



R-matrix with time-dependence calculations for three-sideband RABBITT in helium

A. T. Bondy^{1,2,a}, J. C. del Valle², S. Saha^{2,3}, K. R. Hamilton⁴, D. Bharti⁵, A. Harth^{5,6}, and K. Bartschat²

¹ Department of Physics, University of Windsor, Windsor, ON N9B 3P4, Canada

² Department of Physics and Astronomy, Drake University, Des Moines, IA 50311, USA

³ Department of Physics, Panskura Banamali College (Autonomous), Panskura, West Bengal 721152, India

⁴ Department of Physics, University of Colorado Denver, Denver, CO 80204, USA

⁵ Max-Planck-Institute for Nuclear Physics, 69117 Heidelberg, Germany

⁶ Center for Optical Technologies, Aalen University, 73430 Aalen, Germany

Received 11 April 2024 / Accepted 30 July 2024 / Published online 14 August 2024

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Abstract. Following up on a recent paper (Bharti et al. in Phys Rev A 109:023110, 2024), we compare the predictions from several *R*-matrix with time-dependence calculations for a modified three-sideband version of the “reconstruction of attosecond beating by interference of two-photon transitions” (RABBITT) configuration applied to helium. Except for the special case of the threshold sideband, which appears to be very sensitive to the details of coupling to the bound Rydberg states, increasing the number of coupled states in the close-coupling expansion used to describe the ejected-electron–residual-ion interaction hardly changes the results. Consequently, the remaining discrepancies between the experimental data and the theoretical predictions are likely due to uncertainties in the experimental parameters, particularly the detailed knowledge of the laser pulse.

1 Introduction

The reconstruction of attosecond beating by interference of two-photon transitions (RABBITT) is a widely-employed technique to characterize an attosecond pulse train and measure attosecond time delays in photo-ionization processes, e.g., [1–3]. In the typical RABBITT scheme, photoionization occurs by superposition of an infrared (IR) pulse and an extreme ultraviolet (XUV) pulse, which is composed of odd high-order harmonics of the IR field. The photoelectron spectra generated in this scheme contain one sideband between every two consecutive main peaks generated by the XUV field alone.

In 2019, Harth et al. [4] introduced the 3-SB RABBITT scheme, a variant in which the XUV comb comprises multiple odd harmonics of the frequency-doubled IR field. As a result, the photoelectron spectrum in 3-SB RABBITT exhibits three sidebands between the main peaks. We label these peaks S_l (low), S_c (center), and S_h (high), respectively.

The original idea behind the scheme was to compare the RABBITT phase, extracted from oscillations

in the ejected-electron signal as a function of the delay between the IR and the XUV comb, for the center sideband in both the three-sideband (3-SB) and single-sideband (1-SB) setups. Through this comparison, one could directly obtain information about the continuum-continuum phase Φ_{cc} that is introduced by the additional IR transitions that form the sidebands. In order to extract the Wigner phase, which is associated with the single-photon ionization process and the corresponding photoionization delay, measurements of Φ_{cc} are generally replaced by theoretical assumptions [5–7]. However, a direct measurement of the relative phase between two continuum-continuum transitions was reported by Fuchs et al. [8].

While a direct measurement of Φ_{cc} has not yet been achieved with the 3-SB vs. 1-SB setup, in part due to unexpected complications discovered since the original proposal, the multi-sideband setup was analyzed in more detail theoretically by Bharti et al. [9] with supporting calculations for atomic hydrogen. Then the validity of the scheme was illustrated experimentally first on argon [10] and, most recently, on helium [11]. Both experiments were again supported by numerical calculations, using both single-active-electron (SAE) models and the non-perturbative all-electron *R*-matrix (close-coupling) with time-dependence (RMT) approach [12]. Not surprisingly, only qualitative agreement between experiment and theory was achieved for the

The original online version of this article was revised:
The ORCID of K.Bartschat has been added.

^a e-mail: bondy11u@uwindsor.ca (corresponding author)

argon target, which is still rather complex for a detailed numerical treatment. The agreement improved, to some extent, for the helium target, but the remaining differences between the measurements and the theoretical predictions certainly warrant further investigations.

