

Bound state solution of the Schrödinger equation for Mie potential

Ramazan Sever* and Mahmut Bucurgat

Department of Physics, Middle East Technical University, 06531 Ankara, Turkey
E-mail: sever@metu.edu.tr

Cevdet Tezcan

Faculty of Engineering, Başkent University, Bağlıca Campus, Ankara, Turkey

Özlem Yeşiltaş

Turkish Atomic Energy Authority, Istanbul Road, 30 km Kazan, 06893 Ankara, Turkey

Received 5 January 2007; accepted 24 January 2007

Exact solution of Schrödinger equation for the Mie potential is obtained for an arbitrary angular momentum. The energy eigenvalues and the corresponding wavefunctions are calculated by the use of the Nikiforov–Uvarov method. Wavefunctions are expressed in terms of Jacobi polynomials. The bound states are calculated numerically for some values of ℓ and n with $n \leq 5$. They are applied to several diatomic molecules.

KEY WORDS: Mie potential, diatomic molecules, Schrödinger equation, Nikiforov–Uvarov method

PACS NUMBERS: 03.65.-w, 03.65.Ge, 12.39.Fd

1. Introduction

The study of three-dimensional anharmonic oscillators has raised a considerable amount of interest due to its wide applications in molecular physics [1–4]. The Morse potential is commonly used for anharmonic oscillator. However, its wavefunction does not vanish at the origin. But those of Mie type and pseudo-harmonic potentials do. On the other hand, the Mie type potential possess the general features of the true interaction energy [1]. The Mie type and pseudo-harmonic are two special kinds of exactly solvable power-law and inverse power-law potentials other than the Coulombic and harmonic oscillator. The Hamiltonians with inverse power potential $1/r^n$ are studied in different fields. For instance, path integral, $1/N$ expansion and super-symmetrical approaches

* Corresponding author.

are also studied for this type of potentials [5–8]. Moreover, there are some applications of Mie type potentials such as equation of bulk metallic glass for $Zr_{48}Nb_8Cu_{14}Ni_{12}Be_{18}$ in solid state physics [9], and other applications in solid state physics [10], molecular spectroscopy [11], fluid mechanics [12], the inter-atomic interaction potential in molecular physics [13], $1/r^n$ potential in three dimensions [14].

The Nikiforov–Uvarov (NU) method [15] is introduced for the solution of the hypergeometric type second-order differential equations [16] appeared in the time-independent problems. Recently, NU-method has been used to solve Schrödinger equation for some well known potentials [17–22], Dirac and Klein-Gordon equations for the Coulomb and some exponential potentials. In the present work the Schrödinger equation is solved by the NU method for Mie potential with any value of angular momentum ℓ . As an illustration, energy eigenvalues are computed for N_2 , CO , NO and CH molecules.

The organization of the paper is as follows. In section 2, NU method is briefly introduced. Mie potential calculations are done by using NU method in section 3. Results are discussed in section 4.

2. The Nikiforov–Uvarov method

The NU-method developed by Nikiforov and Uvarov (NU-method) is based on reducing the second order differential equations (ODEs) to a generalized equation of hypergeometric type [15]. It is provided us an analytic solution of Schrödinger equation for certain kind of potentials. It is based on the solutions of general second order linear differential equation with orthogonal function [16]. The one-dimensional Schrödinger equation is reduced to a generalized equation of hypergeometric type with an appropriate coordinate transformation $s = s(r)$. Then, the equation has the form,

$$\psi''(s) + \frac{\tilde{\tau}(s)}{\sigma(s)}\psi'(s) + \frac{\tilde{\sigma}(s)}{\sigma^2(s)}\psi(s) = 0, \quad (1)$$

where $A(s) = \frac{\tilde{\tau}(s)}{\sigma(s)}$ and $B(s) = \frac{\tilde{\sigma}(s)}{\sigma^2(s)}$. In equation (1), $\sigma(s)$ and $\tilde{\sigma}(s)$ are polynomials at most second degree, and $\tilde{\tau}(s)$ is a polynomial with at most first degree [15]. The wave function is constructed as a multiple of two independent parts,

$$\psi(s) = \phi(s)y(s) \quad (2)$$

and equation (1) becomes

$$\sigma(s)y''(s) + \tau(s)y'(s) + \lambda y(s) = 0, \quad (3)$$

where

$$\sigma(s) = \pi(s) \frac{d}{ds}(\ln \phi(s)) \quad (4)$$

and

$$\tau(s) = \tilde{\tau}(s) + 2\pi(s). \tag{5}$$

λ is defined as

$$\lambda_n + n\tau' + \frac{[n(n-1)\sigma'']}{2} = 0, \quad n = 0, 1, 2, \dots \tag{6}$$

