

Shape invariance and the supersymmetry WKB approximation for a diatomic molecule potential

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

2000 J. Phys. A: Math. Gen. 33 6993

(<http://iopscience.iop.org/0305-4470/33/39/313>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.123

The article was downloaded on 02/06/2010 at 08:32

Please note that [terms and conditions apply](#).

Shape invariance and the supersymmetry WKB approximation for a diatomic molecule potential

Chun-Sheng Jia[†], Jia-Ying Wang[‡], Su He[§] and Liang-Tian Sun[†]

[†] The State Key Laboratory of Oil and Gas Reservoir Geology and Exploitation, Southwest Petroleum Institute, Nanchong 637001, People's Republic of China

[‡] Department of Geophysics, China University of Geosciences, Wuhan 430074, People's Republic of China

[§] Scientific Research Affairs Office, Southwest Petroleum Institute, Nanchong 637001, People's Republic of China

E-mail: chshjia@263.net

Received 17 April 2000, in final form 11 July 2000

Abstract. It has been shown that a four-parameter potential for a diatomic molecule is a shape-invariant potential with a translation of parameters. The exact energy spectrum of this potential is obtained by using the shape-invariance approach and the supersymmetry WKB approximation.

There has been a lot of work carried out on the form and computation method of the potential energy function for a diatomic molecule [1–5]. This is because of the need to interpret the spectra of a diatomic molecule in molecular physics and quantum chemistry. The well known Morse potential for a diatomic molecule is a shape-invariant potential with a translation of parameters [6]. The exact energy levels of the Morse potential can be obtained by using the shape-invariance approach [6–8] and the supersymmetry WKB quantization condition [9–11]. The normalized wavefunction can also be obtained with the help of the unified recurrence operator method [12, 13]. Sun [14] has proposed a four-parameter potential for a diatomic molecule, the evaluating accuracy of which, for the experimental RKR curve and the rotational-vibrating level, is of a far higher level than that of the Morse potential. In this paper we show that the four-parameter potential for a diatomic molecule is a shape-invariant potential with a translation of parameters. By using the shape-invariance approach and the supersymmetry WKB quantization condition, we determine the exact energy levels of the four-parameter diatomic molecule potential.

The Schrödinger equation for a particle of mass μ in a one-dimensional potential is

$$\left[-\frac{\hbar^2}{2\mu} \frac{d^2}{dx^2} + V(x) \right] \Psi(x) = E\Psi(x) \quad (1)$$

where $\Psi(x)$ is the wavefunction, $V(x)$ is the potential and E is the energy. The ground-state wavefunction $\Psi_0(x)$ can be written as

$$\Psi_0(x) = N \exp\left(-\frac{\sqrt{2\mu}}{\hbar} \int W(x) dx\right) = N \exp\left(\int Z(x) dx\right) \quad (2)$$

where N is a normalization constant and $W(x) = -\frac{\hbar}{\sqrt{2\mu}}Z(x)$ is called a superpotential in supersymmetric quantum mechanics. Substituting equation (2) into equation (1), one has

$$Z' + Z^2 = v(x) - \varepsilon_0 \quad (3)$$

where $v(x) = \frac{2\mu V(x)}{\hbar^2}$, $\varepsilon_0 = \frac{2\mu E_0}{\hbar^2}$ and E_0 is the ground-state energy. Equation (3) is a nonlinear Riccati equation.

We consider a four-parameter potential energy function for a diatomic molecule proposed by Sun [14]. The potential function

$$V(r) = \frac{D_e(e^\alpha - \lambda)^2}{(e^{\alpha/r_e} - \lambda)^2} - \frac{2D_e(e^\alpha - \lambda)}{(e^{\alpha/r_e} - \lambda)} \quad (4)$$

is defined in terms of four parameters D_e , r_e , α and λ , where D_e is the depth of the potential well and r_e is the equilibrium distance of the two nuclei. Substitution of

$$A = D_e(e^\alpha - \lambda)^2 \quad B = 2D_e(e^\alpha - \lambda) \quad \eta = \alpha/r_e \quad (5)$$

reduces equation (4) to

$$V(r) = \frac{A}{(e^{\eta r} - \lambda)^2} - \frac{B}{(e^{\eta r} - \lambda)}. \quad (6)$$

A particular case is the well known Morse potential, for which the parameters are given by

$$A = D_e e^{2\alpha r_e} \quad B = 2D_e e^{\alpha r_e} \quad \eta = \alpha \quad \lambda = 0. \quad (7)$$

