Hidden Fano interferences in the resonant photoionization of He-like ions

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Total and partial photoionization cross sections of positive He-like ions in their ground states have been evaluated in the vicinity of the $3(1,1)_3\,{}^1P^0$ ("$3s3p$") doubly excited state for nuclear charges ranging from $Z=2$ to $Z=18$. We observe an apparent cancellation of the Fano interferences for $Z\simeq 4$–5, which results in the presence of almost Lorentzian peaks in the photoabsorption spectrum. The origin of this cancellation and the behavior of the Fano and the Starace parameters along Z are discussed.

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The first observation of doubly excited (autoionizing) states in the photoionization of He was made by Madden and Codling [1], thirty years ago. Autoionizing states manifest themselves as very asymmetric peaks in the absorption spectra, which is in contrast with the Lorentzian shapes observed for bound states. In the first theoretical approach to this problem [2,3], the asymmetry (Fano profile) was explained as the result of the interference of a discrete autoionizing state with a smooth continuum background in which the former is embedded. Since then, a lot of experimental and theoretical works have been made in order to understand the role of electron-electron correlations in doubly excited states of He. In particular, the $3(1,1)_3$ resonance of He has been extensively studied both theoretically and experimentally (see, Refs. [4–8], and references therein). In the last years, the experimental effort has been renewed [8–11] by the appearance of high-energy resolution spectrometers using synchrotron radiation. In contrast, experiments on the photoionization of He-like positive ions are very scarce. The only measurements that we are aware of correspond to the photoionization of Li^+ below the $N=2$ threshold [12]. However, with the recent availability of singly and multiply charged ions from electron cyclotron resonance (ECR) or electron-beam ion source (EBIS) sources, photoionization experiments on positive ions are now possible [13].

In this paper, we point out an unexpected phenomenon in the photoexcitation of autoionizing states from the ground state of positive He-like ions above the $N=2$ threshold: The apparent cancellation of the interference between autoionization and (direct) ionization from the ground state. In other words, the resonance peaks in the total cross sections exhibit Lorentzian profiles instead of the Fano ones, and, therefore, except for the presence of a small ionization background—which decreases as Z^{-2}—the corresponding photoabsorption spectra is closer to that of bound states.

We first illustrate the origin of this cancellation by using the Fano parametrization of the total cross section [2]:

$$\sigma(E)=\sigma^0\left[\rho_s^2\frac{(q_s+\epsilon)^2}{1+\epsilon^2}+1-\rho_s^2\right], \tag{1}$$

where $\epsilon=2(E-E_s)/\Gamma_s$, being E_s and Γ_s the energy position and the width of the s resonance, σ^0 is the background nonresonant cross section, q_s is the line profile parameter, and ρ_s^2 is the correlation parameter. The partial cross sections can be parametrized following Starace [14]:

$$\sigma_\mu(E)=\frac{\sigma_\mu^0}{1+\epsilon^2}\{\epsilon^2+2\epsilon(q_s\mathrm{Re}[\alpha_\mu^s]-\mathrm{Im}[\alpha_\mu^s])+1-2q_s\mathrm{Im}[\alpha_\mu^s]-2\mathrm{Re}[\alpha_\mu^s]+(q_s^2+1)|\alpha_\mu^s|^2\}, \tag{2}$$

where σ_μ^0 is the partial background nonresonant cross section and α_μ^s are the Starace parameters. Let us define the interference function:

$$\Xi(E)=\sum_\mu\langle\psi_g|z_1+z_2|\psi_{\mu E}\rangle\langle\psi_{\mu E}|\mathcal{H}|\phi_s\rangle, \tag{3}$$

where ϕ_s is the resonance wave function, $\psi_{\mu E}$ is the nonresonant continuum wave function for channel μ, ψ_g is the ground state, and $\mathcal{H}$ is the Hamiltonian. Ξ represents the global interference between the dipole excitation from the ground state and the autoionizing transition of the resonance to the open continua. Using Eq. (3), q_s, ρ_s^2, and α_μ^s can be written [2,14]:

