Initial Conditions of Closed Classical Orbits from Quantum Spectra

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Abstract

A method is presented for determining the initial conditions of classical orbits from the quantum spectra of the diamagnetic hydrogen atom. Each classical trajectory which is closed at the nucleus produces a sinusoidal fluctuation in the photoabsorption spectrum. The amplitude of each orbit’s contribution appears in the Fourier transform of a spectrum computed at constant scaled energy. For a given initial state, closed-orbit theory gives the dependence of this recurrence amplitude on the initial angle of an orbit. By comparing the recurrence amplitudes for different initial states, the initial conditions of closed classical orbits are determined from quantum spectra.

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1 Introduction

According to the Correspondence Principle, the solutions to Schrödinger’s equation for a given system should contain the classical motion of the same system as a subset (the “classical limit”). In practice, however, gaining information about the classical dynamics of a system from the quantum behavior has proved challenging, particularly for chaotic systems. In some cases, the distribution of eigenvalues can be used to discern whether the classical motion is regular or chaotic [1, 2]. Spectral periodicities are related to periodic orbits [3, 4] and can be used to determine such classical quantities as the period, action, and stability of the periodic orbits [1, 5]. This paper shows that spectral periodicities of the diamagnetic hydrogen atom can be used to determine the initial conditions of the periodic orbits which pass through the origin (closed orbits).
Semiclassical quantization techniques reverse the causal role between quantum and classical behavior by using the classical solutions to construct approximate quantum solutions. EBKM tori quantization [3] gives approximate eigenvalues of conservative integrable systems. Periodic-orbit theory predicts the level density from a sum over periodic orbits and is applicable in regimes of integrable and non-integrable classical motion [3]. The closely related closed-orbit theory [6] predicts photoabsorption spectra from a sum over the orbits which are closed at the nucleus.

Periodic-orbit theory can also be used to glean classical information from quantum level densities [5]. The main result of periodic-orbit theory [3] is an expression for the fluctuating part of the level density,

\[ g_c(E) = \sum_{k} \sum_{n=1}^{\infty} A_{nk} e^{i(nS_k - \alpha_{nk} \pi/2)}, \tag{1} \]

(atomic units). The index \(k\) distinguishes the primitive periodic orbits: the shortest period orbits for a given set of initial conditions. \(S_k\) is the action of a periodic orbit. Each primitive orbit retraces itself, leading to new orbits with action \(nS_k\), where \(n\) is an integer. Hence, every repetition of a periodic orbit is another periodic orbit. The quantity \(A_{nk}\) is related to the stability of an orbit, and \(\alpha_{nk}\) is the orbit’s Maslov index.

## 2 Closed Orbit Theory in Diamagnetic Hydrogen

The Hamiltonian of diamagnetic hydrogen is

\[ H = \frac{p^2}{2} - \frac{1}{r} + \frac{1}{8} B^2 \rho^2, \tag{2} \]

where the magnetic field \(B\) is taken to be along the \(z\) axis. This Hamiltonian can be scaled so that for spectra at constant scaled energy, \(\epsilon = EB^{-2/3}\), the fluctuating part of the level density is [5]

\[ \tilde{g}_c(w) = \sum_{k} \sum_{n=1}^{\infty} \tilde{A}_{nk} e^{i(2\pi nw\tilde{S}_k - \alpha_{nk} \pi/2)}, \tag{3} \]

where \(w = B^{-1/3}\), and \(\tilde{S} = S/(2\pi w)\) is the scaled action. At fixed \(\epsilon\), the classical dynamics has no dependence on \(w\). Consequently, the Fourier transform of an energy level spectrum computed at fixed \(\epsilon\) as a function of \(w\) gives peaks which lie at the scaled action of periodic orbits and whose heights are related to the stability of the orbits [7].
Closed-orbit theory [6] is similar to periodic-orbit theory, except that closed-orbit theory is applicable only to atomic and molecular spectra and yields the oscillator strength density from a specified initial state whereas periodic-orbit theory yields the density of states. Only orbits that begin and end at the nucleus are important in closed-orbit theory. Physically, these are associated with the outgoing waves that are generated when a tightly bound electron is excited to a high-lying state. For diamagnetic hydrogen, every orbit which is closed at the nucleus is also a periodic orbit whose period is equal to either the closure time or twice the closure time.

