

## Lippmann-Schwinger description of multiphoton ionization

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We outline a formalism and develop a computational procedure to treat the process of multiphoton ionization (MPI) of atomic targets in strong laser fields. We treat the MPI process nonperturbatively as a decay phenomenon by solving a coupled set of the integral Lippmann-Schwinger equations. As basic building blocks of the theory, we use a complete set of field-free atomic states, discrete and continuous. This approach should enable us to provide both the total and differential cross sections of MPI of atoms with one and two electrons. As an illustration, we apply the proposed procedure to a simple model of MPI from a square-well potential and to the hydrogen atom.

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### I. INTRODUCTION

In recent years, the process of multiphoton ionization (MPI) of atomic and molecular species has been a subject of intensive experimental and theoretical studies (see reviews by Protopapas *et al.* [1], Lambropoulos *et al.* [2], Chu and Telnov [3], and Posthumus [4], and references therein). Rapid progress in this field has been largely driven by advancement in high-power short-pulse laser techniques. The laser intensities which may go beyond  $10^{13}$  W cm<sup>-2</sup> make it possible to observe many striking phenomena such as MPI and above-threshold ionization.

Accurate theoretical description of ionization processes occurring in laser fields of such intensities should necessarily go beyond a simple perturbative picture. The first nonperturbative theory of MPI was proposed by Keldysh [5], Faisal [6], and Reiss [7]. Their theory (known as KFR) treated the process of MPI as a transition of an electron from an initial bound state into a final state described by the classical Volkov wave function. The KFR approach provided simple analytical formulas for the MPI rate which were found in qualitative agreement with experiment. Various modifications of the KFR theory were made, in particular those accounting for the rescattering process [8,9].

The KFR theory treated the laser field purely classically. The MPI problem can also be formulated in an entirely quantum form. The properties of the scattering matrix in this formulation of the MPI process have been studied starting from the works of Mower [10,11], Gontier *et al.* [12,13], Faisal and Moloney [14], and Jackson and Swain [15]. More recently, Guo and Aberg [16] and Guo, Aberg, and Crasemann [17] put forward an MPI theory (referred to hereafter as GAC) which treats the photoionization process as a QED scattering phenomenon. The emphasis in this theory was placed on a proper QED description of an electron interacting with the laser field (the quantum version of the Volkov states). Further development of the QED picture of the MPI

phenomenon was made by Gao *et al.* [18] and Chen *et al.* [19], who refined the original GAC theory by including the nonlaser modes of the electromagnetic field.

This fully QED approach, although solving the problem in principle, was found to be rather difficult to implement in practice even for the simplest atomic targets such as one- or two-electron atoms. For instance, Chen *et al.* [19] had to make further drastic approximations in order to carry out their calculation of MPI on atomic hydrogen.

One possible solution to this problem is to use some suitable square-integrable basis to represent the Green functions occurring in the theory. Such an approach, using ideas of the complex rotation method, has been proposed by Maquet *et al.* [20]. Another solution is to use the field-free atomic states as building blocks of the theory. Such a choice is particularly advantageous when theory is applied to complex atomic systems with more than one target electron. Such an approach within the context of the complex rotation method has been used by Mercouris and Nicolaiides [21] and Nicolaiides and Mercouris [22]. Description of the quantum-mechanical evolution of an atom coupled to a laser field is also possible in the framework of this method [23].

In the present paper, we outline a quantum formalism for MPI which we intend to use for practical computations on complex atomic systems. The formalism is not entirely new and is based on the ideas expressed earlier in the literature. The main emphasis of this work is on the practical implementation of the formalism and turning it into an efficient computational procedure. In this development, we are inspired by a series of works by Burke and collaborators, who combined the Floquet description of the laser field with the *R*-matrix scattering theory. Following the seminal work [24], this approach has been successfully implemented for calculating the total MPI rate and the level shift in atomic hydrogen [25], helium [26], the negative hydrogen ion [27], and molecular hydrogen [28]. Most recently, the *R*-matrix Floquet theory was combined with the basis spline technique to describe the two-electron MPI from the helium atom in the ground [29] and excited states [30]. In addition to the total MPI rate, some differential cross sections can also be calculated within the Floquet formalism, as was demonstrated for atomic hydrogen by Potvliege and Shakeshaft [31] and Potvliege [32]. It is the most detailed fully differential cross sections that are

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of particular interest to experimentalists and that we intend to evaluate in our approach.

In the present paper, we employ the operator formalism due to Goldberger and Watson [33]. In this formalism, the MPI process is treated as a decay phenomenon. The partial decay rates and the energy level shifts are evaluated via the matrix elements of the transition operator which are found by solving a coupled set of the integral Lippmann-Schwinger equations. In this approach, the matrix elements of the transition operator should be taken between the field-free atomic states accompanied by an integer number of the laser photons.

For one-electron targets, evaluation of the field-free states is trivial. For two-electron targets, an accurate set of target states, both discrete and continuous, can be generated by the so-called convergent-close-coupling (CCC) method. This method has been extensively tested for processes with two electrons in the continuum such as electron scattering on atomic hydrogen [34] and low-field double ionization of helium [35,36]. We intend to use the same set of target states for MPI of He in the nonperturbative strong-field regime.

In our approach, we ignore all the processes of spontaneous emission of photons, which is justified as we are interested in processes induced by strong fields. Since the work of Shirley [37], it is known that if one neglects spontaneous processes in the quantum description of the interaction of laser light and atom, then the quantum picture and the Floquet method of solving the time-dependent Schrodinger equation become equivalent. Therefore, the present approach and those based on the Floquet ansatz (such as [24], for example) are completely equivalent. However, recasting the MPI description in the form presented below may have some practical advantages, especially if we have good means of representing the field-free atomic states for complex atomic systems. This includes, of course, the states belonging to the continuous spectrum. Such means do exist. As mentioned above, the CCC method turned out to be very efficient at representing field-free states of atomic systems. It was the desire to exploit fully the possibilities provided by the CCC technique that largely motivated us to give a formulation of the MPI process presented below.

The rest of the paper is organized as follows. In Sec. II, we give a formulation of the MPI theory in terms of the field-free atomic states. In Sec. II A, we consider a model square-well problem, and in Sec. II B, the MPI of hydrogen. We conclude in Sec. III by outlining a set of problems we intend to consider in the immediate future.

