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δ-Electrons from K- and L-Shell Ionization in Relativistic Systems*

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Inner-shell ionization in adiabatic heavy-ion collisions is calculated within the monopole approximation by using the relativistic united-atom representation for the wave functions. As an example, ionization probability and energy distribution of the δ-electrons is given for the (Pb, Pb) system and compared with experiment.

1. Introduction

The spectroscopy of electrons emitted in slow heavy-ion collisions is one of the tools to study the properties of strongly bound quasi-atomic states. High-energy δ-electrons can be attributed to the high components of the momentum distribution of the initially bound electrons, and provide thus information on their energy and wave function. When using very heavy collision partners the electronic states of superheavy atoms transiently formed during the collision, can be studied.

In the recent years there have been a number of experimental and theoretical approaches to this problem. Starting with the bombardment of heavy ions such as Pb, with lighter projectiles [1] one has now also used heavy projectiles [2] and detected electrons with an energy much higher than the K-shell binding energy of the corresponding united atom. Theoretically, the ionization probability for slow collisions has been estimated in the framework of the atomic model, using Born approximation [3] and adjusting the wave functions to the destorted nuclear field [4]. This method has been applied for asymmetric systems. When the nuclear charges are of equal magnitude the molecular description is preferred, where one chooses the wave functions as eigenstates to the two-center field while the transitions are caused by the change of the field in time. Since the momentum transfer to the electron is large in heavy systems, it has been shown in the case of K-shell ionization that the dominant part of the transition is induced by the monopole expansion term V_0 of the two-center potential [5]. Thus the two-center problem can be reduced to a one-center problem by choosing the wave functions as eigenfunctions to the potential V_0, so that one avoids the problem of calculating two-center continuum states. Another way to get rid of the two-center problem in slow collisions, is to keep the full potential, but take the wave functions as eigenstates to the united atom [6] which is a good approximation since the inner-shell ionization occurs mainly at very small internuclear distances R. Thereby one can include transitions of higher multipolarity which may become important for the excitation of higher p-states.

In our work we combine the two approximations, i.e. we use united-atom wave functions and a monopole potential. Instead of V_0 we take, however, a one-center monopole potential with time-dependent charge. This is justified because the radius of the electron orbit is much larger than R (in the ionization region) such that from the electron point of view the two nuclei are well described by one charge-changing nucleus. Further, the calculations are thereby simplified considerably. In Sect. 2 we derive the cross section for K- and L-shell ionization, and compare in Sect. 3 with other theories and experiment.

2. Theory

In symmetric or near-symmetric collisions the dominant contribution to K-shell ionization comes from the $2p\sigma$ molecular state which correlates to the L_{II}-shell of the united atom, and only a minor fraction comes from $1s\sigma$ ionization.

In the adiabatic perturbation theory the amplitude for direct transitions is given by

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$$a_{fi}=\int_{-\infty}^{\infty} dt\,\langle\psi_f|\frac{\partial V}{\partial t}|\psi_i\rangle\frac{1}{E_f-E_i}\,e^{i/\hbar\int_0^t dt(E_f-E_i)}. \tag{2.1}$$

When one approximates the wave functions ψ and energies E of initial and final state by their time-independent values in the united atom limit [7] (the so-called Briggs model [6]), one obtains by means of partial integration

$$a_{fi}=\frac{1}{i\hbar}\int_{-\infty}^{\infty} dt\,\langle\psi_f|V|\psi_i\rangle\,e^{i/\hbar(E_f-E_i)t}. \tag{2.2}$$

We replace the two-center potential V by a monopole field [8]

$$V(t)=-\frac{Z(R)\,e^2}{r} \tag{2.3}$$

and determine the time-dependent charge by a fit to the $1s\sigma$ level (obtained from a two-center calculation [5] for fixed internuclear distance R) and by means of the relation $Z(E)$ between energy and nuclear charge. In the case of the (Pb, Pb) quasimolecular system, we take

$$Z(R)=Z_2+\begin{cases}84-0.485\,R+3.5\times10^{-3}\,R^2 \\ \qquad R\leqq 45\text{ fm} \\ 77.86/(1+2.76\times10^{-3}\,R) \\ \qquad 45\text{ fm}<R\leqq 60\text{ fm} \\ 104.9/R^{0.1}\,e^{-7.006\times10^{-4}R} \\ \qquad R>60\text{ fm}\end{cases} \tag{2.4}$$

where Z_2 is the target charge. For lighter systems one may obtain $Z(R)$ by means of a variational principle [8].

