

AUTOIONIZATION FROM A SYSTEM WITH LORENTZIAN CONTINUUM

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Abstract. *We discuss a system comprising two autoionizing (AI) levels coupled to the continuum of the Lorentzian structure. The system is irradiated by an external coherent classical field. For such a model, we derive analytical formulas determine the long-time photoelectron spectrum. We show that the parameters that describe the shape of the continuum have a considerable influence on the properties of the discussed spectrum. In particular, the enhancement of the system's sensitivity for the external laser field, additional peak appearance and the confluence of coherences effect, which is related to it, may be apparent.*

I. INTRODUCTION

Systems that contain autoionizing (AI) levels may exhibit very interesting phenomena. Some of them are related to the fact that for such systems we deal with the discrete levels that are located above the ionization threshold (it is possible for many-electron systems). According to the *Fano* theory [1] developed and extended in [2], we can treat such continuum (or continua) and AI levels which interact with them as a one continuum with some structure. Due to the fact that the system can achieve the continuum states via AI levels and by direct transitions, the quantum interferences can occur in the system. Such interference may be manifested by zeros appearing in the photoelectron spectra. Such phenomena have been discussed for various variations of the atomic levels and from various points of view – for instance see [3, 4, 5, 6] *and the references quoted therein*. It should be stressed out that the photoelectron spectra, which exhibit not only Lorentzian shapes but also *Fano profiles*, have been observed experimentally by Journell *et. al.* [7].

In this paper, we shall discuss the system involving two AI levels interacting with the continuum that already has Lorentzian structure, contrary to the model [5] where the flat continuum was considered. For such model we shall derive the analytical formula for the long-time photoelectron spectrum and show that Lorentzian structure of the continuum can change the properties of the system considerably. It's worth noticing that the presence of such structured continuum may lead to the enhancement of the sensitivity of the system for the external field and to the additional peak appearance in the photoelectron spectrum. Moreover, for some values of the parameters, this additional peak will be accompanied by the zero and the *confluence of coherences* effect [3] can be evoked.

II. THE MODEL

We discuss a model with double AI levels and the ground state $|0\rangle$ coupled to the Lorentzian continuum $|C\rangle$ by an external electromagnetic field of constant amplitude (Fig.1). Moreover, the same field couples $|0\rangle$ with two AI levels $|1\rangle$ and $|2\rangle$, respectively,

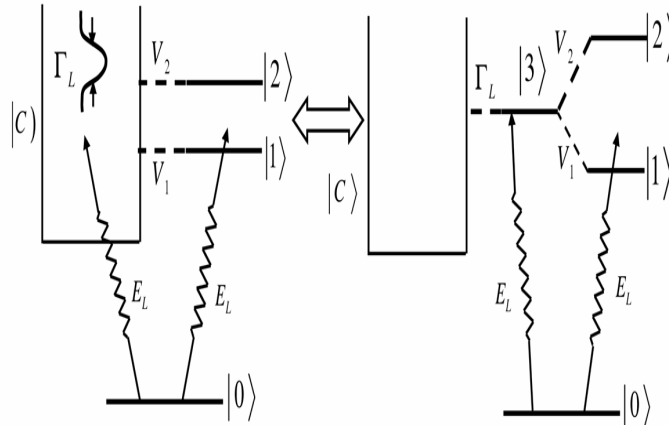


Fig. 1. Atomic level scheme (left) with Lorentzian shaped continuum $|c\rangle$ and coupled to it two AI states $|1\rangle$ and $|2\rangle$. These excited states are coupled to the ground state $|0\rangle$ by an external electromagnetic field of the amplitude E_L . The width of the Lorentzian is equal to Γ_L and the configurational interaction is described by the parameters V_1 and V_2 . The model discussed is equivalent to that with a flat continuum $|c\rangle$ and coupled to it single discrete level $|3\rangle$ (right)

and AI levels interact with the continuum $|C\rangle$ by the configurational interaction. This interaction is described by the matrix elements V_1 and V_2 . In fact, according to the *Fano* theory [1, 2]) the Lorentzian continuum can be replaced by another flat continuum $|C\rangle$ and a single AI level $|3\rangle$. Such replacement is possible if we neglect direct ionization to the flat continuum $|C\rangle$. This corresponds to the situation when we assume high value of the *Fano asymmetry parameter* q (for the discussion of the influence of this parameter on the photoelectron spectra for the systems with double AI levels see [5], for instance, *and the references quoted therein*).

