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Relativity and Screening Effects in Heavy-Ion Collisions

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Diatomic correlation diagrams are the main basis for the description of heavy-ion collisions. We have constructed the first realistic relativistic many-electron correlation diagrams based on nonrelativistic self-consistent-field, Hartree-Fock calculations of diatomic molecules plus relativistic corrections. We discuss the relativistic influences as well as the many-electron screening effects in the I-Au system with a combined charge of $Z=132$ as an example.

The past few years have seen an increasing interest in the atomic phenomena of heavy-ion collisions. Some of the most striking new developments were the first observations of noncharacteristic x rays by Saris *et al.*¹ which they interpreted as transitions between the electronic levels of the states transiently formed during the approach of the two nuclei in the heavy-ion collision at small internuclear distances. The bases for the description of this phenomenon are the correlation diagrams, which were used by Fano and Lichten² in their electron promotion model to explain many aspects of atomic phenomena occurring in the heavy-ion collision. A lot of experimental information has been gathered since,³⁻⁵ and in several cases it was even possible to extract from the experimental data the position of the electronic levels as a function of the internu-

clear distance.⁵ Thus, it now seems possible to make a direct comparison between the experimental and theoretical correlation diagrams.

Theoretical calculations of one-electron correlation diagrams have been done by Helfrich and Hartmann⁶ for the nonrelativistic case and Müller, Rafelski, and Greiner⁷ for the relativistic case. Also for low- Z elements some nonrelativistic, non-self-consistent⁸ as well as self-consistent calculations⁹ of many-electron correlation diagrams have been done. The one-electron correlation diagrams have proved to be very useful in obtaining a qualitative idea of the behavior of the lower levels, but at the present state of the art a quantitative description based on relativistic many-electron correlation diagrams is indispensable. This is especially true since the main interest now has shifted towards *really*

heavy ion collisions because at present the transiently formed system during the collision offers the only way to investigate superheavy quasiatoms where many interesting phenomena are expected to occur.¹⁰

As an example we shall discuss the system I-Au with a combined charge of $Z = 132$ where the first superheavy quasiatomic M x rays have been observed.³ In Fig. 1 we show the result of our nonrelativistic *ab initio* molecular Hartree-Fock calculation for this very heavy system using the program BISON¹¹ which originally was developed for large distances and normal diatomic molecules. The basis set used in the calculation had to be investigated for these heavy atoms. Figure 2 presents the correlation diagram of the same system and the same number of electrons after the correction due to the relativistic effects.

This diagram shows two significant features which are of general importance in very heavy systems. First, because of the interchange of the $2s_{1/2}$ and $2p_{1/2}$ levels in the heavy combined system, there is not even a diabatic crossing of these two levels at every distance. The closest energetical approach of these two levels at $R = 0$ in our case is about 3 keV but increases strongly for even heavier systems. This means that the importance of rotational coupling of these states, which is a mechanism for the creation of a K hole at smaller Z , decreases strongly. Therefore, it

is impossible via this mechanism to bring a hole into the innermost shell, even after multiple collisions. Second, the $3d$ level of the combined system, which is the hole or unoccupied state in the experiment when one observes the quasiatomic M x rays from this system, has a flat wide minimum (which in principle already is explained within the promotion model of Fano and Lichten) at about 0.05 a.u. thus leading to x-ray transitions which are nearly constant in energy even with changing internuclear distance. This is very important because it explains the fact that one observes a peak in the I-Au experiment⁴ instead of a quasicontinuum, which is observed in all other experiments⁵ looking for quasiatomic x rays. This peak-structure behavior is not expected to change even if more than twenty electrons fill the system. What changes with the number of electrons in the system is the extension of the $3d$ minimum. This may be one reason why the cross section of the observed molecular-orbital x rays is much larger than deduced from one-electron correlation diagrams. This also may partially explain why this molecular-orbital x-ray line decreases in intensity for larger energies where the degree of ionization increases and thus the width of the $3d$ minimum decreases.

The number of twenty electrons was chosen on the one hand because of the large computer time required as well as the synopsis of the diagram.

