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A NOTE ON THE JEZIORSKI–PIELA PERTURBATION THEORY

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The general solution for the operator T in the Jeziorski-Piela Perturbation Theory is indicated.

Rayleigh-Schrödinger type perturbation methods for dealing with intermolecular forces were developed by Jeziorski and Piela [1, 2]. One of the important ingredients in their approach is the operator T, (we follow the notation of Refs. [1] and [2]), which is used to divide AH into properly symmetrized $\mathscr{H}_0$ and $\mathscr{V}$. An explicit construction for T is given in Eq. (29) of Ref. [1]. This construction involves an orthonormalization process in the subspace of proper symmetry [1]. In the present note we would like to point out an alternative and simpler method of constructing the operator T. To this effect, we note that whereas T is given in Ref. [1] by Eq. [29], the really important properties of T and the only ones used in the definiton of $\mathscr{H}_0$ and $\mathscr{V}$ are the properties embodied in Eqs. (30)–(32) of Ref. [1]:

$$ST = S, \quad TS = T \tag{1}$$

$$TA = T \quad TQ = 0 \tag{2}$$

$$AT = S \tag{3}$$

$$QT = 0. \tag{4}$$

The operators A, S and Q are defined in [1] and satisfy

$$A^2 = A = A^\dagger \tag{5}$$

$$Q^2 = Q = Q^\dagger \tag{6}$$

$$S^2 = S = S^\dagger = A - Q = AS = SA \tag{7}$$

$$QS = SQ = 0 \tag{8}$$

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It is easy to see (e. g., by using the diagonal representation for S), that the general solution T of Eqs. (1) may be written in the form

$$T = S+(1-S)PS, \tag{9}$$

where P is an arbitrary operator. In view of Eqs. (7) and (8) it is obvious that T of Eq. (9) also satisfies automatically Eq. (2). On the other hand, it cannot satisfy Eqs. (3) and (4) without some specification of the hitherto arbitrary operator P.

It follows from Eqs. (7) that if we satisfy Eq. (4), then Eq. (3) will also be satisfied (and vice versa). We therefore attempt to solve Eq. (4) using the form (9) for T. In view of Eqs. (8), it reduces to

$$QT = QPS = 0. \tag{10}$$

This is an equation for the operator P, which can be solved as

$$P = (1-Q)R, \tag{11}$$

where R is an arbitrary operator. We further note that as a consequence of Eqs. (7) and (8),

$$(1-S)(1-Q) = (1-A). \tag{12}$$

Therefore the general solution for T satisfying Eqs. (1)–(4) is

$$T = S+(1-A)RS, \tag{13}$$

where R is arbitrary and may be used to improve the convergence of the perturbation series.

REFERENCES

[1] B. Jeziorski, L. Piela, *Acta Phys. Pol.* **A42**, 177 (1972).
[2] L. Piela, B. Jeziorski, *Acta Phys. Pol.* **A42**, 185 (1972).