PHYSICAL REVIEW A **68**, 020702(R) (2003)

Unambiguous ionization amplitudes for electron-hydrogen scattering

P. L. Bartlett,* I. Bray, S. Jones† A. T. Stelbovics, A. S. Kadyrov, K. Bartschat,‡ and G. L. Ver Steeg‡
Centre for Atomic, Molecular, and Surface Physics, School of Mathematical and Physical Sciences, Murdoch University, Perth 6150, Australia

M. P. Scott and P. G. Burke
Department of Applied Mathematics and Theoretical Physics, The Queen's University of Belfast, Belfast BT7 1NN, Northern Ireland
(Received 14 April 2003; published 25 August 2003)

According to quantum collision theory, scattering amplitudes are complex numbers, which are completely defined by their magnitude *and phase*. Although the phase information is generally not determined entirely in collision experiments, the phases are well defined and can be used to check computational models. We use four state-of-the-art approaches to calculate the magnitude and phase of the electron-hydrogen ionization amplitude in the Temkin-Poet *S*-wave model. We demonstrate that the correct phase can be extracted for each method by using the appropriate final-state continuum functions.

DOI: 10.1103/PhysRevA.68.020702 PACS number(s): 34.80.Dp

Cross sections alone do not yield the complete information about the complex-valued scattering amplitude that describes the outcome of a collision process resulting in the transition from an initial state before to a final state after the projectile-target interaction. As is well known for the two-body Coulomb collision problem, for example, a classical treatment, the first-order plane-wave Born approximation, and the full quantum-mechanical treatment all yield the same elastic differential Rutherford cross section, but only quantum mechanics predicts the correct phase [1]. The possible importance of the phase of the complex scattering amplitude, and a way to determine it unambiguously (in principle), was emphasized a long time ago by Goldberger, Lewis, and Watson [2]. Denoting the amplitude by $\mathcal{F}(\Delta k)$, they wrote: "... it is $\mathcal{F}(\Delta k)$ rather than the experimentally measured quantity $|\mathcal{F}(\Delta k)|$ that is needed; one must have the phase as well as the magnitude. This troublesome problem arises in many contexts, ranging from chemistry to elementary particle physics."

The difficulties of formal ionization theory were the subject of a recent paper [3], in which the exact asymptotic form of the electron-hydrogen ionization wave function was presented. This work resolved the phase ambiguity of the wave function, which has been a stumbling block in extracting the correct phase of the ionization amplitude due to the long-range correlations of the three Coulomb particles. From the point of view of formal ionization theory, it is therefore of fundamental interest to investigate to what extent computational methods can predict not only the magnitude but also the phase of the complex ionization amplitude. We emphasize once again that, according to quantum mechanics, the phase of this amplitude is unambiguously defined, through the relation between the incoming and the scattered beams. It is *not* the overall free phase by which the total wave function may be multiplied without changing any measurable observables.

The calculation of this phase using a direct finite-difference method (FDM) [4,5], "exterior complex scaling" (ECS) [6], "convergent close coupling" (CCC) [7], and the "intermediate-energy *R*-matrix" (IERM) [8] approach is the topic of this Rapid Communication. As will be shown below, the currently implemented way of extracting the phase in the ECS method is still problematic, but it can easily be rectified for the Temkin-Poet *S*-wave model problem [9,10]. This model, in which only projectile and target states with zero orbital angular momentum are accounted for, is well known to provide an ideal test bed for numerical methods that attempt a solution of the classic three-body breakup problem, electron-impact ionization of atomic hydrogen. In addition to FDM, ECS, CCC, and IERM, it has been used to demonstrate the capabilities of methods such as close coupling with pseudostates [11], hyperspherical close coupling [12], *J*-matrix [13], eigenchannel *R* matrix [14], "*R* matrix with pseudostates" (RMPS) [15], *T*-matrix method [16,17], and time-dependent wave-packet approaches [18–20].

