RELATIVISTIC CALCULATIONS OF SUPER HEAVY QUASI-MOLECULES

W.-D. Sepp and B. Fricke

Physics Department, University of Kassel
D-35oo Kassel, Federal Republic of Germany

Correlation diagrams play an important role in the interpretation of electronic inner shell excitation processes in near adiabatic heavy ion collisions. Two main conditions must be met in the calculation of super heavy quasi-molecules: (i) Since inner shell electrons of heavy atomic systems are involved in the excitation process the problem has to be solved fully relativisticly; (ii) Since the electronic clouds of the two colliding ions (or atoms) strongly overlap all electrons have to be included in order to get the correct electronic screening.

The Dirac-Fock-Slater (DFS) molecular electronic wavefunctions are expanded in (numerically calculated) atomic DFS-wavefunctions of the colliding partners. The advantages of this approach are threefold: (i) The basis states are physically adapted to the quasi-molecular problem; (ii) The basis states are practically orthogonal to the molecular negative energy solutions so we have no 'Brown-Ravenhall' type of disease; (iii) Only a limited number of basis states (typically 5o AO's for a heavy system like Pb-Pb) are needed. Thus the dimensions of the Overlap and Fock matrices are relatively small. The calculation of the Overlap and Fock matrices is done with the Discrete Variational Method (DVM)[1].

Various heavy systems have been calculated[2].

REFERENCES

1. See for the general method: A. Rosén and D.E. Ellis, 1975, J.Chem.Phys. 62, 3o39
2. See e.g.: T. Morović, W.-D. Sepp, and B. Fricke, 1982, Z.Phys. A3o4, 79