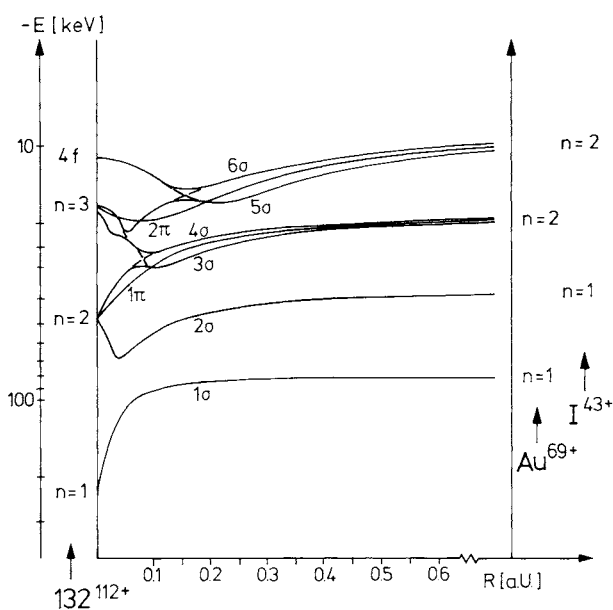


FIG. 1. Nonrelativistic *ab initio* correlation diagrams for the system I-Au (20 electrons).

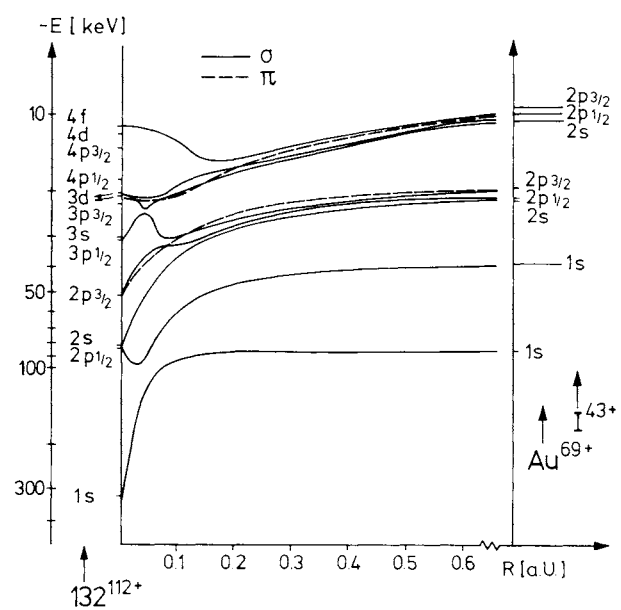


FIG. 2. Relativistic many-electron correlation diagram for the system I-Au (20 electrons) constructed from Fig. 1 including the relativistic effects.

On the other hand, the degree of ionization during the collision is expected to be very high. Using the considerations of the promotion model as well as the experimental experience, the transiently formed I-Au system may possibly possess only as few as forty electrons for high incident energy at the moment of the closest approach.

To give a feeling of the order of magnitude and the importance of the relativistic effects as well as the screening, which are the two physical effects most important in the region of the heavy and superheavy atoms, we show in Fig. 3 the position of the electron levels for nonrelativistic and relativistic, one-electron and many-electron, Hartree-Fock atomic calculations¹² of the combined system I-Au. Only for the lowest level, the 1s state, the shift due to the relativistic effects is of the same order of magnitude or larger than the screening. All other s levels are also strongly shifted to lower energies and together with the strong spin-orbit splitting of the p levels the s and $p_{1/2}$ levels become separated from the levels with the same main quantum number. However, for the outer levels the effect of the screening is large and complicated. For example, the 3d level shifts from about 26 to 10 keV in the two nonrelativistic calculations. One would expect that the relativistic effects increase the bonding, but because of the so-called indirect relativistic effect, which again is an effect of the screening in many-electron atoms, the bonding is not increased but again decreased.

