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Stochastic dynamics of hydrogenic atoms in the microwave field: modelling by maps and quantum description

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Abstract. The motion of an electron of a classical hydrogenic atom in an oscillating electric field is studied theoretically. An analysis is provided, based on the iterative (mapping) forms of the classical equations of motion in perturbation theory and the adiabatic approximation. This greatly facilitates the numerical investigation of stochasticity and the ionisation process and allows the approximate analytical estimation of the threshold field strengths for the onset of chaos and of the diffusion coefficient of the electron in energy space. The method is asymptotically exact at high field frequencies and gives a good approximation for medium and low frequencies. The adiabatic approximation describes well the approach of the stochastic ionisation threshold field strength to the static field ionisation threshold.

From the quantum mechanical point of view the ionisation is a result of the great number of one-photon transitions in the strongly perturbed spectrum of the atom. This results in the diffusion of the electron in energy space identical to the diffusion due to stochastic classical motion. The estimation of the mean time of diffusive ionisation is also given.

1. Introduction

In the last ten years remarkable progress has been made in the study of non-linear dynamical systems. The theory of simple classical non-linear systems with irregular, apparently random, behaviour, known as chaos, has been developed (see, e.g., Lichtenberg and Lieberman 1983, Zaslavskii 1984). The quantum description of such systems is far from complete (see, e.g., Casati 1985). It should be noted that theoretical analysis of the stochastic behaviour of non-linear dynamical systems is mostly carried out for model systems. A highly excited hydrogen atom in the microwave 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 Delone *et al* 1983, Bayfield 1986, Jensen 1986 and references therein). A long series of experiments on non-linear microwave ionisation and transitions in highly excited hydrogen atoms has been performed by Bayfield and Koch (1974), Bayfield and Pinnaduwage (1985a, b), van Leeuwen *et al* (1985) and Bardsley *et al* (1986) in the low-frequency limit (relative frequency $s_0=\omega/\Omega_0\lesssim 1$, where ω is the microwave frequency and $\Omega_0=Z^2/n_0^3$ is the electron orbital frequency of the atom with principal quantum number n_0 and core charge Z). These observations of excitation and ionisation

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rates, which depend strongly on the intensity of the microwave field, provide evidence for stochastic behaivour of weakly bound electrons. The ionisation of Rydberg atoms exhibits a threshold dependence on the electric field amplitude F_0 and appears as a diffusion-like process. The classical calculations carried out for $s_0 \leqslant 1$ using the Monte Carlo method (Leopold and Percival 1978, Jensen 1984, Leopold and Richards 1985, 1986) are in agreement with experiment (van Leeuwen *et al* 1985, Jensen 1986). For $s_0 \gg 1$ the field strengths required for stochastic ionisation of hydrogen atoms and the diffusion coefficient of an electron in the space of the principal quantum numbers of the hydrogen atom can be estimated analytically from the resonance overlap criterion (Delone *et al* 1983, Jensen 1984). On the other hand, at $s_0 \leqslant 1$ the resonance overlap criterion for the scaled critical field amplitude for stochastic ionisation gives the dependence (Shepelyansky 1982, Delone *et al* 1983) $\Phi_0^c = F_0^c n_0^4 / Z^3 \sim s_0^{1/3}$ which disagrees with numerical calculations and experiments and does not explain the increase and approach of the critical field Φ_0^c to the static field ionisation threshold $\Phi_0^{st} = 0.130$ (Jensen 1984) when $s_0 \to 0$. Thus up to now the theory for stochastic ionisation of highly excited hydrogen atoms is developed for the case $s_0 \geqslant 1$ only, while the experiments and numerical calculations have been performed at $s_0 \leqslant 1$. The quantum description of this process has only just begun (Casati *et al* 1984, 1986a, b, Bardsley *et al* 1986, Bardsley and Comella 1986, Jensen 1986).

The purpose of this paper is to develop the method based on the modern mathematical apparatus for studying classical non-linear dynamical systems (described by maps) (Lichtenberg and Lieberman 1983, Zaslavskii 1984) suitable for the approximate description of regular and stochastic dynamics of a highly excited hydrogenic atom in the microwave field. In addition, the relation of the classical ionisation process to the quantum description of the system will be investigated. On the basis of classical perturbation theory we describe the dynamics of the electron of the Rydberg atom in the microwave field by maps (§ 2). This greatly facilitates the numerical investigation of stochasticity and the ionisation process and enables the analytical estimation of the threshold field strength and diffusion coefficient. For low relative frequency the dynamical behaviour of the electron may be described in the adiabatic approximation (§ 3). Section 4 is devoted to the quantum description of the ionisation process. Note that such modelling has been undertaken in a brief report by Gontis and Kaulakys (1987). We mainly restrict our consideration to the one-dimensional model of the hydrogenic atom. That is why the analysis of the one-dimensioinal atom is much more tractable than for the three-dimensional hydrogenic atom but the one-dimensional atom reproduces well the stochastic ionisation process of the hydrogen atom (van Leeuwen *et al* 1985, Jensen 1986). On the other hand the one-dimensional model describes the surface-state electrons bound to the surface of liquid helium by its image charge (Jensen 1984).

2. Classical perturbation theory

The equations of motion of the one-dimensional hydrogenic atom electron in the oscillating electric field are generated by the Hamiltonian (Jensen 1984)

$$H(x, p, t) = \begin{cases} \frac{1}{2}p^2 - Z/x + V(x, t) & x > 0 \\ \infty & x \leqslant 0. \end{cases} \tag{1}$$

In the dipole approximation

$$V(x, t) = xF(t) \qquad F(t) = F_0 \cos(\omega t + \varphi) \tag{2}$$

where x and p are the coordinate and momentum of the electron and F, F_0, ω and φ are the electric field strength, strength amplitude, angular frequency and phase of the electric field, respectively.

