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Delta Electron Emission in Superheavy Quasiatoms with $Z \gtrsim 137$

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Results of coupled channel calculations are presented for total and K-hole coincident δ-electron spectra for the systems I−Pb, I−U and Au−U. Electron screening and vacancy sharing corrections are included. The computed cross sections are compared with the first coincidence measurements of δ-electrons and K-shell vacancies in systems with $Z \gtrsim 137$.

1. Introduction and Theory

In recent years the δ-electron spectroscopy of superheavy quasimolecules and quasiatoms with a total nuclear charge $Z > 100$ has gained widespread interest in experimental as well as in theoretical heavy-ion physics. Experiments of Kozhuharov [1], Güttner et al. [2], Herath-Banda et al. [3], Backe et al. [4, 5], Schweppe et al. [6] and Clemente et al. [7] lead to a new range of atomic physics, and greatly increased our knowledge about atomic systems from $Z = 100$ (Fm) to $Z = 188$ (U+Cm). Due to the strong binding forces electrons of the inner shells display remarkable relativistic features, e.g., rather high momenta components are contained in the electron wavefunctions. This necessitates a theoretical description in a framework employing the Dirac equation. The production cross section of high energy electrons in collisions of very heavy ions is increased by several orders of magnitude due to relativistic effects.

The total δ-electron emission rate as well as the δ-electrons in coincidence with the K-X-rays of both collision partners have been measured by Koenig et al. [3]. The superheavy systems I−Pb, I−U and Au−U were investigated for bombarding energies well below the nuclear Coulomb barrier. We evaluated the total electron spectra and the number of emitted δ-electrons in coincidence with a K-X-ray of the heavier collision partner. In a preceding paper [8] we already presented calculated total electron spectra and double differential cross sections for the lighter systems Br−Pb ($Z = 117$) and Br−U ($Z = 127$). The experimental data of Herath-Banda et al. [3] are well suited to test our theoretical treatment of electron excitations in systems, whose combined nuclear charge exceed $Z = 137$. This is particularly important for the quantitative understanding of the spontaneous positron emission (see e.g. [9]). After the discussion of the basic theoretical ingredients we compare the experimental data with our theoretical results.

The time development of the n-th electron during the collision is described by the time dependent Dirac equation ($\hbar = c = 1$)

$$i \frac{\partial}{\partial t} \psi_n(\mathbf{r}, t) = [\boldsymbol{\alpha} \cdot \mathbf{p} + \beta m + V_{tc}(t)] \psi_n(\mathbf{r}, t). \tag{1}$$

In the present calculations the two-centre potential $V_{tc}(t)$ is approximated by the dominant monopole term [10]. The total electron wavefunction $\psi_n(\mathbf{r}, t)$ is expanded in the basis ϕ_k of adiabatic, molecular wavefunctions, for which the stationary equation holds

$$(\boldsymbol{\alpha} \cdot \mathbf{p} + \beta m + (V_{tc}(t))_{\text{monopole}} + (V_{ee})_{\text{monopole}}) \phi_k(\mathbf{r}, t) = E_k(t) \phi_k(\mathbf{r}, t). \tag{2}$$

The basis functions ϕ_k depend parametrically on time via the dependence of the two-centre potential V_{tc} on the internuclear separation. V_{ee} is the electron-electron potential treated in the framework of the relativistic self-consistent field method [8]. For the exchange term we applied the Slater approximation.

V_{ee} reads

$$V_{ee}(\mathbf{r})=e^2\int\frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\,\mathrm{d}^3r'-\frac{2}{3}\left(\frac{81}{8\pi}\right)^{1/3}e^2(\rho(\mathbf{r}))^{1/3}, \tag{3}$$

where $\rho(\mathbf{r})$ denotes the density of the electron cloud. V_{ee} was calculated using the ground state adiabatic, molecular wavefunctions. To be consistent with our approximation of the two-centre Coulomb potential we restricted V_{ee} to be of monopole type. Our approximation is physically justified since it describes well binding energies and the radial coupling for strongly bound $ns\sigma$- and $np_{\frac{1}{2}}\sigma$-electrons [10]. It is sufficient for our purpose to consider only these states, as they give the dominant contribution to electron emission with electron energies higher than 100 keV. Our model fails, however, to describe electron wavefunctions with angular momentum quantum numbers $|\kappa|>1$ and rotational coupling, due to the spherical symmetry of the monopole term. Thus in the numerical calculations we have restricted our basis to $s_{\frac{1}{2}}\sigma$- and $p_{\frac{1}{2}}\sigma$-states. The expansion is given by

