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Hydrogen in intense laser fields: Radiative close-coupling equations and quantum-defect parametrization

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A system of radiative close-coupling equations for a hydrogen atom in a circularly polarized intense laser field is derived. The radiative scattering matrix is parametrized within a multichannel quantum-defect formalism. The quasienergy spectrum corresponding to nonperturbative shifts and ionization widths of the bound atomic states is computed from the poles of the radiative scattering matrix. For an intensity range up to $\alpha_0 \approx 1.5a_0$ (with α_0 the oscillation amplitude of the free electron in the laser and a_0 the Bohr radius), numerical results are presented in the frequency regime where two-photon ionization and above-threshold ionization of the ground state is possible. For one-photon transitions a stabilization of the atomic states for strong fields is predicted.

I. INTRODUCTION

During recent years there has been increasing interest in multiphoton transitions in atomic and molecular systems induced by intense laser fields. The processes studied include multiphoton ionization [above-threshold ionization (ATI)], harmonic generation, and (low-energy) electron scattering in the presence of a laser field (for a review of recent theoretical work, see Ref. 1). On the theoretical side this has stimulated the development of nonperturbative techniques to model these strong-field interactions. Examples are L^2-basis calculations,[2-5] direct numerical integration of the time-dependent Schrödinger equation for one-dimensional model problems and (realistic) atomic systems,[6-8] variants and improved versions of the Keldysh theory,[9,10] high-frequency approximations,[11,12] and the solution of close-coupling equations.[13-16] In a previous paper we have developed a theory of a hydrogen atom in an intense laser field, based on the following observations.[13]

A free electron in a laser field oscillates with the frequency ω of the light and amplitude α_0 proportional to the electric-field amplitude $\mathcal{E}_0$. Quantum mechanically, this is described by the Volkow solution of the Schrödinger equation. To study the motion of an electron moving both under the influence of a laser and a binding Coulomb potential, it is convenient to transform the Schrödinger equation to a moving frame, to eliminate the asymptotic free-electron oscillations (Kramers-Heisenberg transformation, see references in Ref. 11). By means of a Floquet ansatz in time it will be possible to reduce the time-dependent Schrödinger equation to a system of *radiative close-coupling equations* (RCCE's) for a given quasienergy of the electron.[13-15] The potential in these RCCE's is asymptotically a Coulomb potential (this is a consequence of the fact that the elastic component of the free-electron oscillations has been transformed away). The radiative channels in the close-coupling equations can be identifed as dissociation channels of the electron-ion complex where the electron moving away from the ion has absorbed (or emitted) a definite number of laser photons. The coupling between these radiative channels is induced by the laser field. In our previous work we have argued that for optical frequencies these coupling potentials are finite-range interactions.[13] A radiative scattering matrix that describes transitions between the dissociation channels can be determined from a solution of the RCCE's. In particular, this scattering matrix will exhibit series of laser-induced capture-escape resonances.[14] Widths and shifts of these resonances (determined from the complex energy poles of the S matrix) can be identified with multiphoton ionization rates and ac Stark shifts of the bound atomic states. In practice, solution of the RCCE's can be performed numerically by a suitable truncation of the infinite hierarchy, where the number of channels that must be included depends on the light intensity.

The finite-range character of the radiative interaction leeds to a considerable simplification in solving the RCCE's by allowing us to solve the problem in two steps. As a first step the close-coupling equations must be solved in the radiative interaction region. This gives us at the boundary a short-range reaction matrix which is a smooth function of energy and thus needs to be tabulated only on a coarse energy grid. The second step consists of enforcing the proper asymtotic behavior of the wave function for the open and closed radiative channels. This step can be performed analytically using the properties of the Coulomb functions, and for the closed channels leads to the appearance of a resonance structure. Formally, this is equivalent to applying multichannel quantum-defect theory[17-19] (MQDT) to the radiative interaction problem. Thus the finite-range property of the interaction allows us express the radiative scattering matrix with the help of QDT formulas in terms of a set of intensity dependent smooth MQDT parameters.

The goal is then to compute these parameters directly by solving the RCCE's.

Among the advantages of this theory is that it provides a systematic variational approximation to compute a Coulomb-Volkov solution and the radiative scattering matrix. Furthermore, it accounts properly for the Coulomb potential, and includes and describes analytically the infinite series of Rydberg resonances. This implies, for example, that in the weak-field limit our expression for multiphoton ionization (MPI) rates, etc., reduces exactly to the standard perturbation theory results,[20] including the resonance structure.[21]

In a previous paper we solved the RCCE's by including only open channels in the calculation and applying MQDT to extract the total and partial ionization widths of Rydberg states in strong laser fields (corresponding to ATI) in the range where one-photon ionization is possible.[13] It is the purpose of this paper to extend this work to low-lying atomic states and to present numerical results for hydrogen in circularly polarized light. Inclusion of the low-lying states in the theory is achieved by implementing the concept of deeply bound channels in a QDT formulation.

The paper is organized as follows. In Sec. II the RCCE's are derived and a radiative scattering matrix is defined which is parametrized in terms of a set of smooth quantum defect parameters. Section III presents numerical results for hydrogen in circularly polarized laser light.

II. THE SCHRÖDINGER EQUATION AND WAVE FUNCTION

A. The interaction Hamiltonian

We consider an electron moving under the influence of a Coulomb potential V_c and a laser field which we describe classically. The corresponding Schrödinger equation with minimal coupling Hamiltonian is

$$H_V = \frac{1}{2m}[\mathrm{p} - e\mathbf{A}(\mathbf{x},t)]^2 + V_c(\mathbf{x}), \tag{1}$$

$$i\partial_t \Psi_V(\mathbf{x},t) = H_V \Psi_V(\mathbf{x},t) \ . \tag{2}$$

We take the laser field to be monocromatic and assume the validity of the dipole approximation in the space region of interest. The vector potential corresponding to an electric field $\mathbf{E}(\mathbf{x}=0,t)$ with amplitude $\mathcal{E}_0$, frequency ω, and polarization vector $\boldsymbol{\epsilon}$ is

$$\mathbf{A}(\mathbf{x}=0,t) = \frac{\mathcal{E}_0}{-i\omega}\boldsymbol{\epsilon}\, e^{-i\omega t} + \text{c.c.} \tag{3}$$

The problem simplifies considerably by chosing circularly polarizated laser light, $\boldsymbol{\epsilon} = -(1/\sqrt{2})(\mathbf{e}_x + i\mathbf{e}_y)$. The application of standard multichannel scattering theory below requires us to transform away the asymptotic free-electron oscillations. This is achieved by a time-dependent frame transformation $\Psi_A = e^{i\mathbf{p}\boldsymbol{\alpha}(t)}\Psi_V$ where $\boldsymbol{\alpha}(t)$ is just the solution of Newton's equation $m(d^2/dt^2)\boldsymbol{\alpha}(t) = e\mathbf{E}(t)$ in the oscillating electric field. In the present case of circularly polarized light this gives a circle $\boldsymbol{\alpha}(t) = \alpha_0[\mathbf{e}_x\cos(\omega t) + \mathbf{e}_y\sin(\omega t)]$ with radius $\alpha_0 = \sqrt{2}e\mathcal{E}_0/m\omega^2$. Below α_0 will play the role of an intensity parameter. The new Schrödinger equation for Ψ_A has the Hamiltonian

$$H_A = \frac{1}{2m}\mathbf{p}^{\,2} + V_c(\mathbf{x}+\boldsymbol{\alpha}(t)) + \frac{m}{2}\dot{\boldsymbol{\alpha}}^2 . \tag{4}$$

For large distances $|\,\vec{x}\,|$ a multipole expansion of the oscillating Coulomb potential shows that the leading term is a (time-independent) Coulomb potential, while the next-higher-order term is a dipole oscillating with the amplitude α_0. This identification of the asymptotic interaction as a Coulomb term will be essential below in defining dissociation channels of the electron-ion system in the presence of the laser field.

