An "Effective Hamiltonian" for quasi-degenerate many-body perturbation theory

by

M. N. GITARI MUGAMBI

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ABSTRACT

The Quasi-degenerate Rayleigh - Schrodinger

Perturbation Theory (QD - RSPT) is presented using
an effective operator formalism. The theory is
then applied in the investigation of diagonal
matrix elements that arise at third-order for a
two valence-electron system.

The core-valence separation is shown explicitly up to third-order and the Exclusion Principle Violating remainders carefully analysed.

Cancellation of unlinked folded diagrams is also investigated.