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Quantum chaos in elementary quantum mechanics

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Abstract
We introduce an analytical solution to one of the most familiar problems from the elementary quantum mechanics textbooks. The following discussion provides simple illustrations to a number of general concepts of quantum chaology, along with some recent developments in the field and a historical perspective on the subject.

1. Introduction

Many aspects of the behaviour of quantum systems can be understood and interpreted in terms of the dynamical characteristics of their classical counterparts. It is often possible to obtain *quantitatively* such important attributes of a quantum system as its spectra and even its wavefunction in terms of the appropriate classical quantities [1, 2]. Although the main objects of the classical dynamics, the dynamical trajectories, are not something that can be rigorously used in the context of quantum mechanics, they can often facilitate our understanding of the quantum realm, by providing means for semiclassical interpretation.

As an illustration of this point, let us first look at the infinite square well problem. Let us consider a particle confined in the infinite square well potential,

$$V(x) = \begin{cases} 0, & \text{if} \quad 0 < x < b, \\ \infty, & \text{if} \quad x \leqslant 0 \text{ or } x \geqslant L. \end{cases} \tag{1}$$

Classically, the dynamics of such a particle is as simple as it can possibly be—the particle simply bounces periodically between the two walls. Geometrically its trajectory is a closed loop, which the particle traverses over and over again. The total length of the loop is twice the width of the well, $\mathcal{L} = 2L$, and the period of motion is $T = 2L/v$, where v is the speed of the

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particle. As a result of the wall reflections, the momentum p of the particle changes its sign, but its magnitude never changes.

Quantum mechanically, this system is nearly as simple to describe. The wavefunction $\psi(x)$ in this case is a combination of two plane waves,

$$\psi(x) = A\,e^{ikx} + B\,e^{-ikx}, \tag{2}$$

where $k = p/\hbar$ is the 'wave vector', which must satisfy the boundary conditions $\psi(0) = \psi(L) = 0$. This leads to the quantization condition

$$\sin(kL) = 0, \tag{3}$$

and hence the quantum spectrum k_n of this problem is given by

$$Lk_n = \pi n. \tag{4}$$

Note, that the left-hand side of this equation coincides up to a factor $\hbar$ with the classical action integral,

$$S = \int_\gamma p\,dx = Lp, \tag{5}$$

taken along the trajectory γ that connects the two turning points, and hence the quantization condition (4) implies that the action takes only discrete values, $S_n = \pi\hbar n$. Expressing the de Broglie wavelength λ in terms of the wave vector, $\lambda = 2\pi/k$, relationship (4) can be cast into the form $\mathcal{L}/\lambda_n = n$, which has a simple geometrical meaning. Apparently wave (2) must fit *geometrically n* times onto the (only) classical periodic orbit that has the length $\mathcal{L}$. As the energy of the particle increases, its wavelength becomes smaller and smaller, however the geometrical condition $\mathcal{L}/\lambda_n = n$ always holds.

Such a simple combination of physical and geometrical ideas was used by Bohr and his school in around 1914 to provide the first explanations to one of the most striking features of the quantum mechanical systems—the discrete nature of their energy spectra. According to their views, the discreteness of the quantum spectra is essentially a consequence of the geometrical consistency of wave mechanics.

This 'wave-geometrical' approach proved very successful in early attempts to explain the experimentally observed emission–absorption spectrum of the hydrogen atom. In fact, the results obtained in this way were exact, and that gave reasons to believe that these ideas were adequate to describe the quantum physics of the subatomic world. However, the later attempts of Bohr, Sommerfeld, van Vleck, Born and others [3–5] to continue on with more complicated atoms, failed completely. It was apparently impossible to explain even approximately the experimentally observed spectrum of the helium atom—the next simplest atom after hydrogen in the periodic table of elements and hence the next best candidate for a successful treatment by means of such wave-geometrical quantization. Van Vleck wrote in 1922 [4]:

> *'The conventional quantum theory of atomic structure does not appear able to account for the properties of even such a simple element as helium, and to escape from this dilemma some radical modification in the ordinary conceptions of quantum theory or of the electron may be necessary.'*

What was the nature of the difficulties that required such 'radical' and 'conceptual' modifications? In 1925 Max Born wrote [5]:

> *'...the systematic application of the principles of the quantum theory... gives results in agreement with experiment only in those cases where the motion of a single electron is considered; it fails even in the treatment of the motion of the two electrons in the helium atom.'*

> *This is not surprising, for the principles used are not really consistent . . . . A complete systematic transformation of the classical mechanics into a discontinuous mechanics is the goal towards which the quantum theory strives.'*

Seemingly one makes a very simple and natural move by trying to go from the *exactly solved* hydrogen atom to helium, by adding just one more particle to the two-body nucleus–electron system of hydrogen. However, from the point of view of contemporary classical mechanics, this modest generalization turns an *integrable* two-body system into a *non-integrable* three-body system (a short explanation of the concept of integrability is given in section 5 or for more details see [1]). Hence, in order to impose 'geometrical consistency' on the quantum waves in the helium atom, one would have to deal with the overwhelming geometrical complexity of its classical phase space. It means that all the familiar properties of the generic chaotic systems, such as the exponential proliferation of the periodic orbits associated with extreme complexity of their shapes, would have to be taken into account—something that could hardly had been done in Bohr's time. Indeed, at the beginning of the last century chaos theory was just being developed in the works of Poincaré, Lyapunov, Hadamard, Birkhoff and a few others (see, e.g., [1, 2]). Although the importance of the classical dynamical behaviour for successful quantization was realized by certain researchers [6], it took about 60 years before the first semiclassical quantization procedure for nonintegrable systems was outlined. As for the helium atom, a semiclassical quantization scheme for it was proposed in 1992 [7] using some recent developments of quantum chaos theory [2].

2. Back to 1D potential wells

Surprisingly, the difficulties of the semiclassical quantization of the classically nonintegrable helium atom system can be illustrated by means of elementary quantum mechanics. Below we shall consider a simple modification of system (1) that leads to a transition from classical integrability to non-integrability and clarifies the corresponding outburst of complexity on the quantum level.

Let us add a small step at the bottom of potential (1) and consider a point particle moving in the potential

$$V(x) = \begin{cases} 0, & \text{if} \quad 0 \leqslant x \leqslant b, \\ V, & \text{if} \quad b \leqslant x \leqslant L, \\ \infty, & \text{if} \quad x \leqslant 0 \text{ or } x \geqslant L, \end{cases} \tag{6}$$

shown in figure 1. Seemingly the classical picture does not change much. It appears that if the energy of the particle is higher than V, the particle will oscillate between the points $x = 0$ and $x = L$ just as before, and if its energy is below the potential step height, it will oscillate between $x = 0$ and $x = b$. However, the reality turns out to be much more complicated than that.

