Chapter 3

The “Sommerfeld Puzzle” and Its Extensions

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> *If you want to be a physicist, you must do three things - first, study mathematics, second, study more mathematics, and third, do the same.*
>
> Arnold Sommerfeld

3.1 Abstract

The exact agreement between the Sommerfeld (1916) and Dirac (1928) results for the energy levels of the relativistic hydrogen atom (the so-called “Sommerfeld puzzle”) is analyzed and extended. Werner Heisenberg called this coincidence a ‘miracle’ but Erwin Schrödinger described it as a fortuitous computational accident.

3.2 Introduction

One of the central problems in quantum mechanics is the spectrum of hydrogenlike atoms. The fine structure of hydrogen atom spectral lines was discovered by Albert A. Michelson in 1887: When his ether-wind experiments have failed, he turned to spectroscopy and found that the leading H_α line of the Balmer series comprises a doublet. (The electron was discovered by J. J. Thomson in 1897 and Rutherford’s model of the atom appeared in 1911!)

In 1916 Arnold Sommerfeld [27] applied the quantization rules of the ‘old’ quantum theory to the relativistic hydrogen atom. Exact solution was obtained by C. G. Darwin

[6] and W. Gordon [14] only in 1928 after discovery of the Dirac equation [8–10, 18]: The new answer was precisely the 'old' Sommerfeld formula!

The puzzle had been discussed further in [5, 15, 16, 25, 33] with different interpretations from mathematics, physics, and philosophy. Here, we approach this matter in a systematic and analytic fashion, with some extensions to similar problems in quantum physics.

This work is dedicated to Professor Viktor V. Dodonov on the occasion of his seventy-fifth birthday (diamond jubilee).

3.3 The original "Sommerfeld Puzzle"

3.3.1 WKB approximation in Coulomb problems

Bohr invented his quantization rules for hydrogenlike atoms, based on the classical circular motion of electron in Kepler's problem; whereas Sommerfeld extended these ideas to the relativistic elliptical orbits [22, 29]. Measurement of the fine structure, done by Paschen, was interpreted as an experimental testing of the special theory of relativity [5, 17, 28].

Those phenomenological quantization rules of 'old' quantum mechanics [27, 34] are derived in modern physics from the corresponding wave equations in the so-called semiclassical approximation (WKB method) [4, 13, 20, 21, 24, 26]. (See also [17, 22, 29, 30] for historical reviews.)

In this approximation, for a particle in the central field, one can use a generic radial equation of the form:

$$u''(x) + q(x)\,u = 0, \tag{3.1}$$

where $x^2\,q(x)$ is continuous together with its first and second derivatives (see below) for $0 \le x \le b < \infty$. As is well-known, the traditional semiclassical approximation cannot be used in a neighborhood of $x = 0$. However, the change of variables $x = e^z$, $u = e^{z/2}\,v(z)$ transforms the equation into a new form,

$$v''(z) + q_1(z)\,v = 0, \tag{3.2}$$

where

$$q_1(z) = -\frac{1}{4} + \left(x^2\,q(x)\right)_{x=e^z} \tag{3.3}$$

(Langer's modification [4, 21, 24]). As $z \to -\infty$ (or $x \to 0$), the new function $q_1(z)$ is changing slowly near the constant

$$-1/4 + \lim_{x\to 0} x^2 q(x) \qquad \text{and} \qquad \lim_{z\to-\infty} q_1^{(k)}(z) = 0 \quad (k = 1, 2).$$

Hence the function $q_1(z)$ and its derivatives are changing slowly for large negative z.

The WKB method can be applied to the new equation and, as a result, in the original equation one should replace $q(x)$ with

$$q(x) - 1/(4x^2) = p^2_{\text{effective}}(x) \tag{3.4}$$

(see, for example, [21] and [24] for more details).

For all Coulomb problems under consideration, one may utilize the following generic integral, originally evaluated by Sommerfeld performing complex integration [29]: If

$$p(r) = \sqrt{-A + \frac{B}{r} - \frac{C}{r^2}} \qquad A, C > 0. \tag{3.5}$$

Then

$$\int_{r_1}^{r_2} p(r)\, dr = \pi \left(\frac{B}{2\sqrt{A}} - \sqrt{C} \right) \tag{3.6}$$

provided $p(r_1) = p(r_2) = 0$. (See [2] and appendix for elementary evaluations of this integral.)

The Bohr–Sommerfeld quantization rule takes the form [24, 26]:

$$\int_{r_1}^{r_2} p(r)\, dr = \pi \left(n_r + \frac{1}{2} \right) \qquad (n_r = 0, 1, 2, \dots) \tag{3.7}$$

and, for the energy levels, one gets the following equation:

$$\frac{B}{2\sqrt{A}} - \sqrt{C} = n_r + \frac{1}{2}. \tag{3.8}$$

It is worth noting that a variant of this relation was found by Sommerfeld himself [30], by complex integration, in his original attempt to explain how the quantum rules of the 'old' theory (but only in the cases of the one-dimensional harmonic oscillator and the Kepler problem) are connected with the wave mechanics of Schrödinger.