$$\psi_n(\mathbf{r},t)=\sum\!\!\!\!\!\!\int_k a_{nk}(t)\,\phi_k(\mathbf{r},t)\exp\{-i\chi_k\} \tag{4}$$

with

$$\chi_k=\int_{-\infty}^{t}E_k(t')\,\mathrm{d}t'.$$

The integral sign refers to the continuum states. Projection leads to a set of coupled differential equations for the occupation amplitudes a_{nj}

$$\dot{a}_{nj}(t)=-\sum\!\!\!\!\!\!\int_k a_{nk}(t)\langle\phi_j|\frac{\partial}{\partial t}|\phi_k\rangle\exp\{-i(\chi_k-\chi_j)\}. \tag{5}$$

In the following indices p and q indicate particle and hole states, respectively. Due to reasons stated above, p and q refer either to $s_{\frac{1}{2}}\sigma$- or $p_{\frac{1}{2}}\sigma$-states. The many electron problem can be solved in the framework of the second quantisation formalism. This leads to a simple formula for the number of electrons N_p with a certain energy (either in a discrete or continuous level) per unit energy and per unit solid angle, and for the number of holes N_q in a state [11]. As the hole states are measured via X-ray emission N_q denotes the number of measured characteristic X-ray quanta per unit solid angle.

$$N_p=\sum_{r<F}|a_{rp}(\infty)|^2 \quad \text{for } p>F, \tag{6a}$$

$$N_q=\sum_{s>F}|a_{sq}(\infty)|^2 \quad \text{for } q<F. \tag{6b}$$

F denotes the Fermi surface of initially occupied states. In a similar way one can derive a formula for the coincident rate

$$N_{p,q}=N_p\cdot N_q+|\sum_{r<F}a^*_{rp}(\infty)\,a_{rq}(\infty)|^2. \tag{7}$$

In the formulae (6a) and (6b) the indices r and s indicate particle and hole states with the same angular momentum quantum numbers κ and the same spin. In formula (7) particle and hole have corresponding spins, in the sense that an emitted particle with spin up results in a hole state with spin down. Spin, however, is not measured in this kind of experiments we want to consider. Additionally it is impossible to distinguish electrons emitted from the $1s_{\frac{1}{2}}\sigma$- or the $2p_{\frac{1}{2}}\sigma$-state. This has also to be taken into account in an expression which should describe the experimentally observed coincidence rate. It was also derived in [11] and given there as

$$N_{p=E,q=1s}=N_{E,1s\sigma}+N_{E,2p_{\frac{1}{2}}\sigma}, \tag{8}$$

with

$$N_{E,1s\sigma}=2(N_{Es\sigma,1s\sigma}+N_{Es\sigma}\cdot N_{1s\sigma})+4N_{Ep_{\frac{1}{2}}\sigma}\cdot N_{1s\sigma}, \tag{9a}$$

$$N_{E,2p_{\frac{1}{2}}\sigma}=2(N_{Ep_{\frac{1}{2}}\sigma,2p_{\frac{1}{2}}\sigma}+N_{Ep_{\frac{1}{2}}\sigma}\cdot N_{2p_{\frac{1}{2}}\sigma})+4N_{Es\sigma}\cdot N_{2p_{\frac{1}{2}}\sigma}. \tag{9b}$$

For a discussion of these terms the reader is referred to [11]. All terms in (9) have to be understood as measurable quantities within a solid angular window $\Delta\Omega$ and (for continuum states) a certain energy range ΔE. The formulae, however, represent the result of a limiting process, i.e., the limit of small detector size and high energy resolution. In the case of a realistic finite detector size and energy resolution one has the uncertainties $\Delta p=\Delta E_p\Delta\Omega_p$ and $\Delta q=\Delta\Omega_q$ for the measurement of particles and holes, respectively. These quantities depend entirely on the experimental features like geometry, detectors etc. It can be shown [12] that with non-vanishing Δp, Δq a relation similar to (9) can be derived, offering the possibility to compare uniquely the experimentally measured quantities at given energy resolution ΔE and given solid angular window $\Delta\Omega$ with theoretical calculations. For a more extensive discussion the reader is referred to [12].