We determine $\pi(s)$ and λ by defining

$$k = \lambda - \pi'(s). \tag{7}$$

From equations (4–5), $\pi(s)$ becomes

$$\pi(s) = \left(\frac{\sigma' - \tilde{\tau}}{2}\right) \pm \sqrt{\left(\frac{\sigma' - \tilde{\tau}}{2}\right)^2 - \tilde{\sigma} + k\sigma} \tag{8}$$

$\pi(s)$ has to be a polynomial of degree at most one in equation (8), so the expression under the square root must be the square of a polynomial of first degree [15]. This is simply possible only if its discriminant is zero. After defining k , one can obtain $\pi(s)$, $\tau(s)$, $\phi(s)$ and λ . If we look at equation (4) and the Rodrigues relation

$$y_n(s) = \frac{B_n}{\rho(s)} \frac{d^n}{ds^n} [\sigma^n(s)\rho(s)], \tag{9}$$

where C_n is normalizable constant and the weight function satisfy the relation as

$$\frac{d}{ds} [\sigma(s)\rho(s)] = \tau(s)\rho(s), \tag{10}$$

where

$$\frac{\phi'(s)}{\phi(s)} = \frac{\pi(s)}{\sigma(s)}. \tag{11}$$

3. Mie potential calculations

The Mie-type potentials are given by

$$V(r) = \epsilon \left[\frac{k}{\ell - k} \left(\frac{a}{r}\right)^\ell - \frac{\ell}{\ell - k} \left(\frac{a}{r}\right)^k \right], \tag{12}$$

where ϵ is the interaction energy between two atoms in a solid at $x = a$, and $\ell > k$ is always satisfied.

We solve the one-dimensional Mie potential [1, 2] with $\ell = 2k$ combination. By choosing the special case $k = 1$, corresponding to a Coulombic-type potential with an additional centrifugal potential barrier, we get the following form:

$$V(r) = V_0 \left[\frac{1}{2} \left(\frac{a}{r} \right)^2 - \left(\frac{a}{r} \right) \right], \quad V_0 = 2\epsilon k, \quad (13)$$

where V_0 is the dissociation energy and a is the positive constant which is strongly repulsive at shorter distances. The radial part of the Schrödinger equation for a diatomic molecule potential is

$$\left[-\frac{\hbar^2}{2\mu} \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d}{dr} \right) + \frac{\ell(\ell+1)\hbar^2}{2\mu r^2} + V(r) \right] R_{n\ell}(r) = E_{n\ell} R_{n\ell}(r), \quad (14)$$

where μ is the reduced mass of the diatomic molecules. n denotes the radial quantum number (n and ℓ are named as the vibration-rotation quantum numbers in molecular chemistry). r is the internuclear separation. Substituting the explicit form of $V(r)$, we get

$$\begin{aligned} \frac{d^2 R_{n\ell}(r)}{dr^2} + \frac{2}{r} \frac{dR_{n\ell}(r)}{dr} + \frac{2\mu}{\hbar^2} \left[E_{n\ell} - V_0 \left(\frac{1}{2} \left(\frac{a}{r} \right)^2 - \frac{a}{r} \right) \right] \\ \times R_{n\ell}(r) - \frac{\ell(\ell+1)\hbar^2}{2\mu r^2} R_{n\ell}(r) = 0. \end{aligned} \quad (15)$$

By defining the following variables:

$$\varepsilon^2 = E, \quad (16)$$

$$\beta = -\frac{2\mu}{\hbar^2} V_0 a, \quad (17)$$

$$\gamma = \frac{2\mu}{\hbar^2} \left(\frac{1}{2} V_0 a^2 + \frac{\ell(\ell+1)\hbar^2}{2\mu} \right). \quad (18)$$

