11-1995

Recurrences Associated with a Classical Orbit in the Node of a Quantum Wave Function

John A. Shaw

John B. Delos

William & Mary, jbdelos@wm.edu

Michael Courtney

Daniel Kleppner

Follow this and additional works at: <https://scholarworks.wm.edu/aspubs>

Part of the [Physics Commons](#)

Recommended Citation

Shaw, John A.; Delos, John B.; Courtney, Michael; and Kleppner, Daniel, Recurrences Associated with a Classical Orbit in the Node of a Quantum Wave Function (1995). *Physical Review A*, 52(5), 3695-3703.
<https://doi.org/10.1103/PhysRevA.52.3695>

This Article is brought to you for free and open access by the Arts and Sciences at W&M ScholarWorks. It has been accepted for inclusion in Arts & Sciences Articles by an authorized administrator of W&M ScholarWorks. For more information, please contact scholarworks@wm.edu.

Recurrences associated with a classical orbit in the node of a quantum wave function

John A. Shaw,¹ John B. Delos,^{1,2} Michael Courtney,³ and Daniel Kleppner³

¹Physics Department, College of William and Mary, Williamsburg, Virginia 23185

²Joint Institute for Laboratory Astrophysics, University of Colorado, Boulder, Colorado 80309-0440

³Department of Physics and Research Laboratory for Electronics, Massachusetts Institute of Technology,

77 Massachusetts Avenue, Cambridge, Massachusetts 02139

(Received 2 May 1995)

Absorption spectra of atoms in magnetic fields reveal *recurrences*: manifestations of classical orbits (or quantum wave packets) that go out from the atom and later return. A formula from closed-orbit theory asserts that if the orbit lies on a node of the outgoing wave function, then the strength of the recurrence is zero. New quantum calculations, however, show that the recurrence strength is nonzero, though small. We derive a semiclassical formula for the recurrence strength associated with a classical orbit at a node of the quantum wave function. This formula is compared to the quantum mechanical calculation. Compared to other orbits, the recurrence is about 100 times weaker, and obeys a different classical scaling law.

PACS number(s): 32.60.+i, 05.45.+b, 03.65.Sq

I. INTRODUCTION

If an atom is placed in an electric or magnetic field, and the absorption spectrum to states near the ionization threshold is measured, then the large-scale structure of the spectrum contains oscillations on a smooth background. We call the Fourier-transform of such an absorption spectrum the *recurrence spectrum*. Experiments have shown that this recurrence spectrum consists of peaks at the return times of closed classical orbits of the electron — orbits that go out from the atom and later return [1]. The heights of these peaks are called the recurrence amplitudes, and their absolute squares are called the recurrence strengths.

A semiclassical theory of such recurrence spectra was developed by Du and Delos [2]. This closed-orbit theory asserts that the recurrence strength of any particular classical orbit is related to the angular distribution of the outgoing quantum waves; specifically if a returning orbit lies on a node of the quantum wave function, then that recurrence is not excited — its strength is zero.

In this paper we report quantum calculations of the recurrence strength of an electron orbit in a hydrogen atom in a magnetic field with $3s$ as the initial state. We examine the “quasi-Landau” orbit, which lies in the xy plane perpendicular to the magnetic field. This orbit is responsible for the oscillations in the absorption spectrum that were first observed by Garton and Tomkins [3] and explained by Edmonds [4]. Since the atom is excited from an s state by radiation linearly polarized along the field, the angular distribution of the outgoing wave is a p_z state, which has a node in the xy plane. Therefore, closed-orbit theory predicts a zero recurrence strength, and we can say that the quasi-Landau orbit is “not excited.”

Measurements [5] confirmed that the recurrences associated with this orbit must be very small. Quantum calculations reported here show that the recurrence strength of this orbit is indeed small—about a hundred times smaller than that typical for most orbits—but it is not zero. Therefore closed-orbit theory needs some refinement to describe this situation.

The closed-orbit theory tells us that each recurrence produces a sinusoidal oscillation in the oscillator-strength-density. The recurrence strength of a closed orbit is the square of the amplitude of this oscillation, $C_k^n(E, B)$, which in turn is proportional to the matrix element of the Green's function

$$C_k^n(E, B) = \langle D\Phi_i | G_E^+ | D\Phi_i \rangle \times \text{const}, \quad (1)$$

where Φ_i is the initial state of the atom, D is the dipole operator, and G_E^+ is the constant energy propagator. When this propagator acts on $D\Phi_i$ it produces an outgoing wave which is carried along the classical orbits that turn around in the magnetic field and return to the atom. Each returning wave can be labeled by a discrete index k that identifies a single classical orbit which goes exactly out from and returns exactly to the atomic nucleus. The returning wave is carried not only by this orbit, but also by its neighbors which come back to a region comparable to the size of the initial state. It is these returning waves which interfere with the outgoing waves to give oscillations in the absorption spectrum.

Du and Delos made the approximation that the returning waves are similar to Coulomb scattering waves, and their amplitude is proportional to the amplitude of the outgoing wave at the initial angle of the closed orbit, θ_i . From this approximation, a formula was derived for the recurrence amplitude associated with a closed orbit [6]:

$$C_k^n(E, B) = (E - E_i) 2^{19/4} \pi^{3/2} (\sin \theta_i \sin \theta_f)^{1/2} \times r_o^{-1/4} \left| \frac{d\theta_f}{d\theta_i} \right|^{-1/2} \mathcal{Y}(\theta_i) \mathcal{Y}^*(\theta_f). \quad (2)$$

All notation is defined fully in [2,7]. E is the energy of the active electron, E_i is the energy of the initial state from which excitation takes place, θ_i and θ_f are initial and final directions of the closed orbit relative to the magnetic-field axis, and the angular derivative $d\theta_f/d\theta_i$ evaluated at the return measures the divergence of neighboring trajectories near the closed orbit. The important quantity here is the function $\mathcal{Y}(\theta)$, which is the angular distribution of the outgoing waves. In the present case $\mathcal{Y}(\theta)$ is proportional to

FIG. 1. An initial s state and z -polarized light produces an outgoing wave with odd symmetry with respect to the $z=0$ plane. Zero amplitude goes out along the perpendicular orbit, but the neighbors of the perpendicular orbit produce a small recurrence.