The unperturbed motion of the electron is given by the parametric equations (Landau and Lifshiftz 1975)

$$x = \frac{Z}{-2E}(1-\cos\xi) \qquad t = \frac{Z}{(-2E)^{3/2}}(\xi - \sin\xi) \tag{3}$$

where E is the electron energy, Z is the charge of the core and $\xi(-\infty < \xi < \infty)$ is the parameter. The motion of the electron taking into account the perturbation (2) may be represented by the maps for the energy E and the phase difference θ between the phase of the electric field and phase of the electron's motion (Lichtenberg and Lieberman 1983)

$$\begin{aligned} E_{k+1} &= E_k + \Delta E(E_k, \theta_k) \\ \theta_{k+1} &= \theta_k + \Delta\theta(E_k, \theta_k) \qquad k = 0, 1, 2, \ldots . \end{aligned} \tag{4}$$

It is convenient to choose the period of electron oscillation as a scale of discrete time, i.e. $t_{k+1} - t_k = T_{k+1} \simeq 2\pi Z/(-2E_{k+1})^{3/2}$. Evidently in this case $\Delta\theta \simeq \omega T_{k+1}$ and ΔE may be evaluated from the equation of motion

$$\dot{E} = F\dot{x} \tag{5}$$

according to classical perturbation theory (Lichtenberg and Lieberman 1983). The substitution of equations (2) and (3) into equation (5) and integration over ξ in the interval $-\pi \leqslant \xi \leqslant \pi$ yields

$$\Delta E_{-\pi,\pi} = \frac{\pi Z F_0}{E} J_s'(s) \sin\theta \qquad s = \frac{\omega}{\Omega} = \frac{\omega Z}{(-2E)^{3/2}}. \tag{6}$$

Here $J_s'(z)$ is the derivative of the Anger function

$$J_s'(z) = \frac{1}{\pi}\int_0^{\pi} \sin(sx - z\sin x)\sin x \, dx. \tag{7}$$

The limiting forms of the function $J_s'(s)$ are (Watson 1958, Abramowitz and Stegun 1972)

$$J_s'(s) = \frac{1+\frac{5}{24}s^2}{2\pi(1-s^2)}\sin s\pi \qquad s \leqslant 1 \tag{8}$$

$$J_s'(s) = \frac{b}{s^{2/3}} - \frac{a}{s^{4/3}} - \frac{\sin s\pi}{4\pi s^2} \qquad s \gg 1 \tag{9}$$

where

$$b = \frac{2^{2/3}}{3^{1/3}\Gamma(\frac{1}{3})} \simeq 0.411 \qquad a = \frac{2^{1/3}}{5\times 3^{2/3}\Gamma(\frac{2}{3})} \simeq 0.089. \tag{9'}$$

Accordingly representations (4) in the first approximation are of the following form:

$$\begin{aligned} \varepsilon_{k+1} &= \varepsilon_k + 4\pi\Phi_0\varepsilon_0^2\varepsilon_k^{-1}J_{s_k}'(s_k)\sin\theta_k \\ \theta_{k+1} &= \theta_k + 2\pi/\varepsilon_{k+1}^{3/2}. \end{aligned} \tag{10}$$

Here $\varepsilon = s^{-2/3} = (-2E)/(\omega Z)^{2/3}$, $\Phi_0 = F_0 Z/4E_0^2$, $E_0 = -Z^2/2n_0^2$ with n_0 being the initial principal quantum number of the highly excited atom. Equations (10) represent the iterative form of the classical equations of motion for the electron. At $s \gg 1$ $J_s'(s) = b/s^{2/3}$ and the maps (10) are the area-preserving ones:

$$\frac{\partial(\varepsilon_{k+1}, \theta_{k+1})}{\partial(\varepsilon_k, \theta_k)} = 1. \tag{11}$$

In such a case maps (10) may be transformed to the standard map

$$\begin{aligned} I_{k+1} &= I_k + K \sin \theta_k \\ \theta_{k+1} &= \theta_k + I_{k+1} \end{aligned} \tag{12}$$

by the linearisation procedure, $\varepsilon_k = \varepsilon_0 + \Delta\varepsilon_k$ in the vicinity of the integer $s_0 = \varepsilon_0^{-3/2} = m$ (Lichtenberg and Lieberman 1983). In equations (12) $I_k = -3\pi\Delta\varepsilon_k/\varepsilon_0^{5/2}$ and $K = 12\pi^2 b\Phi_0$. The standard map (12) plays an important role in the consideration of dynamical problems involving instability and the theory of this map has been extensively developed (see Chirikov 1979, Lichtenberg and Lieberman 1983, Zaslavskii 1984, Zheng 1986 and references therein). The criterion of stochasticity for the standard map is $K \geqslant 1$ (Lichtenberg and Lieberman 1983). Accordingly the stochastic ionisation takes place if

$$\Phi_0 = \frac{F_0 n_0^4}{Z^3} \geqslant \Phi_0^c = \frac{1}{12\pi^2 b s_0^{1/3}} \simeq \frac{1}{49}\left(\frac{Z^2}{\omega n_0^3}\right)^{1/3} \qquad s_0 \gg 1 \tag{13}$$

which is identical to the result of Delone *et al* (1983).

