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Scaling relations for the hydrogen atom in a harmonic field: classical chaos and quantum suppression of diffusion

B. Kaulakys [1], V. Gontis
Institute of Theoretical Physics and Astronomy, Lithuanian Academy of Sciences, 232600 Vilnius, Lithuania

G. Hermann and A. Scharmann
I. Physikalisches Institut der Universität Giessen, Heinrich-Buff-Ring 16, W-6300 Giessen, Germany

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Scale transformations for the classical and quantum dynamics of the hydrogen atom in a harmonic field are introduced which reduce the number of parameters, simplify the analysis of the chaotic dynamics and reveal the functional dependences of the classical and quantum processes.

1. Introduction

A highly excited hydrogen atom in a harmonic field is one of the simplest real non-linear systems with stochastic behaviour. That is why great attention is devoted at present to the experimental and theoretical investigation of the dynamics of the electron of the Rydberg atom in the strong microwave field (for a review see refs. [1,2], and references therein). In particular, experimental studies of the microwave ionization of highly excited hydrogen atoms with principal quantum numbers ranging to $n_0=90$ have been performed [3]. One might expect for such quantum numbers the classical theory to be a good approximation for the dynamics of the system. However, quantum analysis [1] has suggested that for the high relative frequency $s_0=\omega n_0^3 \gtrsim 1$ of the microwave field (with ω being the microwave frequency in atomic units) the classical chaotic diffusion is suppressed by a quantum interference effect. This raises the question of the necessary and sufficient conditions for the applicability of the correspondence principle for chaotic systems [2], no longer discussing the problem of "quantum chaos" in general. On the other hand, the modelling by maps of the classical dynamics of a hydrogen atom in a harmonic field is the object of current studies [4–6].

The aim of the present note is to introduce the exact scaling for the description of the hydrogen atom in a harmonic field and to investigate the dependences of the classical and quantum dynamics of the system on the scaled parameters of the problem.

2. Hamiltonian

The Hamiltonian of the hydrogen atom in a linearly polarized microwave field of frequency ω and field strength F in atomic units has the form

$$H=\frac{p^2}{2}-\frac{1}{r}+\frac{M^2}{2r^2}+zF\cos\omega\tilde{t}, \qquad (1)$$

where $\boldsymbol{r}$, $\boldsymbol{p}$ and $\boldsymbol{M}$ are the position, momentum and angular momentum of the electron, respectively.

For the investigation of the ionization process of the hydrogen atom with the initial principal quantum number n_0 one commonly introduces the so-called "scaled field strength and frequency" [1–3,7,8],

[1] Alexander von Humboldt Research Fellow 1990/91 at I. Physikalisches Institut der Universität Giessen.

$$F_0 = n_0^4 F\,, \quad \omega_0 = n_0^3 \omega\,. \tag{2}$$

However, these quantities are rather relative than scaled. The classical dynamics of the one-dimensional hydrogen atom in a harmonic field, as was first shown in ref. [4], for the definite scaled energy $E_s = E/\omega^{2/3}$ depends on a single combination of parameters, i.e. the scaled field strength $F_s = F/\omega^{4/3} = 4F_0 E_{s0}^2$ (see also ref. [5]). Introducing the scale transformation

$$t = \omega\tilde{t}\,, \quad r_s = \omega^{2/3} r\,, \quad p_s = p/\omega^{1/3}\,,$$
$$M_s = \omega^{1/3} M\,, \quad F_s = F/\omega^{4/3}\,, \tag{3}$$

we have from (1)

$$H = \omega^{2/3} H_s\,,$$
$$H_s = \frac{p_s^2}{2} - \frac{1}{r_s} + \frac{M_s^2}{2r_s^2} + z_s F_s \cos t\,. \tag{4}$$

Expressions (3) and (4) show that the classical motion of the electron in the three-dimensional atom with the definite scaled energy E_s and angular momentum M_s depends only on the scaled field strength F_s.