$\cos\theta$, and the quasi-Landau orbit has $\theta_i = \pi/2$, so Eq. (2) gives zero for the recurrence amplitude.

How do we refine this formula so that this orbit produces a nonzero recurrence strength? The point is that the recurrence is produced not by the central orbit alone, but by the family of close neighbors of the central orbit. This family carries that part of the outgoing wave that will later return to overlap the initial state. Usually this family of close neighbors is so narrow that the amplitude of the outgoing wave for the entire family can be replaced by the amplitude of the outgoing wave at the central orbit. However, if that latter amplitude is exactly zero, then the recurrence amplitude will be very small, but it will not be exactly zero because nonzero amplitude is carried by the neighbors (Fig. 1). To find the recurrence amplitude, we need a different approximation for the returning wave: it should be a Coulomb scattering wave having a node at θ_f but nonzero amplitude for θ close to θ_f . Such a wave is constructed in the Appendix, and its recurrence amplitude is derived. First, in Sec. II A, we show the quantum calculation of the recurrence spectrum, and then in Secs. II B and II C, we display and explain the refined semiclassical result.

II. RESULTS AND CONCLUSIONS

A. Quantum calculations

Because of a scaling property of the Hamiltonian, spectra at constant scaled energy [7] yield sharper and more precise recurrences than spectra at a constant field. For this reason, the goal of our quantum calculations is to compute absorption spectra and recurrence spectra at constant scaled energy, $\epsilon = EB^{-2/3}$ [8].

There are a number of techniques for computing the spectra of diamagnetic hydrogen [9–11]. The simplest technique is to diagonalize the Hamiltonian in the zero-field spherical basis, and this technique is applicable to the region of energy and magnetic field of interest here.

FIG. 2. (a) Scaled-variables absorption spectrum for $p \rightarrow s+d$ states, i.e., even-parity final-state excitation. The largest peaks are associated with quantum states that are localized near the perpendicular orbit. (b) Scaled-variables absorption spectrum for $s \rightarrow p$ states, i.e., odd-parity final-state excitations. The large peaks are gone. (c) After multiplication by w^3 , the average oscillator strengths decrease as w^{-1} (dashed line), but the density of states increases proportionately, so the average oscillator-strength-density is constant (heavy line).

For $L_z = 0$, the Hamiltonian for the diamagnetic hydrogen atom is, in atomic units,

$$H = H_0 + H_d, \quad (3)$$

where the unperturbed Hamiltonian is

$$H_0 = \frac{p^2}{2} - \frac{1}{r}, \quad (4)$$

and the diamagnetic perturbation is

$$H_d = \frac{1}{8} B^2 r^2 \sin^2 \theta. \quad (5)$$

H_0 is diagonal in our basis, and the matrix elements of H_0 are the unperturbed energies. The matrix elements of H_d are

$$\frac{1}{8} B^2 \langle n_1 l_1 m | r^2 \sin^2 \theta | n_2 l_2 m \rangle, \quad (6)$$

where n , l , and m are the usual quantum numbers used for the hydrogenic basis. The angular part of the matrix element is given by Clebsch-Gordon coefficients. The radial part is obtained by numerical integration.

Once computed, the Hamiltonian matrix is diagonalized using the Lanczos algorithm [12]. This method can be used to compute the overlap of the eigenvectors with a fixed vector. Oscillator strengths were obtained by choosing this fixed

vector to be the dipole operator acting on the initial state, so that in this case the quantity computed by the diagonalization routine is

$$\langle \Psi_j | z | \Psi_i \rangle = \langle \Psi_j | z | n=3, l=0, m=0 \rangle. \quad (7)$$

Here we chose the initial state to be the $3s$ state of hydrogen because of our interest in ongoing experiments involving the $3s$ state of Li. Oscillator strengths are proportional to the square of the above matrix element,

$$f_{ji} = 2m_e(E_j - E_i) |\langle \Psi_j | z | \Psi_i \rangle|^2 / \hbar^2. \quad (8)$$

The Hamiltonian matrix was diagonalized at a number of closely spaced values of magnetic field, and energy levels and oscillator strengths were obtained in the ranges where the scaled-energy spectra were desired. The energy levels, $E_j(B)$, and oscillator strengths, $f_{ji}(B)$, can be obtained as continuous functions of field by cubic-spline interpolation. Since the lines of constant scaled energy, $E = \epsilon B^{2/3}$, are monotonically decreasing functions of energy (for negative scaled energies), and the energy levels, $E_j(B)$, are monotonically increasing (for $L_z=0$), each line of constant scaled energy crosses each energy level exactly once. The value of $w = 2\pi B^{-1/3}$ at which this occurs is found by fixing ϵ and solving for B in the equation

$$E_j(B) = \epsilon B^{2/3} = \epsilon (2\pi/w_j)^2. \quad (9)$$

The value of the oscillator strength at that field value is found by interpolation. The accuracy of the interpolation can be increased by reducing the spacing between adjacent field points. (Inaccuracies in the interpolation limit the accuracy of the recurrence spectra at high actions, but have little effect at low actions.) A scaled-variables absorption spectrum is shown in Fig. 2. At this scaled-energy, most of the classical trajectories are orderly, and quantum states fall into orderly patterns correlated with regular classical trajectories (tori in phase space). For excitation to even-parity final states, quantum states that are localized near the xy plane produce the

largest orderly sequences of peaks in Fig. 2(a). (These were called “rotators” in [1,13].) For excitations to odd-parity final states, [Fig. 2(b)] these large peaks have disappeared. Periodicities remain, but as we show below, the “fundamental” longest wavelength oscillations have almost vanished.

