenvalues of H_1 are missing. In particular, the energy of the n-th excited state of H_1 is degenerate with respect to the ground state of H_{n+1} and their wave functions are simply related to each other.

2.2. Analytical transfer matrix method

Here we present a brief review of the ATM theory. The ATM quantization condition for an arbitrary one-dimensional potential well takes the form[15]

$$\int_{x_1}^{x_2} \sqrt{E_n - V(x)}\,\mathrm{d}x + \phi_s(n) = (n+1)\pi, \quad n = 0, 1, 2, \ldots, \tag{12}$$

$$\phi_s(n) = \int_{x_1}^{x_2} -\frac{q_n(x)}{q_n'(x)}\,\mathrm{d}\sqrt{E_n - V(x)}, \tag{13}$$

where x_1 and x_2 are the classical turning points, and $\phi_s(n)$ denotes the phase contribution of the scattered subwaves. The ATM condition has some substantial distinctions. The phase contribution of the subwaves, which is always neglected by supersymmetric Wentzel–Kramers–Brillouin (SWKB) and broken supersymmetric Wentzel–Kramers–Brillouin (BSWKB) quantization rules (BSWKB), has been taken into account. In place of the traditional choice $\pi/2$ or any other values, the phase shift at the turning point is definitely equal to π in the ATM condition.

ATM quantization condition is a universal and accurate method of determining energy eigenvalues for any one-dimensional potential. For two-dimensional and three-dimensional potentials, we can transform them into effective one-dimensional ones with some well-known methods. The ATM quantization condition also produces good results for important quantum mechanical systems in the framework of SUSY QM.[12]

3. Application

3.1. Pekeris approximation for the rotating Morse potential

The Morse potential energy function modeling the atom–surface interaction is usually written in the form

$$V(r) = D_\mathrm{e}(\,\mathrm{e}^{-2a(r-r_\mathrm{e})} - 2\,\mathrm{e}^{-a(r-r_\mathrm{e})}), \tag{14}$$

where r is the coordinate perpendicular to the surface, r_e is the equilibrium bond distance, D_e is the well depth, and a controls the width of the potential. These parameters are adjustable. Expression (14) approaches to zero at infinite r and equals D_e at its minimum. It shows that the Morse potential is the combination of a short-range repulsion and a longer-range attractive tail.

The rotating Morse effective potential is described by the sum of Morse potential and the centrifugal barrier as

$$V_\mathrm{eff}(r) = D_\mathrm{e}(\,\mathrm{e}^{-2a(r-r_\mathrm{e})} - 2\,\mathrm{e}^{-a(r-r_\mathrm{e})}) + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}, \tag{15}$$

where l is the angular momentum.

With the Pekeris approximation the centrifugal term can be expanded up to second order in $z = \mathrm{e}^{-a(r-r_\mathrm{e})}$ as follows:[4,18,19]

$$V_\mathrm{eff}(r) = D_\mathrm{e}z^2 - 2D_\mathrm{e}z + A\left(1 - \frac{3}{ar_\mathrm{e}} + \frac{3}{a^2r_\mathrm{e}^2}\right) + A\left(\frac{4}{ar_\mathrm{e}} - \frac{6}{a^2r_\mathrm{e}^2}\right)z + A\left(-\frac{1}{ar_\mathrm{e}} + \frac{3}{a^2r_\mathrm{e}^2}\right)z^2, \tag{16}$$

where

$$A = \frac{\hbar^2}{2m}\frac{l(l+1)}{r_\mathrm{e}^2}. \tag{17}$$

Rearranging Eq. (16), we obtain

$$V_\mathrm{eff}(r) = C_0 - 2C_1z + C_2z^2, \tag{18}$$

where

$$C_0 = A\left(1 - \frac{3}{ar_\mathrm{e}} + \frac{3}{a^2r_\mathrm{e}^2}\right), \tag{19}$$

$$C_1 = D_\mathrm{e} - A\left(\frac{2}{ar_\mathrm{e}} - \frac{3}{a^2r_\mathrm{e}^2}\right), \tag{20}$$

$$C_2 = D_\mathrm{e} + A\left(-\frac{1}{ar_\mathrm{e}} + \frac{3}{a^2r_\mathrm{e}^2}\right). \tag{21}$$