Separating the Hamiltonian (4) into an unperturbed and an interaction part

$$H_0 = \frac{1}{2m}\mathbf{p}^2 + V_c(\mathbf{x}), \tag{5}$$

$$\delta V = V_c(\mathbf{x}+\boldsymbol{\alpha}(t)) - V_c(\mathbf{x}) \ , \tag{6}$$

we have for δV at large distances $r = |\,\mathbf{x}\,|$ a multipole expansion

$$\delta V = \frac{e^2}{4\pi\epsilon_0}\frac{\boldsymbol{\alpha}(t)\mathbf{x}}{r^3} + \cdots \ , \tag{7}$$

which falls off faster than the (time-independent) Coulomb potential in Eq.(5). This property will be essential below in defining radiative reaction channels and a radiative scattering matrix.

B. Ansatz for wave function and close-coupling equations

We separate in Eq.(2) the rapid optical oscillations by means of a Floquet ansatz

$$|\Psi(t)\rangle = \sum_{N=-\infty}^{\infty} \langle N|\Psi(t)\rangle_F e^{-iN\omega t} \ , \tag{8}$$

where the sum over N denotes Fourier componets. $|\Psi(t)\rangle_F$ can be understood as a Floquet vector in a Hilbert space $L^2(\mathbb{R}^3)\otimes\{|N\rangle\}$ with $\{|N\rangle\}$ a Floquet basis ($N = 0, \pm 1, \ldots$). The Floquet state vector satisfies

$$i\partial_t|\Psi(t)\rangle_F = H_F|\Psi(t)\rangle_F \ , \tag{9}$$

with the Floquet Hamiltonian

$$\langle N|H_F|N'\rangle = -N\hbar\omega\delta_{NN'} + \frac{\mathbf{p}^2}{2m}\delta_{NN'} + V^{N-N'}(\mathbf{x}+\boldsymbol{\alpha}(t)) \, . \tag{10}$$

If the field amplitude is assumed to be constant in time the Floquet Hamiltonian is also time independent, which leads to a Floquet-Schrödinger equation (FSE)

$$(E - H_F)\,|\Psi\rangle_F = 0 \tag{11}$$

with E as a quasienergy. In order to get a system of close-coupling equations we expand $|\Psi\rangle_F$ in a basis of spherical harmonics and Floquet states,

$$\langle \vec{x}|\Psi(t)\rangle_F = \sum_{N,l,m} F_{ENlm}(r)/r\,[Y_{lm}(\theta,\varphi)|N\rangle_F]\,e^{-iEt}\,. \tag{12}$$

The collection of quantum numbers $i = \{N, l, m\}$ is a channel index which identifies a radiative reaction channel. As a further step and as a preparation for the MQDT treatment in Sec. II C we write the wave function as a sum of two contributions,[17]

$$|\Psi(t)\rangle_F = \left(\sum_i |\Theta_i\rangle + \sum_\alpha c_\alpha |\varphi_\alpha\rangle\right) e^{-iEt}, \tag{13}$$

$$\langle \mathbf{x}|\Theta_i\rangle = \frac{F_i(r)}{r}\,[Y_i(\theta,\varphi)|N_i\rangle_F]\,, \tag{14}$$

$$\langle \mathbf{x}|\varphi_\alpha\rangle = \frac{P_\alpha(r)}{r}\,[Y_\alpha(\theta,\varphi)|N_\alpha\rangle_F]\,. \tag{15}$$

The first term in Eq.(13) describes the continuum and highly excited atomic states and the nonresonant contributions from closed channels, while the second part is chosen to explicitly display the admixture of a set deeply bound atomic states φ_α with state index $\alpha = 1, \ldots, N_b$ where α includes both an atomic and Floquet label (below we will chose for φ_α the atomic ground state and the first few excited states of the unperturbed atom). We require orthogonality between the two contributions to the wave function, $(F_i|P_\alpha) = 0$, for $N_i = N_\alpha$, $l_i = l_\alpha$, and $m_i = m_\alpha$.

Inserting the ansatz (13)–(15) into the time-independent Schrödinger equation leads us to a system of coupled equations for the radial wave functions $F_i(r)$ and the coefficients c_α of the deeply bound states. These equations can also be obtained from a variational principle[17]

$$\langle \delta\Psi|E - H_F|\Psi\rangle = 0\ , \tag{16}$$

where the scalar product $\langle\ |\ |\ \rangle$ is meant to be in the Floquet Hilbert space and therefore denotes an integration over space and one optical period. The orthogonality condition requires the introduction of Lagrange multipliers $\lambda_{i\alpha}$ if the Floquet and angular part of a channel wave function coincide with one of a bound state. The variation of $F_i(r)$, c_α, and $\lambda_{i\alpha}$ yields

$$\delta F_i : \langle \delta\Theta_i|E - H_F|\Psi\rangle + \sum_\alpha \lambda_{i\alpha}\langle\delta\Theta_i|\varphi_\alpha\rangle = 0, \tag{17}$$

$$\delta c_\alpha : \langle \varphi_\alpha|E - H_F|\Psi\rangle = 0, \tag{18}$$

$$\delta\lambda_{i\alpha} : \langle \delta\Theta_i|\varphi_\alpha\rangle = 0. \tag{19}$$

In order to write the equations for the F_i's explicitly we need the matrix elements of the $(N-N')$-st Fourier coefficient of $V_c(\mathbf{x}+\boldsymbol{\alpha}(t))$ in the basis of spherical harmonics. These are readily read off from a multipole expansion[13]

$$V_c(\mathbf{x},\alpha_0)^{N-N'}_{lml'm'} = \sum_{k=|N-N'|}^{l+l'} d_k^{l,m,l',m',N-N'}\,\frac{r_<^k}{r_>^{k+1}} \tag{20}$$

with $r_< = \min(r,\alpha_0)$, $r_> = \max(r,\alpha_0)$, and

$$d_k^{l,m,l',m',N-N'} = (-1)^{m+N-N'}\sqrt{(2l+1)\,(2l'+1)} \times \begin{pmatrix} l & k & l' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l & k & l' \\ -m & N-N' & m' \end{pmatrix} C_k\left(\frac{\pi}{2},0\right). \tag{21}$$

The C_k's are unnormalized sperical harmonics. Only channels with $m - m' = N - N'$ are coupled. Note that the sum over k is finite. The potential (20) has a cusp at $r = \alpha_0$. Thus Eqs.(17)–(19) reduce to a system of radial close-coupling equations,[17]

$$\sum_j (\mathcal{L}_{ij} + \delta V_{ij})\,F_j = -\sum_\alpha U_{i\alpha}c_\alpha - \sum_\alpha \lambda_{i\alpha}P_\alpha, \tag{22}$$

$$\sum_\beta (\mathcal{H}_{\alpha\beta} - E\delta_{\alpha\beta})\,c_\beta = -\sum_i (U^T)_{\alpha i}|F_i, \tag{23}$$

$$(F_i|P_\alpha) = 0 \tag{24}$$

with

$$\mathcal{L}_{ij} = \left(-\frac{1}{2}\frac{d^2}{dr^2} + \frac{l_i(l_i+1)}{r^2} - \frac{1}{r} - \epsilon_i\right)\delta_{ij}, \tag{25}$$

$$U_{i\alpha} = \delta V_{i\alpha}(r)P_\alpha(r), \tag{26}$$

$$\mathcal{H}_{\alpha\beta} = N_\alpha\omega\delta_{\alpha\beta} + \mathcal{H}^0_{\alpha\beta} + \delta V_{\alpha\beta}\ , \tag{27}$$

