

# 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  $l^{4l}l^{N+2}$  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.

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Received 10 October 1972. Thesis submitted to the University of Canterbury, July 1972. Degree approved, September 1972. Supervisor: Professor B.G. Wybourne.

- [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.