It is now well established that all these methods can predict the total ionization cross section to high precision. The single-differential (with respect to the ejected-electron energy) cross section (SDCS) can be accurately predicted as well, provided that the step-function behavior [21] of the "raw" close coupling (CC) results from methods such as CCC, IERM, and RMPS is properly dealt with. The origin of this step function lies in the different treatment of the two electrons, one through a true continuum function and the other by expansion in a square-integrable basis set. If the step height is nonzero, as in the SDCS for the singlet spin channel, the raw results tend to oscillate around the correct answer. This result is similar to the Gibbs phenomenon known from Fourier analysis, as pointed out by Stelbovics [22]. On the other hand, the zero step in the SDCS for the triplet spin channel yields a nearly monotonic SDCS curve in CC methods, in agreement with the exact result on half the energy range and zero elsewhere.

*Electronic address: bartlett@fizzy.murdoch.edu.au
†Permanent address: Physics Department, University of Missouri-Rolla, Rolla, MO 65409, USA.
‡Permanent address: Department of Physics and Astronomy, Drake University, Des Moines, IA 50311, USA.

Three of the present calculations applied to ionization have been detailed previously, FDM [23], IERM [24], and CCC [25]. However, our ECS method is implemented differently to that used by Baertschy *et al.* [6] or McCurdy *et al.* [26]. The idea of complex scaling is retained, but the scattering wave function $\psi_{sc}^{(+)}(r_1,r_2)=\psi^{(+)}(r_1,r_2)-\psi_0(r_1,r_2)$ for the two electrons with coordinates r_1 and r_2 is calculated by applying a propagation scheme based on that used by Jones and Stelbovics [23]. Here $\psi^{(+)}(r_1,r_2)$ denotes the full wave function with outgoing spherical waves after the collision and $\psi_0(r_1,r_2)$ is the unperturbed initial state.

The ionization amplitude is obtained by using the integral representation

$$I=\int \psi^{(+)}(r_1,r_2)(H-E)\phi^{(-)*}(r_1,r_2)\,dr_1dr_2, \quad (1)$$

where $\phi^{(-)}(r_1,r_2)$ is the final-state wave function with incoming waves, H is the system Hamiltonian, and the total system energy is given by $E=\epsilon_1+\epsilon_2=(k_1^2+k_2^2)/2$.

In the ECS method the above volume integral is converted to a surface integral over the hypersphere with radius $R=\sqrt{r_1^2+r_2^2}$, followed by taking the limit of $R\to\infty$. For large but finite R, this yields the amplitude

$$I(k_1,k_2,R)\sim\frac{R}{2}\int_0^{\pi/2}\left[\phi^{(-)*}(k_1,k_2,R,\alpha)\frac{\partial}{\partial R}\psi_{sc}^{(+)}(R,\alpha)-\psi_{sc}^{(+)}(R,\alpha)\frac{\partial}{\partial R}\phi^{(-)*}(k_1,k_2,R,\alpha)\right]d\alpha, \quad (2)$$

where $\phi^{(-)}(k_1,k_2,R,\alpha)$ is the final-state wave function on the hypersphere and $\alpha=\arctan(r_2/r_1)$ is the hyperangle. In the standard ECS approach, this function is taken as a product of two Coulomb waves with equal charges [26,27]. Note, however, that this choice of two Coulomb waves for the final state is in contrast to the FDM, CCC, and IERM techniques, all of which utilize a plane wave for the fast electron and a Coulomb wave for the slow electron.

The latter choice is the natural one to describe the continuum states for the Temkin-Poet model, as it emerges from the separable nature of the Schrödinger equation [9,10]. It is therefore of interest to apply this final state in the ECS method. Specifically, we use the product of a plane wave, numerically orthogonalized to the first ten $l=0$ bound states of atomic hydrogen, and an $l=0$ Coulomb wave with charge $Z=1$. The orthogonalization of the plane wave is an effective way to reduce spurious oscillations and thereby to improve the convergence of the surface integral. This was also found by McCurdy and Rescigno [28] for a short-range potential problem. Note that in the limit of $R\to\infty$ the surface integrals resulting from a plane wave or an orthogonalized plane wave are identical. We label this procedure ECS2.