## II. NONPERTURBATIVE FRAMEWORK FOR THE DESCRIPTION OF THE MPI PROCESS

Let us consider a system which consists of a number of photons with a given frequency  $\omega$  and momentum vector  $\mathbf{k}$  corresponding to an incident plane wave and a target (atom or ion). We shall describe the field fully quantum mechanically and write the Hamiltonian of the system as

$$\hat{H} = \hat{H}_{\text{atom}} + \hat{H}_{\text{field}} + \hat{H}_{\text{int}}. \quad (1)$$

Here  $\hat{H}_{\text{atom}}$  and  $\hat{H}_{\text{field}}$  have the usual meaning of the Hamiltonians of the atom and the field,

$$\hat{H}_{\text{atom}} = \sum_{i=1}^N \frac{\mathbf{p}_i^2}{2} - \sum_{i=1}^N \frac{Z}{r_i} + \sum_{i,j=1, i>j}^N \frac{1}{r_{ij}},$$

$$\hat{H}_{\text{field}} = \hat{N}\omega. \quad (2)$$

The atomic Hamiltonian is taken in a nonrelativistic form. The number operator  $\hat{N}$  refers to the laser photons only.

The corresponding states of the system consisting of the noninteracting atom and the field are denoted as  $|\alpha\rangle = |a, n\rangle$ , where a set of quantum numbers  $a$  defines a state of the atom and  $n$  is the number of the laser photons. The following notations will be kept throughout the paper: Greek letters will be used to designate the states of a whole system “the atom plus external field,” while the Latin letters will be used for the atomic states. The atomic system of units is in use with  $e = m = \hbar = 1$ .

The part of the Hamiltonian  $\hat{H}_{\text{int}}$  which describes the interaction of the atom and the linearly polarized laser field characterized by angular frequency  $\omega$ , wave vector  $\mathbf{k}$ , and polarization vector  $\mathbf{e}$  can be written as (see, e.g., Sobelman [38])

$$\hat{H}_{\text{int}} = -\frac{1}{c} \sum_{i=1}^N \left( \hat{\mathbf{A}} \cdot \hat{\mathbf{p}}_i - \frac{\hat{\mathbf{A}}^2}{2c^2} \right), \quad (3)$$

where  $\hat{\mathbf{p}}$  is the momentum operator and  $\hat{\mathbf{A}}$  is a quantized vector potential normalized to the unit volume

$$\hat{\mathbf{A}} = \sqrt{\frac{2\pi c^2}{\omega}} e (\hat{a}_{\mathbf{k}}^\dagger e^{i\mathbf{k}\cdot\mathbf{r}} + \hat{a}_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r}}). \quad (4)$$

Here  $\hat{a}^\dagger$  and  $\hat{a}$  have the usual meaning of the operators creating and annihilating a photon. As mentioned above, we are interested in sufficiently strong field intensities, when all processes of spontaneous emission of photons can be neglected. For this reason, only one mode corresponding to the wave vector of the incident laser field is kept in Eq. (4). Therefore, here and below,  $\hat{\mathbf{A}}$  describes the laser photons only. We also restrict ourselves to the dipole approximation in which the operator  $\hat{\mathbf{A}}$  does not act on the atomic coordinates.

The matrix elements of the vector potential operator taken between the noninteracting states of the system “atom plus laser photons” are given by the well-known formulas (see, e.g., Sobelman [38])

$$\langle a, n | \hat{\mathbf{A}} \cdot \hat{\mathbf{a}} | b, n-1 \rangle = \sqrt{\frac{2\pi c^2 n}{\omega}} \langle a | \mathbf{e} \cdot \hat{\mathbf{a}} | b \rangle,$$

$$\langle a, n | \hat{\mathbf{A}} \cdot \hat{\mathbf{a}} | b, n+1 \rangle = \sqrt{\frac{2\pi(n+1)c^2}{\omega}} \langle a | \mathbf{e} \cdot \hat{\mathbf{a}} | b \rangle, \quad (5)$$

where  $\hat{\mathbf{a}}$  is an arbitrary vector operator acting only on the coordinates of the atomic sub-system.

In strong field  $n \approx n-1 \gg 1$  and the coefficients in Eqs. (5) can be simplified to

$$\sqrt{\frac{2\pi n c^2}{\omega}} \approx \sqrt{\frac{2\pi(n+1)c^2}{\omega}} \approx \frac{Fc}{2\omega}, \quad (6)$$

where  $F$  is the electric field strength related to the energy density as  $F^2 = 8\pi m\omega$ . This leads to the following formulas for the matrix elements of the operator  $\hat{H}_{\text{int}}$ :

$$\begin{aligned} \langle a, n | \hat{H}_{\text{int}} | b, n \pm 1 \rangle &= -\frac{F}{2\omega} \langle a | e \cdot \hat{p} | b \rangle, \\ \langle a, n | \hat{H}_{\text{int}} | b, n \pm 2 \rangle &= \frac{F^2}{8\omega^2} \langle a | b \rangle, \\ \langle a, n | \hat{H}_{\text{int}} | b, n \rangle &= \frac{F^2}{4\omega^2} \langle a | b \rangle. \end{aligned} \quad (7)$$

We shall treat the MPI process as a decay phenomenon within the framework of the quantum decay theory as described by Goldberger and Watson [33]. We shall be interested in the following process. At the moment  $t=0$ , the system “atom plus external field” is prepared in the eigenstate  $|\alpha\rangle$  of the Hamiltonian  $\hat{H}_0 = \hat{H}_{\text{atom}} + \hat{H}_{\text{field}}$ . Then interaction  $\hat{H}_{\text{int}}$  between atomic and photon subsystems is switched on. Our aim is to describe possible outcomes of this event. The partial rates of the decay of the initial states  $|\alpha\rangle$  into various open channels  $|\beta\rangle$  are given by the expressions

$$\Gamma_\beta = 2\pi |T^{\beta\alpha}(E)|^2 d\rho(E), \quad (8)$$

Where  $\rho(E)$  denotes the density of states in the final state, and the transition operator  $T$  satisfies the operator equation [33]

$$\hat{T}(E) = \hat{H}_{\text{int}} + \hat{H}_{\text{int}}(1 - \hat{P}_\alpha) \frac{1}{E - \hat{H}_0} \hat{T}(E). \quad (9)$$

