Competition of the Breit interaction in angular anisotropy of Auger electrons

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We study the effects of the Breit interaction on angular emission of Auger electrons emitted from the nonradiative Auger decay $1s2s^22p_{1/2}\,J = 1 \rightarrow 1s^22sJ_f = 1/2$ of berylliumlike high-Z ions excited by electron impact. The Breit interaction is found to contribute to lowering the anisotropy of the Auger electrons, and this effect behaves less prominently with increasing nuclear charge and impact energy for heavier ions than Re^{71+}. This finding is surprisingly different from the conclusion drawn for the case of x-ray photon emission, and, indeed, rather contradicts our common understanding of the role of the Breit interaction in excitation and decay of highly charged heavy ions, for which the contribution of the Breit interaction is ever expected to be more prominent as the nuclear charge and impact energy increase. Our detailed analysis reveals that such an unexpected behavior results from a constructive or more destructive competition of the effects of the Breit interaction on both the excitation and Auger decay of the autoionizing level $1s2s^22p_{1/2}\,J = 1$ of high-Z ions.

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I. INTRODUCTION

The Breit interaction contributes to the leading correction to the Coulomb potential in quantum electrodynamics [1,2], which comprises magnetic interactions and retardation effects in the exchange of a single virtual photon between two interacting electrons [3,4]. The importance of the Breit interaction has been well revealed for energy-level structure and transition properties of heavy atoms and highly charged ions (HCIs) [5–8] and, in particular, for a number of basic atomic processes with free electrons involved, such as elastic electron scattering [9], relativistic transfer ionization [10], dielectronic recombination (DR) [11–14], electron-impact ionization [15], as well as electron-impact excitation (EIE) [16–21]. Moreover, since polarization and angle-resolved properties of characteristic x-rays have been known to be much more sensitive to various physical effects and interactions than total radiative decay rates, their linear polarization and angular distribution have been extensively used as a tool to explore the spin-orbit interaction [22], relativistic effect [23–25], hyperfine interaction [26–28], electron spin-polarization effect [29–31], multipole mixing of radiation fields [32,33], splitting and sequence of overlapping resonances [34–36], spectral formation mechanism [37], as well as the Breit interaction [38–48].

Over the past two decades, the dominance of the Breit interaction has been explored in great detail by analyzing angular and polarization properties of characteristic x-rays radiated from excited HCIs. For example, Nakamura *et al.* [38] found clear evidence in experiments that the importance of the Breit interaction effect on the DR of initially lithiumlike ions increases as the nuclear charge Z increases, which is exceptionally strong for the recombination through the resonant level $1s2s^22p_{1/2}\,J = 1$. Later, Fritzsche *et al.* [39] proposed x-ray measurements on the linear polarization and angular distribution of the $1s2s^22p_{1/2}\,J = 1 \rightarrow 1s^22s^2\,J_0 = 0$ electric-dipole ($E1$) radiation of berylliumlike high-Z ions following the resonant electron capture (i.e., the first step of the DR process) into initially lithiumlike ions. It was found that the Breit interaction significantly dominates the Coulomb repulsion and leads to a qualitative change in the expected x-ray emission pattern, in which its contribution to the linear polarization and angular distribution of the $E1$ radiation indeed becomes larger with increasing nuclear charge. Following this proposal, Hu *et al.* [40] measured the angular distribution of the $E1$ line in the DR of initially lithiumlike Au^{76+} ions at the Tokyo electron-beam ion trap. The experimentally determined angular distribution was found to be consistent with the theoretical prediction [39] and, hence, confirmed the dominance of the Breit interaction. Moreover, the effect of the Breit interaction on both the linear polarization and angular distribution of exactly the same $E1$ line but populated through the EIE of berylliumlike HCIs was investigated as well by us [41,42]. Again, it was shown that the contribution of the Breit interaction becomes more significant with increasing impact electron energy and nuclear charge, respectively, which is rather similar to the case of the DR population mechanism. Since then, a good number of other experimental and theoretical studies have been performed to further explore the role of the Breit interaction in excitation and radiative decay properties of HCIs [43–48].

