RELATIVISTIC MANY-ELECTRON SCF CORRELATION DIAGRAM FOR Pb-Pb

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Correlation diagrams play an important role in the physical understanding and interpretation of colliding atomic systems. In the case of high-energy heavy-ion collisions they have amply shown their validity, as - for examples - in calculation of the well-known $2p_\pi$-$2p_\sigma$ rotational coupling[1], interpretation of MO x-rays[2], or just the empirical connection of anisotropy maxima in the MO x-rays and minima in the correlation diagram[3-4]. With a discrete variational method[5] we have developed a special program to calculate diatomic molecules in a fully relativistic regime, using numerical atomic Dirac-Fock-Slater basis functions of the two colliding atoms as well as of the Z-united atom at the center of gravity. After pre-diagonalization we are able to calculate, with a self-consistent charge procedure, correlation diagrams of very heavy systems. In Figure 1 we present the correlation diagram of Pb on Pb with 96 electrons. A careful comparison with the one-electron correlation diagram given by Kirsch et al[6] shows a number of significant differences and physically important changes:

(a) Even the strongest bound electronic levels are considerably screened. At R = 50fm the binding is lower by 8% for the $1(1/2)_g$, 25% for the $1(1/2)_u$ and 40% for the $3(1/2)_g$ level. By R = 500fm these changes become respectively 13%, 34% and 50%.

(b) Due to the change in screening at small internuclear distances the lowest levels, which correlate to j = 1/2 atomic levels, decrease even steeper at $R \to 0$ when compared with the one-electron correlation diagram.

(c) The $1(1/2)_u$ level (which non-relativistically is called $2p\sigma$) shows a very pronounced minimum at R ≈ 2000fm, the energy eigenvalue being about 120keV. This minimum does not exist in the one-electron correlation diagram given by Kirsch et al[6]. It shows only a region where the $2p_\sigma$ level is relatively constant in energy. This clear minimum in the many-electron correlation diagram is very important since Stoller et al[7] observe an anisotropy maximum near 130 keV in Pb-Pb collisions. According to the interpretation given by Gippner et al[3] and Stoller et al[4] such anisotropy maxima are strongly correlated with the minima in the correlation diagram. The existence of the $2p_\sigma$ minimum is therefore a strong support for this interpretation, which seems also to be valid in the region of such heavy systems.

(d) At small internuclear distances, of ~ 500fm, our many-electron correlation diagram shows pronounced minima for many levels correlating with atomic levels with j > 1/2.

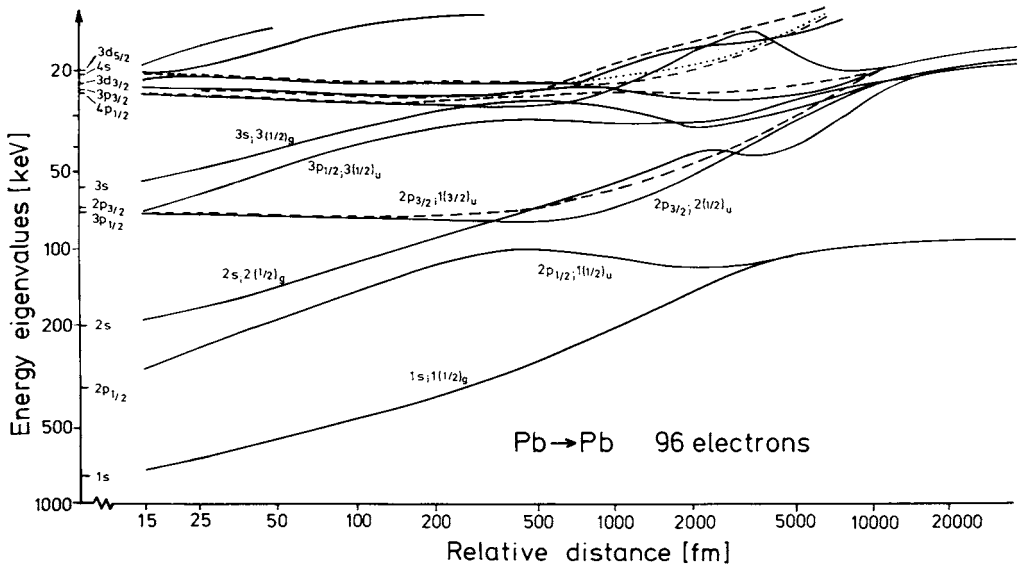

Fig. 1 Self-consistent-charge relativistic Dirac-Fock correlation diagram for Pb on Pb with 96 electrons. The levels are classified on the left according to the Z-united atomic notation; while on the curve the relativistic molecular nomenclature is indicated.

(e) The 'forbidden' crossing between the $1(1/2)_u$ and $2(1/2)_u$ levels is located at R ≈ 500fm with an energy difference ΔE ≈ 20keV. The corresponding values from the 1-electron correlation diagrams are R ≈ 700fm and ΔE ≈ 35keV. A coupled-channel calculation shows an increase of up to nearly an order of magnitude of the hole transfer when going from the one-electron levels to the level-structure in Figure 1.

(f) Due to the strong increase in binding energy for all levels correlating with atomic levels with j = 1/2 at very small internuclear distances, a non-negligible proportion of holes could be transferred from the M-shell via the L-shell into the K-shell of Pb atoms in a single collision process. This is possible due to radial coupling between the $3(1/2)_u$ level and the levels correlating with the M-shell. At very small distances the holes can be transferred from the $3(1/2)_u$ level to the $2(1/2)_u$ and $1(3/2)_u$ levels by respectively radial and rotational coupling. Finally, the crossing between the $2(1/2)_u$ and $1(1/2)_u$ levels as discussed in (e) will allow a large hole transfer into the K-shell of Pb. This coupling increases for even heavier systems because of the increase of the $3p_{1/2}$ Z-united binding. This may be a possible explanation for the unexplained increase of the $1s_\sigma$ ionization in the system Pb-Cm[8].

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