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WKB quantization of the Morse Hamiltonian and periodic meromorphic functions

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Abstract. We show that the well known fact concerning a coincidence between the leading-order WKB and exact quantum mechanical results for an energy spectrum of the Morse Hamiltonian is due to the following property of the bound-state wavefunctions in the complex plane. The logarithmic derivatives of the bound-state eigenfunctions of the Morse Hamiltonian are periodic functions with a pure imaginary period. We show that the Morse potential is the only potential having this property in the following class of potentials: $U(x) = \sum_{n=0}^{n=2m} u_n e^{-anx}$.

1. Introduction

The semiclassical Wentzel–Kramers–Brillouin (WKB) method (Bender and Orzag 1978) provides an efficient tool for finding approximate energy eigenvalues of one-dimensional Hamiltonians. The method was designed to treat quantum mechanical systems in the semiclassical region of large quantum numbers. However, it turned out that for some systems the semiclassical treatment reproduced exact quantum mechanical results. A well known example of a one-dimensional quantum mechanical system for which the standard leading-order WKB quantization condition

$$\int_{x_a}^{x_b} \sqrt{2(E - U(x))}\, dx = \pi(n + \tfrac{1}{2}) \tag{1}$$

yields exact energy spectrum is the harmonic oscillator. Another example is the system described by the Morse Hamiltonian

$$\hat{H} = -\frac{1}{2}\frac{d^2}{dx^2} + D(e^{-2ax} - 2e^{-ax}) \tag{2}$$

where a and D are positive constants. Several modifications of the quantization condition (1) have been proposed in order to enlarge a set of Hamiltonians for which the semiclassical treatment yields exact energy spectrum.

An approach to construct a modified semiclassical quantization condition was realized in the framework of the supersymmetric quantum mechanics (Comtet *et al* 1985, Fricke *et al* 1988, Dutt *et al* 1986, Cooper *et al* 1995). The modified leading-order supersymmetric quantization condition has been shown to reproduce (Eckhardt 1986, Khare 1985, Kasap *et al* 1990) exact energy spectrum for a class of solvable potentials (i.e. solutions can be expressed in terms of easily calculated special functions).

A modified quantization rule proposed by Bruev (1992) reproduces an exact energy spectrum for the same class of solvable one-dimensional Hamiltonians. This modification of the standard WKB quantization procedure has been achieved by taking into account the phase distortions of the WKB functions. Sergeenko (1996) derived a modified wave equation. An application of the leading-order WKB quantization condition to this equation yields exact energy eigenvalues for all solvable spherically symmetric potentials.

In this paper we shall be concerned with the standard leading-order WKB quantization rule (1) and its applications to one-dimensional Hamiltonians. The question we shall be interested in is, why formula (1) reproduces exact energy spectrum for the Morse Hamiltonian.

2. WKB quantization of the Morse Hamiltonian

The well known formula

$$n = \frac{1}{2\pi \mathrm{i}} \int_C \frac{y'}{y}\, \mathrm{d}x \tag{3}$$

yields the number of zeros of $y(x)$ lying inside the closed contour C. Let the function $y(x)$ be a wavefunction of a bound state of some Hamiltonian with the potential $U(x)$ and the contour C in (3) chosen so that it encircles only the real zeros of $y(x)$. It is known (Dunham 1932) that equation (3) can be used for the purposes of a semiclassical quantization. If in addition to all zeros of $y(x)$, the contour C also contains the classical turning points and no other singular points of $y(x)$ then, substituting the leading-order WKB expression for $y(x)$ under integral (3) one obtains the quantization condition (1). Therefore, if the contour of integration in (3) could be chosen so, that substituting the standard leading-order WKB expression for $y(x)$ under the integral, one could obtain the exact value of integral (3), the quantization rule (1) would reproduce exact energy spectrum.

Bertocchi *et al* (1965) have shown that this situation is realized in the case of the harmonic oscillator. All zeros of the bound-state wavefunctions of the harmonic oscillator are on the real axis. Therefore, one can choose as a contour C a circle of an arbitrary large radius $|x| = R$ not changing the value of the integral. One can show that the logarithmic derivative of $y(x)$ in equation (3) satisfies the following estimation:

$$\frac{y'(x)}{y(x)} = \frac{y'^{(1)}(x)}{y^{(1)}(x)} + \mathrm{o}(|x|^{-1})$$

when $|x| \to \infty$. In this expression $y^{(1)}(x)$ is the first-order WKB approximation to the wavefunction of the harmonic oscillator. Thus, substituting the first order WKB wavefunction under the integral (3) and taking the limit $R \to \infty$ one obtains the exact value of the integral. One can show (Ivanov 1996) that the harmonic oscillator and Coulomb potentials are the only potentials belonging to the certain class, for which the bound-state wavefunctions only have a finite number of zeros in the complex plane.

