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ORIGINAL PAPER

D-dimensional energies for scandium monoiodide

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Abstract We solve the Schrödinger equation with the Morse potential energy model in D spatial dimensions. The bound state rotation–vibrational energy spectra have been obtained by using the supersymmetric shape invariance approach. For a fixed vibrational quantum number and various rotational quantum numbers, the energies for the $X^1\Sigma^+$ state of ScI molecule increase as D increases. We observe that the behavior of the vibrational energies in higher dimensions remains similar to that of the three-dimensional system. The dimensional scaling method resembles a translation transformation from the higher dimensions to the actual three dimensions.

Keywords Schrödinger equation · Morse potential energy model · Rotation–vibrational energy · Arbitrary spatial dimensionality · Scandium monoiodide

1 Introduction

Generalizing the Schrödinger equation to an arbitrary spatial dimensionality D has received much attention in chemical physics [1,2]. Louck [3–5] presented detailed derivations for the generalized orbit angular momentum, which are involved in almost all works about higher dimensional wave equations. The dimensional scaling (D-scaling) method involves generalizing the three-dimensional Schrödinger equation

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to D-dimensional space and treating D as a free parameter. The D-scaling method employed in chemical physics today was developed by Herchbach and collaborators [6]. Svidzinsky et al. [7,8] constructed the connection between the classical Bohr quantum mechanical model and the D-scaling model. Serra and Kais [9–12] found that the symmetry breaking of the electronic structure configurations in the large-D limit is completely analogous to the standard phase transitions and critical phenomena in statistical mechanics. With the help of the D-scaling approach, Ferrón et al. [13] investigated stability of two particles in a dipole field. Zhao et al. [14] studied the electron correlation of anisotropic quantum dots in the high-density limit in terms of the D-scaling method. Chen et al. [15] investigated mathematical analysis of the D-scaling method for solving the Schrödinger equation with the Coulomb potentials. A reverse strategy for large-D expansion approach is the program of solving directly the D-dimensional Schrödinger equation. Many efforts have been made to obtain bound state solutions of the D-dimensional Schrödinger equations with typical potential energy models [16–26], which include some diatomic molecule potentials, such as the Morse potential [19], Mie-type potential [20], Schiöberg potential [21], Manning-Rosen potential [22–25], and Pöschl-Teller potential [26]. However, the authors in these works did not report the quantitative investigation on rotation–vibrational energies of real diatomic molecules in higher dimensions. Recently, Hu et al. [27,28] investigated the D-dimensional Schrödinger equations with the improved Manning-Rosen potential and improved Rosen-Morse potential. They observed that the change behavior of the vibrational energies in higher dimensions remains similar to that of the three-dimensional system for the $a^3\Sigma_u^+$ state of $^7\mathrm{Li}_2$ molecule, $3^3\Sigma_g^+$ state of Cs_2 molecule and $5^1\Delta_g$ state of Na_2 molecule. The present main topic is to examine this phenomenon for other diatomic molecule systems.

In 1929, Morse [29] proposed a three-parameter potential energy function for diatomic molecules,

