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Geometric Proof of Exact Quantization Rules in One Dimensional Quantum Mechanics

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Abstract In terms of the construction of vector field with momentum and logarithmic derivative of wavefunction as its components, a geometric proof of an exact quantization rule in one dimensional quantum mechanics systems is given. The quantization rule arises from the $SO(2)$ gauge transformation. In addition, the quantization rule is generalized to the case when the potential function is piecewise continuous between the two turning points.

Keywords Quantization rule · Gauge transformation · Piecewise continuous

1 Introduction

Quantization is a basic concept in quantum theories and a bridge to understanding more clearly the relationship between classical and quantum mechanics. Recently, Ma et al. [1–3] presented an exact quantization rule in studying the bound states of one dimensional quantum mechanics. This quantization rule overcomes the shortcomings of WKB method [4, 5] which is an approximate treatment of the Schrödinger equation and is valid for harmonic oscillator and cases with nearly classical limit of large quantum numbers, namely, the number of nodes of the WKB wave function between the two turning point is large enough. The exact quantization rule demonstrates advantages in obtaining the energy levels and the eigenfunctions of bound states for exactly solvable systems.

Geometric method [6–10] has been considered as so far mathematically most thorough approach to intrinsic understandings and findings to lots of things in the fields of mathematics and physics as well, such as topological invariants, gauge field theories and quantum

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Mechanics. Therefore, it is interesting to find the geometric interpretation of the exact quantization rule. In this paper, we construct a two-dimensional vector field with its components the momentum and logarithmic derivative of wave function, and apply the $SO(2)$ gauge transformation to give a geometric proof of the exact quantization rule. Although Ma et al. consider the discontinuity of potential at turning points, they do not consider the discontinuity between the turning points. So we also investigate the quantization rule of the case when the potential of the system is a piecewise continuous function between the two turning points. We find that the discontinuity of potential contributes a new term to the exact quantization rule. This paper is organized as follows: In Sect. 2, we give a geometric proof of exact quantization rule and generalize it to the case of piece-wise continuous potential. In Sect. 3, we discuss the geometric interpretation of terms in the generalized exact quantization rule.

2 Geometric Proof of Exact Quantization Rule

2.1 Brief Introduction of Exact Quantization Rule

The one dimensional Schrödinger equation of quantum mechanics with energy E is

$$\frac{d^2}{dx}\psi(x) + \frac{2\mu}{\hbar^2}[E - V(x)]\psi(x) = 0, \tag{1}$$

where μ is the mass of the particle, and the potential $V(x)$ is a piecewise continuous real function of space coordinate x. The logarithmic derivative of wave function $\psi(x)$ is defined as

$$\phi(x) = \frac{d\psi(x)/dx}{\psi(x)}. \tag{2}$$

From (1) and (2), we obtain Riccati equations

$$-\frac{d}{dx}\phi(x) = k(x)^2 + \phi(x)^2, \quad E \geq V(x), \tag{3}$$

$$-\frac{d}{dx}\phi(x) = -k(x)^2 + \phi(x)^2, \quad E \leq V(x), \tag{4}$$

in which momentum $k(x)$ is defined as

$$k(x) = \begin{cases} \sqrt{2\mu(E - V(x))}/\hbar, & E \geq V(x), \\ \sqrt{2\mu(V(x) - E)}/\hbar, & E \leq V(x). \end{cases} \tag{5}$$

Note that Schrödinger equation is a second order equation while Riccati equation is a first order one. It is obvious from (3) that $\phi(x)$ decreases monotonically with respect to variable x in the region where $E \geq V(x)$. From (2), $\phi(x)$ has an important property when $E \geq V(x)$ that $\phi(x)$ decrease to $-\infty$, then jumps to $+\infty$ near a zero point of the wave function $\psi(x)$, then it decreases again.