The wavefunctions of the Morse Hamiltonian have an infinite number of zeros in the complex plane. Nevertheless, as we shall see, in this case one can choose the contour of integration in (3) so, that the integral can be evaluated exactly with the help of the leading-order WKB wavefunctions.

Energy spectrum and the bound-state eigenfunctions of the Morse Hamiltonian (2) are given by (Landau and Lifshitz 1977)

$$\begin{aligned} E_n &= -D\left[1 - \frac{a}{\sqrt{2D}}\left(n + \frac{1}{2}\right)\right]^2 \\ y(x) &= \mathrm{e}^{-\xi/2}\xi^s F(-n, 2s+1, \xi) \end{aligned} \tag{4}$$

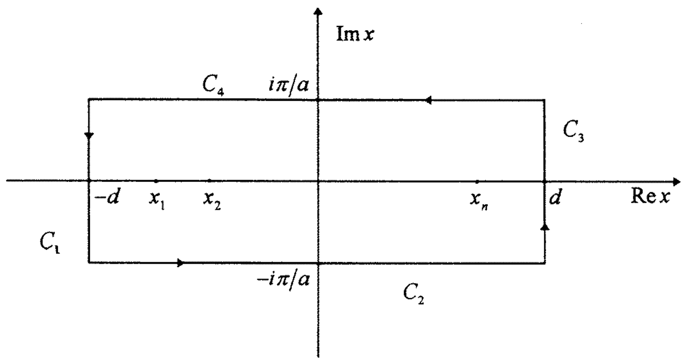

Figure 1. Contour of integration in equation (3).

where: $\xi = \sqrt{8D/a^2}\mathrm{e}^{-ax}$, $s = \sqrt{2D/a^2} - n - \frac{1}{2}$, $F(\alpha, \beta, z)$—a confluent hypergeometric function. The bound-state wavefunctions (4) are entire functions of x. From equation (4) one can see that they possess the following property

$$y\left(x + \frac{2\pi\mathrm{i}}{a}\right) = \mathrm{e}^{\mu} y(x) \tag{5}$$

where μ is some constant. The logarithmic derivative $v(x) = y'(x)/y(x)$ of the function $y(x)$ is therefore a periodic function of x

$$v\left(x + \frac{2\pi\mathrm{i}}{a}\right) = v(x). \tag{6}$$

Let us choose as a contour C in formula (3) the contour shown in figure 1. The parts C_2 and C_4 of this contour are the straight lines $y = \mathrm{i}\pi/a$ and $y = -\mathrm{i}\pi/a$ respectively. The parts C_1 and C_3 are the straight lines $x = -d$ and $x = d$. For sufficiently large d all real zeros of $y(x)$ are situated inside C. Because of the periodicity of $y'(x)/y(x)$ the integrals along C_2 and C_4 are equal in modulus and opposite in sign. Therefore, formula (3) yields

$$n = \frac{1}{2\pi\mathrm{i}}\left(\int_{C_1} \frac{y'}{y}\,\mathrm{d}x + \int_{C_3} \frac{y'}{y}\,\mathrm{d}x\right) = \frac{1}{2\pi\mathrm{i}}\left(\int_{-d+\mathrm{i}\pi/a}^{-d-\mathrm{i}\pi/a} \frac{y'}{y}\,\mathrm{d}x + \int_{d-\mathrm{i}\pi/a}^{d+\mathrm{i}\pi/a} \frac{y'}{y}\,\mathrm{d}x\right). \tag{7}$$

If parameter d is so large that C encircles all real zeros of $y(x)$, integral (7) will not vary if d increases further on. Let us consider first the integral along the contour C_3. The asymptotic form of the logarithmic derivative $v(x)$ of the bound-state wavefunction $y(x)$ of the Morse Hamiltonian can be obtained with the help of the standard methods of the theory of ordinary differential equations (Kamke 1961). One can show that this asymptotic form is

$$v(x) = -\sqrt{-2E} + \mathrm{O}(\mathrm{e}^{-ax}) \qquad x \in C_3 \qquad d \to \infty. \tag{8}$$

The first-order WKB expression for $v(x)$ is given by the known formula (Landau and Lifshitz 1977)

$$v^{(1)}(x) = -\sqrt{2D(\mathrm{e}^{-2ax} - 2\mathrm{e}^{-ax}) - 2E} + \frac{Da}{2}\,\frac{\mathrm{e}^{-2ax} - \mathrm{e}^{-ax}}{D(\mathrm{e}^{-2ax} - 2\mathrm{e}^{-ax}) - E}. \tag{9}$$

Expanding the expression on the right-hand side of equation (9) one can see that

$$v(x) = v^{(1)}(x) + \mathrm{O}(\mathrm{e}^{-ax}) \qquad x \in C_3 \qquad d \to \infty. \tag{10}$$