The purpose of the present follow-up paper, therefore, is a thorough analysis of the sensitivity of the theoretical predictions to changes in the model. While it is not the atomic hydrogen wished for by many theorists, the helium target is very suitable for this, since the ejected-electron–residual-ion interaction is effectively electron scattering from the He^+ target. In addition, the initial state as well as intermediate excited bound states, and even doubly-excited states, can be obtained as solutions of the “collision problem” with slightly modified boundary conditions, hence ensuring consistency between the one-electron target problem (He^+) and the two-electron bound-state and collision models. Since relativistic effects are negligible for the present purposes, and the nonrelativistic one-electron orbitals of He^+ are known analytically, one can perform a convergence study by increasing the number of discrete physical bound states in the close-coupling expansion and supplementing them with short-range pseudostates to account for coupling to high-lying Rydberg states as well as the ionization continuum. This is the idea behind the “convergent close-coupling” (CCC) [13] and R -matrix with pseudostates (RMPS) [14] methods that have been highly successful in describing electron collision and steady-state weak-field photoionization processes for the past nearly three decades.

This paper is organized as follows. We begin in Sect. 2 with a brief review of the RMT approach, with specific emphasis on the models used for this paper. We then present our results in Sect. 3 and summarize our main conclusions in Sect. 4. Unless indicated otherwise, atomic units are used throughout.

2 Theory

We employed the general R -matrix with time dependence (RMT) method [12] to propagate the initial $(1s^2)^1S$ bound state of helium in time under the influence of the time-dependent external electric laser field. In order to do so, the program first needs input from a time-independent code, specifically the basis into which we expand the total wavefunction inside the R -matrix box and the dipole matrix elements between all basis functions. Furthermore, the target orbitals for the $e - \text{He}^+$ collision problem need to be provided. We used the RMATRIX-II code [15], whose output has been interfaced with RMT.

In our recent work [11], we set up the simplest conceivable RMT model, namely a nonrelativistic 1-state approach, which we will label “1st” below. As a follow-up on the previous study to carry out a sensitivity check of our predictions, we now define a 3-state (“3st”), a 6-state (“6st”), and finally a 10-state (“10st”) model. In addition to just the $\text{He}^+(1s)$ ionic ground state in

the 1st approach, the latter models include the excited $n = 2$ (3st) and $n = 3$ (6st) physical excited states, as well as $n = 4$ pseudostates (10st). We used the analytically known $1s, \dots, 3d$ orbitals to represent coupling between the low-lying ionic states. On the other hand, the $n = 4$ orbitals were taken to fall off as $\exp(-1.27r)$, where r is the distance from the origin. Hence, they have a significantly shorter range than the physical $n = 4$ orbitals that fall off as $\exp(-0.5r)$. While introducing even more (pseudo)states would have been desirable, the computational complexity was prohibitive and, as we will see below, largely unnecessary.

While using the $1s$ orbital of He^+ is not optimal to obtain the best ground-state energy in the 1st model, this disadvantage is mitigated already in part by the bound-continuum and continuum-continuum terms in the R -matrix Hamiltonian. In the present extension, the situation is further improved through the additional target orbitals associated with the excited ionic states. In fact, the largest improvement is provided by the $n = 4$ pseudo-orbitals, which lower the theoretical ground-state energy to -2.894 in the 10st model, compared to -2.873 (1st), -2.885 (3st), and -2.887 (6st), respectively. While the RMT code has the option of adjusting the initial state energy to its experimental value of -2.9035 [16], we did not use this option, since (i) we checked that the effect is negligible while (ii) the visibility of the results shown below is better without the adjustment due to the offset caused by the slightly different ionization potentials.

Figure 1 exhibits the pulse used in our calculations, as well as a part of the photoionization spectrum. The central wavelength of the fundamental IR was taken as 1030 nm. As described by Bharti et al. [11], the XUV pulse train was generated as odd harmonics of the frequency-doubled fundamental radiation, i.e., starting with a wavelength of 515 nm. Since an XUV spectrometer was not available for the experiment, the widths and the heights of the various components shown in the center panel of Fig. 1 were estimated based on the measured photoelectron signal. This signal was used to generate an experimental frequency spectrum, which was then Fourier-transformed to provide the electric field as a function of time and read in on a numerical grid. The uncertainty about the pulses, including a chirp in the XUV train, and this being a very challenging experiment, may be significant sources for the remaining discrepancies between experiment and theory discussed below.