$$q_s=[\pi\Xi(E_s)]^{-1}[\langle\psi_g|z_1+z_2|\phi_s\rangle+\mathcal{P}\int\Xi(E')(E_s-E')^{-1}dE'], \tag{4}$$

$$\rho_s^2=2\pi\Xi(E_s)^2\left[\sum_\mu|\langle\psi_g|z_1+z_2|\psi_{\mu E_s}\rangle|^2\Gamma_s\right]^{-1}=\frac{2\pi}{\Gamma_s}\frac{\Xi(E_s)^2}{\sigma^0}, \tag{5}$$

$$\alpha_\mu^s=2\pi\Xi(E_s)\langle\phi_s|\mathcal{H}|\psi_{\mu E_s}\rangle[\langle\psi_g|z_1+z_2|\psi_{\mu E_s}\rangle\Gamma_s]^{-1}. \tag{6}$$

ρ_s is not an independent parameter since

$$\rho_s^2=\frac{1}{\sigma^0}\sum_\mu\sigma_\mu^2|\alpha_\mu^s|^2. \tag{7}$$

However, from Eq. (5), ρ_s is a sort of "normalized" interference function and, therefore, it will be used as a measure of the strength of the Fano interferences. For single channel photoionization, $\Xi\neq0$ for all Z, and, therefore, there is no cancellation. In this case, simple Z-scaling rules applied to the resonance parameters explain the gross features of the photoionization spectra

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along the isoelectronic series [15]. We now examine what happens in multichannel photoionization between the $N=2$ and $N=3$ thresholds. In this case there are four open channels: $1s\epsilon p$, $2s\epsilon p$, $2p\epsilon s$, and $2p\epsilon d$. Writing the dominant configurations as zero-order states for ψ_g, ϕ_s, and $\psi_{\mu E_s}$ together with the corresponding first-order corrections in a perturbative expansion, it can be easily shown that the large-Z behavior of the matrix elements involved in Eqs. (4)–(6) is (see, also, Ref. [15])

$$\langle \psi_g | z_1 + z_2 | \phi_s \rangle \rightarrow \text{const} \times Z^{-2} , \tag{8}$$

$$\langle \phi_s | \mathcal{H} | \psi_{\mu E} \rangle \rightarrow \text{const} , \tag{9}$$

$$\langle \psi_g | z_1 + z_2 | \psi_{\mu E} \rangle \rightarrow \begin{cases} \text{const} \times Z^{-2} \quad \text{for } \mu = 1s\epsilon p \\ \text{const} \times Z^{-3} \\ \text{for } \mu = 2s\epsilon p, 2p\epsilon s, 2p\epsilon d . \end{cases} \tag{10}$$

These are the leading terms in a Z^{-1} expansion. In practice, this behavior is approximately observed for $Z \geq 3$, i.e., Z does not need to be very large. Therefore, the interference function Ξ scales as

$$\Xi(E_s) \rightarrow c_1 Z^{-2} + c_2 Z^{-3} , \tag{11}$$

where the first term comes from $\mu = 1s\epsilon p$ and the second one from $\mu = 2s\epsilon p, 2p\epsilon s, 2p\epsilon d$. When Eq. (11) is exact, c_1 and c_2 are strictly real numbers, since $\Xi(E_s)$ is a real quantity. It is then obvious that