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In sharp contrast to the angular and polarization properties of characteristic x-ray photons, little attention has been paid to those of Auger electrons. As a matter of fact, the (doubly excited) resonant level, $1s2s^22p_{1/2}\,J=1$, can decay not only radiatively with emission of x-ray photons but also nonradiatively with emission of Auger electrons (i.e., the so-called Auger decay, an inverse process of the resonant electron capture). For example, Chen and Reed [49] explored the relativistic effects on the angular distribution of Auger electrons emitted from the Auger decay $1s2s^22p_{1/2}\,J=1 \to 1s^22s\,J_f=1/2$ following EIE of berylliumlike light ions. It was found that the relativistic effects can completely change the characteristics of the angular distribution for those transitions which have many contributing partial waves, even for ions as light as Fe^{22+}. Nevertheless, as a very important part of the relativistic effects, the contribution of the Breit interaction was not considered. Actually, for the Auger decay of ions excited by the EIE mechanism, both the processes have free electrons involved and, thus, the Breit interaction is expected to play a significant role in the angular distribution of the Auger electrons emitted from heavy HCIs. To confirm this, we studied the effect of the Breit interaction on the angular distribution of the Auger electrons emitted in the Auger decay ($1s2s^22p_{1/2}\,J=1 \to 1s^22s\,J_f=1/2$) of low- to high-$Z$ berylliumlike ions following the EIE from their ground state $1s^22s^2\,J_0=0$ [50]. It was found that for low-Z ions the Breit interaction hardly contributes to the angular distribution of the Auger electrons, especially at low impact energies, whereas its contribution becomes more and more prominent as the nuclear charge increases to certain high-Z ions. For even higher-Z ions, however, the angular distribution with the Breit interaction included was found to be nearly independent of the nuclear charge, and even its contribution becomes less prominent as the nuclear charge increases. This finding is surprisingly different from the conclusion drawn for the case of photon emission, irrespective of population mechanism [39–42], and, indeed, contradicts our common understanding of the role of the Breit interaction in excitation and decay of HCIs, for which the Breit interaction is expected to become more prominent as the nuclear charge and impact energy increase.

In this paper, we aim to explore and clarify the reasons for this unexpected behavior of the role of the Breit interaction in the angular emission of Auger electrons following EIE of berylliumlike high-Z ions. To this aim, detailed *ab initio* calculations are performed for selected Nd^{56+}, Ho^{63+}, Re^{71+}, Pb^{78+}, Ra^{84+}, and U^{88+} ions using the multiconfigurational Dirac-Hartree-Fock method and the relativistic distorted-wave theory [2,51]. To be specific, the alignment parameter of the resonant level $1s2s^22p_{1/2}\,J=1$ populated by electron impact and the intrinsic anisotropy parameter of its Auger decay to the ground state $1s^22s\,J_f=1/2$ are calculated at a series of impact energies with and without the inclusion of the Breit interaction, respectively. The anisotropy parameter of the Auger electron emission is further obtained by using both parameters for four different cases (i.e., with and without the Breit interaction considered in the calculation of the two parameters), which is finally used for analyzing the role of the Breit interaction in the angular emission of the Auger electrons. It is shown that the unexpected behavior is caused by a competition of the effects of the Breit interaction on both the EIE population and Auger decay of the resonant level $1s2s^22p_{1/2}\,J=1$ of high-Z ions.

II. THEORY

For (initially) randomly oriented berylliumlike ions and spin-unpolarized impact electrons, if the quantization axis is chosen along the propagation direction of the impact electrons and the detectors used are assumed to be insensitive to spin polarization of electrons, the angular distribution of the Auger electrons emitted in the Auger decay $1s2s^22p_{1/2}\,J=1 \to 1s^22s\,J_f=1/2$ following the EIE $1s^22s^2\,J_0=0 \to 1s2s^22p_{1/2}\,J=1$ of berylliumlike ions can be expressed in the form [52,53]

$$\mathrm{W}(\theta) \propto 1+\beta\, P_2(\cos\theta). \tag{1}$$

Here, $P_2(\cos\theta)$ is the second-order Legendre polynomial as a function of the polar angle θ of the emitted Auger electrons with respect to the quantization axis. β denotes the anisotropy parameter which describes the anisotropy of the Auger electron emission.