Let us first give the quantum mechanical description of the problem. Suppose that the energy E of the particle is above the potential height V. To simplify the notation, we will assume below that $\hbar = 1$ and $m = 1/2$. Then the momentum of the particle in the region $0 \leqslant x \leqslant b$ is $k = \sqrt{E}$, and in the region $b \leqslant x \leqslant 1$ it is $\kappa = \sqrt{E - V}$, and its ψ function consists of two parts,

$$\psi(x) = \begin{cases} \sin(kx), & \text{if} \quad 0 \leqslant x \leqslant b, \\ A \sin[\kappa(L - x)], & \text{if} \quad b \leqslant x \leqslant L, \end{cases} \tag{7}$$
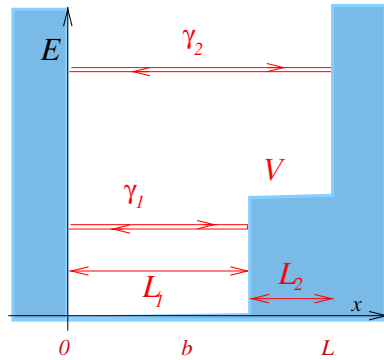
Figure 1. A simple modification of the infinite square well model—a square well with a potential step, along with the two apparent classical trajectories γ_1 and γ_1.
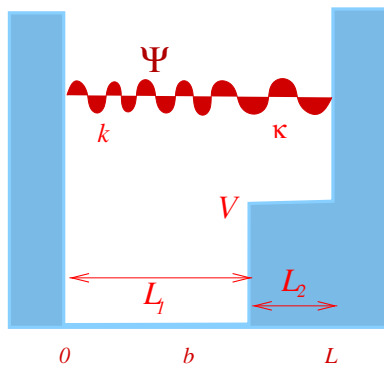

Figure 2. A quantum particle in a square well with a step.

which match continuously at $x = b$, as shown in figure 2. From this continuity requirement one can determine the spectral equation for the spectrum of the problem,

$$\sin(L_1 k + L_2 \kappa) = r \sin[(L_1 k - L_2 \kappa)], \qquad E > V, \qquad (8)$$

where $L_1 = b$ and $L_2 = L - b$ are correspondingly the lengths of the left and the right sides of the well (6) and r is the reflection coefficient

$$r = \frac{k - \kappa}{k + \kappa}. \qquad (9)$$

The $E < V$ case can be treated similarly and basically amounts to substituting $\kappa \rightarrow i\varkappa$, $\varkappa = \sqrt{V - E}$, in expressions (8) and (9). After extracting the complex phase, the spectral equation becomes

$$\sin(L_1 k) = \frac{(-1)^{n+1} k (1 - e^{-2L_2 \varkappa})}{\sqrt{V(1 + e^{-4L_2 \varkappa}) + 2(\varkappa^2 - k^2) e^{-2L_2 \varkappa}}}, \qquad E < V, \qquad (10)$$

where $n = 1, 2 \ldots$, is the root index.

There is an important analogy between (8), (10) and (3)—the arguments of the sine functions in the left-hand sides of these equations are the action lengths $S(E)$ of the classically available regions in the well (6) for $E > V$ and $E < V$ correspondingly,

$$S(k) = \int_\gamma k \, dx = \begin{cases} kL_1 + \kappa L_2, & \text{if} \quad E > V, \\ kL_1, & \text{if} \quad E < V, \end{cases} \qquad (11)$$

which is a continuous and monotonically increasing function of the energy.

On the other hand, it is interesting that unlike (3), equations (8) for $E > V$ and (10) for $E < V$ are *transcendental equations*—that is substantially more difficult to solve. In fact, in the absence of any analytical ways of solving equations (8) and (10) explicitly, all the standard textbooks, e.g. [8, 9], use graphical or numerical methods for approximating its roots, k_n. Notably, there are also no simple 'semiclassical' interpretations similar to (4) for the results of such approximations, which also does not appear important for the purpose of obtaining the numerical values for the roots of the spectral equations (8) and (10).

This is very similar to what happened to the helium atom quantization problem—the 'old quantum theory' treatment became unnecessary once the formalism of the 'new' quantum mechanics of Schrödinger and Heisenberg was established and could be used. The problem of obtaining the energy spectrum of the helium (or in principle any other atom) was reduced to a *technical* problem of diagonalizing the Hamiltonian matrix H_{nm} by means of all sorts of numerical techniques and approximations.

Even without making any historical references, one can note the obvious contrast in the level of complexity between the spectral equations (8), (10) and (3). What is the physical reason for it? Below we shall argue that the complexity of the spectral equations (8), (10) has a deep physical meaning and can be understood from analysing the classical motion of a particle in the potential well (6).

3. The classical limit

To start the discussion of the classical dynamics of a point particle in potential (6), let us note that the reflection coefficient (9) in (8) ($E > V$) does not depend on the Planck constant $\hbar$,

$$r = \frac{1 - \sqrt{1 - V/E}}{1 + \sqrt{1 - V/E}}. \tag{12}$$

Due to this circumstance this quantity (although obtained by purely quantum mechanical means [9]) is in fact quite classical, because one does not need to refer to any quantum mechanical concepts to evaluate r.

This curious fact can be easily interpreted and understood from general principles. Just as any other wave, the probability amplitude (2) gets reflected or diffracted when it encounters inhomogeneities on its way. It is important that the scale of these inhomogeneities should not be too big compared to the wavelength of the wave, otherwise the wave will 'adjust' to the smooth changes of the properties of the media. It is fair to say that in order to induce reflections, the obstacle should appear somewhat 'abruptly' in front of the wave, at a scale d smaller than the characteristic wavelength, $d \ll \lambda$. In our case, since the potential step (6) is defined to be absolutely sharp, changing discontinuously at $x = b$ from 0 to V, the quantum-mechanical wave will always be reflecting from its boundary at $x = b$ with the reflection probability r^2, no matter how small its wavelength is, even *at* the classical limit $\lambda = 0$. In other words, although intuitively one would expect the particle moving with the energy $E > V$ only to change its speed after passing over the point $x = b$, there actually exists a possibility of *classical* (so-called non-Newtonian) backward reflections from the sharp potential barrier edge.

