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A NOTE ON THE USE OF A CONTINUED FRACTION FOR PERTURBATION THEORY

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ABSTRACT. An implicit eigenvalue-eigenvector problem usually solved using perturbation theory is shown to lead to a nonperturbation solution in terms of a continued fraction.

In this note we summarize a method to obtain a nonperturbative solution to the implicit eigenvalue-eigenvector problem arising in nonrelativistic quantum mechanics [1]:

$$(1) \qquad [E - e - t(E)P_0]\ |\alpha\rangle = 0.$$

In equation (1), $t(E)$ is a linear operator in the Hilbert space spanned by the discrete eigenfunctions of the operator H_0 and $t(E)$ satisfies

$$(2) \qquad t(E) = V + VT_0(E)t(E).$$

In equation (2), $T_0(E) = Q_0(E - H_0)^{-1}$ and $P_0 + Q_0 = 1$, $P_0{}^2 = P_0$, $Q_0{}^2 = Q_0$ and $P_0|\alpha\rangle = |\alpha\rangle$, $Q_0|\alpha\rangle = 0$. Now if we solve equation (2) for $t(E)$ we obtain

$$(3) \qquad t(E) = V^{1/2}(1 - V^{1/2}Q_0(E - H_0)^{-1}V^{1/2})^{-1}V^{1/2}.$$

By inspection of the expression for t in equation (3) we see that tP_0 can be expressed as the composition of two successive linear fractional transformations of operator argument:

$$(4) \qquad \begin{aligned} \mathcal{T}_0(U) &= V^{1/2}(1 - U)^{-1}V^{1/2}P_0 \\ \mathcal{T}_1(U) &= V^{1/2}Q_0(U - H_0)^{-1}V^{1/2}. \end{aligned}$$

On the other hand by using the Cauchy formula and multiplying on the left by $\langle\alpha|$ equation (1) may be transformed into

$$(5) \qquad \langle\alpha|E - e - \frac{1}{2\pi i}\oint \frac{t(\epsilon)P_0\, d\epsilon}{\epsilon - E}|\alpha\rangle = 0.$$

The contour includes the eigenvalue E. If we then introduce an equivalent operator h such that $E|\alpha\rangle = (e + h)|\alpha\rangle$, then equation (5) may be written as

$$(6) \qquad \langle\alpha|E - e - \frac{1}{2\pi i}\oint \frac{t(\epsilon)P_0 d\epsilon}{\epsilon - e - h}|\alpha\rangle = 0.$$

This equation will be satisfied if

$$h = \frac{1}{2\pi i} \oint \frac{t(\epsilon) P_0 \, d\epsilon}{\epsilon - e - h} . \tag{7}$$

Now equation (7) together with relations (4) defines a positive definite continued fraction of operator argument [2] under suitable conditions on V and T_0. The study of such continued fractions leads to the development of conditions for the successive approximants of the continued fraction to bracket the limiting value. Instead of our using this theory directly, it has been found easier to use the fact that the operator h satisfies the equation [3]

$$t(e) T_0(e) V^{-1} h^2 + h = t(e) P_0 \tag{8}$$

This quadratic equation may be solved for h by iteration using as a starting estimate $h_0 = t(e) P_0$ and setting

$$\begin{aligned} h_{n+1} &= (1 + t(e) T_0(e) V^{-1} h_n)^{-1} t(e) P_0 \\ &\equiv (1 + B h_n)^{-1} A. \end{aligned} \tag{9}$$

Thus

$$h = (1 + B(1 + B(1 + B(1 + \cdots)^{-1} A)^{-1} A)^{-1} A)^{-1} A; \tag{10}$$

h is therefore expressed by a harmonic continued fraction. A proof of the convergence in the norm of the recursive process of equation (9) has been constructed by modifying the work of McFarland [4].

If we write $V = \lambda V$ then the expansion of the continued fraction for h in a power series in λ yields the familiar Rayleigh-Schrödinger perturbation series. The method described above has been extended to the degenerate case, the time dependent perturbation problem, the general implicit eigenvalue-eigenvector problem and to the solution of the Fredholm equation in terms of a continued fraction. In numerical experiments thus far conducted the continued fraction converges significantly faster than any power series [3].

References

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