As seen clearly from Eq. (1), the angular distribution of the Auger electrons can be uniquely determined once the anisotropy parameter β is known. In fact, the anisotropy parameter β contains all the information about the excitation population and Auger decay of the resonant level $1s2s^22p_{1/2}\,J=1$. For the presently considered case, it is simply expressed as [53,54]

$$\beta=\alpha_2\,\mathcal{A}_{20} \tag{2}$$

with the alignment parameter $\mathcal{A}_{20}$ of the $1s2s^22p_{1/2}\,J=1$ level as well as the intrinsic anisotropy parameter α_2 of the Auger decay $1s2s^22p_{1/2}\,J=1 \to 1s^22s\,J_f=1/2$.

In the density-matrix theory, the alignment parameters are introduced to fully describe the relative population of the magnetic sublevels of any well-defined energy level. Here, the second-rank one, $\mathcal{A}_{20}$, is give by [42]

$$\mathcal{A}_{20}=\sqrt{2}\,\frac{\sigma_{\pm1}-\sigma_0}{2\sigma_{\pm1}+\sigma_0}, \tag{3}$$

where σ_0 and $\sigma_{\pm1}$ represent the partial EIE cross sections for the excitations from the ground state $1s^22s^2\,J_0=0$ to the magnetic sublevels $|M_J=0\rangle$ and $|M_J=\pm1\rangle$ of the autoionizing level $1s2s^22p_{1/2}\,J=1$, respectively. Note that integration over angular and polarization variables of the scattered electrons in the EIE process has been made in obtaining the alignment parameter, as it is assumed to not be observed.

Apart from the alignment parameter $\mathcal{A}_{20}$, the intrinsic anisotropy parameter α_2 is given by [55]

$$\begin{aligned}\alpha_2=&\sqrt{3}N_0^{-1}(-1)^{J+J_f-1/2}\sum_{ll'jj'}[l,l',j,j']^{1/2}\langle l0,l'0|20\rangle\\ &\times\langle\alpha_fJ_f,lj:J\|V_{ee}\|\alpha J\rangle\langle\alpha_fJ_f,l'j':J\|V_{ee}\|\alpha J\rangle^*\\ &\times\begin{Bmatrix}J & j & J_f\\ j' & J & 2\end{Bmatrix}\begin{Bmatrix}l & j & 1/2\\ j' & l' & 2\end{Bmatrix},\end{aligned} \tag{4}$$

which is independent of the prior EIE process but reflects the (initial- and final-state) electronic shell structure of the Auger decay. Here, $[a,b,\ldots]\equiv(2a+1)\times(2b+1)\ldots$ and the standard notations have been employed for both the Clebsch-Gordan coefficients and the Wigner-6j symbols. In addition, $N_0 \equiv \sum_{lj} |\langle \alpha_f J_f, lj : J \| V_{ee} \| \alpha J \rangle|^2 \equiv \sum_{lj} |\langle 1s^2 2s\, J_f = 1/2, lj : J = 1 \| V_{ee} \| 1s2s^2 2p_{1/2}\, J = 1 \rangle|^2$ denotes a normalization constant, which is determined by the reduced Auger decay amplitudes. Note that here there are only two open channels, i.e., $lj = p_{1/2}$ and $p_{3/2}$, due to the conservation laws of parity and total angular momentum of the decay system.

As is well known, both the EIE and Auger decay are mediated by the electron-electron interaction. Its operator, as denoted by V_{ee}, has been derived rigorously within the framework of quantum electrodynamics and applied to a great number of calculations of electronic structure and collisional processes of heavy elements. In the relativistic theory, the frequency-dependent electron-electron interaction operator [39,56]

$$V_{ee} = V_{\mathrm{Coulomb}} + V_{\mathrm{Breit}} = \sum_{p<q} \left[\frac{1}{r_{pq}} - \frac{\boldsymbol{\alpha}_p \cdot \boldsymbol{\alpha}_q}{r_{pq}} \cos(\omega_{pq} r_{pq}) + (\boldsymbol{\alpha}_p \cdot \nabla_p)(\boldsymbol{\alpha}_q \cdot \nabla_q) \frac{\cos(\omega_{pq} r_{pq}) - 1}{\omega_{pq}^2 r_{pq}} \right] \quad (5)$$

consists of both the instantaneous Coulomb interaction (first term) and the Breit interaction, i.e., the magnetic current-current interaction (second term) due to the motion of electrons [57] and the retardation correction (third term) in the exchange of the virtual photon with angular frequency ω_{pq}. Here, $\boldsymbol{\alpha}_p$ denotes the vector of the Dirac matrices associated with the pth electron.