$$U_{\mathrm{M}}(r) = D_e\left(1 - e^{-\alpha(r-r_e)}\right)^2, \tag{1}$$

where D_e is the dissociation energy, r_e is the equilibrium bond length, and α denotes the range of the potential. The Morse potential has been widely used in describing diatomic vibrations [30–35]. In terms of the Pekeris approximation method [36], some authors [37–44] dealt with the centrifugal term of the three-dimensional Schrödinger equation with the Morse potential and other diatomic molecule potentials. Bound state solutions of the three-dimensional Schrödinger equation for the Morse potential have been studied by a number of methods, such as the exact quantization rule method [37], supersymmetric shape invariance approach [38], Nikiforov–Uvarov method [39], asymptotic iteration approach [40], and two-point quasi-rational approximation technique [41]. Miraboutalebi et al. [19] investigated analytical solutions of the N-dimensional Schrödinger equation with the Morse potential based on the Laplace transformation method. By employing the Pekeris approximation approach to deal with the centrifugal term, Jia and Cao [45] studied the bound state solutions of the three-dimensional Klein-Gordon equation for the Morse potential, and calculated the relativistic vibrational transition frequencies for the $X^1\Sigma^+$ state of ScI molecule. The scandium monoiodide molecule is of particular interest because they can be used as prototype for understanding chemical bonding involving d electron. The vibrational and rotational spectra have received much attention [46–49]. A successful empirical potential function should reproduce the experimental Rydberg–Klein–Rees (RKR) [50–52] potential, and satisfy the Lippincott criterion, i.e., an average absolute deviation of less than 1 % of the dissociation energy, D_e [30]. The average deviation σ_{av} is expressed as a percent of D_e, $\sigma_{\text{av}} = 100\sum\left(\left|U_{\exp}(r) - U_{\text{calc}}(r)\right|\right)/N_p D_e$, where N_p is the number of reported points, $U_{\exp}(r)$ and $U_{\text{calc}}(r)$ are the experimentally determined potential and the empirical potential, respectively. The Lippincott criterion has been used by many authors to assess the accuracy of an empirical potential model [32,53]. The average absolute deviation of the Morse potential for the $\mathrm{X}^1\Sigma^+$ state of ScI molecule from the RKR potential reported by Reddy et al. [46] is 0.0344 % of D_e [45]. This average absolute deviation satisfies the Lippincott criterion. The Morse potential is available in yielding the potential energy curve of the $\mathrm{X}^1\Sigma^+$ state of ScI molecule.

In this work, we investigate the bound state solutions of the D-dimensional Schrödinger equation with the Morse potential model. We attempt to explore the properties of the rotation–vibrational energy spectra for the $\mathrm{X}^1\Sigma^+$ state of ScI molecule in higher dimensions.

2 Bound state solutions

The radial part of the D-dimensional Schrödinger equation with a spherical symmetric potential $U(r)$ for a diatomic molecule with reduced mass μ is given by [1,2]

$$\left[-\frac{\hbar^2}{2\mu}\frac{1}{r^{D-1}}\frac{\partial}{\partial r}\left(r^{D-1}\frac{\partial}{\partial r}\right) + U(r) + \frac{\hbar^2 J(J+D-2)}{2\mu r^2}\right]R_{vJ}(r) = E_{vJ}^D R_{vJ}(r), \tag{2}$$

where D is a positive integer and $D \geq 2$, $\hbar$ denotes the reduced Planck constant, E_{vJ}^D is the rotation–vibrational energy of the diatomic molecule system, v and J denote the vibrational and rotational quantum numbers, respectively. By a transformation of $R_{vJ}(r) = r^{-\frac{D-1}{2}}u_{vJ}(r)$, we can write Eq. (2) in the form

$$-\frac{\hbar^2}{2\mu}\frac{d^2u_{vJ}(r)}{dr^2} + \left[U(r) + \frac{K(K+1)\hbar^2}{2\mu r^2}\right]u_{vJ}(r) = E_{vJ}^D u_{vJ}(r), \tag{3}$$

where $K = J + \frac{1}{2}(D-3)$. Taking the spherical symmetric potential $U(r)$ as the Morse potential model (1), we obtain

$$-\frac{\hbar^2}{2\mu}\frac{d^2u_{vJ}(r)}{dr^2} + \left[D_e\left(1 - e^{-\alpha(r-r_e)}\right)^2 + \frac{K(K+1)\hbar^2}{2\mu r^2}\right]u_{vJ}(r) = E_{vJ}^D u_{vJ}(r). \tag{4}$$

Equation (4) can be solved exactly only for the case of $K = 0$. When $K \neq 0$, one can only solve approximately Eq. (4). We take the Pekeris approximation scheme to deal with the centrifugal term [36]. The centrifugal potential is approximately replaced by the following expression [45]

$$\frac{K(K+1)\hbar^2}{2\mu r^2} = \frac{K(K+1)\hbar^2}{2\mu r_e^2}\left(d_0 + d_1 e^{-\alpha r} + d_2 e^{-2\alpha r}\right), \tag{5}$$

where the coefficients d_0, d_1, and d_2 are given by [45]

$$d_0 = 1 - \frac{3}{\alpha r_e} + \frac{3}{\alpha^2 r_e^2}, \tag{6}$$

$$d_1 = 2e^{\alpha r_e}\left(\frac{2}{\alpha r_e} - \frac{3}{\alpha^2 r_e^2}\right), \tag{7}$$

$$d_2 = e^{2\alpha r_e}\left(\frac{3}{\alpha^2 r_e^2} - \frac{1}{\alpha r_e}\right). \tag{8}$$