This curious fact emphasizes an interesting aspect of the connection between classical and quantum mechanics, known as the 'correspondence principle', which was first invoked by Niels Bohr in around 1923. This fundamental principle states that classical mechanics can be understood as a limiting case of quantum mechanics in the so-called 'classical limit', i.e. in the case when the motions are characterized by actions much larger than the value of the Planck constant h. In Bohr's time, the fulfillment of such quantum–classical correspondence
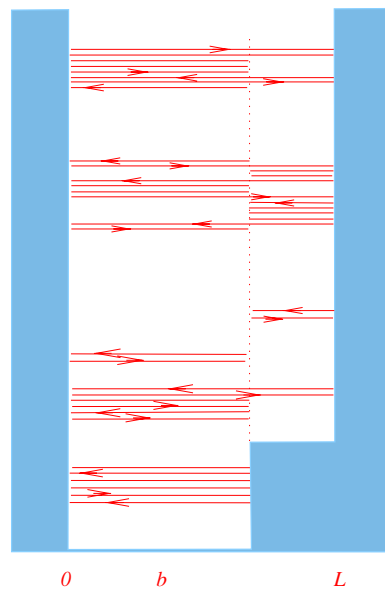
Figure 3. A storm in a coffee cup—non-Newtonian chaos in a one-dimensional step potential. The lines represent examples of non-Newtonian orbits in potential (6). For illustration purposes different trajectories are shown at different energies, as well as different sections of the same trajectories being shifted slightly up and down the energy axis, so that their parts are visible.

was viewed as a natural way to validate meaningfulness and physical consistency of the quantized analogues of familiar classical systems, such as atoms. Hence the correspondence principle is often understood as a naive requirement for the quantum system to reproduce the expected classical behaviour in the limit $h \rightarrow 0$, whereas in fact, there is no such requirement. The appearance of non-Newtonian scattering events is a curious example of a situation when quantum mechanics elucidates a certain implicit aspect of the corresponding classical dynamics, bringing up details that could have been easily overlooked.

Similar considerations can prove that non-Newtonian scattering phenomena can happen for every potential with sharp edges, as some kind of a reminder of the quantum-mechanical legacy of classical mechanics. The fact that we never observe such events in every day life implies that in reality there are no potential changes, sharp on the scale of the quantum wavelengths of the macroscopic objects.

4. Non-Newtonian chaos

Because of the possibility of such classical non-Newtonian reflections, the classical dynamics of a particle in potential (6) is far from trivial. Every time the particle approaches the boundary $x = b$ between the two regions in (6), it can be reflected from it with the probability r^2 and transmitted through it with the probability $t^2 = 1 - r^2$. As a result, instead of a couple of back and forth oscillations which one would naively expect from a particle in potential (6), the actual trajectories of such particle are far more complex. The particle can start, say, in the left side L of the well, move to the boundary $x = b$, reflect back from it, reflect back from the rigid wall at $x = 0$, do this several times, then transmit eventually to the right side R of the well, where it can also perform a number of oscillations before returning to the left side of the well, etc. Any thinkable sequence of oscillations in the right and in the left sides of the potential well (6) represents a possible trajectory of the particle (figure 3). It should also be
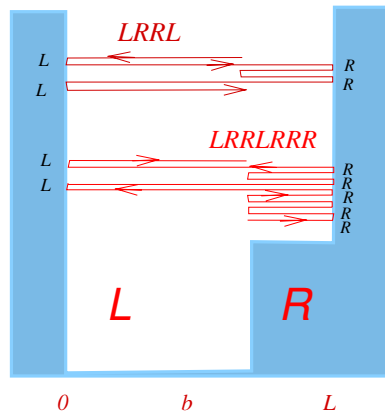
Figure 4. A couple of examples of non-Newtonian orbits in potential (6) marked by their R–L binary codes. Every left swing of the orbit contributes an 'L' to its code and every right one contributes an 'R'. This L–R code representation of the orbits is a simple example of symbolic dynamics over a partition of the phase space [2].

emphasized, that at every reflection or transmission (scattering) event, the particle completely loses its memory about the previous stage of its motion. Given the current position and the momentum of the particle, neither its previous evolution nor its state of motion after the next collision can be reconstructed. Hence, instead of the deterministic evolution we generated a fairly complicated *stochastic* dynamical process by considering a seemingly simple potential (6). It will be argued below that the stochasticity is brought into the classical regime by the semiclassical reflection probabilities, and its ability to generate an infinity of classical orbits makes the system nonintegrable.

Obviously, there can be classical orbits of arbitrary length, and the bigger is the allowed length (or the period) of the trajectory, the larger are the numbers of nontrivial orbits that come into the picture. Is there a way to enumerate all this variety of orbits?

It turns out that the description of the general behaviour of the orbits in this system can be conveniently formalized. Indeed, every orbit can be described by a two-letter code, which would simply tell us in what sequence the orbit swings through the left (L) or the right (R) sides of the well, as shown in (figure 4). Periodic orbits are obviously represented by periodic sequences of symbols. Conversely, any periodic sequence of the symbols (for example, $RLRLRLRLRL\ldots$ or just (RL) for short), unambiguously describes a certain periodic orbit (note however, that two sequences which can be obtained from one another by a cyclical permutation of symbols, correspond to the same periodic orbit). If the orbit swings n_1 times in the left side of the well and n_2 in the right side, its action length is equal

$$S_{orb} = 2n_1 S_1 + 2n_2 S_2, \tag{13}$$

where $S_1 = L_1 k$ and $S_2 = L_2 \kappa$.

The number of periodic orbits increases indefinitely. Their shapes (and correspondingly their L–R binary codes) become more and more complicated, so the classical mechanics in the potential turns out to be surprisingly rich. In fact, the number of geometrically different orbit shapes (or the number of prime periodic orbits, those that never retrace themselves) that include up to m scattering events grows exponentially as

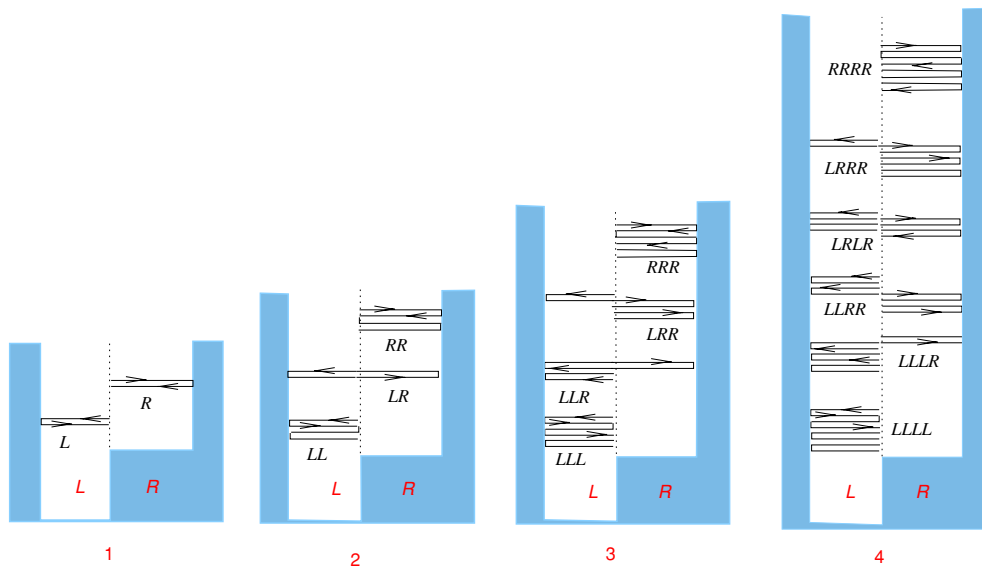$$N \approx \frac{e^{0.7m}}{m}. \tag{14}$$

Figure 5. Exponential proliferation of the orbits in the potential (6). The orbits that undergo 1, 2, 3 and 4 scatterings marked by their R–L binary codes.