Until now we have considered symmetric systems, where created vacancies in the molecular levels are shared equally between the collision partners to create K-holes in the separate atoms. In case of asymmetric systems we have coincidences with the K-X-rays of the collision partner with higher nuclear charge and those with the collision partner with lower nuclear charge. In this paper we consider only coincidences with K-X-rays, which originate from the collision partner with higher nuclear charge. In this case we have to weigh the contributions from the $1s\sigma$- and the $2p_{\frac{1}{2}}\sigma$-molecular levels according to Meyerhof [13]. This yields

$$N_{p=E,\,q=1s}(H)=(1-w)\cdot N_{E,\,1s\sigma}+w\cdot N_{E,\,2p_{\frac{1}{2}}\sigma}. \tag{10}$$

$N_{p=E,q=1s}(H)$ indicates the number of created particles measured in coincidence with the K-X-rays from the collision partner with higher nuclear charge. w is defined by the equations

$$w=\frac{e^{-2x}}{1+e^{-2x}}, \tag{11 a}$$

$$x\equiv\frac{\sqrt{2}\pi(\sqrt{E_H}-\sqrt{E_L})}{\sqrt{m_e}\,v}. \tag{11 b}$$

E_H and E_L denote the energies of the 1 s atomic levels of the collision partners with higher and lower nuclear charge, respectively. m_e is the electron mass and v the projectile velocity. For very asymmetric systems with a large difference $\sqrt{E_H}-\sqrt{E_L}$, the contribution from the $2p_{\frac{1}{2}}\sigma$-hole disappears. The other limit is the case of a symmetric system, where $w=0.5$.

To allow for a comparison with the experimental data of Herath-Banda et al. [3], we still have to perform an integration over the impact parameter b. Thus the double differential cross section for the production of a δ-electron in coincidence with a K-X-ray of the collision partner with the higher nuclear charge reads

$$\frac{d^2\sigma}{dE\,d\Omega}=\int_0^\infty [(1-w)\cdot N_{E,\,1s\sigma}(b)+w\cdot N_{E,\,2p_{\frac{1}{2}}\sigma}(b)]\,2\pi b\,db. \tag{12}$$

2. Discussion and Results

Our calculations were performed using a basis of 8 $s\sigma$-bound and 18 $s\sigma$-continuum states, 6 $p_{\frac{1}{2}}\sigma$-bound and also 18 $p_{\frac{1}{2}}\sigma$-continuum states. V_{ee} was calculated assuming a loss of 50 electrons in the collision system due to pre-collision stripping techniques. All calculations have been performed twice using a Fermi surface of $F=3$ and $F=4$ (i.e., all levels up to $4p_{\frac{1}{2}}\sigma$ and $5p_{\frac{1}{2}}\sigma$, respectively, are filled) to get an estimate of the influence of the Fermi level. The differences in the coincident spectra were of the order of 1%. In the total spectra the contribution of the higher Fermi level varies from 35% in the electron energy region of 200 keV down to 15% at 600 keV. The theoretical spectra presented here have been calculated assuming a Fermi level $F=3$.