Ma et al. pointed out that there exists an exact relation between $k(x)$ and $\phi(x)$, called the exact quantization rule [1].

$$\int_{x_A}^{x_B} k(x)dx - \int_{x_A}^{x_B} \phi(x)\left[\frac{d\phi(x)}{dx}\right]^{-1}\frac{dk}{dx}dx - \left(\arctan\frac{k(x_B)}{\phi(x_B)} - \arctan\frac{k(x_A)}{\phi(x_A)}\right) = N\pi, \tag{6}$$

where x_A and x_B are the turning points determined by $k(x)=0$, $(N-1)$ is the number of node of $\psi(x)$. Equation (6) was deduced in Ref. [1] without any approximation, therefore it is better than both WKB approximation and Bohr-Sommerfeld quantization rules. If the potential $V(x)$ is continuous at the turning points, the momentum $k(x_A)$ and $k(x_B)$ vanish and (6) is just

$$\int_{x_A}^{x_B} k(x)dx - \int_{x_A}^{x_B} \phi(x)\left[\frac{d\phi(x)}{dx}\right]^{-1}\frac{dk}{dx}dx = N\pi, \tag{7}$$

in which the second term in (7) may be regarded as the correction to WKB approximation and Bohr-Sommerfeld quantization rules.

2.2 Geometric Proof of Exact Quantization Rule

The existence of integer N in (6) implies a possibility of geometric interpretation of the quantization rule. In the following, we will give a geometric proof of the quantization rule via construction of vector field and the corresponding gauge transformation. Besides, our proof will generalize the exact quantization rule (6) to the case when potential $V(x)$ has jumping points between the two turning points.

Firstly we construct two dimensional vector field $\vec{e}=(e^1,e^2)$ as the section of a bundle with its base manifold the coordinate space of the quantum mechanics system

$$\begin{aligned} e^1(x) &= (-1)^q\phi(x), \\ e^2(x) &= (-1)^q k(x), \end{aligned} \tag{8}$$

where q is the number of divergent points (or nodes of $\psi(x)$) of the function $\phi(x)$ from the point x_A to x, it is a function of x.

Normalizing vector $\vec{e}$, we get an unit vector field $\overrightarrow{n}=(n^1,n^2)$ with (n^1,n^2) its two components

$$n^1(x)=\lambda(x)(-1)^q\phi(x), \qquad n^2(x)=\lambda(x)(-1)^q k(x), \tag{9}$$

in which

$$\lambda^{-1}(x)=\sqrt{\phi^2(x)+k^2(x)}. \tag{10}$$

Since $\lambda(x)\phi(x)\to 1$ when $\phi\to\infty$ and $\lambda(x)\phi(x)\to -1$ when $\phi\to-\infty$, the factor $(-1)^q$ here realizes the continuousness of component $n^1(x)$ and therefore $\vec{n}(x)$ when $\psi\to 0$, or $\phi\to\pm\infty$. In addition, the factor $(-1)^q$ ensures the unit vector $\vec{n}(x)$ rotates anti-clockwise near the points where $\phi\to\pm\infty$. Clearly, $k(x_i)$ is not well defined from (5) when potential $V(x)$ is jumping at the point x_i. Therefore, vector field $\vec{e}$ is well defined between two turning points except points x_i, the region is defined as $\mathcal{C}=(x_A,x_1)\cup(x_1,x_2)\cup\cdots\cup(x_M,x_B)$. The existence of the jumping points of potential $V(x)$ causes $\vec{n}$ piece-wise continuous from x_A to x_B. These jumping points will contribute to the quantization rule.

The unit vector field $\vec{n}$ can be regarded as the section of sphere bundle. So, we consider the covariant derivative on the area $\mathcal{C}$ which vector $\vec{n}$ is continuous. The covariant derivative Dn^a is defined by $so(2)$ gauge theory

$$Dn^a = dn^a - \omega^{ab}n^b, \quad a,b=1,2 \tag{11}$$

in which gauge potential or connection ω^{ab} is the element of $so(2)$ Lie algebra with property

$$\omega^{ab}=-\omega^{ba}. \tag{12}$$

Obviously the non-vanishing components satisfy $\omega^{12} = -\omega^{21}$. We take the dependent component of connection one form ω^{12} as

$$\omega^{12}(x) = \frac{\phi}{d\phi/dx} dk(x) \tag{13}$$

with which (11) can be written explicitly

$$\begin{aligned} Dn^1 &= dn^1 - \frac{\phi}{d\phi/dx} dk(x) n^2, \\ Dn^2 &= dn^2 + \frac{\phi}{d\phi/dx} dk(x) n^1. \end{aligned} \tag{14}$$