Therefore, for the integral along the contour C_3 one obtains

$$\lim_{d\to\infty}\int_{d-\mathrm{i}\pi/a}^{d+\mathrm{i}\pi/a} v(x)\,\mathrm{d}x = \lim_{d\to\infty}\int_{d-\mathrm{i}\pi/a}^{d+\mathrm{i}\pi/a} v^{(1)}(x)\,\mathrm{d}x = -\sqrt{-2E}\,\frac{2\pi\mathrm{i}}{a}. \qquad (11)$$

Consider now the integral along the contour C_1. For large negative values of x in the classically forbidden region the asymptotic form of $v(x)$ can be shown to be

$$v(x) = \sqrt{2D}\mathrm{e}^{-ax} - \sqrt{2D} + \frac{a}{2} + \mathrm{O}(\mathrm{e}^{ax}) \qquad x \in C_1 \qquad d \to \infty. \qquad (12)$$

The first-order WKB expression for $v(x)$ is given for large negative values of x by the formula

$$v^{(1)}(x) = \sqrt{2D(\mathrm{e}^{-2ax} - 2\mathrm{e}^{-ax}) - 2E} + \frac{Da}{2}\,\frac{\mathrm{e}^{-2ax} - \mathrm{e}^{-ax}}{D(\mathrm{e}^{-2ax} - 2\mathrm{e}^{-ax}) - E}. \qquad (13)$$

From equations (12) and (13) one obtains

$$v(x) = v^{(1)}(x) + \mathrm{O}(\mathrm{e}^{ax}) \qquad x \in C_1 \qquad d \to \infty. \qquad (14)$$

Therefore, for the integral along the contour C_1 one obtains

$$\lim_{d\to\infty}\int_{-d+\mathrm{i}\pi/a}^{-d-\mathrm{i}\pi/a} v(x)\,\mathrm{d}x = \lim_{d\to\infty}\int_{-d+\mathrm{i}\pi/a}^{-d-\mathrm{i}\pi/a} v^{(1)}(x)\,\mathrm{d}x = \frac{2\pi\mathrm{i}}{a}\sqrt{2D}\left(1 - \frac{a}{\sqrt{8D}}\right). \qquad (15)$$

When deriving equation (15) we took into account that integrals of an exponential function along its period vanished and therefore, only the constant terms in equation (12) contributed to integral (15).

Using equations (7), (11) and (15) one obtains finally

$$\sqrt{-2E} = \sqrt{2D} - a(n + \tfrac{1}{2}). \qquad (16)$$

It is easy to see that equation (16) reproduces the correct energy spectrum of the Morse Hamiltonian (2). Since equations (11) and (15) were obtained with the help of the first-order WKB expressions, the WKB quantization rule (1) yields the correct result for an energy spectrum of the Morse Hamiltonian (rule (1) is obtained when first-order approximations of $v(x)$ are used).

3. Uniqueness of the Morse potential

We have seen that the periodicity of the logarithmic derivative of $y(x)$ was crucial for the success of the leading-order WKB quantization formula (1). One should note that this property is quite typical for the certain class of second-order differential equations. Let us consider the one-dimensional Schrödinger equation

$$\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} = 2(U(x) - E) \qquad (17)$$

where $U(x)$ is a meromorphic periodic function of x. Such equations are known in literature as Hill equations (Kamke 1961). In equation (17) we need only consider the case of $U(x)$ having a pure imaginary (or real) period, otherwise the function $U(x)$ would be complex for real values of x.

According to the Floquet theorem (Kamke 1961), equation (17) with periodic function $U(x)$ always has a solution possessing the property of a periodicity of the logarithmic derivative. The problem is, can this solution be made normalizable for some values of E? If it were the case then one might expect the WKB quantization condition (the leading-order rule (1) or its higher-order WKB versions (Kreiger and Rosenzweig 1967)) to reproduce the energy spectrum of equation (17).

We are going to prove the following statement.

Theorem. Let the potential $U(x)$ in equation (17) be the polynomial of a degree k in the variable $u = \mathrm{e}^{-ax} : U(x) = U_k(u)$, where a is a positive constant and k is an even integer. Let an eigenfunction $y(x)$ of the eigenvalue problem (17) have a finite number of zeros in the strip $G : |\,\mathrm{Im}(x)| \leqslant \pi/a$. Then, $y(x)$ can have periodic logarithmic derivatives if, and only if, $U(x)$ is a polynomial of second degree, i.e. $U(x)$ is the Morse potential.

