Recurrence spectroscopy of atoms in electric fields: Scattering in the presence of bifurcations

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Closed-orbit theory gives a semiclassical formula for the photoabsorption oscillator strength density of atoms in external fields. The oscillator strength can be calculated from the properties of the classical orbits of the highly excited electron moving in the combined Coulomb and electric field. The deviation from the Coulomb potential due to an alkali-metal atom core causes scattering between the classical orbits when a closed orbit returns to the origin. Bifurcations of closed orbits happen when a focus moves through the origin and we present a theory that describes the scattering of the electron waves by the alkali-metal core for atoms in external electric fields in the presence of a bifurcation. [S1050-2947(98)03211-9]

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I. INTRODUCTION

Highly excited electronic state atoms in external fields have become good testing grounds for the connection between quantum and semiclassical mechanics. They are amenable to both theoretical calculations and experimental measurement [1–5]. Closed-orbit theory is a semiclassical theory which predicts the positions and amplitudes of peaks in the Fourier transform of the photoabsorption spectrum: The peaks are at the periods of classical orbits that go out and return to the nucleus; the amplitude depends on the divergence rate of the neighbors of the orbits [6,7]. Closed-orbit theory was developed for hydrogen in a magnetic field by Du and Delos [7]. It was applied to alkali-metal atoms in an electric field by Gao and Delos [8]. The general picture of closed-orbit theory, in which waves excited by the laser go out and are turned around in the external fields, was simple. There were, however, the usual problems that occur in any primitive semiclassical formula. The semiclassical approximation for the returning wave near the core could, and would, become infinite as a focus or caustic passed through the origin. These failures occur at the bifurcation energies where closed orbits are created or destroyed as the parameters controlling the classical dynamics vary [9–12]. Uniform approximations to semiclassical wave functions which repair these failures have been developed in the chemical physics and mathematical literature [13–15] and have become better known in atomic physics [16–19]. The nonhydrogenic core of an alkali-metal atom can be treated semiclassically by either propagating trajectories through a model core potential [20] or by a scattering expansion in terms of hydrogenic closed orbits that are coupled together by the core [21]. The closed-orbit approach in Ref. [21] works well for highly excited states where the effective size of $\hbar$ is small and one can partially avoid the neighborhood of bifurcations. It is an open question how to apply this theory near a bifurcation. We present a closed-orbit theory for scattering in alkali-metal atoms in the presence of bifurcations that occur in static electric fields. The theory can be generalized to handle other types of bifurcations in other static fields.

II. RETURNING WAVES FROM CLOSED ORBITS

A. Oscillator strength and the Green's function

The closed-orbit theory starts from a semiclassical approximation for the Green's function in the formula for the average oscillator-strength density. The strength of a transition is proportional to the imaginary part of the overlap matrix

$$\overline{Df} = -2\pi^{-1}(E-E_i)\mathrm{Im}\langle D\psi_i|G_E^+|D\psi_i\rangle, \tag{1}$$

where ψ_i is the initial state, D is the relevant component of the dipole operator of the laser, and G_E^+ is the outgoing Green's function for electrons of energy E. In this formula, $|D\psi_i\rangle$ effectively constitutes a ''source,'' and $G_E^+|D\psi_i\rangle$ are waves that go out at constant energy from this source. Those waves that later return to the source contribute to the integral $\langle D\psi_i|G_E^+|D\psi_i\rangle$ which governs the absorption rate. A ''primitive'' semiclassical approximation to the Green's function will give a sum of returning waves associated with each distinct closed classical orbit. When the closed orbits bifurcate, this approximation that the classical orbits are distinct and isolated breaks down.