The bottom panel of Fig. 1 shows the calculated energy-differential ionization probability. For best visibility, we show it on a linear scale between the first two peaks due to the XUV train, in this case the 11th (H_{11}) and 13th (H_{13}) harmonics of 515 nm. With the XUV only, there would just be two peaks in this part of the ejected-electron spectrum, while adding the fundamental IR results in the above-mentioned sidebands labeled $S_{12,l}$, $S_{12,c}$, and $S_{12,h}$, respectively. In addition to creating sidebands, the IR is strong enough to distort the harmonic peaks. We clearly see that the sideband signal depends on the delay between the XUV and IR laser

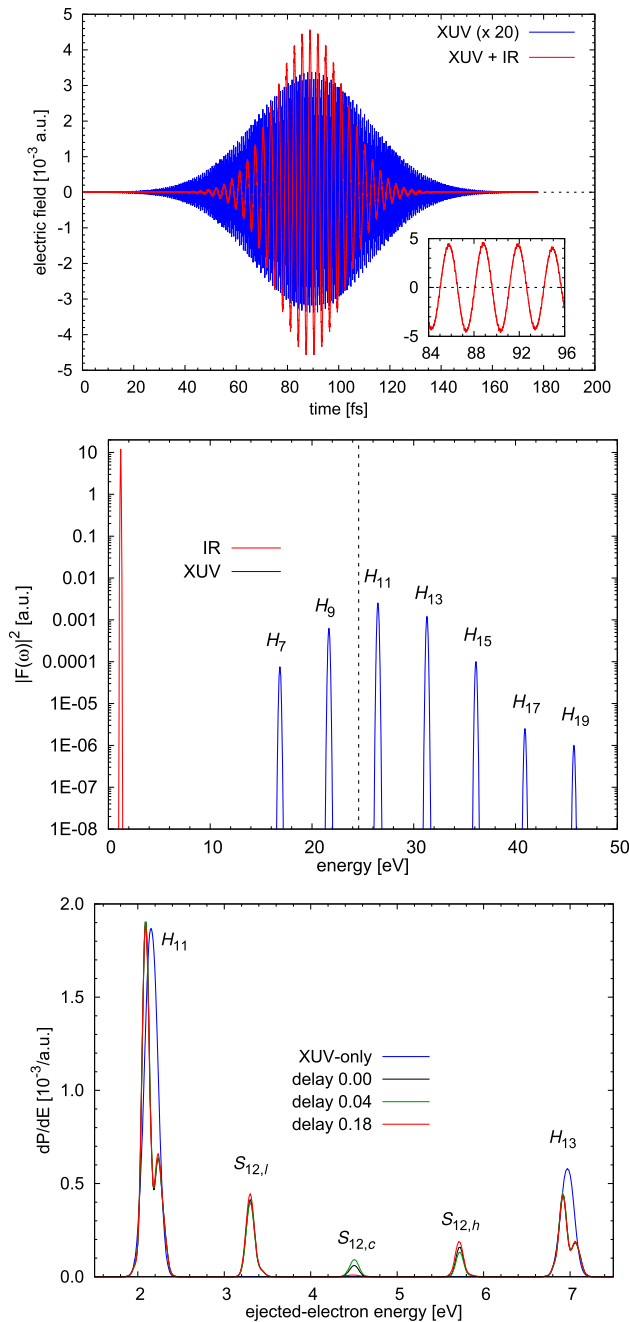


Fig. 1 Top: Electric field for no delay between the fundamental IR and the XUV pulse train. Note that the XUV field was multiplied by 20 for better visibility. The insert shows how small the modification of the IR field by the XUV pulse actually is. In this example, the peak intensity of the IR was set to 7×10^{11} W/cm², while that of the XUV was always kept at 10^9 W/cm². Center: Fourier components of the fields. The XUV pulse trains contains the harmonics $H_7, H_9, \dots, H_{19}$. The heights of the peaks were estimated based on the experimental signal [11]. The vertical dashed line represents the ionization threshold. Bottom: Part of the ejected-electron spectrum. The delays are given in fractions of the fundamental IR period. See text for details

pulses, and also that the center sideband promises the largest contrast. Furthermore, due to both the different strengths of the harmonics and the energy dependence of the photoionization cross section, the heights of the lower and higher sidebands are significantly different.