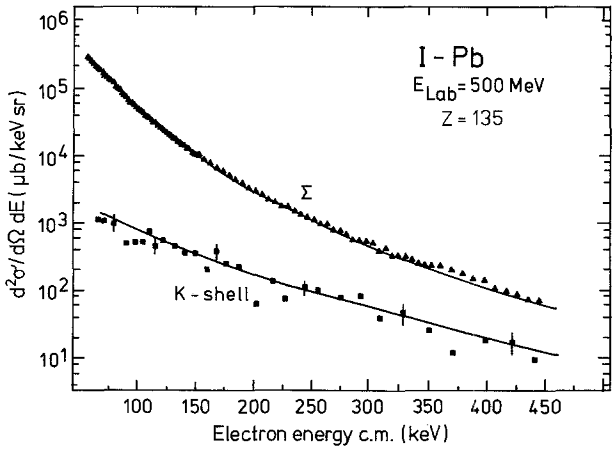

Fig. 1. Experimental double differential cross sections for the total δ-electron yield (Σ, triangles) and for the 1 s-atomic coincident yield (K, squares) versus kinetic electron energy. The system I – Pb at 500 MeV bombarding energy is considered. The full lines are the results of our coupled channel calculations. Experimental data by W. Koenig et al. [3]

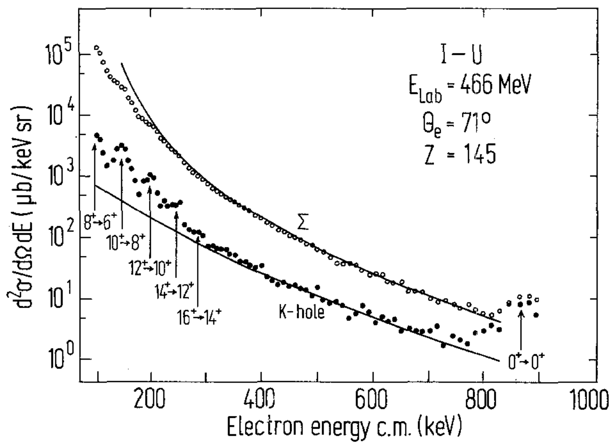

Fig. 2. The same as in Fig. 1 for the colliding system I – U at 466 MeV bombarding energy. Open circles indicate total δ-electron yield, full circles the 1 s-atomic coincident yield

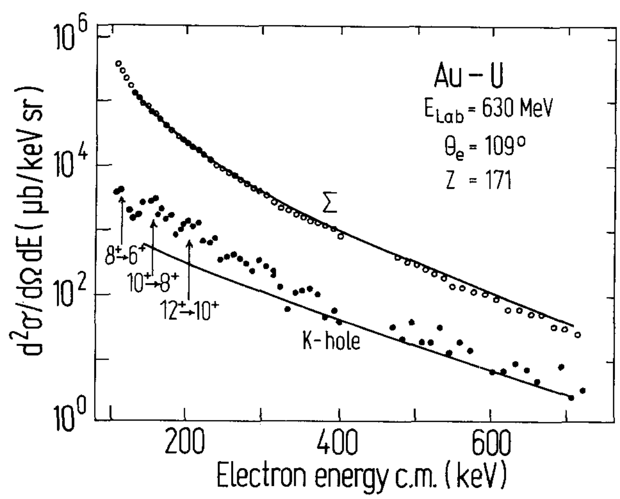

Fig. 3. The same as in Fig. 2 for the colliding system Au – U at 630 MeV bombarding energy

In Figs. 1–3 we compare our results for the double differential cross section with the experimental data of Herath-Banda et al. [3] for the systems I – Pb, I – U and Au – U. The double differential cross section is shown versus the kinetic electron energy in the centre of mass system. The lower curves represent coincidences between electrons and K-holes. The upper curves indicate our result for the total δ-electron emission rate. Remarkable agreement is achieved for the total and the coincident spectra for the slope as well as for the absolute numbers. Note, that in the calculations no scaling or fitting has been applied.

There is no influence of vacancy sharing in the asymmetric systems I – Pb and I – U. For the system Au – U it raises the coincident rate 50% for the low energy part ($\simeq$150 keV) and 20% for the high energy part ($\simeq$600 keV) of the spectrum. The bumps in the coincidence spectra arise from nuclear Coulomb excitation and subsequent internal conversion in the U-nucleus. The corresponding nuclear transitions are indicated. The electrons were observed at certain angles with respect to the beam axis. No anisotropies in the coincidence spectra were detected for these systems, which reflects the validity of the monopole approximation.

In conclusion we may state that our theoretical considerations correctly describe inner-shell excitation and δ-electron production in superheavy systems. The strong relativistic effects are reflected in the rather high production rate of high energy electrons.

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