Pressure Ionization in Partition Function Algebra for Super-Configuration codes

MICHEL BUSQUET, ARTEP, Inc — The phrase “Pressure Ionization” stands for the progressive disappearance, delocalization or hybridization of bound orbitals of atoms immersed in plasmas when density increases. In the ion cell framework, Pressure Ionization is already partly included as orbitals disappear above some density when the one electron energies turns positive or equivalently when the average orbital radius becomes larger than the ion cell radius. However, this simple description yields a non-physical steep variation (with density) of the average $<Z>$ when a whole electron shell vanishes at once. To overcome this problem, several authors proposed to introduce “PIES” (pressure ionized effective statistical weights) $g^* = g \times \pi^*$ in order to obtain a progressive disappearance of the orbitals.

On the other hand, super-shells and super-configurations and partition functions algebra have been introduced by A.Bar-Shalom et al.[1] for a statistical but detailed description of multi-electron, multi-ionized atoms. We present a method that merges pressure ionization and partition functions algebra. We also try to explain why both ionization potential lowering and reduction of statistical weights have to be introduced. A couple of results are presented.


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