Exact classical limit of quantum mechanics: Central potentials and specific states

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A derivation has been performed of some central potentials with no quantum correction to the Hamilton-Jacobi equation. In this exact limit of quantum mechanics, quantum trajectories identical to the classical ones are obtained. Interestingly, some of them are closed orbits. Applications of the found potentials in many areas of physics are also discussed.

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I. INTRODUCTION

Newtonian mechanics can be considered as a limiting case of more general relativistic mechanics since the predictions of the former theory, e.g., trajectories, are derivable from the latter one in the limit of low velocities where v/c≪1. Instead, relations between predictions of Newtonian dynamics and those of quantum mechanics are much more subtle and delicate and, generally speaking, there is not any universal rule leading to the classical dynamics from the quantum one. In particular, taking $\hbar \rightarrow 0$ may be treated as a classical limit, only in a restricted number of cases. In general, each of the possibly considered situations requires special approach. Very often, it means taking large quantum numbers. If, in turn, a particle can be represented by a sharply peaked wave packet, the classical limit is reached by the evolution of averages for the position and momentum according to Ehrenfest's Newton-like equations. Interesting relations are also given by the well-known virial theorem.

All the ways of approaching the classical limit can be summarized in what we have known as Bohr's *correspondence principle*, introduced in the early days of quantum mechanics. It is based on the belief that if quantum mechanics is correct then it must agree with classical mechanics in the appropriate limit [1]. Examples of when it is not possible at all are provided by classically chaotic systems [2]. Detailed discussion [3] of the Arnol'd macroscopic quantum interference state clearly shows the failure of the correspondence principle in such cases. The recent study [4] proves the breakdown of the principle even for large quantum numbers of all long-range potentials of $-C_n/r^n$ with n > 2.

The most important reason for the weakness of the Bohr's principle is the power of the Heisenberg uncertainty relation for position and momentum, which precludes the notion of classical orbits in quantum mechanics. There is, however, a possibility of approaching the classical limit in terms of deterministic trajectories if the so-called generalized Hamilton-Jacobi equation is used. It is easily found if the wave function in polar form

$$\psi(\mathbf{r},t) = R(\mathbf{r},t) \exp[(i/\hbar)\widetilde{S}(\mathbf{r},t)], \tag{1.1}$$

with real functions R and \widetilde{S} , is substituted into the time-

dependent Schrödinger equation and the real and imaginary parts are separated. As a result, we get two equations:

$$\frac{\partial \widetilde{S}}{\partial t} + (1/2m)(\nabla \widetilde{S})^2 + V(r,t) + Q(r,t,\hbar) = 0, \quad (1.2)$$

$$\frac{\partial R^2}{\partial t} + \nabla \cdot (R^2 \nabla \widetilde{S}/m) = 0. \tag{1.3}$$

The first of them is a classical Hamilton-Jacobi equation for the ordinary or outer potential V supplemented by the inner or quantum potential $Q = (-\hbar^2/2m)(\Delta R/R)$. One has to remember taking the limit of $\hbar \to 0$ that R may be a function of Planck constant.

If we introduce a velocity field

$$\boldsymbol{v} = \frac{\boldsymbol{\nabla}\widetilde{S}}{m},\tag{1.4}$$

and take the gradient of Eq. (1.2), the trajectories will evolve according to the Newton's equation under the influence of the force $-\nabla(V+Q)$. The continuity equation (1.3) will then guarantee that if we interpret R^2 as a probability density in a statistical ensemble of the trajectories defined in Eq. (1.4), and if it agrees with the Born probability condition $R^2 = |\psi|^2$ at some initial time, then it will hold for all time.

The idea of using the notion of trajectory in quantum mechanics has been developed by de Broglie and Bohm [5]. It was proved that the description of quantum phenomena with the help of deterministic trajectories (1.4) is consistent with the statistical predictions of ordinary quantum mechanics. A great number of illuminating examples can be found in [6]. Of course, the quantum trajectories have nothing to do with classical trajectories. They would coincide only if the quantum contribution Q to the classical Hamilton-Jacobi equation (1.2) vanished. It is not, however, by taking the limit of $\hbar \rightarrow 0$ but demanding $\Delta R = 0$. Only in this case the classical limit of quantum mechanics is reached exactly.