Such behaviour closely resembles the periodic orbit proliferation scenario that takes place in classically nonintegrable chaotic systems. Hence a particle in potential (6) can be viewed as a simple model of a classically chaotic system (figure 5).

The difference between this and the simple back and forth motion in the square well potential is overwhelming, and provides a simple illustration to the difference between the dynamical behaviour of the integrable and the nonintegrable systems, such as e.g. hydrogen and helium.

Of course the more complex the orbit shape, the smaller is the probability that this particular orbit will be realized. This 'complexity selection' can be easily understood from the point of view of quantum mechanics, where the propagation of the particle is described by the normalized wave (2). It is clear that every reflection or transmission reduces its initial amplitude by the amount of the reflection or transmission coefficient. Hence, it is clear that if a certain prime periodic orbit p (i.e. one that cannot be considered a repetition of a shorter orbit) reflects $\sigma(p)$ times from the either side of the potential barrier at $x = b$, and transmits $\tau(p)$ times through it, its initial amplitude will decrease

$$A_p = (-1)^{\chi(p)} r^{\sigma(p)} (1 - r^2)^{\tau(p)/2} \tag{15}$$

times [11, 12]. Here the factor $(-1)^{\chi(p)}$ keeps track of the sign changes due to the wall reflections and the right reflections from the boundary. If the orbit p is traced over itself ν times, then the corresponding amplitude will be A_p^ν. So the quantity (15) is a certain quantum (and, since r does not depend on $\hbar$, also classical) 'weight' of the orbit.

5. Classical dynamics and quantum spectrum

In the case of a particle moving in the infinite potential well (1), the oscillation between the two walls completely exhausts all the classical dynamical possibilities. At the same time, the magnitude of the momentum $|p|$, is conserved. This illustrates the general situation in the

so-called integrable systems, i.e. those that have as many dynamically conserved quantities (e.g. momentum, angular momentum, etc) as degrees of freedom [6, 10]. These conserved quantities (the action integrals) I_i, $i = 1, \ldots, d$, are quantized according to

$$I_i = h(n_i + \mu_i), \tag{16}$$

where n_i are natural numbers, $n_i = 1, 2, \ldots$, and μ_i is a certain geometrical constant [1]. The energy of these systems is a certain function of the I_i, $E = E(I_1, \ldots, I_N)$, and so the quantization rules (16) immediately produce the semiclassical energy spectrum. For example, for system (1) the action, $I = 2|p|L$, is quantized via $|p| = \hbar\pi n/L$, and yields the quantum energy eigenvalues $E = (\hbar\pi n)^2/2mL^2$. According to this scheme, the 'quantum numbers' n_i are naturally related to the classical integrals of motion I_i.

On the other hand, the classical behaviour of the particle in potential (6) is of manifestly nonintegrable type. The variety of possible dynamical orbits in the potential (6) is much richer than in (1). What information is hidden in this variety of the orbits?

As pointed out above, in the integrable systems there exists a convenient handle—the action integrals, which can be ascribed certain discrete values via the EBK semiclassical quantization procedure. What if the integrals do not exist? What is there in a nonintegrable system that can be used in order to quantize the system semiclassically?

The first answer to this question came in early 1970s, when Gutzwiller [1] showed that a 'handle' for semiclassical quantization of the systems without the sufficient number of the integrals of motion is provided by the so-called density of states—a functional that corresponds a δ-peak to every energy level E_n of the quantum spectrum,

$$\rho(E) \equiv \sum_{n=1}^{\infty} \delta(E - E_n). \tag{17}$$

Gutzwiller provided a semiclassical expansion for $\rho(E)$ (the so-called Gutzwiller trace formula) in terms of the classical quantities related to the periodic orbits,

$$\rho(E) \approx \bar{\rho}(E) + \frac{1}{\pi} \operatorname{Re} \sum_p T_p \sum_{\nu=1}^{\infty} B_p^{\nu} \, \mathrm{e}^{\mathrm{i}\nu S_p(E)}. \tag{18}$$

Here T_p, S_p and B_p are correspondingly the period, the action and a certain weight factor (see below) of the prime periodic orbit p (all classical quantities), and ν is the number of times the orbit p repeats itself. The first term $\bar{\rho}(E)$ represents the non-oscillating part of the density of states.

The gist of the Gutzwiller trace formula is an (almost miraculous) interference effect, produced by the infinity of oscillating terms, one per each periodic orbit, in the sum (18). The statement is that if the energy E in (18) happens to coincide with a *quantum* energy level E_n, then all the terms in the sum (18) will interfere constructively and produce a peak, whereas if there is no E_n there, they will interfere destructively and yield 0.

This is a truly remarkable connection between the classical and the quantum properties of a system. After all, from a formal mathematical perspective, classical characteristics of a system should *a priori* describe only its $\hbar = 0$ limit, whereas according to the trace formula one can use the classical properties of the system to extract the information about its *quantum* properties for $\hbar \neq 0$.

Gutzwiller's formula can also be applied to the 1D system of a particle in the step potential (6). Moreover, it can be shown [11, 12] that for the system (6) the expansion (18) is *exact*. Another important characteristic of the spectrum is the 'spectral staircase' $N(E)$,

$$N(E) \equiv \int_0^E \rho(E') \, \mathrm{d}E' = \sum_n \Theta(E - E_n), \tag{19}$$

where $\Theta(x)$ is Heaviside's theta function,

$$\Theta(x) = \begin{cases} 1, & \text{if} \quad x > 0, \\ 0, & \text{if} \quad x < 0, \end{cases} \tag{20}$$

which gives the number of energy levels in the interval between 0 and E. $N(E)$ can also be expanded into a periodic orbit series,

$$N(E) = \bar{N}(E) + \frac{1}{\pi} \operatorname{Im} \sum_p \sum_{\nu=1}^{\infty} \frac{A_p^\nu}{\nu} e^{i\nu S_p(E)}. \tag{21}$$

What makes expansion (21) particularly convenient for our use, is that the weight factors A_p in it are explicitly given by (15). The first term of $N(E)$ (its non-oscillating part, also known as Weyl's average) is given by

$$\bar{N}(E) = \frac{1}{\pi} S(E) - \gamma_0, \tag{22}$$

where $S(E)$ is the action length (11) of the classically available region of the well, and γ_0 is a small correction term.