At $s \leqslant 1$ the maps (10) are not area-preserving and are not suitable for numerical investigation. However, increasing the accuracy of the iterative expression for the phase θ we can construct the area-preserving maps. The iterative equations on the basis of the classical perturbation theory can be rewritten in the following form (Lichtenberg and Lieberman 1983):

$$\begin{aligned} \varepsilon_{k+1} &= \varepsilon_k + \pi\varepsilon_0^2\Phi_0 f(\varepsilon_{k+1}, \theta_k) \\ \theta_{k+1} &= \theta_k + 2\pi/\varepsilon_{k+1}^{3/2} + \pi\varepsilon_0^2\Phi_0 g(\varepsilon_{k+1}, \theta_k) \end{aligned} \tag{14}$$

where by analogy with equations (10) we obtain

$$f(\varepsilon_{k+1}, \theta_k) = 4\varepsilon_{k+1}^{-1} J'_{s_{k+1}}(s_{k+1}). \tag{15}$$

The function $g(\varepsilon_{k+1}, \theta_k)$ may be obtained from the equation

$$\frac{\partial f}{\partial \varepsilon_{k+1}} + \frac{\partial g}{\partial \theta_k} = 0 \tag{16}$$

which is a consequence of the Liouville theorem for Hamiltonian systems (Lichtenberg and Lieberman 1983). For the analytical construction of the function $g(\varepsilon_{k+1}, \theta_k)$ we can use analytical approximations for the function $J_s'(s)$, e.g.

$$J_s'(s) = \tfrac{1}{2}s - 0.1774\, s^{2.375} \qquad s \leqslant 1.133 \tag{17}$$

and equation (9) for $s > 1.133$. These approximations are consistent with the limiting forms (8) and (9) and represent sufficiently well the function $J_s'(s)$ for any s. Accordingly from equations (15)–(17) we have

$$f(\varepsilon_{k+1}, \theta_k) = \sin\theta_k \begin{cases} 2\varepsilon_{k+1}^{-5/2} - 0.71\,\varepsilon_{k+1}^{-4.5625} & \varepsilon_{k+1} \geqslant 0.92 \\ 4b - 4a\varepsilon_{k+1} - \dfrac{\varepsilon_{k+1}^2}{\pi}\sin\dfrac{\pi}{\varepsilon_{k+1}^{3/2}} & \varepsilon_{k+1} \leqslant 0.92 \end{cases} \tag{18}$$

$$g(\varepsilon_{k+1}, \theta_k) = -\cos\theta_k \begin{cases} 5\varepsilon_{k+1}^{-7/2} - 3.24\varepsilon_{k+1}^{-5.5625} & \varepsilon_{k+1} \geqslant 0.92 \\ 4a + \dfrac{2\varepsilon_{k+1}}{\pi} \sin\dfrac{\pi}{\varepsilon_{k+1}^{3/2}} - \dfrac{3}{2\varepsilon_{k+1}^{1/2}} \cos\dfrac{\pi}{\varepsilon_{k+1}^{3/2}} & \varepsilon_{k+1} \leqslant 0.92. \end{cases} \tag{19}$$

Note that functions (18) and (19) are smoothly varying functions and do not cause the additional stochasticity of the system (14). Thus, maps (14) with equations (18) and (19) are suitable for the numerical investigation of the stochastic ionisation of the highly excited one-dimensional hydrogenic atom in the microwave field. It should be noted that the variable ε_{k+1} in the first of equations (14) is in implicit form but for numerical investigation this is not significant. That is why the quantity ε_{k+1} may be easily obtained by Newton's method of successive approximations.

An approximate criterion for the beginning of local instability for systems (10), (12), (14) according to Zaslavskii (1984) may be written in the form

$$K = \max\left|\frac{\delta\theta_{k+1}}{\delta\theta_k} - 1\right| \geqslant 1 \tag{20}$$

where max means the maximum with respect to θ_k. Substitution of equations (10) into equation (20) yields

$$\Phi_0 \geqslant \Phi_0^c = |12\pi^2 s_0 \boldsymbol{J}'_{s_0}(s_0)|^{-1}. \tag{21}$$

Here it was taken into account that in the limits of perturbation theory $|\varepsilon_{k+1} - \varepsilon_k| \ll \varepsilon_k$. Note that for system (14) criterion (20) gives a result which is close to (21) if $s_0 \geqslant 0.3$. For $s_0 \gg 1$ equation (21) turns into equation (13). This supports the criterion (20). At $s_0 \leqslant 1$ equation (21) overestimates the critical field (see figure 1). However, it is easy to remark that the change of energy of the electron during the period of motion may be greater if the beginning of the motion is $x = 0$, i.e. when ξ in equations (3) change from 0 to 2π. In such a case instead of equation (6) we have

$$\Delta E_{0,2\pi} = \frac{\pi Z F_0}{E} \boldsymbol{J}'_{-s}(s) \sin(\theta + s\pi) \tag{22}$$

and criterion (20) gives

$$\Phi_0 \geqslant \Phi_0^c = |12\pi^2 s_0 \boldsymbol{J}'_{s_0}(s_0)|^{-1}. \tag{23}$$

The limiting forms of this function are

$$\begin{aligned} \boldsymbol{J}'_{-s}(s) &= -\frac{3 - \frac{37}{24}s^2}{2\pi(1 - s^2)} \sin s\pi & s &\leqslant 1 \\ \boldsymbol{J}'_{-s}(s) &= (2b/\sqrt{3}s^{2/3}) \cos(s\pi + \pi/6) & s &\gg 1. \end{aligned} \tag{24}$$

In fact the stochasticity may begin if either of the criteria (21) or (23) is satisfied.