The scaled time-dependent Schrödinger equation can be expressed as

$$\mathrm{i}\omega^{1/3} \frac{\partial \psi}{\partial t} = (H_s^0 + V_s)\psi\,, \tag{5}$$

$$H_s^0 = \frac{\omega^{2/3}}{2}\left[-\frac{1}{r_s^2}\frac{\partial}{\partial r_s}\left(r_s^2 \frac{\partial}{\partial r_s}\right) + \frac{l(l+1)}{r_s^2}\right] - \frac{1}{r_s}\,,$$
$$V_s = z_s F_s \cos t\,. \tag{6}$$

The scaled energy spectrum of the unperturbed scaled hydrogen atom is

$$E_s = -\frac{1}{2\omega^{2/3} n^2} = -\frac{1}{2s^{2/3}}\,, \tag{7}$$

where $s = \omega/(-2E)^{3/2}$ is the ratio of the microwave frequency ω to the Kepler orbital frequency $\Omega = (-2E)^{3/2}$.

We see that the motion of the quantum hydrogen atom in a harmonic field is governed in addition to the scaled field strength by the scaled Planck constant $\hbar_s = \omega^{1/3}$. The increase of the scaled Planck constant with increase of the frequency ω indicates the rise of the quantum properties of the system in the high frequency region.

3. Scaled dynamics

The comparison of the theory with the experimental measurements of microwave ionization shows that a simplified one-dimensional model, in which the electron moves along a straight line in the direction of the field, provides a correct description of the excitation of the real three-dimensional hydrogen atom [1–4]. Therefore, we mainly restrict our subsequent consideration to this model. The scaled Hamiltonian of this model is

$$H_s = \tfrac{1}{2} p_s^2 - 1/x_s + x_s F_s \cos t\,, \quad x_s \geq 0\,. \tag{8}$$

The classical dynamics of the model (8) may be described by a map rather than by the Hamilton equations (see refs. [1,2,4–6]),

$$\bar{E}_s = E_s + \Delta E_s(\bar{E}_s, \vartheta)\,, \tag{9}$$
$$\bar{\vartheta} = \vartheta + 2\pi s + \Delta\vartheta(\bar{E}_s, \vartheta)\,. \tag{9}$$

The energy change ΔE_s of the electron during the period of intrinsic motion depends on the initial coordinate of the electron [4,6]. For motion between two subsequent passages at the aphelion

$$\Delta E_s^{\mathrm{a}} = 2\pi F_s s^{2/3} J_s'(s) \sin\vartheta\,,$$
$$s = (-2\bar{E}_s)^{-3/2}\,, \tag{10}$$

while at the perihelion

$$\Delta E_s^{\mathrm{p}} = 2\pi F_s s^{2/3} J_{-s}'(s) \sin(\pi s + \vartheta)\,, \tag{11}$$

where $J_s'(z)$ is the derivative of the Anger function [4,6]. The phase change $\Delta\vartheta$ can be obtained from the requirement for the area-preserving map (9) [4].

The map at the aphelion, (9), (10), mostly represented for the number of absorbed photons $N = E/\omega$ and called the "Kepler map", is widely used for the analysis of chaotic processes for relatively high frequencies $s \gtrsim 1$ [1,2,4] while the map at the perihelion, (9), (11), stronger reveals the resonance structure of the chaotic dynamics at low frequencies $s \lesssim 1$ [4]. In general, the dynamics of the model (8) is governed by the superposition of both maps and may be described more accurately by the improved mapping equations for the energy changes during the

halves of the intrinsic period [6] (see also ref. [5] for a discussion of the canonical Kepler map).

One can add that the transition to chaos in the low frequency region may be investigated on the basis of the adiabatic map for the phase [4]. The scaled expression of this map has the form

$$\bar{\vartheta}=\vartheta+2\pi s+q\cos\vartheta\,,\quad q=15\pi s^{7/3}F_s\,,$$
$$0.3\lesssim s\lesssim 0.7\,, \tag{12}$$

which is the map of the circle onto itself.