Here  $P_\alpha$  is a projection operator on the initial state  $|\alpha\rangle$ . In Eq. (8), both the matrix element of the transition operator and the density of states are to be computed at the energy, corresponding to the shifted energy of the initial state  $|\alpha\rangle$ :  $E = E_\alpha + \Delta E_\alpha$ . Finally, the energy shift  $\Delta E_\alpha$  of the final state is related to the diagonal matrix element of the transition operator via the implicit equation [33]

$$\Delta E_\alpha = \text{Re } T^{\alpha\alpha}(E). \quad (10)$$

The form of the latter equation suggests the possibility of an iterative scheme for the determination of the level shift. Equations (8)–(10) provide the basis of our calculation scheme for evaluating the rates of various multiphoton processes.

In the alternative formalism [31], when the MPI process is treated as a scattering phenomenon, the expression for the  $T$  operator must be corrected for the virtual transitions between various photodetachment channels. This correction comes from a careful examination of the boundary conditions which must be imposed on a scattering wave function in the Floquet representation. In its simplest form, this can be achieved by dividing the conventional expression for the matrix element of the  $T$  operator by a Bessel function  $J_0$  [31]. The

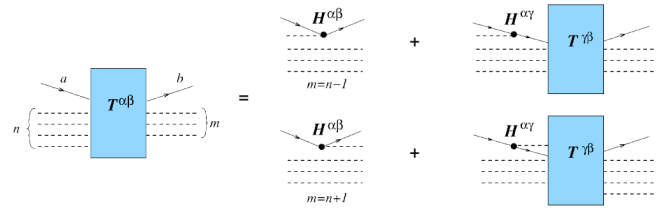


FIG. 1. Diagram representation of the Lippmann-Schwinger equation for multiphoton ionization. The graphical symbols are described in the text.

problem outlined by Eqs. (8)–(10) is a decay, or an initial state, problem. As such, it requires an accurate evaluation of the initial state which subsequently decays into various open channels. Indeed, Eq. (8) is a result of evaluation of the quantum-mechanical amplitude  $\langle \beta | \Psi(t) \rangle$ , where  $\Psi(t)$  evolves from the state  $|\alpha\rangle$  at  $t=0$  [33]. Therefore, no additional correction to the transition amplitudes (9) is needed.

By introducing in Eq. (9) a complete set of states of  $\hat{H}_0$ , this equation can be rewritten in the form of a spectral representation,

$$T^{\beta\alpha} = \hat{H}_{\text{int}}^{\beta\alpha} + \sum_{\gamma \neq \alpha} \frac{\hat{H}_{\text{int}}^{\beta\gamma} T^{\gamma\alpha}}{E_\alpha + \Delta E_\alpha - E_\gamma + i\epsilon}. \quad (11)$$

Here the sign of  $i\epsilon$  gives the rule of bypassing the pole when performing the integration over the continuum spectrum.

The shift of the energy of the initial state is explicitly included into the set of Eqs. (11). This circumstance may be especially important for the atomic systems with more than one electron. When the escaping electron leaves the atomic system, the remaining ion still interacts with the electromagnetic field; the energy shift in Eqs. (11) takes into account effects of this interaction.

In Fig. 1, we give a graphical representation of Eq. (11). Here a straight line with an arrow to the right represents a target atom and the dashed lines are used to depict the photons. A vertex with two electron lines and one photon line represents a dipole matrix element (7) which incorporates many-electron correlation in the target. For simplicity, we do not show the quadrupole and monopole matrix elements (11) which are parametrically small for not very strong fields  $F < 1$ . A rectangular block stands for the  $T$  matrix (11). In the low-field regime, the integral term on the right-hand side of Eq. (11) can be ignored and the atomic ionization is described by the bare matrix element  $\langle a, n | \hat{H}_{\text{int}} | b, n \pm 1 \rangle$ . The strong field effects are incorporated in the integral term and include multiple absorption and emission of the laser photons.

The sum over the spectrum of  $\hat{H}_0$  in Eq. (11) includes summation over various number of photons as well as summation over bound atomic states and integration over the continuous spectrum of the atom. Computation of the integral in Eq. (11) can be greatly simplified by introducing a discrete set of target pseudostates which provides an adequate quadrature rule. As the result of such a discretization, the set of equations (11) becomes a linear system on the unknown elements of the  $T$  matrix. Once this linear system is

solved, all information about the integral and differential features of the MPI process can be obtained from the matrix elements of the  $T$  operator taken at the energy corresponding to the shifted energy of the final state as in Eq. (8) (the so-called on shell matrix elements). We note that in the weak-field limit, summation in Eq. (11) can be restricted to the atomic variables and we arrive at the expression for the dipole matrix element given by Eq. (12) of Kheifets and Bray [35].

### A. Square-well model

To illustrate the feasibility of our approach, we first apply it to a model problem of an MPI process from a one-dimensional square well. It is this model system that was considered by Burke *et al.* [24] in their seminal paper which gave rise to the spectacular success of the  $R$ -matrix Floquet theory. We consider here an electron bound initially in a square-well potential  $V=-2.5$  a.u. for  $0 < x < 1$  and  $V=0$  for  $x > 1$ , with the boundary condition  $R(0)=0$  imposed on the wave functions. This potential supports only one bound state  $a$  with an energy  $E=-0.4657$  a.u. We consider an MPI process when the electric field with the frequency  $\omega=0.2$  is applied such that at least three photons are needed to ionize the system. To solve this problem, we follow the steps outlined in Sec. II. The set of Eqs. (11) is converted into a linear system on the  $T$ -matrix elements by choosing a suitable discretization procedure for the continuous spectrum integration. The summation over a set of intermediate states  $\gamma$  in Eq. (11) is a sum over various numbers of photons  $n_\gamma$  and summation and integration over the set of variables specifying the field-free electron states. For the square-well model, the latter are determined by a single quantum number (momentum of the states belonging to the continuous spectrum or energy of the discrete spectrum). For a given number of photons in the set of intermediate states  $\gamma$ , we first determine if there is a pole in the integral over the continuous spectrum. Similarly to the electron scattering calculations of Bray [34], we divide the momentum integration interval  $(0, \infty)$  into five subintervals.

