Z. Physik A 288, 345–348 (1978)

Zeitschrift
für Physik A

Kinematic Dipole Model for the Anisotropy of Quasimolecular X-Rays*

H. Hartung and B. Fricke
Gesamthochschule Kassel, Theoretische Physik, Kassel, Fed. Rep. Germany

Received May 5, Revised Version July 17, 1978

For the angular dependence of quasimolecular X-ray emission in heavy ion colliding systems we present a semiclassical adiabatic model taking into account spontaneous dipole radiation. Using the most characteristic levels from a DFS-correlation diagram we are able to explain the behaviour of the observed anisotropy.

The question of non-characteristic X-ray anisotropies observed in heavy ion collisions has been discussed for several years [1–4]. Various models have been proposed so far [5–6].
In the following we present the Kinematic Dipole model of the Anisotropy (KDA), which is able to explain the directional behaviour of the MO-X-ray intensity as well as the peak structure of the spectral anisotropy. This quantity is usually defined by

$$A=\frac{S(E_x, 90°)}{S(E_x, 0°)}-1,$$

where $S(E_x, \vartheta)$ is the X-ray intensity for a given X-ray energy E_x and observation angle ϑ. The path of the projectile during the collision can be described by Coulomb trajectories in the field of the effective nuclear charges Z_1^* and Z_2^*.
In slow collisions the electronic orbitals can be treated with great success in the adiabatic approximation [7]. Therefore correlation diagrams play an important role in the interpretation of heavy ion colliding systems [8]. The filling of the inner molecular orbital (MO) levels during the collision leads to the emission of non-characteristic MO-X-ray spectra [9–11].
The selection rules for dipole transitions allow

$$\Delta\Omega=0, \pm 1.$$

Relativistic inner shell transitions as they appear in heavy ion collisions show strong $j-j$ coupling. Thus $\Omega=\frac{1}{2}\rightarrow\Omega=\frac{1}{2}$ transitions lead to an isotropic contribution to the MO spectrum because of an equivalent mixing of $\Delta\Omega=0$ transitions with a $\sin^2\alpha$-photon distribution and $\Delta\Omega=\pm 1$ transitions with a $(1+\cos^2\alpha)$-distribution [12] where α is the angle between the internuclear distance vector **R** and the photon propagation vector **k**.
For $\Omega=\frac{3}{2}\rightarrow\Omega=\frac{1}{2}$ transitions only the case $\Delta\Omega=\pm 1$ appears, leading to an anisotropic photon emission.
In this paper we perform a systematic model study for the anisotropic contributions and their qualitative behaviour with photon energy. The isotropic contributions have, more or less, only quantitative consequences, because the energy dependence of both the anisotropic and isotropic transitions in the same energy region is very similar.
If we integrate incoherently the emitted photon intensity over all Rutherford trajectories and impact parameters, taking into account the angular distribution $1+\cos^2\alpha$ in the molecular rotating frame, we get the angular distribution in the laboratory system. (The effect of the Lorentz transformation into the laboratory system is negligible at these low velocities.) During the integration one has to take into account the radial dependence of first the transition energy ΔE, which one can obtain from a good correlation diagram, second the transition strength, which is proportional to $(\Delta E)^3$ and third the hole probabilities in the initial and final levels.
Furthermore one has to integrate over the azimuth angle ϕ defined by the orientation of the collision plane relative to the plane of observation.
To get an idea of the observable effects of the anisotropy within our model we use a simplified correlation diagram with 5 levels (Fig. 1), which correspond to

* Partially supported by Gesellschaft für Schwerionenforschung, Darmstadt

0340-2193/78/0288/0345/$01.00

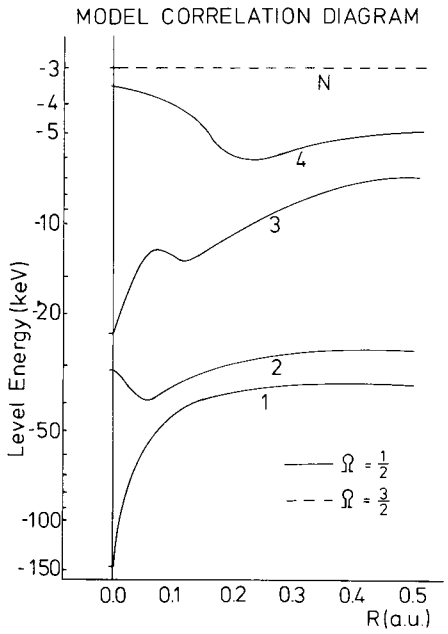

Fig. 1. Model correlation diagram (simplified version of a realistic Xe–Ag relativistic correlation diagram [11])

some typical levels in the correlation diagram Xe –Ag as an example.

The quantum number of level 1 to 4 is $\Omega=\frac{1}{2}$ and level N has $\Omega=\frac{3}{2}$.