III. RESULTS AND DISCUSSION

To analyze the angular distribution of the Auger electrons, both the parameters $\mathcal{A}_{20}$ and α_2 need to be known, as shown in Eqs. (1)–(4), which are traced back to the calculation of the partial EIE cross sections and the Auger decay amplitudes. In the present calculations, configurations $1s^2 2s$, $1s^2 3s$, $1s^2 3d$, $1s^2 2s^2$, $1s^2 2p^2$, $1s^2 2s2p$, and $1s2s^2 2p$ are utilized to generate required wave functions and energy levels of lithiumlike and berylliumlike ions, where the quantum-electrodynamical effects are considered. In addition, maximal partial waves $\kappa = \pm 50$ are adopted to ensure convergence in the calculation of the EIE cross sections. It should be noted that all the calculations of $\mathcal{A}_{20}$ and α_2 are performed twice, i.e., without (labeled by NB) and with (by B) the Breit interaction considered, respectively.

Figure 1 displays the alignment parameter $\mathcal{A}_{20}$ of the autoionizing level $1s2s^2 2p_{1/2}\, J = 1$ populated by the EIE of berylliumlike (high-Z) Nd^{56+}, Ho^{63+}, Re^{71+}, Pb^{78+}, Fr^{83+}, and U^{88+} ions at the impact electron energy of 3.0 times their respective excitation thresholds as an example. Results are presented for both the NB and B cases. It is found that for the NB case the alignment parameter $\mathcal{A}_{20}$ remains almost constant as the nuclear charge increases, whereas a visible Z dependence is obtained for the parameter with the Breit interaction considered, as clearly seen from the figure, which changes from -0.148 for Nd^{56+} to -0.039 for U^{88+}. Moreover, a remarkable decrease of the alignment parameter is found for all the ions considered due to the contribution of the Breit interaction, and such a contribution becomes more prominent for higher-Z ions. For instance, its relative value increases from 69% for Nd^{56+} to 92% for U^{88+} ions. Here, it should be noted that with increasing nuclear charge the alignment parameter for the B case is approaching zero, which means that the population of all the sublevels $|M_J = 0, \pm 1\rangle$ of the autoionizing level $1s2s^2 2p_{1/2}\, J = 1$ becomes nearly identical [cf. Eq. (3)] due to the contribution of the Breit interaction.

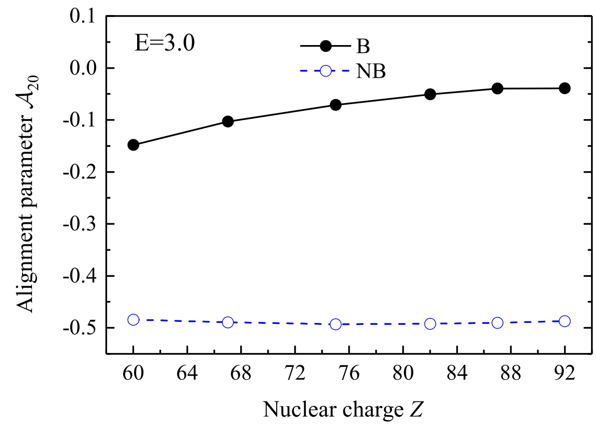

FIG. 1. Alignment parameter $\mathcal{A}_{20}$ of the autoionizing level $1s2s^2 2p_{1/2}\, J = 1$ populated by the EIE of berylliumlike Nd^{56+}, Ho^{63+}, Re^{71+}, Pb^{78+}, Fr^{83+}, and U^{88+} ions at the impact electron energy of 3.0 times their respective excitation thresholds. Results are plotted for both the NB (blue dashed line with hollow circles) and B (black solid line with solid circles) cases for comparison.

