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Extrema in transition energies resulting not in satellites but in dips within spectral lines

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The paper deals with a frequently encountered situation where the energy difference between the terms involved in a radiative transition, being plotted versus the radiator-perturber separation, shows extrema. The paradigm, based on 30 years of theoretical and experimental studies, is that the extrema in the transition energy result in *satellites* in spectral line profiles. In this Rapid Communication we show that this *paradigm breaks down*: the extrema in the transition energy can also result in *dips* in spectral line profiles. Moreover, we demonstrate that if the extremum in the transition energy is due to the *charge exchange*, its spectral signature *most probably should be a dip* rather than a satellite.

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I. INTRODUCTION

It is well known that the shape of spectral lines of a radiating atom/ion (radiator) in a gas or in a plasma depends on the energy terms of the combined quantum system ‘‘radiator+perturber(s).’’ Frequently the energy difference between the terms involved in the radiative transition, being plotted versus the radiator-perturber separation, shows extrema. This situation has been studied for over 30 years, both theoretically and experimentally (see, e.g., [1–11] and reference therein). The paradigm based on these studies is that the extrema in the transition energy result in *satellites* in spectral line profiles [1–11].

In this Rapid Communication we show that the extrema in the transition energy can also result in *dips* in spectral line profiles. Moreover, we demonstrate that for the practically important case where the extremum in the transition energy is due to the *charge exchange*, its spectral signature *most probably should be a dip* rather than a satellite.

This kind of dip has some limited similarity with the dip in the hydrogen line H_α observed in a gas-liner pinch [12]. We discuss in detail several prospective pairs ‘‘radiator-perturber’’ for observing this phenomenon in lines of hydrogenlike ions.

II. SPECTRAL INTENSITY CORRESPONDING TO AN EXTREMUM IN THE TRANSITION ENERGY

We consider a radiative transition between two terms corresponding to some Stark component. We use atomic units and therefore employ the same notation $f(R)$ for both the transition energy and the transition frequency; R is the distance between the radiator and the perturbing atom or ion. We denote as $g(R)$ the area-normalized probability distribution of the quantity R. In the quasistatic approximation, the area-normalized profile $I(\Delta\omega)$ of the Stark component versus the detuning $\Delta\omega$ from the unperturbed frequency ω_0 is usually given by

$$I(\Delta\omega)=\int_0^\infty dR\, G(R)\,\delta[\Delta\omega-f(R)],$$
$$G(R)=g(R)J(R)/J(\infty), \tag{1}$$

where $J(R)$ is a frequency-integrated relative intensity of the Stark component.

We consider a vicinity of some particular distance R_0 corresponding to a small part of the component profile around $\Delta\omega_0=f(R_0)$. In a relatively simple case where $f(R)$ does not have an extremum at $R=R_0$, from Eq. (1) one usually obtains

$$I(\Delta\omega_0)=G(R_0)/|f'(R_0)|. \tag{2}$$

However, if $f(R)$ has an extremum at $R=R_0$, so that the first derivative $f'(R)$ vanishes, then Eq. (2) as well as Eq. (1) at $\Delta\omega=\Delta\omega_0$ becomes inapplicable. Physically this means that some feature in the profile may arise in the vicinity of $\Delta\omega_0$. For obtaining a finite value of $I(\Delta\omega_0)$, one should allow for additional broadening mechanisms and substitute the δ function in Eq. (1) by a more realistic profile, such as a Lorentzian or a Gaussian. For example, for the Lorentzian having a full width at half maximum (FWHM) γ, as shown in Sec. 3.3.2 of the book [13], the intensity $I(\Delta\omega_0)$ becomes

$$\begin{aligned}I(\Delta\omega_0)&\approx G(R_0)\int_{-\infty}^{\infty}d(R-R_0)[\gamma/(2\pi)]/\{(\gamma/2)^2\\&\quad+[f''(R_0)/2]^2(R-R_0)^4\}\\&=G(R_0)\{2/[\gamma|f''(R_0)|]\}^{1/2}.\end{aligned} \tag{3}$$

Result (3) is obtained under the assumption that the function $G(R)$ is the slowest out of two factors in the integrand. The validity of this assumption will be analyzed later on.