For the wave functions ψ we take relativistic functions belonging to an atom with charge Z. In order to obtain the right impact-parameter dependence of the ionization probability with the potential (2.3) it is important to take the charge Z that enters into ψ from (2.4) at the distance of closest approach $R(b, t=0)$. In the case of high-relativistic united atoms where the point-nucleus Dirac wave function is no longer valid, one may introduce an effective charge $Z_{\text{eff}}<137$ into the Dirac function. This Z_{eff} results from a fit of the K-shell ionization probability calculated with Dirac functions (to Z_{eff}) to a calculation using Hartree-Fock wave functions for extended nuclei [9]. For the Pb+Pb united atom ($Z=164$) for example, one finds $Z_{\text{eff}}=134.5$. In this high-Z region, Z_{eff} and thus the wave functions vary slowly with Z. The energy E_i (also to be taken at $R(b, t=0)$) is obtained from a two-center calculation [5]. Actually, since it is only needed for small R, it may also be found from united-atom perturbation theory. $R(t)$ is determined by a Rutherford trajectory.

The advantage of the potential (2.3) together with the use of time-independent energies and wave functions is the splitting of the transition amplitude (2.2) into a time integral $T_{fi}(b)$ and a space integral

$$a_{fi}=-\frac{e^2}{i\hbar}\left(\int_{-\infty}^{\infty} dt\,Z(R)\,e^{i/\hbar(E_f-E_i)t}\right)$$
$$\cdot\left(\int d\mathbf{r}\,\psi^*_{f,jlm}(\mathbf{r},\mathbf{k}_f)\frac{1}{r}\psi_{i,jlm}(\mathbf{r})\right)$$
$$\equiv-\frac{e^2}{i\hbar}T_{fi}(b)\,M_{fi}(\mathbf{Y}_{jlm}(\Omega_{k_f})\,\mathbf{e}) \tag{2.5}$$

which can be evaluated independently. The exact two-center potential factorizes only in momentum space [6], thus involving an extra integral (over momentum).

Using the partial wave expansion of the continuum Dirac functions [10], the angular part of the ejected electron is represented by the spherical harmonic spinor $\mathbf{Y}_{jlm}$ projected on the polarization direction $\mathbf{e}$ of the electron. M_{fi} is the remaining part of the space integral and can be evaluated analytically. The angular integration is trivial since only monopole transitions occur. We take Landau's definition [10] of the relativistic Coulomb waves and normalize them to plane waves:

$$f, g(k_f, r)=2^\gamma\,\pi^{-\frac{1}{2}}(1\pm mc^2/E_f)^{\frac{1}{2}}$$
$$\cdot e^{\pi\nu/2}\frac{|\Gamma(\gamma+1+i\nu)|}{\Gamma(2\gamma+1)}(k_f r)^{\gamma-1}$$
$$\cdot\text{Im, Re}(e^{ik_f r+i\xi}\,{}_1F_1(\gamma-i\nu, 2\gamma+1, -2ik_f r)).$$