Level 1 has its minimum at $R=0$, level 2 has a broad minimum at $R\approx 0.06$ a.u., level 3 is similar to level 1, but includes a maximum and minimum at larger R, and level 4 is a diabatic upper level with a united level energy above the separated atom limit. In this study we regard transitions from level N, which for simplicity is taken as a straight line.

The results are shown in Figure 2 for various transitions within our model correlation diagram. All calculations are done assuming a collision broadening effect according to [11] of 0.5 to 2 keV and projectile impact energy $E_0=27.2$ MeV; for the transition $N\rightarrow 1$ 10 keV (for $E_0=70.8$ MeV) were assumed. The collision broadening is the correction of the adiabatic description due to the dynamics of the collision process. In first order it is proportional to the change of the transition energy with time or internuclear distance respectively. A peak structure behaviour of the anisotropy can be seen in all diagrams. For the transitions into level 1 (Fig. 2a) we get a maximum somewhat below the united atom binding energy E_1^u. The exact position is also dependent on the projectile energy as long as the distance of closest approach is too large to produce the united atom transition energy [13]. For transition energies in the vicinity of the maximum of the anisotropy the internuclear distance vector is mainly perpendicular to the beam axis, which produces the large positive anisotropy. The transitions with the highest X-ray energies originate from backward scattering where the internuclear orientation is more or less parallel to the beam axis thus producing negative anisotropies. Their total contribution of course is small because of the little weighting due to the small impact parameter b. But this negative contribution explains the decrease of the anisotropy at the high energy side. In addition the large collision broadening for this K-transition produces the broad anisotropy peak which usually is observed in the experiment. In a real collision most of the holes in level 1 are created by Coulomb ionization which for small impact parameters shows a distinct maximum [14]. Thus one can expect that the anisotropy will be dominated by contributions from the outgoing parts of trajectories with small impact parameters. This leads to a general increase of the anisotropy. The isotropic contributions on the other hand for $\Omega=\frac{1}{2}\rightarrow\Omega=\frac{1}{2}$ transitions into level 1 in the same energy region again decrease the anisotropy. So the total anisotropy in an actual spectrum is expected to remain in the same order of magnitude as shown in Figure 2a.

For the transition into level 2 (Fig. 2b) we get an anisotropy maximum at energies which correspond to transitions into the minimum of level 2. As a transfer of a hole into this level usually happens by rotational coupling [15] at $R\approx 0$, the main contribution to the anisotropy is expected to originate from the outgoing part (which is shown in Fig. 2b) of the trajectory with a larger weight for small impact parameters. The decrease in the anisotropy usually observed in a real spectrum at the high energy side can easily be interpreted when we go to Figure 2c, where the isotropic part into level 1 together with the anisotropic part into level 2 at these energies sharply reduces the anisotropy.

The maximum anisotropy of transitions into level 3 (Fig. 2d) is again somewhat below the maximum transition energy ΔE_3^u. The maximum and minimum in level 3 causes a deformation of the anisotropy at the low energy region. If this maximum and minimum would be at smaller R it would cause an additional small peak in the anisotropy. The transitions into level 4 (Fig. 2e) show an anisotropy maximum somewhat above the united atom limit. The transition energy maximum at $R\approx 0.22$ a.u. is too far out to produce an anisotropy peak.

To summarize we may say that within our model we can interpret the peak structure behaviour of the anisotropy more or less independently of the hole distribution within the levels:

– we get a maximum near the united atom limits;

– we get a maximum in the anisotropy where a level has an extremum at relatively small R (c.f. level 2).