Substituting expression (5) into Eq. (4) yields the following equation

$$-\frac{d^2 u_{vJ}(r)}{dr^2} + \left(Ae^{-\alpha r} + Be^{-2\alpha r}\right) u_{vJ}(r) = \varepsilon_{vJ} u_{vJ}(r), \tag{9}$$

where A, B, and ε_{vJ} are defined as

$$A = -\frac{4\mu D_e}{\hbar^2} e^{\alpha r_e} + \frac{K(K+1)}{r_e^2} d_1, \tag{10}$$

$$B = \frac{2\mu D_e}{\hbar^2} e^{2\alpha r_e} + \frac{K(K+1)}{r_e^2} d_2, \tag{11}$$

$$\varepsilon_{vJ} = \frac{2\mu}{\hbar^2}\left(E_{vJ}^D - D_e - \frac{K(K+1)\hbar^2}{2\mu r_e^2} d_0\right). \tag{12}$$

We solve Eq. (9) in terms of the supersymmetric shape invariance approach [54–56]. The ground-state wave function $u_{0,J}(r)$ is written in the form of

$$u_{0,J}(r) = \exp\left(-\int W(r)\, dr\right), \tag{13}$$

where $W(r)$ is called a superpotential in supersymmetric quantum mechanics [54]. Substituting Eq. (13) into Eq. (9) leads us to have the following equation satisfied by the superpotential $W(r)$,

$$W^2(r) - \frac{dW(r)}{dr} = Ae^{-\alpha r} + Be^{-2\alpha r} - \varepsilon_{0,J}, \tag{14}$$

where $\varepsilon_{0,J}$ presents the ground-state energy. The superpotential $W(r)$ is written as follows

$$W(r) = C_1 e^{-\alpha r} + C_2, \tag{15}$$

where C_1 and C_2 are two constants. With the help of the superpotential function (16), we yield a pair of supersymmetric partner potentials $U_-(r)$ and $U_+(r)$,

$$U_-(r) = W^2(r) - \frac{dW(r)}{dr^2} = C_2^2 + (2C_1C_2 + \alpha C_1)\,e^{-\alpha r} + C_1^2 e^{-2\alpha r}, \tag{16}$$

$$U_+(r) = W^2(r) + \frac{dW(r)}{dr^2} = C_2^2 + (2C_1C_2 - \alpha C_1)\,e^{-\alpha r} + C_1^2 e^{-2\alpha r}, \tag{17}$$

From supersymmetric partner potential expressions (16) and (17), we have the following relationship

$$U_+(r, a_0) = U_-(r, a_1) + R(a_1), \tag{18}$$

where $a_0 = C_2$, a_1 is a function of a_0, i.e., $a_1 = h(a_0) = a_0 - \alpha$, and the reminder $R(a_1)$ is independent of r, $R(a_1) = a_0^2 - a_1^2$. Equation (18) tells us that the partner potentials $U_-(r)$ and $U_+(r)$ are shape invariant potentials [55]. Making a comparison of Eq. (16) with Eq. (9), we have the following three relationships

$$C_2^2 = -\varepsilon_{0,J}, \tag{19}$$

$$2C_1C_2 + \alpha C_1 = A, \tag{20}$$

$$C_1^2 = B. \tag{21}$$

Substituting expression (15) into expression (13) leads us to rewrite the ground-state wave function $u_{0,J}(r)$ as follows

$$u_{0,J}(r) = e^{-C_2 r} e^{\frac{C_1}{\alpha} e^{-\alpha r}}. \tag{22}$$

We consider the bound state solutions, which demand the wave function $u_{vJ}(r)$ to satisfy the boundary conditions: $u_{vJ}(0) = u_{vJ}(\infty) = 0$. These regularity conditions leads us to have $C_2 > 0$ and $C_1 < 0$. In terms of these restriction conditions, we obtain by solving Eqs. (20) and (21),

$$C_1 = -\sqrt{B}, \tag{23}$$

$$C_2 = \frac{A}{2C_1} - \frac{\alpha}{2}. \tag{24}$$

In terms of the shape invariance approach [55], the energy spectra of the shape invariant potential $U_-(r)$ are given exactly by

