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Multiphoton resonances in $e+H^+$ scattering in a linearly polarized radiation field

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We report a solution of the Gavrila-Kaminski coupled-channel system of equations describing the continuum states of an electron in the combined field of a Coulomb potential and a *linearly polarized* intense radiation field. Convergence was achieved in the number of Floquet states and partial waves for intensities up to 3×10^{14} W/cm^2 at a photon energy of 7.35 eV. In addition, we observed the one- and two-photon capture-escape resonances.

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The approach of Gavrila and Kaminski [1] for determining the bound and continuum states of atomic (ionic) systems in the presence of an intense radiation field has provided [2–8] valuable insights into various phenomena associated with strong laser-matter interactions. In this formulation, a coupled system of differential equations for the Fourier components of the time-dependent wave function in the Kramers-Henneberger gauge [9,10] describes electron scattering by a potential in the presence of a monochromatic laser field. Reliance is made only on a few hypotheses common to many other theories [11], namely, the dipole approximation, a nonrelativistic treatment, and a monochromatic radiation field. Within these limits, the approach is completely general, provided that the solution of the coupled-channel system is carried to convergence. In the high-frequency and high-intensity limit, this system uncouples [1], leading to a description in terms of a single component, which represents elastic scattering. In the past, most applications have dealt with the uncoupled case, and thus represent physical results only under very restricted conditions. Several calculations have been extended to the energetically coupled channels, including the pioneering work of Dimou and Faisal [2], of Franz *et al.* [7], and of Zoller and co-workers [4,8] who employed a multichannel quantum-defect (MCQD) theoretical scheme. However, all of these endeavors have been restricted to circularly polarized radiation fields or to one-dimensional models [12]. This may be a serious restriction since, in the case of circularly polarized field, the one-electron Schrödinger equation can immediately be reduced to a time-independent form in a rotating frame, which is not the typical case. In addition, the system can reach a very limited set of intermediate (virtual) states due to angular momentum conservation requirements. Therefore, in order to exhibit the full power of this technique, we have extended calculations in the coupled-channel formulation to a linearly polarized external field. In this paper, we report the solution of the Gavrila-Kaminski coupled-channel problem for linearly polarized external radiation field. We observe the one- and two-photon capture-escape resonances in the elastic-scattering cross section of an electron by a proton (i.e., for a Coulomb potential) in the presence of a strong, linearly polarized radiation field, similar to those explored for circularly polarized light. These resonances arise from the formation of a temporary bound state of the electron-proton system in the presence of the laser field accompanied by the emission and subsequent absorption of one or two photons.

We follow the basic formulation of Gavrila and co-workers [1,3,6] and Pont [5] and use the Kramers-Henneberger gauge for the time-dependent Schrödinger equation that describes the interaction of an electron with a proton in the presence of an oscillating electric field. The results of these manipulations in atomic units (a.u.) yield

$$[-\tfrac{1}{2}\nabla^2+V(\mathbf{r}+\boldsymbol{\alpha}(t))]\psi=i\frac{\partial\psi}{\partial t}\,, \tag{1}$$

where $\boldsymbol{\alpha}(t)$ is the classical radius vector of the electron under the influence of only the radiation field, and $V(\mathbf{x})$ represents the Coulomb interaction, $-1/|\mathbf{x}|$. By choosing $\mathbf{A}=\mathbf{a}\sin\omega t$ for the vector potential of the radiation field, we obtain,

$$\boldsymbol{\alpha}(t)=\frac{\mathbf{a}}{\omega}\cos(\omega t)\equiv\boldsymbol{\alpha}_0\cos(\omega t)\,. \tag{2}$$

We conveniently select the polar axis to lie along the radius vector ($\boldsymbol{\alpha}_0=\alpha_0\hat{\mathbf{z}}$). We invoke the usual Floquet ansatz and expand the periodic part of the wave function in a Fourier series. In addition, we make a single-center expansion of the spatial function as

$$\psi(\mathbf{r},t)=e^{-iEt}r^{-1}\sum_{n=-\infty}^{\infty}e^{-in\omega t}\sum_{l_n,m_n}f_{nl_nm_n}(r)Y_{l_nm_n}(\hat{\mathbf{r}}) \tag{3}$$

with E serving as the quasienergy and $\hat{\mathbf{r}}$ representing the angular coordinates (θ,ϕ), θ referring to the angle between $\boldsymbol{\alpha}_0$ and $\mathbf{r}$. Substituting Eq. (3) into (1), multiplying through by a specific Fourier and angular component $\exp(in'\omega t)Y_{l_{n'}m_{n'}}(\hat{\mathbf{r}})$, and integrating over a period of the field ($T=2\pi/\omega$) as well as angle, we derive a set of coupled second-order differential equations,