3.3.2 Exact solutions: Nikiforov-Uvarov approach

Generalized equation of the hypergeometric type [24],

$$u'' + \frac{\widetilde{\tau}(x)}{\sigma(x)} u' + \frac{\widetilde{\sigma}(x)}{\sigma^2(x)} u = 0 \tag{3.9}$$

(σ, $\widetilde{\sigma}$ are polynomials of degrees at most 2, $\widetilde{\tau}$ is a polynomial at most first degree), by the substitution

$$u = \varphi(x) y(x) \tag{3.10}$$

can be reduced to the form

$$\sigma(x) y'' + \tau(x) y' + \lambda y = 0 \tag{3.11}$$

if:

$$\frac{\varphi'}{\varphi} = \frac{\pi(x)}{\sigma(x)}, \qquad \pi(x) = \frac{1}{2}\left(\tau(x) - \widetilde{\tau}(x) \right) \tag{3.12}$$

(or, $\tau(x) = \widetilde{\tau} + 2\pi$, for later),

$$k = \lambda - \pi'(x) \qquad (\text{or, } \lambda = k + \pi'), \tag{3.13}$$

and

$$\pi(x) = \frac{\sigma' - \widetilde{\tau}}{2} \pm \sqrt{\left(\frac{\sigma' - \widetilde{\tau}}{2} \right)^2 - \widetilde{\sigma} + k\sigma} \tag{3.14}$$

is a linear function. (Use the choice of constant k to complete the square under the radical symbol; see [2, 11, 24] for more details.)

In Nikiforov-Uvarov's method, the energy levels can be obtained from the quantization rule:

$$\lambda + n\tau' + \frac{1}{2}n\,(n-1)\,\sigma'' = 0 \qquad (n = 0, 1, 2,\ ...) \tag{3.15}$$

and the corresponding square-integrable solutions are classical orthogonal polynomials, up to a factor. They can be found by the Rodrigues-type formula:

$$y_n(x) = \frac{B_n}{\rho(x)}\left[\sigma^n(x)\rho(x)\right]^{(n)}, \qquad (\sigma\rho)' = \tau\rho, \tag{3.16}$$

where B_n is a constant. Each infinite (countable) set of these square-integrable solutions is complete [24].

3.3.3 The Sommerfeld-type potentials in the Nikiforov-Uvarov approach

Let us choose

$$\begin{aligned} \sigma(x) &= x, \qquad \widetilde{\tau}(x) = 0, \\ \widetilde{\sigma}(x) &= -ax^2 + bx - c + \frac{1}{4}. \end{aligned} \tag{3.17}$$

Then

$$\pi(x) = \frac{1}{2} \pm \sqrt{ax^2 + (k-b)x + c}. \tag{3.18}$$

When $k = b \pm 2\sqrt{ac}$, one can complete the square and obtain

$$\pi = \frac{1}{2} \pm \left(\sqrt{a}x \pm \sqrt{c}\right), \qquad \tau = 2\pi. \tag{3.19}$$

We may choose

$$\tau' = -2\sqrt{a} < 0 \qquad \text{and} \qquad \lambda = b - 2\sqrt{ac} - \sqrt{a}. \tag{3.20}$$

As a result, for all Sommerfeld-type potentials, by the Nikiforov-Uvarov quantization rule (3.15) one obtains

$$\frac{b}{2\sqrt{a}} - \sqrt{c} = n + \frac{1}{2}, \tag{3.21}$$

as an equation for the exact energy levels. (It is worth noting that Sommerfeld had obtained a similar relation in special cases [30].)

3.3.4 The puzzle resolution

By (3.8) and (3.21), we arrive at the following result.

Theorem 3.3.1.

$$a = A, \qquad b = B, \qquad c = C. \tag{3.22}$$

Thus, the equations for energy levels are identical in both, exact and approximate, approaches for all central potentials discussed by Sommerfeld. According to our analysis, the equivalence of the energy levels for all Sommerfeld-type potentials occurs as a result of mathematical coincidence as earlier stated by Schrödinger [5, 35] (see below).

On the contrary, Heisenberg writes [16]: "*It would be intriguing to explore whether this is about a miracle or it is the group-theoretical approach which leads to this formula.*"

3.4 Examples

We discuss several typical cases when the energy levels coincide in both, exact and approximate, approaches for the Sommerfeld-type potentials.

