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Can Bohmian trajectories account for quantum recurrences having classical periodicities?

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Abstract

Quantum systems in specific regimes display recurrences at times matching the period of the closed trajectories of the corresponding classical system. This is the case of the excited hydrogen atom in a magnetic field, that we investigate from the point of view of the de Broglie–Bohm (BB) interpretation of quantum mechanics. *Individual* BB trajectories do not possess the classical periodicities and cannot account for the quantum recurrences, that can only be explained by considering the statistical *ensemble* of trajectories.

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1. Introduction

The manifestation of classical orbits has been found in a host of quantum systems, displaying features such as scars of wavefunctions along periodic orbits of the corresponding classical system or time recurrences appearing at the periods of classical closed orbits [1]. These features have been observed experimentally in systems such as mesoscopic devices or atoms in external fields. From within a pure Schrödinger based approach, these phenomena may appear as coming out of the blue. They are however well understood by performing asymptotic $\hbar$ expansions. In particular it is straightforward to show (e.g. [2]) that the evolution operator obtained from the path integral expression becomes to first order in $\hbar$

$$\langle x_2, t_2|e^{-iH(t_2-t_1)/\hbar}|x_1, t_1\rangle = (2i\pi\hbar)^{-D/2}\sum_k \left|\det\frac{\partial^2 R_k}{\partial x_2 \partial x_1}\right|^{1/2} \times \exp\left(\frac{i}{\hbar}\left[R_k(x_2, x_1; t_2-t_1) - \phi_k\right]\right) + O(\hbar). \quad (1)$$

We have assumed for simplicity a time-independent Hamiltonian H in D-dimensional configuration space. The sum runs on the *classical paths* k connecting x_1 and x_2 and R_k is the classical action along the trajectory k; it satisfies the Hamilton–Jacobi equation of classical mechanics [3]

$$\frac{\partial R(x,t)}{\partial t} + \frac{(\nabla R(x,t))^2}{2m} + V(x) = 0. \quad (2)$$

The determinant is linked to the classical density and ϕ_k is an additional phase that keeps track of the points where the classical amplitude is singular. The physical meaning of Eq. (1) is simple: when $\hbar/R$ is small (a situation to be termed here 'semi-classical regime') propagation in configuration space takes place only along the classical paths, the sum reminding us that the *wave* takes all the *paths* simultaneously with a given weight—the classical amplitude.

An alternative interpretation of quantum phenomena hinges on the existence of point-like particles following a well-defined space–time trajectory—a *quantum trajectory*. The de Broglie–Bohm (BB) theory is by far the best-known and most developed of hidden-variables theories, and BB trajectories have been computed for a wide range of quantum systems (see [4] and references therein as well as more recent work e.g. [5–7]). One of the main motivations behind the BB theory is to bridge

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the gap between classical and quantum mechanics. Indeed the interpretation of quantum phenomena by way of a statistical distribution of particles moving along well-defined quantum trajectories appears as an attractive manner of understanding how classical mechanics can emerge from quantum phenomena.

The main concern of this work is to analyze the role of quantum trajectories as predicted by the de Broglie–Bohm interpretation in quantum systems displaying the fingerprints of classical trajectories. In such systems, the wavefunction is carried by classical trajectories, and it is therefore of interest to compare and contrast classical and quantum trajectories. This will be done for a well known prototypical system, an excited hydrogen atom in a magnetic field [8]. This system has been heavily investigated, both theoretically and experimentally, in the past 20 years and the success of its semiclassical analysis has converted this system into a paradigm of "quantum chaos". We will briefly present the main characteristics of this system in Section 2. We will then summarize the main properties of BB trajectories and their expected behaviour in the semiclassical regime. Specific quantum trajectories for the hydrogen atom in a magnetic field will be computed in Section 4. We will see that observable quantum recurrences are ruled by the periodicity of the periodic orbits of the corresponding classical system; the role of the quantum trajectories in accounting for the recurrences will be discussed in Section 5.