Below we will show angle-integrated results from theoretical calculations for the sideband groups S_{12}, S_{14}, S_{16} , and S_{18} , as well as angle-differential results from theory and experiment for S_{12}, S_{14} . For S_{16} in the angle-differential case we show theoretical predictions only since there was insufficient signal in the experiment to obtain meaningful data for the latter group. Even though the absolute heights of the peaks vary, we will see that the RABBITT phases Φ_R , which are extracted from the respective signals by fitting each of them to the functional form

$$S(\tau, \theta) = A(\theta) + B(\theta) \cos(4\omega\tau - \Phi_R(\theta)), \quad (1)$$

largely follow the predictions from the decomposition approximation described in Ref. [9]. In Eq. (1), τ is the delay between the IR and the XUV, while A is the average signal and B is the amplitude of the oscillation. These parameters depend on the energy of the ejected electron (i.e., the specific sideband of interest), and one can do the fitting with the angle-integrated signal or pick a particular angle θ or angular range.

3 Results and discussion

3.1 Angle-integrated RABBITT phase

Figure 2 shows our results for the RABBITT phase Φ_R extracted from the angle-integrated ionization signals. The top panel of the graph is for an IR peak intensity of 7×10^{11} W/cm², as obtained in the 1st, 3rd, 6th, and 10th models. The points are not at the same energy due to the theoretical binding energy being different in each model, with the smallest binding energy found in the 1st model and the largest in the 10th model. Consequently, the latter has the peaks in the ejected-energy spectrum at the lowest energy in each group.

There are a number of interesting observations to be made. To begin with, except for the threshold sideband S_{th} , which is the higher sideband of the S_{10} group and the only one above the ionization threshold, we see only a minor dependence on the number of states included in the close-coupling expansion. The main reason for the model sensitivity of the S_{th} RABBITT phase appears to be the fact that this sideband is affected by the XUV-harmonic H_9 , which moves the active electron into a virtual or possibly even a physical state of the Rydberg series. Furthermore, the center sideband, which lies in the Rydberg spectrum, may also come into play for S_{th} in a three-photon process, namely by two IR emissions from H_{11} followed by an absorption. Hence, only a small change in the theoretical model, which will change the ionization potential and the position of the Rydberg states, can have a significant effect on the coupling