3.4.1 Nonrelativistic Coulomb problem

In the well-known case of nonrelativistic Coulomb's problem, one gets

$$u'' + \left[2\left(\varepsilon_0 + \frac{Z}{x}\right) - \frac{(l+1/2)^2}{x^2}\right]u = 0 \tag{3.23}$$

$$\left(\varepsilon_0 = \frac{E}{E_0},\ E_0 = \frac{e^2}{a_0},\ a_0 = \frac{\hbar^2}{me^2},\ x = \frac{r}{a_0}\right)$$

(in dimensionless units with Langer's modification).

Thus, $A = -2\varepsilon_0$, $B = 2Z$, $C = (l+1/2)^2$ and in view of the quantization rule [30]:

$$\frac{Z}{\sqrt{-2\varepsilon_0}} - l - \frac{1}{2} = n_r + \frac{1}{2}. \tag{3.24}$$

As a result, we obtain exact energy levels for the nonrelativistic hydrogenlike problem:

$$\varepsilon_0 = \frac{E}{E_0} = -\frac{Z^2}{2(n_r+l+1)^2}. \tag{3.25}$$

Here, $n = n_r + l + 1$ is the principal quantum number [19].

3.4.2 Relativistic Schrödinger equation

In the case of the relativistic Schrödinger equation, one should write [2, 7, 24, 26, 30]:

$$u'' + \left[\left(\varepsilon + \frac{\mu}{x}\right)^2 - 1 - \frac{(l+1/2)^2}{x^2}\right]u = 0 \tag{3.26}$$

$$\left(\varepsilon = \frac{E}{mc^2},\quad \mu = \frac{Ze^2}{\hbar c},\quad x = \frac{mc}{\hbar}r\right).$$

Here, $A = 1 - \varepsilon^2$, $B = 2\mu\varepsilon$, and $C = (l+1/2)^2 - \mu^2$ (with Langer's modification). The combined quantization rule implies

$$\frac{\mu\varepsilon}{\sqrt{1-\varepsilon^2}} = n_r + \nu + 1, \quad \nu = -\frac{1}{2} + \sqrt{\left(l+\frac{1}{2}\right)^2 - \mu^2} \tag{3.27}$$

and the formula for the relativistic energy levels is given by [7, 26, 30]:

$$\begin{aligned}\frac{E_{n_r,\,l}}{mc^2} &= \frac{1}{\sqrt{1+\dfrac{\mu^2}{\left[n_r+\frac{1}{2}+\sqrt{\left(l+\frac{1}{2}\right)^2-\mu^2}\right]^2}}} \qquad (3.28)\\ &= 1-\frac{\mu^2}{2n^2}-\frac{\mu^4}{2n^4}\left(\frac{n}{l+1/2}-\frac{3}{4}\right)+\mathrm{O}\left(\mu^6\right),\end{aligned}$$

where the expansion, in the limit $\mu=(Ze^2)/(\hbar c)\to 0$, when $c\to\infty$, can be derived by a direct Taylor's formula and/or verified by a computer algebra system. Here, $n=n_r+l+1$ is the corresponding nonrelativistic principal quantum number. The first term in this expansion is simply the rest mass energy $E_0=mc^2$ of the charged spin-zero particle, the second term coincides with the energy eigenvalue in the nonrelativistic Schrödinger theory and the third term gives the so-called fine structure of the energy levels, which removes the degeneracy between states of the same n and different l.

3.4.3 Dirac equation

Sommerfeld's fine structure formula for the relativistic Coulomb problem [27, 29], can be thought of as the main achievement of the 'old' quantum mechanics. Here, we will derive this result in a semiclassical approximation for the radial Dirac equations (separation of variables in spherical coordinates is discussed in detail elsewhere; see for instance [1, 3, 6, 14, 31]). In the dimensionless units, one of these second-order differential equations has the form

$$v_1''+\frac{(\varepsilon^2-1)x^2+2\varepsilon\mu x-\nu(\nu+1)}{x^2}\,v_1=0 \qquad (3.29)$$

and the second equation can be obtained from the first one by replacing $\nu\to-\nu$. By Langer's modification, we obtain

$$p(x)=\left[\left(\varepsilon+\frac{\mu}{x}\right)^2-1-\frac{(\nu+1/2)^2+\mu^2}{x^2}\right]^{1/2}. \qquad (3.30)$$

For the Dirac equation, $A=1-\varepsilon^2$, $B=2\mu\varepsilon$, $C=(\nu+1/2)^2$. The relativistic energy levels of an electron in the central Coulomb field are given by [6, 14, 27, 29]:

$$E=E_{n_r,\,j}=\frac{mc^2}{\sqrt{1+\mu^2/\left(n_r+\nu\right)^2}} \quad (n_r=0,1,2,\ \ldots). \qquad (3.31)$$

Here, $\mu=(Ze^2)/(\hbar c)$ and in Dirac's theory,

$$\nu=\nu_{\text{Dirac}}=\sqrt{\left(j+1/2\right)^2-\mu^2}, \qquad (3.32)$$

where $j=1/2,3/2,5/2,\ \ldots$ is the total angular momentum including the spin of the relativistic electron.