The model can be described by the following Hamiltonian (we use units $\hbar = 1$):

$$\begin{aligned}
 H = & (E_0 + E_L)|0\rangle\langle 0| + E_1|1\rangle\langle 1| + E_2|2\rangle\langle 2| + \int dE E|C\rangle\langle C| + \\
 & + \sum_{j=\{1,2\}} \left[\Omega_j|j\rangle\langle 0| + \int dE F(E) V_j|C\rangle\langle j| + \int dE F(E) \Omega_c|C\rangle\langle 0| + H.c. \right] , \quad (1)
 \end{aligned}$$

where E_k ($k = \{0, 1, 2\}$) denote energies of the levels $|0\rangle$, $|1\rangle$ and $|2\rangle$, respectively. The parameters $\Omega_{1,2}$ and Ω_c are the *Rabi* frequencies that are defined by the matrix elements $\langle k| - \vec{d} \cdot \vec{E}|0\rangle$ ($k = \{1, 2, c\}$) which describe atom-external electric (laser) field interaction within the dipole and rotating wave approximations. Moreover, V_j ($j = \{1, 2\}$) correspond

to the configurational interaction that couples Lorentzian continuum $|C\rangle$ with two AI levels $|1\rangle$ and $|2\rangle$. The shape of the continuum $|C\rangle$ is defined by the function $F(E)$, which appears in the Hamiltonian (1) and is defined by:

$$|F(E)|^2 = \frac{1}{\pi} \frac{\Gamma_L}{(E - E_m)^2 + \Gamma_L^2} , \quad (2)$$

the position of the Lorentzian maximum is determined by the value of E_m and its width is equal to Γ_L . This Lorentzian shape is a special case of the *Fano profile* [1] for the cases when we neglect the direct ionization to the flat continuum.

In this paper, we shall neglect all incoherences and damping processes in our model and therefore, the time-evolution of the system can be described by the wave-function. It can be expressed in the following form:

$$|\psi(t)\rangle = a(t) e^{-i(E_0 + E_L)t} |0\rangle + b_1(t) e^{-iE_1 t} |1\rangle + b_2(t) e^{-iE_2 t} |2\rangle + \int dE b_E(t) e^{-iEt} |C\rangle , \quad (3)$$

where $a(t)$, $b_1(t)$, $b_2(t)$ and $b_E(t)$ are the complex probability amplitudes corresponding to the states $|0\rangle$, $|1\rangle$, $|2\rangle$ and $|C\rangle$, respectively. To determine them, we apply the standard procedure and the time-dependent Schrödinger equation. In consequence, we get the following set of differential equations (in the rotating frame) that are equations of motion for the system discussed here:

$$i \frac{da'}{dt} = \Omega_1 b'_1 + \Omega_2 b'_2 + \int dE F^*(E) \Omega_c b'_E , \quad (4a)$$

$$i \frac{db'_1}{dt} = \Omega_1 a' + \delta_1 b'_1 + \int dE F^*(E) V_1 b'_E , \quad (4b)$$

$$i \frac{db'_2}{dt} = \Omega_2 a' + \delta_2 b'_2 + \int dE F^*(E) V_2 b'_E , \quad (4c)$$

$$i \frac{db'_E}{dt} = F(E) [\Omega_c a' + V_1 b'_1 + V_2 b'_2] + (\Delta_1 + \delta_1) b'_E , \quad (4d)$$

where we have introduced the following detunings

$$\delta_1 = E_1 - E_0 - E_L, \quad \delta_2 = E_2 - E_0 - E_L, \quad \Delta_1 = E - E_1, \quad \Delta_2 = E - E_2 \quad (5)$$

and the new probability amplitudes in the form

$$a'(t) = a(t), \quad b'_1(t) = b_1(t) e^{-\delta_1 t}, \quad b'_2(t) = b_2(t) e^{-\delta_2 t}, \quad b'_E(t) = b_E(t) e^{-(\delta_1 + \Delta_1)t} \quad (6)$$