We have also performed numerical investigation of the transition to the chaos in system (14) with equations (18) and (19). The results of this investigation are shown in figures 1-3. We see that analysis of equations (14) allows us to estimate the threshold field strengths for the onset of chaos (figure 1). The dependence of the critical field on the relative frequency is not smooth but has a rather complicated structure. Such a structure is related to the resonance island structure visible in figures 2 and 3, where we can see not only the resonance corresponding to the integer values of the relative frequency (first-order resonances) but also the resonances corresponding to the fractional frequencies (second-order resonances). The overlap of such resonances is the reason for global stochasticity. Figure 2 illustrates making distinct and broadening

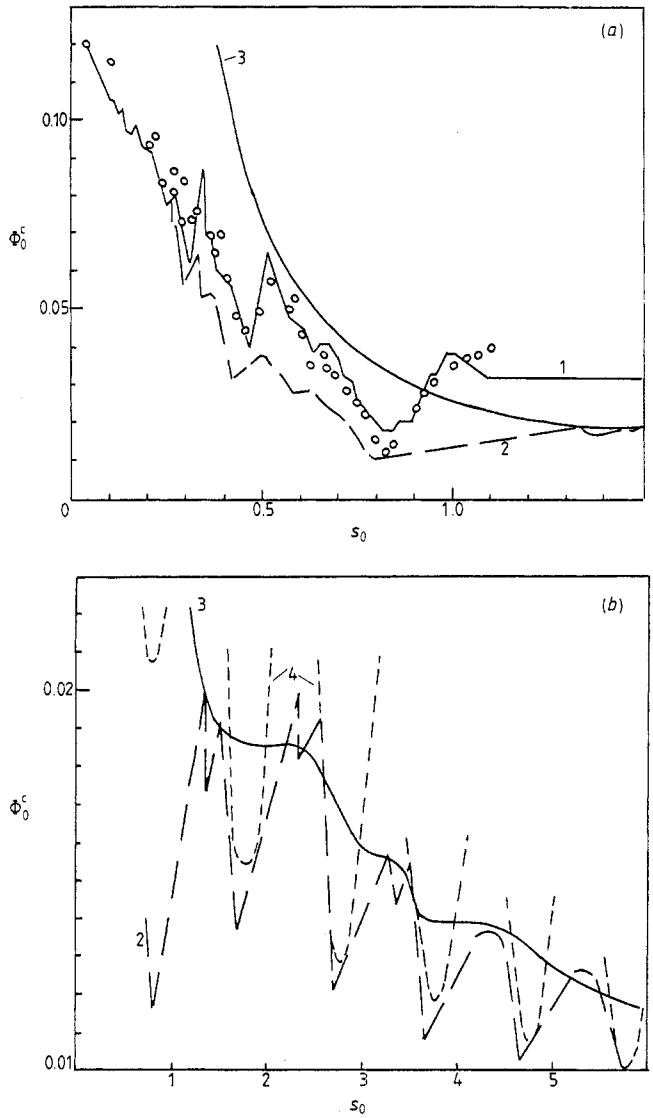

Figure 1. Scaled threshold field strengths for the onset of chaos $\Phi_0^c = F_0^c n_0^4/Z^3$ against relative microwave frequency $s_0 = \omega n_0^3/Z^2$. The open circles represent the experimental values for 10% ionisation (van Leeuwen *et al* 1986, Jensen 1986); curve 1, classical calculations of electron trajectories (Jensen 1986); curve 2, numerical investigation of map (14) with equations (18) and (19); curve 3, equation (21); curve 4, equation (23); curve 5, adiabatic approximation (equation (41)); curve 6, numerical investigation of equation (43). Parts (*a*), (*b*) and (*c*) show extent of curves.

the fractional resonances for $s \lesssim 1$ with increase of the electric field strength. In figure 3 we see an overlap of resonances corresponding to $s = 7$ and $s = 8$ and distinct second-order resonances at $s = \frac{13}{2}, \frac{19}{3}, \ldots$.

Analytical estimation of the critical field according to criterion (20) gives the smooth dependence of the threshold field strengths on frequency (equation (21)). This analytical estimation gives a good fit at $s_0 \gg 1$, but overestimates the critical field at $s_0 \lesssim 1$. It

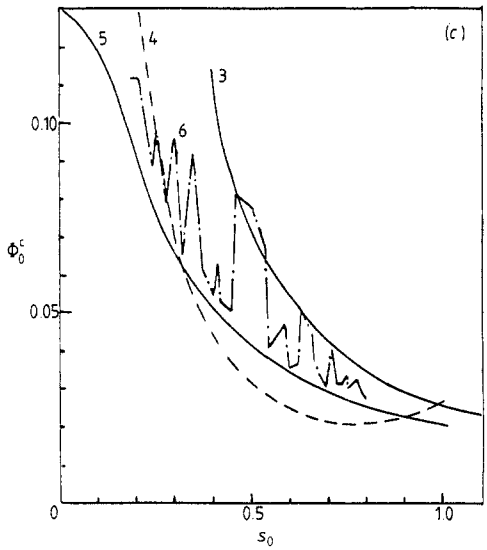

Figure 1. (continued).

is interesting to note that criterion (23) considerably specifies the threshold field strengths for $s_0 \sim 1$.