and $\delta V_{ij} = V^{N_i-N_j}_{l_im_il_jm_j}(r,\alpha_0) - V_c(r)\delta_{ij}$. Here ϵ_i is the electron energy in the radiative channel i, defined by $E = -N_i\hbar\omega + \epsilon_i$ with $-N_i\hbar\omega$ the channel threshold. For a given energy E a radiative channel can be open ($\epsilon_i > 0$) or closed ($\epsilon_i < 0$). The set of indices i of open and closed channels will be denoted by $\mathcal{O}$ and $\mathcal{C}$, respectively. In practice, the RCCE has to be truncated to a finite number N of channels $|\Theta_i\rangle$, depending on the light intensity. We call N_o the number of open and N_c the number of closed channels ($N = N_o + N_c$). $\mathcal{H}$ is a Hamiltonian matrix between N_b bound states (in the calculations of Sec. II C below we will take the bound channels functions as eigenfunctions of the unperturbed atomic Hamiltonian H_0 [see Eq.(25)] with energy $E^{(0)}_\alpha$ and belonging to the Floquet state $|\ N_{\alpha F}\rangle$). $U_{i\alpha}$ describes the coupling of the bound states to the channels $|\Theta_i\rangle$. In writing Eqs. (25)–(27) we have adopted atomic units.

C. Radiative reactance and scattering matrix

To solve the RCCE's (23)–(25) we have to specify boundary conditions for large and small r.[17,18] At the origin $r = 0$ we require the physical solutions $F_i(r)$ to be regular. For large r Eq. (23) is dominated by a (diagonal) Coulomb potential. Thus, for a given energy E, the components of the wave function $F_i(r)$ in the open channels ($\epsilon_i > 0$) will be linear combinations of the regular and irregular Coulomb functions for $r \to \infty$, and will be exponentially decaying in the closed channels ($\epsilon_i < 0$),

$$F^{R}_{ij}(r) \longrightarrow \begin{cases} s_i(r)\delta_{ij} + c_i(r)R_{ij} \quad (i \in \mathcal{O}) & (28) \\ 0 \quad (i \in \mathcal{C})\,. & (29) \end{cases}$$

$s_i(r) \equiv s(\epsilon_i, l_i, r)$ and $c_i(r) \equiv c(\epsilon_i, l_i, r)$ denote the regular and irregular Coulomb functions in the fragmentation channel $i = \{N_i, l_i, m_i\}$ with energy ϵ_i.[17] For N_o open channels the RCCE's have N_o independent solutions (specified by the second wave-function index j). Equation (28) defines a radiative reaction matrix R with dimension $N_o \times N_o$. In a similar way solutions with scattering boundary conditions are

$$F^{S}_{ij}(r) \longrightarrow \begin{cases} \varphi^{-}_i(r)\delta_{ij} - \varphi^{+}_i(r)S_{ij} \quad (i \in \mathcal{O}) & (30) \\ 0 \quad (i \in \mathcal{C})\,, & (31) \end{cases}$$

with $\varphi^{\pm}(\epsilon, l, r) = c(\epsilon, l, r) \pm is(\epsilon, l, r)$ outgoing (ingoing) Coulomb waves. S is a radiative scattering matrix that is related to the reactance matrix by $S = (1 - iR)/(1 + iR)$.

The matrix element S_{ij} describes the scattering of electrons from the radiative dissociation channel i to channel j, which is accompanied by the absorption of $N_j - N_i$ laser photons. The scattering matrix S will, as a function of energy E, display series of Rydberg resonances. These resonances are associated with laser-induced recombination resonances of the electron-ion complex, i.e., they correspond to the decay of quasibound states in the closed channels to the continuum due to (multiphoton) ionization. Below we will concentrate on calculating the width and shift of these states as a function of laser intensity, particularly in the region of intense light fields where perturbation theory becomes questionable.

To parametrize these series of Rydberg resonances we use MQDT.[17,18] The application of QDT is possible in the present case because of the finite range of the radiative interaction, i.e., we can effectively set $\delta V_F(r) = 0$ for $r > r_c$. In discussing the physical wave functions in (30) and (31) we had to distinguish between open ($i \in \mathcal{O}$) and closed ($i \in \mathcal{C}$) channels. In addition, QDT subdivides the closed channels into weakly closed and deeply closed channels: weakly closed channels are defined as channels with energies $\epsilon_i < 0$ just below threshold in the energy region of the highly excited Rydberg states, such that the outer classical turning point of the Coulomb wave function for the given ϵ_i is much larger than the range of the interaction r_c; deeply closed channels have large negative values of ϵ_i. We denote the set of channel indices corresponding to the weakly and deeply closed channels by $\mathcal{C}_w$ and $\mathcal{C}_d$, respectively, where $\mathcal{C}_w \cup \mathcal{C}_d = \mathcal{C}$. MQDT considers solutions $\mathcal{F}_{ij}(r)$ of the RCCE's with asymptotic behavior for $r > r_c$ where *the weakly closed channels are forced to be open*,

$$\mathcal{F}^{\chi}_{ij}(r) = \varphi^{-}_i(r)\delta_{ij} - \varphi^{+}_i(r)\chi_{ij} \quad (i \in \mathcal{O} \cup \mathcal{C}_w), \tag{32}$$

$$\mathcal{F}^{\chi}_{ij}(r) \longrightarrow 0 \quad (i \in \mathcal{C}_d), \tag{33}$$

with $j \in \mathcal{O} \cup \mathcal{C}_w$. χ ($\mathcal{R}$) is a smooth radiative scattering (reactance) matrix as it is built up from a finite interaction region $r < r_c$. $\mathcal{F}_{ij}(r)$ will in general contain exponentially growing terms in the weakly closed channels. To relate the QDT wave function (32) and (33) to the N_o physical solutions $F_{ij}(r)$, MQDT eliminates the diverging components by forming appropriate linear combinations of the $\mathcal{F}_{ij}(r)$. This gives an expression for the scattering (reactance) matrix in terms of the smooth MQDT scattering (reactance) matrices,

$$R = \mathcal{R}_{oo} - \mathcal{R}_{oc}\left[\tan(\pi\nu) + \mathcal{R}_{cc}\right]^{-1}\mathcal{R}_{co}, \tag{34}$$

$$S = \chi_{oo} - \chi_{oc}\left(e^{-2\pi i\nu} - \chi_{cc}\right)^{-1}\chi_{co}. \tag{35}$$

The subscripts o and c refer to the partitioning of $\mathcal{R}$ in block matrices, with respect to open and weakly closed channels. ν is a diagonal matrix of effective quantum numbers with dimension equal to the number of closed channels N_c, $\epsilon_i = -1/2\nu_i^2$. Equations (34) and (35) provide us with an analytical parametrization of the resonance structure in terms of a smooth χ or $\mathcal{R}$ matrix. The widths and shifts of these resonances may be found from the complex energy poles in the scattering matrix S. The goal of solving the radiative interaction problem is then to determine these smooth MQDT parameters directly.

In a previous paper[13] we reported such a calculation for hydrogen by solving the RCCE's above threshold at a single energy, keeping only open channels, and extrapolating $\mathcal{R}$ to the bound-state region to extract in a single step the partial ionization widths of all Rydberg states. There are several limitations in this previous work: first of all, extrapolation is possible only in a energy range smaller than the optical frequency, i.e., one is limited to predict (above-threshold) ionization rates in a regime where one-photon ionization from the Rydberg states is possible; and, second, there is the question regarding contributions from the closed channels.