To solve these equations, we apply standard Laplace transform procedure. We assume that the system initially was in its ground state $|0\rangle$, *i.e.* $a'_0 = 1$ and $b'_1 = b'_2 = b'_E = 0$ for the time $t = 0$. Thus, after eliminating the probability amplitude $b'_E(t)$ Laplace transform (corresponding to the continuum states), we get the following set of algebraical equations:

$$-A[z + \Gamma_0 K(z)] + B_1[i\Omega_1 + \Gamma_{01} K(z)] + B_2[i\Omega_2 + \Gamma_{02} K(z)] = 1 , \quad (7a)$$

$$-A[i\Omega_1 + \Gamma_{01} K(z)] + B_1[z + i\delta_1 + \Gamma_1 K(z)] + B_2 \Gamma_{12} K(z) = 0 , \quad (7b)$$

$$-A[i\Omega_2 + \Gamma_{02} K(z)] + B_1 \Gamma_{12} K(z) + B_2[z + i\delta_2 + \Gamma_2 K(z)] = 0 , \quad (7c)$$

where $A(z)$, $B_1(z)$ and $B_2(z)$ are the Laplace transforms of the probability amplitudes $a'(t)$, $b'_1(t)$ and $b'_2(t)$, respectively. The parameter $K(z)$ is defined as:

$$K(z) = \frac{1}{\pi} \int dE \frac{|F(E)|^2}{z + i(\Delta_1 + \delta_1)} \quad , \quad (8)$$

and we have introduced the following widths:

$$\Gamma_0 = \pi \Omega_2^2 \quad , \Gamma_{12} = \pi V_1 V_2 = \sqrt{\Gamma_1 \Gamma_2} \quad , \quad (9a)$$

$$\Gamma_k = \pi V_k^2 \quad \Gamma_{0k} = \pi \Omega_c V_k \quad k = \{1, 2\} \quad (9b)$$

The widths Γ_1 and Γ_2 can be related to the autoionization widths commonly discussed in the literature, although one should keep in mind that the latter were defined for the interaction with the flat continuum, whereas those defined here correspond to the discrete level – *structured* continuum interactions.

To find the explicit formula for the parameter $K(z)$ we need to find the integral appearing in eq.(8). Therefore, we extend the integration over the energies from minus to plus infinities. This corresponds to the assumption of neglecting all threshold effects. In practice, we assume that all discrete levels embedded in the continuum are located high enough to be far from the ionization threshold. Such assumption is commonly applied in the discussions about the models with AI levels (for instance, see the classical paper [3]). For the case discussed here $K(E)$ can be expressed in the following form:

$$K(z) = \frac{1}{\pi} \frac{1}{z + \Gamma_L + i\delta} \quad , \quad (10)$$

where the detuning $\delta = E_m - E_L - E_0$.

The equations (7) can be easily solved analytically. Due to the fact that the analytical expressions are very long for the discussed model, we don't give it here. Of course, it is possible to calculate the inverse Laplace transforms from the obtained results presented above in finding the solutions for the probability amplitudes that determine the dynamic of the system discussed. However, the main aim of this paper is to check whether the Lorentzian structure of the continuum can influence the long-time photoelectron spectrum. Hence, we shall concentrate on the solutions within this limit.