To conclude this section we shall present the derivation of expressions for the diffusion coefficient of the electron in energy space and the mean time of the diffusive ionisation. Using the random-phase assumption for global stochasticity (Lichtenberg and Lieberman 1983) from equations (6) and (22), by definition (see e.g. Lifshitz and Pitayevsky 1979, Kaulakys and Čižiūnas 1987), we have

$$B(E) = \frac{\overline{(\Delta E)^2}}{2T_k} = \frac{\pi Z F_0^2}{2(-2E)^{1/2}} \begin{cases} [J'_{-s}(s)]^2 & s \leqslant 1 \\ [J'_s(s)]^2 & s \geqslant 1. \end{cases} \tag{25}$$

The diffusion coefficient in the space of the principal quantum numbers when $|\Delta n| \ll n$ is related to the diffusion coefficient in energy space as

$$B_n = B(E) n^6 / Z^4 \qquad E = -Z^2/2n^2. \tag{26}$$

If $s \gg 1$ $J'_s(s) = b/s^{2/3}$ (equation (9)) and equations (25) and (26) give the expression

$$B_n = \tfrac{1}{2}\pi b^2 F_0^2 n^3 / (\omega Z)^{4/3} \qquad \omega n^3 Z^{-2} \gg 1 \tag{27}$$

which agrees with the result of Delone *et al* (1983) and Jensen (1984).

The expressions for the mean time of diffusive ionisation have been derived by Kaulakys and Čižiūnas (1987):

$$\tau_d = \frac{(\omega^4 Z)^{1/3}(-8E_0)^{1/2}}{\pi (bF_0)^2} = \frac{2 n_0^3 s_0^{4/3}}{\pi (bZ\Phi_0)^2} \qquad \omega n_0^3 Z^{-2} \geqslant 1. \tag{28}$$

This means that the ionisation takes place on average after

$$\nu = (12\pi)^2 s_0^3 / \kappa^2 \simeq 1421 s_0^3 / \kappa^2 \qquad s_0 \geqslant 1 \tag{29}$$

field oscillations. Here $\kappa = F_0/F_0^c = \Phi_0/\Phi_0^c$ with Φ_0^c given by equation (13). Expression (29) is in reasonable agreement with the findings of the numerical investigation of system (14) and the results of the paper by Leopold and Richards (1985). Note that the mean ionisation time increases strongly with the increase of the initial relative frequency of the field if the field strengths are close to the threshold field strengths.

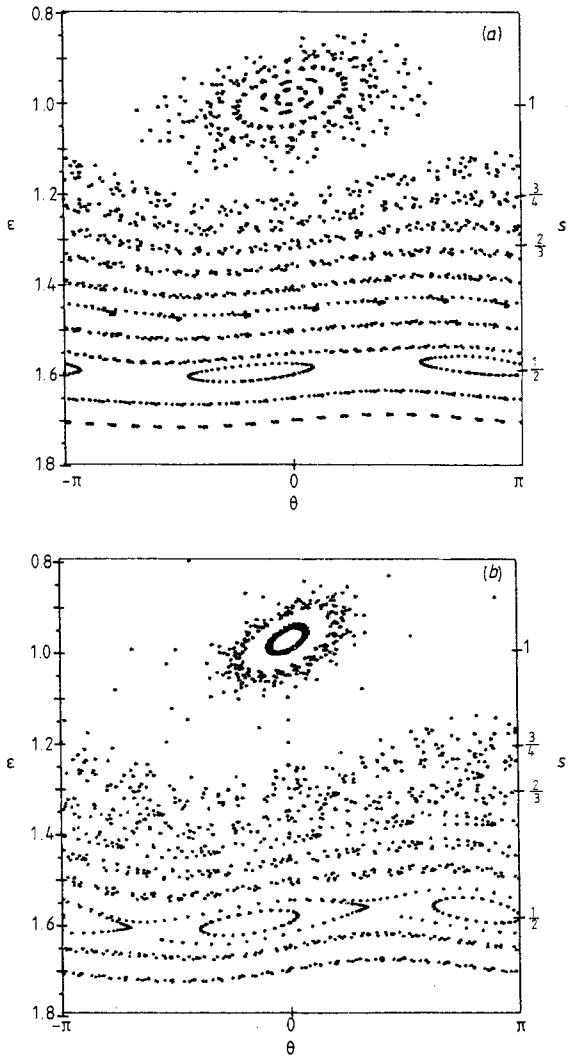

Figure 2. Trajectories for the map (14) with equations (18) and (19) on the phase plane (θ, ε). (a) $\pi\varepsilon_0^2\Phi_0 = 0.06$; (b) $\pi\varepsilon_0^2\Phi_0 = 0.12$. The initial conditions are $\theta_0 = 0$, $\varepsilon_0 = 1.7 - 0.05i$ $(i = 0, 1, 2, \ldots)$.

Thus the time corresponding to 300 oscillations of the microwaves (van Leeuwen *et al* 1985, Jensen 1986) is insufficient for the estimation of threshold field strengths for the onset of chaos at $s_0 \gtrsim 1$. That is why the threshold field strengths obtained in the present paper by carrying out 2000 iterations of system (14) are slightly smaller than those of Jensen (1986) (see figure 1).