According to closed-orbit theory, the average oscillator strength density at constant \( \epsilon \) is given by a smooth background plus an oscillatory sum of the form [6]

\[
f(w) = \sum_k \sum_{n=1}^{\infty} D_{nk}^i \sin(2\pi nw \tilde{S}_k - \phi_{nk}).
\] (4)

\( \phi_{nk} \) is a phase that depends on the Maslov index and other details of the orbit. \( D_{nk}^i \) is the recurrence amplitude of a closed orbit for a given initial orbit (labeled \( i \)). It contains information about the stability of the orbit, its initial and final directions, and the matrix element of the dipole operator between the initial state and a zero-energy Coulomb wave. The Fourier transform of an oscillator strength spectrum computed at fixed \( \epsilon \) as a function of \( w \) is called a recurrence spectrum, because it gives peaks which correspond to the scaled action of closed orbits and whose heights correspond to \( D_{nk}^i \).

### 3 Method for Determining Initial Angles

The dependence of the recurrence amplitude \( D_{nk}^i \) on the initial and final angles of an orbit can be used to determine these angles from computed photoabsorption spectra. We can write the recurrence amplitude as

\[
D_{nk}^i = F^i(\theta_i, \theta_f)G_{nk},
\] (5)

where \( \theta_i \) and \( \theta_f \) are the initial and final angles the orbit makes with the \( z \) axis at the origin. (For a specified scaled energy, the initial conditions of a closed orbit are completely determined by its initial angle.) The dependence on the initial and final angles of the orbit and on the initial state is completely contained in the function \( F^i(\theta_i, \theta_f) \). \( G_{nk} \) is related to the stability of the orbit [6]. Several factors simplify the discussion for the scaled energy (\( \epsilon = -0.7 \)) considered here [8]. The dynamics is near integrable in this regime and all closed orbits have either \( \theta_f = \theta_i \) or \( \theta_f = \pi - \theta_i \). Furthermore,
Fig. 1: Predicted ratios of recurrence amplitudes from different initial states.

\[ F^i(\theta_i, \theta_f) = F^i(\theta_i, \pi - \theta_f). \]

Consequently, the angular dependence can be considered a function of a single angle, \( \theta \).

The form of \( F(\theta) \) for a given initial state can be obtained from Du and Delos [6]. For \( m = 0 \) final states,

\begin{align*}
F^{3s}(\theta) &= 0.625 \sin \theta [P_1(\cos \theta)]^2 \quad (6) \\
F^{2p}(\theta) &= 0.5797 \sin \theta [P_2(\cos \theta) + P_0(\cos \theta)/4]^2 \quad (7) \\
F^{3d}(\theta) &= 0.8505 \sin \theta [P_3(\cos \theta) + 2P_1(\cos \theta)/9]^2, \quad (8)
\end{align*}

where the \( P_l(\cos \theta) \) are Legendre polynomials. (For orbits parallel to the field, there is no \( \sin \theta \) term.) The angular functions are normalized [9] such that

\[ \int_0^\pi F^i(\theta) \, d\theta = 1. \quad (9) \]

Since all the dependence on the initial state is contained in \( F^i(\theta) \),

\[ \frac{D^n_{nk}}{D^i_{nk}} = \frac{F^i(\theta)}{F^j(\theta)}. \quad (10) \]

Consequently, the ratio \( F^i(\theta)/F^j(\theta) \) for a particular closed orbit can be determined by dividing the recurrence amplitudes for the corresponding peak in the computed recurrence spectrum.