If the pole is present in the integral, the first two subintervals are chosen to be  $(0, k_{\text{pole}})$  and  $(k_{\text{pole}}, 2k_{\text{pole}})$  with a typical number of 60 momentum points in each interval. Then the  $\delta$ -function singularity is isolated and the remaining principal value integral is evaluated by a modified Simpson's rule [34]. The remaining part of the momentum integral is divided as follows:  $(2k_{\text{pole}}, 4)$  (50 integration points),  $(4, 10)$  (40 points), and  $(10, 350)$  (40 points). These intervals are pole-free and the integration is performed by using a conventional Simpson's rule. If there is no pole in a given channel, the integration procedure remains essentially the same except for the boundary of the first and second intervals, which is chosen at one atomic unit of momentum. In this case, the conventional Simpson's rule is used throughout.

We retained various numbers of photons in the intermediate state of Eq. (11). For simplicity, we count this number from the baseline of three photons in the initial state, which we denote as  $\alpha=|a, 3\rangle$ . In the intermediate and final states, we can then have negative numbers of photons. For example,

$n=-1$  in the final state  $|\gamma\rangle$  would mean that four photons have been absorbed. Using this convention, the calculations we performed can be denoted as  $(n^{\text{min}}, n^{\text{max}})$ , meaning that the number of photons in the intermediate and final states ranges from  $n^{\text{min}}$  to  $n^{\text{max}}$ .

The problem which arises immediately when one tries to apply Eqs. (11) for the square-well model is the singularity of the matrix elements  $\hat{H}_{\text{int}}^{\beta\alpha}$  when both states  $\alpha, \beta$  lie in the continuum. This is, of course, a consequence of the choice of the gauge of the vector potential in formulas (3). Fortunately, as we shall show in the section, this problem can be avoided for real atomic systems by choosing the interaction Hamiltonian in the Kramers-Hennerberger (acceleration) form. For the square-well potential, such a choice of the interaction Hamiltonian is not possible due to the singular character of the potential. We shall have, therefore, to devise a suitable procedure of the regularization of the matrix elements of operator (3) when both states belong to the continuous spectrum. There is a vast amount of literature devoted to the study of such matrix elements for various potentials (e.g., [39–41]). We dealt with this problem along the lines described in the paper by Mercouris *et al.* [23]. One can show that for any potential for which the asymptotic behavior of the continuous wave function is given by  $R_k \propto \sin(kr + \delta)$ , the following result holds:

$$\int_0^\infty R_{k_i}(r) \frac{d}{dr} R_{k_f}(r) dr = V(k_i, k_f) + \frac{\cos(\delta_i - \delta_f)}{2} \text{P} \frac{1}{k_i - k_f}. \quad (12)$$

Here  $V(k_i, k_f)$  is a regular function and the symbol P has the usual meaning of the principal value integral. Note that this divergence is present only when the velocity form (as in the present paper) or the length form are used for the electromagnetic interaction operator; it is absent if the acceleration form is used. The presence of the singularity in the matrix elements in the velocity and length gauges is a consequence of the use of the spectral representation for the Green function in Eq. (11) and should disappear from the final result after the summation over the whole spectrum is carried out. A convenient way to deal with such integrals is to introduce a suitable regularization procedure. Different procedures of this sort can be devised. We shall illustrate the use of the two simplest methods.

The first regularization scheme consists in computing all the divergent integrals over some finite interval  $(0, D)$ , hoping that the final results depend only very weakly upon  $D$  if its value is suitably chosen. That this is indeed so can be seen from the results for the level shift presented in Table I. According to Eq. (10), this quantity is related to the real part of the diagonal matrix element of the  $T$  operator.

To determine the shift, we devised a simple iterative procedure, based on Eq. (10). The linear system (11) was solved with a trial value  $\Delta E_\alpha=0$ , then the value given by the right-hand side of Eq. (10) was adopted as a new trial value for  $\Delta E_\alpha$ . The procedure was repeated until convergence was achieved. Typically, three iterations were sufficient to achieve convergence on the level of a fraction of a percent.

TABLE I. Dependence of the level shift from the  $(-4,4)$  calculation upon the regularization parameter  $D$  (in a.u.).

$D$	$F=0.06$ a.u.	$F=0.1$ a.u.	$F=0.14$ a.u.	$F=0.2$ a.u.
30	-0.023307	-0.065753	-0.13132	-0.28124
40	-0.023305	-0.065704	-0.13045	-0.27645
50	-0.023311	-0.065794	-0.13245	-0.29102
60	-0.023316	-0.065743	-0.13386	-0.29239
70	-0.023313	-0.065749	-0.13193	-0.29839

The results of a  $(-4,4)$  calculation using this strategy are shown in Table I. The calculation was performed for different values of the cutoff parameter  $D$ . As one can see, the values for the level shift are fairly stable with respect to the variations of the regularization parameter  $D$ . The stability of the results with  $D$  becomes somewhat worse for very strong fields ( $F=0.2$  a.u. in Table I). This, however, is to be expected as for such strong fields the  $(-4,4)$  calculation is probably too small and a larger number of photons should be included to obtain more accurate results. Results in Table I should be compared with the plot illustrating the level shift as a function of the electric field strength from the time-dependent  $R$ -matrix calculation of Burke and Burke [42]. Although the numerical values are not reported in this paper, a visual comparison of our data with the plot is quite satisfactory.

Another regularization scheme, which we found to give somewhat more stable results for the ionization rates, is based on the regularization formula for a principal value integral,

$$P \frac{1}{k_i - k_f} = \lim_{\epsilon \rightarrow 0} \frac{k_i - k_f}{\epsilon^2 + (k_i - k_f)^2}. \quad (13)$$

Again, one can hope that if the regularization is properly implemented, the final results do not depend upon the regularization parameter  $\epsilon$ . We analyze these results in the form of the partial ionization rates computed according to Eq. (8). The momentum  $k_f$  of the final state is determined via the

TABLE II. Convergence of the partial ionization rates  $\Gamma_3, \Gamma_4, \Gamma_5$  from the  $(-3,3)$  calculation with respect to the regularization parameter  $\epsilon$  in 13. The field strength is  $F=0.1$  a.u.

