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Inelastic scattering effects in recurrence spectra of He atoms in a magnetic field

L.B. Zhao [a,*], M.L. Du [b]

[a] *Department of Physics and Astronomy and the Center for Simulational Physics, University of Georgia, Athens, GA 30602-2451, USA*
[b] *Institute of Theoretical Physics, Chinese Academy of Sciences, PO Box 2735, Beijing 100080, China*

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Abstract

We report recurrence spectra of He atoms in a magnetic field near the second and third ionization thresholds. The analysis of the recurrence spectra reveals the presence of new peaks. It is shown that these peaks are signatures of inelastic (interchannel) scattering events of active electrons by the atomic cores and they correspond to combinations of electron closed-orbits in different channels. Our calculations are based on a formulation combining the standard closed-orbit theory away from the core region with the close-coupling R-matrix theory in the core region.

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The understanding of quantal behaviors of classical chaotic systems (see, e.g., [1]) has been the driving force in the early studies of Rydberg atoms in strong external fields. Garton and Tomkins were the first to observe oscillations in absorption spectra near ionization thresholds for atoms in a strong magnetic field, and more experimental measurements with much higher energy resolution were made later [2]. A closed-orbit theory (COT) describing the oscillations was developed by Du and Delos [3]. COT relates each oscillation in the absorption spectra to a classical closed-orbit beginning and ending near the nucleus. Gao and Delos [4] introduced a quantum defect into COT in the study of non-hydrogen atoms in an electric field. However, they found the effect to be negligible in their problem. The importance of core scattering was later demonstrated for He atoms in external fields [5], and additional peaks beyond the standard COT were observed in the recurrence spectra. Dando et al. [6] extended COT to describe the recurrence spectra of atoms in external fields by including core-scattered waves. In this extension, the core produces a phase shift in the electron wave function, but the core is frozen and is not allowed to change in the photoabsorption process.

What happens to the recurrence spectra of complex atoms in external fields when the atomic cores can be excited to several quantum states? In a recent study of Rydberg molecules in an external field, effects of inelastic scattering of active electrons by the molecular cores have been observed [7]. This method developed for molecules cannot be directly applied to complex atoms in an external field because the dynamics of atoms in the short-range interaction regions differs from that of molecules, and therefore a different treatment is required for atomic systems. Progress has been made with respect to complex atoms in an external field by Granger and Greene [8]. However, they used a scattering matrix formalism in both small r and large r regions, which deviates from the quantum scattering approach of the standard COT near atomic cores. The scattering matrix formalism has so far been applied only to hydrogen atoms in external fields. The results are being debated vigorously and the formulations are being questioned by Main and Wunner, and Matzkin [9]. This Letter reports calculations of recurrence spectra of He atom in a magnetic field near

* Corresponding author.
E-mail address: zhao@physast.uga.edu (L.B. Zhao).

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the second and third ionization thresholds based on a formulation that combines the closed-orbit theory away from the core region with the close-coupling R-matrix theory in the core region.

The spirit of our method is consistent with the approaches by Dando et al. [6] and Matzkin et al. [7]. The configuration space of atoms in external fields is divided into the inner and outer regions. In the inner region, effects of external fields on quantum systems are negligible, and thus the wavefunctions can be evaluated in fully quantum-mechanical methods. We further divide the inner region into the short-range interaction region and Coulomb region. It is assumed that all the complex dynamics occurs in a small short-range region near the nucleus, while in the Coulomb region the active electron feels only the Coulomb potential. This scheme to divide the configuration space makes it convenient to evaluate the wavefunctions in the inner region using the close-coupling R-matrix method. When the electron is in the outer region, only the Coulomb potential and the magnetic field act on the active electron, the wavefunctions of the active electron can be accurately obtained using the semiclassical method [3]. Then the wavefunctions in the inner and outer regions are matched in the Coulomb region. Below we sketch the physical picture and the matching procedure.

Atoms in a magnetic field, when irradiated by a laser, may absorb photons and produce steady outgoing waves in each channel. We assume that the magnetic field is in the z direction, and use Ψ_{ini} as the wave function of the initial atomic state and D as the dipole operator. The total atomic wave function Ψ describing the photo-absorption satisfies an inhomogeneous Schrödinger equation with a source term $(E-H)\Psi = D\Psi_{\text{ini}}$. The wave function near the source can be separated into a direct part and a returning part $\Psi = \Psi_{\text{dir}} + \Psi_{\text{ret}}$. The direct part Ψ_{dir} represents initial outgoing electron waves in all concerned channels after absorbing photons, and it can be obtained by solving the inhomogeneous Schrödinger equation neglecting the external field. The returning part Ψ_{ret} represents waves of the electron first going away from and then returning back to the source region by the Coulomb potential and the magnetic field. The absorption intensity is essentially determined by the imaginary part of an overlapping integral, $-\operatorname{Im}\int\langle D\Psi_{\text{ini}}|\Psi\rangle$. The direct part and the returning part give, respectively, the smooth background and the oscillations in the absorption spectra [3]. When the initial outgoing waves propagate into the outer region, where the magnetic field cannot be neglected, a semiclassical approximation is utilized to describe the waves of active electrons in each channel. The semiclassical wave function can be constructed from classical electron trajectories [3]. The waves propagating along closed orbits in each channel will return to the core region. In the case of H atoms, the returning waves are scattered only by the Coulomb field; in the present case, the returning waves in *each channel* can be scattered by both the Coulomb field and the core to produce the Coulomb-scattered and core-scattered waves in *all channels*. The wavefunctions for the active electron including both incoming and scattering terms in the matching region can be written as,