The equivalent potential for the radial motion is given by

$$V_l(r) = V(r) + \frac{l(l+1)\hbar^2}{2\mu r^2} \quad (8)$$

where μ is the reduced mass. For the s state ($l = 0$), the corresponding $v(r)$ in equation (3) is

$$v(r) = \frac{2\mu V(r)}{\hbar^2} = \frac{a}{(e^{\eta r} - \lambda)^2} - \frac{b}{(e^{\eta r} - \lambda)} \quad (9)$$

where $a = \frac{2\mu A}{\hbar^2}$ and $b = \frac{2\mu B}{\hbar^2}$. Putting $Z(r) = \frac{P}{e^{\eta r} - \lambda} + Q$ and substituting this into equation (3) yields

$$P^2 - \eta\lambda P = a \quad 2PQ - \eta P = -b \quad Q^2 = -\varepsilon_0. \quad (10)$$

The radial wavefunction $R(r)$ for the ground state can be expressed as

$$\begin{aligned} R(r) &= \frac{N}{r} \exp\left(\int Z(r) dr\right) = \frac{N}{r} \exp\left[\int \left(\frac{P}{e^{\eta r} - \lambda} + Q\right)\right] \\ &= N \frac{1}{r} (e^{\eta r} - \lambda)^{P/\eta\lambda} e^{(Q-P/\lambda)r}. \end{aligned} \quad (11)$$

In view of the wavefunction $R(r)$ satisfying the standard conditions, that is when $r \rightarrow 0$, $R(r)$ is finite, and when $r \rightarrow \infty$, $R(r)$ becomes $R(r) \rightarrow 0$, and solving equation (10) we obtain

$$\begin{aligned} P &= \begin{cases} \frac{\eta\lambda + \sqrt{\eta^2\lambda^2 + 4a}}{2} & \lambda > 0 \\ \frac{\eta\lambda - \sqrt{\eta^2\lambda^2 + 4a}}{2} & \lambda < 0 \end{cases} \\ Q &= \frac{P^2 - a - b\lambda}{2\lambda P} \\ \varepsilon_0 &= -Q^2. \end{aligned} \quad (12)$$

The corresponding superpotential $W(r)$ and the ground-state energy E_0 are given by

$$W(r) = -\frac{\hbar}{\sqrt{2\mu}} Z(r) = -\frac{\hbar}{\sqrt{2\mu}} \left(\frac{P}{e^{\eta r} - \lambda} + Q \right) \tag{13}$$

$$E_0 = \frac{\hbar^2}{2\mu} \varepsilon_0 = -\frac{\hbar^2}{2\mu} Q^2 = -\frac{\hbar^2}{2\mu} \left(\frac{P^2 - a - b\lambda}{2\lambda P} \right)^2. \tag{14}$$

Using equations (13) and (10), the corresponding supersymmetry partner potentials $V_+(r)$ and $V_-(r)$ can be written in terms of the superpotential $W(r)$ as

$$\begin{aligned} V_+(r) &= W^2(r) + \frac{\hbar}{\sqrt{2\mu}} W'(r) \\ &= \frac{\hbar^2}{2\mu} \left[\frac{(P^2/\lambda)e^{\eta r}}{(e^{\eta r} - \lambda)^2} + \frac{-a/\lambda - b}{e^{\eta r} - \lambda} + Q^2 + \frac{\eta P e^{\eta r}}{(e^{\eta r} - \lambda)^2} \right] \end{aligned} \tag{15}$$

$$\begin{aligned} V_-(r) &= W^2(r) - \frac{\hbar}{\sqrt{2\mu}} W'(r) \\ &= \frac{\hbar^2}{2\mu} \left[\frac{(P^2/\lambda)e^{\eta r}}{(e^{\eta r} - \lambda)^2} + \frac{-a/\lambda - b}{e^{\eta r} - \lambda} + Q^2 - \frac{\eta P e^{\eta r}}{(e^{\eta r} - \lambda)^2} \right]. \end{aligned} \tag{16}$$

Putting $a_0 = P$, the shape-invariance condition can be expressed as

$$V_+(r, a_0) = V_-(r, a_1) + R(a_1) \tag{17}$$

where $a_1 = P + \eta\lambda = a_0 + \eta\lambda$ and

$$R(a_1) = \frac{\hbar^2}{2\mu} \left[\left(\frac{a_0^2 - a - b\lambda}{2\lambda a_0} \right)^2 - \left(\frac{a_1^2 - a - b\lambda}{2\lambda a_1} \right)^2 \right].$$