III. RESULTS FOR EXTREMA CAUSED BY AN AVOIDED CROSSING

We are interested primarily in the situation where an extremum in the energy difference between an upper term *a*

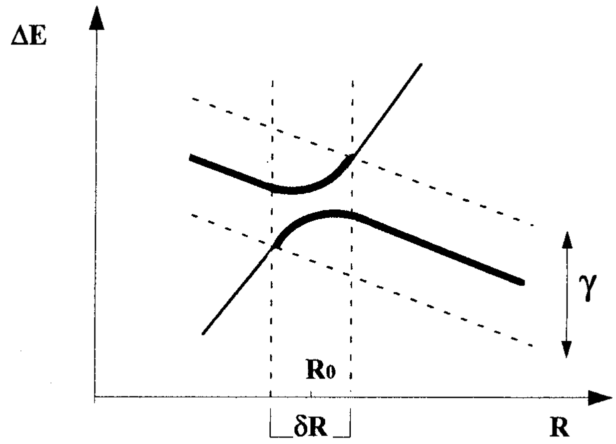

FIG. 1. Transition energies $f_-(R) = E_a - E_{ao}$ and $f_+(R) = E_{a'} - E_{ao}$ versus the radiator-perturber separation R, plotted in a vicinity δR of an avoided crossing of the perturber's term a' with the radiator's term a at $R = R_0$ in the course of the radiative transition from the term a to the term a_0. The transition energy $f_-(R)$ actually occupies a band of a width γ (shown by dashed lines) controlled primarily by the dynamical broadening caused by electron and ion microfields in a plasma. The radiator's transition energy modified by the avoided crossing is shown by the bold line. In the interval δR, the transition energy has two branches, corresponding to the fact that the wave function of the radiator's term in this interval is a linear combination of wave functions of two different energies.

and a lower term a_0 is caused by an avoided crossing of the radiator's term a with some perturber's term a'. We denote as $f_-(R)$ the transition frequency between the *original* terms a and a_0 at $R \leqslant R_0$ and as $f_+(R)$ the transition frequency between the *original* terms a' and a_0 at $R \geqslant R_0$. Here by ''original'' we mean the terms as they would be if the terms a and a' would not be coupled and therefore would cross (Fig. 1).

In the vicinity of $R = R_0$, as a result of the avoided crossing, there occurs a transition of the energy difference from $f_-(R_0)$ to $f_+(R_0)$ as well as a transition of the slope from $f'_-(R_0)$ to $f'_+(R_0)$. If $f'_-(R_0)$ and $f'_+(R_0)$ have the opposite signs, the avoided crossing causes an extremum in the energy/frequency difference (Fig. 1).

Combining Eqs. (2) and (3), it is easy to calculate the ratio of the true intensity $I(\Delta\omega_0)$ to the original intensity $I_0(\Delta\omega_0)$ (that is, the intensity $I_0(\Delta\omega_0)$ which would be if it were no coupling of the a and a' terms):

$$I(\Delta\omega_0)/I_0(\Delta\omega_0) = |f'_-(R_0)|\{2/[\gamma|f''(R_0)|]\}^{1/2}. \tag{4}$$

Here we come to the following *central point*. From Eq. (4) it is clear that if $|f'_-(R_0)|$ would be relatively large and/or $\gamma|f''(R_0)|$ would be relatively small, we would have $I(\Delta\omega_0)/I_0(\Delta\omega_0) > 1$, thus indicating the formation of a peak (satellite). However, if $|f'_-(R_0)|$ is relatively small and/or $\gamma|f''(R_0)|$ is relatively large, we have $I(\Delta\omega_0)/I_0(\Delta\omega_0) < 1$, thus indicating the formation of a *dip*, rather than a satellite. This result *disproves the existing paradigm* in accordance to which any extremum in the transition energy/frequency could manifest only as a satellite.