B. Isolated semiclassical returning waves

Isolated recurrences can be labeled by the two indices (k,n), where k labels the particular closed orbit and n is the number of the return to the origin. For an isolated orbit, the returning part of the wave function $G_E^+|D\psi_i\rangle$, call it $\Psi_{\mathrm{return}}^{k,n}(r,\theta)$, can be written as a partial-wave expansion in the regular zero-energy radial functions [22] and spherical harmonics:

$$\Psi_{\mathrm{return}}^{k,n}(r,\theta) = N_k^n \sum_{l\geq|m|} d_{l,m}\sqrt{8}R_l^{\mathrm{reg}}Y_{l,m}(\theta,0), \tag{2}$$

where N_k^n is a matching constant depending on the semiclassical amplitude and phase of the returning wave. Formulas for these constants were derived in [7,8] and explicit expressions are given in [23]. They contain the actions and amplitudes of the classical closed orbits, and the initial angular distribution of the waves excited by the laser, $\mathcal{Y}(\theta_i)$. The coefficients $d_{l,m}$ are chosen to give an azimuthally rotated incoming zero-energy Coulomb wave coming in from the direction θ_f:

$$d_{l,m} = \frac{4\pi}{\sqrt{2}}(-1)^{l-m}e^{i\delta_l}Y_{l,m}^*(\theta_f,0), \tag{3}$$

where $\delta_l=\pi\mu_l$ are the quantum defects. This coefficient will be important later when we calculate the partial-wave expression for the uniform returning waves. The wave function in Eq. (2) contains both incoming and outgoing parts. The outgoing part has both a core-scattered and Coulomb-scattered component: the $e^{i\delta_l}$ in Eq. (3) combines with the asymptotic form of $R_l^{\rm reg}$ in Eq. (2) to give a T matrix for scattering off the core, Eq. (10).

We define

$$R_k^n \equiv \langle D\phi_i | \Psi_{\rm return}^{k,n} \rangle, \tag{4}$$

which we call the ''(k,n) recurrence integral.'' Formulas for these recurrence integrals were developed in [7,8]. One finds, using Eqs. (2), (3), (4), and the initial state wave function, that

$$R_k^n = \frac{4\pi}{\sqrt{2}} \tilde{\mathcal{Y}}(\theta_f^{k,n}) N_k^n . \tag{5}$$

The overlap in Eq. (1) is then approximated by

$$\overline{Df} = -2\pi^{-1}(E-E_i)\,{\rm Im} \sum_{k,n} R_k^n . \tag{6}$$

When core scattering is included, returning waves on the kth closed orbit create core-scattered outgoing waves which will go out on every closed orbit. A portion of the core-scattered wave goes out in the direction of the Coulomb-scattered wave of the kth orbit, this constitutes the ''shadowing'' of the kth orbit by the core because the Coulomb-scattered wave is reduced by the interference with the core-scattered wave. The rest of the core-scattered wave goes out and is a source of waves on all other orbits. These core-scattered outgoing waves are again turned around by the external fields and return to the atom where they produce a whole new set of recurrences. These ''combination-recurrences'' are labeled by both of the hydrogenic orbits $(k_2 n_2; k_1 n_1)$: the recurrence produced by the n_2th return of the k_2th closed orbit which itself had been initiated by the core-scattered wave produced on the n_1th return of the k_1th closed orbit. This describes a single scattering event and for double scattering and multiple scattering we need labels $k_1,k_2,k_3,\ldots$ and $n_1,n_2,n_3,\ldots$. Multiply-scattered recurrence integrals will be denoted $R_{\mathbf{k}}^{\mathbf{n}}$, with bold $(\mathbf{k},\mathbf{n})$. Then we define

$$R_{\mathbf{k}}^{\mathbf{n}} = R_{k_{J+1}}^{n_{J+1}} \left[\prod_{j=0}^{J} (F_{k_{j+1}k_j}^{n_j} R_{k_j}^{n_j}) \right], \tag{7}$$

where J is the total number of core scatterings. If $J=0$, we take the quantity in the square brackets to be ''one'' and the result reduces to the previous formula for Eq. (6). The formula for the modulations in oscillator strength from the closed orbits for an alkali-metal atom is then

$$\overline{Df} = -\frac{2}{\pi}(E-E_i)\,{\rm Im} \sum_{\mathbf{n},\mathbf{k}} R_{\mathbf{k}}^{\mathbf{n}} . \tag{8}$$