$\epsilon \times 10^2$	$\Gamma_3(10^{-4}$ a.u.)	$\Gamma_4(10^{-6}$ a.u.)	$\Gamma_5(10^{-6}$ a.u.)
100	1.582	1.7958	5.584
50	1.829	0.9439	5.866
25	2.045	0.2198	6.165
12.5	2.216	0.1252	6.518
6.25	2.334	0.4667	6.552
3.125	2.404	0.7188	6.529
1.563	2.441	0.8496	6.547
0.781	2.454	0.9187	6.578
0.390	2.456	0.9537	6.610
0.195	2.460	0.9682	6.622

energy of the initial state  $\alpha$ , number of photons in the final state  $n_f$ , and the energy shift  $\Delta E$ , given by Eq. (10),

$$\frac{k_f^2}{2} = E_\alpha + \Delta E - n_f \omega. \quad (14)$$

The total ionization rate is the sum of the partial rates over all the open channels.

In Table II, we show the partial ionization rates  $\Gamma_3, \Gamma_4, \Gamma_5$  from our  $(-3,3)$  calculation. The data presented in the table clearly indicate convergence as  $\epsilon \rightarrow 0$ . In Table III, we present the partial ionization rates  $\Gamma_i$ , where  $i$  denotes the number of absorbed photons for the field strength  $F=0.1$  a.u. We used a different number of laser photons ( $n^{\min}, n^{\max}$ ), with  $n^{\max}=3,4$  and  $n^{\min}=-4,-3,-2,-1,0$ . In these calculations, the number of open channels may differ. For example, in the  $(-4,3)$  calculation, one may have the final states with three, four, five, six, or seven photons absorbed. We remind the reader that we count the number of photons from the baseline of three photons in the initial state.

As one can see, the partial rates corresponding to processes with a large number of photons absorbed (four and five) show a certain stability with respect to the number of photons included in the calculation, which gives us confidence in the results obtained for these partial rates. One may note, in particular, that for  $F=0.1$  a.u., the partial rate  $\Gamma_5$  becomes larger than the rate  $\Gamma_4$ .

The partial contribution of various open channels to the total ionization rate can be judged from the data presented in Fig. 2, where we plot the branching ratios for the channels with various numbers of photons in the final state. Again, one can see that for not very large field strengths ( $F < 0.05$  a.u.), the contributions of the channels with more than three photons absorbed (labeled  $n=4$  and  $n=5$  in the figure) can be neglected, though for larger fields their effect is becoming increasingly important.

TABLE III. Ionization rates for  $F=0.1$  a.u.

$n^{\min}, n^{\max}$	$\Gamma_3(10^{-4}$ a.u.)	$\Gamma_4(10^{-6}$ a.u.)	$\Gamma_5(10^{-6}$ a.u.)
-2,3	2.4586	1.0628	6.7172
-3,3	2.4562	0.9537	6.6101
-4,3	2.4569	0.9644	6.5025
-2,4	2.3228	0.8676	6.6303
-3,4	2.3208	0.7817	6.5132

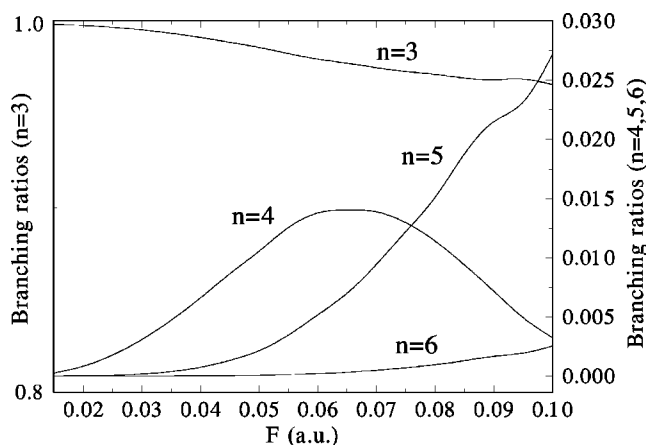


FIG. 2. Branching ratios of the partial ionization rate to the total rate for various open channels in the square-well model.

Incidentally, one may note that even the (0,3) calculation would not correspond exactly to the third-order perturbation theory. Indeed, solution of the coupled set of Eq. (11) amounts effectively to summation of an infinite subset of the perturbation theory terms, as is illustrated in Fig. 1.

The situation becomes somewhat more complicated for stronger fields ( $F > 0.1$  a.u.) where the level shift is so large that the channel closing may occur. A look at the data for the shift presented in Table I shows that when  $F \approx 0.14$  a.u., the energy of the initial bound state  $\alpha$  is  $E \approx -0.6$  a.u. and absorption of the three photons is no longer sufficient to ionize the system. A more precise value of the field for which the channel corresponding to absorption of the three photons closes is  $F \approx 0.1435$  a.u., as shown by Burke and Burke [42]. A rich variety of phenomena may occur when the field approaches this critical value (and larger ones, corresponding to closing of other channels), in particular ionization rates as functions of electric field intensity may have discontinuities [42].

In Fig. 3, we plot the total ionization rate as a function of the field strength from the  $(-4,3)$  calculation. The same data for the total ionization rate are presented in Table IV. In the figure, we make a comparison with the time-dependent

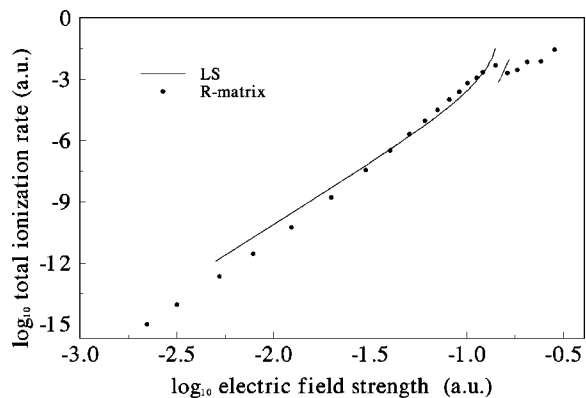


FIG. 3. Total ionization rate as a function of the field strength. The solid line shows the present  $(-4,3)$  calculation. Results of the time-dependent  $R$ -matrix calculation of Burke and Burke [42] are shown as points.