$$\Xi(E_s) = 0 \quad \text{if } Z = -c_2/c_1 . \tag{12}$$

Then, cancellation of the interference function may be possible for a *unique* value of Z provided that $-c_2/c_1 > 0$. It must be noted that $\Xi = 0$ implies $q_s = \pm\infty$, $\rho_s^2 = 0$, and $\alpha_\mu^s = 0$. [See Eqs. (4)–(16).] Therefore, the shape of the resonance peak in the total cross section will be Lorentzian [see Eq. (1)]. On the other hand, substitution of $q_s = \pm\infty$ and $\alpha_\mu^s = 0$ in Eq. (2) does not lead to Lorentzian profiles for the partial cross section. This means that the interference of the doubly excited state with each continuum state $\psi_{\mu E}$ considered separately do not vanish, so that the partial cross sections still exhibit asymmetric peaks for the resonances. For the $3(1,1)_3\,{}^1P^0$ doubly excited state of He [16] (shortly $3s3p$), $\text{sign}(c_1) = -\text{sign}(c_2)$, but, as can be inferred from the existing experiments, condition (12) is not satisfied at all for He. However, there might be other He-like ions with $Z > 2$ for which such a condition could be satisfied. In particular, the "equivalent" $3s3p$ states of these ions ($Z > 2$) should be good candidates to explore possible cancellations of the interference function Ξ.

For this purpose, we have evaluated total and partial photoionization cross sections in the vicinity of the $3s3p$ resonance of He, Li^+, Be^{2+}, B^{3+}, C^{4+}, N^{5+}, O^{6+}, F^{7+}, Ne^{8+}, Si^{12+}, and Ar^{16+}, which corresponds to the range of nuclear charges $Z = 2$–$10, 14, 18$. We have used the L^2-integrable method of Ref. [6], which is based on the Feshbach formalism and whose accuracy has been shown in previous studies on the photoionization of the helium atom from the ground state as well as from metastable states [6,17]. Interchannel couplings are fully taken into account by solving the K-matrix equations in a representation of discretized uncoupled continuum states. Except for the limited size of the basis sets used in the calculations, no other approximations are made. A detailed description of the method can be found in our previous work on He [6]. Calculations for the other members of the isoelectronic series have been made with the Slater-type orbital (STO) bases reported in [6], which were optimized for He and, therefore, can also be expected to be optimum for $Z > 2$, since electron correlation is less important. In particular, the basis set used for the ground state ensures that the virial theorem is satisfied with a relative accuracy of 10^{-5} for all systems. An appealing feature of the theoretical method is that no fitting procedure is needed to evaluate the resonance parameters, which are directly obtained for $E = E_s$. In the present work, we have used the equations reported in Ref. [6] to evaluate (in the length gauge) the Fano and the Starace parameters for the $3s3p$ Feshbach resonance. Our calculated parameters remain practically constant around E_s, and take into account the effect of neighboring reso- neighboring resonances.

In Fig. 1 we have plotted the resonance parameters q_s, ρ_s^2, $|\alpha_\mu^s|$, and Γ_s as functions of Z. Figure 1(a) shows that q_s presents an asymptote for $Z \simeq 4$–5, and, therefore, there is a cancellation of the interference function around this value of the nuclear charge. Also for $Z \simeq 4-5$, one can see in Figs. 1(b) and 1(c) that $\rho_s^2 \simeq 0$ and $\alpha_\mu^s \simeq 0$ for all μ, in agreement with our previous reasonings. Therefore, for B^{3+} and, to a lesser extent, for Be^{2+}, the corresponding resonance peak in the total cross section must be almost Lorentzian. This is further illustrated in Fig. 2, where we present the shape of the $3s3p$ resonance for He, B^{3+}, and Si^{12+}. For He and Si^{12+}, the resonance exhibits typical Fano profiles: A "window" followed by a peak at larger energies in the case of He (since $q_s > 0$), and the opposite in the case of Si^{12+} (since $q_s < 0$).

We have determined c_1 and c_2 in Eq. (12) assuming that our calculated matrix elements for $Z = 18$ verify Eqs. (8)–(10) exactly. The corresponding result is $c_1 = -0.003\,345$, $c_2 = 0.013\,41$. These values indicate that $\Xi(E_s)$ should vanish at $Z = 4.01$, which is coherent with our results of Fig. 1 and, therefore, supports the interpretation that the Fano interferences are hidden for $Z \simeq 4-5$ because of the different scaling properties of the dipole matrix elements [see Eqs. (10) and (11)].