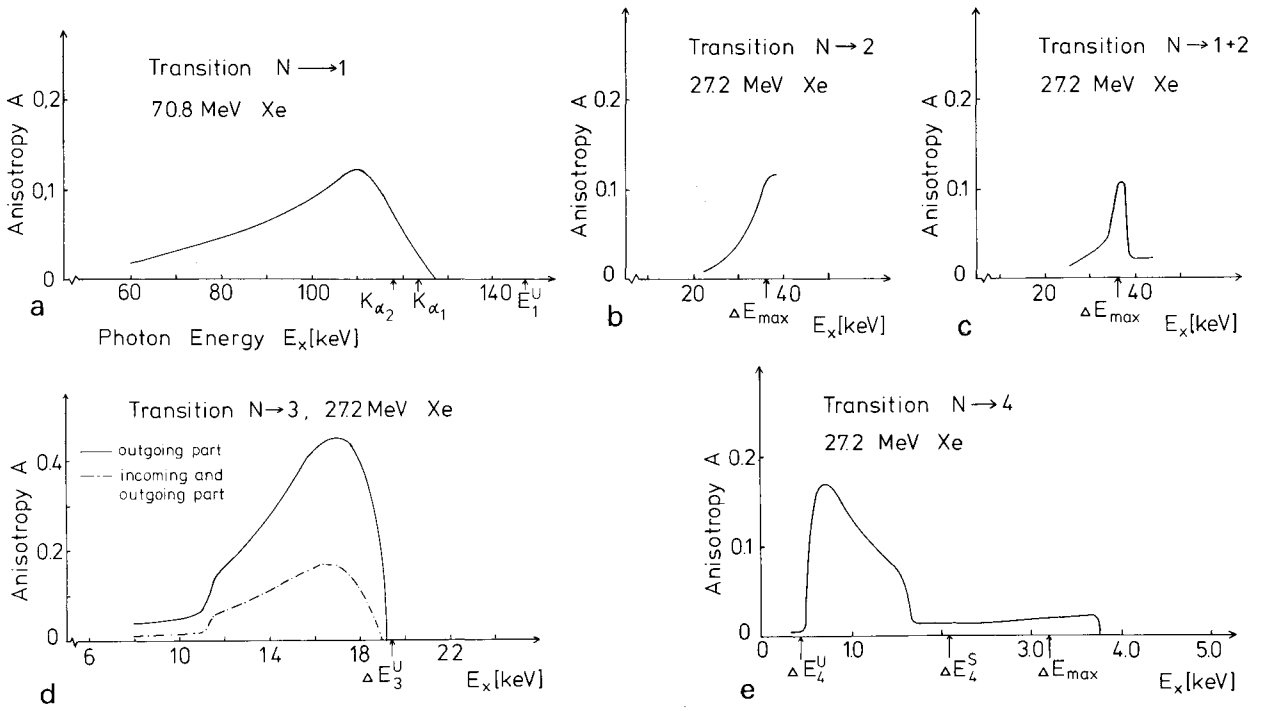

Fig. 2a–e. Spectral anisotropy for various transitions. **a** Transition $N \rightarrow 1$ for 70.8 MeV impact energy. A collision broadening of 10 keV was assumed. **b** Transition $N \rightarrow 2$ with contributions only from the outgoing parts of the trajectories: 2 keV collision broadening was included. **c** Combined anisotropy curve for transitions $N \rightarrow 1$ plus $N \rightarrow 2$. **d** Transition $N \rightarrow 3$. The dip below 12 keV results from the two extrema in level 3. **e** Transition $N \rightarrow 4$ with contributions only from the outgoing parts of the trajectories; 0.5 keV collision broadening was assumed. ΔE_4^s-transition energy of the separated system

This should make it possible to extract from good experimental data information about the united atom limits of the quasi-atoms, which would turn out to be a spectroscopy of superheavy elements [16–17]. In addition we get information of the structure and details of the correlation diagram at small R in the quasi-molecule. To separate quasi-atomic from quasi-molecular structures one needs good and realistic relativistic many-electron correlation diagrams.

Of course, within our model the maximum possible anisotropy is $+100\%$, which in reality is much smaller due to contributions from all parts of the Rutherford trajectory. For high impact energies and small Z the maxima of the observed anisotropies may come up to 240% as can be seen by Wölfli et al. [18]. We believe that in this case the explanation of Wölfli et al. [18] will be correct, who assumes a transition from a non-adiabatic electron with a translational factor e^{+ikr} into a bound state leading to a transition with a $\sin^2\vartheta$ angular distribution where ϑ is the angle between the beam axis and the k-vector of the emitted photon. In a real collision the contributions of both effects are strongly dependent on the impact energy and the initial and final states, respectively. In the adiabatic limit the anisotropies become as small as our values, as it is experimentally seen by Wölfli et al. [18].

We would like to thank Prof. Wölfli for many stimulating discussions on this subject.

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H. Hartung
B. Fricke
Theoretische Physik
Gesamthochschule Kassel
Heinrich-Plett-Straße 40
D-3500 Kassel
Federal Republic of Germany

Note Added in Proof. As an example for a very heavy system we have performed calculations of the anisotropy spectrum for Pb on Pb within the KDA model. Using the simple one-electron two-center correlation diagram of Soff et al. [19] which we have partially corrected for many-electron effects we get the spectrum shown in Figure 3, where the transitions into the three innermost $\Omega = 1/2$ levels are taken into account. The energetical position as well as detailed structure of the peaks may still be somewhat uncertain because of the unrealistic correlation diagram. Because this heavy system is strongly governed by relativistic effects, all $\Omega = 1/2$ to $1/2$ transitions will be isotropic. Only the transitions with $\Delta\Omega = \pm 1$ lead to anisotropic contributions. This is the reason that in this system the anisotropy maxima will be at or below 10 %.

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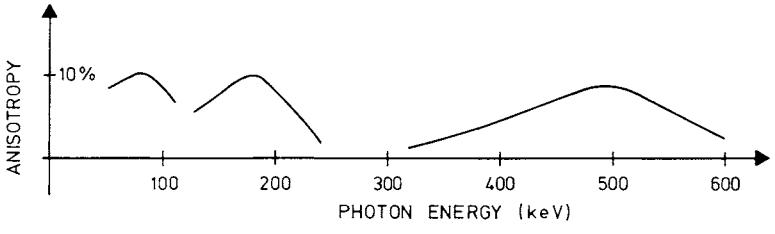

Fig. 3. Calculated anisotropy spectrum for the system Pb → Pb at 4.8 MeV/amu taking into account transitions into the three innermost $\Omega = 1/2$ levels