Apart from the alignment parameter $\mathcal{A}_{20}$, the intrinsic anisotropy parameter α_2 of the nonradiative Auger decay $1s2s^2 2p_{1/2}\, J = 1 \rightarrow 1s^2 2s\, J_f = 1/2$ is shown in Fig. 2 as well for the six berylliumlike ions. Again, the results are given for both cases. The Coulomb interaction alone results in a large positive value of the intrinsic anisotropy parameter for all the ions, which decreases only slightly from 0.682 for Nd^{56+} to 0.410 for U^{88+}, whereas a quite remarkable decrease

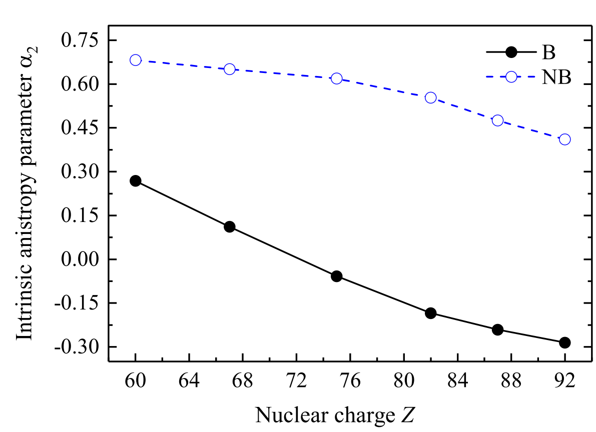

FIG. 2. Intrinsic anisotropy parameter α_2 of the Auger decay $1s2s^2 2p_{1/2}\, J = 1 \rightarrow 1s^2 2s\, J_f = 1/2$ of berylliumlike Nd^{56+}, Ho^{63+}, Re^{71+}, Pb^{78+}, Fr^{83+}, and U^{88+} ions. Results are given for both the NB (blue dashed line with hollow circles) and B (black solid line with solid circles) cases for comparison.

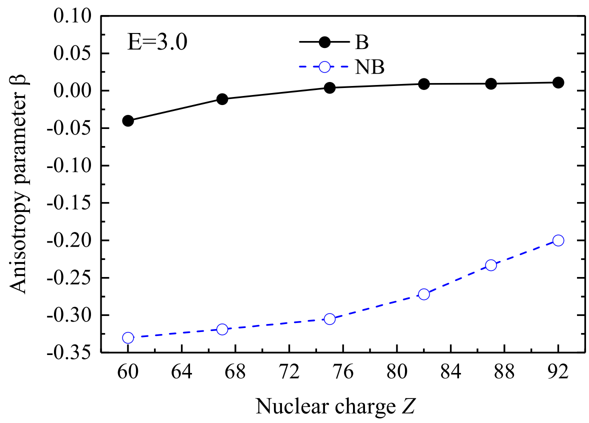

FIG. 3. Anisotropy parameter β of the Auger electrons emitted from the Auger decay $1s2s^22p_{1/2}\,J=1 \rightarrow 1s^22s\,J_f=1/2$ following the EIE of Nd^{56+}, Ho^{63+}, Re^{71+}, Pb^{78+}, Fr^{83+}, and U^{88+} ions at the impact electron energy of 3.0 times their respective excitation thresholds. Results are given for both the NB (blue dashed line with hollow circles) and B (black solid line with solid circles) cases for comparison.

of the parameter is found for the case with the Breit interaction incorporated and, in particular, changes its sign from positive to negative at about $Z = 72$. Such a change in the sign will result in a qualitative change in the angular emission pattern of the Auger electrons. Moreover, similar to the case of the alignment parameter, the contribution of the Breit interaction to the intrinsic anisotropy parameter also becomes more and more prominent as the nuclear charge increases. To be specific, the relative contribution increases quickly from 61% for Nd^{56+} to 169% for U^{88+} ions.