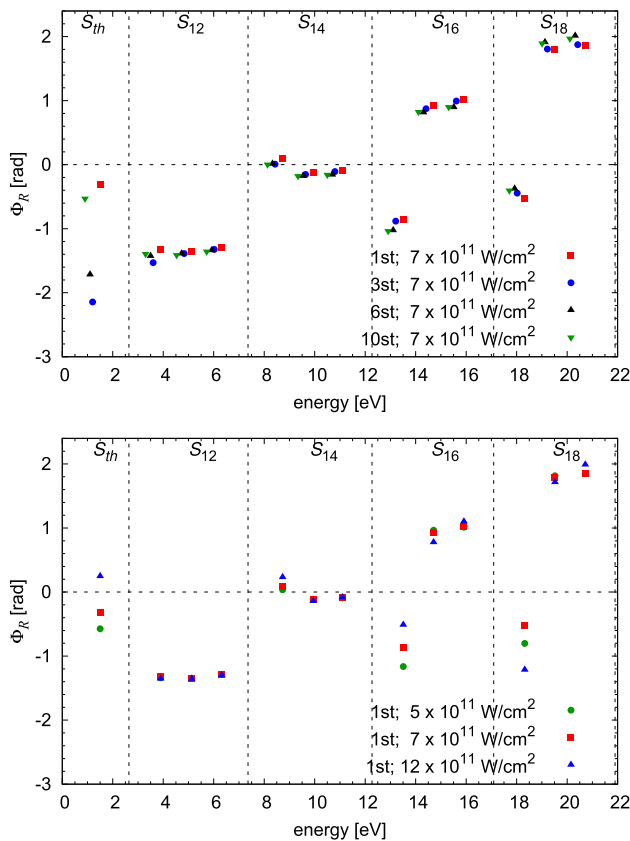


Fig. 2 Top: Absolute angle-integrated RABBITT phases, as obtained in the RMT models with a different number of coupled states for a peak intensity of $7 \times 10^{11} \text{ W/cm}^2$. The vertical dashed lines indicate the approximate positions of the XUV harmonics to guide the eye to the sideband groups. Bottom: Absolute angle-integrated RABBITT phases, as obtained in the RMT-1st model for three different intensities

in the so-called “under-threshold RABBITT” scenario. Experimentally, this sideband also presents exceptional challenges. These are currently being addressed in a follow-up experiment. We expect the results to be reported in a future publication.

Moving on to the sideband groups S_{12} and S_{14} , we essentially see a confirmation of the “decomposition approximation” [9], which predicts the RABBITT phases in each of the three sidebands of a group to be identical, except for a trivial phase π between the center and the lower/higher sideband, which has been compensated for in the graph to show the resemblance clearly. Indeed, the approximation is fulfilled very well. On the other hand, the RABBITT phases for the lower sidebands in both the S_{16} and S_{18} groups differ significantly (by about two radians) from those for the center and higher sidebands. While we do not have an explanation for the size of the difference, the most likely reason for the discrepancy from the predicted similarity of all three phases is the fact that the lower sideband is also coupled to a relatively strong next-lower rather than just the adjacent harmonic in the XUV

comb. It may be possible to gain further insights by applying the analysis suggested by Lucchini [17]. This effect is further enhanced, albeit only slightly, by the decreasing cross section with increasing ejected-electron energy. We emphasize that this effect was also seen in the experimental data presented by Bharti et al. [11]. We do not show these experimental data here, because we can extract the RABBITT phases from absolute delays between the IR and the XUV train. These absolute delays are known theoretically from our construction of the pulses, whereas there is a free offset in the presentation of the experimental data. The latter would reduce the visibility of the results and create a potential source of confusion if other groups were to try similar calculations as those presented here.

Given that the results for an IR peak intensity of $7 \times 10^{11} \text{ W/cm}^2$ generally showed a small dependence on the number of states in the close-coupling expansion, and RABBITT calculations are computationally expensive due to the many delays that need to be scanned through, we only show results from the 1st model in the bottom panel of Fig. 2, but this time for three different IR peak intensities, namely $5 \times 10^{11} \text{ W/cm}^2$, $7 \times 10^{11} \text{ W/cm}^2$, and $12 \times 10^{11} \text{ W/cm}^2$, respectively. The results confirm the general conclusions drawn above. In the S_{12} and S_{14} sideband groups, as well as the center and higher sidebands of the S_{16} and S_{18} groups, where the decomposition approximation seems to be fulfilled very well, there is also only a weak intensity dependence in the extracted RABBITT phase. On the other hand, a much stronger dependence on the IR intensity is seen in the threshold sideband and also in the lower members of the S_{16} and S_{18} groups. The former result can be understood from the fact that the ponderomotive potential will couple the Rydberg spectrum in a slightly different way to the formation of S_{th} if the IR intensity is varied, and the same coupling to the harmonics of very different strength that caused the unusual behavior in $S_{16,l}$ and $S_{18,l}$ for $7 \times 10^{11} \text{ W/cm}^2$ will likely also be the reason at these intensities.

3.2 Angle-differential RABBITT phase

We now move on to the angle-differential case. Figure 3 shows the experimental results [11] in comparison with theoretical predictions for IR peak intensities of $5 \times 10^{11} \text{ W/cm}^2$, $7 \times 10^{11} \text{ W/cm}^2$, and $12 \times 10^{11} \text{ W/cm}^2$, respectively. We concentrate on the S_{12} and S_{14} sideband groups, since experimental data are available for these cases.