The sum in Eq. (8) is shorthand for

$$\sum_{\mathbf{n},\mathbf{k}} R_{\mathbf{k}}^{\mathbf{n}} = \sum_{n_1,k_1} R_{k_1}^{n_1} + \sum_{n_2,k_2} \sum_{n_1,k_1} R_{k_2}^{n_2} F_{k_2k_1}^{n_1} R_{k_1}^{n_1} + \sum_{n_3,k_3} \sum_{n_2,k_2} \sum_{n_1,k_1} R_{k_3}^{n_3} F_{k_3k_2}^{n_2} R_{k_2}^{n_2} F_{k_2k_1}^{n_1} R_{k_1}^{n_1} + \cdots . \tag{9}$$

The scattering between each pair or orbits k to k' is described by the T-matrix-like quantity [24]

$$F_{k',k}^{n} = \frac{i}{\tilde{\mathcal{Y}}(\theta_f^{k,n})\mathcal{Y}(\theta_i^{k'})} \frac{1}{4\pi} \sum_{l \geq |m|} (e^{2i\delta_l}-1) \times Y_{lm}^*(\theta_f^{k,n},0) Y_{lm}(\theta_i^{k'},0). \tag{10}$$

C. Uniform semiclassical returning waves

Bifurcations occur when two or more closed orbits merge with or are created from one another as the parameters controlling the classical dynamics are changed. Whether a closed orbit is isolated or not depends on its action difference in units of $\hbar$ from its neighboring orbits. In the Coulomb plus electric field problem, orbits are created from the orbit parallel to the electric field axis ($\theta_i=0$ on the $+z$ axis). At the bifurcation energy they are identical to the parallel orbit, but then move away from the parallel orbit, to increasing θ_i and to increasing actions, S. At energies less than $E=-2\sqrt{F}$ the orbits can reach $\theta=\pi$ radians and collide with the orbit which is along the $-z$ axis and be destroyed by merger with that orbit. This is the inverse of the bifurcation that created the orbit. These are the only times orbits in this system can bifurcate, so we need uniform approximations which are valid for the''uphill'' and ''downhill'' orbits and the neighborhood of the $\pm z$ axes.

To describe the wave function near the bifurcations, we first define semiparabolic coordinates:

$$\begin{aligned} \hat{r} &= \tfrac{1}{2}(u^2+v^2), \quad \hat{r} = rF^{1/2}, \\ \hat{z} &= \tfrac{1}{2}(u^2-v^2), \quad \hat{z} = zF^{1/2}, \\ \frac{d\hat{t}}{d\tau} &= u^2+v^2, \quad \hat{t} = tF^{3/4}. \end{aligned} \tag{11}$$

The Hamiltonian in these scaled semiparabolic coordinates is

$$\hat{H} = \tfrac{1}{2}(p_u^2+p_v^2) + \frac{m^2}{2u^2} + \frac{m^2}{2v^2} - \epsilon(u^2+v^2) + \tfrac{1}{2}(u^4-v^4) = 2, \tag{12}$$

where $\hat{m}=mF^{1/4}$ is the scaled z component of the angular momentum, ϵ is the scaled energy, and p_u and p_v are $du/d\tau$ and $dv/d\tau$, respectively. We can now derive Hamilton's equations of motion and calculate the closed orbits in the (u,v) space. Since we are interested in the orbits on the $\pm z$ axis, we take $m=0$ and start the orbits from $u=v=0$ and launch them at an initial angle $\theta_i = 2\ \tan^{-1}(p_{v_i}/p_{u_i})$ with $0 \leq p_{v_i} \leq 2$ and $p_{u_i} = \sqrt{4-p_{v_i}^2}$. We define a Poincaré surface of section, (p_v, v) with $u=0$, and record p_{v_f} and v_f when

the trajectory crosses the surface in either direction. For the downhill orbit, we must define a surface of section, (p_u,u) with $v=0$. The following discussions will also hold for the downhill orbit if we replace (p_v,v) by (p_u,u) everywhere.