In Dirac's theory the nonrelativistic limit has the form

$$\frac{E_{n_r,\,j}}{mc^2}=1-\frac{\mu^2}{2n^2}-\frac{\mu^4}{2n^4}\left(\frac{n}{j+1/2}-\frac{3}{4}\right)+\mathrm{O}\left(\mu^6\right),\quad \mu\to 0, \tag{3.33}$$

where $n=n_r+j+1/2$ is the principal quantum number of the nonrelativistic hydrogenlike atom. Once again, the first term in this expansion is the rest mass energy of the relativistic electron, the second term coincides with the energy eigenvalue in the nonrelativistic Schrödinger theory and the third term gives the so-called fine structure of the energy levels — the correction obtained for the energy in the Pauli approximation which includes the interaction of the spin of the electron with its orbital angular momentum. The total spread in the energy of the fine structure levels is in agreement with experiments.

The maximum spreads of the fine-structure levels occur when $l=0$, $l=n-1$ and $j=1/2$, $j=n-1/2$ for the Schrödinger (3.28) and Dirac (3.33) theories, respectively. Therefore, for the quotient, one gets

$$\frac{\Delta E_{\text{Schrödinger}}}{\Delta E_{\text{Sommerfeld}}}=\frac{4n}{2n-1}\qquad (n=2,3,\,...). \tag{3.34}$$

(See [2, 7, 26, 30] for more details.)

In connection with Sommerfeld's fine structure formula Erwin Schrödinger writes, *inter alia*, in a letter dated 29th February, 1956 [5, 35]: *"... you are naturally aware of the fact that Sommerfeld derivation of the fine-structure formula provides only fortuitously the result demanded by the experiment. One may notice then from this particular example that newer form of quantum theory (i.e., quantum mechanics) is by no means such an inevitable continuation of the older theory as is commonly supposed. Admittedly the Schrödinger theory, relativistically framed (without spin), gives a formal expression of the fine-structure formula of Sommerfeld, but it is incorrect owing to the appearance of half-integers instead of integers. My paper in which this is shown has ... never been published; it was withdrawn by me and replaced by non-relativistic treatment... The computation [by the relativistic method] is far too little known. It shows in one respect how necessary Dirac's improvement was, and on the other hand it is wrong to assume that the older form of quantum theory is 'broadly' in accordance with the newer form. "*

It took two quantum revolutions, from 1916 until 1928, in order to derive Sommerfeld's formula in the Dirac theory of the relativistic hydrogen atom!

3.4.4 Kratzer potential

In order to investigate the vibrational-rotational spectrum of a diatomic molecule, the following potential

$$U(r)=-2D\left(\frac{a}{r}-\frac{1}{2}\frac{a^2}{r^2}\right),\qquad D>0, \tag{3.35}$$

with a minimum $U(a)=-D$ and $0<r<\infty$, has been used [11, 12].

We are looking for solutions of the Schrödinger equation in spherical coordinates and introduce the dimensionless quantities:

$$x=\frac{r}{a},\qquad \beta^2=-\frac{2ma^2}{\hbar^2}\,E,\qquad \gamma^2=\frac{2ma^2}{\hbar^2}\,D \tag{3.36}$$

together with the standard substitution: $R(r) = u(x)$.

For bound states $E < 0, \beta > 0$ and the radial equation takes the form

$$u'' + \left[-\beta^2 + \frac{2\gamma^2}{x} - \frac{\gamma^2 + l(l+1)}{x^2} \right] u = 0. \tag{3.37}$$

Here, $A = -\beta^2$, $B = 2\gamma^2$, and $C = \gamma^2 + (l + 1/2)^2$ with Langer's modification.

As a result, the bound states are given by

$$E_{n,l} = -\frac{2ma^2 D^2}{\hbar^2} \frac{1}{(\nu + n)^2}, \tag{3.38}$$

where

$$\nu = \frac{1}{2} + \sqrt{\gamma^2 + \left(l + \frac{1}{2} \right)^2}, \qquad \gamma^2 = \frac{2ma^2}{\hbar^2} D. \tag{3.39}$$

(For further details and applications, see [11, 12] and the references therein.)

3.5 n-Dimensional Problems

3.5.1 Separation of variables

For hyperspherical coordinates in $\mathbb{R}^n$, when $\mathbf{x} = r\mathbf{s}$, $\mathbf{s}^2 = 1$, the Laplace operator take the form [23]:

$$\Delta = \Delta_r + \frac{1}{r^2} \Delta_{\mathbf{s}}, \tag{3.40}$$

where

$$\Delta_r = \frac{1}{r^{n-1}} \frac{\partial}{\partial r} \left(r^{n-1} \frac{\partial}{\partial r} \right) \tag{3.41}$$

and

$$\Delta_{\mathbf{s}} Y + \lambda Y = 0, \quad \lambda = l\,(l + n - 2)\,, \quad l = 0, 1, 2, \ \ldots \tag{3.42}$$

for a set of hyperspherical harmonics $Y(\mathbf{s}) = Y_{l,\{l_k\}}(\mathbf{s})$ corresponding to a given tree [23, 32].