Recurrence spectra were obtained by scaling the absorption spectrum, subtracting the smooth background, and then computing the Fourier transform. The scaling and subtraction is done in the following way. If the absorption spectrum is measured at fixed B as a function of energy, then the average oscillator-strength-density near threshold is essentially constant, independent of E and B for small E and B . We denote this average oscillator-strength-density D_{Ef} and we recognize that it is a derivative $(\partial f(E, B)/\partial E)_B$. In scaled-variables experiments [1,5], the oscillator-strength-density is measured using steps in w at fixed ϵ ,

$$D_w f = \left| \frac{\partial f(\epsilon, w)}{\partial w} \right| = \left| \frac{\partial f(E, B)}{\partial E} \right| \left| \frac{\partial E}{\partial w} \right|_B = D_{Ef} \left(\frac{8\pi^2 \epsilon}{w^3} \right). \quad (10)$$

It follows that at fixed ϵ , the average oscillator-strength-density falls off as w^{-3} , so if we multiply all oscillator strengths by $w^3/8\pi^2\epsilon$, then the background will be independent of w and ϵ . This is illustrated in Fig. 2(c). We subtract the background, multiply by $e^{i\hat{S}w}$, integrate over a large but finite range of w , and take the absolute square of this Fourier transform. This gives what we define as the “quantum scaled-variables recurrence spectrum.”

Such a recurrence spectrum is shown in Fig. 3. This result (for hydrogen) is very comparable to the recurrence spectrum observed for He in [5]. We see a number of large recurrences for $\hat{S} > 4$. However, only small regularly spaced recurrences are present for $\hat{S} < 4$.

Classical calculations show that at these energies the system has two short orbits that go out from and later return to the atom: one parallel to the magnetic field (up or down) and one perpendicular to the field. The parallel orbit produces the larger set of small peaks, at multiples of $\hat{S} = 0.83$. The smallest set of peaks, at multiples of $\hat{S} = 0.77$ are connected with

FIG. 3. Quantum recurrence spectrum at $\epsilon = -0.70$. In the lower part of the graph recurrence strengths are inverted and multiplied by 10. Weak recurrences due to the parallel, V_n , and perpendicular orbits, R_n , are visible.

the perpendicular orbit. However this orbit lies on a node of the quantum wave function, so closed-orbit theory predicted that its recurrence strength should be zero. This observation motivated us to refine the theory for this case.

B. Semiclassical formula for the recurrence strength

The closed-orbit theory asserts that the oscillator-strength density is a smooth background plus a sum of sinusoidal terms,

$$\overline{D_{Ef}}(E, B) = D_{Ef_0}(E, B) + D_{Ef_1}(E, B). \quad (11)$$

D_{Ef_0} is the smooth background representing the average absorption in the absence of recurrences. D_{Ef_1} is the superposition of sinusoidal oscillations, one for each return (n) of each closed orbit (k)

$$D_{Ef_1}(E, B) = \sum_{k,n} C_k^n(E, B) \sin \Delta_k^n(E, B). \quad (12)$$

The phase of the oscillation is

$$\Delta_k^n(E, B) = S_k^n(E, B)/\hbar - \mu_k^n \frac{\pi}{2} - \phi_k, \quad (13)$$

where $S_k^n(E, B)$ is the classical action for n passages around the k th closed orbit (starting and ending at the nucleus), μ_k^n is the Maslov index for the returning wave on that orbit, and ϕ_k is an additional phase: for the zero-degree orbit ($k=0$) $\phi_0 = \pi/4$, while for all other orbits except at a node $\phi_k = 3\pi/4$. $C_k^n(E, B)$ is the recurrence amplitude for the n th return of the k th closed orbit. For the zero-degree orbit the amplitude is

$$C_0^n(E, B) = 2^{9/2} (E - E_i) \pi r_o^{-1/2} \times \left| \frac{d\theta_f}{d\theta_i} \right|^{-1} \mathcal{Y}(\theta_i=0) \mathcal{Y}^*(\theta_f=0), \quad (14)$$

while for all others except those at a node it is given by Eq. (2).

The above results were derived in previous papers. In this paper we show that when the atom is excited from an s to a p state, so that the perpendicular orbit ($k=1$) lies in a node, and Eq. (2) yields zero, then its recurrence amplitude is

$$C_1^n(E, B) = 2^{13/4} (E - E_i) \pi^{1/2} r_o^{-3/4} \left| \frac{d\theta_f}{d\theta_i} \right|^{-3/2} |I(n_i, 0, 1)|^2 \quad (15)$$

and the additional phase is

$$\phi_1 = \frac{\pi}{4} - \frac{\pi}{2} \left[\operatorname{sgn} \left(\frac{d\theta_f}{d\theta_i} \right)_n - 1 \right], \quad (16)$$

where $\operatorname{sgn}(d\theta_f/d\theta_i)_n$ is the sign of the derivative of θ_f with respect to θ_i on the n th closure of the perpendicular orbit [$I(n_i, l, l')$ is a matrix element defined in Du and Delos [2], and n_i is the principal quantum number of the initial state]. These formulas are derived in the Appendix.