Gao and Delos showed that for hydrogen the uniform approximation for the returning wave for the $k=0$ near a bifurcation can be written as

$$\Psi^{0,n}_{\rm unif}=D'\int_{p_v}A(p_v)\exp(iF(p_v))\times\mathcal{Y}(\theta_i)J_0(p_v v/\hat{\hbar})J_0(p_u u/\hat{\hbar})p_v dp_v, \quad (13)$$

where

$$A(p_v)=\left|\frac{p_{v_i}}{p_{v_f}}\frac{\partial p_{v_i}}{\partial p_{v_f}}\right|^{1/2}, \quad (14)$$

$$F(p_v)=\left\{\tilde{S}^n_0(\epsilon)-\frac{a_1(\epsilon)}{2}p_v^2-\frac{a_3(\epsilon)}{4}p_v^4\right\}\Big/\hat{\hbar}-\nu\frac{\pi}{2}, \quad (15)$$

and the final momenta in $A(p_v)$ and in the integral are evaluated on the surface of section $u=0$. The constant D' is $-\pi 2^{3/2}$ if the index ν is chosen to be $\nu=\mu_0+2$, where μ_0 is a constant equal to the Maslov index of the central orbit before the bifurcation creates (or after the bifurcation destroys) the new orbits.

We show in the Appendix that this returning wave function has a partial-wave expansion

$$\Psi^{0,n}_{\rm unif,pw}=D'\int_{p_v}A(p_v)\mathcal{Y}(\theta_i)\exp(iF(p_v))\times\left\{\sum_l d_{l0}\sqrt{8}R^{\rm reg}_l Y_{l0}(\theta,0)\right\}p_v dp_v, \quad (16)$$

where d_{l0} is given by Eq. (3). This is an important result — the uniform wave function is constructed by superimposing the azimuthally rotated zero-energy incoming waves with amplitudes and phases determined by the diffraction integral. The exact form of $F(p_v)$ and $A(p_v)$ depends on the type of bifurcation, but Eq. (16) only depends on the principle of superposition and the azimuthal symmetry.

This wave function also includes the outgoing scattered wave: the $e^{i\delta_l}$ in $d_{l,0}$ combines with the asymptotic form of $R^{\rm reg}_l$ to give the T matrix connecting the incoming waves to the outgoing core-scattered wave.

To check Eq. (16), we show that it reduces to the formulas derived in Ref. [19]. We can form the overlap of Eq. (16) with $\langle D\phi_i|$ to get the uniform recurrence integral analogous to Eq. (4) for the primitive semiclassical recurrence. Repeating the procedure that leads to Eq. (5), we have

$$R^n_{k,\rm unif}=\frac{4\pi}{\sqrt{2}}D'\int_{p_v}g(p_v)\exp(iF(p_v))p_v dp_v, \quad (17)$$

where

$$g(p_v)\equiv A(p_v)\mathcal{Y}(\theta^{k,n}_i)\tilde{\mathcal{Y}}(\theta^{k,n}_f). \quad (18)$$

The index k here does not necessarily refer to an isolated orbit, but is a bookkeeping device referring to the central orbit. The angles $\theta^{k,n}_i$ and $\theta^{k,n}_f$ are functions of p_v on the nth return of the central orbit. The uniform recurrence strength in Eq. (17) is similar to the results derived by Gao and Delos [19] and used in [23], but now the $\mathcal{Y}$'s are complex and contain the quantum defects. Now let us examine the scattered portion of the wave and its effect on the recurrence spectrum.

D. Scattering of uniform wave function

The core-scattered wave can be extracted from the asymptotic form of the partial-wave expansion Eq. (16) for the outgoing wave. The result is

$$\Psi^{\rm core,+}_{\rm unif}(r,\theta)=2^{1/4}\pi^{1/2}D'\frac{\exp(i(\sqrt{8r}-3\pi/4))}{r^{3/4}}\times\int A(p_v)e^{iF(p_v)}\mathcal{Y}(\theta_i)\sum_{l\geqslant|m|}Y^*_{l0}(\theta_f)\times(e^{2i\delta_l}-1)Y_{l0}(\theta)p_v dp_v. \quad (19)$$