The complexity of our task of describing the spectrum in (6) can already be appreciated from expansions (18) and (21): every non-Newtonian orbit that exists in (6) explicitly contributes to these expansions.

In addition to the huge number of periodic orbits, there are many other subtle dynamical effects that contribute to the complexity of expansions (18) and (21). For instance, it was mentioned above that as the energy of the particle passes from above to below V, the particle becomes classically unable to penetrate into the right section of the well, $b < x < L$. However, there remains the possibility of quantum tunnelling into the region R, described semiclassically as motion with imaginary momentum, $\kappa \to i\varkappa$. With this change, the formal structure of the Gutzwiller formula remains the same, so expansions (18) and (21) can be used, with due care, both for $E > V$ and for $E < V$. For example, actions (13) of the orbits that 'tunnel' under the step are imaginary, $S_{orb} = 2S_1 n_1 + i2n_2 S_2$ (such orbits are called 'ghost orbits' [2]). This point will be discussed in more detail below. This illustrates the point that as the energy of the particle changes, the physical characteristics of the orbits (and therefore of the expansion terms in (18)) may change.

6. Obtaining the spectrum

Since the right-hand side of expansion (18) can be obtained from considering the classical motion of the particle, expansion (18) provides a clear connection between the dynamical characteristics of the system and its spectrum in the quantum regime. The energy levels of the quantum system are obtained according to (18) as the poles (delta spikes) produced by the periodic orbit sum [1]. It is important however, that by using this approach, one cannot tell *when* these poles will appear prior to performing the summation of the periodic orbit series (18). Without having any extra information about the system, the only *a priori* strategy for obtaining E_n is to scan the energy axis by summing the series (18) for every value of E to find out whether or not the sum produces a δ-peak.

This illustrates the fact that $\rho(E)$ is a *global* characteristic of the spectrum. Both $\rho(E)$ and its expansion (18) describe the whole spectrum at once, rather than the specific individual energy levels, in contrast to the case of the integrable systems, where every action integral I_i is quantized directly (16) and *separately* from the rest of the degrees of freedom.

Actually, it is possible to extract the information about the individual energy levels E_n out of $\rho(k)$ without such tedious 'energy axis scanning'—if only one knows where to look.
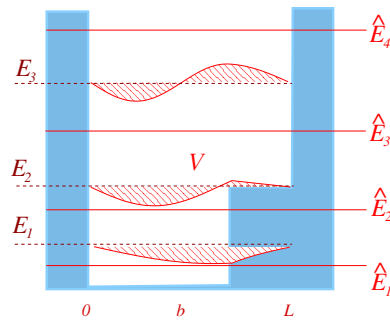
Figure 6. The energy separators $\hat{E}_n$ (their values on the energy scale are shown by solid lines) define the upper and the lower bounds for the quantum energy levels E_n, shown by the dashed lines.

Indeed, if for instance we would happen to know that some energy level E_n is the *only* level that lies between two points $\hat{E}_n^+$ and $\hat{E}_n^-$ (and hence $\rho(E)$ has only one δ-peak between these points), then the integral

$$E_n = \int_{\hat{E}_n^-}^{\hat{E}_n^+} E\rho(E)\, \mathrm{d}E, \tag{23}$$

would produce the E_n. Since we know the expansion of $\rho(E)$ in terms of the periodic orbits this integration can be performed.

Hence, solving the spectral problem is equivalent to finding two 'separators', $\hat{E}_n^+$ and $\hat{E}_n^-$, for *every* energy level E_n. Apparently, for the purpose of separating one level from another, it is enough to assume that $\hat{E}_{n-1}^+ = \hat{E}_n^-$, so basically we are looking for a sequence of points $\hat{E}_n$ that interweaves the sequence of the energy levels and separates one energy level from another [11, 12]. In other words, we need to establish a partition of the E-axis into the intervals $[\hat{E}_{n-1}, \hat{E}_n]$, each one of which contains exactly one energy level (figure 6).

Note however, that even if that could be achieved, one would still have just an algorithmic recipe for evaluating E_n rather than a *formula* of the type $E_n = \dots$. In order to get such a formula, we would need to find *a global function* $\hat{E}(n)$ that depends explicitly on n and produces all the separating points in their natural sequence *as a function of their index*,

$$\hat{E}_n = \hat{E}(n). \tag{24}$$

Once such a functional dependence of the separators on their index is established, integral (23) would turn the index n into a *quantum number* and give us a complete solution to the spectral problem in the form $E_n = \dots$.

Although generally finding a sequence (24) is not an easy task, it can be obtained for the particle in potential (6).

7. Spectral equation

In order to get this information, let us examine closely the spectral equations (8) and (10). Since the quantity that we are after, the classical action $S(E)$ defined by (11) is in the arguments of the sines in the left-hand sides of the equations (8) and (10), we can formally invert them to obtain

$$S(E) = \pi \left(n - \frac{1}{2}\right) - \begin{cases} (-1)^n \left(\arcsin\left(r\sin(S_1 - S_2) + \frac{\pi}{2}\right)\right), & \text{if } E > V, \\ \arctan(\varkappa(1 + \mathrm{e}^{-2S_2})/k(1 - \mathrm{e}^{-2S_2})), & \text{if } E < V, \end{cases} \tag{25}$$

where $n = 1, 2, \dots$.

It is important to note that the two terms in (25) behave quite differently. While the first term, $\pi\left(n - \frac{1}{2}\right)$, increases regularly with n, it is much harder to follow the behaviour of the second term of this equation. On the other hand, since the inverse trigonometric functions are bounded, $-\frac{\pi}{2} \leqslant \arcsin(x), \arctan(x) \leqslant \frac{\pi}{2}$, the second term always contributes less to the solution than the first term. Indeed, when the index n in equation (25) changes by 1 as we go from the level n to $n + 1$, the first term increases by π, which is generically (that is almost always) *more* than what the arcsine or arctangent can provide.