We thus have the set of three coupled partial differential equations [Eqs. (1.2) and (1.3), and $\Delta R = 0$] for three unknown functions R, \widetilde{S} , and V. In this way, one can look for special potentials V and the states ψ of (1.1) with the property that the quantum trajectories are identical to the classical ones. It was Rosen who first raised this problem and found few potentials with the above property [7]. In the ensuing

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years, more examples of this kind have been derived [6,8–11] and some general formulas covering known cases and suggesting new ones were also found [12,13].

In this paper, we shall attempt to obtain an important subclass of such potentials, possibly all central potentials and states in them, leading to the identical classical and quantum motions. This will be the subject of Sec. II. Then, in Sec. III, we discuss general properties of the special potentials and related states, among them, the shapes of trajectories. Discussion of results and some physical applications of the derived potentials are given in Sec. IV.

II. CENTRAL POTENTIALS

The set of the partial differential equations mentioned above can be solved exactly only in some cases. If we restrict ourself to the potentials independent of time, then we may assume in Eqs. (1.2) and (1.3) that $\partial R/\partial t = 0$ and $\widetilde{S}(\mathbf{r},t) = -Et + S(\mathbf{r})$. This simplifies the set to the form

$$V = E - (1/2m)(\nabla S)^2,$$
 (2.1)

$$\nabla \cdot (R^2 \nabla S) = 2R \nabla R \cdot \nabla S + R^2 \Delta S = 0, \qquad (2.2)$$

$$\Delta R = 0, \tag{2.3}$$

where the functions R and S have to be real functions of their arguments.

Solutions of the Laplace equation (2.3), which guarantee that the quantum potential Q is exactly zero, are to be inserted to the continuity equation (2.2), which, in turn, guarantees conservation of probability flow. Finally, the solutions for S can be used to derive potentials V from Eq. (2.1).

A. Two-dimensional (2D) potentials

Let us use $x = \rho \cos \varphi$, $y = \rho \sin \varphi$ with $\rho = ix + jy$, and observe that for the 2D central potentials to appear, the quantity $(\nabla S)^2$ in Eq. (2.1) has to be a function of ρ only, say $f(\rho)$. Instead of Eqs. (2.1)–(2.3), we thus now have

$$(\nabla S)^2 = \left(\frac{\partial S}{\partial \rho}\right)^2 + \frac{1}{\rho^2} \left(\frac{\partial S}{\partial \varphi}\right)^2 \equiv f(\rho), \tag{2.4}$$

$$2\frac{\partial S}{\partial \rho}\frac{\partial R}{\partial \rho} + 2\frac{1}{\rho^2}\frac{\partial S}{\partial \varphi}\frac{\partial R}{\partial \varphi} + R(\rho,\varphi)\left(\frac{\partial^2 S}{\partial \rho^2} + \frac{1}{\rho}\frac{\partial S}{\partial \rho} + \frac{1}{\rho^2}\frac{\partial^2 S}{\partial \varphi^2}\right)$$

$$= 0, \tag{2.5}$$

$$\frac{\partial^2 R}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial R}{\partial \rho} + \frac{1}{\rho^2} \frac{\partial^2 R}{\partial \phi^2} = 0. \tag{2.6}$$

The elliptic type Laplace's equation (2.3) or (2.6) separates in eleven different orthogonal coordinates [14] and the general solution of Eq. (2.6) can be written as

$$R(\rho,\varphi) = (a\varphi + b)(c \ln \rho + d) + \sum_{k} (a_k \rho^k + b_k \rho^{-k})$$
$$\times (A_k \cos k \varphi + B_k \sin k \varphi). \tag{2.7}$$

The first term corresponds to k=0 and the sum is over $k=\pm 1,\pm 2,\ldots,\pm \infty$. There can be, also, solutions of Eq. (2.6), which do not have the form of the product of functions of ρ and of φ . We have found an example of such solution that reads

$$R(\rho, \varphi) = \alpha \ln \rho - \beta (\ln \rho)^2 + \beta \varphi^2 + \gamma \varphi + \delta. \tag{2.8}$$

All letters not explained herein (e.g., a,b,c,d) are to be understood as real constants since R and S were determined as real functions. We should emphasize at this point that amplitudes R of the states ψ in Eq. (1.1), for the potentials we are looking for, have to belong to the class of functions in Eq. (2.7) or, in case of need, to those presented in Eq. (2.8).