Having both the alignment parameter $\mathcal{A}_{20}$ and the intrinsic anisotropy parameter α_2 available, the anisotropy parameter β, or equivalently, the angular distribution of the Auger electrons emitted from the nonradiative Auger decay $1s2s^22p_{1/2}\,J=1 \rightarrow 1s^22s\,J_f=1/2$, can be easily obtained by means of Eq. (2). As an example, Fig. 3 displays the anisotropy parameter of berylliumlike Nd^{56+}, Ho^{63+}, Re^{71+}, Pb^{78+}, Fr^{83+}, and U^{88+} ions calculated at the impact electron energy of 3.0 times their respective excitation thresholds. Once again, results are plotted for both cases. As shown in the figure, the Breit interaction contributes to remarkably decreasing the anisotropy parameter of all the ions, i.e., making the Auger electron emission much less anisotropic, which is indeed similar to the effect of the Breit interaction on both parameters $\mathcal{A}_{20}$ and α_2, as discussed above. Nevertheless, the anisotropy parameter with the Breit interaction included is surprisingly found to remain almost constant (in particular, beyond about $Z = 75$) rather than to be strongly Z dependent as the nuclear charge Z increases. What is even more surprising is that the contribution of the Breit interaction to the anisotropy parameter β becomes less prominent with increasing nuclear charge. Such an unexpected behavior contradicts what has been known on the role of the Breit interaction in excitation and decay of heavy (few-electron) HCIs [13,38–44].

In order to understand how the Breit interaction affects the anisotropy parameter (or, equivalently, the angular

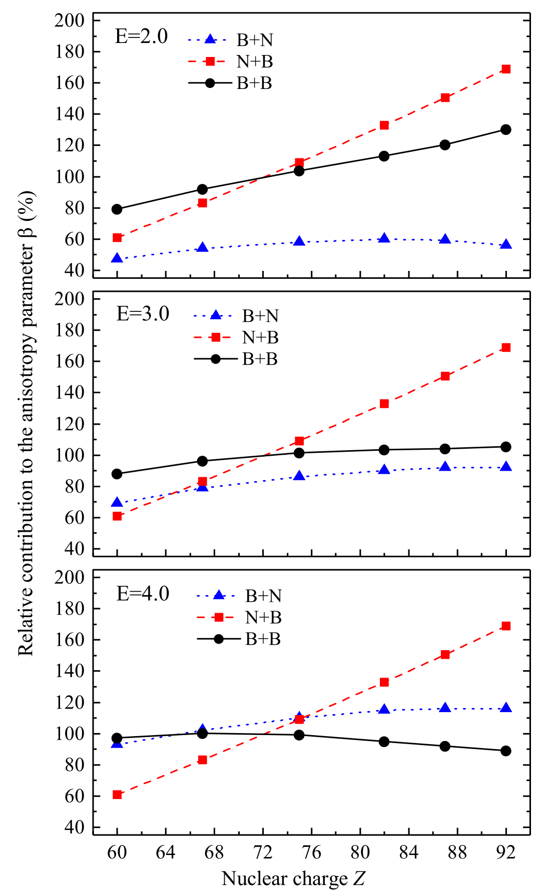

FIG. 4. Relative contribution of the Breit interaction to the anisotropy parameter β of the Auger electrons with respect to the results without the Breit interaction considered in both the alignment parameter and the intrinsic anisotropy parameter (as denoted by N + N), calculated at three impact electron energies of 2.0 (top panel), 3.0 (middle), and 4.0 (bottom) times their respective excitation thresholds. Results are plotted for three cases, i.e., B + N (blue dotted line with triangles), N + B (red dashed line with squares), and B + B (black solid line with circles), for comparison. B + N denotes the relative contribution for the case with the Breit interaction included in the calculation of the alignment parameter but without in the intrinsic anisotropy parameter, while the other two cases have similar meanings.

distribution) of the Auger electrons through the alignment parameter and the intrinsic anisotropy parameter and, thereby, clarify the reasons for the unexpected behaviors of the role of the Breit interaction, the anisotropy parameter is calculated at a series of impact electron energies for four different cases, i.e., with and without the Breit interaction considered in the calculation of one or both of the parameters in sequence. For example, Fig. 4 illustrates the relative contribution of the Breit interaction to the anisotropy parameter with respect to the results without the Breit interaction included in both the alignment parameter and the intrinsic anisotropy parameter (as denoted by N + N). Results are plotted here for three cases (i.e., B + N, N + B, and B + B) for comparison. B + N denotes the relative contribution for the case with the Breit interaction included in the calculation of the alignment parameter $\mathcal{A}_{20}$ but without in the intrinsic anisotropy parameter α_2, and similar meanings hold true for the other two cases.