Fig. 1 shows \( F^{2p}(\theta)/F^{3s}(\theta) \) and \( F^{3d}(\theta)/F^{3s}(\theta) \). These ratios are symmetric about 90°. A given ratio corresponds to either two or four possible initial angles, but since a closed orbit of diamagnetic hydrogen with initial angle \( \theta \) has a symmetric partner of the same shape with initial angle \( \pi - \theta \), only the range from 0 \( \leq \theta \leq \pi/2 \) is of interest. This leaves either one or two possible initial angles, depending on the value of the ratio, but this ambiguity can be resolved by looking at both ratios.
Fig. 2: Recurrence amplitude for odd-parity, $m = 0$ final states at $\epsilon = -0.7$ excited from the 3s initial state. (The recurrence amplitude is the square root of the power spectrum.)

4 Recurrence Spectra

We now turn to the recurrence spectra. A number of methods are available for computing spectra of diamagnetic hydrogen [2, 10, 11]. Diagonalizing the Hamiltonian matrix in a spherical hydrogenic basis is adequate for $\epsilon = -0.7$ [12]. The oscillator strength spectrum, $f(w)$, is multiplied by $w^3$ to remove the global variation of oscillator strength over the range of fields ($31 < w < 133$) and normalized so that

$$\int_{w_{\text{min}}}^{w_{\text{max}}} w^3 f(w) \, dw = 1.$$  \hspace{1cm} (11)

This produces narrower peaks in the recurrence spectrum and allows for comparison with recurrence spectra of different initial states. (In principle, one can obtain arbitrarily high resolution in the recurrence spectrum by computing spectra to very large $w$. This allows identification of orbits arbitrarily close in action.)

The $m = 0$ odd-parity recurrence spectrum for the 3s initial state is shown in Fig. 2. (van der Veldt et al. have analyzed a similar experimental recurrence spectrum for the 2s initial state in helium [13].) To interpret the spectrum, it is helpful to recall the basic structure of closed orbits in diamagnetic hydrogen. At large negative scaled energies, there are three primitive short-period orbits: one moves on the $\rho$ axis, and two move on the $\pm z$ axis [1]. Most longer-period primitive closed orbits are created by bifurcations of these orbits and their repetitions.

The orbits on the $\rho$ axis and those which bifurcate from them are called rotators. Peaks corresponding to these orbits will be labeled $R_n^\rho$, where $n$
Fig. 3 Top: Recurrence amplitude for even-parity, $m = 0$ final states at $\epsilon = -0.7$ excited from the 2$p$ initial state. Bottom: Recurrence amplitude for odd-parity, $m = 0$ final states at $\epsilon = -0.7$ excited from the 3$s$ initial state. This recurrence spectrum is multiplied by $-1$ for comparison.

denotes the repetition of the orbit on the $\rho$ axis from which the orbit bifurcated, and $b$ distinguishes between different orbits which bifurcated from the same parent. The orbits on the $z$ axis and those which bifurcated from them are called vibrators. Recurrences corresponding to these orbits are labeled $V_n^b$, where $n$ and $b$ have the same meaning as for the rotators. For $\breve{S} < 4$ the recurrence spectrum is dominated by repetitions of the perpendicular and parallel orbits (labeled $R_n$ and $V_n$, respectively) [13]. For $\breve{S} > 4$ other orbits are present which were born by bifurcations of these orbits, and the recurrence spectrum becomes more complicated.

## 5 Determination of Initial Angles

This method for determining initial angles can be tested by considering recurrence spectra for $9.9 < \breve{S} < 12.4$, which are shown in Fig. 3 for the 2$p$ and 3$s$ initial states. This range of action has a number of orbits with non-trivial (not 0° or 90°) initial angles and is sufficiently low that the density of orbits allows most recurrences to be resolved.