The stationary Schrödinger equation, in a central field,

$$\widehat{H}\Psi = E\Psi, \quad \widehat{H} = -\frac{\hbar^2}{2m}\Delta + V(r)\,, \tag{3.43}$$

admits a separation of the variables in hyperspherical coordinates:

$$\Psi = R(r)\, Y(\mathbf{s})\,. \tag{3.44}$$

The radial equation in $\mathbb{R}^n$ when $\mathbf{x} = r\mathbf{s}, \mathbf{s}^2 = 1$, take the form

$$\begin{aligned} \frac{1}{r^{n-1}} \frac{d}{dr} \left(r^{n-1} \frac{dR}{dr} \right) - \frac{l(l+n-2)}{r^2} R & \\ + \frac{2m}{\hbar^2} \left[E - V(r) \right] R = 0. & \end{aligned} \tag{3.45}$$

The following identities

$$\begin{aligned}\frac{1}{r^{n-1}}\frac{d}{dr}\left(r^{n-1}\frac{dR}{dr}\right) &= \frac{1}{r^{(n-1)/2}}\left(r^{(n-1)/2}R\right)'' \\ &\quad -\frac{(n-1)(n-3)}{4r^2}R\end{aligned} \tag{3.46}$$

and

$$\begin{aligned}l(l+n-2)+\frac{(n-1)(n-3)}{4} &= \left(l+\frac{n-3}{2}\right)\left(l+\frac{n-1}{2}\right) \\ &= \left(l+\frac{n-2}{2}\right)^2-\frac{1}{4}\end{aligned} \tag{3.47}$$

are easily verified. As a result, if $\chi = r^{(n-1)/2}R$:

$$\chi'' + \left[\frac{2m}{\hbar^2}\left(E-V(r)\right) - \frac{\left(l+(n-3)/2\right)\left(l+(n-1)/2\right)}{r^2}\right]\chi = 0 \tag{3.48}$$

as an extension of the radial equation in $\mathbb{R}^3$ to $\mathbb{R}^n$. The following special cases of the centrifugal term were discussed by Sommerfeld [30]:

$$\left(l+\frac{n-3}{2}\right)\left(l+\frac{n-1}{2}\right) = \begin{cases} 0,\ n=1, l=0 & \text{in } \mathbb{R}^1 \\ l^2-\frac{1}{4},\ n=2 & \text{in } \mathbb{R}^2 \\ l(l+1),\ n=3 & \text{in } \mathbb{R}^3 \end{cases}. \tag{3.49}$$

One can see that the radial equation (3.48) can be solved for the Sommerfeld-type potentials, thus extending the puzzle to $\mathbb{R}^n$. Moreover, in the radial equation, $\mathbb{R}^3 \to \mathbb{R}^n$ provided

$$l \to l + \frac{n-3}{2}, \tag{3.50}$$

which allows to extend all exactly solvable in $\mathbb{R}^3$ potentials into $\mathbb{R}^n$.

3.5.2 Kepler problems

For the nonrelativistic Coulomb problem in $\mathbb{R}^n$, one gets in dimensionless units:

$$u'' + \left[2\left(\varepsilon_0+\frac{Z}{x}\right) - \frac{\left(l+(n-3)/2\right)\left(l+(n-1)/2\right)}{x^2}\right]u = 0$$

$$\left(\varepsilon_0 = \frac{E}{E_0},\ E_0 = \frac{e^2}{a_0},\ a_0 = \frac{\hbar^2}{me^2},\ x = \frac{r}{a_0}\right). \tag{3.51}$$

With the Langer modification: $A = -2\varepsilon_0$, $B = 2Z$, $C = (l+(n-2)/2)^2$. In view of the quantization rule (3.8) one gets:

$$\frac{Z}{\sqrt{-2\varepsilon_0}} - l - \frac{n-2}{2} = n_r + \frac{1}{2}. \tag{3.52}$$

As a result, we obtain exact energy levels for the n-dimensional nonrelativistic hydrogen-like problem:

$$\varepsilon_0 = \frac{E}{E_0} = -\frac{Z^2}{2(n_r+l+(n-1)/2)^2} \tag{3.53}$$

in the WKB approximation, which is identical to the exact solution.