Figure 1 also shows the behavior of the Fano and the Starace parameters when $Z \rightarrow \infty$. Using the Z scaling rules of Eqs. (8)–(10) in Eqs. (4)–(6), we obtain, for large Z:

$$q_s \rightarrow \text{const}, \tag{13}$$

$$\rho_s^2 \rightarrow \text{const}, \tag{14}$$

$$\alpha_\mu^s \rightarrow \begin{cases} \text{const} \quad \text{for } \mu = 1s\epsilon p \\ \text{const} \times Z \quad \text{for } \mu = 2s\epsilon p, 2p\epsilon s, 2p\epsilon d , \end{cases} \tag{15}$$

which is in agreement with our findings of Fig. 1(a)–(c). In particular, two important limit values are $q_s \simeq -2.3$ and $\rho_s^2 \simeq 0.007$. Also, Eq. (9) implies that the resonance width Γ_s tends to a constant value [$\Gamma_s \simeq 0.44$ eV, see Fig. 1(d)], and σ^0 behaves as Z^{-2}.

To conclude, we have shown that photoionization of

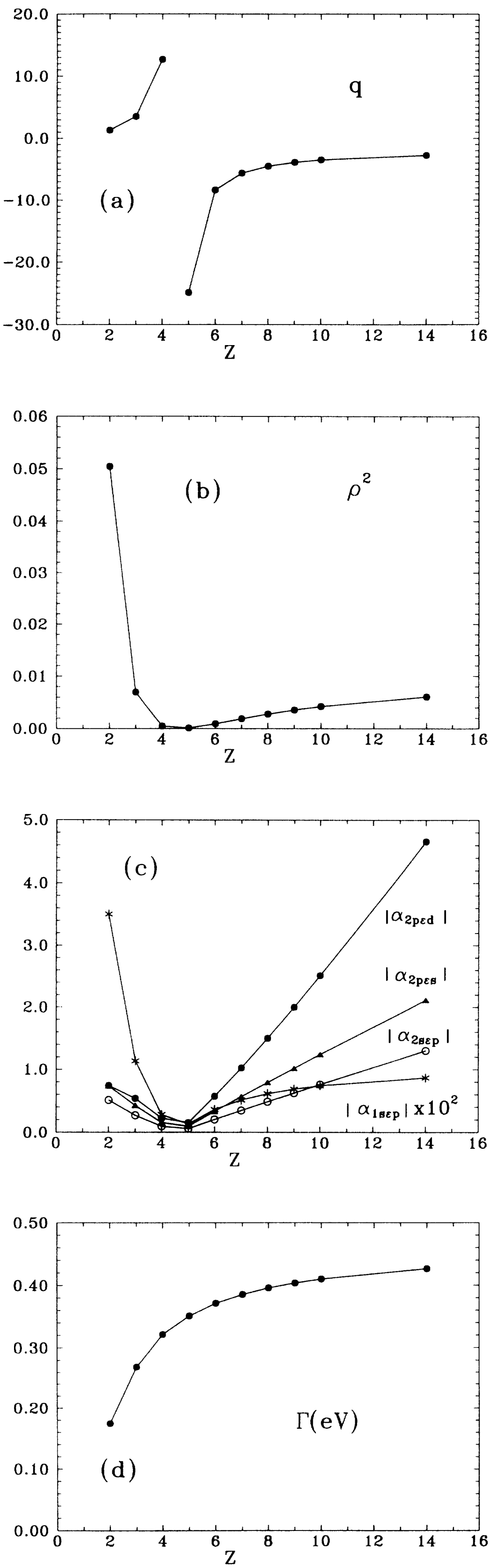

FIG. 1. Resonance parameters of the $3s3p$ doubly excited state in the photoionization spectrum of He-like ions. (a) line profile parameter q_s, (b) correlation parameter ρ_s^2, (c) Starace parameters $|\alpha_{1s\epsilon p}^s|, |\alpha_{2l\epsilon l'}^s|$, and (d) total autoionization width Γ_s.