The method for determining the initial angle of an orbit is demonstrated by considering the peak at $\breve{S} = 10.0661$. The amplitudes for the 2$p$ and 3$s$ initial states are $D^{2p} = 0.0361$ and $D^{3s} = 0.0294$. Their ratio corresponds to $F^{2p}(\theta)/F^{3s}(\theta) = 1.228$. Two initial angles give this ratio: $\theta = 28.51°$ and
Table 1: Predicted initial angles from two different amplitude ratios are compared with actual classical initial angle, \( \theta_{cl} \). All angles are in degrees.

| \( S \)  | \( D_{2p}^{3} \) | \( \theta_{2p/3s} \) | \( D_{3d}^{3} \) | \( \theta_{3d/3s} \) | \( \theta_{cl} \) | orbit |
|---------|----------------|----------------|----------------|----------------|----------------|-------|
| 10.066  | 1.228          | 28.51          | 0.615          | 29.07          | 29.10          | \( V_{12} \) |
| 10.140  | 1.815          | 12.04          | 2.209          | 12.88          | 14.23          | \( V_{12} \) |
| 10.266  | 0.406          | 45.64          | 0.086          | 46.28          | 45.35          | \( R_{13} \) |
| 10.485  | 1.181          | 29.54          | 0.481          | 30.68          | 31.00          | \( R_{13} \) |
| 10.895  | 1.195          | 29.23          | 0.557          | 29.74          | 29.47          | \( V_{13} \) |
| 10.979  | 1.671          | 17.27          | 1.758          | 17.69          | 18.05          | \( V_{13} \) |
| 11.080  | 0.583          | 41.85          | 0.012          | 40.14          | 41.84          | \( R_{14} \) |
| 11.312  | 1.172          | 29.73          | 0.488          | 30.58          | 30.71          | \( R_{14} \) |
| 11.724  | 1.182          | 29.52          | 0.577          | 29.52          | 29.71          | \( V_{14} \) |
| 11.816  | 1.487          | 22.44          | 1.406          | 21.09          | 20.71          | \( V_{14} \) |
| 11.898  | 0.707          | 39.29          | 0.043          | 38.62          | 39.31          | \( R_{15} \) |
| 12.140  | 1.191          | 29.31          | 0.495          | 30.49          | 30.52          | \( R_{15} \) |

\( \theta = 73.47^\circ \). This ambiguity can be resolved by considering the amplitude for the 3d initial state. \( D_{3d}^{3} = 0.0181 \) which corresponds to \( F_{3d}^{3}(\theta)/F_{3s}^{3}(\theta) = 0.615 \). Once again, two initial angles give this ratio: \( \theta = 29.07^\circ \) and \( \theta = 53.90^\circ \). Consequently, the initial angle is determined to be near \( \theta = 28.51^\circ \). This is in good agreement with the actual initial angle, \( \theta_{cl} = 29.10^\circ \).

This method can be used to determine the initial angle of the closed orbits corresponding to many of the peaks in Fig. 3. Table 1 shows that this method gives agreement with the initial angles obtained classically. Some of the closed orbits corresponding to peaks in Fig. 3 are shown in Fig. 4.

The initial angles with the largest errors are for orbits where one or more of the recurrence amplitudes is small or where the ratio \( F_{i}(\theta)/F_{j}(\theta) \) has a small slope. If the recurrence amplitudes themselves are small, there is a larger relative error in the computed amplitudes due to noise in the Fourier transform. There is also a larger relative error in the semiclassical approximations for small recurrences, because the semiclassical approximations used to derive Eq. 5 neglect the contribution of a closed orbit’s neighbors to the angular dependence of its recurrence strength [14]. The error in the predicted initial angle is large if the ratio of angular functions has a small slope because a small error in the computed recurrence amplitudes or in the semiclassical angular functions leads to a large error in angle. In principle, the errors in the semiclassical approximations become smaller as \( \hbar \to 0 \). This limit can be approached practically in diamagnetic hydrogen by look-
ing at smaller magnetic fields at a given scaled energy. The difficulty of small slopes in the angular ratios can be remedied by considering a range of initial states so that, for every angle, at least one of the angular ratios has a large slope. A weighted average over many initial states should produce more accurate initial angles than consideration of a few initial states.

