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Theoretical spectroscopy of autoionization resonances in spectra of lanthanide atoms

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Abstract
A theoretical study of the autoionization resonances in the spectra of lanthanide atoms (ytterbium) was carried out within the relativistic many-body perturbation theory and the generalized relativistic energy approach (the Gell-Mann and Low *S*-matrix formalism). The accurate results on the autoionization resonance energies and widths in ytterbium are presented with correctly accounting for the exchange correlation and relativistic corrections and are compared with the other available theoretical and experimental data.

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1. Introduction

The investigation of spectra (optical and spectral), radiative and autoionization characteristics of heavy elements atoms and multicharged ions has traditionally been of great interest for the further development of quantum atomic optics and atomic spectroscopy and their different applications in plasma chemistry, astrophysics, laser physics, etc (see [1–14]). Different atomic spectroscopy methods have been used to study the radiative and autoionization characteristics of atomic systems. The well-known classical multi-configuration Hartree–Fock method (as a rule, the relativistic effects are taken into account in the Pauli approximation or Breit Hamiltonian, etc.) allowed to obtain a great deal of useful spectral information about light and non-heavy atomic systems, but in fact it provides only a qualitative description of spectra of heavy atoms and ions. The multi-configuration Dirac–Fock method is the most reliable version of calculation for multielectron systems with a large nuclear charge. In these calculations, one- and two-particle relativistic effects are taken into account practically precisely. In this sense, special attention should be given to the two very general and important computer systems for relativistic and QED calculations of atomic and molecular properties that were developed in the Oxford group and are known as GRASP ('GRASP', 'Dirac'; 'BERTHA', 'QED') (see [1–8] and references therein). In particular, the BERTHA program embodies a new formulation of relativistic electron structure theory within the framework of relativistic QED. This leads to a simple and transparent formulation of the Dirac–Hartree–Fock–Breit (DHFB) self-consistent field equations along with algorithms for molecular properties, electron correlation and higher order QED effects. The DHFB equations are solved by a direct method based on a relativistic generalization of the McMurchie–Davidson algorithm for the electron integrals that economize memory requirements and is not significantly more expensive computationally than comparable nonrelativistic calculations [1–3].

Studying spectra, radiative and autoionization characteristics of heavy atoms and ions is quite a complicated task because of the need for correctly accounting for the exchange correlation and relativistic corrections (and also radiative and nuclear effects in the case of superheavy atomic systems). In this paper, we report our theoretical study of the autoionization resonances in spectra of lanthanide atoms (the ytterbium atom), which was carried out within the relativistic many-body perturbation theory (PT) and the generalized relativistic energy approach (the Gell-Mann and Low *S*-matrix formalism) [4, 9–19]. Accurate results on the autoionization resonance energies and widths in the ytterbium are presented with correctly accounting for the exchange correlation and relativistic corrections and compared with the other available theoretical and experimental data.

2. The relativistic energy approach and optimized many-body perturbation theory (PT)

A generalized gauge-invariant relativistic energy approach in the case of the multielectron atomic systems has been developed by Glushkov–Ivanov–Ivanova (see [9–12]).

The approach is based on the Gell-Mann and Low *S*-matrix formalism and the relativistic many-body PT using the optimized one-quasiparticle (QP) representation and an accurate account of the relativistic and exchange-correlation effects. In the relativistic case, the Gell-Mann and Low formula expressed an energy shift ΔE through the QED scattering matrix including the interaction with a photon vacuum field as the laser field [9–16]. The wave function zeroth basis is found from the Dirac equation with a potential, which includes the *ab initio* optimized model (Ivanov–Ivanova-type [20]) potential or density functional (DF) potentials, the electric potential of a nucleus (the Gaussian form of the charge distribution in a nucleus is usually used by us) [5]. The PT second and higher order corrections are taken into account by using the polarization and screening density functionals and potentials (from [11–14]). Generally speaking, the majority of complex atomic systems possess a dense energy spectrum of interacting states with essentially relativistic properties. In the theory of the non-relativistic atom a convenient field procedure is known for calculating the energy shifts ΔE of degenerate states. The procedure is connected with the secular matrix M diagonalization [8]. In constructing M, the Gell-Mann and Low adiabatic formula for ΔE is used. In contrast to the non-relativistic case, the secular matrix elements are already complex in the second order of the electrodynamical PT (first order of the interelectron interaction). Their imaginary part of ΔE is connected with the radiation decay (radiation) possibility. In this approach, the entire calculation of the energies and decay probabilities of a non-degenerate excited state is reduced to the calculation and diagonalization of the complex matrix M. In papers of different authors, the $\mathrm{Re}\,\Delta E$ calculation procedure has been generalized for the case of nearly degenerate states, whose levels form a more or less compact group. One of these variants has been introduced previously [9–12, 17–22]: for a system with a dense energy spectrum, a group of nearly degenerate states is extracted and their matrix M is calculated and diagonalized. If the states are well separated in energy, the matrix M reduces to one term, equal to ΔE. The non-relativistic secular matrix elements are expanded in a PT series for the interelectron interaction. The complex secular matrix M is represented in the form [9–11, 17–19]