III. PHOTOELECTRON SPECTRUM

For the model discussed here the long-time photoelectron spectrum can be defined as $W(E) = \lim_{t \rightarrow \infty} |b_E(t)|^2$. As we shall concentrate on the long-time limit the spectrum can be determined by the direct application of the obtained analytical expressions. It can be written particularly as

$$W(E) = \left| F(E) \left[\Omega_c A(z) + V_1 B_1(z) + V_2 B_2(z) \right] \right|_{z=-i(\Delta_1+\delta_1)}^2 \quad . \quad (11)$$

If we assume that the Lorentzian shape is very broad, *i.e.* $\Gamma_L \gg \Gamma_0, \Gamma_k$ ($k = \{1, 2\}$) (from the definitions (9) we can write the analogous inequalities for Γ_{12} and Γ_{0k} ($k =$

$\{1, 2\}$)), the results presented here should be identical to those discussed in [5]. Therefore, we define the new Rabi frequency (analogous to [3] and [5]) as:

$$\Omega = \sqrt{4\pi\Gamma} (Q + i) \Omega_c e^{i\phi} \quad (12)$$

with some phase ϕ (we choose the value of ϕ in such a way that Ω is assured to be real), the effective width $\Gamma = \Gamma_1 + \Gamma_2$ and *effective* asymmetry Fano parameter Q . The latter can be expressed by the autoionization widths and usual asymmetry parameters in the following way:

$$Q = \frac{q_1\Gamma_1 + q_2\Gamma_2}{\Gamma} \quad . \quad (13)$$

For the model discussed here the asymmetry parameters q_1 and q_2 can be written as:

$$q_i = \frac{\Omega_i}{\pi\Omega_c V_i} \quad (i = 1, 2) \quad . \quad (14)$$

In fact, these parameters describe the ratio between the probabilities of the direct transition from the ground state to the one of AI states and the analogous transition via the continuum. Therefore, if we neglect the direct ionization, the asymmetry parameters are assumed to be large.

As it was mentioned above, for the limit $\Gamma_L \rightarrow \infty$, our spectrum should tend to that discussed in [5]. Therefore, we need the proper normalization of our result. To ensure nonvanishing $W(E)$ for such limit we need to redefine the matrix elements (and in consequence, the appropriate widths) that corresponds to the transitions to (from) the continuum states. They should be normalized by Γ_L in the following way:

$$\Omega'_c = \frac{\Omega_c}{\sqrt{\pi\Gamma_L}} \quad , \quad (15a)$$

$$V_i = \frac{V_i}{\sqrt{\pi\Gamma_L}} \quad (i = 1, 2) \quad . \quad (15b)$$

Thus, Fig.2 shows the photoelectron spectra for weak external excitation ($\Omega = 1$), high values of the asymmetry parameters ($q_1 = q_2 = 100$) and various values of the Lorentzian width Γ_L . We assume that the energies of both AI levels are equal and the external field is tuned exactly to the transition from the ground state $|0\rangle$ to the AI states – $E_0 = 0$, $E_1 = E_2 = E_L = 1$. As we have assumed high values for q -parameters, we do not observe the usual Fano zeros. Moreover, since both degenerated AI levels are characterized by the same AI widths ($\Gamma_1 = \Gamma_2 = 0.5$) and both q -parameters are identical, we do not observe additional zeros in the spectrum as well. This is the same behaviour as that discussed in [5]. The spectrum consists of only one, broad peak, with the energy equal to both: energy of AI levels and energy $E_0 + E_L$. located at the position corresponding to the tuning of the external field. If Γ_L decreases, the spectrum changes considerably. Firstly, two additional, satellite peaks appear in the spectrum. They are usual Autler-Townes doublet peaks commonly discussed in the literature (for instance see [3, 4, 5, 6] *and the references quoted therein*). Their separation and heights increase as the value of Γ_L decreases. Usually, such peaks can be observed in the photoelectron spectra when atomic systems interacts with high external fields. This fact indicates that the finite width of the continuum leads to the enhancement of the sensitivity of the system for the external field. Moreover, we see that,

as values of Γ_L decrease, the central peak becomes narrower and its position is shifted toward the position of the Lorentzian maximum $E_m = 1.25$.