We need to reexpress these equations in terms of scaled variables. Define scaled variables as

$$\hat{q} = \frac{q}{2} B^{2/3},$$

$$\hat{p} = p B^{-1/3}, \quad (17)$$

$$\hat{t} = \frac{t}{2} B,$$

to get the scaled Hamiltonian and scaled action,

$$\hat{H} = H B^{-2/3}, \quad (18)$$

$$\hat{S}_k^n(\epsilon) = \frac{B^{1/3}}{2\pi} S_k^n(E, B), \quad (19)$$

$$w = 2\pi B^{-1/3}. \quad (20)$$

Then the action at fixed scaled energy changes with B as

$$S_k^n(E, B) = \hat{S}_k^n(\epsilon) w. \quad (21)$$

Finally, we write

$$Df_1(w; \epsilon) = D_{Ef_1}(E(w, \epsilon), B(w, \epsilon)), \quad (22)$$

i.e., $Df_1(w; \epsilon)$ is $D_{Ef_1}(E, B)$ re-expressed as a function of w and ϵ , and we define the reduced absorption rate as

$$R(w; \epsilon) \equiv B^{-1/6} \frac{\bar{D}f_1(w; \epsilon)}{(E - E_i)}. \quad (23)$$

Combining all of the above formulas, this reduced absorption rate as a function of ϵ and w for an s to p state transition is

$$\begin{aligned} R(w; \epsilon) &\equiv B^{-1/6} \frac{\overline{Df_1}(w; \epsilon)}{(E - E_i)} \\ &= \sum_n (2\pi/w)^{1/2} D_0^n(\epsilon) \sin[\Delta_0^n(w; \epsilon)] \\ &\quad + \sum_n (2\pi/w) D_1^n(\epsilon) \sin[\Delta_1^n(w; \epsilon)] \\ &\quad + \sum_n \sum_k D_k^n(\epsilon) \sin[\Delta_k^n(w; \epsilon)], \end{aligned} \quad (24)$$

where

$$D_0^n(\epsilon) \equiv B^{-1/3} \frac{g_0 C_0^n(E, B)}{(E - E_i)},$$

$$D_1^n(\epsilon) \equiv B^{-1/2} \frac{g_1 C_1^n(E, B)}{(E - E_i)},$$

$$D_k^n(\epsilon) \equiv B^{-1/6} \frac{g_k C_k^n(E, B)}{(E - E_i)}, \quad k \neq 0, 1 \quad (25)$$

and

$$\hat{\Delta}_k^n(\epsilon) = \hat{S}_k^n(\epsilon) w - \mu_k^n \frac{\pi}{2} - \phi_k. \quad (26)$$

FIG. 4. Quantum (heavy line) and semiclassical (light line) recurrence spectra at several scaled energies are compared. For most recurrences, the two are so close that the difference is invisible. Here we see on an expanded scale the weak recurrences associated with the first five returns of the parallel and perpendicular orbits. The larger peaks, occurring near $\hat{S} = 0.83n$, $n = 1, \dots, 5$, arise from the parallel orbit, and the smaller peaks, near $\hat{S} = 0.77n$, arise from the perpendicular orbit. As the scaled energy increases, the fifth recurrence of the perpendicular orbit grows (arrow), and becomes very large at $\epsilon = -0.698$, where a period-5 bifurcation creates a new orbit. That recurrence was seen in experimental measurements [5], and it was called a “ghost” of the orbit that was yet to come [14].

The “reduced” amplitudes $D_k^n(\epsilon)$ are independent of w and the phases $\Delta_k^n(w; \epsilon)$ are linear in w . Hence it follows from the last term in Eq. (24) that each return (n) of each orbit (k) gives a perfectly sinusoidal oscillation in the reduced absorption rate $R(w; \epsilon)$. (This is why the scaled-variables method gives especially clean Fourier transforms.) The parallel ($k=0$) and perpendicular ($k=1$) orbits are exceptions. Because it lies on the axis of cylindrical symmetry, the parallel orbit produces oscillations that are relatively weak, and which decrease with increasing w as $(2\pi/w)^{1/2}$ [first term in Eq. (24)]. The perpendicular orbit, when it lies on a node of the outgoing wave, gives oscillations that decrease as $(2\pi/w)$ [second term in Eq. (24)].

The square of the Fourier transform of $R(w; \epsilon)$, $|\tilde{R}(\hat{S}; \epsilon)|^2$, is the semiclassical recurrence strength.

C. Comparison of quantum and semiclassical results

The semiclassical recurrence strength is compared to the quantum calculation in Fig. 4. The figure shows the quantum calculation in thick lines and the semiclassical calculation in

thin lines. As mentioned previously, the peaks due to the perpendicular orbit are the smallest features at $\hat{S} = 0.75, 1.5, 2.3, 3.05$, and 3.8 . The agreement between the two calculations is quite good for actions below $\hat{S} = 3.5$ at the lower scaled energies in Fig. 4. This confirms the validity of the formula. (Presently there are no experiments that have measured these small recurrences—they are at the noise level of present observations, but we expect them to become visible in the future.)

Figure 4 shows another interesting phenomenon. As the scaled energy increases the predicted recurrence strength of the fifth return of the perpendicular orbit near $\hat{S} = 3.8$ grows much larger than the quantum prediction. The fifth return of the perpendicular orbit undergoes a bifurcation at $\epsilon = -0.698$, just above the highest energy displayed in Fig. 4. At that energy a new orbit splits out of the perpendicular orbit, creating therefore a new peak in the recurrence spectrum. At the bifurcation energy, there is a cusplike focus which causes semiclassical formulas to diverge. Near such a classical bifurcation the quantum recurrence strength increases significantly, but remains finite. A peak at $\hat{S} = 3.8$, $\epsilon = -0.70$ has been seen in experimental measurements [5] and in calculations [14]. This peak is called a “ghost” because, presuming that the perpendicular orbit produces zero recurrence, the peak is a “shadow” or precursor of the new orbit which is about to be created. In Fig. 4, the ghost is the very large peak marked with an arrow.

This interpretation is correct, but it is not the entire story: This peak actually represents the combined effect of the small but nonzero recurrence of the perpendicular orbit plus the ghost of the bifurcation that is about to occur. Therefore this peak is also continuously connected with all of the other weak recurrences of the perpendicular orbit.

As stated before, since our semiclassical formulas diverge at the bifurcation, they overestimate the recurrence strength near the bifurcation. This is visible in Fig. 4 for $\hat{S} = 3.85$, $\epsilon > -0.73$. In other papers we have shown how to repair similar divergences to obtain a finite recurrence strength at a bifurcation [15,16].