To extend this work to the low-lying atomic resonances, for example, to describe MPI from the ground state, it is convenient to introduce these states in the calculation explicitly as bound states φ_α [compare Eq.(15)]. Below we derive, following Seaton, the corresponding parametrization of the $S(R)$ matrix; the relation to the time-dependent treatment and construction of an effective Hamiltonian for bound states by projection operator techniques is discussed in Sec. II D. We write the solution of Eq.(22) as the sum of two contributions,

$$F_{ij}(r) = F^0_{ij}(r) + \sum_\alpha F^1_{i\alpha} c_{\alpha j} \ , \tag{36}$$

where we require F^0 and F^1 to satisfy the equations

$$\sum_j \mathcal{L}_{ij} F^0_{jk} = -\sum_\alpha \lambda^0_{ik\alpha} P_\alpha \ , \tag{37}$$

$$\sum_j \mathcal{L}_{ij} F^1_{j\alpha} = -\sum_\beta \lambda^1_{i\alpha\beta} P_\beta - U_{i\alpha} \ , \tag{38}$$

with asymptotic behavior

$$F^{0R}_{ij}(r) = s_i(r)\delta_{ij} + c_i R^0_{ij} \ , \quad F^{1R}_{i\alpha}(r) = c_i R^1_{i\alpha}; \tag{39}$$

$$F^{0S}_{ij}(r) = \varphi^-_i(r)\delta_{ij} - \varphi^+_i S^0_{ij} \ , \quad F^{1S}_{i\alpha}(r) = \varphi^+_i S^1_{i\alpha} \tag{40}$$

for $r > r_c$ and with $i,j = 1,\ldots,N$ and $\alpha = 1,\ldots,N_b$. F^0 is a solution with the coupling to the bound states projected out. S^0 is the corresponding contribution to the scattering matrix. F^1, on the other hand, arises from a coupling of bound states to free channels and consists of outgoing waves with amplitude S^1. We eliminate the c_α's in Eq.(39) by inverting Eq.(23),

$$c^S = (E - \mathcal{H} - D^S)^{-1} B^S \tag{41}$$

with

$$B^S_{\beta j} = \sum_i (U)^T_{\beta i} \mid F^{S_0}_{ij} \tag{42}$$

photoionization transition matrix elements from bound states to the continuum dressed by the laser, and

$$D^S_{\alpha\beta} = (U^T_{\alpha i} \mid F^{S1}_{i\beta}), \tag{43}$$

a matrix describing the ionization width and Stark shifts of the bound states due to the coupling to the continuum. Furthermore, using Eq.(37) one finds the relation[17]

$$S^1 = i\frac{\pi}{2}(B^S)^T. \tag{44}$$

Inserting the coefficients c_α's in Eq.(36) gives in matrix notation the wave function

$$F^S(r) = F^{S0}(r) + F^{S1}(r)(E - \mathcal{H} - D^S)^{-1} B^S \ , \tag{45}$$

which exhibits a resonance structure due to admixture of the bound states. Analogous results can be derived for the standing-wave solutions replacing the superscript S by R in Eqs.(41)–(45). Finally, the reactance and scattering matrix are

$$R = R^0 - \frac{1}{\pi} R^1 \left(E - \mathcal{H} - D^R\right)^{-1} R^{1^T}, \tag{46}$$

$$S = S^0 - \frac{2i}{\pi} S^1 \left(E - \mathcal{H} - D^S\right)^{-1} S^{1^T}, \tag{47}$$

respectively, where B and D play the role of smooth MQDT parameters. The scattering matrix exhibits poles as a function of energy E at the eigenvalues of

$$\det[E - \mathcal{H}^{\text{eff}}(E)] = 0 \tag{48}$$

with

$$\mathcal{H}^{\text{eff}}(E) = \mathcal{H} + D^S(E), \tag{49}$$

a non-Hermitian effective Hamiltonian in the N_b-dimensional subspace of the bound states. Note that $\mathcal{H}^{\text{eff}}$ is a slowly varying function of energy so that, in principle, Eq.(48) is a transcendental equation in energy. Diagonalizing $\mathcal{H}^{\text{eff}}$ gives

$$\mathcal{H}^{\text{eff}} A = A\left(E^{\text{res}} - i\tfrac{1}{2}\gamma\right) \tag{50}$$

with $A^{-1} = A^T$ the transformation to dressed bound states. E^{res} and γ are diagonal matrices containing the shifted resonance energies $E^{\text{res}}_{\tilde\alpha}$ and total ionization width $\gamma_{\tilde\alpha}$ ($\tilde\alpha = 1,\ldots,N_b$), respectively. This allows the scattering matrix (47) to be written as

$$S = S^0 - \frac{2i}{\pi}(S^1 A)(E - E^{\text{res}} + i\tfrac{1}{2}\gamma)^{-1}(AS^1)^T. \tag{51}$$

For *isolated resonances*, or in the limit of weak ionization, we identify

$$\gamma_{i\tilde\alpha} = \frac{2}{\pi}\left|\sum_\alpha S^1_{i\alpha} A_{\alpha\tilde\alpha}\right|^2 \tag{52}$$

as the partial ionization rate (ATI rate) from the dressed state $\tilde\alpha$ to the dissociation channel i. This is consistent with the interpretation of $\gamma_{\tilde\alpha}$ in Eq.(50) as total ionization rate

$$\gamma_{\tilde\alpha} = \sum_i \gamma_{i\tilde\alpha}. \tag{53}$$

Equation (53) may be derived with the help of

$$F^{1S} = F^{1R} + iF^{0R}(1 - iR^0)^{-1} R^1 \ , \tag{54}$$

which gives

$$\text{Im}(\mathcal{H}^{\text{eff}}) = -\frac{1}{\pi}(R^1)^T[1 + (R^0)^2]^{-1} R^1 = -\frac{i}{\pi} S^{1^\dagger} S^1. \tag{55}$$

It is straightforward to generalize Eqs.(46) and (47) to the case when some of the free channels are closed. In this case one finds for the reaction matrix R in terms of the smooth reaction matrices $\mathcal{R}^0$ and $\mathcal{R}^1$

$$R = \mathcal{R}^0_{oo} - \mathcal{R}^0_{oc}\left[\tan(\pi\nu) + \mathcal{R}^0_{cc}\right]^{-1}\mathcal{R}^0_{co} - \frac{1}{\pi}\left\{\mathcal{R}^1_{ob} - \mathcal{R}^0_{oc}\left[\tan(\pi\nu) + \mathcal{R}^0_{cc}\right]^{-1}\mathcal{R}^1_{cb}\right\}$$
$$\times\left\{E - \mathcal{H}_{bb} - D_{bb} - (1/\pi)\mathcal{R}^1_{bc}\left[\tan(\pi\nu) + \mathcal{R}^0_{cc}\right]^{-1}\mathcal{R}^1_{cb}\right\}^{-1}$$
$$\times\left\{\mathcal{R}^1_{bo} - \mathcal{R}^1_{bc}\left[\tan(\pi\nu) + \mathcal{R}^0_{cc}\right]^{-1}\mathcal{R}^0_{co}\right\}\ , \tag{56}$$

where the second term is the contribution from the Rydberg resonances (34) and the third term can be interpreted as bound resonances interacting with Rydberg resonances and the continuum (final-state interaction). Again a similar result is derived for the S matrix. For the rate from the dressed bound states $\tilde{\alpha}$ to the continuum including a final-state interaction with Rydberg states one finds

$$\gamma_{i\tilde{\alpha}} = 2/\pi \mid \{[S^1_o - \chi_{oc}(e^{-i\pi\nu} - \chi_{cc})^{-1}S^1_c]A\}_{i\tilde{\alpha}} \mid^2 \quad (i \in \mathcal{O}). \tag{57}$$

D. Connections with a time-dependent treatment

MPI is an intrinsically time-dependent problem. Initially atoms are prepared in the atomic ground state and the ejected electrons are measured after the laser pulse has passed the atom. Thus, in principle, a proper formulation of MPI requires a solution of the time-dependent Schrödinger equation with appropriate initial conditions. A description of MPI in terms of rates as in Sec. II D is approximate and is valid only under certain conditions. Resonantly enhanced MPI (REMPI) is an example of a process with (in general) more complicated time dynamics. Below we relate the theory of Sec. II C to a time-dependent treatment, in particular to the theory of REMPI formulated with the help of projection-operator theory and — as a limiting case of weak fields — perturbation theory. We close with comments on treating Rydberg resonances. Since these formulations belong to the standard repertoire of the theory of MPI,[21] we confine ourself to an outline of basic principles.