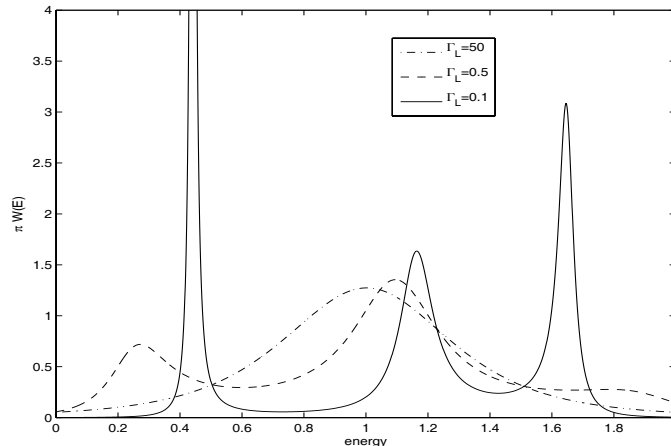


Fig. 2. The photoelectron spectra for weak excitation case $\Omega = 1$ and various values of the Lorentzian widths Γ_L . The energies of the two AI levels are identical and equal to 1. The laser is tuned to the $|0\rangle \leftrightarrow |1\rangle$ and $|0\rangle \leftrightarrow |2\rangle$ transitions. The widths $\Gamma_1 = \Gamma_2 = 0.5$, $E_m = 1.25$, and $q_1 = q_2 = 100$.

Fig.3 shows the analogous situation to that depicted in Fig.2, but, for this case, the energies of AI levels are not identical ($E_1 = 1$, $E_2 = 1.5$). Since we deal with two separate AI levels, the zero appears in the spectrum and is located at the energy $E = (E_1 + E_2)/2$. This the same energy as that of the central peak related to the Lorentzian maximum at $E = E_m = 1.25$. Such convergence of the energies leads to the *confluence of coherences* effect [3, 4, 5] appearance – the zero is accompanied by a sharp peak. This effect becomes more and more pronounced as the width Γ_L decreases.

IV. CONCLUSION

In this paper, we have discussed the model involving two AI levels and one continuum with Lorentzian structure. For such a system, we have derived the analytical formula for the long-time photoelectron spectrum and discussed its properties showing that the structure of the continuum can influence the spectrum considerably. In particular, we have shown that thanks to the Lorentzian shape of the continuum and its finite width, the system becomes more sensible for the interaction with external field as we observe Autler-Townes doublets even for the weak field cases. Moreover, additional peak, related to the continuum structure can be visible in the spectrum. For the cases when the interference zero is present in the spectrum, this peak can lead to the *confluence of coherence* effect appearance. We have shown that changes in the position of the Lorentzian maximum can alter the spectrum considerably, as well. Those effects justify the statements that the autoionization processes strongly depends on the continuum shape and that the photoelectron spectrum can be changed considerably by variations of the parameters describing this shape.

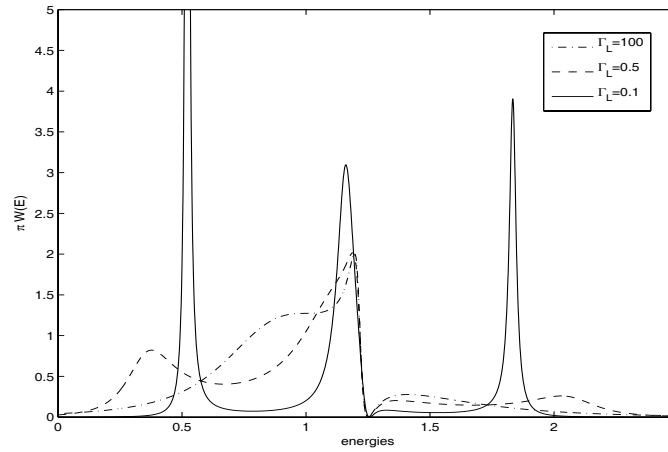


Fig. 3. The same as in Fig.2 but AI levels have energies: $E_1 = 1$, $E_2 = 1.25$. The remaining parameter are the same as in Fig.2.

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