Physically, the above findings can be illustrated as follows. Let us consider again the starting formula (1) for $I(\Delta\omega)$, but with the δ-function substituted by a more realistic profile (e.g., by the Voigt profile). If the extremum in the transition energy/frequency is ''gradual'' [i.e., $|f''(R_0)|$ is relatively small], then in the course of integration over R around R_0, the frequency remains in the vicinity of $\Delta\omega_0$ ''longer'' than at the absence of the extremum. Therefore, more intensity gets accumulated at $\Delta\omega_0$ than it would be at the absence of the extremum, thus resulting in a peak (satellite). However, if the extremum in the transition energy/frequency is ''sharp'' [i.e., $|f''(R_0)|$ is relatively large], then in the course of integration over R around R_0, the frequency remains in the vicinity of $\Delta\omega_0$ ''shorter'' than at the absence of the extremum. Therefore, less intensity gets accumulated at $\Delta\omega_0$ than it would be at the absence of the extremum, thus resulting in a dip.

The absolute value of the second derivative $f''(R_0)$ can be estimated as

$$f''(R_0) \approx [f'_+(R_0) - f'_-(R_0)]/\delta R, \tag{5}$$

where δR is the interval where there occurs the conversion of the original radiator's term a into a'. The interval δR can be found from the following considerations.

Due to the dynamical broadening by electron and ion microfields in a plasma and the radiative broadening (the latter resulting in a ''natural'' width), the radiator has a finite lifetime $1/\gamma$. Consequently, the transition energy of the radiator actually *occupies a band of the width* γ (see Fig. 1). Therefore, it is easy to find that

$$\delta R = \gamma/|f'_+(R_0) - f'_-(R_0)|. \tag{6}$$

Thus, the ratio $I(\Delta\omega_0)/I_0(\Delta\omega_0)$ can be represented in the form

$$I(\Delta\omega_0)/I_0(\Delta\omega_0) = 2^{1/2}|f'_-(R_0)/[f'_+(R_0) - f'_-(R_0)]|. \tag{7}$$

Clearly, the right-hand side of Eq. (7) is controlled by the inverse value of the *relative change of the derivative of the transition energy* at the crossing and does not depend on the dynamical width γ. If the relative change of this derivative is small, there forms a satellite. However, if the relative change of this derivative is large, we find again that the *existing paradigm breaks down*: there forms a *dip* (rather than a satellite).

IV. RESULTS FOR AVOIDED CROSSINGS DUE TO CHARGE EXCHANGE IN PLASMAS

From now on we focus specifically at the avoided crossings in the system of two Coulomb centers (dicenters) ZeZ'. We would like to remind that terms of the dicenter may indeed cross: the well-known noncrossing rule [14] is inapplicable because the system possesses an algebraic symmetry higher than the geometrical symmetry [15]. However, due to the charge exchange some of the crossings transform into avoided crossings [16,17].

We consider a radiative transition in a hydrogen/hydrogenlike atom/ion of the nuclear charge Z at the presence of the nearest perturber which is a fully stripped ion of the charge $Z' \neq Z$ located at the distance R. The upper (term a) and the lower (term a_0) states involved in the radiative transition have the principal quantum numbers n and n_0, respectively. At some distance R_0, a Z term of the principal quantum number n (term a) experiences an avoided crossing with a Z' term of the principal quantum number n' (term a').

We are going to show that when an extremum in the transition energy is due to a charge-exchange-caused avoided crossing, which occurs at a relatively large distance

$$R \gg \max(n^2/Z, n'^2/Z'), \tag{8}$$

then *practically always it results in a dip* in the profile of the corresponding Stark component of the spectral line, rather than in a satellite. In other words, we are going to show that in this situation, practically always we have $I(\Delta\omega_0)/I_0(\Delta\omega_0) < 1$.

Indeed, condition (8) allows to treat separately a set of Z terms (perturbed by the Z' ion) and a set of Z' terms (perturbed by the Z ion) as well as to use $1/R$ expansion for the transition energies $f_-(R)$ and $f_+(R)$. In this way, we find the following first nonvanishing terms for the derivatives of the transition energies:

$$f'_-(R) = -3Z'(nq - n_0q_0)/(ZR^3),$$
$$F'_+(R) = -(Z'-Z)/R^2 - 3(n'q'Z/Z' - n_0q_0Z'/Z)/R^3. \tag{9}$$

Here, $q = n_1 - n_2$, $q_0 = n_{01} - n_{02}$, $q' = n'_1 - n'_2$ are electric quantum numbers expressed via the corresponding parabolic quantum numbers.