3.5.3 Harmonic oscillators

In $\mathbb{R}^n$, when $\mathbf{x} = r\mathbf{s},\ \mathbf{s}^2 = 1$, and

$$V(r) = \frac{1}{2} m\omega^2 r^2 \tag{3.54}$$

the radial equation takes the form

$$\chi'' + \left[\frac{2m}{\hbar^2} \left(E - \frac{1}{2} m\omega^2 r^2 \right) - \frac{(l + (n-3)/2)\,(l + (n-1)/2)}{r^2} \right] \chi = 0. \tag{3.55}$$

The Bohr-Sommerfeld quantization rule, with Langer's modification, is given by

$$\begin{aligned} &\int_{r_1}^{r_2} \sqrt{\frac{2m}{\hbar^2} \left(E - \frac{1}{2} m\omega^2 r^2 \right) - \frac{(l + (n-2)/2)^2}{r^2}}\, dr \\ &= \pi \left(n_r + \frac{1}{2} \right). \end{aligned} \tag{3.56}$$

Transforming the integral into a Sommerfeld-type form,

$$\int_{r_1}^{r_2} \sqrt{\frac{2mE}{\hbar^2 r^2} - \frac{m^2\omega^2}{\hbar^2} - \frac{(l + (n-2)/2)^2}{r^4}}\ (r dr), \tag{3.57}$$

one can introduce the new variable $\xi = r^2$ and conclude that

$$A = \frac{m^2\omega^2}{4\hbar^2}, \quad B = \frac{mE}{2\hbar^2}, \quad C = \frac{1}{4} \left(l + \frac{n-2}{2} \right)^2. \tag{3.58}$$

As a result, in WKB approximation, the energy levels are given by

$$E_{n_r} = \hbar\omega \left(2n_r + l + \frac{1}{2} \right), \quad n_r = 0, 1, 2, \ldots\ . \tag{3.59}$$

On the contrary, introducing the dimensionless units

$$\frac{\kappa^2}{2\mu} = \varepsilon = \frac{E}{\hbar\omega}, \quad \mu = \frac{m\omega}{\hbar}, \quad \xi = \mu r^2 \tag{3.60}$$

we arrive at the generalized equation of hypergeometric type with the following coefficients

$$\begin{aligned} \sigma(\xi) &= \xi, \qquad \widetilde{\tau}(\xi) = \frac{1}{2}, \\ \widetilde{\sigma}(\xi) &= \frac{1}{4} \left[(2\varepsilon)\xi - \xi^2 - \left(l + \frac{n-3}{2} \right) \left(l + \frac{n-1}{2} \right) \right] \end{aligned} \tag{3.61}$$

and the Nikiforov-Uvarov approach results in the same eigenvalues.

Indeed, one may choose, in a generic form,

$$\begin{aligned} \sigma(\xi) &= \xi, \qquad \widetilde{\tau} = \frac{1}{2} \\ \widetilde{\sigma}(\xi) &= b\xi - a\xi^2 - c + \frac{1}{16}. \end{aligned} \tag{3.62}$$

Then

$$\pi(\xi) = \frac{1}{2} \pm \left(\sqrt{a}\ \xi \pm \sqrt{c}\right), \quad k - b \pm 2\sqrt{ac}. \tag{3.63}$$

We may choose $k = b - 2\sqrt{ac}$ and $\pi(\xi) = \frac{1}{2} + \sqrt{c} - \sqrt{a}\ \xi$. Then

$$\begin{aligned} \lambda &= k + \pi' = b - 2\sqrt{ac} - \sqrt{a} \\ \tau(\xi) &= \widetilde{\tau} + 2\pi = \frac{3}{2} + 2\sqrt{c} - 2\sqrt{a}\ \xi \end{aligned} \tag{3.64}$$

and the quantization rule, once again, is given by

$$\frac{b}{2\sqrt{a}} - \sqrt{c} = n_r + \frac{1}{2}. \tag{3.65}$$

For the WKB solutions, in the radial equation:

$$u'' + \frac{1}{2\xi} u' + \frac{b\xi - a\xi^2 - c + 1/16}{\xi^2} u = 0, \tag{3.66}$$

in the dimensionless units, one can use a back substitution $u(\xi) = v(\eta)$ and $\eta = \sqrt{\xi}$. Then

$$v'' + 4\frac{b\eta^2 - a\eta^4 - c + 1/16}{\eta^2} v = 0. \tag{3.67}$$

With the Langer-type modification, the Bohr-Sommerfeld rule reads

$$\begin{aligned} \pi\left(n_r + \frac{1}{2}\right) &= \int_{\eta_1}^{\eta_2} p(\eta)\ d\eta = 2\int_{\eta_1}^{\eta_2} \sqrt{b - a\eta^2 - \frac{c}{\eta^2}}\ d\eta \\ &= \int_{\eta_1}^{\eta_2} \sqrt{-a + \frac{b}{\eta^2} - \frac{c}{\eta^4}}\ 2(\eta d\eta) \\ &= \int \sqrt{-a + \frac{b}{\xi} - \frac{c}{\xi^2}}\ d\xi = \pi\left(\frac{b}{2\sqrt{a}} - \sqrt{c}\right) \end{aligned} \tag{3.68}$$

and we arrive to the energy equation (3.65) once again. Use

$$a = \frac{1}{4}, \quad b = \frac{\varepsilon}{2}, \quad c = \frac{1}{4}\left(l + \frac{n-2}{2}\right)^2 \tag{3.69}$$

in order to obtain the corresponding exact energy levels (3.59).

