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Supersymmetric WKB solutions for pseudoharmonic and Mie-type potentials

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Using the supersymmetric WKB approach, we have obtained exact energy spectra for a pseudoharmonic and a Mie-type potential in three dimensions.

Supersymmetric quantum mechanics [1,2] (SUSYQM) offers an alternative approach for analysing dynamical problems in quantum mechanics. The supersymmetric WKB method [1–4] (SWKB) is one of the most useful techniques for reproducing the spectra of all analytically solvable potentials. Recently, it was shown that the leading-order ($\hbar^0$) SWKB quantization condition gives exact bound-state spectra for shape-invariant potentials [2–4].

In this paper, we have applied the SWKB method for the first time in three dimensions for the Mie-type [5] and pseudoharmonic [6] potentials, which have the property of shape-invariance. Note that the standard WKB method does not give exact results for the Mie-type and pseudoharmonic potentials unless it is supplemented by a Langer-like correction [7].

The study of three-dimensional anharmonic oscillators has raised a considerable amount of interest because of its varied applications in molecular physics [8]. The Morse potential is commonly used for an anharmonic oscillator. However, its wavefunction does not vanish at the origin, but those for Mie-type and pseudoharmonic potentials do. The Mie-type potential possesses the general features of the true interaction energy [8], inter-atomic and inter-molecular, and dynamical properties of solids [9]. On the other hand, the pseudoharmonic potential may be used for the energy spectrum of linear and non-linear systems [6]. The Mie-type and pseudoharmonic are two special kinds of analytically solvable power-law and inverse power-law potentials other than the Coulombic and harmonic oscillator; for these reasons, we have chosen them in the application of the SWKB method.

The non-relativistic Hamiltonian is

$$\tilde{H} = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x) \tag{1}$$

and $\tilde{E}_0$, $\tilde{\Phi}_0$ the true ground-state energy and corresponding eigenfunction of $\tilde{H}$. In SUSYQM, the structure of the Hamiltonian is given by $H \equiv \tilde{H} - \tilde{E}_0$, and the ground-state energy of H is precisely zero [1,2]. It is easy to see that H can be written formally in either of the pair-Hamiltonian $H_\pm$ forms,

$$H \equiv H_\pm = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V_\pm(x) \tag{2}$$

and, hence, the Schrödinger equation for the ground state is

$$H_-\Phi_0(x) = \left(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V_-(x)\right)\Phi_0(x) = 0 \tag{3}$$

and, consequently,

$$H_- = \frac{\hbar^2}{2m}\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{\Phi_0''(x)}{\Phi_0(x)}\right). \tag{4}$$

Here, $\Phi_0(x)$ is the normalizable ground-state eigenfunction of the Hamiltonian H_-. For unbroken su-

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persymmetry, choosing $H=H_-$ is convenient [3], and general results [1] indicate that the spectrum of H_+ is identical to that of H_- except for $E_0^- = 0$. The primes in eq. (4) denote the second derivative with respect to the coordinate x.

Let

$$A=\frac{\hbar}{\sqrt{2m}}\left(\frac{\mathrm{d}}{\mathrm{d}x}-\frac{\Phi_0'}{\Phi_0}\right) \tag{5a}$$

and its Hermitian conjugate

$$A^+=\frac{\hbar}{\sqrt{2m}}\left(-\frac{\mathrm{d}}{\mathrm{d}x}-\frac{\Phi_0'}{\Phi_0}\right). \tag{5b}$$

These give

$$A^+A\equiv H_-\,,$$

$$AA^+\equiv H_+=-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}+V_+(x)\,, \tag{6}$$

where

$$V_+(x)=V_-(x)-\frac{\hbar}{\sqrt{2m}}\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\Phi_0'}{\Phi_0}\right). \tag{7}$$

The potentials V_+ and V_- are called supersymmetric partner potentials. Also one can see that the relation between the partner potential V_- and the actual potential V is $V_-=V-\bar{E}_0$.