ACKNOWLEDGMENTS

The work at MIT was supported by NSF Grant No. 9221489-PHY and ONR Grant No. N00014-90-J-1322. The work at William and Mary was supported by NSF Grant No. 930568-PHY and ONR Grant No. N00014-94-1-0930. J.B.D. thanks JILA for their hospitality.

APPENDIX: DERIVATION OF EQ. (15)

A. Recurrence amplitude and phase for the nodal orbit

The recurrence amplitude and phase are evaluated by the method given in [2]. The problem is divided into distinct regions of space and we use the appropriate Green’s function to propagate the wave function in each region. (1) Near the nucleus, the Coulomb Green’s function is used to propagate waves outward. (2) Far from the nucleus a semiclassical approximation is used to propagate the wave function in the combined Coulomb and magnetic fields. (3) These two regions overlap for intermediate distances and we can connect

the wave functions together on a spherical boundary. In practice the boundary between the inner and outer regions is picked to be $(20-50) a_0$. (4) When the waves return to the nucleus, the semiclassical returning waves in the external region are joined to an appropriate Coulomb-scattering wave in the internal region, and the overlap with $D\Phi_i$ is calculated.

The first three steps are identical to the calculation in [2], and are summarized in Eqs. (A1)–(A12) below.

1. Outgoing waves

The dipole operator of the laser's electromagnetic field produces transitions between the initial state of the atom and states near the ionization threshold. If we consider light linearly polarized along the field, a transition from an s state gives an outgoing p wave with the final m quantum number of zero. In the inner region, where the external magnetic field is weak compared to the Coulomb field, the wave function is given by a Coulomb Green's function acting on the dipole modified initial state:

$$\Psi_{\text{out}}(q') = \int G(q', q'') D(q'') \Phi(q'') dq''. \quad (\text{A1})$$

The Green's function $G(q', q'')$ propagates the wave at q'' to the point q' . Near the nucleus, the Green's function can be separated into radial and angular parts and expanded in the eigenfunctions of the zero-energy Schrödinger equation:

$$G(q', q'') = \sum_{lm} Y_{lm}(\theta', \phi') g(r', r'') Y_{lm}^*(\theta'', \phi''), \quad (\text{A2})$$

$$g(r', r'') = -2\pi i \frac{H_{2l+1}^+(\sqrt{8r'}) J_{2l+1}(\sqrt{8r''})}{\sqrt{r' r''}}, \quad r' > r''. \quad (\text{A3})$$

$J_{2l+1}(\sqrt{8r'})$ and $H_{2l+1}^+(\sqrt{8r''})$ are the regular Bessel function and the outgoing Hankel function, respectively. The initial state can also be separated into radial and angular parts so that $\phi(q'') = R_{ni}(r'') Y_{lm}(\theta'', \phi'')$ and $D(q'') = r'' \cos(\theta'')$. Integrating the asymptotic form of the Hankel function [17] for large r' yields the outgoing wave as a function of r' and θ' :

$$\Psi_{\text{out}}(r', \theta') = -i\pi^{1/2} 2^{3/4} \frac{e^{i\sqrt{8r'}}}{r'^{3/4}} e^{-i3\pi/4} \mathcal{Y}(\theta'). \quad (\text{A4})$$

$\mathcal{Y}(\theta')$ contains both the radial wave function integrals and the spherical harmonics. Explicitly,

$$\mathcal{Y}(\theta') = \sum_{l'} (-)^{l'} I(n, l, l') b_{l'm} Y_{l'm}(\theta', 0), \quad (\text{A5})$$

where

$$I(n, l, l') = \int_0^\infty R_{ni}(r'') r''^3 \frac{J_{2l'+1}(\sqrt{8r''})}{r''^{1/2}} dr''. \quad (\text{A6})$$

The dipole selection rules give $l' = l \pm 1$. Any dipole transition from an initial s state has $\mathcal{Y}(\theta')$ proportional to $\cos \theta'$ and a node in the x - y plane when $\theta' = \pi/2$. For example,

$$2s: \mathcal{Y}(\theta') = -I(2, 0, 1) \frac{1}{\sqrt{3}} \frac{1}{2} \left(\frac{3}{\pi} \right)^{1/2} \cos \theta',$$

$$I(2, 0, 1) = 4.6888. \quad (\text{A7})$$

The result for a $3s$ initial state is exactly the same with $I(2, 0, 1)$ replaced by $I(3, 0, 1) = 9.1804$. We will write the radial integral from the n th s state as $I(n, 0, 1)$.

2. Semiclassical returning waves

The semiclassical approximation relates the wave function $\Psi(r, \theta)$ at an arbitrary "field point" r, θ to the wave function at a corresponding "source point" r', θ' on the initial surface and to properties of the (presumably unique) classical trajectory that goes from the source point to the field point. Using this approximation

$$\Psi_{\text{ret}}(r, \theta) = A_2(r, \theta) \frac{r'}{r} \left[\frac{\sin \theta'}{\sin \theta} \right]^{1/2} \times \exp[i[S_2(r, \theta) - \mu\pi/2]] \Psi_{\text{out}}(r', \theta'). \quad (\text{A8})$$

The classical action S_2 is given by

$$S_2 = \int_{q'}^q \vec{p} \cdot d\vec{q}, \quad (\text{A9})$$

evaluated along the closed trajectory. The semiclassical amplitude A is

$$A_2 = \left| \frac{J_2(t=0)}{J_2(t=T)} \right|^{1/2}, \quad J_2(t) = \frac{\partial(r, \theta)}{\partial(t, \theta')}, \quad (\text{A10})$$

where $J_2(t)$ is the two-dimensional Jacobian evaluated at the initial and final times. The Maslov index, μ , is an integer which counts the number of caustics encountered along the trajectory.