The initial outgoing wave produced by the laser is

$$\Psi_{\rm out}(\theta)=-i\pi^{1/2}2^{3/4}r^{-3/4}\exp\left[i\left(\sqrt{8r}-\frac{3\pi}{4}\right)\right]\mathcal{Y}(\theta), \quad (20)$$

so the core-scattered wave can be rewritten as

$$\Psi^{+}_{\rm unif}(\theta)=\Psi_{\rm out}(\theta)\frac{4\pi}{\sqrt{2}}D'\int g(p_v)e^{iF(p_v)}F(\theta^{k,n}_f,\theta)p_v dp_v. \quad (21)$$

Here $F(\theta^{k,n}_f,\theta)$ is the analog of Eq. (10) where we have not yet taken θ to be $\theta^{k'}_i$ and $\theta^{k,n}_f$ is integrated over the range of p_v. The portions of this scattered wave that go out in the direction of another closed orbit of the system can be propagated again to get the ''combination'' recurrence. So the combination recurrence formed by scattering the uniform wave function into the direction $\theta^{k'}_i$ is

$$R^{n',n}_{k';k,\rm unif}=R^{n'}_{k'}\frac{4\pi}{\sqrt{2}}D'\int g(p_v)F(\theta^{k,n}_f,\theta^{k'}_i)e^{iF(p_v)}p_v dp_v \quad (22)$$

for scattering into the direction leading to an isolated closed orbit. If $F(\theta^{k,n}_f,\theta^{k'}_i)$ could be factored out from under the integration, Eq. (22) could be written as $R^{n'}_{k'}F^n_{k',k}R^n_{k,\rm unif}$ using Eq. (17) for the uniform recurrence integral. However, $F(\theta^{k,n}_f,\theta^{k'}_i)$ depends on p_v through $\theta^{k,n}_f$ and this cannot in general be done. It is a nice shorthand when manipulating the scattering series, if we remember that it is just a symbolic representation of Eq. (22). It can also be shown that

$R^{n'}_{k'}F^{n}_{k',k}R^{n}_{k,\mathrm{unif}}$ and $R^{n'}_{k',\mathrm{unif}}F^{n}_{k',k}R^{n}_{k}$ are equivalent when the uniform approximation is needed for k' instead of k.

The combination recurrence formed by coupling two bifurcating orbits is given by

$$R^{n',n}_{k',\mathrm{unif};k,\mathrm{unif}} = 8\pi^2 D'^2 \int_{p_v'} g(p_{v'}) e^{iF(p_{v'})} \times \int_{p_v} g(p_v) F(\theta_f^{k,n}, \theta_i^{k'}) e^{iF(p_v)} p_v dp_v p_{v'} dp_{v'} \tag{23}$$

for scattering into an orbit labeled by (k',n').

In the isolated orbit limit the integrals in Eqs. (22) and (23) can be evaluated by stationary phase and they reduce to the primitive semiclassical scattering formula for a single scattering off the core, Eq. (7) with $J=1$.

We can now write the scattering series, Eq. (9), and symbolically replace R^n_k by $R^n_{k,\mathrm{unif}}$ wherever there is a bifurcation. In practice, it is easier to extract the s, p, and d components of the scattered wave by interchanging the order of summation and integration in Eq. (19). In the electric field, where $A(p_v)$ and $F(p_v)$ are given by Eqs. (14) and (15), the diffraction integrals over p_v for each angular momentum l are evaluated at the real and complex stationary phase points by the methods in Ref. [23]. These components are then used to calculate the scattered wave in a direction θ from Eq. (21). This scattered wave is now a source of outgoing waves on all closed orbits of the system. Again it is necessary to include the effect of the scattered wave on the subsequent returns of the orbit that underwent the bifurcation, i.e., shadowing when $k=k'$ in Eq. (9), but now the scattered wave $F^n_{k',k}R^n_{k,\mathrm{unif}}$ contains contributions from both the central orbit and the adjacent stationary phase points. Also, when the combination recurrences formed by coupling other orbits, i.e., $k\neq k'$ in Eq. (9), to the uniform recurrence are computed, they will contain contributions from both central and adjacent stationary phase points. Thus we label the uniform recurrence by $\theta_f^{k,n}$ of the central orbit when the uniform recurrence is the source of the outgoing wave and by $\theta_i^{k'}$ when the uniform recurrence is the recipient of the outgoing wave and this properly accounts for the combined effects of the central and adjacent orbits. Comparisons of the recurrence spectra computed with this improved semiclassical approximation and quantum calculations are given in the next section.

