Comments on properties of projected spectra

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We note that $\alpha_{10} = \alpha_{20}$ and we have one of the functionals first given by Wright and Scadron (1964) and α_{30} is the other functional given by these authors.

A detailed study of the properties of these sequences and their applications to quantum scattering theory is in progress and will be reported in due course.

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NEWTON, R. G., 1966, *Scattering Theory of Waves and Particles* (New York: McGraw-Hill).
WRIGHT, J. A., and SCADRON, M., 1964, *Nuovo Cim.*, **34**, 1571–81.

Comments on properties of projected spectra

Abstract. Arguments are presented leading to the rejection of the result of Warke and Gunye that the energies of eigenstates of angular momentum $\boldsymbol{J}^2$, projected from a Hartree–Fock state which is an eigenstate of J_z, are monotonic in J.

In Hartree–Fock calculations for light nuclei one frequently employs a solution Ψ which is an eigenstate of J_z:

$$J_z\Psi = K\Psi$$

but not of $\boldsymbol{J}^2$. The physical states are obtained by projecting from Ψ the eigenstates ϕ_I of $\boldsymbol{J}^2$, where

$$\Psi = \sum_I a_I\phi_I.$$

In what follows we take $K = 0$ and so have only even values of I. This is the case most frequently studied. In practice it is found that when $I_2 > I_1$, $E_{I_2} > E_{I_1}$. Warke and Gunye (1967) claim that this is a necessary consequence of having $E_0 < E_{\mathrm{HF}}$, that is to say that, if the energy of the projected state with $I = 0$ is less than the Hartree–Fock energy, then E_I is a monotonic increasing function of I.

The first step in their argument is to show that the sign of $E_{I_2} - E_{I_1}$ (for $I_2 > I_1$) is always the same. We show that this has not been proved. We may note that the monotonicity result, if true, would be of some interest. For example, it would indicate that the spectrum retains some qualitative resemblance to a rotational spectrum, and also could be a possible way of criticizing an approximate projection method, by requiring it to give this result.

The starting point in the argument uses the product projection operator (Löwdin 1964)

$$P_{I_1} = \frac{\prod\limits_{i\neq 1}\{J^2 - I_i(I_i+1)\}}{\prod\limits_{i\neq 1}\{I_1(I_1+1) - I_i(I_i+1)\}}. \tag{1}$$

For any particular Ψ the range of i values will be finite, up to n say. Using (1) one may write

$$E_{I_2}-E_{I_1} = \{I_2(I_2+1)-I_1(I_1+1)\}\frac{N}{D} \tag{2}$$

where N and D are functions of I_1 and I_2 defined in terms of expectation values $\langle\rangle$ in the state Ψ, namely

$$N = \langle H\alpha\rangle\langle J^2\alpha\rangle - \langle HJ^2\alpha\rangle\langle\alpha\rangle$$

and

$$D = \{\langle J^2\alpha\rangle - I_1(I_1+1)\langle\alpha\rangle\}\{\langle J^2\alpha\rangle - I_2(I_2+1)\langle\alpha\rangle\}$$

where the operator α is

$$\alpha = \alpha(1,2) = \prod_{i\neq 1,2}\{J^2-I_i(I_i+1)\}.$$

It is stated that the fact that Ψ is not an eigenstate of H or J^2 leads to the consequence that N cannot be zero, and therefore $E_{I_2}-E_{I_1}$ will not vanish for $I_2 \neq I_1$; thus E_I is either an increasing or a decreasing function of I.

But, since N is a function of discrete variables I_1 and I_2, the fact that N cannot be zero does not imply that N cannot change sign.† Nor has anything been said to show that D cannot change sign. In fact, examination of D shows that for fixed I_1 the sign of D changes with each step $I_2 \to I_2+2$. For one can readily see that

$$\langle\alpha\rangle = a_{I_1}{}^2\prod_{i\neq 1,2}\{I_1(I_1+1)-I_i(I_i+1)\}+a_{I_2}{}^2\prod_{i\neq 1,2}\{I_2(I_2+1)-I_i(I_i+1)\}$$

and that $\langle J^2\alpha\rangle$ has two similar terms, each with an additional factor $I_1(I_1+1)$ or $I_2(I_2+1)$. Hence

$$D = -\{I_1(I_1+1)-I_2(I_2+1)\}^2 a_{I_1}{}^2 a_{I_2}{}^2\prod_{i\neq 1,2}\{I_1(I_1+1)-I_i(I_i+1)\}$$
$$\times\prod_{i\neq 1,2}\{I_2(I_2+1)-I_i(I_i+1)\}. \tag{3}$$

Let us now consider fixed I_1 and $I_2 > I_1$. Then, as $I_2 \to I_2+2$, only the last product in (3) can change sign. It contains $n-\frac{1}{2}I_2$ negative terms, of which the first

$$I_2(I_2+1)-(I_2+2)(I_2+3)$$

is replaced when $I_2 \to I_2+2$ by the positive term $(I_2+2)(I_2+3)-I_2(I_2+1)$. So sign changes are bound to occur in D. Further, we note that evaluation of N, in the manner leading to equation (3) for D, can only lead back to equation (2).

We conclude that it has yet to be proved that the projected spectra must be monotonic in I.

In a later paper (Warke and Khadkikar 1968) justification is sought for a phenomenological expression, derived from (2),

$$E_{I_2}-E_0 = \frac{A(I_2)I_2(I_2+1)}{1-BI_2(I_2+1)}. \tag{4}$$

It is stated that, in (4), B can be treated as only weakly dependent on I_2. B is defined as the ratio, evaluated for $I_1 = 0$, of $\langle\alpha\rangle$ to $\langle J^2\alpha\rangle$. Insensitivity to I_1 or I_2 in expressions such as $\langle\alpha\rangle$ is stated to be likely if all I_i are equally represented in Ψ. We take

† This point has also been made by H. A. Lamme (private communication). An example of non-monotonic behaviour is to be found in work by Lamme and Boeker (1969).

this to mean that B is expected to be least sensitive to I_2 when all a_I are equal and $I_n \gg I_2$. However, we find, taking $a_0 = a_2 = a_4$ and $I_n = 20$, that the ratio of values of B for $I_2 = 2$ and $I_2 = 4$ is about $-9{\cdot}5$.

It thus appears that any use of equation (2) to derive qualitative properties of the projected spectrum is risky.

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Lamme, H. A., and Boeker, E., 1969, *Nucl. Phys.*, **136,** A609–23.
Löwdin, P.-O., 1964, *Rev. Mod. Phys.*, **36,** 966–76.
Warke, C. S., and Gunye, M. R., 1967, *Phys. Rev.*, **155,** 1084–9.
Warke, C. S., and Khadkikar, S. B., 1968, *Phys. Rev.*, **170,** 1041–6.