3. Returning Coulomb waves

The semiclassical approximation diverges as $r \rightarrow 0$ for the returning wave. Therefore it is necessary to match Ψ_{ret} in Eq. (A8) to a quantum solution for an incoming Coulomb scattering wave before calculating the overlap. In [2], that Coulomb scattering wave was obtained by the following procedure. They started from a zero-energy Coulomb wave that is incoming along the negative z axis. In parabolic coordinates this solution is the zero-order Bessel function,

$$\Psi_c = J_0(2\sqrt{\xi}), \quad \xi = r - z. \quad (\text{A11})$$

This wave function was rotated so that the direction of the incoming wave matched the direction of the returning classical trajectory, and then to regain cylindrical symmetry it was spun about the z axis by integrating over the coordinate ϕ_k . Taking the asymptotic form of Eq. (A11) and performing the integration over ϕ_k by stationary phase, they ob-

tained the analytic form of an incoming Coulomb wave at the boundary radius r_b [Eq. (4.23a) in [2]],

$$\Psi_{c,\text{inc}} = e^{i\pi/2} 2^{-3/2} \pi^{-1} \frac{e^{-i2\sqrt{r}[1+\cos(\theta-\theta_f)]}}{\sqrt{r \sin\theta \sin\theta_f}}. \quad (\text{A12})$$

The magnitude of the wave in the interior was then taken to be proportional to the ratio of Eq. (A8) and Eq. (A12), evaluated on the boundary sphere r_b at the angle of the returning orbit, θ_f ,

$$\begin{aligned} N &\equiv \Psi_{\text{ret}}/\Psi_{c,\text{inc}}|_{r_b, \theta_f} \\ &= 2^{3/2} \pi e^{-i\pi/2} A_2(r_b, \theta_f) r_b^{1/2} (\sin\theta_f \sin\theta_i)^{1/2} \\ &\quad \times e^{i\sqrt{8}r} \exp\{i[S_2(r_b, \theta) - \mu\pi/2]\} \Psi_{\text{out}}(r_b, \theta_i). \end{aligned} \quad (\text{A13})$$

In the present case, this constant is exactly zero because $\Psi_{\text{out}}(r_b, \theta')$ is proportional to $\cos\theta'$, and for the perpendicular orbit $\theta_i = \pi/2$. Furthermore, Eq. (A12) has the wrong dependence on θ : it is nonzero and smoothly varying near $\theta = \theta_f = \pi/2$, where we need a returning wave that has a node at $\pi/2$. Therefore we go back to Eq. (A11) and start from a different ansatz.

A solution with the right behavior begins from a wave function that has a node on the incoming axis. Such a wave function is proportional to the first-order Bessel function

$$\Psi_{c,\text{node}} = \eta^{1/2} J_1(2\sqrt{\xi}) e^{i\phi}, \quad \xi = r - z, \quad \eta = r + z. \quad (\text{A14})$$

To rotate this result to arbitrary incoming directions, we replace $\xi = r - z$ by $\xi = r - \hat{\mathbf{k}} \cdot \mathbf{r}$ and $\eta = r + z$ by $\eta = r + \hat{\mathbf{k}} \cdot \mathbf{r}$ and “spin” the wave function by integrating over ϕ_k to restore cylindrical symmetry. Repeating the asymptotic expansion and evaluating the integral in ϕ_k by stationary phase, the new analytic form for the incoming wave is

$$\Psi_{c,\text{inc}}^{\text{node}} = \frac{\mp \sqrt{1 - \cos(\theta - \theta_f)}}{2^{3/2} \pi} \frac{e^{-i2\sqrt{r_b}[1+\cos(\theta-\theta_f)]}}{\sqrt{\sin\theta \sin\theta_f}}. \quad (\text{A15})$$

The positive sign corresponds to $\theta > \theta_f$ and the negative sign to $\theta < \theta_f$. This function goes linearly through zero at θ_f , consistent with the odd parity wave function.

The matching constant N_{node} is

$$\begin{aligned} N_{\text{node}} &= \lim_{\theta \rightarrow \theta_f} [\Psi_{\text{ret}}(r_b, \theta) / \Psi_{c,\text{node}}(r_b, \theta)] \\ &= -i2^{9/4} \pi^{3/2} (\sin\theta_f \sin\theta_i)^{1/2} r_b^{-3/4} A_2(r_b, \theta_f) \\ &\quad \times \exp\{i[S_2(r_b, \theta_f) + 2\sqrt{8}r_b - \mu\pi/2 - 3\pi/4]\} \\ &\quad \times \lim_{\substack{\theta \rightarrow \theta_f \\ \theta' \rightarrow \theta_i}} \frac{\mathcal{Z}(\theta')}{\mp \sqrt{1 - \cos(\theta - \theta_f)}}, \end{aligned} \quad (\text{A16})$$

where we have combined Eqs. (A4), (A8), and (A15). To

take the limit, Taylor expand $\mathcal{Z}[\theta'(\theta)]$ in the vicinity of $\theta = \pi/2$ so Eq. (A7) becomes

$$\begin{aligned} \mathcal{Z}[\theta'(\theta)] &= -I(n, 0, 1) \frac{1}{\sqrt{3}} \frac{1}{2} \left(\frac{3}{\pi}\right)^{1/2} \cos\theta' \approx \\ &\quad -I(n, 0, 1) \frac{1}{\sqrt{3}} \frac{1}{2} \left(\frac{3}{\pi}\right)^{1/2} \frac{\partial\theta'}{\partial\theta} \cos\theta. \end{aligned} \quad (\text{A17})$$