$$M = M^{(0)} + M^{(1)} + M^{(2)} + M^{(3)}, \tag{1}$$

where $M^{(0)}$ is the contribution of the vacuum diagrams of all orders of PT, and $M^{(1)}$, $M^{(2)}$, $M^{(3)}$ those of the one-, two- and three-QP diagrams, respectively. $M^{(0)}$ is a real matrix, proportional to the unit matrix. It determines only the general level shift. We have assumed that $M^{(0)} = 0$. The diagonal matrix $M^{(1)}$ can be presented as a sum of the independent one-QP contributions. For simple systems (such as alkali atoms and ions), the one-QP energies can be taken from the experiment. Substituting these quantities into (1), one could have summarized all the contributions of the one-QP diagrams of all orders of the formally exact QED PT. However, the necessary experimental quantities are very often not available. The first two order corrections to $\mathrm{Re}M^{(2)}$ have been analyzed previously [19] using Feynman diagrams. The contributions of the first-order diagrams have been completely calculated. In the second order, there are two kinds of diagrams: polarization and ladder ones. The polarization diagrams take into account the QP interaction through the polarizable core, and the ladder diagrams account for the immediate QP interaction. Some of the ladder diagram contributions as well as some of the three-QP diagram contributions in all PT orders have the same angular symmetry as the two-QP diagram contributions of the first order. These contributions have been summarized by a modification of the central potential, which must now include the screening (anti-screening) of the core potential of each particle by two others. The additional potential modifies the one-QP orbitals and energies. Then the secular matrix is as follows:

$$M \to \tilde{M}^{(1)} + \tilde{M}^{(2)}, \tag{2}$$

where $\tilde{M}^{(1)}$ is the modified one-QP matrix (diagonal), and $\tilde{M}^{(2)}$ the modified two-QP one. $\tilde{M}^{(1)}$ is calculated by substituting the modified one-QP energies, and $\tilde{M}^{(2)}$ by means of the first PT order formulae for $M^{(2)}$, putting the modified radial functions of the one-QP states in the radial integrals.

Let us recall that in the QED theory, the photon propagator $D(12)$ plays the role of this interaction. Naturally, the analytical form of $D(12)$ depends on the gauge, in which the electrodynamical potentials are written. The inter-QP interaction operator with accounting for the Breit interaction has been taken as follows [9–11]:

$$V\left(r_i r_j\right) = \exp(\mathrm{i}\omega r_{ij})\frac{\left(1-\alpha_i\alpha_j\right)}{r_{ij}} + V^{w}_{ee}, \tag{3}$$

where, as usual, α_i are the Dirac matrices. In general, the results of all approximate calculations depended on the gauge. Naturally, the correct result must be gauge-invariant. The gauge dependence of the amplitudes of the photo-processes in the approximate calculations is a well-known fact and was investigated in detail by Grant, Armstrong, Aymar and Luc–Koenig, Glushkov and Ivanov, and others (see [1–4, 9–11, 21–25]). Grant has investigated the gauge connection with the limiting non-relativistic form of the transition operator and has formulated the conditions for approximate functions of the states, in which the amplitudes of the photo-processes are gauge invariant. These results remain true in the energy approach because the final formulae for the probabilities coincide in both approaches. Glushkov–Ivanov have developed a new relativistic gauge-conserved version of the energy approach [11]. Here we have applied this approach (relativistic energy approach, REA) to generate the optimized relativistic orbitals basis in the zeroth approximation of the optimized many-body PT (REA-OMBPT).