It is the practice to use the superpotential, $W(x)$, rather than the ground-state eigenfunction, Φ_0, of H_- [1–4]. The relation between $W(x)$ and Φ_0 is given by

$$W(x)=-\frac{\hbar}{\sqrt{2m}}\left(\frac{\Phi_0'}{\Phi_0}\right) \tag{8}$$

and the pair of Hamiltonians $H_\pm$ are written as

$$H_\pm=-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}+W^2(x)\pm\frac{\hbar}{\sqrt{2m}}W'(x)\,. \tag{9}$$

To find $W(x)$, the Ricatti equation must be solved for the potential in eq. (9),

$$V_\pm(x)=W^2(x)\pm\frac{\hbar}{\sqrt{2m}}W'(x)\,. \tag{10}$$

Application of this general relation to different potentials $V_\pm$ may be simple, if one knows the actual ground-state energy.

The SWKB quantization condition to leading order in $\hbar$ is [3]

$$\int_a^b\{2m[E_n^- - W^2(x)]\}^{1/2}\mathrm{d}x=n\pi\hbar\,,$$

$$n=0,1,2,... \tag{11}$$

and the turning points a and b are given by

$$W^2(a)=W^2(b)=E_n^-=E\,. \tag{12}$$

Similarly, for H_+ one can obtain

$$\int_a^b\{2m[E_n^+ - W^2(x)]\}^{1/2}\mathrm{d}x=(n+1)\pi\hbar\,,$$

$$n=0,1,2,...\,, \tag{13}$$

where $E_n^\pm$ are the energy eigenvalues of the supersymmetric partner potentials $V_\pm$. From eqs. (11) and (13), the level degeneracy $E_{n+1}^-=E_n^+$ holds; also this condition is a result of the general structure of SUSYQM [1–4].

We first consider a special case of the Mie-potential which has been solved by other methods [10,11]. The general form of the Mie-type potential is [5]

$$V(r)=D_0\left[\frac{n}{m-n}\left(\frac{\sigma}{r}\right)^m-\frac{m}{m-n}\left(\frac{\sigma}{r}\right)^n\right], \tag{14}$$

where D_0 is the interaction energy between two atoms in a molecular system at $r=\sigma$, and $m>n$ is always satisfied. If we take $m=2n$ and $n=1$, (14) reduces to

$$V(r)=\frac{A}{r^2}-\frac{B}{r}\,, \tag{15}$$

where $A=D_0\sigma^2$ and $B=2D_0\sigma$. This potential includes the terms which give the representation of both the steep repulsive branch and the long-range attraction. A single minimum occurs at $r=\sigma$ where the energy is $-D_0$.

The effective Hamiltonian is

$$H_{\mathrm{eff}}=-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\frac{l(l+1)\hbar^2}{2mr^2}+\frac{A}{r^2}-\frac{B}{r}\,. \tag{16}$$

One obtains the superpotential for eq. (16) by eqs. (10) and (15)

$$W(r)=\frac{B/2}{\alpha+(\alpha^2+C)^{1/2}}-\frac{\alpha+(\alpha^2+C)^{1/2}}{r}, \quad (17)$$

where $\alpha=(\hbar^2/8m)^{1/2}$ and $C=[l(l+1)\hbar^2+2mA]/2m$. From eqs. (9) and (17), we can rewrite the effective Hamiltonian H_{eff} as

$$H_{\text{eff}}=-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}+W^2(r)-\frac{\hbar}{\sqrt{2m}}W'(r)$$
$$-\frac{B^2/4}{[\alpha+(\alpha^2+C)^{1/2}]^2}. \quad (18)$$

From eqs. (11) and (18), we then obtain the exact spectrum of the potential in eq. (15) as

$$E_n=-\left(\frac{B/2\alpha}{2n+1+[(2l+1)^2+A/\alpha^2]^{1/2}}\right)^2,$$
$$n=0, 1, 2, ... \quad (19)$$

and from eqs. (8) and (17), the exact ground-state wavefunction of eq. (15), without the necessity of considering the Langer correction [7], as

$$\Phi_0^-=r^{1/2\{1+[(2l+1)^2+A/\alpha^2]^{1/2}\}}$$
$$\times\exp\left(-\frac{Br/4\alpha^2}{1+[(2l+1)^2+A/\alpha^2]^{1/2}}\right). \quad (20)$$