$$\begin{aligned}\mathcal{F}^{+}_{\alpha',\alpha m_\ell} = {}& \sum_{\ell}(-1)^{\ell-m_\ell} Y^{*}_{\ell m_\ell}(\theta_{\alpha,f},0)\sum_{\ell' m_{\ell'}} Y_{\ell' m_{\ell'}}(\hat{r}) \\ & \times\left[\frac{i}{2r}\left(\varphi^{-}_{\alpha'\ell'}-\varphi^{+}_{\alpha'\ell'}\right)\delta_{\alpha'\alpha}\delta_{\ell'\ell}\delta_{m_{\ell'}m_\ell} \right. \\ & \left. + \frac{i}{2r}T(\alpha'\ell' m_{\ell'};\alpha\ell m_\ell)\varphi^{+}_{\alpha'\ell'}\right], \end{aligned} \qquad (1)$$

where α is the quantum number of target states [10], $\varphi^{\pm}_{\alpha\ell}(r) = -i\sqrt{2r}H^{(1,2)}_{2\ell+1}(\sqrt{8r})$ with $H^{(1,2)}_{2\ell+1}(\sqrt{8r})$ being the Hankel function of the first and second type, $T(\alpha'\ell' m_{\ell'};\alpha\ell m_\ell) = \delta_{\alpha'\alpha}\delta_{\ell'\ell}\delta_{m_{\ell'}m_\ell} - S(\alpha'\ell' m_{\ell'};\alpha\ell m_\ell)$ with S being the scattering matrix element in the uncoupling representation, $\varphi^{-}_{\alpha\ell}$ corresponds the returning wave at channel αm_ℓ, $\varphi^{+}_{\alpha\ell}$ the Coulomb-scattered wave, and $T(\alpha'\ell' m_{\ell'};\alpha\ell m_\ell)\varphi^{+}_{\alpha'\ell'}$ the core-scattered wave. The scattering matrix elements in the uncoupling representation can be obtained from those in the coupling representation by a representation transformation. If $T=0$, Eq. (1) is reduced to Eq. (4.22c) of Du and Delos's [3] except for a factor $1/2\pi$ which is introduced here for convenience of calculations.

The core-scattered waves in Eq. (1) include the elastic and inelastic components. The inelastic part accompanies a change of core states or channel numbers before and after scattering and is therefore named interchannel scattering, while the core states remain the same before and after an elastic scattering and is therefore named intrachannel scattering. The Coulomb-scattered waves retrace the closed orbits in reverse and lead to oscillations associated with repetitions of orbits when returning to the nucleus. The outgoing core-scattering waves on each closed orbit of each channel may be turned back once more to the core, and therefore additional oscillations associated with intrachannel and interchannel scattering may be produced. Such processes are repeated with increasing time. We match the quantal incoming waves with the semiclassical returning waves at each channel at a sphere of radius (∼30–50 a.u.) dividing the inner and outer regions, as done by Du and Delos [3]. Up to this step, the central effort of describing complex atoms in a magnetic field has been completed. We should mention that when only a single channel is involved, our expressions for the matching of the wavefunctions are reduced to those of Dando et al. [6]. In terms of the solutions obtained from matching, one readily obtains the average oscillator-strength density, the absorption rate and the recurrence spectra.

Using the method described above, we calculated and analyzed the recurrence spectra of He from the metastable 1s2s ^1S state to Rydberg states of He near the second and third ionization thresholds. The two thresholds have an energy difference $\Delta E = 3.4363\ \text{cm}^{-1}$. We assume that He atoms are irradiated by a linearly polarized laser in the z direction, thus $M_L = 0$ for all the final states. We have included the five channels: I 1s$[^2S(0)]a\ell$, II 2s$[^2S(0)]a\ell$, III 2p$[^2P(1)]a\ell$, IV 2p$[^2P(0)]a\ell$, and V 2p$[^2P(-1)]a\ell$, where $a\ell$ represents active electron states, the numbers in the round brackets denote the magnetic quantum numbers M_{L_α}. We found that the outgoing electron $a\ell$ in channel I cannot be returned back by a magnetic field of a few Teslas because of its huge kinetic energy, and as a consequence channel I does not contribute