Below we will be interested in studying the spectra of the autoionization resonances in the ytterbium atom and in calculating their energies and widths. The excited states of the ytterbium atom can be treated as the states with the two-QP (also three-QP) above the electron core $[\mathrm{Xe}]4\mathrm{f}^{14}$. Within the energy approach [8–11] the radiative and autoionization widths are determined by the square of an electron interaction matrix element having the form

$$V^{\omega}_{1234} = [(j_1)\,(j_2)\,(j_3)\,(j_4)]^{1/2}\sum_{\lambda\mu}(-1)^{\mu}\begin{pmatrix} j_1\, j_3 & \lambda \\ m_1 - m_3 & \mu \end{pmatrix} \times Q_{\lambda}\,(1234)\,. \tag{4}$$

The real part of the electron interaction matrix element is determined using expansion in terms of Bessel functions [17–19, 26]:

$$\frac{\cos|\omega| r_{12}}{r_{12}} = \frac{\pi}{2\sqrt{r_1 r_2}} \sum_{\lambda=0} (\lambda)\, J_{\lambda+1/2}(|\omega| r_<)\, J_{-\lambda-1/2}(|\omega| r_>) \\ P_\lambda(\cos \mathbf{r}_1 \mathbf{r}_2)\,. \tag{5}$$

The Coulomb part Q_λ^{Qul} is expressed in terms of radial integrals R_λ, angular coefficients S_λ :

$$Q_\lambda^{\mathrm{Qul}} = \frac{1}{Z}\{R_l(1243)S_\lambda(1243) + R_\lambda(\tilde{1}\tilde{2}43)S_\lambda(\tilde{1}\tilde{2}43) \\ + R_\lambda(1\tilde{2}\tilde{4}3)S_\lambda(1\tilde{2}\tilde{4}3) + R_\lambda(\tilde{1}\tilde{2}\tilde{4}\tilde{3})S_\lambda(\tilde{1}\tilde{2}\tilde{4}\tilde{3})\}. \tag{6}$$

As a result, the autoionization decay probability is expressed in terms of $Q_\lambda(1243)$ matrix elements. Below is given the example

$$\mathrm{Re}\, R_\lambda(1243) = \iint \mathrm{d}r_1 r_1^2 r_2^2 f_1(r_1)\, f_3(r_1)\, f_2(r_2)\, f_4(r_2) \\ Z_\lambda^{(1)}(r_<)\, Z_\lambda^{(1)}(r_>)\,, \tag{7}$$

where f is the large component of the radial part of the single electron state Dirac function and the function Z is connected with the Bessel functions. The angular coefficient is defined by a standard method as above [13]. The Breit part of Q is defined in a similar way as above, but the contribution that is of our interest is a real part. The Breit interaction is known to change considerably the Auger decay dynamics in some cases (see, e.g., [9]). Determination of the radiation decay probabilities (oscillator strengths) results in calculating the imaginary matrix elements of the interaction (3). According to the Ivanov *et al* [13] method, calculation of the integrals $\mathrm{Re}\, R_\lambda(1243)$ is reduced to solving a system of differential equations:

$$\left.\begin{aligned} y_1' &= f_1 f_3 Z_\lambda^{(1)}(\alpha|\omega| r)\, r^{2+\lambda}, \\ y_2' &= f_2 f_4 Z_\lambda^{(1)}(\alpha|\omega| r)\, r^{2+\lambda}, \\ y_3' &= [y_1 f_2 f_4 + y_2 f_1 f_3]\, Z_\lambda^{(2)}(\alpha|\omega| r)\, r^{1-\lambda}. \end{aligned}\right\} \tag{8}$$

In addition, it is easy to show that

$$y_3(\infty) = \mathrm{Re}\, R_\lambda(1243), \quad y_1(\infty) = X_\lambda(13). \tag{9}$$