It is seen from Eq. (9) that, given condition (8), the absolute value of the slope of $f_+(R)$ is much greater than the absolute value of the slope of $f_-(R)$. Further, we substitute expressions (9) in Eq. (7) and obtain

$$I(\Delta\omega_0)/I_0(\Delta\omega_0) \approx [2^{1/2}3Z'/(ZR_0)]|(nq - n_0q_0)/(Z-Z')|. \tag{10}$$

Thus, in view of condition (8), we have indeed proven the above statement that $I(\Delta\omega_0)/I_0(\Delta\omega_0) \ll 1$, which means the formation of a dip. We call this charge exchange caused dip an ''x dip.''

Result (10) is applicable to the Stark components of $nq - n_0q_0 \neq 0$ (i.e., for lateral Stark components, which constitute the majority of the components). For the Stark components of $nq - n_0q_0 = 0$ (central components), a similar result could be also obtained.

As a measure of the ''contrast'' of the x dips, we introduce a quantity called ''visibility'' defined as follows:

$$V \equiv \left| 1 - \left[I_k J_k(\infty) + \sum_{i \neq k} I_{0,i} J_i(\infty) \right] \Big/ \sum_{\text{all } i} I_{0,i} J_i(\infty) \right|$$
$$\approx \left| (1 - I_k/I_{0k}) \Big/ \left[\sum_{\text{all } i} J_i(\infty)/J_k(\infty) \right] \right|. \tag{11}$$

Here $I_k J_k(\infty)$ is the intensity of the Stark component number k at $\Delta\omega = \Delta\omega_0$, in whose profile the x dip occurs; $I_{0,i} J_i(\infty)$ is the original intensity of the Stark component number i of this spectral line at $\Delta\omega = \Delta\omega_0$.

V. DENSITY RANGE FOR OBSERVING x FEATURES

There are upper and lower limits which determine the range of electron densities, where the x features can be observed. The upper limit N_e^{upper} physically comes from the condition that the dynamical broadening should not be so large as to wash out the x feature. Mathematically, for the derivation of $I(\Delta\omega_0)$ in Sec. II to be valid, it is required that the characteristic interval ΔR_G of a significant change of the ''slow'' function $G(R)$ would be greater than the characteristic interval ΔR_γ of a significant change of the ''fast'' quasi-Lorentzian. Since $\Delta R_\gamma = \delta R$, the requirement $\Delta R_\gamma < \Delta R_G$ translates into the condition

$$\gamma < |f'_+(R_0) - f'_-(R_0)|/[2G(R_{\text{peak}})], \tag{12}$$

where R_{peak} is the location of the peak of $G(R)$.

The lower limit of electron densities N_e^{lower} physically comes from the requirement that the crossing distance R_0 should not differ too much from the most probable interperturber distance [otherwise, R_0 would belong to a very low-weight part of the function $G(R)$]. More rigorously, the ratio of the original intensity of the Stark component at $\Delta\omega_0$ to its peak intensity should exceed certain threshold what can be written, using Eqs. (1) and (2), as

$$G(R_0)|f'_-(R_0)|^{-1}/[G(R_{\text{peak}})|f'_-(R_{\text{peak}})|^{-1}] > \epsilon, \tag{13}$$

where, say, $\epsilon \sim 0.1$. We note that for relatively large Z (typically, for $Z \geq 8$), the dynamical width is relatively small, so that condition (13) controls both the lower and the upper limits of the density range.