This fact allows one to obtain the set of separating points discussed in the previous section. Indeed, since the irregular terms in (25) are different from 0, the values $\hat{S}_n = \pi(n - 1/2)$ *themselves* are never the solutions to (25). Hence, since the difference between the two consecutive points $\hat{S}_n$ is always bigger than the second term in (25), so the roots S_n of (25) will be locked inside the intervals

$$\pi\left(n - \tfrac{1}{2}\right) < S_n < \pi\left(n + \tfrac{1}{2}\right). \tag{26}$$

Thus, the first discrete quantum action value will be locked between $\pi/2$ and $3\pi/2$, the second one between $3\pi/2$ and $5\pi/2$, and so on. So we run immediately into the separating points for the quantum values of action,

$$\hat{S}_n = \pi(n - 1/2), \qquad n = 1, 2, \ldots, \tag{27}$$

or the *action separators*. One can now either extract the energy separators $\hat{E}_n$ from $S(\hat{E}_n) = \pi(n - 1/2)$, and obtain the energy spectrum via (23), or alternatively, one can first obtain the actual quantum levels of action and then extract the quantum energy levels from them. In the latter case one needs to introduce a 'density of the action states', $\rho(S)$, defined as $\rho(S)\,\mathrm{d}S = \rho(E)\,\mathrm{d}E$,

$$\rho(S) \equiv \sum_{n=1}^{\infty} \delta\left(S - S_n\right) \frac{\mathrm{d}E}{\mathrm{d}S}, \tag{28}$$

and use the same approach that was outlined in the previous section for $\rho(E)$.

It is possible then to obtain the discrete quantum action values S_n via

$$S_n = \int_{\pi(n-1/2)}^{\pi(n+1/2)} S\rho(S)\,\mathrm{d}S = SN(S)\Big|_{\pi(n-1/2)}^{\pi(n+1/2)} - \int_{\pi(n-1/2)}^{\pi(n+1/2)} N(S)\,\mathrm{d}S, \tag{29}$$

where we used the identity

$$\rho(S) = \frac{\mathrm{d}N(S)}{\mathrm{d}S}. \tag{30}$$

Using the relationship $N(\hat{S}_n) = n$ (there are exactly n roots s_n below the nth separator) and the expansion (21), we get

$$S_n = 2\pi n - \frac{\pi}{2} - \int_{\pi(n-1/2)}^{\pi(n+1/2)} \bar{N}(S)\,\mathrm{d}S - \frac{1}{\pi}\,\mathrm{Im}\sum_{p,\nu} \int_{\pi(n-1/2)}^{\pi(n+1/2)} \frac{A_p^\nu}{\nu}\,\mathrm{e}^{\mathrm{i}\nu S_p}\,\mathrm{d}S, \tag{31}$$

where the weight factors A_p are given by (15).

Note, that (4) gives exactly the first term of expansion (31). Hence the oscillatory terms in (31), with their amplitudes proportional to the non-Newtonian reflection amplitudes, are indeed due to the 'nonintegrability' of (6).

Since all of quantities on the right-hand side of (31) are known, this formula provides an explicit representation of the discrete quantum values of the action functional in terms of the geometric and dynamical characteristics of potential (6). Formula (31) allows the computation of the action corresponding to every quantum level *individually*, *explicitly* and *exactly* in terms of the classical parameters, indexed by its 'quantum number' n.

It should be mentioned however, that the quantum number n in (4) and in (31) has rather different origins. Formula (31) does not have such a direct geometrical interpretation as (4). While in (4) the number n is the number of waves that fit the trajectory, in the case of the step potential (6) n is the index of the cell (26) that contains the corresponding action value S_n.

So once again, we arrive at defining the quantum energy spectrum via a discrete set of allowed values of the action functional, $S_n = S(E_n)$. This relationship (which is yet to be presented explicitly) can be viewed as a direct generalization of (4).

Of course, for using the periodic orbit expansions in practice, one needs to know how to truncate the series (18) or (31) to obtain finite order approximations to S_n. Since usually the periodic orbit series are not absolutely convergent, the order in which the expansion terms are incorporated into the sum (31) is important. It turns out [11, 12], that the correct way to obtain the mth approximation to the exact value of S_n is to include into sum (31) all the trajectories that reach the point $x = b$ m times or less.

8. Overview and an example

Let us summarize the steps for obtaining the mth correction to S_n using the semiclassical periodic orbit expansion technique.

1. Write down all the m-letter sequences (words) w_m. For example, there are two words, (L) and (R), for $m = 1$, four words (LL), (LR), (RL) and (RR) for $m = 2$, eight words (LLL), (LLR), (LRL), (RLL), (RLR), (RRL), (LRR) and (RRR) for $m = 3$ and so on. (To do the same thing geometrically—draw all possible periodic orbits similar to the ones shown in figure 4 that include exactly m transmissions and reflections.)

2. Find which w are cyclic permutations of one another—all these sequences represent the same orbit, so pick one and discard its replicas. From the above examples, both $m = 1$ orbits will remain, for $m = 2$ we may keep (LL), (LR) and (RR), for $m = 3$ we keep (LLL), (LLR), (RLR) and (RRR). (Geometrically: find out which loops represent the same sequence of left and right swings. Pick one and discard its replicas.)

3. Count the number n_L of L and n_R of R in w and find the action S_w of the orbit w according to

$$S_w = 2n_R S_1 + 2n_L S_2. \tag{32}$$

Remember that if $E < V$ then $S_2 = i\sqrt{V - E} L_2$.

4. Assuming that the first symbol in w cyclically follows the last one, find out which of the remaining sequences w are prime sequences and which ones are repetitions of a shorter code. Find the repetition number ν_w for each orbit (use $\nu_w = 1$ if the orbit is prime). For example, for $m = 2$ the orbit $\nu_{LR} = 1$, $\nu_{RR} = \nu_{LL} = 2$, and for $m = 3$ $\nu_{LLL} = \nu_{RRR} = 3$, $\nu_{LLR} = \nu_{RLR} = 1$. (Geometrically, find out how many times each orbit traverses over itself.)