We can obtain a new form of approximate effective potential which is equivalent to that of the Morse potential for $l = 0$ after some transformations

$$V_\mathrm{eff}\,(r) = C_0 + D_\mathrm{e}'\left(z'^2 - 2z'\right), \tag{22}$$

where

$$D_\mathrm{e}' = C_1^2/C_2, \tag{23}$$

$$z' = \mathrm{e}^{-a\left(r-r_\mathrm{e}'\right)}, \tag{24}$$

$$r_\mathrm{e}' = r_\mathrm{e} + a^{-1}\ln\left(\mathrm{C}_2/C_1\right). \tag{25}$$

Applying the Pekeris approximation to the rotating Morse potential in the framework of SUSY QM, we can obtain the hierarchy of SUSY partner potentials from Eqs. (10) and (15),

$$V_n(r) = V_{n-1}(r) - \frac{\hbar^2}{\mu}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\ln\psi_0^{(n-1)}(r), \tag{26}$$

where $\psi_0^{n-1}(r)$ is the ground state wave function of the $(n-1)$-th Hamiltonian partner.

With $z_n = \mathrm{e}^{-a(r-r_n)}$, we have

$$V_n(r) = D_{n-1}(z_{n-1}^2 - 2z_{n-1}) + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2} - \frac{\hbar^2}{m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\ln\psi_0^{(n-1)}(r). \quad (27)$$

Hence, using the Pekeris wave function of the $(n-1)$-th Morse SUSY partner potential

$$\psi_0^{(n)}(r) = N_{ol}^{(n)}\,\mathrm{e}^{-Q^n z_n/2}(Q_n z_n)^{m_n^{(0)}} \quad (28)$$

in Eq. (27), we have

$$V_n(r) = D_{n-1}(z_{n-1}^2 - 2z_{n-1}) + \frac{\hbar^2}{2\mu}\frac{l(l+1)}{r^2} + \frac{\hbar^2 a^2}{2\mu}Q_{n-1}z_{n-1}, \quad (29)$$

$$V_n(r) = D_n(z_n^2 - 2z_n) + \frac{\hbar^2}{2\mu}\frac{l(l+1)}{r^2}, \quad (30)$$

where

$$Q_n^2 = \frac{4}{a^2}\left[\frac{l(l+1)}{r_n^2}(3b_n^2 - b_n) + \frac{2\mu D_n}{\hbar^2}\right], \quad (31)$$

$$b_n = \frac{1}{ar_n}, \quad (32)$$

$$D_n = D_{n-1}\left(1 - \frac{\hbar^2 a^2 Q_{n-1}}{4\mu D_{n-1}}\right)^2, \quad (33)$$

$$r_n = r_{n-1} - a^{-1}\ln\left(1 - \frac{\hbar^2 a^2 Q_{n-1}}{4\mu D_{n-1}}\right), \quad n = 1, \ldots, N-1, \quad (34)$$

with

$$D_0 = D_\mathrm{e}, \quad (35)$$

$$r_0 = r_\mathrm{e}. \quad (36)$$

The first few effective SUSY partner potentials for $l = 5$ are plotted in Fig. 1. The potential wells become more and more shallow as the order of the partner potential increases. It also indicates that the number of states supported by each partner potential decreases.

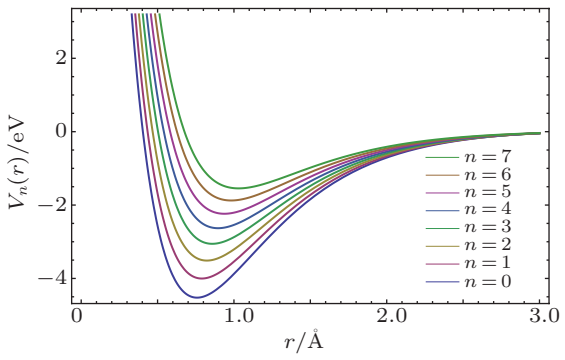


Fig. 1. (colour online) Effective supersymmetric partner potentials $V_n(r)$, $n = 0, \ldots, 7$ of H_2 for $l = 5$. $D_{\mathrm{e}1} = 4.7446$ eV, $a = 1.9425$ Å^{-1} (1 Å=0.1 nm), $r_{\mathrm{e}1} = 0.7416$ Å, $M = 2\mu/\hbar^2 = 241.09$ eV^{-1}·Å^{-2}.