Now, we have to find functions S obeying Eqs. (2.5) or (2.2). Since we are interested only in those that satisfy additionally Eq. (2.4), this allows us to look for special forms of S instead of trying to find a general solution. To this end, we have tried S as a function of ρ only, of φ only, and finally, all possible functions dependent of both ρ and φ and satisfying Eqs. (2.4) and (2.5).

For example, when $S = S(\rho)$, Eq. (2.4) is obviously obeyed, and Eq. (2.5) reduces to the form

$$\frac{\partial^2 S}{\partial \rho^2} + \frac{\partial S}{\partial \rho} \left(\frac{1}{\rho} + \frac{2}{R} \frac{\partial R}{\partial \rho} \right) = 0. \tag{2.9}$$

It can be solved with the result

$$S(\rho) = C_1 \int (\rho R^2)^{-1} d\rho + C_2.$$
 (2.10)

The phase S is a function of ρ only if it is also the case for R. It follows from Eqs. (2.7) and (2.8) that this will happen if $R(\rho) = C \ln \rho + d$. Then, from Eq. (2.10), we have $S(\rho) = -C_1/CR(\rho)$. Finally, from Eq. (2.1), we have the first example of the searched potentials, i.e.,

$$V(\rho) = E - \frac{C_1^2}{2m} \frac{1}{\rho^2 (C \ln \rho + d)^4},$$
 (2.11)

and the amplitude R and the phase S of the function ψ in Eq. (1.1).

Further derivations are tedious and more involved and that is why we present just the final results. Table I gives all 2D central potentials and wave functions we were able to find

B. Three dimensional potentials

It is natural now to use the spherical coordinates: $x = r \sin \theta \cos \varphi$, $y = r \sin \theta \sin \varphi$, $z = r \cos \theta$ with r = ix + jy + kz. An exact solution of the 3D Laplace equation (2.3) has known form of the product of functions, each dependent on only one variable

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Potential	R(ho, arphi)	S(ho, arphi)
$\overline{V_1(\rho) = E - (C_1^2/2m)(1/\rho^2 R_1^4)}$	$R_1 = C \ln \rho + d, C \neq 0$	$S_1 = -C_1/CR_1, C \neq 0$
$ \frac{V_2^{(A)}(\rho) = E - (C_2^2/2m)(1/\rho^2)}{V_2^{(B)}(\rho) = E - (C^2/m)(1/\rho^2)} $	$R_2^{(A)} = R_1$ $R_2^{(B)} = R_1 + C\varphi$	$S_2^{(A)} = C_2 \varphi$ $S_2^{(B)} = R_1 - C \varphi$
$\overline{V_3(\rho) = E - (1/2m)(C_1^2/\rho^2 R_1^4 + C_2^2/\rho^2)}$	$R_3 = R_1, C \neq 0$	$S_3 = C_2 \varphi - C_1 / CR_1, C \neq 0$
$ \frac{V_4^{(k)}(\rho) = E - (\alpha_k^2/2m)\rho^{2k}}{\alpha_k^2 = (k+1)^2(A_k^2 + B_k^2)} \\ k = 1,2,3, \dots $	$R_4^{(k)} = \rho^{k+1} [A_k \sin(k+1)\varphi$ $-B_k \cos(k+1)\varphi]$ $k = 1, 2, 3, \dots$ $R_4 = \text{const}$	$S_4^{(k)} = \rho^{k+1} [A_k \cos(k+1)\varphi + B_k \sin(k+1)\varphi]$ $k = 1, 2, 3, \dots$ $S_4^{(k)}$
$V_5^{(k)}(\rho) = E - (\beta_k^2/2m)\rho^{-2k}$ $\beta_k^2 = (k-1)^2(a_k^2 + b_k^2)$ $k = 2,3,4,$	$R_5^{(k)} = \rho^{-k+1} [a_k \sin(k-1)\varphi$ $-b_k \cos(k-1)\varphi]$ $k = 2,3,4, \dots$ $R_5 = \text{const}$	$S_5^{(k)} = \rho^{-k+1} [a_k \cos(k-1)\varphi + b_k \sin(k-1)\varphi]$ $k = 2,3,4, \dots$ $S_5^{(k)}$

