Quantum Manifestations of Bifurcations of Classical Orbits: An Exactly Solvable Model

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We examine photodetachment of H^- in parallel electric and magnetic fields, $h\nu + H^- \rightarrow H + e^-$ using semiclassical approximations. The fields cause the electron to return to the atom, producing recurrences that are visible as interference oscillations in the photodetachment cross section. As the energy is varied, new returning orbits are created through bifurcations. Each such new recurrence increases the complexity of the absorption spectrum, and each bifurcation causes a local failure of the semiclassical approximation. The failure is repaired by a Fresnel diffraction integral.

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Periodic orbits play a central role in nonlinear dynamics—in Poincaré's words, they offer "the only opening through which we might try to penetrate the fortress (Chaos) which has the reputation of being impregnable." This classical statement holds also in quantum mechanics, wherein the periodic orbit theory [1] of Gutzwiller, Balian, and Bloch and Berry provides a general theoretical framework for studying quantum manifestations of classical chaos. Periodic orbits produce scars in wave functions and oscillations in the density of states, while closed orbits produce oscillations in absorption spectra and real-time recurrences that have been observed in many atoms and molecules.

Bifurcations of periodic orbits and of closed orbits are of particular interest [2]. A bifurcation is defined as the creation of new periodic orbits as a fixed parameter of the system is varied (such as the total energy or the magnetic field strength). Bifurcations are readily observable because they create new recurrences in absorption spectra, and because at a bifurcation observed recurrences are especially strong. In fact, semiclassical theory predicts that the recurrence strength diverges at every bifurcation, because a bifurcation is correlated with a focus of classical orbits. We have seen many such cases in atomic spectra. This is a deep problem for periodic orbit theory, because every stable periodic orbit produces such focusing effects, which in turn lead to vanishing denominators in the periodic orbit sum.

We consider photodetachment of an electron from a negative ion, $h\nu + H^- \rightarrow H + e^-$, in the presence of static parallel electric and magnetic fields [3]. This system constitutes a key model which opens the door to the solution of the above problems. This model has the following properties: (1) The relevant parts of the model are exactly solvable. Whereas the mathematical theory of bifurcations is very abstract, everything in the present system can be understood by elementary methods. (2) It admits a simple structure of closed orbits and their associated recurrences, and it possesses an orderly sequence of bifurcations. (3) At each bifurcation a certain geometrical structure—a cylindrically focused cusp—passes through the origin. This causes the semiclassical approximation to fail. (4) The failure is repaired by a simple diffraction function, a Fresnel integral. The integral provides a uniform approximation which is always finite and which behaves correctly in all limiting cases. (5) The focused cusp is sufficiently similar to the structures found in excitation of neutral atoms that the present model has helped us to derive appropriate formulas for those more difficult cases. (6) Finally, the model accurately represents a system on which experimental measurements can test the predictions.

Following conventional ideas, we describe electron detachment by saying that the active electron is initially loosely bound to the hydrogen atom by a short-range, spherically symmetric potential. The Hamiltonian governing this electron is [4]

$$H = \frac{1}{2m}\left(p_\rho^2 + \frac{L_z^2}{\rho^2}\right) + \frac{\omega_c L_z}{2} + \frac{1}{8}m\omega_c^2\rho^2 + \frac{1}{2m}p_z^2 + eF_0 z - eV_b(r). \quad (1)$$

If the active electron absorbs a photon, it leaves the atom traveling radially outward in any direction, but with a fixed initial speed. Outside the short range of the binding potential $V_b(r)$, the electron feels only the static parallel electric and magnetic fields. Accordingly, the z-motion is uniform acceleration, and the motion in ρ and φ is a circular motion at the cyclotron frequency ω_c

$$\begin{aligned} z(t) &= t(2E/m)^{1/2}\cos\theta_0 - t^2 eF_0/2m, \\ p(t) &= (2/\omega_c)(2E/m)^{1/2}\sin\theta_0\,|\sin\omega_c t/2|, \\ \varphi(t) &= \frac{\omega_c t}{2} + \varphi_0, \end{aligned} \quad (2)$$

where θ_0, φ_0 are the polar and azimuthal angles defining the initial outward motion.