3.6 Some Extensions

3.6.1 Trigonometric case: Pöschl-Teller potential hole

The following generic integral,

$$I(A) = \int_{\theta_1}^{\theta_2} \sqrt{A - \frac{B}{\cos^2\theta} - \frac{C}{\sin^2\theta}}\ d\theta, \tag{3.70}$$

with the aid of substitution $T=\cos 2\theta$, can be transformed into the sum of two similar Sommerfeld-type integrals:

$$\begin{aligned} I\left(A\right) &= \frac{\pi}{2\sqrt{2}}\left(\frac{\left(A-B+C\right)}{\sqrt{2A}}-\sqrt{2C}\right) \\ &\quad +\frac{\pi}{2\sqrt{2}}\left(\frac{\left(B-C+A\right)}{\sqrt{2A}}-\sqrt{2B}\right) \\ &= \frac{\pi}{2}\left(\sqrt{A}-\sqrt{B}-\sqrt{C}\right). \end{aligned} \tag{3.71}$$

(For an independent evaluation, see also appendix below.) As a result, the Bohr-Sommerfeld quantization rule gives

$$\sqrt{A}=\sqrt{B}+\sqrt{C}+2n+1. \tag{3.72}$$

The stationary Schrödinger equation for the familiar Pöschl-Teller potential takes the form [11, 12]:

$$\frac{d^2\psi}{dx^2}+\frac{2m}{\hbar^2}\left[E-U\left(x\right)\right]\psi=0, \tag{3.73}$$

where $0<x<\pi/(2\alpha)$ and

$$U\left(x\right)=\frac{V_0}{2}\left[\frac{a\left(a-1\right)}{\sin^2\left(\alpha x\right)}+\frac{b\left(b-1\right)}{\cos^2\left(\alpha x\right)}\right], \quad V_0=\frac{\hbar^2\alpha^2}{m}. \tag{3.74}$$

Here, with the help of the Langer-type modification: $a\left(a-1\right)\rightarrow\left(a-1/2\right)^2$ and $b\left(b-1\right)\rightarrow\left(b-1/2\right)^2$. One gets

$$A=\frac{2mE}{\alpha^2\hbar^2}, \quad B=\left(b-\frac{1}{2}\right)^2, \quad C=\left(a-\frac{1}{2}\right)^2 \tag{3.75}$$

and

$$E_n=\frac{V_0}{2}\left(a+b+2n\right)^2. \tag{3.76}$$

In our consideration, the WKB method results in the exact energy levels derived in [11, 12]. (The mathematical motivation of the Langer-type modification will be discussed elsewhere.)

Conclusion. We have demonstrated that for a large class of exactly solvable potentials the approximate WKB energy levels coincide with exact ones. Most of these problems have different symmetry groups.

3.6.2 Hyperbolic case: modified Pöschl-Teller potential hole

For a modified potential,

$$U\left(x\right)=-\frac{V_0}{\cosh^2\left(\alpha x\right)} \qquad (-\infty<x<\infty), \tag{3.77}$$

the Bohr-Sommerfeld quantization rule with the help of the integral (3.94) below result in $(\varepsilon=-E/V_0)$:

$$E_n=-\frac{\hbar^2\alpha^2}{2m}\left[\frac{\sqrt{2mV_0}}{\hbar\alpha}-\left(n+\frac{1}{2}\right)\right]^2, \tag{3.78}$$

which is a bit different from the exact values given by

$$E_n = -\frac{\hbar^2\alpha^2}{2m}\left[\frac{1}{2}\sqrt{\frac{8mV_0}{\hbar^2\alpha^2}+1}-\left(n+\frac{1}{2}\right)\right]^2. \tag{3.79}$$

(See [11–13] for details.)

3.7 Appendix A: Integral Evaluations

On a contrary, one can use a technique of differentiation with respect to parameters for the familiar integrals related to the Bohr-Sommerfeld quantization rule. As is well-known, if

$$J(x) = \int_{f(x)}^{g(x)} F(x,y)\ dy, \tag{3.80}$$

then

$$\frac{dJ}{dx} = \int_{f(x)}^{g(x)} \frac{\partial F(x,y)}{\partial x}\ dy + F(x,g(x))\frac{dg}{dx} - F(x,f(x))\frac{df}{dx}. \tag{3.81}$$

In the WKB case, the last two terms vanish because the limits are the turning points when the integrand equals zero [13]. In the following examples, we utilize this procedure for the integrals occurring in the "Sommerfeld-type puzzle" cases discussed in this note.