Then, the radial integrals involved are of the following type

$$I(n)=\int_0^{\infty} dr\,r^{2\gamma-n}\,e^{-\alpha_0 r}\,e^{ik_f r}$$
$$\cdot\,{}_1F_1(\gamma-i\nu, 2\gamma+1, -2ik_f r)$$
$$=\Gamma(2\gamma-n+1)(\alpha_0-ik_f)^{-2\gamma+n-1}$$
$$\cdot\,{}_2F_1\left(\gamma-i\nu, 2\gamma-n+1, 2\gamma+1, \frac{-2ik_f}{\alpha_0-ik_f}\right) \tag{2.6}$$

where the hypergeometric function ${}_2F_1$ simplifies for $n=0$ to

$${}_2F_1(n=0)=\left(1+\frac{2ik_f}{\alpha_0-ik_f}\right)^{-\gamma+i\nu}.$$

In the case of $1s_{1/2}$ and $2p_{1/2}$ initial states, $\gamma=\sqrt{1-(Z_{\text{eff}}e^2/\hbar c)^2}$, α_0 is the inverse shell radius ($\alpha_0^s=Z_{\text{eff}}/a_0$, $\alpha_0^p=\alpha_0^s(2+2\gamma)^{-1/2}$, $a_0=\hbar^2/me^2$), k_f and E_f the momentum and energy of the ejected electron,

respectively, and $v=Z_{\text{eff}}\, e^2 E_f/((\hbar c)^2 k_f)$. The space integral M_{fi} is given by the sum of the matrix elements of the large and small component of ψ:

$$M_{f,1s_{1/2}}=N_i^s N_f[\sqrt{(1+\gamma)(1+mc^2/E_f)}$$
$$\cdot \operatorname{Im}(e^{i\xi_s} I_s(n=1))$$
$$-\sqrt{(1-\gamma)(1-mc^2/E_f)}\operatorname{Re}(e^{i\xi_s} I_s(n=1))]$$
$$M_{f,2p_{1/2}}=N_i^p N_f\left\{\sqrt{(1+g_2/2)(1+mc^2/E_f)}\right.$$
$$\cdot\left[(g_2-2)\operatorname{Im}(e^{i\xi_p} I_p(n=1))\right.$$
$$\left.-\frac{2(g_2-1)\alpha_0^p}{2\gamma+1}\operatorname{Im}(e^{i\xi_p} I_p(n=0))\right]$$
$$-\sqrt{(1-g_2/2)(1-mc^2/E_f)}\left[g_2\operatorname{Re}(e^{i\xi_p} I_p(n=1))\right.$$
$$\left.\left.-\frac{2(g_2-1)\alpha_0^p}{2\gamma+1}\operatorname{Re}(e^{i\xi_p} I_p(n=0))\right]\right\} \tag{2.7}$$

where $g_2=(2+2\gamma)^{1/2}$. In (2.7) enters the real and imaginary part of $I(n)$ from (2.6), evaluated with α_0^s and α_0^p, respectively.

$$\exp(i\xi_s)=((\gamma+iv)/(-1+ivmc^2/E_f))^{\frac{1}{2}},$$
$$\exp(i\xi_p)=((\gamma+iv)/(1+ivmc^2/E_f))^{\frac{1}{2}},$$

and the normalization constants are

$$N_i^s=\left[(2\alpha_0^s)^{2\gamma+1}\frac{1}{2\Gamma(2\gamma+1)}\right]^{\frac{1}{2}}$$
$$N_i^p=\left[(2\alpha_0^p)^{2\gamma+1}\frac{2\gamma+1}{4\Gamma(2\gamma+1)\,g_2(g_2-1)}\right]^{\frac{1}{2}}$$
$$N_f=\pi^{-\frac{1}{2}}/\gamma\, e^{\pi\nu/2}(2k_f)^{\gamma-1}\,|\Gamma(\gamma+1+iv)|$$

where Γ is the gamma function.
The transition probability differential in electron momentum is given by

$$\frac{dP(b)}{dk_f}=2k_f^2\int d\Omega_{k_f}\sum_e |a_{fi}|^2. \tag{2.8}$$

The factor 2 accounts for the 2 electrons in the initial state (=sum over the spin states). The integral over electron angle is trivial since the monopole approximation corresponds to isotropically distributed electrons (as long as the initial state is not polarized). We get from (2.5)

$$\frac{dP(b)}{dk_f}=2k_f^2(e^2/\hbar\, T_{fi}(b)\, M_{fi})^2. \tag{2.9}$$

From this we obtain the double differential cross section by multiplying it with the elastic Rutherford cross section

$$\frac{d^2\sigma}{d\Omega\, dk_f}=\frac{dP(b)}{dk_f}\frac{d\sigma_R}{d\Omega}. \tag{2.10}$$