Every classical orbit that subsequently returns to the atom produces a recurrence that may be visible either in real time or as oscillations in the photoabsorption cross section. What are the closed orbits? We find them easily from Eqs. (2). For the z-motion, the time required to go from $z = 0$ up against the electric force and then return to $z = 0$ is $t^z_{\rm ret} = 2(2mE)^{1/2}\cos\theta_0/eF_0$. The motion in $\rho(t)$ is a sinusoidal oscillation and represents cyclotron motion in the magnetic field. The electron returns to $\rho = 0$ at each cyclotron period $t^\rho_{ret} = 2n\pi/\omega_c$. A closed orbit occurs whenever the electron goes out with energy and direction of motion such that $t^z_{\rm ret} = t^\rho_{ret}$.

It follows that one returning orbit always exists: it lies on the positive z axis, and at very low energies this is the only orbit that can exist. The return time for ρ motion is the fixed cyclotron time, independent of the energy and independent of the radius of the motion. However, the return time for z motion cannot exceed $t_\parallel(E) = 2(2mE)^{1/2}/eF_0$, which at small E may be much less than the cyclotron time. Therefore, for energies such that $t_\parallel(E) < 2\pi/\omega_c$, the only possible returning orbit lies on the positive z axis.

If we increase the electron's energy, the return time of the parallel orbit also increases until, at the first "bifurcation energy," it is exactly equal to one cyclotron time. At this point, a new returning orbit is created. Increasing the energy further, the return time of the parallel orbit continues to increase. However, by "aiming" the electron at a different angle, we put less energy into the z motion and more into the ρ motion. Above the first bifurcation energy there always exists an initial direction that divides the energy between the two modes in such a way that the z return time equals the ρ return time $2\pi/\omega_c$ so the orbit goes up and down in z while simultaneously executing a single circle in (x, y).

We may say that the new orbit is created out of the parallel orbit, and it moves away as the energy is increased. This phenomenon is what we define as a *bifurcation of an orbit closed at the origin.*

As we increase the energy further, a second bifurcation energy occurs, at which the return time of the parallel orbit is exactly twice the cyclotron period. At this point another new returning orbit is created, which undergoes two cyclotron circles in (x, y) while simultaneously moving up and down in z. As we continue to increase the energy, a sequence of bifurcations occurs, with the nth bifurcation occurring at $E_n = n^2\pi^2(eF_0)^2/2m\omega_c^2$, where $t_\parallel(E)$ is n cyclotron times. Resulting closed orbits are drawn in Fig. 1.

We need to know exactly what happens to the whole family of outgoing trajectories at a bifurcation. As stated earlier, each family is defined by the condition that the electron begins at the origin ($\rho = 0$, $z = 0$) with fixed speed moving in any direction. For low energies we have the families of trajectories depicted in Fig. 2. Caustics (boundaries between allowed and forbidden regions where trajectories cross over each other and semiclassical approximations diverge) are apparent in the figure. In the lower part of the left-hand figure, caustics come together to form an upward-pointing cusp, whose tip is located at $z \approx -1.8 \times 10^3$ a.u. Since φ is an ignorable coordinate this cusp is actually a three-dimensional structure, which we call a focused cusp, obtained by rotating the two-dimensional cusp through 2π. This focused cusp is directly connected with the bifurcations of the parallel orbit. As we increase the energy this cusp rises toward the origin, and there exists an energy at which the tip of the cusp precisely touches the origin. This energy is exactly the first bifurcation energy, where a new closed orbit is created. On the right, we show the family of trajectories at an energy above the first bifurcation energy but below the second. The new orbit created at the first boundary energy is shown along with the parallel orbit. Another cusp at $z \approx -4.2 \times 10^3$ a.u. has appeared. As we increase the energy to the second bifurcation energy $E_{b=2}$ this cusp will eventually touch the origin, and the second new orbit is created. This sequence of events continues and produces all the other bifurcations. At every bifurcation a focused cusp touches the origin.

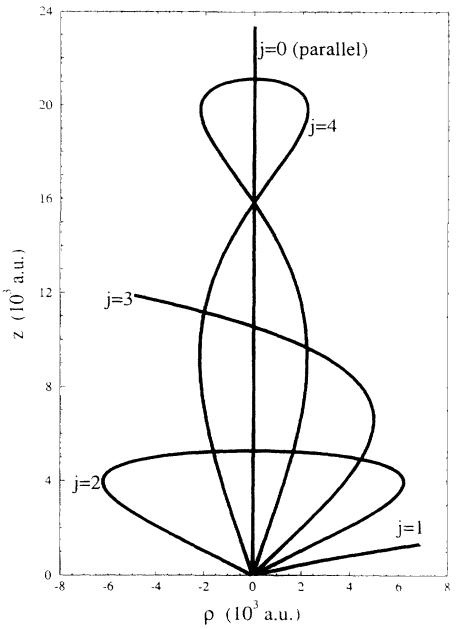

FIG. 1. Some orbits closed at the nucleus for parallel electric and magnetic fields.