We consider MPI from a low-lying atomic state $|g\rangle$. We solve the FSE with initial condition for the Floquet state $|g, N=0\rangle$ at $t=0$ with energy E_g. Let us suppose now that in the excitation sequence to the continuum a couple of resonances occur, i.e., the Floquet energies of these states are nearly degenerate with E_g (for the moment we exclude high-lying Rydberg states, see below). These resonant states define a N_b-dimensional subspace of the Floquet Hilbert space. Denoting by P a Feshbach projection operator on these resonantly coupled states, and $Q = 1 - P$ its compliment, the FSE can be partitionated according to

$$i\frac{\partial}{\partial t}P|\Psi(t)\rangle_F = (PH_FP)P|\Psi(t)\rangle_F + (PH_FQ)Q|\Psi(t)\rangle_F\ , \tag{58}$$

$$i\frac{\partial}{\partial t}Q|\Psi(t)\rangle_F = (QH_FQ)Q|\Psi(t)\rangle_F + (QH_FP)P|\Psi(t)\rangle_F\ , \tag{59}$$

which should be compared with the RCCE's (22) and (23) where bound states have been projected out. The wave function in Q space can be eliminated in Eq.(58) by formally integrating Eq.(59) and substituting the result into Eq.(58). Within a Markov (or pole) approximation this integro-differential equation for $P|\Psi(t)\rangle_F$ simplifies to equations for the N_b level system:

$$i\frac{\partial}{\partial t}P|\Psi(t)\rangle_F = \left(PH_FP + PH_FQ\frac{1}{E_g - QH_FQ + i\eta}QH_FP\right)P|\Psi(t)\rangle_F \equiv \mathcal{H}^{\text{eff}}P|\Psi(t)\rangle_F \tag{60}$$

and

$$Q|\Psi(t)\rangle_F = \frac{1}{E_g - QH_FQ + i\eta}(QH_FP)P|\Psi(t)\rangle_F \tag{61}$$

with $\eta \to 0+$. This simplification is valid provided the self-energy [the second term in Eq.(60)] is a smooth function of the energy E_g. Equation (60) defines an effective non-Hermitian Hamiltonian $\mathcal{H}^{\text{eff}}$ in the subspace of resonantly coupled states.[20] We note that this effective Hamiltonian is identical to the $\mathcal{H}^{\text{eff}}$ introduced in Eq.(49) when parametrizing resonances in the S matrix due to the deeply bound states. In the standard theory of REMPI the Q space is defined as the space of nonresonant and continuum states and the coupling from P to Q space (ionization of resonant states) and within the Q space (continuum-continuum processes) is treated in lowest-order perturbation theory. The RCCE's allow us to calculate this effective Hamiltonian in a nonperturbative way, including, for example, continuum-continuum transitions summed up to infinite order (within the set of channels included in the calculation). Obviously, in the weak-field limit these results agree with those derived in perturbation theory. In addition, the Schrödinger equation (60) can be integrated in time for a realistic laser pulse envelope, i.e., without the assumption of a square or adiabatic pulse.

A further simplification occurs when the ground state is only weakly coupled to the higher-lying bound and continuum states. This is the case of MPI via a few nonresonant steps which provides a bottleneck in the excitation process. The P space reduces to the ground state and therefore $P = |g, N=0\rangle\langle g, N=0|$. In the quasienergy spectrum this manifests itself as an eigenvalue $E_g - (i/2)\gamma_g$ with small imaginary part γ_g and an eigenvector dominantly composed of the atomic ground state. It is not difficult to show that γ_g may be identified with the total ionization rate given by

$$\gamma_g = \sum_i \gamma_{ig} \tag{62}$$

and with partial (ATI) ionization rates:

$$\gamma_{ig} = \left| \sum_j \left\langle F_{ij}^{S\dagger} | \delta V_{Fj}^b | g, N=0 \right\rangle \right|^2 \tag{63}$$

and $\left|F^S\right\rangle$ a solution of Eq.(37) describing a final-state interaction with the light field. The expression (63) for the ionization rate is the starting point of many theories of nonresonant MPI, which differ in the approximation for the final state dressed by the light field.[9,10,12] We emphasize that the RCCE's provide us with numerically exact solutions for γ_i (including the resonant structure of intermediate states).

In the weak-field limit Eq.(63) agrees with standard perturbation theory where the radiative transition matrix elements are in acceleration form.[21] Perturbation theory is most easily derived by converting the RCCE to an integral equation and iterating this equation (see Appendix A). Let us consider the two-photon ionization rate as an example.[22] We have in second order

$$\gamma_g = 2\pi \left| \langle f | (\alpha_0 \boldsymbol{\epsilon} \cdot \mathbf{p}, H_0)\, G_0^+(E_g + \omega)\, (\alpha_0 \boldsymbol{\epsilon} \cdot \mathbf{p}, H_0) | g \rangle + \langle f | \left[\alpha_0 \boldsymbol{\epsilon} \cdot \mathbf{p}\, (\alpha_0 \boldsymbol{\epsilon} \cdot \mathbf{p}, H_0) \right] | g \rangle \right|^2 , \tag{64}$$

which in view of gauge invariance of the radiative interaction can be shown to be the same as the rate derived using the dipole interaction Hamiltonian,

$$\gamma_g = 2\pi \left| \left\langle f | e\mathbf{x} \cdot \boldsymbol{\epsilon}\, \mathcal{E}_0\, G_0^+(E_g + \omega)\, e\mathbf{x} \cdot \boldsymbol{\epsilon}\, \mathcal{E}_0 | g \right\rangle \right|^2, \tag{65}$$

with G_0^+ the Coulomb Green function. In a similar way, the Stark shift of level $|g\rangle$, which appears as a shift of the resonance in the radiative scattering matrix and as a shifted eigenvalue of the effective Hamiltonian (49), is in second-order perturbation theory

$$\begin{aligned} \delta E_g = {} & \langle g | \tfrac{1}{2} [i\alpha_0 \boldsymbol{\epsilon} \cdot \mathbf{p}, (i\alpha_0^* \boldsymbol{\epsilon}^* \cdot \mathbf{p}, H_0)] | g \rangle + \langle g | \tfrac{1}{2} [i\alpha_0^* \boldsymbol{\epsilon}^* \cdot \mathbf{p}, (i\alpha_0 \boldsymbol{\epsilon} \cdot \mathbf{p}, H_0)] | g \rangle \\ & + \langle g | (i\alpha_0^* \boldsymbol{\epsilon}^* \cdot \mathbf{p}, H_0) G_0^+(E_g + \hbar\omega)(i\alpha_0 \boldsymbol{\epsilon} \cdot \mathbf{p}, H_0) | g \rangle + \langle g | (i\alpha_0 \boldsymbol{\epsilon} \cdot \mathbf{p}, H_0) G_0^+(E_g - \hbar\omega)(i\alpha_0^* \boldsymbol{\epsilon}^* \cdot \mathbf{p}, H_0) | g \rangle \ , \end{aligned} \tag{66}$$

which as expected agrees with the Stark shift calculated in the dipole interaction form

$$\begin{aligned} \delta E_g = {} & \langle g | e\mathbf{x} \cdot \boldsymbol{\epsilon}^* \mathcal{E}_0^* G_0^+(E_g + \hbar\omega) e\mathbf{x} \cdot \boldsymbol{\epsilon} \mathcal{E}_0 | g \rangle \\ & + \langle g | e\mathbf{x} \cdot \boldsymbol{\epsilon} \mathcal{E}_0 G_0^+(E_g - \hbar\omega) e\mathbf{x} \cdot \boldsymbol{\epsilon}^* \mathcal{E}_0^* | g \rangle \ . \end{aligned} \tag{67}$$

Furthermore, it is possible to derive an MQDT parametrization for the Rydberg resonances in the perturbation-theory transition rates. This is obtained by specializing the MQDT parametrization for Eq.(57) to weak fields, in agreement with results derived in Ref. 20.