TABLE IV. Total ionization rate from the  $(-4,3)$  calculation.

$F$ (a.u.)	$\Gamma$ (a.u.)	$F$ (a.u.)	$\Gamma$ (a.u.)
0.025	$0.192 \times 10^{-7}$	0.14	$0.237 \times 10^{-1}$
0.05	$0.135 \times 10^{-5}$	0.15	$0.119 \times 10^{-2}$
0.075	$0.291 \times 10^{-4}$	0.16	$0.358 \times 10^{-2}$
0.1	$0.254 \times 10^{-4}$	0.175	$0.356 \times 10^{-1}$
0.125	$0.279 \times 10^{-2}$		

$R$ -matrix calculation by [42] which was found to be almost identical to the earlier Floquet  $R$ -matrix results by Bruke *et al.* [24].

Our data show a certain trend to deviate from those obtained in Bruke and Bruke [42] and Bruke *et al.* [24] for smaller field intensities, around  $F \approx 0.02$  a.u. This deviation could probably be attributed to difficulties of numerical character which are due to the necessity to manipulate the divergent integrals. These are most difficult to cope with for smaller fields when rates are small. These difficulties may easily be avoided for “real world” problems. For any realistic atomic system, writing the electromagnetic interaction operator in the acceleration form would make all the integrals well-defined and convergent.

## B. Hydrogen atom

We turn now to a more realistic system—the hydrogen atom in the presence of a monochromatic linearly polarized laser field. As we mentioned above, this system is in some sense simpler than the model square-well problem, as we can use the Kramers-Henneberger form of the interaction Hamiltonian [43,44], which, as we shall see, allows us to avoid all the problems of divergence of the matrix elements.

If the electromagnetic field is treated classically, the Kramers-Henneberger Hamiltonian can be obtained from the minimal-coupling Hamiltonian  $\hat{H}_{\min}$  given by Eqs. (2) and (3) by means of a canonical transformation  $\hat{H}_{\text{KH}} = e^{i\hat{T}} \hat{H}_{\min} e^{-i\hat{T}} - \partial\hat{T}/\partial t$  generated by the operator [44]

$$\hat{T} = -\frac{1}{c} \int_0^t \mathbf{A}(\tau) \mathbf{p} \, d\tau + \frac{1}{2c^2} \int_0^t \mathbf{A}^2(\tau) d\tau, \quad (15)$$

where  $\mathbf{A}$  is the vector potential and  $\mathbf{p}$  is the momentum operator.

In the present approach, when the electromagnetic field is described quantum mechanically, we need a quantum analog of the transformation (15). Such a transformation is known as the Pauli-Fierz canonical transformation [45]. For the case of the sufficiently intense linearly polarized monochromatic light, when all the processes of spontaneous radiation are neglected and the quantized vector potential is given by Eq. (4), with only the laser mode photons preserved in the expansion, this transformation assumes the form [46]

$$\mathbf{r} = \mathbf{r}' + \frac{\mathbf{a}}{\omega} \hat{Q},$$

$$\mathbf{p} = \mathbf{p}',$$

$$\begin{aligned}\hat{Q} &= \hat{Q}', \\ \hat{P} &= \hat{P}' - \frac{\mathbf{a}\mathbf{p}'}{\omega},\end{aligned}\quad (16)$$

where  $\mathbf{a} = 2e\sqrt{\pi/\omega}$ ,  $\mathbf{e}$  is the polarization vector, and the operators  $\hat{Q}'$  and  $\hat{P}'$  are expressed in terms of creation and annihilation operators in Eq. (4) via

$$\begin{aligned}\hat{a}_k &= \frac{1}{\sqrt{2}}(\hat{P} + i\hat{Q}), \\ \hat{a}_k^\dagger &= \frac{1}{\sqrt{2}}(\hat{P} - i\hat{Q}).\end{aligned}\quad (17)$$

In Eqs. (16) and (17), primed quantities refer to the original (laboratory) frame, and nonprimed to the Kramers-Henneberger frame.

Under the transformation (16), the minimal-coupling Hamiltonian (2) becomes

$$\hat{H}_{\text{KH}} = \frac{\mathbf{p}^2}{2} - \frac{1}{r} + \hat{H}_{\text{field}} + \hat{H}_{\text{intKH}},\quad (18)$$

where  $\hat{H}_{\text{field}}$  has the same meaning as in Eq. (2) and the interaction Hamiltonian has the form

$$\hat{H}_{\text{intKH}} = -\frac{1}{|\mathbf{r} + \hat{\boldsymbol{\alpha}}|} + \frac{1}{r},\quad (19)$$

where the operator  $\hat{\boldsymbol{\alpha}} = \hat{\mathbf{F}}/\omega^2$  is related to the operator of the electric field intensity  $\hat{\mathbf{F}}$ .

A certain amount of care should be taken when physically relevant information is to be extracted from the transformed Hamiltonian  $\hat{H}_{\text{KH}}$ , in particular when our aim is to study the time evolution of a quantum system prepared at the moment  $t=0$  in a given eigenstate of the field-free Hamiltonian. The Kramers-Henneberger transformation consists, basically, in transforming the Schrödinger equation into a noninertial frame moving with an electron oscillating in the field [in the quantum version of this transformation, this can be seen from the first of Eqs. (16), the quantity on the right-hand side of this equation being essentially an electric field operator]. Both the initial- and final-state vectors must then be transformed accordingly [47,48]. This circumstance may introduce additional complexity in the problem. Below, we report results on the total ionization rate for multiphoton ionization of a hydrogen atom. One can present the following argument showing that if we are interested in integral characteristics, such as total ionization rate, one need not transform initial and final states. Indeed, the solution of the set of Eqs. (11) with the Kramers-Henneberger Hamiltonian (18) and (19) is essentially a study of the singular points of the resolvent operator  $(E - \hat{H}_{\text{KH}})^{-1}$  (we will be looking, of course, for the points lying on the unphysical sheets of the Riemann surface). The total ionization rate from the ground state of hydrogen obtained below from such a study of the Hamiltonian  $\hat{H}_{\text{KH}}$  is in fact related to an imaginary part of one such sin-

gular point. On the other hand, the total ionization rate obtained using the minimal-coupling Hamiltonian is related to a singular point of the resolvent operator  $(E - \hat{H}_{\text{min}})^{-1}$ , which is connected to the resolvent operator  $(E - \hat{H}_{\text{KH}})^{-1}$  by means of the canonical transformation (16). The latter transformation does not change the position of singular points, hence a study of the singular points  $H_{\text{KH}}$  alone [by means of solving the set of Eqs. (11)] should give us a correct value for the total ionization rate.