$$\varepsilon_{0,J}^{(-)} = 0, \tag{25}$$

$$\begin{aligned}\varepsilon_{vJ}^{(-)} &= \sum_{k=1}^{v} R\left(a_k\right) = R\left(a_1\right) + R\left(a_2\right) + \cdots + R\left(a_v\right) \\ &= a_0^2 - a_1^2 + a_1^2 - a_2^2 + \cdots + a_{v-1}^2 - a_v^2 = a_0^2 - a_v^2 = C_2^2 - \left(C_2 - v\alpha\right)^2, \end{aligned} \tag{26}$$

where the quantum number $v = 0, 1, 2, \ldots$. From Eqs. (9), (14) and (16), we have the following relationship for ε_{vJ},

$$\varepsilon_{vJ} = \varepsilon_{vJ}^{(-)} + \varepsilon_{0,J}. \tag{27}$$

Substituting Eqs. (19) and (26) into Eq. (27) and using expression (24), we obtain

$$\varepsilon_{vJ} = -\left(\frac{A}{2C_1} - \frac{\alpha}{2} - v\alpha\right)^2. \tag{28}$$

Substituting expression (23) into expression (28) and employing expressions (10)–(12), we obtain the rotation–vibrational energy spectra for the diatomic molecule presented by the Morse potential energy model in higher dimensions,

$$\begin{aligned}E_{vJ}^{D} &= D_e + \frac{K\left(K+1\right)\hbar^2}{2\mu r_e^2} d_0 \\ &\quad - \frac{\hbar^2}{2\mu}\left(\frac{\frac{2\mu}{\hbar^2}\left(2D_e e^{\alpha r_e} - \frac{K(K+1)\hbar^2}{2\mu r_e^2} d_1\right)}{2\left(\frac{2\mu}{\hbar^2} D_e e^{2\alpha r_e} + \frac{K(K+1)}{r_e^2} d_2\right)^{\frac{1}{2}}} - \left(v + \frac{1}{2}\right)\alpha\right)^2. \end{aligned} \tag{29}$$

In terms of the superpotential $W\left(r\right)$ given in expression (15) and the ground-state wave function $u_{0,J}\left(r\right)$ given in expression (22), we can yield the excited state wave functions by employing the explicit recursion operator approach [57,58]. The unnormalized wave functions are given by [57]

$$u_{v+1,J}\left(r, a_0\right) = A^{+}\left(r, a_0\right) u_{v,J}\left(r, a_1\right), \tag{30}$$

where the operator $A^{+}\left(r, a_0\right)$ is given by [57]

$$A^{+}\left(r, a_0\right) = -\frac{d}{dr} + W\left(r, a_0\right). \tag{31}$$

Considering $a_0 = C_2$ and $a_1 = a_0 - \alpha = C_2 - \alpha$, and using expressions (15) and (22), we obtain the following expression from recursion relation (30),

$$\begin{aligned} u_{1,J}(r) &= \left(-\frac{d}{dr}+C_1e^{-\alpha r}+C_2\right)e^{-(C_2-\alpha)r}e^{\frac{C_1}{\alpha}e^{-\alpha r}} \\ &= \left(2C_2-\alpha+2C_1e^{-\alpha r}\right)e^{-(C_2-\alpha)r}e^{\frac{C_1}{\alpha}e^{-\alpha r}}. \end{aligned} \tag{32}$$

From expressions (8), (11) and (23), we have

$$C_1=-\frac{e^{\alpha r_e}}{r_e}\sqrt{\frac{2\mu r_e^2D_e}{\hbar^2}+K\left(K+1\right)\left(\frac{3}{\alpha^2r_e^2}-\frac{1}{\alpha r_e}\right)}. \tag{33}$$

With the help of expressions (7), (10), (24) and (33), we obtain

$$C_2=\frac{\frac{4\mu r_e^2D_e}{\hbar^2}-K\left(K+1\right)\left(\frac{4}{\alpha r_e}-\frac{6}{\alpha^2r_e^2}\right)}{2r_e\sqrt{\frac{2\mu r_e^2D_e}{\hbar^2}+K\left(K+1\right)\left(\frac{3}{\alpha^2r_e^2}-\frac{1}{\alpha r_e}\right)}}-\frac{\alpha}{2}. \tag{34}$$

Substituting expressions (33) and (34) into expression (32) lead us to obtain the following expression for the first excited state wave function under the replacements of $\alpha\to\frac{\alpha}{r_e}$ and $r\to r_e\left(r+1\right)$,

$$u_{1,J}\left(r\right)=\frac{\alpha}{r_e}e^{-\frac{\alpha}{2}(k_N-3)}\left(k_N-2-\frac{2\eta_N}{\alpha}e^{-\alpha r}\right)e^{-\frac{\alpha}{2}(k_N-3)r}e^{-\frac{\eta_N}{\alpha}e^{-\alpha r}}, \tag{35}$$

where $k_N=\frac{2\xi_N^2}{\alpha\eta_N}$, η_N and ξ_N are defined by expression (28) of Ref. [19]. Employing the same procedure, one can produce the other excited state wave functions.