III. COMPARISON WITH QUANTUM CALCULATIONS

Quantum calculations for the triplet helium $m=0$ recurrence spectra were done at several scaled energies between $-3.0<\epsilon<-2.0$ where both the uphill and downhill orbits exist and undergo numerous bifurcations. The principal quantum numbers of the states were in the range $20<n<30$, which leads to relatively large electric field strengths and sizes of the effective Planck's constant, $\hat{\hbar}=\hbar F^{-1/4}$. Triplet helium has fairly large s and p phase shifts from the quantum defects, $\delta_0=0.30\pi$ and $\delta_1=0.07\pi$.

Figure 1 shows the semiclassical recurrence spectrum at scaled energy $\epsilon=-2.70$ compared with a quantum calculation of the recurrence spectrum. In Fig. 1(a), the primitive semiclassical recurrence spectrum shows extreme overestimates of the recurrence strengths at scaled actions starting from $\hat{S}=5.3$ near a bifurcation of the 13th return of the uphill orbit ($\epsilon_{\mathrm{bif}}=-2.773$) and at $\hat{S}=6$ from a bifurcation of the 13th return of the downhill orbit ($\epsilon_{\mathrm{bif}}=-2.703$). These divergent amplitudes are then coupling through scattering to all other orbits at higher actions and thus the recurrence spectrum for actions larger than $\hat{S}=5.3$ is completely wrong in the primitive semiclassical approximation with scattering. By including the uniform approximation for the divergent amplitudes of the 13th returns of the uphill and downhill orbits and the ''shadowing'' effects of the core, but neglecting the core-scattered combination orbits, Fig. 1(b) shows an improved semiclassical recurrence spectrum which is no longer divergent. However, it is only when both shadowing and combination orbits are included that the semiclassical spectrum agrees with the quantum calculation, see Figs. 1(c) and 1(d). Clearly the combination orbits give new peaks in the spectrum, see $\hat{S}=6.4$, 7.6, and 8.1 in Figs. 1(b) and 1(c) for example, but they also interfere destructively with the uni-

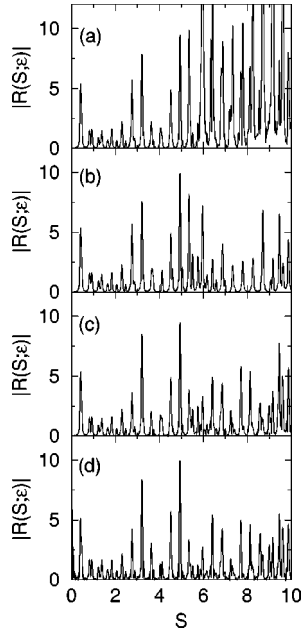

FIG. 1. The recurrence spectrum for helium triplet $m=0$ at $\epsilon=-2.70$ is calculated in several approximations, (a)–(c), and compared to the quantum recurrence spectrum, (d). In (a) the primitive semiclassical approximation is used with core scattering included, Eq. (9) [21]. The divergent amplitudes at $\hat{S}=5.4$ and 6 from the bifurcations of the uphill and downhill orbits become mixed throughout the spectrum. In (b) the primitive semiclassical amplitudes for these orbits are replaced by the uniform amplitudes, but combination orbits are not included. The divergences are removed, but combination recurrence peaks are missing and the interference effects of the combination recurrences are absent. The core scattering is included in the *shadowing* of the orbits. In (c) both the combination recurrences and the shadowing are included. There is now good agreement. The principal quantum numbers for all spectra were in the range $20<n<30$ and the average electric field strength was $F=661$ V/cm.