Excitation of Rydberg resonances invalidates the Markov (or pole) approximation in Eq.(60). In this case the self-energy term $D^S(E)$ in the effective Hamiltonian $H_{\text{eff}}(E)$ becomes a rapdily varying function of energy, reflecting the resonance structure in the weakly closed channels. In a recent paper[23] we have outlined how the time evolution of the bound-state wave function can be calculated. The idea is to derive a system of RCCE's by Laplace transformation of the time-dependent Schrödinger equation [Eq.(5) of Ref. 23]. Eliminating the open and weakly bound channels gives an expression for the Laplace transformed bound-state amplitudes (corresponding to P space) where the Rydberg resonances can be parametrized with the help of MQDT [Eqs. (14) and (15) of Ref. 23]. This Laplace transform can be inverted giving either a dressed-state representation, corresponding to a sum over eigenstates of the bound states mixed by the laser into the Rydberg states, or — close to threshold — in terms of a multiple scattering (or classical path) expansion.

The conclusion of this section is that the radiative MQDT parameters of Sec. II C can be used as input for a time-dependent calculation of MPI transition probabilities.

III. RESULTS AND DISCUSSION

We have solved the RCCE (22) for hydrogen in circularly polarized laser light numerically. The differential equations were converted to scattering integral equations (see Appendix A) which were solved by iteration. This provides us directly with the smooth radiative QDT parameters $R^0, R^1, D, \mathcal{H}$. The multichannel wave function was tabulated on a grid in the interaction region of radius r_c, where typically $0 \le r \le r_c \approx 50 - 120 a_0$. The number of radiative open and closed channels included in the calculation was increased systematically until, for a given intensity and laser frequency, convergence of the radiative reaction matrix was achieved. For a given energy range there are resonances in the scattering matrix corresponding to MPI of deep-lying atomic states. The corresponding eigenstates of the unperturbed Hamiltonian were projected out as bound channels $|\varphi_\alpha\rangle$.

As our first example we discuss the elastic transtion amplitude $T(E) = (1/2\pi i)[S(E) - 1]$ for the frequency $\omega = 0.27$ and energy range where two-photon ionization (2PI) of the 1s and one-photon ionization (1PI) of the p states is possible. The schematic representation of this process is shown in Fig. 1. Note that for this frequency the excitation step from the 1s to the p states is nonresonant. Figure 2 corresponds to a (relatively small)

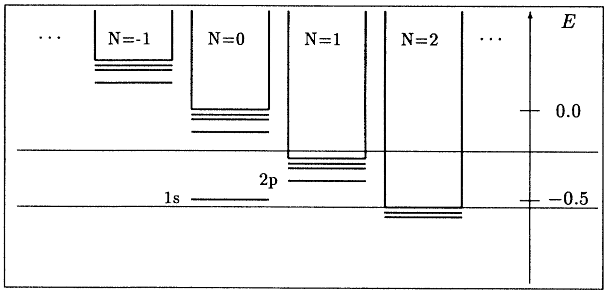

FIG. 1. Schematic representation of 2PI of the hydrogenic ground state.

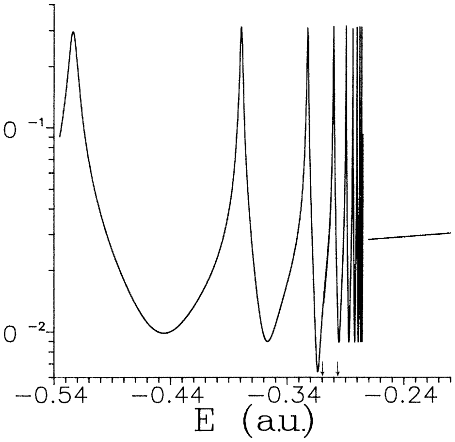

FIG. 3. Same as Fig. 2 with $\alpha_0 = 0.7$ (a.u.) ($I = 1.8\ 10^{14}$ W/cm^2).

intensity parameter $\alpha_0 = 0.2$ (a.u.), $I = 1.5 \times 10^{13}$ W/cm^2. In the calculation the states ($1s, N = 0$) and ($2p - 4p, N = 1$) were projected out as deeply bound states $|\varphi_\alpha\rangle$, and the np, $n > 4$, were treated as a weakly closed channel, the total number of channels was 15 ($-4 \leq N \leq 4$, $l \leq 4$). The leftmost resonance in Fig. 2 is associated with the 2PI of the $1s$ state; the other resonances belong to the 1PI of the np Rydberg series. In the energy range $-0.54 \leq E \leq -0.31$ the $1s$, $2p$, and $3p$ resonances were calculated according to the parametrization (47), while the Rydberg resonances $n \geq 4$ were obtained by solving the RCCE's above the Rydberg threshold, and extrapolating the QDT parameters to the bound region using Eq.(35). In Fig. 2 the line profile in the energy region around the $4p$ resonances was calculated using both procedures (marked by the arrow). The good agreement is an indication of the weak energy dependence of the QDT parameters. Figure 3 is the analogous plot for $\alpha_0 = 0.7$ (a.u.). Our results for the elastic scattering amplitudes are consistent with those of Franz *et al.*,[15] who have solved the RCCE's in the neighborhood of the $1s$ and $2p$ resonances and the first few members of the Rydberg series for intensities up to $\alpha_0 \leq 0.2$.

The line profiles in Figs. 2 and 3 are series of isolated resonances so that the widths reflect the ionization lifetime of the atomic states. The partial and total ionization rates are given by Eqs. (52) and (53), respectively. According to Figs. 2 and 3 the ionization width of the $1s$ state increases with intensity. The dependence of the total and ATI partial rates ($N = 2, 3, 4$) of $1s$ on the light intensity is shown in Fig. 4. As expected, for low intensities we get an I^N dependence consistent with perturbation theory for N photon absorption. For higher intensities a deviation from the power-law behavior is observed. It is suprising that for intensities, where the par-

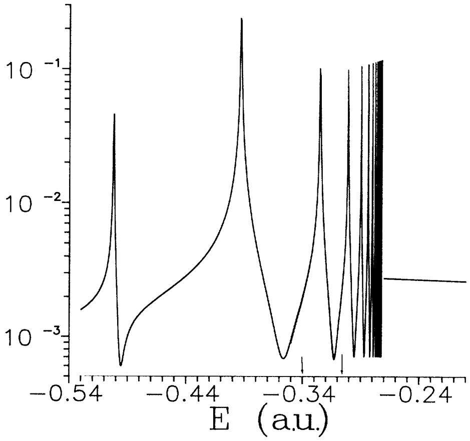

FIG. 2. The modulus of the elastic transition amplitude $| T(E) |$ for ($N = 2, l = 2, m = 2$) $\rightarrow$ ($N = 2, l = 2, m = 2$) is plotted as a function of energy E (a.u.). The parameters are $\alpha_0 = 0.2$ (a.u.) and $\omega = 0.27$ (a.u.) ($I = 1.5\ 10^{13}$ W/cm^2).