Expressions (9)–(12) show that the classical motion of the one-dimensional hydrogen atom in a harmonic field in fact depends on a single parameter – the scaled field strength F_s. The transition between a regular and stochastic motion may be characterized by a scaled threshold field strength as a function of a scaled energy or scaled frequency: $F_s^c=f(s)$. Note that F_0 according to (2) is related to F_s by virtue of $F_0=s_0^{4/3}F_s$. Thus, in the high scaled frequency limit the threshold field strengths for the onset of classical chaos can be estimated from the map (9), (10) [4],

$$F_s^c\simeq\frac{1}{12\pi^2 s^{7/3}J_s'(s)}\simeq\frac{1}{12\pi^2 b s^{5/3}}\,,\quad F_0^c\simeq\frac{1}{49 s_0^{1/3}}\,,$$
$$J_s'(s)\simeq\frac{b}{s^{2/3}}\,,\quad b\simeq 0.411\,,\quad s\gg 1\,. \tag{13}$$

For low scaled frequency $s\lesssim 1$ the detailed resonance structure of the chaotic dynamics follows from the numerical analysis of the maps (9)–(12) and the improved mapping equations [6].

Considerably more complicated is the quantum dynamics of the model (8) which, besides the scaled field strength F_s, depends on the scaled Planck constant $\hbar_s=\omega^{1/3}$. Moreover, the quantum localization phenomenon that limits the diffusive process is essential and may determine the ionization probability [1].

The energy spectrum of the unperturbed one-dimensional hydrogen atom is given also by expression (7). The transition $n\to n'$ frequency is found to be $\Delta E_s/\hbar_s=\Delta n/s$ and the equations of motion are then

$$\frac{\mathrm{d}a_{n'}}{\mathrm{d}t}=-\mathrm{i}F_q\cos t\times\sum_n\langle n'|x_s|n\rangle\exp[\mathrm{i}(\Delta n/s)t]a_n\,, \tag{14}$$

where the wavefunction is given in terms of the unperturbed states $|n\rangle$ of system (8) by

$$\psi(t)=\sum_n|n\rangle\exp(-\mathrm{i}E_s t/\omega^{1/3})a_n(t) \tag{15}$$

and the quantum scaled field strength $F_q=F_s/\omega^{1/3}=F/\omega^{5/3}$ was introduced. Since the matrix element $\langle n'|x_s|n\rangle$ for $|\Delta n|\ll n, n'$ in accordance with refs. [4,6] depends only on s and Δn for $|\Delta n|\gtrsim 1$ can be written as

$$\langle n'|x_s|n\rangle=-\frac{s^{2/3}}{\Delta n}J'_{\Delta n}(\Delta n)\simeq-\frac{bs^{2/3}}{|\Delta n|^{5/3}}\,, \tag{16}$$

eq. (14) shows that the transition probabilities with definite Δn and s depend only on the quantum scaled field strength F_q.

It has been shown in ref. [4] that the one-photon transitions in the strongly perturbed spectrum of the atom result in the diffusion coefficient of the electron in energy space being identical to the diffusion coefficient due to the stochastic classical motion. Later analysis revealed the importance and convenience of the photonic basis for the quantum dynamics of the model (8) [1,2,7–9]. The corresponding equations for the transition amplitudes between the photonic states may be approximated by

$$\frac{\mathrm{d}b_{N'}}{\mathrm{d}t}=\mathrm{i}\sum_N\frac{F_q\cos t}{s^{1/3}\Delta N}J'_{s\Delta N}(s\Delta N)\exp(\mathrm{i}\Delta N t)b_N\,. \tag{17}$$