6 Conclusion

In summary, a method is presented for determining the initial conditions of classical orbits from the quantum spectra of the diamagnetic hydrogen atom. However, this quantum mechanical method is an inefficient choice for searching for closed classical orbits. More efficient classical methods are available for finding closed and periodic orbits by directly integrating Hamilton’s equations [15]. This development of a quantum mechanical method of finding closed orbits is a practical step toward understanding how the solutions to Schrödinger’s equation yield the solutions to Hamilton’s equations in the classical limit. It has been shown to be accurate in the near-integrable regime of diamagnetic hydrogen. A simple generalization should be applicable in more strongly chaotic regimes.

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References

[1] H. Hasegawa, M. Robnik, and G. Wunner, No. 98, New Trends in Chaotic Dynamics of Hamiltonian Systems, Progress in Theoretical Physics, Supplement, pp. 198 (1989); H. Friedrich and D. Wintgen, Phys. Rep. 183, 38 (1989).
[2] D. Delande and J. C. Gay, Phys. Rev. Lett. 57, 2006 (1986).

[3] Chaos in Classical and Quantum Mechanics, M. C. Gutzwiller, Springer-Verlag (1990).

[4] A. Holle, J. Main, G. Wiebusch, H. Rottke, and K. H. Welge, Phys. Rev. Lett. 61, 161 (1988).

[5] D. Wintgen, Phys. Rev. Lett. 58, 1589 (1987).

[6] M.L. Du and J.B. Delos, Phys. Rev. A 38, 1896 (1988); 38, 1913 (1988); J. Main, G. Wiebusch, K. Welge, J. Shaw, and J. B. Delos, Phys. Rev. A 49, 847 (1994).

[7] This technique can be generalized to non-scaling systems by treating $\hbar$ as a variable parameter and computing the spectrum of $1/\hbar$ at constant $E$. The Fourier transform of the $1/\hbar$ spectrum gives peaks at the action of periodic orbits and whose heights correspond to $A_{nk}$ in Eq. 1.

[8] One might object that inserting classical information at this point invalidates the claim of being able to determine the initial angles from the spectra. The relationship between the initial and final angles simplifies the discussion, but it is not necessary for determining the initial conditions. A more general technique which does not rely on this relationship will be published elsewhere.

[9] This approach also works by comparing absolute recurrence amplitudes with absolute angular distributions. However, absolute recurrence amplitudes are prohibitively difficult to measure experimentally. Normalizing the angular distributions and recurrence amplitudes circumvents this difficulty and provides a technique for determining the initial angles of closed orbits experimentally.

[10] D. Wintgen and H. Friedrich, Phys. Rev. A 35, 1464 (1987).

[11] C.W. Clark and K.T. Taylor, J. Phys. B. 15, 1175 (1982).

[12] M.L. Zimmerman, J.C. Castro, and D. Kleppner, Phys. Rev. Lett. 40, 1083 (1978).

[13] T. van der Veldt, W. Vassen, and W. Hogervorst, Europhys. Lett. 21, 9 (1993).
[14] Note the small peaks corresponding to the first few repetitions of the perpendicular orbit. Closed-orbit theory predicts zero amplitude for this orbit. ($P_1 (\cos \theta) = \cos \theta$, and $\theta = \pi/2$.) This is because closed-orbit theory makes the assumption that the recurrence amplitude carried by the neighboring trajectories has the same initial angle as the closed orbit. This approximation fails when the angular dependence of the closed orbit is exactly zero, as in this case. John Shaw and John Delos have modified closed-orbit theory to account for the contribution of neighboring orbits whose initial angles do not give a zero in the angular dependence of the recurrence amplitude (private communication).

[15] M. Baranger, K. T. R. Davies, and J. H. Mahoney, Ann. Phys. 186, 95 (1988).