3. Adiabatic approximation

Classical perturbation theory does not explain the approach of the critical field Φ_0^c to the static field ionisation threshold $\Phi_0^{st} = 0.130$ when $s_0 \to 0$. As follows from the above consideration the main information about the transition to chaos is contained in the

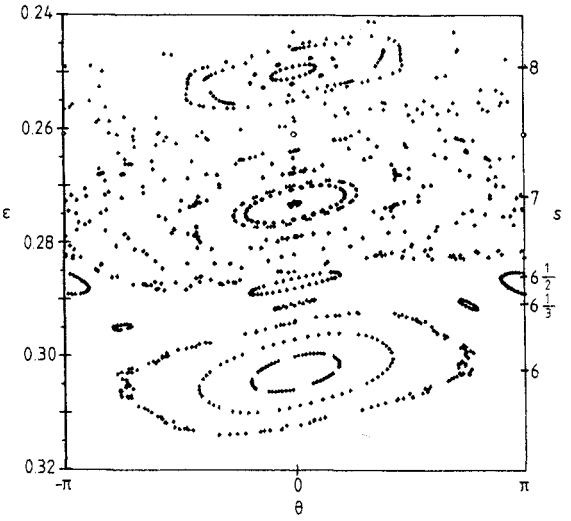

Figure 3. As for figure 2, but here $\pi\varepsilon_0^2\Phi_0 = 0.035$ and the initial conditions are $\theta_0 = 0$, $\varepsilon_0 = 0.3\text{-}0.003i$.

iterative relation for the phase. More exactly, the map for the phase may be written in the form

$$\theta_{k+1} = \theta_k + \omega T(n, \theta_k) \qquad T(n, \theta_k) = 2\pi/\Omega(n, \theta_k) \tag{30}$$

where $\Omega(n, \theta_k)$ and $T(n, \theta_k)$ are the frequency and period of the motion of the electron taking into account the influence of the electric field. If the perturbation is sufficiently slow then the action of the perturbed oscillator will remain an adiabatic invariant (Landau and Lifshitz 1973):

$$j = \pi^{-1}\int_0^{x_1} p(x)\,\mathrm{d}x \qquad p(x) = [2(E + Z/x + Fx)]^{1/2} \tag{31}$$

where x_1 is the classical turning point, $p(x_1) = 0$. Since j is assumed to be an adiabatic invariant, it is equal to the initial action which coincides with the initial principal quantum number n_0 (Jensen 1984). By evaluating the integral (31) we have

$$n_0 = Z\left(\frac{1+y}{-2E}\right)^{1/2} F(\tfrac{1}{2}, -\tfrac{1}{2}; 2; y) \qquad y = \frac{1-(1-4ZFE^{-2})^{1/2}}{1+(1-4ZFE^{-2})^{1/2}} \tag{32}$$

where $F(a, b; c; y)$ is a hypergeometric function. Thus equations (32) define the relation between the initial principal quantum number of the highly excited hydrogenic atom and the energy of the electron in the electric field, if the field is turned on slowly. From equations (32) we have

$$E = -\frac{Z^2}{2n_0^2} - \frac{3n_0^2}{2Z}F + \ldots \qquad |F| \ll Z^3/16n_0^4 \tag{33a}$$

$$E = -(8Z/3\pi n_0)^2 \qquad F = F^{\mathrm{st}} = E^2/4Z. \tag{33b}$$

For $F = F^{\mathrm{st}}$ the turning point x_1 coincides with the maximum of the potential barrier (Jensen 1984). Thus the threshold for classical ionisation in an adiabatically varying electric field is $F^{\mathrm{st}} = 2^{10}Z^3/(3\pi n_0)^4 \simeq 0.130Z^3/n_0^4$.

The period of motion of the electron in the Coulomb and static electric fields may be obtained from equation (31) according to Landau and Lifshitz (1973):

$$T = 2\pi \frac{\partial n}{\partial E} = 2\pi Z \left(\frac{1+y}{-2E}\right)^{3/2} F(\tfrac{3}{2}, \tfrac{1}{2}; 2; y). \tag{34}$$

Here we have used the Gauss relations among the contiguous hypergeometric functions (Abramowitz and Stegun 1972). From equation (34) it follows that

$$T = \frac{2\pi Z}{(-2E)^{3/2}}\left(1 + \frac{15ZF}{2(-2E)^2}\right) \qquad |F| \ll \frac{Z^2}{16n_0^4} \tag{35a}$$

$$T = 4Z\left(\frac{1+y}{-2E}\right)^{3/2} [4\ln 2 - 2 - \ln(1-y)] \qquad F \to F^{st}\ (y \to 1). \tag{35b}$$

In this way $T \to \infty$ by a logarithmic law when $F \to F^{st}$.

Equations (30), (32), (34) define the iterative relation for the phase θ of the electron moving in the slowly varying field if $F = F_0 \cos\theta_k$. From equations (32) we have

$$\Phi_0 = \frac{F_0 n_0^4}{Z^3} = \frac{y}{4\cos\theta_k}[F(\tfrac{1}{2}, -\tfrac{1}{2}; 2; y)]^4$$
$$y = [1-(1-4ZF_0\cos\theta_k/E^2)^{1/2}]/[1+(1-4ZF_0\cos\theta_k/E^2)^{1/2}]. \tag{36}$$

An approximate criterion for stochasticity for the map (30) is given by equation (20). Substitution of equations (30) and (34) into equation (20) gives

$$\left|\frac{3\pi s_0 y \tan\theta_k [F(\frac{3}{2}, \frac{1}{2}; 2; y) + [(1+y)/4]\, F(\frac{5}{2}, \frac{3}{2}; 3; y)]}{(1-y)[F(\frac{1}{2}, -\frac{1}{2}; 2; y)]^2}\right| = 1. \tag{37}$$

Phase θ_k must be chosen from the requirement of the minimum of the field Φ_0 given by equation (36). Note that according to equation (37) $y \to 1$ if $s_0 \to 0$ and $y \to 4/15\pi s_0 \tan\theta_k$ if $s_0 \geqslant 1$. This allows us to simplify equation (37) keeping the main terms only:

$$\left|\frac{yd\tan\theta_k}{1-y}\right| = 1 \qquad d = \frac{15\pi s_0}{4}. \tag{38}$$