The system of differential equations includes equations for the functions $f/r^{|æ|-1}$, $g/r^{|æ|-1}$, $Z_\lambda^{(1)}$, $Z_\lambda^{(2)}$. The formulae for the autoionization (Auger) decay probability include the radial integrals $R_\alpha(\alpha k \gamma \beta)$, where one of the functions describes an electron in the continuum state. When calculating this integral, the correct normalization of the function Ψ_k is a problem. The correctly normalized function should have the following asymptotic at $r \to 0$:

$$\left.\begin{matrix} f \\ g \end{matrix}\right\} \to (\lambda\omega)^{-1/2} \begin{cases} \left[\omega + (\alpha Z)^{-2}\right]^{-1/2} \sin(kr+\delta)\,, \\ \left[\omega - (\alpha Z)^{-2}\right]^{-1/2} \cos(kr+\delta)\,. \end{cases} \tag{10}$$

When integrating the master system, the function is calculated simultaneously:

$$N(r) = \left\{\pi\omega_k\left[f_k^2\left[\omega_k + (\alpha Z)^{-2}\right] + g_k^2\left[\omega_k + \left(\alpha Z^{-2}\right)\right]\right]\right\}^{-1/2}. \tag{11}$$

It can be shown that at $r \to \infty$, $N(r) \to N_k$, where N_k is the normalization of functions f_k, g_k of the continuous spectrum satisfying the condition (10). It is important to also note that the calculation is carried out in the *jj*-coupling scheme representation. The transition to the intermediate coupling scheme has been realized by diagonalization of the secular matrix. Indeed, only $\mathrm{Re}\, M$ should be diagonalized. The imaginary part is converted by means of the matrix of eigenvectors $\{C_{mk}\}$, obtained by diagonalization of $\mathrm{Re}\, M$:

$$\mathrm{Im}\, M_{mk} = \sum_{ij} C_{mi}^*\, M_{ij}\, C_{jk}. \tag{12}$$

M_{ij} are the matrix elements in the *jj*-coupling scheme, and M_{mk} are those in the intermediate coupling scheme representation. This procedure is correct to terms of the order of $\mathrm{Im}\, M/\mathrm{Re}\, M$ [8]. More details can be found in [9–14, 17–19, 23–29].

3. Results

In table 1 we present the experimental (compilation) [34] (www.nist.gov/physlab/data/asd.cfm) and theoretical data for energies (accounted for from the ground state: $4f^{14}6s^2{}^1S_0$) of some YbI singly excited states: MCHF-BP—the data [35] obtained on the basis of the multiconfiguration Hartree–Fock (MCHF) method within the framework of Breit–Pauli (BP) relativistic corrections developed by Fischer [36] (A, B+D, D different sets of configurations considered in MCHF-BP calculation [35]); HFR—the data [35] obtained on the basis of Cowan's relativistic Hartree–Fock method; EA-MMBPT ($E1$)—the data [18, 30, 31] obtained by Ivanov *et al* on the basis of the model many-body PT and energy approach (EA-MMBPT); '[37]'—the data of the analysis by Wyart–Camus and this work (REA-OMBPT method, $E2$).

In table 2 we present the experimental (Letokhov *et al*) and theoretical data [18, 30, 31, 34] for energies and widths of the excited (autoionization) states of the 7s6p configuration in the spectrum of YbI (accounted for from the ground state: $4f^{14}6s^2{}^1S_0$Yb): $E1$, $\Gamma 1$—the EA-MMBPT method data of Ivanov *et al* [18, 30, 31]; $E2$, $\Gamma 2$—this work (REA-OMBPT method); $E3$—the MCHF-BP data of [35] (the classification in [35] differs from the classification in [18] and our classifications). A scheme of YbI energy levels and experimentally studied transitions is presented in figure 1.

An analysis reveals quite physically reasonable agreement between the values of energies $E1$, $E2$, E_{exp}; however, the values of the widths $\Gamma 1$, Γ_{exp} significantly differ. In our opinion, this fact is explained by insufficiently exact estimates of the radial integrals, using the non-optimized bases and some other additional calculation approximations. This is true in the case of the analysis of the MCHF and HFR data. In our calculations, the optimized bases of the orbitals and more accurately accounting for important multi-body exchange-correlation effects is performed. In table 3 the

Table 1. Energies E (cm^{-1}) of the YbI singly excited states.