TABLE I. The 2D central potentials and related wave functions. The functions R and S are, respectively, the amplitude and the phase of the function defined in Eq. (1.1), where for E=0, we have $\tilde{S}=S$.

$$R_{kl}(r,\theta,\varphi) = [e_1 \cos(l\varphi) + e_2 \sin(l\varphi)]$$

$$\times (e_3 r^k + e_4 r^{-k-1}) P_k^l(\cos\theta), \quad (2.12)$$

where $l \le k$, and $l, k = 0, 1, 2, \ldots$, the symbol P_k^l stands for the associated Legendre polynomials, and e_j (j = 1, 2, 3, 4) are real constants. The general solution is obtained, as summations over k and l are performed.

This case is much more restrictive than the 2D one. To get a central potential, $(\nabla S)^2$ in Eq. (2.1) has to be a function of r only, say g(r). In spherical coordinates, we obtain

$$(\nabla S)^2 = \left(\frac{\partial S}{\partial r}\right)^2 + \frac{1}{r^2} \left(\frac{\partial S}{\partial \theta}\right)^2 + \frac{1}{r^2 \sin^2 \theta} \left(\frac{\partial S}{\partial \varphi}\right)^2 \equiv g(r). \tag{2.13}$$

The form of $(\nabla S)^2$ strongly restricts admissible solutions of Eq. (2.2) for S with R given in Eq. (2.12). A systematic review of various possible dependences of the functions R and S on r, θ , and φ we have performed, shows that the case of R = const and $S = \alpha/r$ (α is a real constant) is likely the only one leading to a central potential in the 3D case. We will get now [7]

$$V_6(r) = E - \frac{a^2}{2m}r^{-4}. (2.14)$$

III. PROPERTIES

There are two integrals of the motion for conservative systems in central potentials: the total energy E and angular momentum E. This is the case in our study too. One can solve the stationary Schrödinger equation for the potentials we have found and obtain all possible states corresponding to these attractive potentials with E=0. There is, among them, a very restricted number of specific states for which the quantum contribution E0 to the classical Hamilton-Jacobi equation (1.2) is exactly zero. Thus, we can derive trajecto-

ries identical in both classical and quantum cases.

A. Trajectories

From the integral of energy $(m/2)(\dot{\rho}^2 + \rho^2 \dot{\varphi}^2) + V(\rho) = E$, we can find the motion $\rho = \rho(\varphi)$, and from the angular momentum $L \equiv L_z = m\rho^2 \dot{\varphi} = \text{const}$, its time dependence. The case of L=0 leads to $\varphi = \text{const}$ and thus to lines starting from the scattering center where $\rho = 0$. The motion can be found equivalently also from the guidance relation (1.4), which now reads $\dot{\rho} = (1/m)\nabla S$ with S given in the third column of Table I for the 2D potentials.

The latter method, gives at once for $V_1(\rho)$, a family of straight lines y=Ax, converging to the center of coordinates $\rho=\sqrt{x^2+y^2}=0$. For $V_2(\rho)$, in turn, it is convenient to integrate the equation for energy E. The result is $\rho_2(\varphi)=\rho_0\exp[-(1/L)\sqrt{C_2^2-L^2}\varphi]$, with $C_2^2\!\!>\!\!L^2$. If $C_2^2\!\!=\!\!L^2$, we have a closed orbit $\rho_2^{(A)}\!=\!\rho_0$ which is a circle of radius ρ_0 . This corresponds to the phase $S_2^{(A)}$ in Table I. Moreover, if $C_2^2\!=\!2L^2\!=\!2C^2$, then a particle is falling down to the center along a logarithmic spiral given above. This case corresponds to the phase $S_2^{(B)}$ in Table I.

The next potential, $V_3(\rho)$, combines two previous ones, and in this case, the fastest way of deriving the corresponding trajectory is using the guidance equation in polar coordinates. We thus have $C_2(C\ln\rho+d)^3=3CC_1\varphi$, where again $C_2=L$, and for the vanishing C_1 or C_2 , we will get the already discussed orbits. Otherwise, we have a spiral $\rho_3(\varphi)=\rho_0\exp(q\varphi^{1/3})$ with q being a real constant different from zero.