As an explicit example, we consider the *S*-wave model of *e*-H ionization by 4 Ry incident electrons where the total spin-dependent ionization cross sections are near their maxima. Figure 1 shows the familiar results for the single-differential cross section obtained by the FDM method [5], the ECS approach developed during the present work, and the CCC and IERM methods, respectively. The IERM calculations were performed with an *R*-matrix box radius of $100a_0$ (Bohr radii). Further runs with box radii of $155a_0$ and $185a_0$, respectively, showed an increase in the number of oscillations in the singlet spin channel due to the additional number of pseudostates in the CC expansion, while the triplet results, as well as the predictions from a smoothing procedure for the singlet channel (not shown), are essentially converged. It is seen from the figure that our ECS results are in excellent agreement with the FDM predictions, which we take to be the benchmark since they were obtained by matching to the correct boundary conditions for this problem. The ECS results were obtained at a hyper-radius of $400a_0$, and are much the same whether a Coulomb wave or an orthogonalized plane wave is used for the fast electron. The CCC and IERM calculations exhibit a qualitatively similar step-function behavior. As expected [22], the singlet results converge to around one quarter of the true value at equal-energy sharing. For the triplet case, all four calculations are in excellent agreement on the first half of the energy range, but then CCC and IERM yield negligible cross sections on the second half.

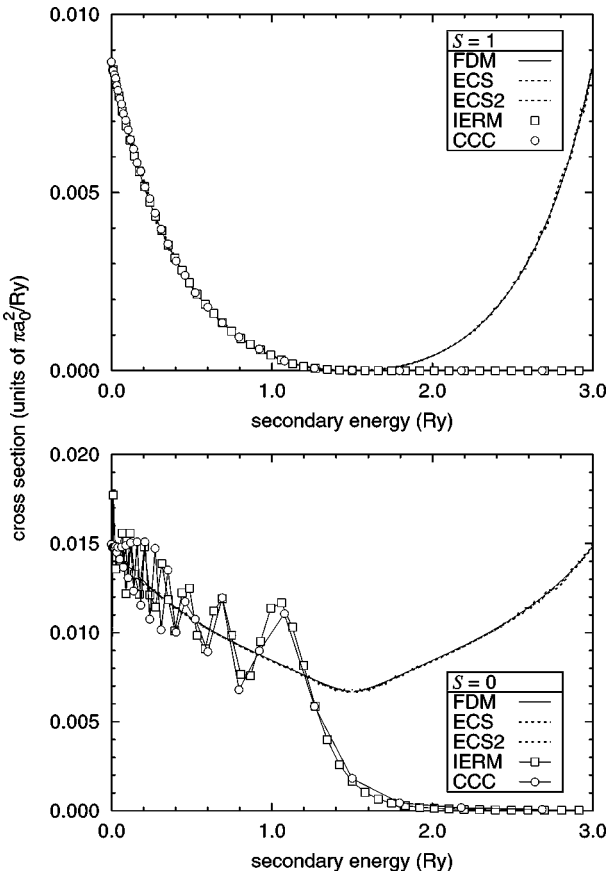

FIG. 1. Single-differential cross section for *e*-H ionization by 4 Ry incident electrons for the two total spin channels $S=1,0$ in the *S*-wave model. The theoretical methods are described in the text. The symbols correspond to the cross sections evaluated at the pseudostate energies. The FDM and the two ECS curves (see text) are barely distinguishable.

