Sequences of functionals for the evaluation of eigenvalues of the Lippmann-Schwinger kernel

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Letters to the Editor

Sequences of functionals for the evaluation of eigenvalues of the Lippmann–Schwinger kernel

Abstract. Three sequences of functionals which are stationary at the eigenvalues of the Lippmann–Schwinger kernel are constructed. In addition to providing estimates of the eigenvalues, variations of these functionals also provide approximations to the eigenvectors and some interesting transforms of the eigenvectors.

The evaluation of the eigenvalues of the Lippmann–Schwinger kernel is of considerable importance in quantum scattering theory, particularly in the study of resonances (see, for example, Newton 1966). If $\hat{H}_0 + \lambda\hat{H}_1$ is the Hamiltonian of a quantum system and if E is its total energy, then the Lippmann–Schwinger kernel $\hat{K}$ is given by

$$\hat{K} = \frac{\hat{H}_1}{E'-\hat{H}_0} = \hat{G}_0\hat{H}_1 \tag{1}$$

where

$$E' = E \pm \mathrm{i}\epsilon \tag{2}$$

ϵ being an arbitrarily small real positive quantity which assures the existence of $\hat{K}$ near the given energy.

Three sequences of functionals have been constructed such that each functional is stationary at the eigenvalues of $\hat{K}$. The stationary values are, in general, neither maxima nor minima. A variation of these functionals provides not only the estimates of the eigenvalues, but also those of the eigenvectors $\psi(E)$ and some interesting transforms of the eigenvectors such as $\hat{G}_0{}^{\pm n}\psi(E)$ and $\hat{H}_1{}^{-n}\psi(E)$ for positive integral values of n. Since it is easy to verify that the claims made in this paragraph are correct, it is sufficient to reproduce the expressions for the sequences; they are, for $n = 0, 1, 2, \ldots,$

$$\alpha_{1n}(\chi) = \frac{\langle\chi|\hat{G}_0{}^{-n}\hat{H}_1\hat{G}_0{}^{-n}|\chi\rangle}{\langle\chi|\hat{G}_0{}^{-(2n+1)}|\chi\rangle} \tag{3}$$

$$\alpha_{2n}(\chi) = \frac{\langle\chi|\hat{H}_1{}^{2n+1}|\chi\rangle}{\langle\chi|\hat{H}_1{}^{n}\hat{G}_0{}^{-1}\hat{H}_1{}^{n}|\chi\rangle} \tag{4}$$

and

$$\alpha_{3n}(\chi) = \frac{\langle\chi|\hat{G}_0{}^{n}\hat{H}_1\hat{G}_0\hat{H}_1\hat{G}_0{}^{n}|\chi\rangle}{\langle\chi|\hat{G}_0{}^{n}\hat{H}_1\hat{G}_0{}^{n}|\chi\rangle}. \tag{5}$$

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)

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