Likewise for θ near $\theta_f = \pi/2$, $\mp \sqrt{1 - \cos(\theta - \theta_f)} \approx -2^{-1/2} \cos\theta$, so N_{node} becomes

$$\begin{aligned} N_{\text{node}} &= -i2^{7/4} \pi (\sin\theta_f \sin\theta_i)^{1/2} r_b^{-3/4} A_2(r_b, \theta_f) \frac{\partial\theta'}{\partial\theta} \\ &\quad \times \exp\{i[S_2(r_b, \theta_f) + 2\sqrt{8}r_b - \mu\pi/2 \\ &\quad - 3\pi/4]\} I(n, 0, 1) \end{aligned} \quad (\text{A18})$$

as long as $\partial\theta/\partial\theta'$ is nonzero. It can be shown [6] that $A_2(r_b, \theta_f) \approx |\partial\theta'/\partial\theta|^{1/2}$ so

$$\begin{aligned} N_{\text{node}} &= -i2^{7/4} \pi (\sin\theta_f \sin\theta_i)^{1/2} r_b^{-3/4} |A_2(r_b, \theta_f)|^3 \\ &\quad \times \exp\left\{i\left[S_2(r_b, \theta_f) + 2\sqrt{8}r_b - \mu\pi/2\right.\right. \\ &\quad \left.\left.- 3\pi/4 + \frac{\pi}{2} \left[\text{sgn}\left(\frac{\partial\theta'}{\partial\theta}\right) - 1\right]\right\} I(n, 0, 1). \end{aligned} \quad (\text{A19})$$

The wave function near the nucleus due to the returning waves is the partial wave expansion of Eq. (A14) multiplied by the constant N_{node} .

4. Partial wave expansion of the returning Coulomb waves

Before deriving the partial-wave expansion, let us specialize to the case $\theta_f = \pi/2$. Then Eq. (A15) becomes

$$\Psi_{c,\text{inc}}^{\text{node}}(r_b, \theta) \approx \frac{\left(\theta - \frac{\pi}{2}\right)}{4\pi} \exp\left\{-i\sqrt{8}r_b \left[1 - \frac{1}{8} \left(\theta - \frac{\pi}{2}\right)^2\right]\right\} \quad (\text{A20})$$

for θ near $\pi/2$ (we have used a Taylor expansion about $\pi/2$).

Any exact solution to the zero-energy Schrodinger equation with $B=0$ and $m_l=0$ has the partial-wave (pw) expansion

$$\Psi_c^{pw,\text{node}} = \sum_l T_l \frac{J_{2l+1}(\sqrt{8}r)}{r^{1/2}} Y_{l,0}(\theta, \phi). \quad (\text{A21})$$

We want to evaluate T_l for that function $\Psi(r, \theta)$ whose incoming part goes to Eq. (A20) for r near r_b and θ near $\pi/2$. By orthonormality

$$\begin{aligned} T_l \left[\frac{J_{2l+1}(\sqrt{8}r_b)}{r_b^{1/2}} \right]_{\text{inc}} &= \int Y_{l,0}^*(\theta, \phi) \Psi_{c,\text{inc}}^{\text{node}}(r_b, \theta) \\ &\quad \times \sin\theta \, d\theta \, d\phi. \end{aligned} \quad (\text{A22})$$

Substituting Eq. (A20) into Eq. (A22), we find that the integral has a stationary-phase point at $\theta = \pi/2$, so we can use a Taylor expansion of everything in the integrand. We only want odd-parity $m=0$ states, so we set $l=2k+1$. Then from familiar properties of Legendre polynomials, Eq. 8.6.3 in [17], one can show that

$$Y_{2k+1}^0(\theta, \phi) \approx \left[(-)^{k+1} \sqrt{\frac{4k+3}{4\pi}} 2\pi^{-1/2} \frac{\Gamma(k+3/2)}{\Gamma(k+1)} \right] \times \left(\theta - \frac{\pi}{2} \right). \quad (\text{A23})$$

With this substitution, let $x = \theta - \pi/2$, the integral in Eq. (A22) reduces to the simple form

$$\int x^2 e^{i\alpha x^2} dx = \frac{\pi^{1/2}}{2\alpha^{3/2}} e^{i3\pi/4}, \quad \alpha > 0. \quad (\text{A24})$$

The incoming part of the Bessel function is

$$[J_{2l+1}(\sqrt{8r_b})]_{\text{inc}} = (2\pi)^{-1/2} (8r_b)^{-1/4} e^{-i[\sqrt{8r_b} - (2l+1)\frac{\pi}{2} - \frac{\pi}{4}]}, \quad (\text{A25})$$

so, incorporating all constants,

$$T_{2k+1} = (-)^k \sqrt{2\pi(4k+3)} \quad 2\pi^{-1/2} \frac{\Gamma(k+3/2)}{\Gamma(k+1)} \quad (\text{A26})$$

and in particular

$$T_1 = \sqrt{2\pi} \quad 3^{1/2}. \quad (\text{A27})$$

5. Recurrence strength of the returning waves

We can now calculate the matrix elements, Eq. (1). The wave function near the origin is $N_{\text{node}} \Psi_{c,\text{inc}}^{pw,\text{node}}$, Eq. (A19) times Eq. (A21):

$$\Psi_{c,\text{node}} = N_{\text{node}} \Psi_{c,\text{node}}^{pw} = N_{\text{node}} \sum_l T_l \frac{J_{2l+1}(\sqrt{8r})}{r^{1/2}} Y_{l,m}(\theta, \phi). \quad (\text{A28})$$