$$\left[\frac{d^2}{dr^2}-\frac{l_{n'}(l_{n'}+1)}{r^2}-k_n^2\right]f_{\Gamma'}(r)=\sum_{\Gamma}U_{\Gamma'\Gamma}(r)f_{\Gamma}(r)\,, \tag{4}$$

where $k_n^2=(E+n\omega)$,

$$U_{\Gamma'\Gamma}(r)=\sum_{\lambda}\left[\frac{2l_n+1}{2l_{n'}+1}\right]^{1/2}C(l_n\lambda l_{n'}|m_n0m_n)\times C(l_n\lambda l_{n'}|000)v_\lambda^{n'n}(r)\,, \tag{5}$$

and

$$v_\lambda^{n'n}(r)=\frac{(2\lambda+1)}{\pi}\int_0^\pi dv\,P_\lambda(v)\times\int_{-1}^{1}du\frac{V(\mathbf{r}+\boldsymbol{\alpha}_0u)T_{n'-n}(u)}{(1-u^2)^{1/2}},\tag{6}$$

with $u\equiv\cos(\omega t)$, $v\equiv\cos(\theta)$, and $T_k(u)$ $[P_k(v)]$, the Chebyshev [Legendre] polynomial of order k. The Clebsch-Gordan coefficients are given by $C(l_1l_2l_3|m_1m_2m_3)$, and the channels $\Gamma=(n,l_n)$ are labeled by a Floquet-state quantum number n and its associated angular momentum quantum number l_n. We extract the scattering information by matching the asymptotic form of these radial components to the usual K-matrix conditions from which we also calculate the S and T matrices. We associate several important properties with these equations. First, they are block diagonal in the azimuthal quantum number ($m_n=m_{n'}\equiv m$) although all Fourier components couple. Therefore, the coupled equations may be solved independently for each value of m. Second, only those channels with the same parity, determined by whether $n+l_n$ is even or odd, couple. Third, the equations bear a striking similarity to those for electron scattering from a linear ionic diatomic molecule in the static approximation for electronic transitions between alternating σ_g and σ_u states. We have used this resemblance to check many of the programming details.

We solve Eq. (4) numerically in the close-coupling (CC) approximation in which the expansion is truncated at a finite number of channels, N. In the inner region ($r\leq\alpha_0$), we convert Eq. (4) to a system of coupled integral equations and effect a solution by means of a linear algebraic (LA) prescription [13]. In the outer region, we employ an R-matrix propagation scheme [14] to extend the solution into the asymptotic regime. For electron-proton scattering, the potential is local, and we could employ the R-matrix propagation for all radial values. However, we have utilized the LA method in the inner region to demonstrate the versatility of our approach. As has been demonstrated for electron-molecule collisions [13,14], this technique can just as easily handle multielectron and nonlocal effects. In addition, the formulation admits the use of different gauges in various spatial regimes [12]. A direct correlation exists between the displacement α_0 and the size of the expansion basis in Eq. (3) needed for convergence. In close analogy to the internuclear separation in electron-molecule collisions, the displacement represents the separation of "effective charges"—the more extended this separation, the larger the corresponding basis required to span the regime. Displacements of the order of 5 bohrs ($5a_0$) are easily tractable on most supercomputers such as a Cray Y-MP with single symmetries requiring a few minutes. Removing the single-center expansion should allow the exploration of a more extensive range of α_0. We recall that the restriction rests with a ratio of the intensity to frequency (E_0/ω^2). Therefore, we can treat very intense fields as long as the frequency is high. We have checked the programs in several ways. First, for the elastic scattering ($n-n'=0$), we have closed all channels and solved for the bound eigenstates of U_{nn}. For a selection of values of α_0, we obtain excellent agreement with the results of other investigators [3] for the ground σ_g state. Second, we have employed the $e^-+H_2^+$ paradigm to examine an analogous multistate coupling scheme, obtaining agreement for all scattering quantities with earlier molecular collision programs [15]. We have in all cases assiduously checked the convergence of the scattering quantities as a function of the number of channels N, the number of mesh points, and the matching radius, pushing the convergence to better than a few percent. For the parameters considered, we generally found that at least a nine-state ($n\leq|4|$) CC calculation was required with three to four ($l\leq5$ or 7) partial waves for each state ($27\leq N\leq33$) for this level of convergence.