According to equations (36) and (38) we have

$$\Phi_0 = \frac{\cos\theta_k + 2d\sin\theta_k}{8(\cos\theta_k + d\sin\theta_k)^2}. \tag{39}$$

Here we have used an approximation

$$[F(\tfrac{1}{2}, -\tfrac{1}{2}; 2; y)]^4 \simeq 1 - \tfrac{1}{2}y \qquad y \leqslant 1. \tag{40}$$

From equation (39) it follows that $\Phi_0^c = \Phi_0^{min} = \frac{1}{8}$† at $\theta_k = 0$ if $d < 2^{-1/2}$. If $d \geqslant 2^{-1/2}$ Φ_0 is minimal when $\tan\theta_k = (2d^2-1)/3d$ and

$$\Phi_0^c = \frac{(4d^2+1)(4d^4+5d^2+1)^{1/2}}{32d(d^2+1)^2} \qquad d = \frac{15\pi s_0}{4} \geqslant 1/2^{1/2}. \tag{41}$$

Approximately, we have

$$\Phi_0^c = \frac{1}{15\pi s_0}\left(1 - \frac{2}{(5\pi s_0)^2}\right) \qquad s_0 \geqslant 0.2. \tag{42}$$

† The difference of this value of the critical field from the static field threshold $\Phi_0^{st} = 0.130$ is due to approximation (40) only.

The adiabatic critical field for stochastic ionisation as a function of relative frequency is shown in figure 1.

It should be noted that the derivation of equation (37) was fulfilled by the variation of equation (30) over θ_k according to equation (20) at the constant energy but not the action. Variation of equations (30), (34) over θ_k at the constant action yields equations similar to (37)-(42) but then in equations (38)-(42) $d = 3\pi s_0/2$. This means that the motion of the electron of the hydrogenic atom in the low-frequency field is more stable for adiabatic perturbations then for unadiabatic ones.

For $|F| \ll F^{st}$ the iterative relation for the phase according to equations (30) and (35*a*) is

$$\theta_{k+1} = \theta_k + 2\pi s_0 + q \cos \theta_k \qquad q = 15\pi s_0 \Phi_0 \tag{43}$$

which is the map of the circle onto itself. The theory of this map has been extensively developed (see e.g. Chirikov 1979, Martínez-Mekler *et al* 1986, Umberger *et al* 1986 and references therein). Equation (43) may be used for evaluation of the critical field for stochastic ionisation at $0.3 \leqslant s_0 \leqslant 0.7$. Criterion (20) for such a case gives $q = 1$, which is consistent with equation (42). More precisely, the threshold field strengths for the onset of chaos for map (43) may be obtained numerically. The results of numerical analysis are also shown in figure 1. We see a rather complicated dependence of the threshold field strengths on the frequency. For $s_0 = \frac{1}{4}, \frac{1}{3}, \frac{1}{2}, \frac{2}{3}, \frac{3}{4}, \ldots$ the ionisation is suppressed by the persistence of resonance island structures visible in figure 2. The positions of the islands of regular motion depend slightly on the field strength. We see that criterion (20) for map (43) is rather approximate.

The comparison of the adiabatic critical field with numerical calculations, perturbation theory and experimental values shows that the adiabatic approximation may be used for the estimation of the critical field for $s_0 \leqslant 1$. The adiabatic approximation overlaps with the perturbation approximation at $0.3 \leqslant s_0 \leqslant 0.7$.

4. Quantum dynamics for the electron

Already early experiments on the microwave ionisation of highly excited hydrogen atoms have shown that this ionisation cannot be treated as a usual multiphoton process (see Delone *et al* 1983) and a mechanism of quantum diffusion of the electron over the excited states has been suggested (Delone *et al* 1978). The diffusion over the excited states is a result of the one-photon transitions among the strongly perturbed states. The one-photon transitions caused by the non-resonant field may occur if the broadening and shift of the atomic levels are comparable to the distance between the unperturbed levels. That is why we suppose that the broadening and shift of the atomic levels caused by the electromagnetic field are strong and the spectrum of the hydrogen atom in the microwave field is nearly continuous. The transition rate between the energy states E and E' is (Landau and Lifshitz 1960)

$$\mathrm{d}W(E, E') = 2\pi |V_{E,E'}|^2 \delta(\omega \pm \omega_{E,E'})\, \mathrm{d}E' \tag{44}$$

where $\omega_{E,E'} = E' - E$ and $V_{E,E'}$ is the Fourier component of the matrix element of the perturbation operator (2)

$$V_{E,E'} = \tfrac{1}{2}\langle E|x|E'\rangle F_0. \tag{45}$$

The matrix element $\langle E|x|E'\rangle$ is usually related to the matrix element between the discrete states:

$$|\langle E|x|E'\rangle|^2\,\mathrm{d}E' = |\langle n|x|n'\rangle|^2 Z(-2E')^{-3/2}\,\mathrm{d}E'. \tag{46}$$

The matrix element $\langle n|x|n'\rangle$ may be evaluated using the semiclassical wavefunctions

$$R_n(x) = \left(\frac{2}{\pi n^3}\right)^{1/2} \frac{Z}{x\sqrt{p_n}} \cos\left(\int_0^x p_n\,\mathrm{d}x - \frac{\pi}{4}\right) \qquad 0 < x < \frac{2n^2}{Z}$$
$$p_n = (2Z/x - Z^2/n^2)^{1/2}.$$