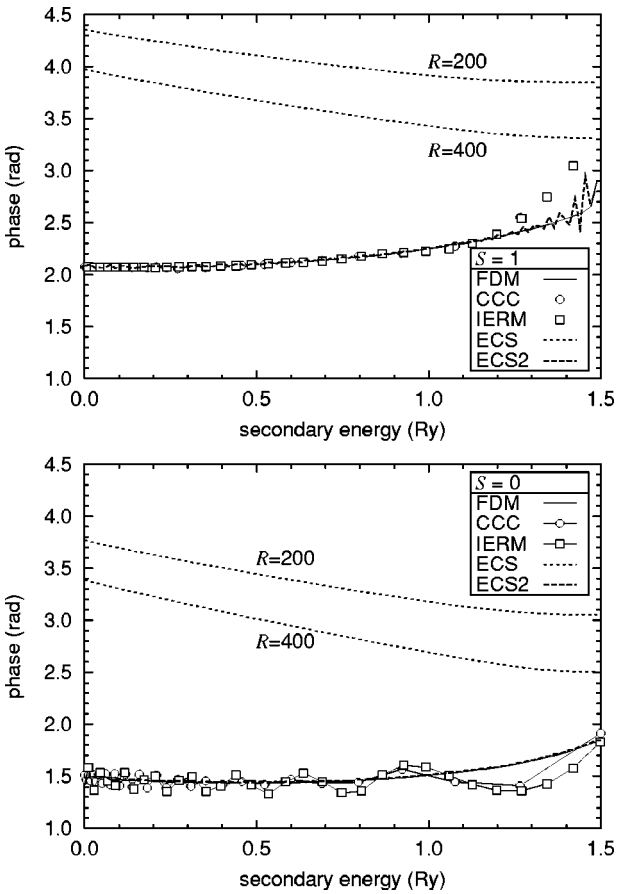

FIG. 2. The phases corresponding to the SDCS of Fig. 1 on the first half of the secondary energy range. The Coulomb phases have not been included. Predictions from the standard ECS method, evaluated with two Coulomb waves in the final state, are shown for hyperradii of $200a_0$ and $400a_0$, respectively. The curve labeled ECS2 is obtained when an ''orthogonalized'' plane wave and a Coulomb wave are used in the final state to form the ECS amplitudes.

No oscillations are expected here due to the zero height of the step.

Figure 2 displays the corresponding phases of the ionization amplitude (the underlying T^S matrix). Contributions from the Coulomb phase(s) are omitted from the presentation due to the known oscillatory behavior at small energies. Because of the step function in the raw CCC and IERM results, the amplitudes only have physical meaning on the first half of the secondary energy range. Consequently, we present results up to equal-energy sharing. (As for the SDCS, the FDM and ECS results will be symmetric with regard to the equal-energy sharing point, while CCC and IERM would need to be explicitly symmetrized.)

There is excellent agreement between the phase of the ionization amplitude extracted from the FDM method and from the ECS2 approach, in which the orthogonalized plane wave is used. The CCC and IERM phases also agree well with these predictions, with the singlet results once again oscillating around the exact results. On the other hand, the ECS phase extracted with two Coulomb waves in the final state is R dependent and exhibits an entirely different behavior as a function of the secondary energy. This lack of convergence in the phase is not surprising, since it is well known that the use of Coulomb waves with fixed rather than screened charges leads to divergent phases in the full e-H ionization amplitude [29–31].

In conclusion, the advanced time-independent methods such as FDM, CCC, IERM, and ECS can, indeed, predict not only the magnitude but also the phase of the complex ionization amplitude. On the other hand, the standard procedure in the ECS method to define the ionization amplitude, with two Coulomb waves in the final state, leads to the correct magnitude but a completely different and diverging phase, which varies slowly with the hyper-radius R at which the amplitude is extracted from the ECS wave function.

In the future, it will be of interest to investigate the phase of the full e-H ionization amplitude. For this problem, we already have strong indications that the magnitudes of the ionization amplitudes are in good agreement between CCC and ECS. However, the phase associated with the ECS final state of two Coulomb waves should again be divergent. Moreover, the continuum final state appropriate for the Temkin-Poet model will not suffice. Instead, the states of Ref. [3] will need to be employed to ensure convergence in the phase extracted from the FDM and ECS methods.

We acknowledge the Merit Allocation Scheme on the National Facility of the Australian Partnership for Advanced Computing. This work was supported, in part, by the Australian Research Council (I.B., A.T.S., A.S.K., and K.B.), the National Science Foundation (K.B. and G.L.V.), and the United Kingdom EPSRC (M.P.S. and P.G.B.). K.B. and G.L.V. would like to thank Murdoch University for the hospitality received during their visit jointly sponsored by international travel grants from the ARC and the NSF.

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