Configuration	J	MCHF+BP(A)	MCHF+BP(C)	MCHF+BP(BD)	HFR	EA-MMBPT	This work	[38]	[34, 35]
$6s^2_{1/2}$*	0	0	0	0	0	0	0	0	0
$6s_{1/2}6p_{1/2}$	0	18 087	17 262	18 730	17 320	17 400	17 310	17 312	17 288
$6s_{1/2}6p_{1/2}$	1	18 174	17 568	18 813	17 954	18 100	18 008	17 962	17 992
$6s_{1/2}6p_{3/2}$	1	24 614	26 667	25 257	25 069	25 500	25 094	25 075	25 068
$6s_{1/2}6p_{3/2}$	2	18 357	18 249	18 999	19 710	19 800	19 715	19 716	19 710
$6s_{1/2}5d_{3/2}$	1	24 094	28 871	23 740	24 489	23 900	24 410	24 489	24 489
$6s_{1/2}5d_{3/2}$	2	24 505	28 973	24 172	24 484	24 600	24 824	24 751	24 752
$6s_{1/2}5d_{5/2}$	2	26 984	29 633	26 841	27 677	26 100	26 970	27 654	27 678
$6s_{1/2}5d_{5/2}$	3	25 860	29 374	25 500	25 271	24 900	25 098	25 270	25 271

* Note: $E = -148\,710\,cm^{-1}$; $E1 = -148\,700\,cm^{-1}$; $E2 = -148\,695\,cm^{-1}$ [34].

Table 2. Energies $E(cm^{-1})$ and widths $\Gamma(cm^{-1})$ of the YbI 7s6p configuration states.

Term	Theory $E3$	Theory $E1$	Theory $\Gamma 1$	Theory $E2$	Theory $\Gamma 2$	Expt E_{exp}	Expt Γ_{exp}
$^3P^0_0$	61 233	59 800	0.7	59 450	1.25	59 130.5	1.1
$^3P^0_1$	62 085	60 000	3.0	60 315	1.10	60 428.7	0.95
$^3P^0_2$	62 423	62 600	0.7	62 587	1.51	62 529.1	1.6
$^1P^0_1$	64 216	63 600	1.8	63 613	2.48	63 655.8	2.6

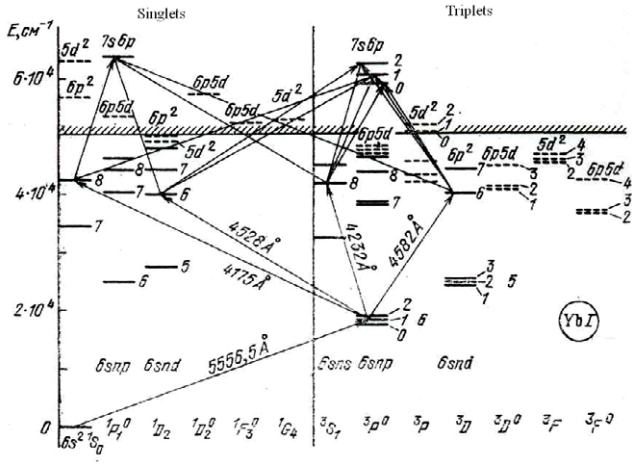

Figure 1. Scheme of the YbI energy levels and experimentally studied transitions.

energies (accounted for from the Yb $4f^{14}$ core energy) of the YbI excited states with a doubly excited valence shell are listed: $E1$—the EA-MMBPT data (from [18, 31, 34]); $E2$—the REA-OMBPT present data. In table 4 the same data are listed for other similar states. The presented EA-MMBPT and REA-OMBPT data on the energies are in physically reasonable agreement with the experimental data. However, a comparison of the corresponding results for widths demonstrates again a sufficiently large discrepancy.

In table 5 we list the widths (cm^{-1}) of the YbI autoionization states with a doubly excited valence shell. Analysis shows that the state $5d_{3/2}5d_{5/2}$ ($J = 1$) is really autoionizative (hitherto this question has remained opened). Its anormal smallness can be explained by the fact that its decay is forbidden in the nonrelativistic limit.

In conclusion, it should be noted that the autoionization resonances studied (Rydberg states are more preferable) in the lanthanides atoms can be very useful, for example, in the new optimal laser photo-ionization schemes of separating heavy isotopes and nuclear isomers [30–33, 13]. For example,

Table 3. Energies (in $10^2\,cm^{-1}$) of some YbI excited states with a doubly excited valence shell.

