Treatment of the hole states in CI+MBPT method

The particle-hole formalism allows more efficient treatment of the states with more-than-half filled shells. It is particularly useful for almost filled shells with not more than one hole. General MBPT formalism for states with valence particles and holes is well known [1]. Explicit expressions for the particle-hole and particle-particle-hole cases were derived in Refs. [2, 3] respectively. For the former case we can define effective Hamiltonian which includes only one-body (Σ_1) and two-body (Σ_2) types of corrections. In the latter case there is, strictly speaking, also three-body term Σ_3. This term is usually small [4] and we can still use the same form of the effective Hamiltonian, as for particle-hole case.

Generalization of the CI+MBPT approach to the systems with holes requires certain modifications. The main problem here is avoiding of double counting. In this method we divide the whole Hilbert space into valence subspace P and complementary subspace Q. It is assumed that there is energy gap between subspaces P and Q. In the valence subspace we use direct diagonalization of the effective Hamiltonian, while in the subspace Q we use perturbation theory. This way we account for all possible interactions in the system and avoid double counting. In the standard CI+MBPT approach valence subspace is defined as no-holes subspace. Respectively, the complementary subspace Q includes all basis states with at least one hole. Conventional MBPT expressions remain practically unchanged for such definition of the valence space: we simply exclude all terms which do not have holes in intermediate states. Below we will call this standard rule.

If the energy gap between core and valence shells is small, we may want to treat some hole states non-perturbatively. Thus, we include them in the valence space P. Now we need to use more complicated rules to exclude these states from MBPT expressions. It may be difficult to formulate such rules for the general case. However, it can be done for the specific case of one electron above the core (Yb^+). Here valence space includes one-particle states and particle-particle-hole states (States with more than one hole lie high and can be treated perturbatively). That means that two-body terms in the Hamiltonian appear only for states with one hole. Therefore, when we calculate matrix elements of Σ_2 for two particles we use standard rule (at least one hole in intermediate states). As long as there is one more hole spectator, such configurations belong to subspace Q. When we calculate particle-hole matrix elements we require either two holes in intermediate states, or one hole from the inner core shells, which are not included in the valence space (non-standard rule). Particle matrix elements of Σ_1 have to be calculated in two ways: standard rule apply for configurations with one hole and non-standard rule for configurations without holes. Hole matrix elements of Σ_1 are always calculated with non-standard rule formulated above. The number of matrix elements for Σ_1 is much smaller, than for Σ_2, so this doubling of matrix elements will not lead to significant increase in calculational costs.

References

[1] I. Lindgren and J. Morrison, *Atomic many-body theory*, vol. 13 of *Springer series in Chemistry Physics* (Springer-Verlag, Berlin, 1982).

[2] E. Avgoustoglou, W. R. Johnson, D. R. Plante, J. Sapirstein, S. Sheinerman, and S. A. Blundell, Phys. Rev. A **46**, 5478 (1992).

[3] U. I. Safronova, W. R. Johnson, M. S. Safronova, and J. R. Albritton, Phys. Rev. A **66**, 042506 (2002).

[4] V. A. Dzuba, V. V. Flambaum, and M. G. Kozlov, Phys. Rev. A **54**, 3948 (1996).