To apply the strategy based on Eqs. (11) to the system described by the Kramers-Henneberger Hamiltonian, one should be able to compute the matrix elements of the operator (19). The procedure which we devised for this purpose is described below.

### 1. Calculation of matrix elements of $\hat{H}_{\text{int}}$

We shall need the following formula for the matrix elements of the operator of the electromagnetic field, which can be obtained analogously to Eqs. (5):

$$\langle a, n | \mathbf{a} \cdot \hat{\mathbf{F}} | b, m \rangle \approx \frac{1}{2} \langle a | \mathbf{a} \cdot \mathbf{F} | b \rangle, \quad n \rightarrow \infty, \quad |m - n| = 1,$$

$$\langle a, n | \mathbf{a} \cdot \hat{\mathbf{F}} | b, m \rangle = 0, \quad |m - n| \neq 1. \quad (20)$$

In Eq. (20),  $\mathbf{F}$  is the classical vector of electric field strength and  $\mathbf{a}$  is an arbitrary vector operator not acting on the photon variables. The correction term to the nonzero matrix element in Eq. (20) is of the order of  $n^{-1/2}$  and is negligible in the limit of large intensities, which is of interest to us in the present paper.

Consider first the matrix element

$$M_{mp} = \langle n + p | (\mathbf{a} \cdot \hat{\mathbf{F}})^m | n \rangle. \quad (21)$$

We are interested now only in photonic variables, therefore we omitted in Eq. (21) any reference to atomic variables. It is easy to see that  $M_{mp} \neq 0$  only if  $m = p + 2k$  with an integer non-negative  $k$ . If this condition is satisfied, it is easy to show using Eqs. (7) and simple combinatorial analysis that

$$M_{mp} = \left(\frac{\mathbf{a} \cdot \mathbf{F}}{2}\right)^m \frac{m!}{\left(\frac{m+p}{2}\right)! \left(\frac{m-p}{2}\right)!}. \quad (22)$$

We can now compute a more complicated matrix element,

$$\langle n - p | \exp\{\mathbf{a} \cdot \hat{\mathbf{F}}\} | n \rangle. \quad (23)$$

By expanding the exponential function in the above expression, with the use of Eq. (21) and the known series expansion for the Bessel function  $I_p(x)$  [49],

$$I_p(x) = \left(\frac{x}{2}\right)^p \sum_{k=0}^{\infty} \frac{\left(\frac{x}{2}\right)^{2k}}{k! \Gamma(k+p+1)}, \quad (24)$$

we can obtain the following expression:

TABLE V. Matrix elements of the operator (3) for  $F=0.0534$  a.u.

Angular frequency	$\langle 1s, n=1   \hat{H}_{\text{int}}   2p, n=0 \rangle$		$\langle 1s, n=1   \hat{H}_{\text{int}}   kp, n=0 \rangle$	
	Present	PT	Present	PT
0.65	0.03070	0.03118	0.02126	0.02143
0.184	0.04678	0.08261	0.11335	0.26796

$$\langle n+p | \exp\{\mathbf{a} \cdot \hat{\mathbf{F}}\} | n \rangle = I_p(\mathbf{a} \cdot \mathbf{F}), \quad (25)$$

where  $I_p(x)$  is a modified Bessel function of order  $p$  [49].

We may now turn to the computation of the matrix elements of the operator (3). Representing Eq. (3) as a Fourier transform,

$$\frac{1}{|\mathbf{r}_i + \hat{\boldsymbol{\alpha}}|} = \frac{1}{2\pi^2} \int \frac{e^{i\mathbf{q} \cdot (\mathbf{r} + \hat{\boldsymbol{\alpha}})}}{q^2} d\mathbf{q}, \quad (26)$$

using expression (25) and the known integral representation for the modified Bessel function  $I_p(x)$  [49],

$$I_p(x) = \frac{1}{\pi} \int_0^\pi e^{x \cos \theta} \cos p\theta d\theta, \quad (27)$$

one can obtain the following formula:

$$\left\langle n+p \left| \frac{1}{r_i} - \frac{1}{|\mathbf{r}_i + \hat{\mathbf{F}}/\omega^2|} \right| n \right\rangle = \frac{1}{\pi} \int_0^\pi \cos p\theta \left( \frac{1}{r_i} - \frac{1}{|\mathbf{r}_i + \mathbf{F} \cos \theta/\omega^2|} \right) d\theta. \quad (28)$$

To proceed further, we use a spherical harmonics expansion [50],

$$\frac{1}{|\mathbf{r}_i + \mathbf{F} \cos \theta/\omega^2|} = \sum_{k=0}^{\infty} \sqrt{\frac{4\pi}{2k+1}} \frac{r_{<}^k}{r_{>}^{k+1}} [-\text{sgn}(\cos \theta)]^k Y_{k0}(\mathbf{r}), \quad (29)$$

where  $r_{<}(r_{>})$  is the smaller (greater) of  $r_i$  and  $F \cos \theta/\omega^2$ . Here the field  $\mathbf{F}$  is directed along the  $z$  axis. Equation (29) allows separation of the radial and angular variables. Angular parts are evaluated analytically using integrals of products of several spherical functions [50],

$$\begin{aligned} & \int Y_{l_1 m_1}(\boldsymbol{\Omega}) Y_{l_2 m_2}(\boldsymbol{\Omega}) Y_{l_3 m_3}(\boldsymbol{\Omega}) d\boldsymbol{\Omega} \\ &= \sqrt{\frac{(2l_1+)(2l_2+1)(2l_3+1)}{4\pi}} \begin{pmatrix} l_1 & l_2 & l_3 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & l_3 \\ m_1 & m_2 & m_3 \end{pmatrix}. \end{aligned} \quad (30)$$

Radial integrals are computed numerically.