The Schrödinger equation takes the simple form:

$$\left[\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} + \frac{1}{r^2} (\varepsilon^2 r^2 - \beta r - \gamma) \right] R_{n\ell}(r) = 0. \quad (19)$$

From equation (19), it is clear that $\sigma(r) = r$, $\tilde{\tau} = 2$, $\tilde{\sigma} = \varepsilon^2 r^2 - \beta r - \gamma$. We find $\pi(r)$ as

$$\pi(r) = -\frac{1}{2} \pm \begin{cases} i\varepsilon r + \frac{1}{2}\sqrt{4\gamma+1}, & k_1 = -\beta + \varepsilon\sqrt{-1-4\gamma}, \\ i\varepsilon r - \frac{1}{2}\sqrt{4\gamma+1}, & k_2 = -\beta - \varepsilon\sqrt{-1-4\gamma} \end{cases} \quad (20)$$

and $\tau(r)$ can be written as

$$\tau(r) = \begin{cases} 1 + 2i\varepsilon r + \sqrt{4\gamma+1}, & k_1 = -\beta + \varepsilon\sqrt{-1-4\gamma}, \\ 1 - 2i\varepsilon r + \sqrt{4\gamma+1}, & k_2 = -\beta - \varepsilon\sqrt{-1-4\gamma} \end{cases} \quad (21)$$

For appropriate solutions $\tau'(r) < 0$ [15]. Therefore we use $k_2 = -\beta - \varepsilon\sqrt{-1 - 4\gamma}$, $\pi_2 = -\frac{1}{2} - i\varepsilon r - \frac{1}{2}\sqrt{1 + 4\gamma}$ and $\tau(r) = 1 - 2i\varepsilon r + \sqrt{1 + 4\gamma}$ for obtaining eigenvalues and eigenfunctions. Using equations (6–7) we find energy spectrum as

$$E_n = -\left(\frac{2\mu V_0 a}{\hbar^2}\right)^2 \left[2n + 1 + \sqrt{1 + \frac{8\mu}{\hbar^2} \left(\frac{V_0 a^2}{2} + \frac{\ell(\ell + 1)\hbar^2}{2\mu} \right)} \right]^{-2}. \tag{22}$$

Wavefunction is calculated from equations (9–11).

$$\phi(r) = r^{\frac{1}{2}(-1 + \sqrt{1 + 4\gamma})} e^{-i\varepsilon r}, \tag{23}$$

and

$$\rho(r) = r^{\sqrt{1 + 4\gamma}} e^{-2i\varepsilon r}, \tag{24}$$

and the radial part of the wavefunction becomes

$$R_{n,\ell} = C_n r^{\frac{1}{2}(-1 + \sqrt{1 + 4\gamma})} e^{-i\varepsilon r} L_n^{\sqrt{1 + 4\gamma}}(2i\varepsilon r). \tag{25}$$

Table 1

Calculated energy eigenvalues of the Mie potential for N_2 , CO , NO and CH diatomic molecules with different values of n and ℓ in eV. The data for potential parameters are taken from Ref. [22].

State (n)	ℓ	N_2	CO	NO	CH
0	0	0.00271631	0.0254063	0.0205538	0.0416018
1	0	0.0810235	0.0756383	0.0611503	0.120556
	1	0.0810268	0.0758723	0.0613568	0.122185
2	0	0.13411	0.125172	0.101132	0.194768
	1	0.134351	0.125403	0.101335	0.1963
	2	0.134833	0.125867	0.101742	0.199356
3	0	0.186486	0.17402	0.140511	0.264609
	1	0.186719	0.174248	0.140712	0.266052
	2	0.187194	0.174704	0.141112	0.26893
	3	0.187907	0.175387	0.141713	0.273228
4	0	0.238152	0.222196	0.1793	0.330417
	1	0.238385	0.222421	0.179498	0.331777
	2	0.238854	0.22287	0.179892	0.334491
	3	0.239557	0.223544	0.180484	0.338544
	4	0.240495	0.224442	0.181272	0.343916
5	0	0.28913	0.269712	0.217511	0.392495
	1	0.289361	0.269933	0.217705	0.393779
	2	0.289824	0.270377	0.218094	0.396341
	3	0.290518	0.271041	0.218677	0.400166
	4	0.291443	0.271927	0.219453	0.405238
	5	0.292599	0.273036	0.220424	0.41153