By analogy with papers by Davydkin and Zon (1982) and Goreslavsky *et al* (1982) we have

$$\langle n|x|n'\rangle \simeq \frac{Z^2}{\pi \bar{n}^3} \int_0^{2\bar{n}^2/Z} \frac{x}{p_{\bar{n}}} \cos\chi(x)\,\mathrm{d}x$$
$$\chi(x) = \int_0^x (p_n - p_{n'})\,\mathrm{d}x \simeq \tfrac{4}{3} s u^{3/2} F(\tfrac{1}{2}, \tfrac{3}{2}; \tfrac{5}{2}; u). \tag{47}$$

Here $s = |n' - n| \ll n$, $\bar{n} = \sqrt{nn'}$ and $u = Zx/2n^2$. The limiting forms of the matrix element (47) are

$$\langle n|x|n'\rangle = \begin{cases} \dfrac{3}{2}\dfrac{nn'}{Z} & s \ll 1 \\ -\dfrac{bnn'}{Zs^{5/3}} & s \gg 1 \end{cases} \tag{48}$$

where b is defined by equation (9'). From comparison of equation (48) with limiting forms of the derivatives of the Anger functions (9) and (24) it can be written

$$\langle n|x|n'\rangle \simeq -\frac{nn'}{Zs} \begin{cases} \boldsymbol{J}'_{-s}(s) & s \leqslant 1 \\ \boldsymbol{J}'_s(s) & s \geqslant 1. \end{cases} \tag{49}$$

Equation (49) may be treated as a combination of the results given by Davydkin and Zon (1981) and Goreslavsky *et al* (1982)†.

Substitution of equations (45) and (46) into equation (44) gives

$$\mathrm{d}W(E, E') = \frac{\pi F_0^2 |\langle n|x|n'\rangle|^2 Z}{2(-2E')^{3/2}} \delta(\omega \pm \omega_{E,E'})\,\mathrm{d}E'. \tag{50}$$

The diffusion coefficient of the electron in energy space by analogy with equation (25) is

$$B(E) = \frac{1}{2}\int \omega_{E,E'}^2\,\mathrm{d}W = \tfrac{1}{2}\pi F_0^2 |\langle n|x|n'\rangle|^2 s^2 (-2E)^{3/2}/Z. \tag{51}$$

Substitution of equation (49) into equation (51) gives equation (25). Thus the great number of uncorrelated one-photon transitions results in diffusion of the electron in the energy space identical to the diffusion due to the stochastic classical motion.

For the three-dimensional hydrogenic atom in the linearly polarised electromagnetic field all considerations are the same but the matrix element $|\langle n|x|n'\rangle|^2$ must be replaced by

$$\sum_{l'm'} |\langle nlm|z|n'l'm'\rangle|^2 = \sum_{l'm'} |\langle lm|C_0^{(1)}|l'm'\rangle|^2 (R_{nl}^{n'l'})^2$$

† One should notice some contradictions between the results of these papers, but the correctness of the limiting forms (48) are beyond doubt (see e.g. Bethe and Salpeter 1957, Landau and Lifshitz 1975).

where $C_0^{(1)}$ is the component of the spherical function and $R_{nl}^{n'l'}$ is the radial matrix element. The matrix element $\langle lm|C_0^{(1)}|l'm'\rangle$ is not equal to zero only if $l' = l \mp 1$ and $m' = m$ and is given by the expression (Bethe and Salpeter 1957)

$$|\langle lm|C_0^{(1)}|l \mp 1\, m\rangle|^2 = \frac{l_{\max}^2 - m^2}{(2l+1)(2l'+1)} \qquad l_{\max} = \max(l, l').$$

The radial matrix element $R_{nl}^{n'l'}$ is exponentially small if $s \gg 1$ and $l \sim n$ (Goreslavsky *et al* 1982). For $l \ll n$ $R_{nl}^{n'l'}$ depends slightly on l and $(R_{nl}^{n'l'})^2 \simeq |\langle n|x|n'\rangle|^2$ where $\langle n|x|n'\rangle$ is given by equation (49) (Davydkin and Zon 1981, Goreslavsky *et al* 1982). Finally for $m = 0$ we have

$$\sum_{l'm'} |\langle nl0|z|n'l'm'\rangle|^2 \simeq \tfrac{1}{2}|\langle n|x|n'\rangle|^2.$$

So, the diffusion coefficient for the three-dimensional atom in the linearly polarised microwave field is approximately twice as small as for the one-dimensional atom.

5. Conclusions

We have studied theoretically the dynamics of hydrogenic atoms in an oscillating electric field. In classical perturbation theory and adiabatic approximations we have derived iterative (mapping) forms of the classical equations of motion. This allows us to analyse the regular and stochastic dynamics of the highly excited hydrogenic atom in a microwave field on the basis of modern mathematical apparatus for studying classical non-linear dynamical systems. Such a method considerably facilitates the numerical investigation of transition to chaotic motion and the ionisation process, and allows the analytical estimation of the threshold field for the onset of chaos and the diffusion coefficient of the electron in energy space. The iterative method, in contrast to the resonance-overlap theory, covers all frequencies of the microwave field (from the static field limit to high frequencies, where the resonance-overlap theory is suitable). We also have estimated the mean time of the diffusive ionisation and shown that, when the field strength is close to the threshold field strength, the ionisation time increases strongly with increasing relative frequency of the field.

We have indicated that from the quantum mechanical point of view the ionisation of the atom is a result of the great number of accidental one-photon transitions in the strongly perturbed spectrum of the atom. Such a model results in the diffusion of the electron in energy space of the atom identical to the diffusion due to the stochastic classical motion. In addition, the diffusion coefficient for the three-dimensional hydrogenic atom is approximately twice as small as for the one-dimensional atom and the diffusion takes place mainly over states with small orbital momentum.

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