Semiclassical methods give a simple formula for the photodetachment cross section: $\sigma(E) = \sigma_0(E) + \sum_{j=0}^{n}\sigma^j_{\rm ret}(E)$, where $\sigma_0(E)$ is the cross section in the absence of fields, and $\sigma^j_{\rm ret}(E)$ is the oscillatory contribution to the cross section arising from the jth closed orbit. We find [4,5]

$$\sigma^{j=0}_{\rm ret} = -\frac{3}{2}\sigma_0\left(\frac{\hbar\omega_c}{2E}\right)\frac{1}{\sin[\omega_c(2mE)^{1/2}/eF_0]} \times \sin\Phi_0\,, \tag{3a}$$

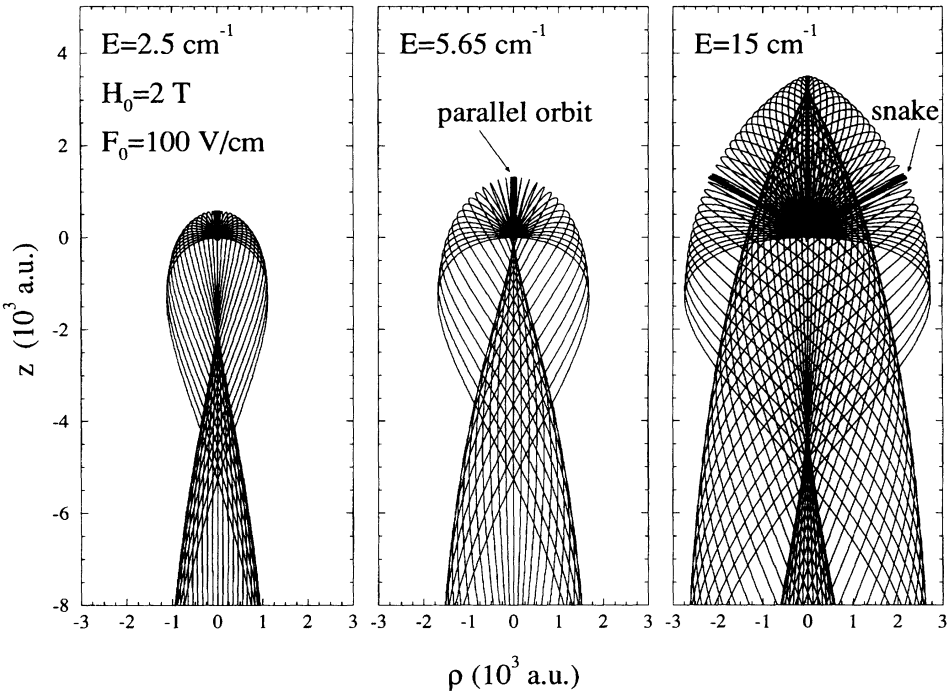

FIG. 2. Families of trajectories outgoing from the origin with fixed speed at three different energies.

$$\sigma^j = -3\sigma_0\left[\left(\frac{\hbar\omega_c}{2E}\right)\frac{(eF_0/\omega_c)\pi}{\sqrt{2mE}}\right]^{1/2} \times (\cos\theta_0^j)^{3/2}\sin(\Phi_j - \pi/4), \quad (3b)$$

where $\Phi_j = S_j/\hbar - \mu_j\pi/2$ is the action around the jth closed orbit corrected by the Maslov index μ_j, and where $j = 0$ refers to the parallel orbit.

Equations (3) say that the recurrence amplitude of the parallel orbit [defined as the prefactor of $\sin\Phi_0$ in Eq. (3a)] diverges at every bifurcation because of the sin in the denominator. Those divergences are visible in Fig. 3, and they identify the bifurcation energies. This prediction is of course incorrect. To fix it we need an accurate wave function of the cylindrically focused cusp, which can be constructed using Maslov's methods. By re-expressing the Schroedinger wave function in the mixed position-momentum space

A representative calculation is shown in Fig. 3. Superimposed on a gradually rising photodetachment cross section there are oscillations connected with each closed orbit. Close to $E = 0$ is a simple pattern, then at each of the bifurcation energies a new oscillation appears, and the pattern grows steadily more complex as the energy increases.