Example 1. For the Sommerfeld-type integrals,

$$I = \int_{r_1}^{r_2} p(r)\ dr, \qquad p(r) = \sqrt{-A+\frac{B}{r}-\frac{C}{r^2}} \quad (A, C > 0), \tag{3.82}$$

provided $p(r_1) = p(r_2) = 0$, one gets

$$\begin{aligned} \frac{dI}{dB} &= \frac{1}{2}\int_{r_1}^{r_2} \frac{dr}{\sqrt{-Ar^2+Br-C}} \\ &= \frac{1}{2\sqrt{A}}\int_{r_1}^{r_2} \frac{dr}{\sqrt{\dfrac{B^2-4AC}{4A^2}-\left(r-\dfrac{B}{2A}\right)^2}} \\ &= \frac{1}{2\sqrt{A}}\arcsin\left(\frac{2Ar-B}{\sqrt{B^2-4AC}}\right)\Bigg|_{r_1}^{r_2} = \frac{\pi}{2\sqrt{A}}. \end{aligned} \tag{3.83}$$

As a result,

$$\frac{dI}{dB} = \frac{\pi}{2\sqrt{A}}, \qquad I\left(B_0 = 2\sqrt{AC}\right) = 0 \tag{3.84}$$

and, by integration,

$$I = \pi\left(\frac{B}{2\sqrt{A}}-\sqrt{C}\right). \qquad \blacksquare \tag{3.85}$$

Example 2. Our trigonometric integral,

$$I(A) = \int_{\theta_1}^{\theta_2} \sqrt{A - \frac{B}{\cos^2\theta} - \frac{C}{\sin^2\theta}}\, d\theta = \frac{\pi}{2}\left(\sqrt{A} - \sqrt{B} - \sqrt{C}\right), \tag{3.86}$$

can be evaluated in a similar fashion:

$$\frac{dI}{dA} = \frac{\pi}{4\sqrt{A}}, \quad I\left(A_0 = \sqrt{B} + \sqrt{C}\right) = 0. \tag{3.87}$$

Indeed, if $T = \cos 2\theta$ one gets

$$I(A) := \frac{1}{2}\int_{T_1}^{T_2} \sqrt{(A - 2B - 2C) + 2(B - C)T - AT^2}\, \frac{dT}{1 - T^2}, \tag{3.88}$$

where

$$T_1 = \frac{B - C - \sqrt{(A - B - C)^2 - 4BC}}{A}, \quad T_2 = \frac{B - C + \sqrt{(A - B - C)^2 - 4BC}}{A}. \tag{3.89}$$

Thus

$$\frac{dI}{dA} = \frac{1}{4}\int_{T_1}^{T_2} \frac{dT}{\sqrt{(A - 2B - 2C) + 2(B - C)T - AT^2}} = \frac{1}{4\sqrt{A}} \arcsin\left(\frac{AT - B + C}{\sqrt{(A - B - C)^2 - 4BC}}\right)\Bigg|_{T_1}^{T_2} = \frac{\pi}{4\sqrt{A}}. \tag{3.90}$$

Simple integration results in

$$I(A) = \frac{\pi}{2}\left(\sqrt{A} - \sqrt{B} - \sqrt{C}\right), \tag{3.91}$$

where we have used the initial condition (3.87). ■

Example 3. The hypergeometric integral

$$J(\varepsilon) = \int_{-x_0(\varepsilon)}^{x_0(\varepsilon)} \sqrt{\operatorname{sec\,h}^2 x - \varepsilon}\, dx, \quad J(1) = 0. \tag{3.92}$$

Here $0 \leq \varepsilon \leq 1$ and $x_0(\varepsilon) = \operatorname{sech}^{-1}\sqrt{\varepsilon}$:

$$\frac{dJ}{d\varepsilon} = -\frac{1}{2}\int_{-x_0(\varepsilon)}^{x_0(\varepsilon)} \frac{dx}{\sqrt{\operatorname{sec\,h}^2 x - \varepsilon}} = -\frac{1}{2\sqrt{\varepsilon}} \arcsin\left(\sqrt{\frac{\varepsilon}{1 - \varepsilon}} \sinh x\right)\Bigg|_{-x_0(\varepsilon)}^{-x_0(\varepsilon)} = -\frac{\pi}{2\sqrt{\varepsilon}}, \qquad J(\varepsilon) = \pi\left(1 - \sqrt{\varepsilon}\right). \tag{3.93}$$

Thus

$$\int_{-x_0}^{x_0}\sqrt{\sec\mathrm{h}^2 x-\varepsilon}\;dx=\pi\left(1-\sqrt{\varepsilon}\right). \qquad \blacksquare \tag{3.94}$$

(See also [13].)

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