3.2. Energy eigenvalues for the supersymmetric partner potentials by ATM condition

The Schrödinger equation for the rotating Morse potential is given by[4,20]

$$H_1\psi_{vl}^{(1)} = \left(-\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + V_\mathrm{eff}(r)\right)\psi_{vl}^{(1)} = E_{vl}\psi_{vl}^{(1)}. \quad (37)$$

In this section, we apply the ATM condition to the effective supersymmetric partner potentials. Following the ATM method,[12–15] we truncate the profile of the partner potentials $V_n(r)$ at two appropriate points r_m and r_p, which are far away from the turning points r_1 and r_2, which is shown in Fig. 2. The turning points of the approximate effective potentials can be obtained from Eq. (22). The effects of the truncation will be negligible if the potentials at the truncation points are much larger than the energies of relevant levels.

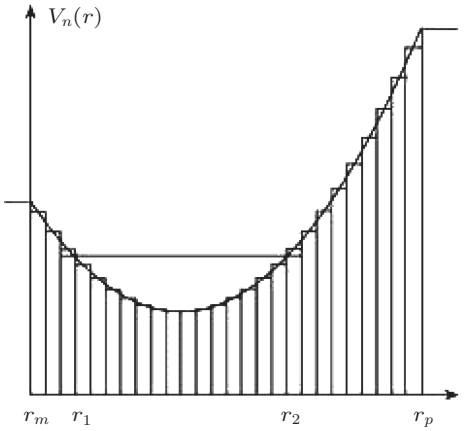


Fig. 2. Energy variation of an arbitrary potential $V_n(r)$ with coordinate r.

In order to obtain the accurate energy eigenvalues for the rotating Morse potential, the first step is to obtain the exact hierarchy of rotating Morse partner potentials with no approximation in the framework of SUSY QM. Then we apply the Pekeris approximation to each member of the hierarchy. In this way, the position of the minimum and the well depth are modified for each SUSY partner potential. We do not apply the Pekeris approximation to the original potential directly, but we calculate higher states of the Morse potential partners with the application of the Pekeris approximation, which may allow us to obtain the results with a better accuracy.

Table 1. Energy levels for the H_2 molecule, calculated by the Pekeris approximation and the hierarchy of supersymmetric Morse potentials with ATM condition, with physical parameters being $D_{e1} = 4.7446$ eV, $a = 1.9425$ Å^{-1}, $r_{e1} = 0.7416$ Å, $M = 2\mu/\hbar^2 = 241.09$ eV^{-1}·Å^{-2}.