VI. FUTURE EXPERIMENTAL APPLICATIONS

For applying our theory to particular ZeZ' systems it is important to use the following selection rule for the charge exchange in such systems. For each Z' term (n'_1, n'_2, m'), the charge exchange, also manifested as an avoided crossing, is possible with no more than one Z term, namely: either with the Z term of the following parabolic quantum numbers [16,17]

$$n_1 = n'_1, \quad m = m', \quad n_2 = n - n'_1 - |m'| - 1 \tag{14}$$

or not at all, if the set (n_1, n_2, m) given by Eq. (14) does not correspond to any Z term. Physically, this selection rule follows from the picture of the charge exchange as the corresponding interaction of states in two adjacent potential wells (one is centered at the charge Z, another at the charge Z') and from the fact that for such interaction to be possible, the radial wave functions of these states should have the same number of nodes [16,17].

Now we provide examples of prospective ZeZ' systems for observations of x dips in laser-produced plasmas of multicharged ions, resulting from extrema in the transition energy of radiators. In our calculations we took into account both the electron and ion dynamical broadenings; the ion dynamical contribution was calculated using analytical results of paper [18]. The first example concerns the L_β line of O VIII ($Z=8$, $\lambda_0=16.0$ Å) perturbed by fully stripped Si($Z'=14$). Avoided crossings of some of the $Z=8$ terms of $n=3$ with some of the $Z'=14$ terms of $n'=5$ occur in a vicinity of $R_0\approx 16$. This distance is about nine times greater than the size n'^2/Z' of the largest out of the two separate states (Z,n) and (Z',n'). More specifically, the avoided crossing of the (Z,n) term of $q=-2$ with the (Z',n') term of $q'=-4$ results in extrema in the transition energy of the radiator. Applying our formulas from Sec. IV, we find that this crossing should translate into a dip of the visibility $V\approx 25\%$. The dip is located at $\Delta\lambda\approx 3.7$ mÅ (i.e., on the red side). In addition, the avoided crossing of the (Z,n) term of $q=-1$ with the (Z',n') term of $q'=-3$ also results in extrema in the transition energy of the radiator. Applying our formulas from Sec. IV, we find that this crossing should translate into a dip of the visibility $V\approx 9\%$. The dip is located at $\Delta\lambda\approx 1.8$ mÅ (i.e., on the red side). Using the results of Sec. V, we obtain the range of densities where these two x dips could be observed (for $T\sim 500$ eV): $N_e^{\mathrm{upper}}\sim 7\times 10^{21}$ cm^{-3}, $N_e^{\mathrm{lower}}\sim 1\times 10^{19}$ cm^{-3}.

The second suggestion deals with the L_γ line of Na XI ($Z=11$, $\lambda_0=8.03$ Å) perturbed by fully stripped Cl ($Z'=17$). Avoided crossings of some of the $Z=11$ terms of $n=4$ with some of the $Z'=17$ terms of $n'=6$ occur in a vicinity of $R_0\approx 25$. This distance is about 12 times greater than the size n'^2/Z' of the largest out of the two separate states (Z,n) and (Z',n'). More specifically, the avoided crossing of the (Z,n) term of $q=-2$ with the (Z',n') term of $q'=-4$ results in extrema in the transition energy of the radiator. Applying our formulas from Sec. IV, we find that this crossing should translate into a dip of the visibility $V\approx 13\%$. The dip is located at $\Delta\lambda\approx 4.4$ mÅ, (i.e., on the red-side). In addition, the avoided crossing of the (Z,n) term of $q=-3$ with the (Z',n') term of $q'=-5$ also results in extrema in the transition energy of the radiator. Applying our formulas from Sec. IV, we find that this crossing should translate into a dip of the visibility $V\approx 10\%$. The dip is located at $\Delta\lambda\approx 6.5$ mÅ (i.e., on the red side). Using the results of Sec. V, we obtain the range of densities where these two x dips could be observed (for $T\sim 800$ eV): $N_e^{\mathrm{upper}}\sim 2\times 10^{22}$ cm^{-3}, $N_e^{\mathrm{lower}}\sim 2\times 10^{20}$ cm^{-3}.

Finally, we emphasize that the phenomenon of x dips is of a great physical interest from both theoretical and experimental viewpoints. The experimental study of x dips would serve for producing not-yet-available fundamental data on the charge exchange between multicharged ions, virtually inaccessible by other experimental methods.

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