Another $so(2)$ connection [6] one form $\widetilde{\omega}^{12}$ defined by the unit vector field $\vec{n}(x)$ is

$$\widetilde{\omega}^{12} = n^1 Dn^2 - n^2 Dn^1. \tag{15}$$

According to $so(2)$ gauge theory, $\widetilde{\omega}^{12}$ and ω^{12} are related by gauge transformations

$$\widetilde{\omega}^{12} - \omega^{12} = d\theta \tag{16}$$

where θ is gauge transformation parameter determined by

$$d\theta = n^1 dn^2 - n^2 dn^1. \tag{17}$$

The parameter θ is nothing but the angel change of unit vector $\vec{n}$,

$$\tan\theta = \frac{n^2}{n^1}.$$

Putting (9) and (14) into (15), and noticing $(-1)^{2q} = 1$, we obtain

$$\begin{aligned} \widetilde{\omega}^{12} &= \lambda\phi \left[d(\lambda k) + \left(\frac{\phi}{d\phi/dx} dk(x) \right) \lambda\phi \right] - \lambda k \left[d(\lambda\phi) - \left(\frac{\phi}{d\phi/dx} dk(x) \right) \lambda k \right] \\ &= \lambda^2 \left[\phi dk - k d\phi + \frac{\phi}{d\phi/dx} (\phi^2 + k^2) dk \right]. \end{aligned} \tag{18}$$

From Riccati equation (3), the first term cancels with the last term, then we have

$$\widetilde{\omega}^{12} = \lambda^2 [-k d\phi].$$

Further using the definition of λ in (10) as well as Riccati equation (3), we finally obtain

$$\widetilde{\omega}^{12} = k dx. \tag{19}$$

Therefore if $\frac{\phi}{d\phi/dx} dk$ can be taken as an $so(2)$ connection, or gauge potential, kdx can be taken as another one as well.

Putting (19) and (13) into (16), we obtain

$$k dx - \frac{\phi dk}{d\phi/dx} = d\theta. \tag{20}$$

The vector $\vec{n}$ and $so(2)$ connection are well defined along $\mathcal{C} = (x_A, x_1) \cup (x_1, x_2) \cup \cdots \cup (x_M, x_B)$, so is the following integral

$$\int_{\mathcal{C}} k dx - \int_{\mathcal{C}} \frac{\phi dk}{d\phi/dx} = \int_{\mathcal{C}} d\theta. \tag{21}$$

Since potential $V(x)$ at the turning points may not be continuous, let's define

$$\lim_{x \to x_A^+} \arctan\left(\frac{k(x)}{\phi(x)}\right) = \arctan\left(\frac{k(x_A)}{\phi(x_A)}\right),$$
$$\lim_{x \to x_B^-} \arctan\left(\frac{k(x)}{\phi(x)}\right) = \arctan\left(\frac{k(x_B)}{\phi(x_B)}\right).$$

Now the integral in the right side of (21) can be obtained as

$$\begin{aligned}\int_{\mathcal{C}} d\theta &= \lim_{x \to x_B^-} \theta(x) - \lim_{x \to x_A^+} \theta(x) - \sum_i \beta_i \\ &= N\pi - \sum_i \beta_i + \arctan\left(\frac{k(x_B)}{\phi(x_A)}\right) - \arctan\left(\frac{k(x_A)}{\phi(x_B)}\right),\end{aligned} \tag{22}$$

where N is the zero points of $\phi(x)$, β_i is the angle change of θ at the point x_i where vector $\vec{n}(x)$ is not continuous. Rigorously speaking, β_i is the angle from vector $\vec{n}(x_i - \epsilon)$ to $\vec{n}(x_i + \epsilon)$ with ϵ tends to zero.

$$\beta_i = \lim_{\epsilon \to 0} (\theta(x_i + \epsilon) - \theta(x_i - \epsilon)). \tag{23}$$

The term β_i originates from the potential $V(x)$ jumping at the point x_i.

