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The supersymmetric WKB approximation for Hartmann potential *

Chen Gang (陈 刚)†

Department of Physics, Shaoxing College of Arts and Sciences, Shaoxing 312000, *China*

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Using the method of supersymmetric WKB approximation, the energy spectrum of some noncentral separable potentials can be exactly obtained in r and θ dimensions. We take the Hartmann potential as an important example for its validation, and the result is consistent with that obtained by using the supersymmetric quantum mechanics and shape invariance.

Keywords: Hartmann potential, energy spectrum, supersymmetric WKB approximation
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1. Introduction

Supersymmetric was first studied in the simplest case of supersymmetric quantum mechanics by Witten,[1] and Cooper and Freeman.[2] It was realized that supersymmetric gives insight into the factorization method of Infeld and Hull.[3] In 1983, the concept of shape invariant potential was introduced by Gendenstein.[4] It was readily shown that, for any shape invariant potential, the energy spectrum can be obtained algebraically.[5] In 1985, Comtet *et al* suggested the supersymmetric WKB approximation based on supersymmetric quantum mechanics.[6] With the ideas of the supersymmetric WKB approximation, a number of potentials can also be solved exactly.[7–9] Although most of these potentials are either one-dimensional or central potential, there are some non-central separable (in spherical polar coordinates) potentials. Those potentials have supersymmetric and shape invariance and can be exactly solved in terms of the supersymmetric quantum mechanics and shape invariance.[10] In this paper, we suggest that the energy spectra of those potentials can also be obtained by the supersymmetric WKB quantization condition, and choose the Hartmann potential as an important example to show that.

The Hartmann potential was introduced in quantum chemistry to describe ring-shaped molecules like benzene. It is given by the following expression:

$$V(r,\theta)=\frac{\alpha}{r}+\frac{\beta}{(r\sin\theta)^2}, \tag{1}$$

where $\alpha=-\eta\sigma^2e^2$, $\beta=-\eta^2\sigma^2\hbar^2/2\mu$, η and σ are positive real parameters, which range from 1 to 10 in theoretical chemistry applications. The limiting case $\beta=0$ corresponds to the well-known Coulomb potential, which has been investigated in many articles and textbooks.

2. Separable potentials in spherical polar coordinates

In spherical polar coordinates the most general potential, for which the Schrödinger equation is separable, is given by [11]

$$V(r,\theta,\phi)=V(r)+\frac{V(\theta)}{r^2}+\frac{V(\phi)}{r^2\sin^2\theta}, \tag{2}$$

where $V(r)$, $V(\theta)$, $V(\phi)$ are arbitrary functions of their argument. If one writes the wavefunction $\Psi(r,\theta,\phi)$ as

$$\Psi(r,\theta,\phi)=\frac{R(r)}{r}\frac{H(\theta)}{(\sin\theta)^{1/2}}K(\phi), \tag{3}$$

then the following equations (in units of $2\mu=\hbar=1$) are obtained:

$$-\frac{\mathrm{d}^2K(\phi)}{\mathrm{d}\phi^2}+V(\phi)K(\phi)=m^2K(\phi), \tag{4}$$

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†E-mail: Chengang@zscas.edu.cn

$$-\frac{\mathrm{d}^2H(\theta)}{\mathrm{d}\theta^2}+\left[V(\theta)+\left(m^2-\frac{1}{4}\right)\csc^2\theta\right]H(\theta)=l^2H(\theta), \tag{5}$$

$$-\frac{\mathrm{d}^2R(r)}{\mathrm{d}r^2}+\left[V(r)+\frac{l^2-1/4}{r^2}\right]R(r)=ER(r), \tag{6}$$

where m^2 and l^2 are separation constants.

For the Hartmann potential we have

$$V(r)=\frac{\alpha}{r},\quad V(\theta)=\beta\csc^2\theta,\quad V(\phi)=0, \tag{7}$$

hence we can get three Schrödinger equations as follows:

$$-\frac{\mathrm{d}^2K(\phi)}{\mathrm{d}\phi^2}=m^2K(\phi), \tag{8}$$

$$-\frac{\mathrm{d}^2H(\theta)}{\mathrm{d}\theta^2}+\left[\left(m^2+\beta-\frac{1}{4}\right)\csc^2\theta\right]H(\theta)=l^2H(\theta), \tag{9}$$

$$-\frac{\mathrm{d}^2R(r)}{\mathrm{d}r^2}+\left[\frac{\alpha}{r}+\frac{l^2-1/4}{r^2}\right]R(r)=ER(r). \tag{10}$$

Though solution of $K(\phi)$ cannot be given by supersymmetric quantum mechanics, we can get it through direct integration. Its solutions are

$$K(\phi)=\frac{1}{\sqrt{2\pi}}\mathrm{e}^{\mathrm{i}m\phi},\quad m=0,\pm1,\pm2,\cdots \tag{11}$$

In the following sections we will use the supersymmetric WKB quantization condition to get the energy spectrum of the Hartmann potential in r and θ dimensions.