5. Scan each word w_m (again, the first symbol of w follows the last one) and write down the weight A_w according to the substitutions

$$LR \to t, \qquad RL \to t, \qquad LL \to r, \qquad RR \to -r, \tag{33}$$

plus each wall reflection contributes a sign change. For example, for $m = 1$, $A_L = -r$, $A_R = r$, for $m = 2$ $A_{LR} = t^2$, $A_{RR} = A_{LL} = r^2$, and for $m = 3$ we have $A_{LLL} = -r^3$, $A_{RRR} = r^3$, $A_{LLR} = -rt^2$, $A_{RLR} = rt^2$. (Geometrically: assign a factor t to every transmission, a factor -1 to every wall reflection, a factor r to every left side reflection and a factor $-r$ to every right side reflection.)
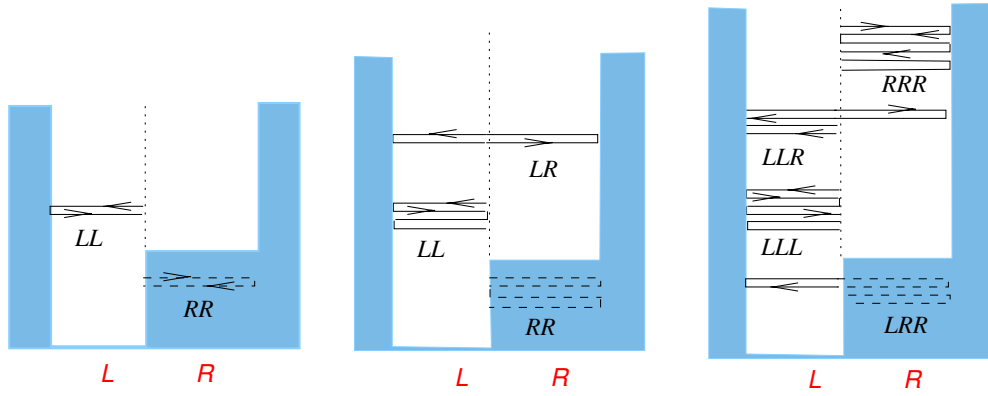
Figure 7. The orbits required for evaluating the first three periodic orbit expansion approximations to the S_n. Since the evaluation of the low levels which correspond to the energy $E < V$ will require ghost orbits, a few ghost orbits are also illustrated. The tunnelling parts of the ghost orbits are shown with dashed lines.

6. For every orbit, find the corresponding term in expansion (31),

$$\int_{\pi(n-1/2)}^{\pi(n+1/2)} \frac{A_w}{v_w} \, e^{iS_w(S)} \, dS, \tag{34}$$

and integrate.

If all the words up to length m are considered, the result will produce the mth approximation to the exact discrete sequence of actions.

All the non-Newtonian orbits described in the previous sections contribute to the expansion of each eigenvalue S_n. One can now appreciate the complexity of solving analytically equations (8) and (10) compared to solving the simple equation (3), by comparing the complexities of the corresponding classical dynamics.

8.1. An example

As an example, let us compute the first three approximations to a few momentum eigenvalues, using the orbits that include up to three scattering events, outlined in the summary and shown in figure 7. We have according to (31) that the first three corrections will be:

$$S_n = 2\pi n - \frac{\pi}{2} - \int_{\pi(n-1/2)}^{\pi(n+1/2)} \bar{N}(S) \, dS - \text{Im} \int_{\pi(n-1/2)}^{\pi(n+1/2)} \left(r \, e^{i2S_1 k} - e^{i2S_2 k} r \right) \, dS$$

$$- \text{Im} \int_{\pi(n-1/2)}^{\pi(n+1/2)} \left(\frac{1}{2} r^2 \, e^{4iS_1} + t^2 \, e^{i2S_1 + i2S_2} + \frac{1}{2} \, e^{4iS_2} r^2 \right) \, dS$$

$$- \text{Im} \int_{\pi(n-1/2)}^{\pi(n+1/2)} \left(\frac{1}{3} r^3 \, e^{6iS_1} + t^2 r \, e^{i(2S_2 + 4S_1)} - t^2 r \, e^{i(2S_1 + 4S_2)} - \frac{1}{3} r^3 \, e^{6iS_2} \right) \, dS. \tag{35}$$

In order to use formula (35), one needs to specify the parameters of the potential well (6). In particular, it is a specific value of V that determines at what energy the periodic orbits will acquire tunnelling parts. For simplicity, let us consider the case of a symmetrical well, when $L_1 = L_2 = 1$. Then the action S defined by (11) will be

$$S(E) = \begin{cases} k + \kappa, & \text{if } E > V, \\ k, & \text{if } E < V, \end{cases} \tag{36}$$

Table 1. The results of the periodic orbit expansion approximations to the exact values of s_n. The first $m = 0$ column gives the Weyl $s_n^{(m=0)}$ estimate for the roots of the spectral equation, and the following columns show the corrections to it due to the $m = 1$, $m = 2$ and $m = 3$ code length orbits. Note that the third periodic orbit expansion approximation to s_2 comes out higher than the critical value, $s_2^{(m=3)} > s_{crit} = 5$, whereas the actual root s_2 is smaller than s_{crit}. Hence more periodic orbit expansion terms are needed to capture the correct qualitative behaviour of s_2.

Root	$m = 0$	$m = 1$	$m = 2$	$m = 3$	Exact
s_1	2.4354	2.6198	2.6173	2.605	2.595 878 720 129 5728
s_2	6.1601	5.5789	5.2366	5.1434	4.945 531 691 438 1690
s_{17}	53.4071	53.405	53.404	53.406	53.403 119 615 030 526

in terms of which

$$\begin{cases} r = \frac{V}{S^2}, \quad t^2 = \left(1 - \frac{V^2}{S^4}\right), \quad \gamma_0 = \frac{1}{2}, & \text{if } E > V, \\ r = e^{2i\pi\gamma_0}, \quad \gamma_0 = \frac{1}{\pi}\arctan\frac{\sqrt{V-S^2}}{S}, \quad t^2 = (1 - e^{2i\pi\gamma_0}), & \text{if } E < V. \end{cases} \tag{37}$$

Note γ_0 also appears in the Weyl average (22).

Next, let us pick a certain value for the potential step height, say $V = 25$. This will set the $E_{crit} = 25$ and $k_{crit} = 5$ to be the 'critical values' of energy and the momentum—that is if we are looking for an energy level below $E = V = 25$, then the tunnelling effects have to be taken into account. Correspondingly, the critical value for the action will be $S_{crit} = k_{crit}L_1 = 5$, and so one should use different parts of formulae (36) to extract the E_n or k_n out of S_n, depending on whether a particular s_n is smaller or greater than 5.

After the height of the potential step has been chosen, certain general statements about the behaviour of the quantum S_n levels can be made. For the specific case $V = 25$, the first and the second separators, $\hat{S}_1 = \frac{\pi}{2}$ and $\hat{S}_2 = \frac{3\pi}{2}$, will be smaller than S_{crit}, and so the level contained between them will correspond to the energy $E_1 < V$. The third action separator is bigger than k_{crit}, $\hat{S}_3 = 5\pi/2 > 5$, so we will be in a better position to judge the location of the second level $\hat{S}_2 < S_2 < \hat{S}_3$ after computing corrections (35). All the other levels S_n, for $n > 2$, have energies higher than V.