The standard WKB results of the potential in eq. (15) is

$$E_n=-\left(\frac{B/2\alpha}{2n+1+[4l(l+1)+A/\alpha^2]^{1/2}}\right)^2,$$
$$n=0, 1, 2.... \quad (21)$$

As can be seen from eqs. (19) and (21), if $l(l+1)$ is replaced by $(l+\frac{1}{2})^2$ in the WKB solution, eq. (21), one obtains the SWKB solution, eq. (19), exactly. Furthermore, for $A=0$ (in eqs. (16) and (19)) the results become identical with the exact spectrum of the three-dimensional Coulomb potential.

The other combinations of the Mie-type potential, namely $m>2$, $n>1$, are non-shape-invariant types. However, exact energy spectra are not obtainable and consequently it is necessary to go beyond the leading-order SWKB calculation.

As a second application, the SWKB approach can also be applied to obtain the exact spectrum of the pseudoharmonic potential which has also been solved by other methods [6]; this potential has the form

$$V(r)=V_0\left(\frac{r}{r_0}-\frac{r}{r}\right)^2. \quad (22)$$

This can be used to calculate the vibrational energies of diatomic molecules with the equilibrium bond length r_0 and force constant $k=8V_0/r_0^2$. Its effective Hamiltonian is

$$H_{\text{eff}}=-\frac{\hbar^2}{2m}-\frac{d^2}{dr^2}+\frac{l(l+1)\hbar^2}{2mr^2}+Br^2+\frac{A}{r^2}-2V_0, \quad (23)$$

where $A=V_0r_0^2$ and $B=V_0/r_0^2$. Taking the superpotential for eq. (22)

$$W(r)=\sqrt{B}r-\frac{\alpha+(\alpha^2+C)^{1/2}}{r}, \quad (24)$$

where $C=[l(l+1)\hbar^2+2mA]/2m$, we can rewrite H_{eff} as

$$H_{\text{eff}}=-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}+W^2(r)-\frac{\hbar}{\sqrt{2m}}W'(r)$$
$$+2\sqrt{B}[\alpha+(\alpha^2+C)^{1/2}]-2V_0. \quad (25)$$

From eqs. (11) and (25), the exact spectrum of the potential in eq. (22) is obtained as

$$E_n=2\alpha\sqrt{B}\{4n+2$$
$$+[(2l+1)^2+A/\alpha^2]^{1/2}\}-2V_0,$$
$$n=0, 1, 2, ... \quad (26)$$

and from eqs. (8) and (24) the exact ground-state wave function of eq. (22), without applying any correction [7], as

$$\Phi_0^-=r^{1/2\{1+[(2l+1)^2+A/\alpha^2]^{1/2}\}}$$
$$\times\exp\left(-\frac{\sqrt{B}r^2}{4\alpha}\right). \quad (27)$$

The standard WKB results of the same potential, eq. (22) are

$$E_n=2\alpha\sqrt{B}\{4n+2$$
$$+[4l(l+1)+A/\alpha^2]^{1/2}\}-2V_0,$$
$$n=0, 1, 2, ... \quad (28)$$

The replacement by $(l+\frac{1}{2})^2$ of $l(l+1)$ in the WKB solution, eq. (28), produces the same result of the SWKB solution, eq. (26), as obtained above for the

Mie-type potential. If one takes $A=0$ in eqs. (23) and (26), then eq. (26) becomes the exact energy spectra of the three-dimensional harmonic oscillator potential.

The WKB method gives reasonable results for higher states for the potential functions studied in this work. However, the SWKB method gives correct spectra for the whole range of the spectrum for the shape-invariant potential functions. This is one of the most important points of superiority of the SWKB method to the WKB method.

Summarizing, we have obtained the exact spectra, without applying any correction, of a pseudoharmonic and a Mie-type potential using the SWKB method in three dimensions. The present SWKB results for both potentials agree with the previous calculations [6,10,11].

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