v	l	$E^{(0)}_{v,l}$	$E^{(1)}_{v,l}$	$E^{(2)}_{v,l}$	$E^{(3)}_{v,l}$	$E^{(4)}_{v,l}$	$E^{(5)}_{v,l}$	$E^{(6)}_{v,l}$	$E^{(7)}_{v,l}$	HV
	0	–4.47601								–4.47601
	5	–4.25880								–4.25901
0	10	–3.72193								–3.72473
	15	–2.95158								–2.96635
	20	–2.02864								–2.08401
	0	–3.96231	–3.96231							
	5	–3.75714	–3.75358							
1	10	–3.23572	–3.23817							
	15	–2.49192	–2.50175							
	20	–1.59819	–1.62918							
	0	–3.4799	–3.4799	–3.4799						
	5	–3.27878	–3.28001	–3.2804						
2	10	–2.78081	–2.78634	–2.78844						
	15	–2.06355	–2.08068	–2.08894						
	20	–1.19904	–1.2438	–1.26957						
	0	–3.0288	–3.0288	–3.0288	–3.0288					
	5	–2.83573	–2.83775	–2.83882	–2.83915					
3	10	–2.3572	–2.36581	–2.37056	–2.37236					
	15	–1.66649	–1.6909	–1.7054	–1.71239					
	20	–0.83119	–0.889727	–0.927184	–0.948845					
	0	–2.60901	–2.60901	–2.60901	–2.60901	–2.60901				
	5	–2.42398	–2.42679	–2.42854	–2.42946	–2.42976				
4	10	–1.96489	–1.97659	–1.98399	–1.98809	–1.98964				
	15	–1.30072	–1.33242	–1.35315	–1.36551	–1.37149				
	20	–0.494643	–0.566959	–0.61611	–0.647757	–0.666208				
	0	–2.22051	–2.22051	–2.22051	–2.22051	–2.22051	–2.22051			–2.22051
	5	–2.04353	–2.04712	–2.04955	–2.05107	–2.05188	–2.05214			–2.05285
5	10	–1.60389	–1.61866	–1.62873	–1.63512	–1.63866	–1.64002			–1.65265
	15	–0.96626	–1.00525	–1.03221	–1.04993	–1.06054	–1.06054			–1.11167
	20	–0.18940	–0.27549	–0.336334	–0.37797	–0.40502	–0.40502			–0.52372
	0	–1.86332	–1.86332	–1.86332	–1.86332	–1.86332	–1.86332	–1.86332		–1.86332
	5	–1.69439	–1.69876	–1.70188	–1.70531	–1.70531	–1.70602	–1.70602		–1.70687
6	10	–1.27418	–1.29204	–1.30476	–1.31899	–1.31899	–1.32208	–1.32208		–1.33633
	15	–0.66310	–0.70937	–0.74257	–0.78090	–0.78090	–0.79011	–0.79467		–0.84224
	20	–0.08454	–0.01532	–0.08786	–0.17514	–0.17514	–0.19863	–0.21282		–0.31794
	0	–1.53743	–1.53743	–1.53743	–1.53743	–1.53743	–1.53743	–1.53743	–1.53743	–1.53743
	5	–1.37654	–1.38171	–1.38550	–1.39004	–1.39004	–1.39004	–1.39182	–1.39203	–1.39263
7	10	–0.97578	–0.99672	–1.01210	–1.03061	–1.03061	–1.03061	–1.03817	–1.03923	–1.05265
	15	–0.39125	–0.44480	–0.48424	–0.53255	–0.53255	–0.53255	–0.55393	–0.55804	–0.60673
	20	0.32718	0.21354	–0.12931	0.02343	0.02343	0.02343	–0.02839	–0.04140	–0.14869

Substituting the approximate effective potential into the ATM quantum condition, we can have the energy eigenvalues for the partner potentials. We calculate the rovibrational energy eigenvalues of the H_2 molecule for which accurate numerical values have been obtained by other methods. In Table 1 we list the energy eigenvalues for the corresponding partner Hamiltonians for relatively high vibrational and rotational quantum numbers, and compare our results with those obtained by the hypervirial perturbation (HV) method. The HV method gives results that are indistinguishable from those obtained with numeri-

cal methods.[21] In order to illustrate the performance of our method, we take different values of ν in Table 1. The ATM method produces good results for the quantum number $l = 0$. The results $E^0_{v,l}$ in this table correspond to the original Pekeris approximation. It indicates that our improved approximation gives the results with reasonable accuracy for the relatively small quantum number $l = 5$. Although for higher states with $l = 10$, $l = 15$, and $l = 20$, the improved approximation method loses its accuracy, it is consistently much better than the original Pekeris approximation. For $v = 1$, $v = 2$, $v = 3$, and $v = 4$, there are no results available from other methods for comparison. The energy eigenvalues in the table are calculated by the ATM method and they are original. It is demonstrated that the energy eigenvalues of the original Hamiltonian improve as we evaluate them indirectly through the energy eigenvalues of the higher SUSY partners Hamiltonians.

4. Conclusion

In our work, we use ATM condition to obtain the energy eigenvalues of the rotating Morse potential. With the combination of SUSY QM and the Pekeris approximation, we can obtain accurate results for the energies of rovibrational states of the hydrogen molecule from the ATM condition.

Comparison of the results with those from accurate numerical calculations shows that the accuracy of the eigenvalues of the rotating Morse potential under Pekeris approximation can be improved by SUSY QM. We obtain the exact hierarchy of SUSY partner potentials for the rotating Morse potentials with no approximation and then apply the Pekeris approximation to each member of the hierarchy. With the Pekeris approximation, the turning points of the partner potentials can be obtained. The ATM condition can be used to calculate the energy eigenvalues for the partner potentials. It is demonstrated that the calculation of the higher rovibrational states of the original Morse potential with Pekeris approximation produces better results than applying the approximation directly to the original potential.

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