2. The hydrogen atom in a magnetic field

The Hamiltonian describing the hydrogen atom in a magnetic field is given by (e.g. the review paper [8])

$$H = \frac{p^2}{2m} + \left(\frac{qBL_z}{2mc} - \frac{q^2}{r} + \frac{(x^2+y^2)q^2B^2}{8mc^2} \right), \tag{3}$$

where B is the strength of the magnetic field oriented in the z direction, m the mass of the electron, and r the distance of the electron relative to the nucleus. The spherical symmetry of the Coulomb field is broken by the magnetic field, leaving an axial symmetry (invariance around the z axis). We will take $L_z = 0$ in what follows and we will assume B is sufficiently strong so that perturbation theory is not necessarily valid. It can be shown that H possesses a scaling property, from which it follows that the classical dynamics does not depend independently on the values of the energy E and of the intensity B of the field but on the ratio $\epsilon = EB^{-2/3}$ known as the scaled energy. For $\epsilon \to -\infty$ the dynamics is near-integrable whereas phase space is fully chaotic for $\epsilon \gtrsim -0.1$ and of mixed nature for $-0.8 \gtrsim \epsilon \gtrsim -0.1$.

The Schrödinger equation, obtained from the standard quantization of H, is simplified by eliminating the trivial azimuthal angle. We are left with a nonseparable 2-dimensional (ϱ, z) problem which does not admit analytical solutions; ϱ, z are the rectangular (cylindrical) coordinates in the axial plane. Obtaining the bound energies E_n and the eigenfunctions $\psi_{E_n}(\varrho, z)$ for highly excited states therefore involves numerical computations with large basis sizes. We will employ atomic units, the energies of the electron being labeled by $E_n = -1/2n^2$ (where n is of course not an integer). For small ϵ the energy eigenvalues follow the well known pattern given by perturbation theory (Zeeman effect) but as ϵ increases the spectrum becomes very complex, as the spherical n/L degeneracy of the free-field atom is totally broken and thousands of energy levels appear. The interpretation of individual levels becomes meaningless, but it was gradually realized that well-resolved peaks are visible by taking a Fourier transform of the photoabsorption spectrum (obtaining what is called a recurrence spectrum). These peaks, related to the large scale fluctuations of the spectrum, appear at times corresponding to periods of classical orbits closed at the nucleus.

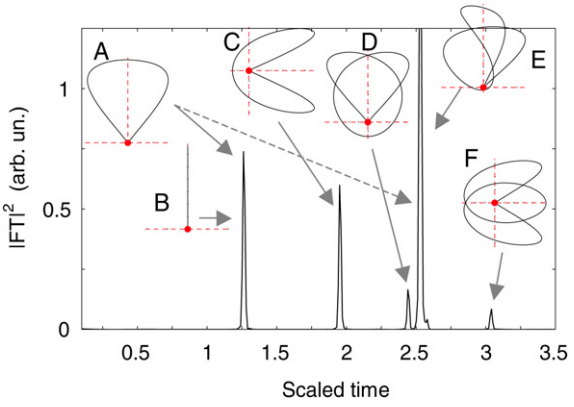

Fig. 1. Recurrence spectrum of the hydrogen atom in a magnetic field obtained from quantum computations (Fourier transform of the computed photoabsorption spectrum excited from the ground state with the laser polarized along the field axis). The excitation energy spans the interval $77 < n < 155$ and the magnetic field varies accordingly so that the scaled energy stays fixed at $\epsilon = -0.3$, thereby obtaining a *scaled* spectrum. The diagrams show the shape of the orbits closed at the nucleus of the corresponding (scaled) classical problem in the (ϱ, z) plane (B is along the vertical z axis). The arrows indicate the orbit whose period matches the time of a given peak in the recurrence spectrum. Note that more than one orbit can contribute to a given peak, and that the repetitions of an orbit contribute to peaks appearing at multiple integer times of the fundamental period (e.g., dotted arrow for the orbit A).

A typical computed recurrence spectrum involving photoabsorption from the ground state of the hydrogen atom is given in Fig. 1. Sharp peaks are visible. Above each peak, we have drawn the shape of the classical orbit whose period matches the recurrence time of the peak. This plot arises from quantum calculations, but recurrence spectra have been experimentally observed in hydrogen [9] as well as other species of one electron ('Rydberg') atoms [10] and molecules [11] in external fields.[1] Purely semiclassical calculations have also been undertaken, reaching an excellent agreement with experimental observations and exact quantum calculations. The semiclassical formalism, known as 'Closed orbit theory' [12], starts from the semiclassical propagator (1) and explains the recurrences observed with classical periodicity by the propagation of the

[1] The recurrence spectrum shown in Fig. 1 arises from the Fourier transform of a *scaled-energy* photoabsorption spectrum where both the energy E and field B are varied so as to keep the scaled energy ϵ constant (in a standard spectrum, B is fixed and only E varies). This results in considerably narrow peaks, instead of wide overlapping structures that would be harder to resolve (most experiments reported in [9,10] were performed employing scaled energy spectroscopy techniques).