The dipole modified initial state,

$$D\Psi_i = r \cos\theta R_{n,l_i}(r) Y_{l_i,m_i}(\theta, \phi), \quad (\text{A29})$$

is overlapped with this wave function. Therefore

$$\begin{aligned} \langle D\Psi_i | \Psi_{c,\text{node}} \rangle &= N_{\text{node}} \sum_{lm} T_l \int_r R_{n,l_i}(r) \frac{J_{2l+1}(\sqrt{8r})}{r^{1/2}} r^3 dr \\ &\times \int_{\theta,\phi} \cos\theta Y_{l_i,m_i}(\theta, \phi) Y_{lm}(\theta, \phi) \\ &\times \sin\theta d\theta d\phi, \end{aligned} \quad (\text{A30})$$

which simplifies to

$$\begin{aligned} \langle D\Psi_i | \Psi_{c,\text{node}} \rangle &= N_{\text{node}} \sum_{lm} T_l I(n, l_i, l) [b_{lm} \delta_{l,l_i+1} \delta_{m,m_i} \\ &+ b_{lm} \delta_{l,l_i-1} \delta_{m,m_i}], \end{aligned} \quad (\text{A31})$$

where b_{lm} are Clebsch-Gordon coefficients [2], Eqs. (4.2) and (4.3). For the transitions of interest here with initial states $2s$ or $3s$ these selection rules give only a single term, $l=1$, $m=0$, and $b_{10} = 1/\sqrt{3}$. The initial and final angles are taken to $\theta_i = \theta_f = \pi/2$. The overlap is

$$\begin{aligned} \langle D\Psi_i | \Psi_{c,\text{node}} \rangle &= -2^{9/4} \pi^{3/2} r_b^{-3/4} |A_2(r_b, \theta_f)|^3 \\ &\times \exp \left(i \left\{ S_2(r_b, \theta_f) + 2\sqrt{8r_b} - \mu\pi/2 \right. \right. \\ &\left. \left. - \pi/4 + \frac{\pi}{2} \left[\text{sgn} \left(\frac{\partial\theta'}{\partial\theta} \right) - 1 \right] \right\} \right) |I(n, 0, 1)|^2, \end{aligned} \quad (\text{A32})$$

and the oscillatory part of the oscillator strength is

$$\begin{aligned} Df_1(E) &= -\frac{2}{\pi} (E - E_i) \text{Im} \{ \langle D\Psi_i | \Psi_{c,\text{node}} \rangle \} \\ &= \sum_n 2^{13/4} (E \\ &\quad - E_i) \pi^{1/2} r_b^{-3/4} |A_1^n(r_b, \pi/2)|^3 |I(n, 0, 1)|^2 \\ &\quad \times \sin \left\{ S_1^n(r_b, \pi/2) + 2\sqrt{8r_b} - \mu_1^n \pi/2 \right. \\ &\quad \left. - \pi/4 + \frac{\pi}{2} \left[\text{sgn} \left(\frac{\partial\theta'}{\partial\theta} \right) - 1 \right] \right\}. \end{aligned} \quad (\text{A33})$$

Notation here has changed, for example from S_2 (which means two-dimensional action) to S_1^n (which means the two-dimensional action on the n th return of orbit number 1, by convention the perpendicular orbit). The recurrence amplitudes and phases are

$$C_1^n = 2^{13/4} (E - E_i) \pi^{1/2} r_b^{-3/4} |A_1^n(r_b, \pi/2)|^3 |I(n, 0, 1)|^2,$$

$$\Delta_1^n = nS_1^1 - \mu_1^n \pi/2 - \pi/4 + \frac{\pi}{2} \left[\text{sgn} \left(\frac{\partial\theta'}{\partial\theta} \right)_n - 1 \right]. \quad (\text{A34})$$

S_k^n is defined as the two dimensional action from origin to origin, not stopping at the boundary. The action of the n th return of an orbit is $S_1^n = nS_1^1$ (however this is not true for the Maslov indices [6,7], $\mu_i^n \neq n\mu_1^1$). This completes the derivation of the recurrence amplitude and phase, Eq. (15), for the quasi-Landau orbit when it lies in the node.

- [1] A. Holle, J. Main, G. Weibusch, H. Rottke, and K. H. Welge, *Phys. Rev. Lett.* **61**, 161 (1988).
- [2] M. L. Du and J. B. Delos, *Phys. Rev. A* **38**, 1896 (1988); **38**, 1913 (1988).
- [3] W. R. S. Garton and F. S. Tomkins, *Astrophys. J.* **158**, 839 (1969).
- [4] A. R. Edmonds, *J. Phys. (Paris) Colloq.* **31**, C4-71 (1970).
- [5] T. van der Veldt, Ph.D thesis, Vrije Universiteit te Amsterdam, 1993 (unpublished); T. van der Veldt, W. Vassen, and W. Hogervorst, *Europhys. Lett.* **21**, 903 (1993).
- [6] J.-M. Mao, J. Shaw, and J. B. Delos, *J. Stat. Phys.* **68**, 51 (1992).
- [7] J. Main, G. Wiebusch, K. H. Welge, J. Shaw, and J. B. Delos, *Phys. Rev. A* **49**, 847 (1994).
- [8] Here we use atomic units defined such that 1 a.u. of magnetic field = 2.35×10^5 T. Many other papers [2,13] use the “Gaussian form” of atomic units in which $B/c \equiv \gamma$ appears everywhere.
- [9] D. Delande, A. Bommier, and J. C. Gay, *Phys. Rev. Lett.* **66**, 141 (1991).
- [10] C. W. Clark and K. T. Taylor, *J. Phys. B* **15**, 1175 (1982).
- [11] M. L. Zimmerman, M. M. Kash, and D. Kleppner, *Phys. Rev. Lett.* **45**, 1092 (1980).
- [12] C. Lanczos, *J. Res. Natl. Bur. Stand.* **45**, 255 (1950).
- [13] J. B. Delos, S. K. Knudson, and D. W. Noid, *Phys. Rev. A* **30**, 1208 (1984).
- [14] M. Kus, F. Haake, and D. Delande, *Phys. Rev. Lett.* **71**, 2167 (1993).
- [15] A. Peters, C. Jaffe, and J. Delos, *Phys. Rev. Lett.* **73**, 2825 (1994).
- [16] J. Gao, Ph.D thesis, College of William and Mary, 1994 (unpublished).
- [17] M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions* (National Bureau of Standards, Washington, D.C., 1964).