The energy eigenvalues of Hamiltonian $H_- = -\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + V_-(r)$ are given by

$$E_0^{(-)} = 0 \tag{18}$$

$$\begin{aligned} E_n^{(-)} &= \sum_{k=1}^n R(a_k) = R(a_1) + R(a_2) + \dots + R(a_n) \\ &= \frac{\hbar^2}{2\mu} \left[\left(\frac{a_0^2 - a - b\lambda}{2\lambda a_0} \right)^2 - \left(\frac{a_1^2 - a - b\lambda}{2\lambda a_1} \right)^2 + \left(\frac{a_1^2 - a - b\lambda}{2\lambda a_1} \right)^2 \right. \\ &\quad \left. - \left(\frac{a_2^2 - a - b\lambda}{2\lambda a_2} \right)^2 + \dots + \left(\frac{a_{n-1}^2 - a - b\lambda}{2\lambda a_{n-1}} \right)^2 - \left(\frac{a_n^2 - a - b\lambda}{2\lambda a_n} \right)^2 \right] \\ &= \frac{\hbar^2}{2\mu} \left[\left(\frac{a_0^2 - a - b\lambda}{2\lambda a_0} \right)^2 - \left(\frac{a_n^2 - a - b\lambda}{2\lambda a_n} \right)^2 \right] \\ &= \frac{\hbar^2}{2\mu} \left[\left(\frac{a_0^2 - a - b\lambda}{2\lambda a_0} \right)^2 - \left(\frac{(a_0 + n\eta\lambda)^2 - a - b\lambda}{2\lambda (a_0 + n\eta\lambda)} \right)^2 \right]. \end{aligned} \tag{19}$$

Combining equations (3) and (16), we can obtain the relation between $V(r)$ and $V_-(r)$,

$$V(r) = \frac{A}{(e^{\eta r} - \lambda)^2} - \frac{B}{(e^{\eta r} - \lambda)} = V_-(r) + E_0. \tag{20}$$

Hence, the energy levels of the potential expressed in equation (6) for the s state can be computed as

$$\begin{aligned}
 E_n &= E_n^{(-)} + E_0 \\
 &= \frac{\hbar^2}{2\mu} \left[\left(\frac{a_0^2 - a - b\lambda}{2\lambda a_0} \right)^2 - \left(\frac{(a_0 + n\eta\lambda)^2 - a - b\lambda}{2\lambda(a_0 + n\eta\lambda)} \right)^2 \right] - \frac{\hbar^2}{2\mu} \left(\frac{a_0^2 - a - b\lambda}{2\lambda a_0} \right)^2 \\
 &= -\frac{\hbar^2}{8\mu\lambda^2} \frac{[(a_0 + n\eta\lambda)^2 - a - b\lambda]^2}{(a_0 + n\eta\lambda)^2} \\
 &= -\frac{\hbar^2}{8\mu\lambda^2} \frac{[(P + n\eta\lambda)^2 - a - b\lambda]^2}{(P + n\eta\lambda)^2}
 \end{aligned} \tag{21}$$

$$n = 0, 1, 2, 3, \dots$$

From the above study, we suggest that the four-parameter potential for a diatomic molecule is a shape-invariant potential with a translation of parameters. For the shape-invariant potentials of translational type, the exact energy spectrum can be obtained by using the supersymmetry WKB quantization condition [9]

$$\int_{x_L}^{x_R} \sqrt{2\mu[E_n^{(-)} - W^2(x)]} dx = n\pi\hbar \quad n = 0, 1, 2, \dots \tag{22}$$

where the two turning points x_L and x_R are given by $[E_n^{(-)} - W^2(x)] = 0$. The energy $E_n^{(-)}$ in equation (22) is the energy level of the supersymmetry partner potentials $V_-(x)$. Substituting the superpotential given in equation (13) into the SWKB quantization condition, equation (22), gives

$$\int_{r_L}^{r_R} \sqrt{2\mu \left[E_n^{(-)} - \frac{\hbar^2}{2\mu} \left(\frac{P}{e^{\eta r} - \lambda} + Q \right)^2 \right]} dr = n\pi\hbar. \tag{23}$$