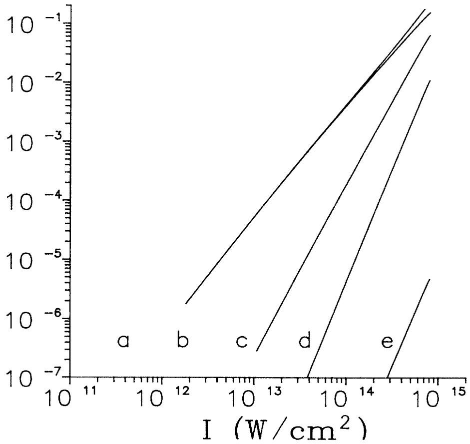

FIG. 4. Ionization rate of hydrogen $1s$ by a circulary polarized laser with frequency $\omega = 0.27$ (a.u.) (2PI). (a) Total rate; ATI rates: ionization into channel (b) $N = 2$, $l = 2$; (c) $N = 3$, $l = 3$; (d) $N = 4$, $l = 4$; (e) $N = 4$, $l = 2$. (The value of $\alpha_0 = 1$ corresponds to $I = 3.7 \times 10^{14}$ W/cm^2.)

tial rates already deviate significantly from lowest-order perturbation theory ($\alpha_0 \approx 1$), the total rate still shows an I^N ($N = 2$) dependence. There is no point to calculate ionization rates for higher intensities than those given in Fig. 4 in the present case, since the total rate becomes comparable to the frequency (ionization within one optical cycle), which is not consistent with the present formulation. The rates shown in Fig. 4 were computed ignoring the energy dependence of the effective Hamiltonian (49), i.e., setting $\mathcal{H}^{\text{eff}}(E) = \mathcal{H}^{\text{eff}}(E = -0.5)$ in Eq.(48). Again this is justified by the weak energy dependence of the QDT parameters. This approximation is not possible, however, when channels becomes closed due to the Stark shift.

Figure 5 is a plot of the ac Stark shift of the 1*s* state as a function of α_0. Obtaining correct Stark shifts in the acceleration form interaction Hamiltonian is a nontrivial task, especially for *s* states. The problem becomes apparent already in the weak-field limit, where perturbation theory is valid. The second-order Stark shift in the acceleration and dipole interaction forms has been given in Eqs. (66) and (67), respectively. The first and second term in Eq.(66) is the shift in the high-frequency limit that as a function of the light intensity shifts upwards.[11] On the other hand, it is obvious from (67) that for frequencies below the 1*s*-2*p* transition the 1*s* state will shift downwards. Consequently, in Eq.(66) the upward shift of the first two terms has to be compensated by the last two terms involving the Green function. In practice, both contributions are of same order of magnitude but have different signs which leads to an almost complete cancellation. Thus an approximate representation of the Green function (for example, a truncated summation over bound eigenstates of the atomic Hamiltonian — which is a reasonable approximation in the dipole form) will lead to even qualitatively incorrect results. One consequence of this observation for our present calculation is that the wave function in the closed channels [see Eq.(13)] cannot be represented by a superposition of a few eigenstates of the unperturbed Hamiltonian. In Fig. 5 the intensity dependence of the Stark shift of the 1*s* state is shown for various sets of channel configurations: curve *a* is the results of second-order perturbation theory (in length and acceleration form); curve *b* is our "best" calculation with 15 channels ($-4 \leq N \leq 4$, $l \leq 4$). We note a surprising agreement between these two curves up to $\alpha_0 \approx 0.8$. In contrast, curves *c* and *d* correspond to six- and four-channel models (which obviously have not converged). Curve *e* was obtained by representing the $s, N = 0$ channel in the RCCE by a single 1*s* state; obviously (see the inset in Fig. 5) this gives the correct low-intensity limit $\alpha_0 \leq 0.02$ but predicts (incorrectly) a positive Stark shift for $\alpha_0 > 0.12$. Finally, curve *f* assumes a wave function with only $N \geq 0$ channels included, which predicts a positive shift for all α_0.

We recall from Fig. 4 that the 2PI ionization rate of the 1*s* state increases with intensity. In contrast, for the same frequency we find a stabilization of the 2*p* state (1PI) above $I = 10^{14}$ W/cm^2 (Fig. 6). Our calculations predicts an analogous narrowing of the resonances for all *p* states. A similar suppression of 1PI occurs for the 1*s* state and $\omega = 0.51$ (Fig. 7). This is consistent with the recent L^2-basis calculation by Dörr, Potvliege, and Shakeshaft,[2] who for the case of linear polarization find decreasing rates for $\alpha_0 \approx 1$. We emphasize that in the present case this behavior cannot be explained by a Stark shift towards the ionization threshold where the transition matrix elements vanish as for negative ions.[24]

Finally, in Fig. 8 the elastic scattering amplitude is shown for $\omega = 0.49$ (a.u.) as a function of energy. This corresponds to a frequency where the ground state is

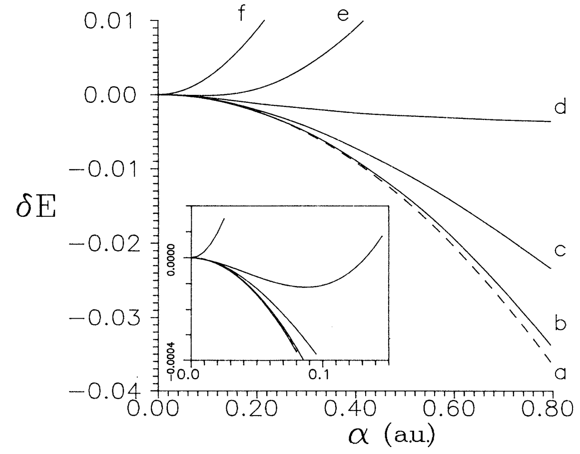

FIG. 5. ac Stark shift of the 1*s* (relative to the thresholds) for various channel configurations [$\omega = 0.27$ (a.u.)]. (a) Second-order perturbation theory; (b) 15 channels (see Fig.2); (c) 6 channels (without $N = 3, 4$); (d) 4 channels (without $N = -2, l = 2$ and $N = 0, l = 2$); (e) 3 channels (without $N = 0, l = 0$); (f) 2 channels (without $N = -1, l = 1$).

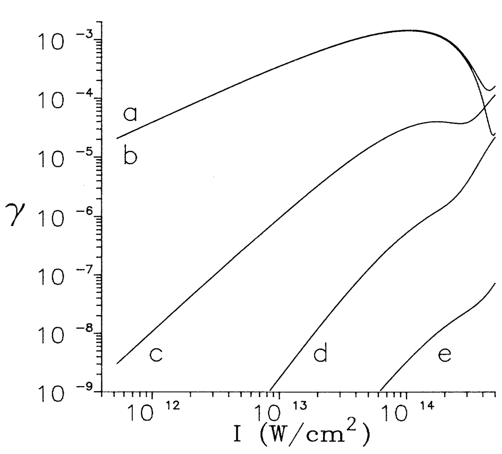

FIG. 6. Total and partial rates of the 2*p* for $\omega = 0.27$ (a.u.) where 1PI is allowed. (a) Total rate; (b) - (e) ATI rates as described in Fig.4.