From expression (31) of Ref. [19], we obtain the first excited state wave function,

$$R_{\lambda,1}\left(r\right)=N_1\left(\frac{2\eta_N}{\alpha}\right)^{\frac{\alpha}{2}(k_N-3)}\left(k_N-2-\frac{2\eta_N}{\alpha}e^{-\alpha r}\right)e^{-\frac{\alpha}{2}(k_N-3)r}e^{-\frac{\eta_N}{\alpha}e^{-\alpha r}}. \tag{36}$$

Except the normalization constant, expression (35) is the same with expression (36). They give the same unnormalized wave function.

3 Discussion

The equilibrium force constant k_e is defined as the second derivates of the potential energy function $U\left(r\right)$ for diatomic molecules,

$$\left.\frac{d^2U(r)}{dr^2}\right|_{r=r_e}=k_e=\mu\omega_e^2, \tag{37}$$

where ω_e denotes the equilibrium harmonic vibrational frequency. Employing the above definition, we obtain the expression for the parameter α in the Morse potential model, $\alpha=\sqrt{\frac{k_e}{2D_e}}$.

When $D=3$, the rotation–vibrational energy spectrum expression (29) becomes the following form

$$E_{vJ}^{D}=D_e+\frac{J\left(J+1\right)\hbar^2}{2\mu r_e^2}d_0-\frac{\hbar^2}{2\mu}\left(\frac{\frac{2\mu}{\hbar^2}\left(2D_e e^{\alpha r_e}-\frac{J(J+1)\hbar^2}{2\mu r_e^2}d_1\right)}{2\left(\frac{2\mu}{\hbar^2}D_e e^{2\alpha r_e}+\frac{J(J+1)}{r_e^2}d_2\right)^{\frac{1}{2}}}-\left(v+\frac{1}{2}\right)\alpha\right)^2, \tag{38}$$

which presents rotation–vibrational energy levels of the diatomic molecule in the presence of the Morse potential energy model in three spatial dimensions. Rotation–vibrational energy expression (38) is in consistent with that given in Eq. (27) of Ref. [40]. Bayrak and Boztosun [40] solved the three-dimensional Schrödinger equation with the Morse potential by employing the asymptotic iteration method.

In the special case of $D=3$ and $J=0$, the rotation–vibrational energy spectrum expression (29) can be deduced to the following form

$$E_{vJ}^{D}=\left(v+\frac{1}{2}\right)\hbar\omega_e-\left(v+\frac{1}{2}\right)^2\frac{\hbar^2\omega_e^2}{4D_e}, \tag{39}$$

where we have used the relationship of $\alpha=\sqrt{\frac{\mu\omega_e^2}{2D_e}}$. Expression (39) coincides with expression (13) of Ref. [29].

In view of $K=J+\frac{1}{2}\left(D-3\right)=J-1+\frac{1}{2}\left(D+2-3\right)$, we obatin $E_{vJ}^{D}=E_{v,J-1}^{D+2}$ from expression (38). This shows that an isomorphism exists for the Mors potential in D dimensions between spatial dimension and orbital angular momentum, i.e., the rotation–vibrational energy keeps invariant for a molecule presented by the Morse potential model under a transformation of an increase in the spatial dimension by two ($D\rightarrow D+2$) and a decrease the orbital angular momentum by one ($J\rightarrow J-1$). For this molecular system presented by the Morse potential, the states connected by the dimensional link in Eq. (38) are exactly degenerate. This is so-called inter-dimensional degeneracy symmetry as discussed in literature [59,60].

We consider the $X^1\Sigma^+$ state of ScI molecule. The molecular constants for this molecular state are taken from the literature [46]:$D_e=2.858\,\text{eV}$, $r_e=2.6078$ Å, and $\omega_e=277.18\,\text{cm}^{-1}$. Taking these experimental values as inputs, we can determine the value of the potential parameter α in terms of $\alpha=\omega_e\sqrt{\frac{\mu}{2D_e}}$.