For two families of potentials, i.e., $V_4^{(k)}(\rho)$ and $V_5^{(k)}(\rho)$, the motions can be found, e.g., by integrating the equation for energy E. The results are given by

$$\rho_4^{(k)}(\varphi) = \left\{ \frac{L}{\alpha_k \cos[(k+1)(\varphi - \varphi_0)]} \right\}^{1/(k+1)},$$

$$k = 1, 2, 3, \dots, \tag{3.1}$$

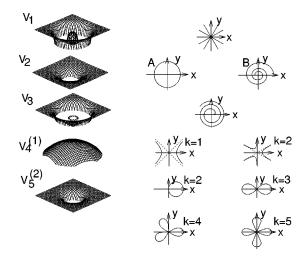


FIG. 1. An illustration of the content of Table I. The sketches represent 2D central potentials in the vicinity of the beginning of coordinates and trajectories corresponding in each case to the states where the quantum correction Q [Eq. (1.2)] to the Hamilton-Jacobi equation is exactly zero. The free constants are positively determined and their numerical values are chosen for convenience. Except for $V_4^{(k)}$, all the remaining potentials are singular for $\rho = 0$. Two of them, V_1 and V_3 , have another singularity for $\rho = \exp[-d/C]$. Contrary to the case of V_3 , the former singularity is not visible in the plot of V_1 . The highest values of this potential are obtained for $\rho = \exp[-(2+d/C)]$, which in the plot is very close to the value of $\rho = 0$.

$$\rho_5^{(k)}(\varphi) = \left\{ \frac{\beta_k}{L} \cos[(k-1)(\varphi - \varphi_0)] \right\}^{1/(k-1)},$$

$$k = 2, 3, 4, \dots$$
(3.2)

In the case of $\rho_4^{(k)}(\varphi)$ we derive from Eq. (3.1) a hyperbola (k=1), and for $k \ge 2$, figures composed of k+1 open arcs. For the last family of potentials, $V_5^{(k)}(\rho)$, all trajectories are represented by closed curves. Correspondingly, we will get from Eq. (3.2) the circle (k=2), the Bernoulli lemniscate (k=3), and (k-1)-leaved roses for $k \ge 4$.

What we have said above is summarized in Fig. 1, where plots of the 2D central potentials are given together with classical orbits related to the states listed in Table I. No plot is given for $V_6(r)$. In this case, the trajectories are straight lines crossing the beginning of coordinates.

B. Wave functions

The states generating trajectories in Fig. 1 do not have extrema. Their existence is precluded by the structure of Laplace equation, that the amplitudes R of our wave functions must obey. Further, if we accept the definition that bound states are represented by those solutions of the Schrödinger equation for which the usual normalization integral is finite, then obviously our states do not belong to this class. Rather they represent special stationary states of scattering potentials with closed orbits for some of them.

To see how exceptional the states are, we shall consider an example in more detail. Let us choose the potential $V_4^{(1)}(\rho) = E - (\alpha_1^2/2m)\rho^2 \equiv V_0 - (1/2)m\gamma^2\rho^2$ and write its

special state in the Cartesian coordinates x and y. From Table I, we have

$$\psi(x,y) = [2A_1xy - B_1(x^2 - y^2)] \exp\{(i/\hbar)[A_1(x^2 - y^2) + 2B_1xy]\}.$$
(3.3)

This potential has been a subject of many intensive studies (see the next section) and its wave functions and eigenvalues are well known [15]. The solutions can be separated into two groups: those belonging to complex-energy eigenvalues and being also the eigenstates of orbital angular momentum

$$E_1 = V_0 \mp i(n_x + n_y + 1)\hbar \gamma,$$
 (3.4)

$$U_1 = C_1 \exp[\pm (i/2)\beta^2(x^2 + y^2)] H_{n_x}^{\pm}(\beta x) H_{n_y}^{\pm}(\beta y),$$
(3.5)

and infinitely degenerate states with some of them having the real-energy eigenvalue V_0 ,

$$E_2 = V_0 \mp i(n_x - n_y) \hbar \gamma, \tag{3.6}$$

$$U_2 = C_2 \exp[\pm (i/2)\beta^2(x^2 - y^2)]H_{n_x}^{\pm}(\beta x)H_{n_y}^{\mp}(\beta y).$$
(3.7)