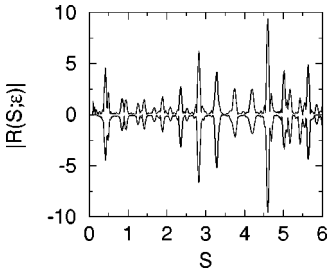

FIG. 2. The recurrence spectrum for helium triplet $m=0$ at $\epsilon=-2.61$ from a quantum calculation (top) is compared to the uniform semiclassical calculation (bottom). The principal quantum numbers for this calculation are in the range $20<n<30$ and the average electric field strength was $F=708$ V/cm. The peak at $\hat{S}=2.82$ is the sixth return of the downhill orbit and is treated by a uniform approximation in the semiclassical spectrum. The peaks at $\hat{S}=3.3$ and $\hat{S}=3.8$ are sensitive to the combination recurrences formed by scattering from the uniform return at $\hat{S}=2.8$ and the agreement with the quantum spectrum is good.

form recurrence peaks at $\hat{S}=5.3$ and 6, further suppressing their contributions to the spectrum. Both the bifurcations of the uphill and downhill orbits at this scaled energy have complex stationary phase points.

A similar calculation at $\epsilon=-2.61$ also shows good agreement with the quantum calculations, Fig. 2. The sixth return of the downhill orbit, at $\hat{S}=2.82$, has a bifurcation at $\epsilon=-2.636$. Above $\epsilon=-2.636$ the stationary phase points of the diffraction integral are real. Below $\epsilon=-2.636$ the stationary phase points are complex. The recurrence strength of the peaks at $\hat{S}=3.28$ and 3.75 at $\epsilon=-2.61$ is sensitive to the coherent sum of the combination recurrences formed from the uniform recurrence (both the central orbit and the real stationary phase points) plus the first and second returns of the uphill orbits. The agreement between the uniform semiclassical spectrum and the quantum spectrum for these peaks is quite good.

At some scaled energies the semiclassical recurrence spectra do show discrepancies in the peak amplitudes when compared to the quantum spectra. Approximations have been made in the program that calculates the combination recurrences. For example, the current programs calculate the shadowing effects of the core recursively at the average field strength to get the shadowed recurrence strengths for each return of an orbit. The uniform scattering in this part of the code is treated exactly. The program then couples these shadowed recurrence strengths up to a maximum in J, see Eq. (7), to get the combination recurrences. In this part of the code the shadowed recurrences are coupled by $F^{n}_{k',k}$, which is only an approximation when one of the shadowed recurrences is a shadowed uniform recurrence. The good agreement shown in Figs. 1 and 2 and other calculations show that this method does describe the essential physics of the scattering system. Further comparisons of the quantum and semiclassical recurrence spectra are being made.

IV. CONCLUSIONS

A method of calculating the scattered wave near a classical bifurcation energy has been developed for alkali-metal atoms in external electric fields. The form of this approximation, a partial wave expansion of the outgoing wave whose coefficients depend on the diffraction integral, Eq. (16), should be generalizable to other types of bifurcations that occur in magnetic and combined electric and magnetic fields by changing the form of the diffraction integral. This should allow the computation of the recurrence spectra in the presence of bifurcations and scattering in other atom-field systems.

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APPENDIX: PARTIAL-WAVE EXPANSION OF UNIFORM WAVE FUNCTION

To calculate the uniform wave function near the nucleus, we would like to find the expansion of the product of Bessel functions $J_0(p_u u/\hbar)J_0(p_v v/\hbar)$ in semiparabolic coordinates in terms of the regular radial functions $R_l^{\rm reg}(r)Y_{lm}(\theta,\phi)$, in spherical coordinates.

The wave functions in the outer region must smoothly connect to the solutions in the inner region. If we require the incoming parts of these functions (denoted by a superscript ''inc'') to be equal, $\psi^{\rm inc}_{\rm s.c.}=\psi^{\rm inc}_{\rm pw}$, in the region $r=50a_0$, then

$$[J_0(p_u u/\hbar)J_0(p_v v/\hbar)]^{\rm inc}=\left[\sum_l C_l\sqrt{8}R_l^{\rm reg}(r)Y_{l0}(\theta,0)\right]^{\rm inc}, \tag{A1}$$

where the coefficients C_l are to be determined and the regular radial functions are defined in terms of the zero-energy solutions of the Schrödinger equation as [8,22]

$$R_l^{\rm reg}(r)=\cos\delta_l\frac{J_{2l+1}(\sqrt{8r})}{\sqrt{8r}}-\sin\delta_l\frac{Y_{2l+1}(\sqrt{8r})}{\sqrt{8r}}. \tag{A2}$$