Proof of the theorem. Since $U(x)$ is also an entire function, $y(x)$ is also an entire function. The function $v(x) = y'(x)/y(x)$—logarithmic derivative of $y(x)$—is a meromorphic function of x having poles at the points where $y(x)$ has zeros. For the polynomial in $u = \mathrm{e}^{-ax}$ potential $U(x)$ the semiclassical approximation is valid for $y(x)$ when $|x| \to \infty$ remaining in the strip G. Since $y(x)$ is presumed to be normalizable, the leading-order WKB formulae for $v(x)$ yield:

$$v(x) \sim c_1 \qquad |x| \to \infty\, \mathrm{Re}(x) > 0 \qquad x \in G \tag{18a}$$

$$v(x) \sim c_2 \exp\left(-\frac{kax}{2}\right) \qquad |x| \to \infty\, \mathrm{Re}(x) < 0 \qquad x \in G \tag{18b}$$

where c_1, c_2 are some constants. Thus, the function $v(x)$ tends to a constant when $|x| \to \infty$, $x \in G$, $\mathrm{Re}(x) > 0$, and $v(x)$ tends to infinity when $|x| \to \infty$, $x \in G$, $\mathrm{Re}(x) < 0$. In addition, in the conditions of the theorem, $v(x)$ is a meromorphic function having a finite number of zeros in the strip $G : |\,\mathrm{Im}(x)| \leqslant \pi/a$. We shall now use the known result of the theory of meromorphic functions (Markushevitch 1968), stating that the meromorphic function $v(x)$ possessing the above-listed properties must be a rational function of the variable $u = \mathrm{e}^{-ax}$

$$v(x) = \frac{p_0 + p_1 u + \cdots + p_m u^m}{q_0 + q_1 u \cdots + q_n u^n} = \frac{P_m(u)}{Q_n(u)} \tag{19}$$

where $P_m(u)$,$Q_n(u)$ are some polynomials. The result, quoted from Markushevitch (1968), can be understood if one considers the following change of the variable: $-ax = \ln t$. One can show that under this change of the variable, $v(x)$ goes onto the meromorphic function $\tilde{v}(t)$. Conditions (18) expressed in terms of the variable t imply that the function $\tilde{v}(t)$ is regular or has a pole at $t = \infty$. The well known result of the theory of meromorphic functions is that a meromorphic function which is either regular or has a pole at infinity must be a rational function.

Consider the Riccati equation for $v(x)$ following from equation (17)

$$\frac{\mathrm{d}v}{\mathrm{d}x} + v^2 = 2(U(x) - E). \tag{20}$$

Substituting expression (19) into equation (20) one obtains after simple calculation

$$-au\left(\frac{\mathrm{d}P_m}{\mathrm{d}u} Q_n - P_m \frac{\mathrm{d}Q_n}{\mathrm{d}u}\right) + P_m^2 = 2Q_n^2(U_k - E). \tag{21}$$

The coefficient p_m of the polynomial $P_m(u)$ can always be made equal to unity by dividing $P_m(u)$ and $Q_n(u)$ by p_m. Therefore in equation (21) there are $m + n + 2$ variables (m coefficients of $P_m(u)$, $n + 1$ coefficient of $Q_n(u)$ and energy E). To satisfy equation (18b) one should demand: $m = n + k/2$. Therefore, the maximum degree of the polynomials in equation (21) is $2n + k$ and equation (21) yields $2n + k + 1$ equations for $m + n + 2 = 2n + 2 + k/2$ variables. For these equations to have solutions we should demand

$$2n + k + 1 \leqslant 2n + 2 + \frac{k}{2} \Rightarrow k \leqslant 2. \tag{22}$$

Since in the conditions of the theorem k was assumed to be an even number, there is only a possibility of satisfying equation (21): $k = 2$, the polynomial $U_2(u)$ is the Morse potential.

As we have seen, equation (17) with a periodic potential $U(x)$ always has a solution having a periodic logarithmic derivative. The proven theorem allows us to conclude that for all even-degree polynomial in $u = e^{-ax}$ potentials, except the Morse potential, these solutions always have an infinite number of zeros in the strip $G : |\,\mathrm{Im}(x)| \leqslant \pi/a$. If the number of zeros in the strip G is infinite, integral (3) cannot be used for quantization. Therefore, in the general case of even-degree polynomial in $u = e^{-ax}$ potentials, one can expect the WKB quantization rule to reproduce exact energy spectrum only in the case of the Morse potential.

4. Remarks and prospects

We have shown that the success of the WKB quantization rule for the Morse Hamiltonian was due to the periodicity property of the logarithmic derivatives of the Morse Hamiltonian eigenfunctions. We have shown that this property of wavefunctions singles out the Morse potential from the class of even-degree polynomial in the variable $u = e^{-ax}$ potentials. Whether one can enlarge this class or find other potentials having the property that the logarithmic derivatives of the bound-state wavefunctions are periodic functions, is an interesting question. We believe it deserves further consideration.

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