3. Results and Comparison with Experiment

The total probability $P(b)$ for inner-shell ionization calculated from (2.9) is shown in Fig. 1 for the $1s\sigma$ and $2p\sigma$ initial states. As an example, the system (Pb, Pb) was chosen at a projectile energy of 4.7 MeV/amu corresponding to $v/c=0.1$ which is much smaller than the orbiting velocity of the inner-shell electron such that the adiabatic description is valid. For comparison, Fig. 1 shows also the results from a two-center calculation [5]. The $1s\sigma$ ionization probability can be reproduced very well within our monopole model while in the $2p\sigma$ case only the relative dependence on impact parameter is the same but the absolute values are a factor of 3 too low. The better agreement in the $1s\sigma$ case is due to the choice of the potential (2.3) which is deduced from ground state properties. For higher states, the two-center character of the potential becomes more important even if one only retains its monopole expansion term as done in [5].
The experiments were performed with the Unilac accelerator in Darmstadt. Both ionization probability

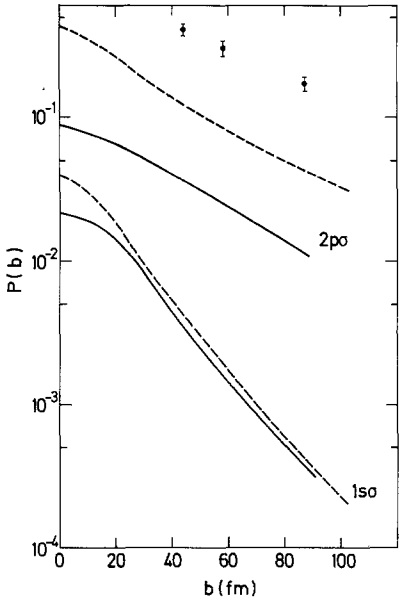

Fig. 1. Ionization probability for the Pb + Pb system (4.7 MeV/amu projectile energy) versus impact parameter. Full lines correspond to the ionization of $1s\sigma$ and $2p\sigma$ states calculated in the monopole approximation, dashed lines are the calculations from [5]. Experimental data (sum of $1s\sigma$ and $2p\sigma$) are taken from [11]

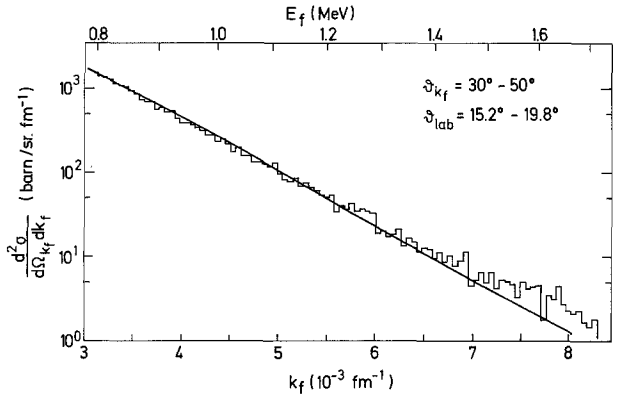

Fig. 2. Differential cross section for δ-electron emission in 4.7 MeV/amu (Pb, Pb) collisions as a function of electron momentum k_f. The data are from [12]. Theory is normalized to experiment