In the formulas: $\beta = \sqrt{m\gamma/\hbar}$, the signs +/- correspond to the outward/inward moving particles, the functions U are generalized functions in a Schwartz space of the Gel'fand triplet $\mathcal{S}(\mathbb{R}^2) \subset \mathcal{L}^2(\mathbb{R}^2) \subset \mathcal{S}(\mathbb{R}^2)^x$ [15], and the polynomials H_n^{\pm} can be found from the relation [16]

$$H_n^{\pm}(\xi) = (\mp i)^n \exp(\mp i \xi^2) \frac{d^n}{d\xi^n} \exp(\pm i \xi^2).$$
 (3.8)

The first few polynomials are: $H_0^{\pm}(\xi) = 1$, $H_1^{\pm}(\xi) = 2\xi$, $H_2^{\pm}(\xi) = 4\xi^2 \mp 2i$, $H_3^{\pm}(\xi) = 8\xi^3 \mp 12i\xi$, and $H_n^{\pm}(\xi)^* = H_n^{\mp}(\xi)$.

We can now try to detect the state (3.3) from among the states U_1 and U_2 . Since in our case $E=V_0$, this can only take place when $n_x=n_y=n$ in Eqs. (3.6) and (3.7). Now, for n=1 we have $U_2(n=1)=\psi_{B_1=0}(x,y)$ if $A_1=\pm\hbar\beta^2/2$ and $C_2=A_1/2\beta^2$. It follows from Eq. (3.3) that we have found additional solutions for the potential under consideration, i.e., $\psi_{A_1=0}(x,y)$ and, of course, the full solution $\psi(x,y)$, both not derivable by the method of separation of variables used in Ref. [15]. For any real values of A_1 and B_1 , the function $\psi(x,y)$ does not produce any quantum correction Q in Eq. (1.2).

The phase $S_4^{(1)}$ of the solution $\psi(x,y)$ [Eq. (3.3)] gives a stationary flow that moves along the hyperbola as shown in Fig. 1. A similar type of motion (now y = C/x) is also obtained when in Eq. (3.7) we set $n_x = n_y = n = 0$. This case corresponds to $R_4 = \text{const}$ and $S = S_4^{(1)}$ with $B_1 = 0$ in Table I. Of course, we will get again Q = 0 in Eq. (1.2). When $B_1 \neq 0$ we also have another solution not found in Ref. [15] for which Q = 0.

Authors of the work [15] observed...that the velocities... in both cases (n=0,1)...do not contain any order of

 \hbar at all. They concluded that...this fact indicates that these flows will have a kind of classical property. Our paper clearly shows what this sentence really means. We have also shown that the above property can also be observed for some states not being in the form of a product of single-variable functions of x and of y only.

IV. DISCUSSION

We have presented a search for central potentials, with the property that some of their states generate quantum trajectories identical to the classical ones. Found examples are listed in Table I. It is, of course, an open question, whether we have discovered all of them. The set of the partial differential equations (2.1)-(2.3) is too intricate to be solved exactly and to get a decisive answer in this way. We have also found the wave functions and the corresponding trajectories for each of the potentials. It is interesting that in the limit of continuous spectrum (E=0) some orbits can be closed curves.

The potential $V_4^{(1)}(\rho)$, chosen for more detailed discussion in Sec. III B, has been studied in the 1D version for a long time, as the simplest model of an unstable system in quantum mechanics [16–21]. It was recently used to the description of unstable states of some chemical reactions [22].

A number of 2D potentials is also used in the description of low-dimensional quantum dots. Few examples are discussed in Sec. 4.2 of Ref. [23]. The 3D potential in Eq. (2.14), sometimes called the Maxwell potential, is widely utilized in the collision theory (see, e.g. Ref. [24]).

The threshold value of E=0, which separates the boundstate spectrum from the continuum, is singled out to effect our work's purpose. Behavior of quantum systems near the threshold was recently the subject of a quite strong activity. This is motivated by advances in cold-atom collisions [25] as well as by the need for a deeper understanding of the semiclassical limit of some repulsive and attractive central potentials [26].

As a final conclusion, we can state that in most cases, quantum systems do not obey the correspondence principle and it is argued [2,3] that quantum mechanics is, therefore, incomplete. There can exist, however, some states of the known central potentials for which the correspondence principle is obeyed exactly.

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