3. Supersymmetric WKB approximation in θ dimension

If put $B(B-1)=\beta+m^2-\frac{1}{4}$ or $B=\sqrt{\beta+m^2}+\frac{1}{2}$, Eq.(9) becomes

$$-\frac{\mathrm{d}^2H(\theta)}{\mathrm{d}\theta^2}+[B(B-1)\csc^2\theta]H(\theta)=l^2H(\theta). \tag{12}$$

In order to use the supersymmetric WKB quantization condition, its superpotential $W(\theta)$ has to be known. From Refs.[12–14], we can easily obtain the superpotential $W(\theta)$. Its superpotential $W(\theta)$ and ground state E_0 are respectively given by

$$W(\theta)=-B\cot\theta,\quad E_0=B^2. \tag{13}$$

The supersymmetric WKB quantization condition is [6]

$$\int_{x_\mathrm{L}}^{x_\mathrm{R}}\sqrt{[E_n^{(-)}-W^2(x)]}=n\pi,\quad n=0,1,2,\cdots, \tag{14}$$

where two turning points x_L and x_R are given by $[E_n^{(-)}-W^2(x)]=0$, the energy $E_n^{(-)}$ being the energy level of the supersymmetric partner potential $V_-(x)$. Substituting the superpotential given by Eq.(13) into the supersymmetric WKB quantization condition, we obtain

$$\int_{\theta_\mathrm{L}}^{\theta_\mathrm{R}}\sqrt{[E_s^{(-)}-B^2\cot^2\theta]}=s\pi,\quad s=0,1,2,\cdots. \tag{15}$$

With a change of variables $y=-\cot\theta$, Eq.(15) becomes

$$B\int_{y_\mathrm{L}}^{y_\mathrm{R}}\frac{1}{1+y^2}\sqrt{(y_\mathrm{R}-y)(y-y_\mathrm{L})}\mathrm{d}y=s\pi, \tag{16}$$

where two turning points are given by $y_\mathrm{L}=-\sqrt{E_s^{(-)}}/B$ and $y_\mathrm{R}=\sqrt{E_s^{(-)}}/B$. Using the integral expression [8] and by simple computation, we obtain

$$E_s^{(-)}=(B+s)^2-B^2. \tag{17}$$

For the energy spectrum $E_s=E_s^{(-)}+E_0$, we obtain

$$l=(B+s). \tag{18}$$

4. Supersymmetric WKB approximation in r dimension

From Refs.[12–14], superpotential $W(r)$ and ground state E_0 in Eq.(10) are respectively given by

$$W(r)=-\left[\frac{\alpha}{2\left(l+\frac{1}{2}\right)}+\frac{\left(l+\frac{1}{2}\right)}{r}\right],$$
$$E_0=-\frac{\alpha^2}{4\left(l+\frac{1}{2}\right)^2}. \tag{19}$$

Substituting $W(r)$ of Eq.(19) into the supersymmetric WKB quantization condition (14), we obtain

$$\int_{r_\mathrm{L}}^{r_\mathrm{R}}\sqrt{E_n^{(-)}-\left[\frac{\alpha}{2\left(l+\frac{1}{2}\right)}+\frac{\left(l+\frac{1}{2}\right)}{r}\right]^2}\,\mathrm{d}r=n\pi,$$
$$n=0,1,2,\cdots. \tag{20}$$

With a change of variable $\rho=-\frac{1}{r}$, Eq.(20) becomes

$$\left(l+\frac{1}{2}\right)\int_{\rho_\mathrm{L}}^{\rho_\mathrm{R}}\frac{1}{\rho^2}\sqrt{(\rho_\mathrm{R}-\rho)(\rho-\rho_\mathrm{L})}\mathrm{d}y=n\pi, \tag{21}$$

where the two turning points are given by

$$\rho_{\rm L} = -\frac{1}{\left(l+\frac{1}{2}\right)}\sqrt{E_n^{(-)}} - \frac{\alpha}{2\left(l+\frac{1}{2}\right)^2}$$

and

$$\rho_{\rm R} = \frac{1}{\left(l+\frac{1}{2}\right)}\sqrt{E_n^{(-)}} - \frac{\alpha}{2\left(l+\frac{1}{2}\right)^2}.$$

Using the integral expression [8] and by simple computation, we obtain

$$E_n^{(-)} = -\frac{\alpha^2}{4\left(n+l+\frac{1}{2}\right)^2} + \frac{\alpha^2}{4\left(l+\frac{1}{2}\right)^2}. \qquad (22)$$

For the energy spectrum $E_n = E_n^{(-)} + E_0$, we obtain

$$E_n = -\frac{\alpha^2}{4\left(n+l+\frac{1}{2}\right)^2}. \qquad (23)$$

Finally, comparing Eq.(23) with Eq.(18), we obtain the exact energy spectrum of the Hartmann potential:

$$E_{n,s} = -\frac{\alpha^2}{4(n+\sqrt{\beta+m^2}+s+1)^2}. \qquad (24)$$

It can be seen that the result of Eq.(24) is consistent with that of Ref.[10]

5. Conclusion

In this paper, we have presented the full energy spectrum of the Hartmann potential in terms of the supersymmetric WKB approximation. The energy spectrum is exactly solved and the result is consistent with that of the supersymmetric quantum mechanics and shape invariance. By using the supersymmetric WKB approximation, we believe that the noncentral separable potentials have exact energy spectrum and the method in this paper will probably be extended to any noncentral separable potential.

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