$\tilde{\Psi}(p_x, p_y, z)$ and using cylindrical coordinates in that space, the wave function and the resulting photodetachment cross section can easily be reduced to a Fresnel integral [6]. Using the definitions given in Ref. [7], the contribution to the photodetachment cross section arising from the combined effects of the parallel orbit and the nth new orbit at energies close to the nth bifurcation is [7]

$$\sigma = -3\sigma_0(meF_0/p^3\cos^3\theta_0)^{1/2}\,\mathrm{Im}\left[e^{i\beta}\int_{u_0}^{\infty} e^{iu^2}\,du\right].$$

This formula is finite at all energies and reduces to Eq. (2a) plus (2b) (with $j = n$) when z_c is sufficiently far from the origin.

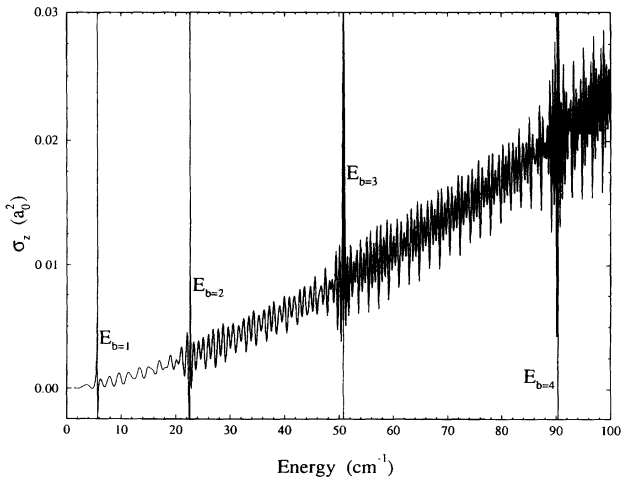

FIG. 3. Photodetachment cross section according to semiclassical formula. Each bifurcation leads to a divergence followed by a more complicated oscillatory structure.

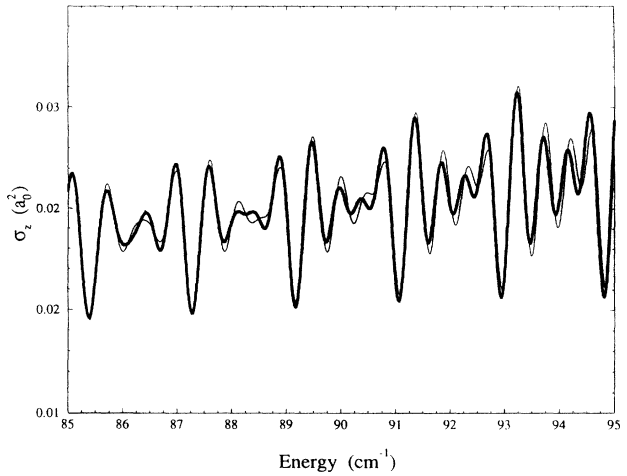

FIG. 4. Photodetachment cross section near the fourth bifurcation using exact quantum theory (heavy line) and uniform semiclassical approximation (light line).

Results are shown in Fig. 4. From the corrected formula, we find that (1) generally the recurrence amplitude of the parallel orbit is much less than that of the other orbits, but (2) near a bifurcation they become comparable, and (3) exactly at each bifurcation, the combined recurrence amplitude of the parallel orbit and the new orbit together is precisely half the recurrence amplitude of the new orbit by itself.

All of these consequences of the model can be tested experimentally, preferably by scaled-variable spectroscopy.

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[2] J.-M. Mao and J. B. Delos, Phys. Rev. A **45**, 1746 (1992); J.-M. Mao, K. A. Rapelje, S. J. Blodgett-Ford, J. B. Delos, A. König, and H. Rinneberg, Phys. Rev. A **48**, 2117 (1993); J. Gao and J. B. Delos, Phys. Rev. A **49**, 869 (1994). Other important studies of the behavior near bifurcations are as follows: C. P. Malta, M. A. M. deAguiar, and A. M. Ozorio de Almeida, Phys. Rev. A **47**, 1625 (1993); M. Kus, F. Haake, and D. Delande, Phys. Rev. Lett. **71**, 2167 (1993); M. W. Beims and G. Alber, Phys. Rev. A **48**, 3123 (1993).