With a change of variables $y = \frac{1}{e^{\eta r} - \lambda}$, equation (23) becomes

$$\int_{y_L}^{y_R} \sqrt{2\mu \left[E_n^{(-)} - \frac{\hbar^2}{2\mu} (Py + Q)^2 \right]} \frac{-4\lambda}{\eta[(2\lambda y + 1)^2 - 1]} dy = n\pi\hbar. \tag{24}$$

By putting $\rho = 2\lambda y + 1$ and after algebraic simplification, equation (24) can be expressed as

$$\int_{\rho_L}^{\rho_R} \frac{-\hbar P}{\eta\lambda} \frac{1}{\rho^2 - 1} \sqrt{(\rho - \rho_L)(\rho_R - \rho)} d\rho = n\pi\hbar \tag{25}$$

where the two turning points are given by

$$\rho_L = 1 - \frac{2\lambda Q}{P} - \frac{2|\lambda|}{\hbar P} \sqrt{2\mu E_n^{(-)}}$$

and

$$\rho_R = 1 - \frac{2\lambda Q}{P} + \frac{2|\lambda|}{\hbar P} \sqrt{2\mu E_n^{(-)}}.$$

For computing the integral in equation (25), we use the integral expression [11]

$$\int_{z_L}^{z_R} \frac{1}{z^2 - 1} \sqrt{(z - z_L)(z_R - z)} dz = \frac{\pi}{2} \left[\sqrt{(z_L + 1)(z_R + 1)} - \sqrt{(z_L - 1)(z_R - 1)} + 2 \right]^{1/2} \tag{26}$$

where the limits z_L, z_R are real numbers, with $z_L < z_R$. Comparing equation (25) with equation (26), and solving for $E_n^{(-)}$ gives

$$E_n^{(-)} = -\frac{\hbar^2}{8\mu\lambda^2} \frac{[(P + n\eta\lambda)^2 - P(P - 2\lambda Q)]^2}{(P + n\eta\lambda)^2} + \frac{\hbar^2}{2\mu} Q^2 \quad n = 0, 1, 2, 3, \dots \quad (27)$$

Substituting $P(P - 2\lambda Q) = a + b\lambda$ into equation (27) and combining equation (14), it can be seen that the result in equation (27) is consistent with the result in equation (19).

From equation (21), the energy E_n can be written in the form

$$E_n = -\frac{\hbar^2\eta^2}{8\mu} \frac{[n^2 + 2nP/\eta\lambda + P^2/\eta^2\lambda^2 - a/\eta^2\lambda^2 - b\lambda/\eta^2\lambda^2]^2}{(n + P/\eta\lambda)^2}. \quad (28)$$

By using equations (12) and (5) and $a = \frac{2\mu A}{\hbar^2}$ and $b = \frac{2\mu B}{\hbar^2}$, we can obtain

$$\begin{aligned} \frac{a}{\eta^2\lambda^2} &= \frac{2\mu D_e r_e^2 (e^\alpha - \lambda)^2}{\hbar^2 \alpha^2 \lambda^2} = \delta^2 \\ \frac{b}{\eta^2|\lambda|} &= \frac{4\mu D_e r_e^2 (e^\alpha - \lambda)}{\hbar^2 \alpha^2 |\lambda|} = \gamma^2 \\ \frac{P}{\eta\lambda} &= \frac{1}{2} + \sqrt{\frac{1}{4} + \delta^2} = m. \end{aligned} \quad (29)$$

Substituting the above expressions into equation (28) and using $\delta^2 = m^2 - m$, it follows that

$$\begin{aligned} E_n &= -\frac{\hbar^2\alpha^2}{8\mu r_e^2} \frac{[n^2 + m(2n + 1) - \gamma^2]^2}{(n + m)^2} & \lambda > 0 \\ E_n &= -\frac{\hbar^2\alpha^2}{8\mu r_e^2} \frac{[n^2 + m(2n + 1) + \gamma^2]^2}{(n + m)^2} & \lambda < 0. \end{aligned} \quad (30)$$

These results are the same as those in equations (13) and (19) in [14] through solving the hypergeometric equation. For the convenience of solving equations (7) and (15) in [14], Sun took the approximate boundary conditions, which are $\lambda = 1$ and $\frac{|\lambda|}{1+|\lambda|} = 1$ when $r \rightarrow 0$ for $\lambda > 0$ and $\lambda < 0$, respectively. However, these approximations are not needed in the present treatment. The normalized wavefunctions for the four-parameter diatomic molecule potential can be obtained by using the unified recurrence operator method [13].