Configuration	J	Theory		Expt E_{exp}
	.	$E1$	$E2$	
$6p^2_{1/2}$	0	−1067	−1064	−1062, 7
$6p^2_{3/2}$	2	−987	−1004	−1008.9
$6p_{1/2}6p_{3/2}$	1	−1054	−1050	−1049
$6p_{1/2}6p_{3/2}$	2	−1032	−1036	−1039.5
$5d^2_{3/2}$	2	−1034	−1032	−1010.76
$5d_{3/2}5d_{5/2}$	2	−994	–995	−994.63
$5d_{3/2}5d_{5/2}$	3	−1030	−1032	−1032.47

Table 4. Theoretical energies (in $10^2\,cm^{-1}$) of the YbI excited states with a doubly excited valence shell.

Configuration	J	$E1$	$E2$	Configuration	J	$E1$	$E2$
$6p^2_{1/2}$	0	−1067	−1064	$6p_{3/2}5d_{5/2}$	3	−963	–962
$6p^2_{3/2}$	0	−920	–918	$6p_{3/2}5d_{5/2}$	4	−1062	−1061
$6p^2_{3/2}$	2	−987	−1004	$5d^2_{3/2}$	0	−981	–982
$6p_{1/2}6p_{3/2}$	1	−1054	−1050	$5d^2_{3/2}$	2	−1034	−1032
$6p_{1/2}6p_{3/2}$	2	−1032	−1036	$5d^2_{5/2}$	0	−961	–963
$6p_{1/2}5d_{3/2}$	1	−1077	−1072	$5d^2_{5/2}$	2	−970	–968
$6p_{1/2}5d_{3/2}$	2	−1075	−1069	$5d^2_{5/2}$	4	−861	–859
$6p_{1/2}5d_{5/2}$	2	−1007	−1004	$5d_{3/2}5d_{5/2}$	1	−980	–982
$6p_{1/2}5d_{5/2}$	3	−1119	−1115	$5d_{3/2}5d_{5/2}$	2	−994	–995
$6p_{3/2}5d_{3/2}$	0	−1020	−1017	$5d_{3/2}5d_{5/2}$	3	−1030	−1032
$6p_{3/2}5d_{3/2}$	1	−1014	−1012	$5d_{3/2}5d_{5/2}$	4	−1024	−1026
$6p_{3/2}5d_{3/2}$	2	−914	–913	$7s_{1/2}6p_{1/2}$	0	−889	−886.4
$6p_{3/2}5d_{3/2}$	3	−1039	−1035	$7s_{1/2}6p_{1/2}$	1	−887	−886
$6p_{3/2}5d_{5/2}$	1	−949	–948	$7s_{1/2}6p_{3/2}$	1	−851	–849
$6p_{3/2}5d_{5/2}$	2	−1118	−1116	$7s_{1/2}6p_{3/2}$	2	−861	−860

the laser photo-ionization scheme with autoionization of the excited ytterbium atoms (with an optimal set of energetic and radiative parameters: pulse form, duration, energetic for

Table 5. The widths (cm^{-1}) of the YbI autoionization states with a doubly excited valence shell.

Configuration	J	Term	$\Gamma 1$	$\Gamma 2$
$6p^2_{3/2}$	0	$^1S_0$	5.4	5.69
$6p_{3/2}5d_{5/2}$	1	$^1P^0_1$	5.7	5.95
$6p_{3/2}5d_{5/2}$	3	$^1F^0_3$	1.60	1.98
$5d^2_{3/2}$	0	$^3P_0$	0.01	0.05
$6p_{3/2}5d_{3/2}$	2	$^1D^0_2$	0.20	0.52
$5d_{3/2}5d_{5/2}$	1	$^3P_1$	1(−4)	8(−4)
$5d^2_{5/2}$	0	$^1S_0$	3.30	3.63
$5d^2_{5/2}$	2	$^3P_2$	0.40	0.73
$5d^2_{5/2}$	4	$^1G_4$	0.90	1.74

Note: $0.0008 = 8(-4)$.

laser and electric field pulses, etc) could provide significantly higher yield and effectiveness of the entire process of isotope separation in comparison with the standard two- or three-stepped schemes with direct excitation and ionization by two laser pulses [13, 31, 38, 39].

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