## 2. Numerical results

We first illustrate our procedure of the calculation of the matrix elements of the interaction Hamiltonian. With the help of the formulas (28) and (29), we calculated the inte-

grals  $\langle a, n+p | \hat{H}_{\text{int}} | b, n \rangle$ . In the case of a hydrogen atom, the atomic states  $|a\rangle$  are characterized by energies and angular momenta. We computed integrals for a sufficiently dense grid of energies. As for the range of momenta and a number of photons retained in the calculation, their upper limits depend on the value of the electric field strength. For moderately high field strengths ( $F \approx 0.1$  a.u.), it was sufficient to compute integrals with  $l < l_{\text{max}}=3$  and  $p < p_{\text{max}}=7$ . The integrals were computed and stored on a disk.

As one can see from Eq. (28), in the weak field limit  $p=1$  and the interaction Hamiltonian in the Kramers-Hennerberger form reduces to the operator  $\hat{\mathbf{F}}\mathbf{r}/r^3\omega^2$ , which is commonly used in the first-order calculations performed in the acceleration gauge. The parameter which measures the departure of the matrix element of operator (28) from the first-order result is the ratio  $F/\omega^2$ . This departure can be quite significant. To give an illustration of the relative role of the higher-order corrections in Eq. (28), we present in Table V few values of the matrix elements  $\langle 1s, n=1 | \hat{H}_{\text{int}} | 2p, n=0 \rangle$  and  $\langle 1s, n=1 | \hat{H}_{\text{int}} | kp, n=0 \rangle$  with momentum  $k=1$  a.u. for different frequencies and electric field strength of  $F=0.0534$  a.u. First-order matrix elements are also given in Table V (marked as PT). As can be seen, for small frequencies the deviation of the matrix elements from the first-order values can be significant.

To facilitate comparison with the literature, we performed a series of calculations for the same set of laser field strengths and frequencies as reported by Dorr *et al.* [27], who used a combination of the Floquet ansatz and the  $R$ -matrix methods. Our results for the level shift and total ionization rate together with the literature values are summarized in Table VI.

When presenting their data for the level shifts, Dorr *et al.* [27], who performed their calculation in the length gauge, subtracted the ponderomotive energy  $E_p = F^2/4\omega^2$  from the total shift. Since the level shifts in the acceleration and the length gauge are related as  $\Delta E^A = \Delta E^L - E_p$  [24], the two sets of data are directly comparable.

We consider first the case of the laser field with  $\omega = 0.65$  a.u. and  $F=0.0534$  a.u. As noted by Dorr *et al.* [27], this is still a perturbative regime. In Eqs. (11), we need not, therefore, retain a very large set of intermediate states  $\gamma$  to achieve convergence.

In the sum over the intermediate states we included the hydrogen atom states with orbital momentum  $l=0,1$  and a set of photonic states with numbers of photons ranging from  $n_{\text{min}}=-2$  to  $n_{\text{max}}=3$ . Counting the photons, we use here the same convention we used in the previous section when dealing with the square-well potential model. We count the total



TABLE VI. Total ionization rates and shifts for atomic hydrogen in a linearly polarized field of frequency  $\omega$  and strength  $F$  (a.u.). Numbers in parentheses represent data of Dorr *et al.* [27].

Angular frequency	Field strength	Total ionization rate		Shift	
		Present	Dorr <i>et al.</i> [27]	Present	Dorr <i>et al.</i> [27]
0.65	0.0534	0.00263	0.00256	0.000364	0.000360
	0.754	0.13	0.14	0.176	0.195
0.184	0.0169	$9.2 \times 10^{-6}$	$8.8 \times 10^{-6}$	-0.002910	-0.002543
	0.0534	$1.33 \times 10^{-3}$	$1.40 \times 10^{-3}$	-0.0280	-0.0257

number of photons in the system from the minimal number of photons needed to ionize the initial state. Thus, for the angular frequency  $\omega=0.65$  and the ground state of the hydrogen atom, we have one photon in the initial state. The state with  $n=-1$  will then correspond to the state in which two photons have been absorbed.

As one can see from Table VI, we achieve quite a good agreement with the data of Dorr *et al.* [27], both for the total rate and level shift. For a much larger field and the same frequency  $\omega=0.65$  a.u., we need a larger set of intermediate states to be included, Eq. (11). Convergence was achieved when we included the hydrogen atom states with  $l < l_{\max}=4$  and photonic states with numbers of photons ranging from  $n_{\min}=-2$  to  $n_{\max}=3$ .

For the process of genuine multiphoton ionization ( $\omega=0.184$ ), we also have reasonably good agreement with the results of the Floquet  $R$ -matrix calculation [27]. For the field strength  $F=0.0169$ , we used atomic states with angular momenta  $l < 4$  and photonic states with  $n_{\min}=-1$  and  $n_{\max}=5$ . This field value is still in the perturbative regime.

Truly nonperturbative effects appear for larger field strengths. To obtain the values of the shift and total rate for  $F=0.0534$ , we used atomic states with  $l < 4$  and photonic states with  $n_{\min}=-2$  and  $n_{\max}=5$ .

### III. CONCLUSION

We developed a nonperturbative formalism which describes the MPI process by a set of coupled integral equa-

tions of the Lippmann-Schwinger type. In contrast to the scattering formalism given in the literature [9,16,17,19], we do not rely on the field modified Volkov states. Instead, we employ a more convenient set of the field-free atomic states which is particularly advantageous for complex atomic systems with more than one target electron. This approach, however, can only be realized if one is able to generate a complete set of discrete target pseudostates providing an accurate quadrature rule. In this respect, we rely on the CCC method, which demonstrated its ability to build an efficient pseudostate basis for one- and two-electron targets. This gives us confidence that we can implement our computational scheme for nonperturbative description of MPI in complex atomic systems such as the helium atom. Thus we should be able to extend a very successful application of the CCC method to the weak-field double photoionization to the strong-field domain.

We demonstrated the utility of our approach for a model problem of a square-well potential and a hydrogen atom. Also, we demonstrated that the partial ionization rates, computation of which is usually the most difficult part of the problem, remain stable with respect to the number of photons retained in the calculation.

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