If we rewrite equation (22) in atomic units, we obtain

$$E_n = -V_0^2 a^2 \left(2n + 1 + \sqrt{(2\ell + 1)^2 + 2V_0 a^2} \right)^{-2}. \quad (26)$$

4. Conclusions

We have investigated the analytical solution of the Schrödinger equation for Mie potential. By using a special case of Mie potential as $m = 2k$ and $k = 1$, the problem is reduced to a Coulombic potential with the additional centrifugal barrier. Energy eigenvalues and corresponding eigenfunctions are obtained by the NU method. Energy eigenvalues are computed for N_2 , CO , NO and CH molecules. They are listed in table 1.

Acknowledgments

This research was partially supported by the Scientific and Technological Research Council of Turkey.

References

- [1] G. Mie, Ann. Phys. (Leipzig)II, 657 (1903).
- [2] G.C. Maitland, M. Rigby, E.B. Smith and W.A. Wakeham, *Intermolecular forces* (Oxford Univ. Press, Oxford, 1987).
- [3] See for example, *Rare Gas Solids*, edited by M.L. Klein and J.A. Vemebles, (Academic Press, New York, 1976), Vol.1.
- [4] I.I. Goldman and V.D. Krivchenkov, *Problems in quantum mechanics* (Pergamon Press, New York, 1961); Y. Weissman and J. Jortner, Phys. Lett. A 70 (1979) 177; M.L. Seze, Chem. Phys. 87 (1984) 431; M. Sato and J. Goodisman, Am. J. Phys. 53 (1985) 350; Ş. Erkoç, R. Sever, Phys. Rev. A 37 (1988) 2687.
- [5] Ş. Erkoç and R. Sever, Phys. Rev. D 30 (1984) 2117.
- [6] Ş. Erkoç and R. Sever, Phys. Rev. D 33 (1986) 588; F.M. Fernandez et al., Phys. Rev. D 36 (1987) 650.
- [7] B. Gonul et al., J. of Phys. A: Math. Gen. 34 (2001) 8271.
- [8] E. Kasap et al., Chem. Phys. Lett. 172 (1990) 499.
- [9] S. Ozder et al., Chem. Phys. Lett. 135 (1987) 582.
- [10] R.W. Hasse, Phys. Lett. A 161 (1991) 130.
- [11] J. Plieva, J. Mol. Spectrosc. 193 (1997) 7.
- [12] Y.K. Toubin et al., J. Eng. Phys. Thermophys. 76 (2003) 619.
- [13] R.J. LeRoy and W. Lam, Chem. Phys. Lett. 71 (1970) 544; R.J. LeRoy and R.B. Bernstein, J. Chem. Phys. 52 (1970) 3869.
- [14] S. Ozcelik and M. Simsek, Phys. Lett. 152 (1991) 145.
- [15] A.F. Nikiforov and V.B. Uvarov, *Special Functions of Mathematical Physics* (Birkhäuser, Basel, 1988).
- [16] G. Szego, *Orthogonal polynomials* (American Mathematical Society, New York, 1959) (revised edition).

- [17] D. Gomez-Ullate, N. Kamran and R. Milson, ArXiv:nlin.SI/0401030.
- [18] N.W. Evans, Phys.Rev. A 41 (1990) 5666; Group Theory of the Smorodinsky-Winternitz System; J. Math. Phys. 32 (1991) 3369; Super-Integrability of the Winternitz System; Phys. Lett. A 147 (1990) 483.
- [19] Shi-Hai Dong, G. Sun and M. Lozada-Cassou, Phys. Lett. A 340 (2005) 94.
- [20] Shi-Hai Dong, Physica Scripta, 65 (2002) 289; Shi-Hai Dong and Zhong-Qi Ma, Shi-Hai Dong, J. Phys. A: Math. Gen. 31 (1998) 9855; C.Y. Shen, S.H. Dong, Phys. Lett. A 335 (2005) 374.
- [21] A.K. Chattopadhyay, Phys. Lett. A 357 (2006) 108.
- [22] C. Berkdemir, A. Berkdemir, J. Han, Chem. Phys. Lett. 417 (2006) 326.