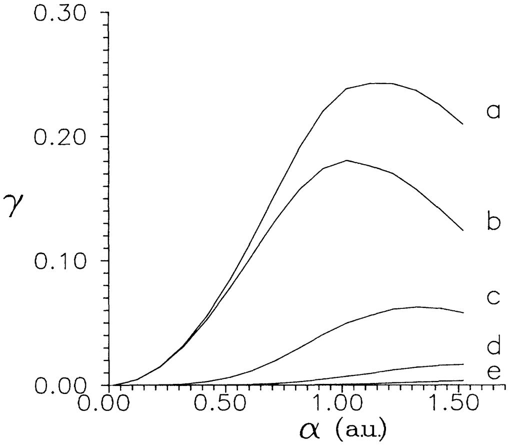

FIG. 7. Ionization of the hydrogenic ground state for $\omega = 0.51$ (a.u.) where 1PI is allowed. 15 channels have been included in the calculation (see Fig.2). (a) Total rate; (b) – (e) ATI rates to $N = 1, l = 1$ and $N = 4, l = 4$.

mixed into the Rydberg series around $10p$, a situation analogous to an (autoionizing) complex resonance where a bound state autoionizes to a continuum via the coupling to many Rydberg states. In this case the time-dependent ionization probability should be calculated according to the methods of Ref. 23.

IV. CONCLUSIONS

In this paper we have derived a system of radiative close-coupling equations for hydrogen in circularly polarized laser light. We have solved these equations numerically increasing systematically the number of closed and open radiative channels kept in the calculation until for a given intensity convergence was achieved. This provides us with the best variational approximation for the radiative scattering matrix. Due to the finite-range character of the radiative interaction, the close-coupling equations can be solved in two steps: first, a set of radiative quantum-defect parameters (the reaction matrix, etc.) is determined and tabulated on a coarse energy grid by solving the RCCE's in the interaction region; in the second step, the proper asymtotic behavior of the wave function and physical reaction matrix is constructed using multichannel quantum-defect theory. The complex quasienergies (shifts and ionization widths) are computed as poles of the scattering matrix using the quantum-defect formalism. In extension our previous work,[13] we have included closed channels in the calculation and found them to be very important. In this work we have presented detailed numerical results for elastic e-p scattering for frequencies, where the $2p$ and $1s$ states couple to the continuum by one- and two-photon transitions as well as higher-order processes, and have computed the corresponding quasienergy spectrum predicting (partial) ionization rates and shifts in the strong-light-field limit $\alpha_0 \approx 1$.

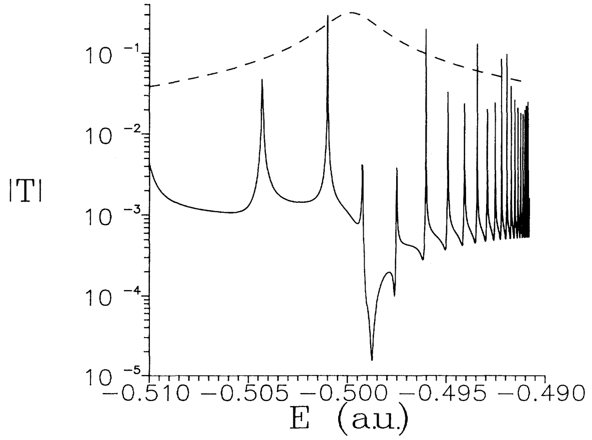

FIG. 8. Elastic transition amplitude $T(E)$ for $(N, l = 2) \to (N, l = 2)$ where the 1s couples resonantly to many Rydberg states around $10p$ [$\omega = 0.49$ (a.u.)].

The present work is based on a spherical expansion of the wave function in the oscillating coordinate system. We have found contributions from (deeply) closed channels to be of crucial importance to achieve convergence, in particular in computing the Starkshift of the s states. This indicates that the interaction region close to the atomic core should be treated in a coordinate that is better adapted to the physical situation, or by working inside the interaction region in the dipole length form of the field-atom interaction. One possiblity is to include "oscillating" basis function, moving with the atomic core, in the variation principle when deriving the close-coupling equations;[25] the radiative coupling between these oscillating orbitals is then given in the dipole length form which should significantly improve convergence with the number of channels. Physically, this corresponds to a frame transformation where the electron in the laser field is described far from the atomic core in a frame moving with the wiggling motion of the free electron and close to the atomic core, where the electronic motion is dominatly governed by the atomic forces, in an nucleus-fixed frame.

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APPENDIX: INTEGRAL EQUATION FOR THE SCATTERING WAVE FUNCTION

We convert the the differential equations (37) and (38) to an integral equation. First we construct a Green function of $\mathcal{L}_i^0 g_i(r, r') = -\delta(r - r')$ for the zero-order Coulomb problem with proper boundary conditions for the open and closed channels. For the open channels we choose a

Green function with standing-wave boundary conditions,

$$g_i(r,r') = 2\ s_i(r_<)\ c_i(r_>)/W(s_i,c_i) \quad (\epsilon_i > 0), \tag{A1}$$

where $r_< = \min(r,r')$ and $r_> = \max(r,r')$, and s (c) regular (irregular) Coulomb functions (31) normalized to a Wrosnki determinant $W(s_i,c_i) = -\pi$. For the closed channels we have

$$g_i = 2\ s_i(r_<)\ \theta_i(r_>)/W(s_i,\theta_i) \quad (\epsilon_i < 0)\ , \tag{A2}$$

with θ_i the asymptotically decaying Coulomb (Whittaker) function. The required integral equation is

$$\begin{aligned} F^0_{ij} = {} & s_i(r)\delta_{ij} + \sum_\alpha \int_0^\infty dr'\ g_i(r,r')\lambda^\alpha_{ij} P_\alpha(r') \\ & + \sum_l \int_0^\infty dr'\ g_i(r,r')\delta V_{il}(r') F^0_{lj}(r'). \end{aligned} \tag{A3}$$

We eliminate the λ^α_{ij} in Eq.(70) by means of Eq.(24),

$$\lambda^0_{kj\alpha} = -\sum_l \int_0^\infty dr\ P_\alpha(r)\delta V_{kl}(r) F^0_{lj}(r), \tag{A4}$$

which gives

$$F^0_{ij} = s_i(r)\delta_{ij} + \sum_l \int_0^\infty dr'\ \bar{g}_i(r,r')\delta V_{il}(r') F^0_{lj}(r'), \tag{A5}$$

with new Green function

$$\overline{g}_i = g_i - \sum_\alpha \frac{P_\alpha(r)\ P_\alpha(r')}{\epsilon_i - \epsilon_\alpha}. \tag{A6}$$

If instead of (A1) and (A2) we use the spectral representation

$$g_i(r,r') = \sum\!\!\!\!\!\!\!\int_n \frac{P_{nl_i}(r)\ P_{nl_i}(r')}{\epsilon_i - \epsilon_{nl_i}}\ , \tag{A7}$$

with $\sum\!\!\!\!\!\!\!\int$ a sum over a complete set of Coulomb eigenstates, the poles in $g_i(r)$ corresponding to the energies $\epsilon_i = \epsilon_\alpha$ are seen to cancel. This yields a smooth reactance matrix $R^0(E)$

$$R^0_{ij} = -\frac{2}{\pi} \sum_k \int_0^{r_c} dr\ s_i(r)\delta V_{ik}(r) F^0_{kj}(r) \tag{A8}$$

(in MQDT the cutoff radius has to be chosen large enough so that no bound state contributes to the asymptotics). In a similar way an integral equation is derived for F^{R1} [Eq.(39)]

$$\begin{aligned} F^{R1}_{i\alpha} = {} & \int_0^\infty dr'\ \overline{g}_i(r,r') U_{i\alpha}(r) \\ & + \sum_l \int_0^\infty dr'\ \overline{g}_i(r,r')\delta V_{il}(r') F^{R1}_{l\alpha}(r'). \end{aligned} \tag{A9}$$

Iteration of these integral equations in δV_F gives a perturbation expansion in the light field in terms of acceleration form matrix elements.

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