Putting (22) into (21), we have

$$\int_{\mathcal{C}} k dx - \int_{\mathcal{C}} \frac{\phi dk}{d\phi/dx} + \sum_i \beta_i - \arctan\left(\frac{k(x_B)}{\phi(x_B)}\right) + \arctan\left(\frac{k(x_A)}{\phi(x_A)}\right) = N\pi. \tag{24}$$

This quantization rule is obtained by a geometric method, therefore each term has a geometric interpretation.

2.3 New Term of Quantization Rule

Comparing (24) with (6), we find there is a new term $\sum_i \beta_i$ in (24), which arises from the discontinuity of potential $V(x)$. This generalization is helpful sometimes since there does exist models in quantum mechanics in which the potential $V(x)$ is piece-wisely continuous between the two turning points. For example, in one-dimensional system, consider a finite square well with a square barrier whose potential is low than that of the boundary of the well, for definiteness,

$$V(x) = \begin{cases} V_A, & x \le -\pi \\ 0, & -\pi < x < x_C \\ \delta, & x_C \le x \le x_D \\ 0, & x_D < x < x_B \\ V_B, & x_B < x \end{cases} \tag{25}$$

with energy $\delta < E < V_A$ and $\delta < E < V_B$. In this model, the sign of β_C is opposite to that of β_D.

3 Discussions and Conclusions

In the following, we give some discussions and conclusions.

The first two terms in equation (24) are formally regarded as two $so(2)$ connections. If kdx can be taken as a non-vanishing component of $so(2)$ connection, the other one form $\frac{\phi dk}{d\phi/dx}$ should also be a connection component, which are related to the former one by gauge transformation in (16). This is the geometric reason that the right side of (24) is an integer multiplied by π. As $so(2)$ Lie algebra is isomorphic to $U(1)$ Lie algebra, the terms have also an interpretation of $U(1)$ connections, which is consistent with the fact that wave functions are the sections of line bundle with one dimensional space as its base manifold.

There are contributions from angles jumping in (24) $(\arctan(\frac{k(x_A)}{\phi(x_A)}) - \arctan(\frac{k(x_B)}{\phi(x_B)}))$ and $\sum_i \beta_i$. They both originate from the discontinuity of potential function $V(x)$. To see clearly how the vector (n^1, n^2) rotate in the fiber space, we consider a potential without jumping points both at the turning points and between the turning points. So the last three terms in the right side of (22) vanish and we have

$$\int_{x_A}^{x_B} d\theta = N\pi \tag{26}$$

which shows that the vector (n^1, n^2) rotates $N/2$ circles when x goes from turning point A to B. By Sturm-Liouville theorem, the number N increases as the eigenvalue of energy E increases. Here we find the number $N/2$ plays the role like winding number. For even parity of wavefunction ψ, the right side of (26) is an integer multiplied by 2π.

Ma et al. also discussed some three dimensional systems such as three-dimensional harmonic oscillator and hydrogen atom. Since such systems are spherically symmetric, they are actually one-dimensional systems with radial coordinates. It is still an open question to generalize the quantization rule to arbitrary two or three dimensional systems whose turning points form one dimensional curve or two dimensional surface. In our intuitive opinion, the momentum $k(x)$ defined in (5) should be generalized to two or three dimensional vector and the corresponding quantization rule should reflect this property.

In Ref. [1] and Ref. [3], they presented some arguments that the term $\int_{x_A}^{x_B} \frac{\phi dk}{d\phi/dx}$ is invariant for the exactly solvable systems. And by calculating ϕ directly from the Riccati equation, lots of examples are checked that $\int_{x_A}^{x_B} \frac{\phi dk}{d\phi/dx}$ is really independent on the number of the nodes(or the energy level) of eigenfunction. As far as we know, a proof has not been given yet now. It is also known that wave functions and the energy levels for the exactly solvable systems can also be solved by the supersymmetric mechanics [11] for shape invariant potential [12], in which ϕ is nothing but the superpotentials. Careful analysis of supersymmetric mechanics may lead to a proof of invariance of $\int_{x_A}^{x_B} \frac{\phi dk}{d\phi/dx}$. Alternatively, a deep investigation of relationship between geometric method and supersymmetric mechanics with shape invariant potentials, provides perhaps some clues to this issue.

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