We first note that, as in the angle-integrated case, there is only a small dependence on the number of states in the close-coupling expansion. Consequently, the theoretical predictions are likely converged to a higher extent than the remaining differences between the experimental data and the corresponding prediction. Regarding the overall trend, there is qualitative agreement between the data and the RMT results in that the RABBITT phase for the higher sideband in each group drops first with increasing detection angle,

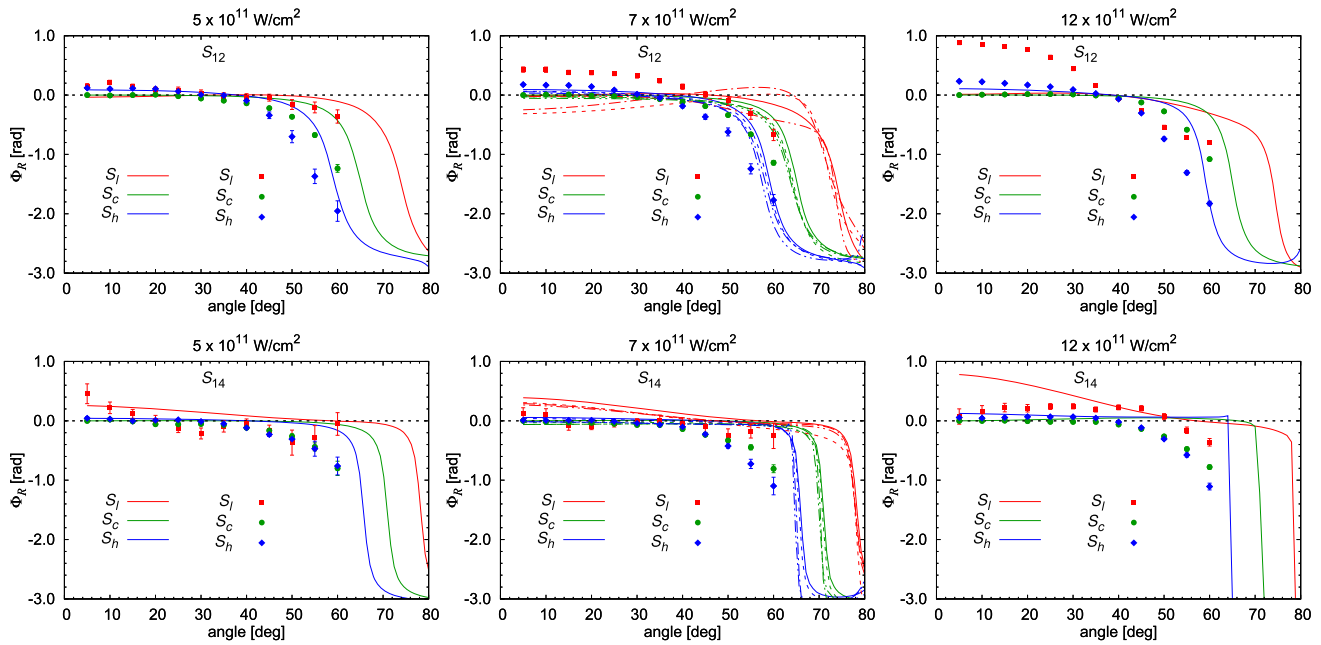


Fig. 3 Angle-differential results for the RABBITT phase in comparison with experiment. The experimental data are represented by the symbols, while the lines representing the theoretical predictions are distinguishable by their color and by the first one to drop rapidly with increasing angle is representing S_h , followed by S_c , and lastly S_l . For the peak intensities of $5 \times 10^{11} \text{ W/cm}^2$ and $12 \times 10^{11} \text{ W/cm}^2$, we only show the 1st results. For $7 \times 10^{11} \text{ W/cm}^2$, we add RMT predictions from models with a different number of coupled states. The linetypes are: solid (1st), dashed (3st), dash-dot (6st), dash-dot-dot (10st). Due to the unknown absolute phase in the experiment, Φ_R for the center sideband is offset to start at zero. Also, to simulate the experimental situation, a 10° window ($\pm 5^\circ$ about the nominal angle) and the energy range of the peak were integrated over

followed by the phase for the center and, finally, the one for the lower sideband. However, the drop in Φ_R (by about π) occurs over a much narrower angular range in the theoretical curves compared to experiment. It is generally sharper in the S_{14} group compared to S_{12} , and it is particularly sharp for the center and higher sidebands in S_{14} .