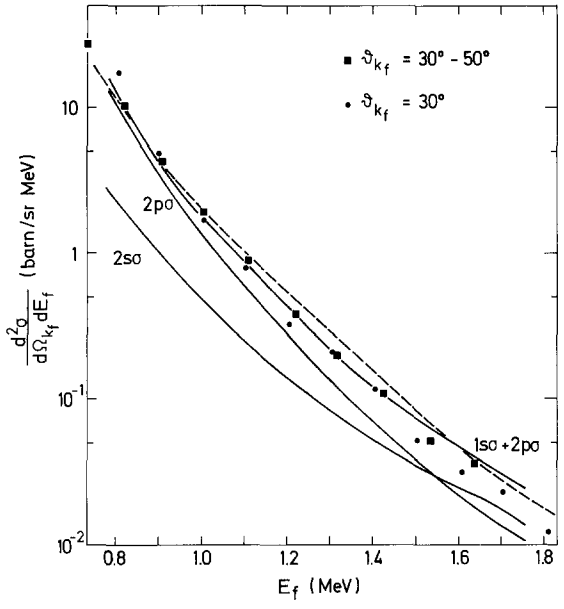

Fig. 3. Differential cross section for δ-electrons emitted in 4.7 MeV/amu (Pb, Pb) collisions as a function of total electron energy E_f. The full lines are calculations within the monopole approximation, and the dashed line is the sum of $1s\sigma$ and $2p\sigma$ direct excitation from a two-center calculation (Soff). The experimental data are from Kienle et al. (■) [12] and from Walcher et al. (●) [13]. Theory is normalized to experiment (see text)

[11] and high-energy electron spectra in coincidence with K-X-rays [2] were measured. The shape of the impact-parameter dependence of the ionization probability is well described by theory (Fig. 1). However, aside from the direct ionization, there may also be contributions from transitions to higher bound states which are emptied previous in the collision, or from multistep processes that could account for the discrepancy in absolute value. Also experimental background effects cannot be excluded.

Figure 2 shows the differential cross section for electron emission obtained from a coincidence experiment where besides the electron momentum k_f and emission angle ϑ_{k_f} also the scattering angle ϑ_{lab} is measured. The theoretical curve is the sum of the $1s\sigma$ and $2p\sigma$ ionization calculated from (2.10) and normalized to experiment at $E_f = 0.8$ MeV.

In Fig. 3 the differential cross section is summed over all scattering angles and the experimental data are compared with the results from our monopole model (multiplied by a factor of 34.4) and from the two-center calculation (multiplied by 13.8). We find a good agreement in the energy dependence of the ejected electrons. Also shown are the separate contributions from the $1s\sigma$ and $2p\sigma$ ionization. While for lower electron energies the $1s\sigma/2p\sigma$ fraction is around 0.2–0.3, the $1s\sigma$ ionization becomes of equal importance for small impact parameters ($b \lesssim 20$ fm) when E_f exceeds ≈ 1.2 MeV. Contributions from other initial states are neglected since they would involve multistep processes to create a K-vacancy.

The energy dependence of the δ-electrons mirrors thus mainly the behaviour of the $2p\sigma$ electrons and can be used to determine their momentum distribution. If one is interested in the $1s\sigma$ state, one must either choose asymmetric systems where the spacing between the projectile and target $1s_{1/2}$ state is large enough to prevent vacancy sharing, while another possibility would be to measure at very small impact parameters and high electron energy and use only slightly asymmetric systems (to avoid the symmetrization between projectile and target).

It has also been attempted to measure the δ-electron spectrum at different electron angles ϑ_{k_f}. Theoretically, one expects a nearly isotropic distribution since monopole transitions are dominant for the $j = 1/2$ states in K and L shell. Further, in the united-atom representation, dipole transitions cancel for symmetric systems. There may be an anisotropy originating from the fact that the electron cannot adjust completely to the two-center field, thus leading to a finite dipole transition. Since the ratio of v and v_p, the orbiting velocity of the united atom $2p_{1/2}$ electron, is below 0.3, this effect should be small. A relativistic investigation of this problem is in progress.

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