So let us find the discrete quantum action values S_1, S_2 and (for example) S_{17}, and the corresponding quantum momentum eigenvalues, k_1, k_2 and k_{17}. Using expressions (35), (36), (37) and integrating from $\pi/2$ to $3\pi/2$, from $3\pi/2$ to $5\pi/2$ and from $33\pi/2$ to $35\pi/2$ (using some numerical integration software is highly recommended) we find the values shown in table 1.

Note that in the second case the integration in (35) should be split into two parts,

$$\int_{3\pi/2}^{5\pi/2} N(S)\,dS = \int_{3\pi/2}^5 N^{(E<S)}(S)\,dS + \int_5^{5\pi/2} N^{(E>V)}(S)\,dS, \tag{38}$$

in order to follow the changes in the structure of the expansion terms described by (36) and (37). Note also that the column to column changes are more significant for the second root—this indicates that the 'spectral fluctuations' for this root are high due to the orbit metamorphosis that takes place at $E = V$, inside the integration interval $\hat{E}_2 < E_2 < \hat{E}_3$. This also indicates that more periodic orbit expansion terms are needed to get a more precise position of s_2 with respect to V.

After the allowed values S_n for the action are found, the quantum levels of the momentum can be obtained by inverting the relationship (36),

$$k = \begin{cases} \frac{s^2-V}{2s}, & \text{if } s_n > V, \\ s, & \text{if } s_n < V. \end{cases} \tag{39}$$
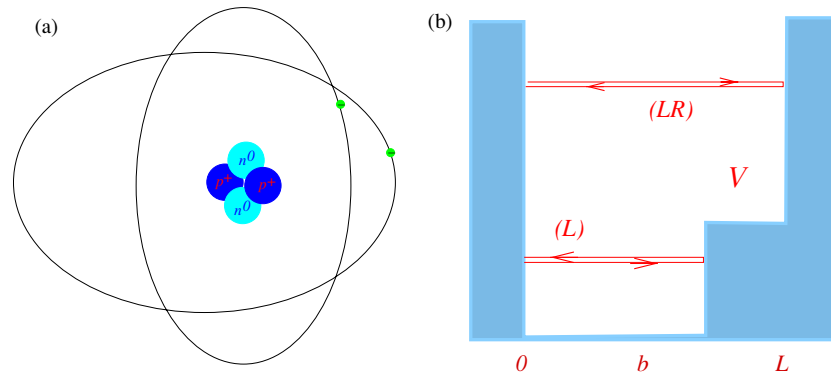
Figure 8. The familiar schematic picture of the helium atom (a), which was also used as the physical model in 1920s, is analogous to using only Newtonian trajectories in the potential (6), shown in (b). This scheme completely ignores the actual classical dynamical complexity. Compare (b) to figures 3 and 5.

According to (1) one has from (39):

$$k_1 = 2.605, \qquad k_2 = 5.0020, \qquad k_{17} = 26.4689. \qquad (40)$$

This demonstrates how the periodic orbit expansion quantization rule (31) gives the explicit solution to our spectral problem.

9. Discussion

We have studied an elementary example of a classically nonintegrable (quantum stochastic) system in potential (6). Despite the simplicity of the setup, the classical dynamics of the particle in the potential (6) turns out to be quite complicated, and this complexity is manifested in its spectral properties in the quantum regime. Surprisingly, in studying this most elementary example, one runs into essentially all the dynamical and physical effects (integrability versus nonintegrability, the exponential proliferation of the periodic orbits in the nonintegrable case, periodic orbit expansions, the use of symbolic dynamics, orbit metamorphosis, tunnelling, ray splitting, etc) that appear in semiclassical analysis of more realistic physical systems. Usually these phenomena are investigated via a rather involved mathematical apparatus, whereas in our example they can be analysed by elementary means. Due to its illustrative simplicity, this and similar [11, 12] systems can be thought of as the 'harmonic oscillators' of quantum chaos.

On the other hand, this problem is rich enough to illustrate the essence of the difficulties associated with the semiclassical quantization of chaotic dynamical systems, such as the helium atom. As mentioned above, the early attempts to quantize the helium atom failed because the qualitative difference in the dynamical complexity between hydrogen and helium was overlooked. The attempts to quantize a chaotic system within the framework of Bohr–Sommerfeld or EBK quantization theory using only a few integrable-like trajectories can be compared to considering just the two 'naive' (Newtonian) classical trajectories in potential (6), (L) for $E < V$ and (LR) for $E > V$ (figure 8). From the structure of the exact result (31) it is clear that such a consideration would produce only very approximate results, far from the real complexity of the problem.

Formula (31) represents an example of the 'modification' of the EBK quantization condition (4) mentioned in the Van Vleck citation above, for the simple case of the potential (6), in an explicit and self-contained form. Certainly, obtaining the semiclassical spectrum in

the form $E_n = \ldots$ for more complicated systems such as the helium atom is a much more difficult task. However, this result creates an interesting precedent that may indicate new directions in semiclassical quantization theory and related fields.

Acknowledgments

References

[1] Gutzwiller M C 1990 *Chaos in Classical and Quantum Mechanics* (New York: Springer)
[2] Cvitanović P, Artuso R, Mainieri R, Tanner G and Vattay G *Classical and Quantum Chaos* www.nbi.dk/ChaosBook/, Niels Bohr Institute (Copenhagen 2001)
[3] Bohr N 1924 *On the Application of the Quantum Theory to Atomic Structure* (Cambridge: Cambridge University Press)
[4] van Vleck J H 1922 *Phil. Mag.* **44** 842
[5] Born M 1925 *Vorlesungen über Atommechanik* (Berlin: Springer)
    Born M 1927 *Mechanics of the Atom* (New York: Ungar) (Engl. Transl.)
[6] Einstein A 1917 Zum quantensatz von Sommerfeld und Epstein *Verh. Deutsch. Phys. Ges.* **19** 82–92
[7] Wintgen D, Richter K and Tanner G 1992 *CHAOS* **2** 19
[8] Griffith D J 1995 *Introduction to Quantum Mechanics* (Englewoods Cliff, NJ: Prentice-Hall)
[9] Landau L D and Lifshitz E M 1977 *Quantum Mechanics* (New York: Pergamon)
[10] Keller J B 1958 *Ann. Phys., NY* **4** 180
[11] Dabaghian Yu, Jensen R V and Blümel R 2001 *JETP Lett.* **74** 235
    Dabaghian Yu, Jensen R V and Blümel R 2002 *JETP* **121** 1–16
[12] Blümel R, Dabaghian Yu and Jensen R V 2002 *Phys. Rev. Lett.* **88** 044101
    Blümel R, Dabaghian Yu and Jensen R V 2002 *Phys. Rev.* E **65** 046222