In equation (6), if we make the replacements, $A = 0$, $B = V_0$ and $\lambda = 1$, then equation (6) becomes

$$V(r) = -\frac{V_0}{e^{\eta r} - 1} \quad (31)$$

which is the Hulthen potential, a shape-invariant potential with a translation of parameters [15]. Substituting $a = \frac{2\mu A}{\hbar^2} = 0$ into equation (12), we can obtain $P = \eta\lambda$. With this and $b = \frac{2\mu V_0}{\hbar^2}$ and by taking $\lambda = 1$, we can obtain the energy spectrum for the Hulthen potential from equation (21):

$$E_n = -\frac{\hbar^2\eta^2}{8\mu} \frac{[(n + 1)^2 - 2\mu V_0/\hbar^2\eta^2]^2}{(n + 1)^2} \quad n = 0, 1, 2, 3, \dots \quad (32)$$

This is consistent with that in equation (68.14) in [3] obtained with the help of the factorization method.

Using the four-parameter diatomic molecule potential and the Morse potential, Sun [14] computed the errors of fitting the RKR potential curves for two kinds of metal dimers and six kinds of non-metal diatomic molecules. The results show that the average errors given by the four-parameter diatomic molecule potential are between 0.370% and 2.66%, and that the average errors produced by the Morse potential are between 0.860% and 16.1%. For fitting the experimental RKR potential curve of the $X^1\Sigma_g^+$ ground state of ${}^7\text{Li}_2$ observed by Barakat *et al* [16], the average error is 2.12% produced by the four-parameter diatomic molecule potential, and 8.38% given by the Morse potential [14]. We suggest that the four-parameter diatomic-molecule potential model can produce theoretical values which are in better agreement with the experimental spectrum data than the Morse potential model.

We have presented the full energy computation for the four-parameter potential of a diatomic molecule with the help of a shape-invariance approach. We have also presented the supersymmetry WKB approximation treatment for the four-parameter potential, with exact SWKB energy levels. Comparing the superpotential of the four-parameter diatomic molecule potential with the superpotential of the Hulthen potential, we put forward the four-parameter diatomic molecule potential and the Hulthen potential belonging to the same type of shape-invariant potentials with a translation of parameters.

Acknowledgments

CSJ thanks the Geophysics Department of the China University of Geosciences for their warm hospitality. Financial support from the Southwest Petroleum Institute is gratefully acknowledged. This work is supported by the Visiting Scholar Foundation of the Key Laboratory in the University.

References

- [1] Morse P M 1929 *Phys. Rev.* **34** 57
- [2] Dunham J L 1932 *Phys. Rev.* **41** 721
- [3] Flugge S 1974 *Practical Quantum Mechanics* (Berlin: Springer)
- [4] Nieto M M and Simmons L M Jr 1979 *Phys. Rev. A* **19** 438
- [5] Znojil M 1994 *J. Phys. A: Math. Gen.* **27** 7491
- [6] Gendenshtein L E 1983 *Sov. Phys.-JETP Lett.* **38** 356
- [7] Cooper F, Ginocchio J N and Khare A 1987 *Phys. Rev. D* **36** 2458
- [8] Cooper F, Khare A and Sukhatme U 1995 *Phys. Rep.* **251** 267
- [9] Comtet A, Bandrank A and Campbell D K 1985 *Phys. Lett. B* **150** 159
- [10] Dutt R, Khare A and Sukhatme U 1986 *Phys. Lett. B* **181** 295
- [11] Hruska M, Keung W Y and Sukhatme U 1997 *Phys. Rev. A* **55** 3345
- [12] Dabrowska J W, Khare A and Sukhatme U P 1988 *J. Phys. A: Math. Gen.* **21** L195
- [13] Chun-Sheng Jia, Xiao-Guo Wang, Xiao-Ke Yao, Pu-Chun Chen and Wei Xiao 1998 *J. Phys. A: Math. Gen.* **31** 4763
- [14] Jiu- Xun Sun 1999 *Acta Phys. Sin.* **48** 1992
- [15] Chun-Sheng Jia, Xiao-Guo Wang, Qiu-Bo Yang, Su He and Hao Li 1998 *Commun. Theor. Phys.* **30** 305
- [16] Barakat B, Bacis R, Carrot F, Churassy S, Crozet P and Martin F 1986 *Chem. Phys.* **102** 215