One of the most interesting phenomena predicted by the circular-polarized calculations is the capture-escape resonance in which the electron emits a specific number of photons, becomes temporarily trapped in one of the bound states, and then absorbs an equivalent number of photons to escape. Therefore we expect such a situation to arise when the energy difference between the electron and n photons approximately equals the binding energy of a bound state. The "binding potential" ($V_{\Gamma\Gamma}$; $n=n'=0$) determines to a large extent the location of the resonance energy while the strength of the coupling matrix elements ($V_{\Gamma\Gamma'}$) to the decay states establishes the width. Since both of these quantites depend strongly on laser intensity, the resonance will exhibit a position shifted relative to the hydrogenic bound state and a variable width as the field strength increases. In Fig. 1, we present the magnitude of the elastic-scattering T-matrix element $[(0,2)\rightarrow(0,2)]$ as a function of the quasienergy E for an electric field E_0 of 0.0207 a.u. ($I=1.5\times10^{13}$ W/cm^2) and a frequency of $\omega=0.27$ a.u. (7.35 eV) with $m=0$ and even parity. This case, which yields a displacement of $0.284a_0$, has been extensively studied for circularly polarized light [7,8]. We note immediately the presence of the capture-escape resonances. The lowest peak corresponds to the temporary capture of the incident electron into the ground $1s$ state of

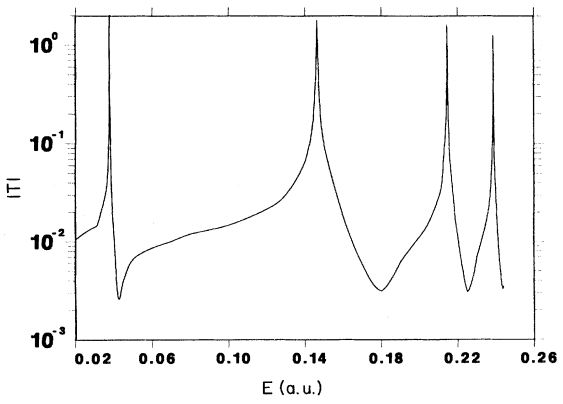

FIG. 1. The magnitude of the elastic-scattering T-matrix element $(0,2)\rightarrow(0,2)$ as a function of the quasienergy E for $E_0=0.0207$ a.u. (1.5×10^{13} W/cm^2) and $\omega=0.27$ a.u. (7.35 eV) for $n\leq|5|$ and $N=33$.

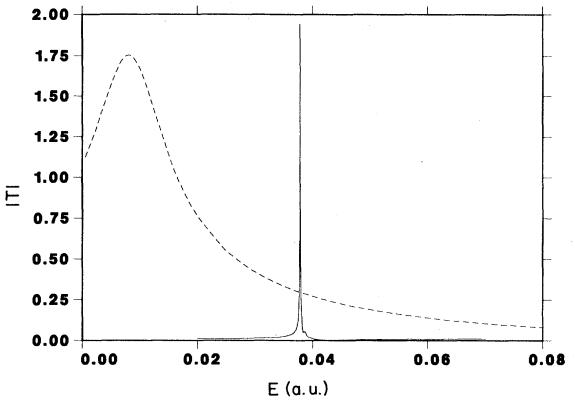

FIG. 2. Same as Fig. 1 for solid line but with $E_0=0.0952$ a.u. (3×10^{14} W/cm^2) for the dashed curve.

H by two-photon emission. The expected position is 0.04 a.u., and we notice a distinct downward shift. For the five-state case ($n\leq|2|$), the lowest coupling order at which double-photon processes can appear, we observed an upward shift. However, as more states are included ($N\rightarrow 11$), the position moves below 0.04 a.u., demonstrating the great importance of the inclusion of a large CC basis. The remaining series of resonances are associated with single-photon transitions to the excited states of H with principal quantum numbers equal to 2, 3, and 4, respectively. The positions of these resonances shift to higher energies than expected from pure energy conservation, indicating the strong interaction among the various channels. This series, of course, converges on the ionization limit at 0.27 a.u. and forms an ideal candidate for a MCQD approach suggested by Marte and Zoller [8]. In Fig. 2, we examine the effects of increasing field strength on the resonance parameters. For the same frequency, we increase the field to 0.0926 a.u. ($I=3\times10^{14}$ W/cm^2) and observe that the position of the two-photon resonance shifts down and the width considerably broadens. The one-photon resonances for this intensity also broaden but shift to higher energies. We note that the eigenphase sum also reveals the resonance structure described above and can be used to determine widths and shifts. Finally, for the frequency considered, we have not reached the intensity regime where stabilization [16] begins for the low-lying states of hydrogen. However, with this approach such phenomena can be investigated, which we shall pursue in future studies.

We have extended the approach of Gavrila and Kaminski to the solution of the Schrödinger equation in the Kramers-Henneberger gauge for electron-proton scattering in an intense *linearly polarized* radiation field using a Floquet-Fourier expansion and solving the resulting set of coupled differential equations. We observed the one- and two-photon capture-escape resonances and examined their behavior as a function of field strength.

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