Abstracts of Australasian PhD Theses

Quantum mechanics and many-body problems. Effective operators in atomic energy level Z-expansion calculations

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Rajnak and Wybourne's effective operators are generalized to degenerate ground configurations l^N and $l'^4 l' l^{N+2}$ as well as by removing the assumption of a Hartree-Fock basis. Explicit calculation of discrete radial integrals and energy denominators permits calculation of the discrete part of E_2 in Layzer's Z-expansion. Specific application is made to the carbon isoelectronic sequence. Ground state energies obtained are not as low as Hartree-Fock values, but term structure prediction is better. Continuum contributions are estimated to be fifteen percent of E_2.

First and second-order fine structure calculations are too large. Reasons why third-order is expected to be important are given.

The possibility of Z-expansions with non-hydrogenic basis is considered.

References

[1] David Layzer, "On a screening theory of atomic spectra", *Ann. Phys.* 8 (1959), 271-276.

[2] K. Rajnak and B.G. Wybourne, "Configuration interaction effects in ℓ^N
       configurations", *Phys. Rev.* 132 (1963), 280-290.

[3] K. Rajnak and B.G. Wybourne, "Electrostatically correlated spin-orbit
       interactions in ℓ^N-type configurations", *Phys. Rev.* 134A (1964),
       596-600.