As seen explicitly from the figure, the Breit interaction affects the anisotropy parameter β of the Auger electrons in rather different ways through each of the two parameters $\mathcal{A}_{20}$ (i.e., the EIE population) and α_2 (i.e., the Auger decay) or both of them, which depends on the impact energy and, in particular, strongly on the nuclear charge of the ions. In general, the relative contribution of the Breit interaction to the anisotropy parameter due to its inclusion in the calculation of the intrinsic anisotropy parameter α_2 (i.e., for the case $\mathrm{N+B}$) becomes much more prominent as the nuclear charge increases, which increases from 61% for Nd^{56+} to 169% for U^{88+} ions. By sharp contrast, the relative contribution changes slowly due to the inclusion of the Breit interaction in the alignment parameter (i.e., for the case $\mathrm{B+N}$), which increases from 47% to 56%, from 69% to 92%, and from 93% to 116% for the impact energies of 2.0, 3.0, and 4.0 times their excitation thresholds, respectively. In addition, regarding to the case with full consideration of the Breit interaction in both the EIE and Auger decay amplitudes (i.e., the case $\mathrm{B+B}$), the relative contribution behaves (as a function of the nuclear charge Z) rather differently for different impact electron energies. To be specific, at the energies of 2.0 and 3.0 times the thresholds it increases smoothly from 79% for Nd^{56+} to 130% for U^{88+} and from 88% to 106%, respectively, whereas at the higher energy of 4.0 times considered the relative contribution decreases unexpectedly from 100% for Ho^{63+} to 89% for U^{88+} ions. These specific data indeed indicate that the contribution of the Breit interaction to the anisotropy parameter (i.e., the angular distribution) of the Auger electron emission is not always the most prominent for the heaviest U^{88+} ions and the highest impact electron energy considered, which contradicts our common understanding of the role of the Breit interaction in excitation and decay of heavy HCIs, as discussed above.

From the above analysis, it is shown that this unexpected behavior results from a constructive or destructive competition of the effects of the Breit interaction on the EIE population and Auger decay of the autoionizing level $1s2s^22p_{1/2}\,J=1$ of high-Z ions. To be specific, for Nd^{56+} and Ho^{63+}, the Breit interaction contributes constructively to lowering the angular anisotropy β of the Auger electrons through the parameters $\mathcal{A}_{20}$ and α_2 at all the impact energies considered, although such a constructive contribution becomes less constructive as the energy increases. In contrast, for other higher-Z ions considered the Breit interaction contributes destructively to the angular anisotropy, which becomes more destructive as the nuclear charge Z and the impact energy increase, respectively. Take U^{88+}, for example: at the energy of 4.0 times the threshold the relative contribution of the Breit interaction to the anisotropy parameter is as high as 116% and 169% for the $\mathrm{B+N}$ and $\mathrm{N+B}$ cases, respectively, whereas the contribution is only 89% for the $\mathrm{B+B}$ case, i.e., the case with the Breit interaction included in both the EIE and Auger decay amplitudes.

IV. CONCLUSION

To summarize, we studied the effect of the Breit interaction on the angular distribution of the Auger electrons emitted in the Auger decay $1s2s^22p_{1/2}\,J=1 \rightarrow 1s^22s\,J_f=1/2$ of berylliumlike high-Z ions populated by electron impact. It was found that the Breit interaction makes the angular distribution much less anisotropic for all the ions and impact energies considered. For Z ions higher than about $Z=75$, moreover, the absolute and relative contribution of such an effect becomes less prominent as the nuclear charge and the impact energy increase, respectively. This finding is surprisingly different from the conclusion drawn for the case of x-ray photon emission [39–42], and, indeed, contradicts our common understanding of the role of the Breit interaction in excitation and decay of HCIs, for which the Breit interaction is ever expected to become more prominent with increasing nuclear charge and impact energy. From a detailed analysis, it was revealed that such an unexpected behavior results from a constructive or destructive competition of the effects of the Breit interaction on the EIE population and Auger decay of the autoionizing level $1s2s^22p_{1/2}\,J=1$ of berylliumlike high-Z ions.

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