The triple problem of convergence in the perturbation expansions with non-diagonal propagators

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THE TRIPLE PROBLEM OF CONVERGENCE IN THE PERTURBATION EXPANSIONS WITH NON-DIAGONAL PROPAGATORS;

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Let us consider the standard perturbation theory of the Rayleigh-Schrödinger type, with the Hamiltonian split

$$H = H_o + g H_1 \qquad /1/$$

and pair of ansatzs

$$E = E_o + g E_1 + g^2 E_2 + \dots .$$
$$|\psi\rangle = |\psi_o\rangle + g|\psi_1\rangle + \dots . \qquad /2/$$

Their insertion in the Schrödinger equation $H|\psi\rangle = E|\psi\rangle$ leads to a RS hierarchy of relations

$$H_o |\psi_o\rangle = E_o |\psi_o\rangle \qquad /3/$$

and

$$H_o|\psi_k\rangle + H_1|\psi_{k-1}\rangle = E_o|\psi_k\rangle + \dots + E_k |\psi_o\rangle \qquad /4/$$

with k = 1, 2, ...

In a textbook spirit, we may interpret E_1, E_2, ... as abbreviations,

$$E_1 = \frac{1}{\langle\psi_0|\psi_0\rangle} \langle\psi_0|\left(H_0|\psi_1\rangle + H_1|\psi_0\rangle - E_0|\psi_1\rangle\right), \ldots \qquad /5/$$

and, inserting them in /4/, eliminate formally also the wavefunction corrections,

$$|\psi_1\rangle = \frac{1}{E_0 - H_0}\left(H_0|\psi_0\rangle - E_1|\psi_0\rangle\right), \ldots . \qquad /6/$$

In this way, perturbation theory may be interpreted as a reduction of the full problem to its simplified version /3/.

The "simplicity" of H_0 is usually specified as a possibility of its complete diagonalisation. In the modified RS /MRS/ approach[1], the "simplicity" of H_0 is weakened: in a given "unperturbed" basis $|0\rangle$, $|1\rangle$, ..., we admit all operators $H_0 = T + |0\rangle g \langle 0|$ with a free parameter g and "invertible" matrix T, i.e., with such a matrix that we may obtain also an explicit form of the operator R /with, say, $R = 1/(E_0 - T)$ where E_0 is a function of g/.

The main MRS idea is simple - we have noticed that an explicit knowledge of R and V specifies already all the corrections /5/ and /6/, while a presence of a free parameter g enables us also to get rid of the eigenvalue problem /3/[1]. Indeed, we may write, in an explicit manner,

$$|\psi_0\rangle = R|0\rangle g \langle 0|\psi_0\rangle, \quad \langle 0|\psi_0\rangle \neq 0 \qquad /7/$$

$$g = g(E_0) = 1/\langle 0|R(E_0)|0\rangle .$$

In practice, it is useful to write $g = g(E_0)$ and treat E_0 as a free parameter itself.

There is one important reason for using non-diagonal T in the split /1/ - we may make $H - H_0$ as small as necessary for a good convergence of the expansions /2/. There is a price to be paid of course - we must guarantee a quick practical convergence also in a transition $T \rightarrow R$ and in the corresponding MRS forms of prescriptions /5/ and /6/.

1. The $T \rightarrow R$ convergence.

The simplest way how to define R is a brute-force numerical inversion of the truncated matrices N x N. In Ref.[1], the related $N \rightarrow \infty$ convergence has been reduced to a continued-fractional convergence, by means of a restriction of T´s to tridiagonal matrices. In Ref.[2], this procedure has been extended to 2s+1 - diagonal T´s. An alternative, purely non-numerical type of the $T \rightarrow R$ transition[3] represents one of the possible final solutions of this problem - we may reconstruct any trial T' into an "invertible" one simply by its fixed-point re-arrangement $T' = T +$ corrections. Numerically, this has been illustrated elsewhere[3] - we may only summarize here that there are no problems with the first, $N \rightarrow \infty$ type of convergence in practice, since its "residuum" may simply be incorporated in the perturbation itself.

2. The intermediate-summation convergence.

Each MRS contribution, say, E_k , is defined as a RS-type sum over intermediate states. Each insertion of R represents a single summation in the RS formalism - here, the summation goes over the two /left and right/ indices. The related "additional" convergence problem may again be eliminated in the same manner as above - we may modify the input unperturbed propagator R' /general matrix/ and use its 2t+1 - diagonal part only, $R' \to R^{/t/}$, $t < \infty$. Again, the related modification of $T' \to T^{/t/}$ (= a general matrix now) is, in effect, again a mere re-definition of the perturbation.

The numerical tests of the above idea may again be found elsewhere[4] and illustrate, for the cut-offs t dedreasing from infinity, an emergence of the RS-type asymptotic-series divergence, especially for small t (= 0 or 1). In an opposit setting, the analysis of the $t \to \infty$ limit supports a hypothesis of the MRS convergence - see Table 1 here, which lists the "optimal orders" /giving the optimal asymptotic-series MRS results/for anharmonic oscillators as analysed in Ref.[4].

Table 1. An "optimal order" N_0 as a function of t.

t	0	1	3	5	7
N_0	2	2	4	6	10

3. The numerical indications of the MRS convergence of energies.

For any coupling λ of anharmonicity x^4, we may choose H with another coupling λ_0 as a matrix T. For a broad range of λ's, we obtain results exemplified here in Figure 1.

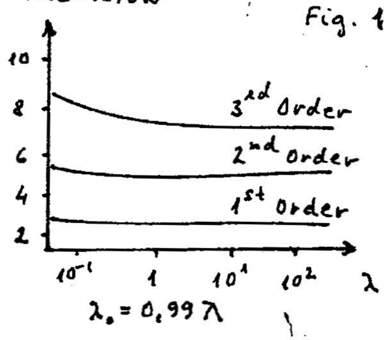

Fig. 1

A similar pattern is obtained also for the very broad range of parameters E_0. For the variable λ_0 we obtain the dependence illustrated here in Figure 2 for $\lambda = 1$.

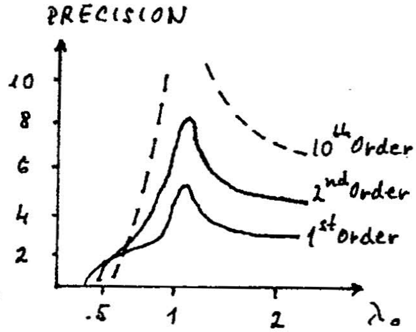

Fig. 2

We may see that the $\lambda_0 < 1$ part of the latter Figure is a curve with an inflection point which is almost order-independent. - We believe that the MRS convergence is very good for $\lambda_0 > \lambda^{(inflection)}$ and conjecture that $\lambda_0^{(inflection)} \leq 1$ is a "natural" boundary of the convergence domain, or at least of a domain of a reliable use of the MRS asymptotic series.

References.

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