This consideration shows that an attempt to obtain relativistic many-electron correlation diagrams (as long as *ab initio* relativistic molecular Hartree-Fock calculations are not available) should be done by calculating nonrelativistic correlation diagrams which then have to be corrected for relativistic effects. The relativistic corrections in Fig. 2 were incorporated in the following way. For the two extreme cases in the correlation diagram, the united- and separate-atom limits, we do, of course, know the exact results. For the intermediate region we get a good scaling by comparing the exact nonrelativistic and relativistic one-electron calculations and taking into account an assumption of the indirect relativistic effect which we know very well from atomic Dirac-Fock calculations.¹²

We conclude that it is very important to have as exact correlation diagrams as possible. The procedure used here, which yields already very different but much more realistic correlation diagrams than the ones used before, is a step in

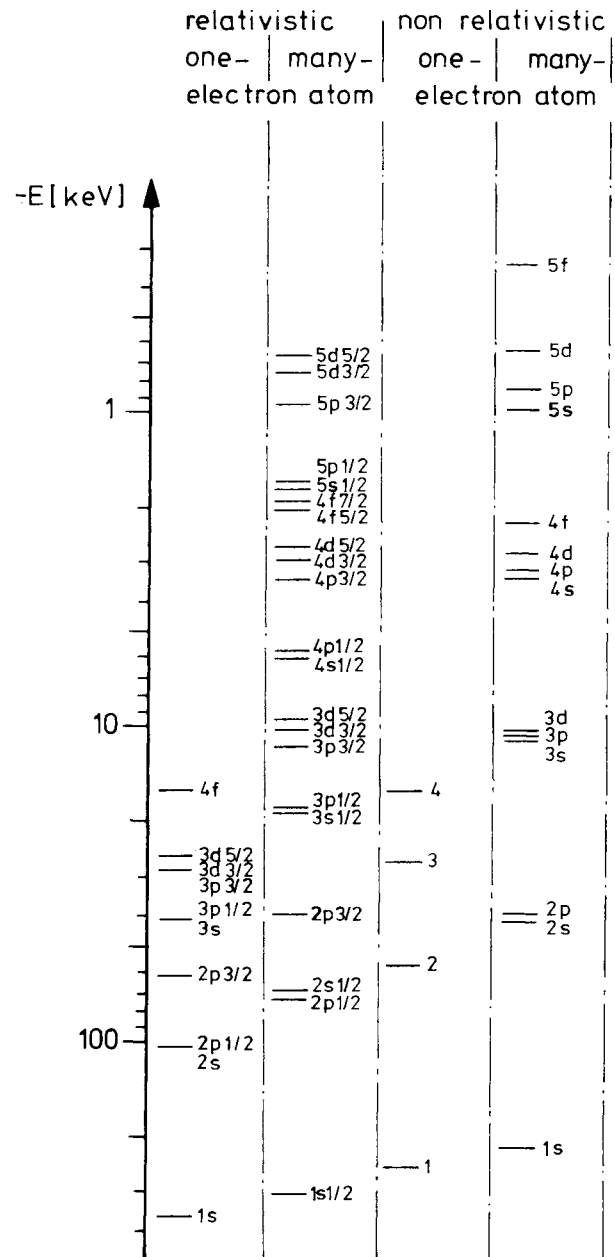


FIG. 3. A comparison of the levels of the system $Z = 132$ (the combined system of I-Au) using nonrelativistic and relativistic, one-electron and many-electron, atomic calculations. The hydrogenic values, which are used in the one-electron correlation diagrams, are shown only as a reference to see the magnitude of the relativistic and screening effects.

this direction. The main hope is to extract from the comparison of the experimental results and the theoretical correlation diagrams information on the levels of the combined system. This is very important for very heavy systems because of the possible large additional energetic correc-

tions due to the self-energy, vacuum polarization, magnetic interaction, and retardation. Nearly all of these corrections have been calculated by expansions in terms of the parameter $Z\alpha$, but experiments are already being conducted in the region where $Z\alpha > 1$. This is a great challenge to the theory. An approach to *ab initio* relativistic many-electron molecular Hartree-Fock calculations is under way.

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