There is also some disagreement between experiment and theory in the relationship between the RABBITT phases for the various sidebands at small angles. In particular, the experimental data for the lower sideband indicate a strong deviation from the other two, particularly in $S_{12,1}$ at the highest IR peak intensity of $12 \times 10^{11} \text{ W/cm}^2$. Even though the model sensitivity of the theoretical predictions is generally small, it is visible particularly in the lower sideband of both groups. The largest effect is seen in $S_{12,1}$, where the presumably more accurate calculations (6st and 10st) predict Φ_R to start *below* the other two, while the experimental data have it starting *above* them. We currently do not have an explanation for this discrepancy. Since this problem is highly tractable with regard to the underlying theory, effectively electron scattering from a He^+ target, we are confident that our converged calculations are accurate within the assumed input parameters. These calculations involve, of course, some idealizations whose accuracy regarding the physics is limited by the knowledge of and, subsequently, the ability to properly model all the intricacies in the actual experiment.

We finish, once again, with an illustration of the model sensitivity in the results presented above. Figure 4 exhibits the signal as a function of the delay between the IR and the XUV train for both the angle-integrated cases as well as ejected-electron angles of 30° , 45° , and 60° . In the S_{12} and S_{14} groups, one can clearly see the phase of π predicted in the decomposition approximation between the center sideband and the other two. In S_{16} , on the other hand, that phase is there between the center and the higher sideband, while the lower sideband is clearly different.

Finally, we note that it is not always the center sideband that shows the highest contrast, in particular by reaching almost zero intensity for some delays. Sometimes, the higher sideband assumes this role. In all cases, the lower sideband is the strongest, while its oscillation amplitude relative to the average background is generally the smallest of the three. Nevertheless, the delay-dependence of all signals is sufficient to allow a highly accurate fit to the expected signal and hence to extract the RABBITT phase.

4 Conclusions and outlook

In this paper, we discussed the model sensitivity of our theoretical description of a recent three-sideband RABBITT experiment in helium [11]. Except for the