He-like ions above the $N=2$ threshold can lead to the cancellation of the Fano interferences for a given nuclear charge. The origin of this phenomenon is the different Z-scaling law and opposite phase of the dipole transition matrix elements for the different outgoing channels. Such a cancellation yields photoelectron spectra that do not present any more asymmetric profiles for the resonances. As a consequence, different ions with almost similar electron correlation properties can exhibit quite different spectra. This is in contrast with the photoion-

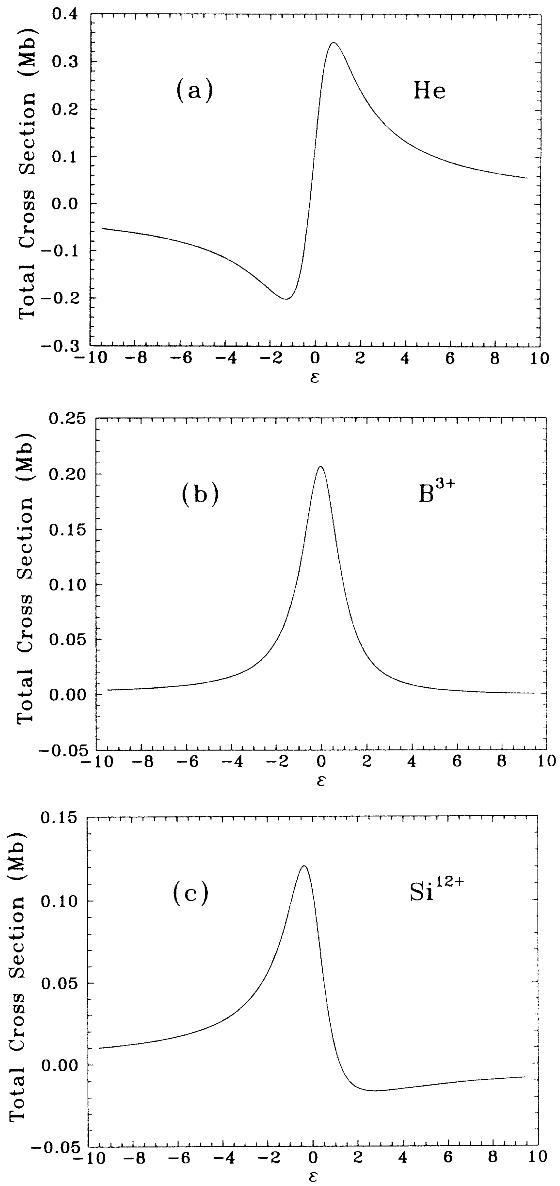

FIG. 2. Total photoionization cross sections of (a) He, (b) B^{3+}, and (c) Si^{12+} in the vicinity of the $3s3p$ resonance. In order to make the comparison more apparent, we have plotted $\sigma(E)-\sigma^0(E)$ (i.e., the smooth decreasing background has been subtracted) and the resulting cross sections have been multiplied by Z^2. The background cross sections for $E=E_s$ are $\sigma^0=1.0007$ Mb for $Z=2$, $\sigma^0=0.1183$ Mb for $Z=5$, and $\sigma^0=0.01331$ Mb for $Z=14$.

ization below the $N=2$ threshold, where most of physics can be understood by using a more simple Z-scaling analysis. The existence of symmetric (Lorentzian) resonances provides us with ideal systems where energy positions and widths can be accurately determined from experiments by simply fitting a two-parameter formula to the cross sections.

Although the present analysis has been restricted to the $3(1,1)_3\ {}^1P^0$ "$3s3p$" resonance, cancellation of interferences can also occur for more excited resonances. In particular, it would be very interesting to see if they exist for all values of the K,T correlation quantum numbers [16], or if there are selection rules which prevents their existence for some resonance series.

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