In Fig. 1, we plot the rotation–vibrational energy versus the spatial dimension D. From Fig. 1, we observe that for fixed v and various J, the energies for the $X^1\Sigma^+$ state of ScI molecule diverge as D increases.

In Fig. 2, we plot the pure vibrational energy versus the vibrational quantum numbers v. The experimental data [46] determined by using the RKR method for the $X^1\Sigma^+$ state of ScI molecule in three-dimension case are also depicted. We find that the difference between the two adjoint states increases as D increases. The results presented in Fig. 2 reveal that the behavior of the vibrational energies for the $X^1\Sigma^+$ state of ScI molecule in higher dimensions remains similar to that of the three-dimensional

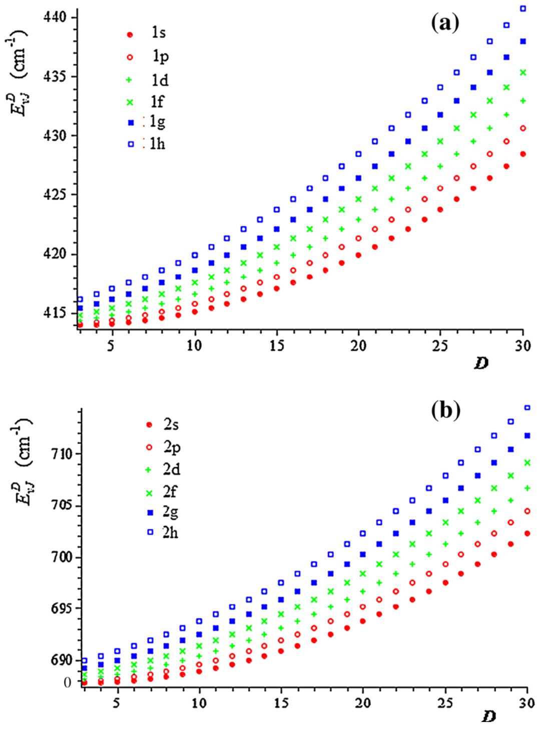

Fig. 1 (Color online) Energy for the $X^1\Sigma^+$ state of ScI molecule versus D for $v = 1, 2$ and various J

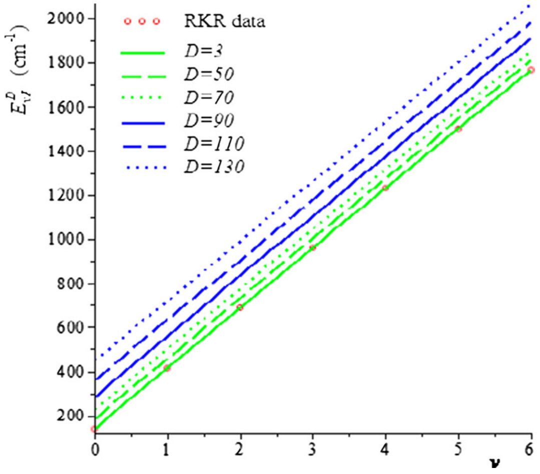

Fig. 2 (Color online) Energy for the $X^1\Sigma^+$ state of ScI molecule versus v for $J = 0$ and various D

system. This phenomena provides an explanation for the physical foundations of the D-scaling method, namely that the D-scaling approach resembles a translation transformation from the higher dimensions to the actual three dimensions. In Figs. 1 and 2, we do not consider the case $D = 2$. The reason is that there is a singular point at this point as addressed in [2].

4 Conclusions

In this work, we have studied the bound state solutions of the Schrödinger equation with the Morse potential energy model in D dimensions. By employing the Pekeris approximation method to deal with the centrifugal term, we obtain analytically the rotation–vibrational energy spectra of the diatomic molecule presented by the Morse potential model in terms of the supersymmetric shape invariance approach. For the $X^1\Sigma^+$ state of ScI molecule, we observe that for a fixed v and various J the rotation–vibrational energies diverge as D increases, and also observe that the behavior of the vibrational energies in higher dimensions remains similar to that of the three-dimensional system. For the special case $D = 3$, the present results agree well with those obtained by other methods.

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