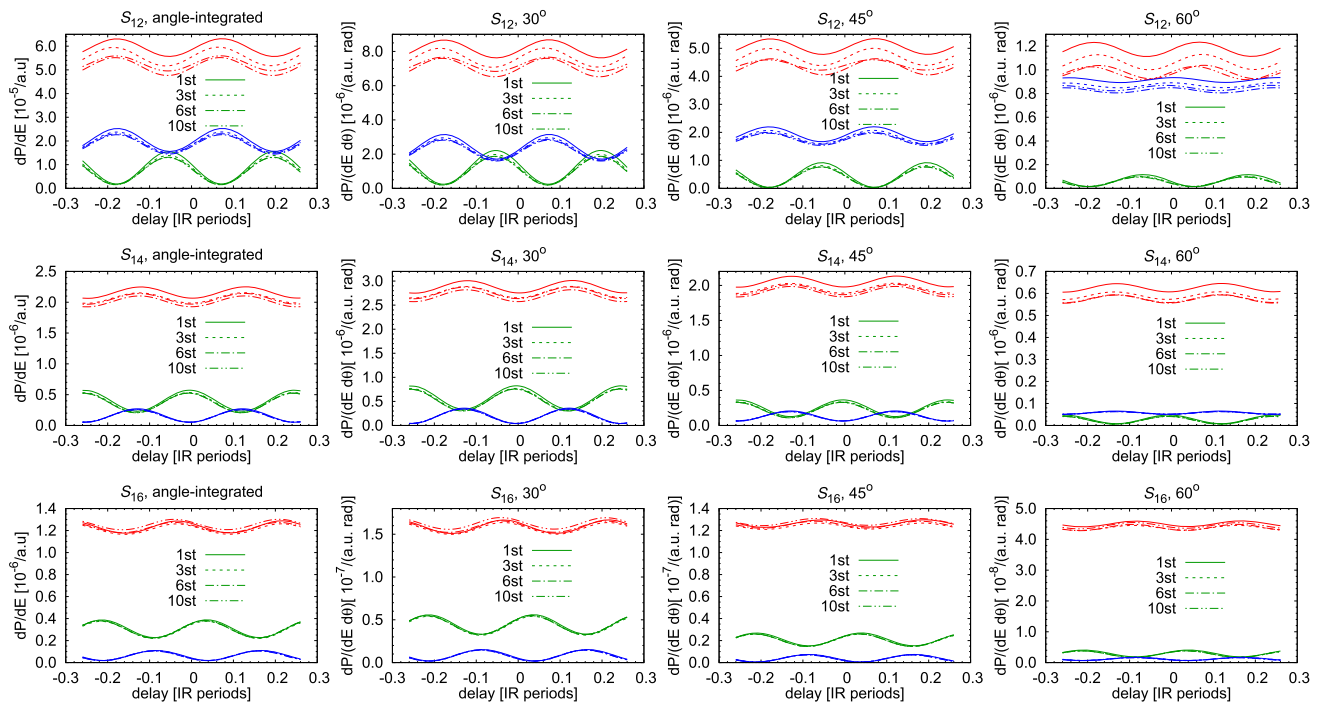


Fig. 4 Predicted signal oscillations for a peak intensity of $7 \times 10^{11} \text{ W/cm}^2$ in the S_{12} , S_{14} , and S_{16} sideband groups. The left column shows the oscillations in the angle-integrated case, while the other columns are for selected ejection angles of 30° , 45° , and 60° , respectively. Again, a 10° window and the energy range of the peak were integrated over. Each panel contains 1-state, 3-state, 6-state, and 10-state results to illustrate the sensitivity of the predictions to changes in the model. In all panels, the lower sideband (in red) has the largest magnitude. In S_{12} , the higher sideband (in blue) is the second-largest, while the center sideband (in green) is the second-largest in S_{14} and S_{16} , except at 60° in S_{14}

threshold sideband, which will be analyzed in a separate study to be carried out in the future, we found that R -matrix with time-dependence calculations in the simplest form of a 1-state model should be sufficient to reproduce the principal characteristics of the process. These include the dependence of the RABBITT phase on the laser intensities involved, as well as the angle dependence of the phases in the three sidebands. We found good agreement with the predictions of the decomposition approximation [9] for two sideband groups, and significant aberrations in the two higher groups, where the weak XUV harmonics and the diminishing photoionization cross section apparently lead to significant deviations in the lower sideband. We note, however, that these deviations were indeed confirmed by experiment [11].

Looking back at the recent experiment and the present paper, we conclude that the 3-SB setup still contains a few surprises that warrant further investigation. The helium target is promising in this respect, since several theoretical groups around the world should be able to carry out calculations of similar sophistication as the ones reported here.

Of particular interest is the under-threshold RABBITT case. With the present laser parameters, the first sideband just above threshold is coupled to the Rydberg spectrum, and hence the results become very sensitive to details of the model and the laser param-

eters. We hope that the present paper will stimulate further investigations of this topic.

Acknowledgements A.T.B., J.C.d.V., S.S., K.R.H., and K.B. acknowledge funding from the NSF through grant No. PHY-2110023 and PHY-2408484 as well as the Frontera Pathways allocation PHY-20028. A.T.B. is grateful for funding through NSERC. The calculations were performed on Stampede-2 and Frontera at the Texas Advanced Computing Center in Austin (TX). The experimental part of this work was supported by the DFG-QUTIF program under Project No. HA 8399/2-1 and IMPRS-QD.

Author contributions

A.T.B. and K.B. wrote the initial draft of the manuscript. A.T.B., S.S. and J.C.d.V. carried out the calculations. A.T.B. performed theoretical analysis. K.R.H. provided guidance in using RMT to carry out the calculations. D.B. generated the experimental data that appear in this work. A.H. conceived of and supervised the experiment. K.B. oversaw the theoretical portion of the paper. All authors contributed to manuscript editing and submission.

Data Availability Statement Data will be made available on reasonable request. [Author's comment: The data

sets generated during the current study will not be deposited, but they are available from the corresponding author upon reasonable request.]

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