The transition probabilities $P_{N,N'}$ between the photonic states during the period of intrinsic motion for high frequencies $s\gtrsim 1$ may be evaluated by means of Presnyakov and Urnov's model [10],

$$P_{N,N'}=J^2_{N'-N}(K)\,,\quad K=2\pi F_q s^{2/3}J_s'(s)\,. \tag{18}$$

Using the expression $\sum_n n^2J_n^2(K)=\frac{1}{2}K^2$ we may formally evaluate the local diffusion coefficient of the electron in the scaled energy space,

$$B(E_s)\equiv\frac{1}{2T_s}\sum_{N'}(E_s'-E_s)^2P_{N,N'}=\tfrac{1}{2}\pi F_s^2 s^{1/3}J_s'^2(s)\,, \tag{19}$$

where $T_s = 2\pi s$ is the scaled period of the electron intrinsic motion and the approximation of uncorrelated transitions was used. Therefore, the local quantum diffusion coefficient depends only on the scaled field strength and scaled frequency and agrees with the classical diffusion coefficient [4].

However, in order to be a quantal transition process similar to the classical one it has to include at least a few quantum states. In our case this corresponds to the condition $K \gtrsim 1$, i.e.

$$F_q^a \gtrsim (2\pi b)^{-1} \simeq 0.4 ,$$
$$F_0^a \gtrsim 0.4 s_0^{5/3}/n_0 , \quad s \gtrsim 1 . \tag{20}$$

On the other hand, condition (20) coincides with the requirement for the classical energy change (10) to be larger than the photon energy, $\Delta E_s^a > \omega^{1/3}$ (see also ref. [7] for comparison of the classical and quantum dynamics of system (8)).

For high scaled frequencies $s \gg 1$, $K = 2\pi b F_q$ in (18) is a constant and the transition probabilities (18) coincide with the probabilities for the kicked rotator model [11]. The same result (18) may also be obtained from the quasiclassical approximation for the map (9), (10) based on the appropriate kicked model Hamiltonian [12]. In addition, the structure (18) for transition probabilities is common for all kicked models and for the non-linear Hamiltonians $H^0(N)$ results in the quantum localization of classical chaos with localization length $l_N \equiv \Delta N = \frac{1}{2}K^2$ [1,11-13]. Thus, for the diffusive achievement of a given distance l_N the quantum scaled field strength

$$F_q^{l_N} = \sqrt{2 l_N}/2\pi b , \quad s \gg 1 , \tag{21}$$

is needed. A comparison of the localization length with the ionization bound distance $N_i = E/\omega = E_s/\omega^{1/3}$ yields the following critical value of the field strength for quantal diffusive ionization,

$$F_q^i = 1/2\pi b n \omega^{1/2} , \quad F_0^i = s_0^{7/6}/(6.6 n_0)^{1/2} , \tag{22}$$

which is the well known result of Casati et al. [13].

Thus, our scaled analysis enables one to clarify "the not clear relation between the two conditions" (20) and (22) [14]. Of course, the detailed investigation of the quantum chaos needs numerical analysis, but the scale transformations (3)-(7) reduce the space of parameters and reveal the functional dependences.

4. Conclusions

Introduction of the scale transformation for the description of the hydrogen atom in a harmonic field enables one to maximally simplify the analysis of the dynamical processes and to reduce the number of parameters of the problem. The classical motion depends only on the scaled field strength $F_s = F/\omega^{4/3}$ while the quantum dynamics depends in addition on the scaled Planck constant $\hbar_s = \omega^{1/3}$. However, the transition amplitudes between the states of the unperturbed hydrogen atom as well as between the "photonic states" depend also only on one parameter - the quantum scaled field strength $F_q = F/\omega^{5/3}$. Note that $F_0 = F_q s_0^{4/3} \omega^{1/3}$ and, therefore, the relative (see (2)) quenching field strength F_0^{quen} depends not only on the relative frequency s_0 but also on the absolute field frequency ω. This is in agreement with the experimental results [3].

The quantal diffusive ionization is a result of the kinetical delocalization of the quantum localization of chaotic diffusion and depends on both scaled parameters. The application of the scaling for the stabilization of atoms in the problem of superintense laser fields (see e.g. ref. [15]) is also relevant and, in our opinion, useful.

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