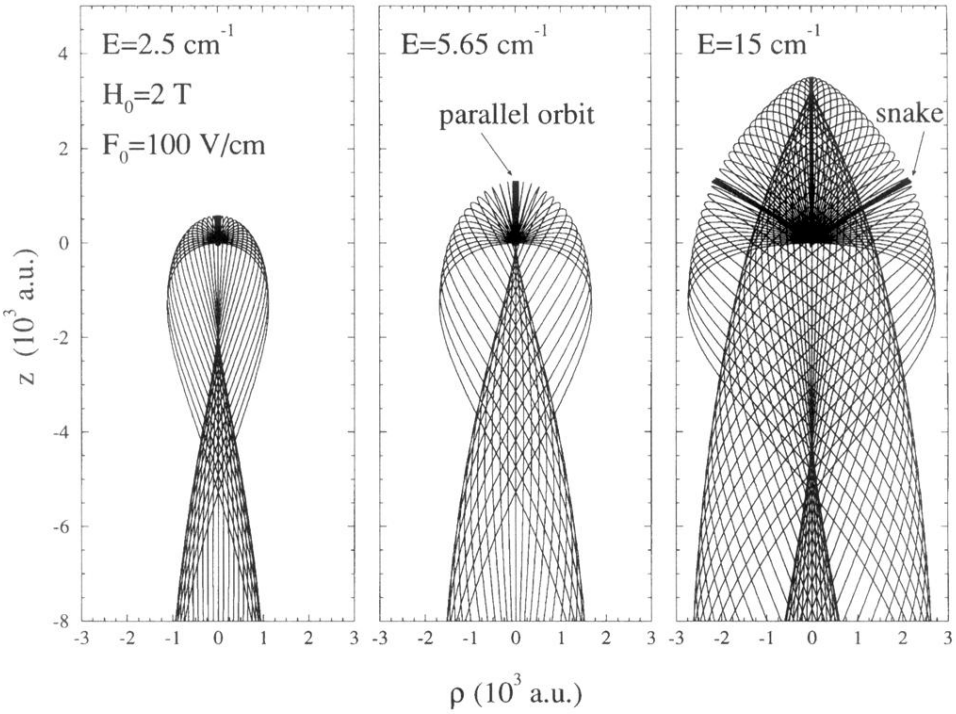
[3] This system was previously considered by M. L. Du, Phys. Rev. A **40**, 1330 (1989) and by I. I. Fabrikant, Phys. Rev. A **43**, 258 (1991), but their fully quantum treatment did not display any connection with classical orbits.

[4] e is the absolute value of the electron charge, ω_c is the cyclotron frequency eH_0/mc, F_0 and H_0 are the applied electric and magnetic field strengths, $V_b(r)$ is the effective atomic potential that binds the active electron to the hydrogen atom, and $L_z = xp_y - yp_x$ is the conserved z component of the angular momentum, which we take to be zero.

[5] A full derivation will be published elsewhere.

[6] Proof: The generator of the Lagrangian manifold for a two-dimensional cusp is the function $\tilde{S}(p_x, z) = \sqrt{2mE - p_x^2}(z - z_c) + \alpha p_x^4$ and the associated wave function in configuration space is known as a Pearcy function. However, for a cylindrically focused cusp, replace p_x^2 by $p_x^2 + p_y^2$, and the wave function in configuration space is $\Psi(xyz) = \int \exp\{i[p_x x + p_y y + \tilde{S}(p_x, p_y)]/\hbar\} dp_x\, dp_y$. We need to evaluate it at the origin $x = 0$, $y = 0$, and $z = 0$. Use cylindrical coordinates for the integration, expand the square root in powers of $(p_x^2 + p_y^2)$, and (voilà) there is the Fresnel integral.

[7] Im means imaginary part, $p = \sqrt{2mE}$, $\beta = pz_c - meF_0 z_c^2/4\,\mathrm{p}\cos^3\theta_0\hbar - (\mu_0 - 1)\pi/2$, $u_0 = -(z_c/2) \times (meF_0/p\hbar\cos^3\theta_0)^{1/2}$, θ_0 is the initial angle of the new orbit after the bifurcation, or zero before the bifurcation, $z_c = z(nt_c)$ is the location of the cusp at the given energy.



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