By orthogonality of the spherical harmonics we have (dropping the ''inc'' temporarily to simplify the equations)

$$C_l\sqrt{8}R_l^{\rm reg}(r)=\int_\Omega Y^*_{l0}(\theta,0)J_0(p_u u/\hbar)J_0(p_v v/\hbar)d\Omega. \tag{A3}$$

We can evaluate this integral by the following substitutions:

$$p_u=|P|\cos\Theta_p,\quad p_v=|P|\sin\Theta_p, \tag{A4}$$

$$u=R\cos\Theta,\quad v=R\sin\Theta,$$

$$d\Omega=\sin\theta d\theta d\phi=4\cos\Theta\sin\Theta d\Theta d\phi, \tag{A5}$$

where we have used $R=\sqrt{u^2+v^2}$ and $\theta=2\Theta$. This gives

$$C_l\sqrt{8}R_{nl}^{\rm reg}(r)=8\pi\int \cos\Theta\sin\Theta Y_{l0}^*(2\Theta)$$
$$\times J_0(PR/\hat{\hbar}\cos\Theta_p\cos\Theta)$$
$$\times J_0(PR/\hat{\hbar}\sin\Theta_p\sin\Theta)d\Theta. \quad \text{(A6)}$$

Now we expand both sides of this equation asymptotically [25]. The incoming part of $\psi_{\rm s.c.}$ in Eq. (A6) becomes

$$\psi_{\rm s.c.}^{\rm inc}=2\pi\int_0^{\pi/2}\sqrt{\frac{\cos\Theta\sin\Theta}{\cos\Theta_p\sin\Theta_p}}\left(\frac{2}{\pi}\frac{\hat{\hbar}}{PR}\right)Y_{l0}^*(2\Theta)$$
$$\times(\exp\{-i[PR/\hat{\hbar}\cos(\Theta_p-\Theta)-\pi/2]\}$$
$$+\text{terms in }(\Theta_p+\Theta)). \quad \text{(A7)}$$

The incoming part of ψ_{pw} in Eq. (A6) becomes

$$\psi_{pw}^{\rm inc}=C_l 2\pi^{-1/2}\left(\frac{\hat{\hbar}}{PR}\right)^{3/2}$$
$$\times(-)^l\{\exp[-i(PR/\hat{\hbar}-3\pi/4+\delta_l)]\}, \quad \text{(A8)}$$

where we have used the identity $PR/\hat{\hbar}=\sqrt{8r}$ (valid when we can neglect the potential). If we evaluate the integral in Eq. (A7) by stationary phase about $\Theta_p=\Theta$, then

$$\psi_{\rm s.c.}^{\rm inc}=2^{5/2}\pi^{1/2}Y_{l0}^*(2\Theta_p)\left(\frac{\hat{\hbar}}{PR}\right)^{3/2}$$
$$\times\exp(-i(PR/\hat{\hbar}-3\pi/4)). \quad \text{(A9)}$$

If we set Eq. (A8) equal to Eq. (A9), then the coefficients C_l are

$$C_l=2^{3/2}\pi(-)^l e^{i\delta_l}Y_{l0}^*(\theta_f), \quad \text{(A10)}$$

since $2\Theta_p$ is the angle of the incoming trajectory θ_f. This is exactly $d_{l,m}$ for $m=0$, the formula for an azimuthally rotated incoming zero-energy Coulomb wave when there is an alkali-metal core.

If we insert Eq. (A10) into Eq. (A1) and then insert Eq. (A1) back into Eq. (13) we can prove Eq. (21). If the isolated orbit approximation holds, then the p_v integral evaluated by stationary phase is just a complex multiplicative constant evaluated for the (k,n) orbit coming in from θ_f. We get the matching constants N_k^n back. If the orbit is not isolated, we do the Fresnel integrals and get the uniform recurrence formula back.

With the explicit form of the coefficients that go into the partial-wave expansion of the uniform wave function, we can calculate the scattered component of that wave.

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