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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

$$H = H_0 + g H_1 \quad /1/$$

and pair of ansatzs

$$E = E_0 + g E_1 + g^2 E_2 + \dots$$

$$|\psi\rangle = |\psi_0\rangle + g |\psi_1\rangle + \dots \quad /2/$$

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

$$H_0 |\psi_0\rangle = E_0 |\psi_0\rangle \quad /3/$$

and

$$H_0 |\psi_k\rangle + H_1 |\psi_{k-1}\rangle = E_0 |\psi_k\rangle + \dots + E_k |\psi_0\rangle \quad /4/$$

with $k = 1, 2, \dots$

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

$$E_n = \frac{1}{\langle \psi_0 | \psi_0 \rangle} \langle \psi_0 | (H_0 | \psi_n \rangle + H_1 | \psi_0 \rangle - E_0 | \psi_n \rangle), \dots /5/$$

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

$$| \psi_n \rangle = \frac{1}{E_0 - H_0} (H_0 | \psi_0 \rangle - E_n | \psi_0 \rangle), \dots \quad /6/$$

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/ approach¹, the "simplicity" of H_0 is weakened: in a given "unperturbed" basis $|0\rangle, |1\rangle, \dots$, 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,

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

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

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 $N \times N$. 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 $T \rightarrow R$ transition³ 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 $T' = T + \text{corrections}$. Numerically, this has been illustrated elsewhere³ - 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, $R' \rightarrow R'^t$, $t < \infty$. Again, the related modification of $T' \rightarrow T'^t$ (= 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 elsewhere⁴ and illustrate, for the cut-offs t decreasing from infinity, an emergence of the RS-type asymptotic-series divergence, especially for small t (= 0 or 1). In an opposite setting, the analysis of the $t \rightarrow \infty$ 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_0 's, we obtain results exemplified here in Figure 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 $\lambda = 1$.

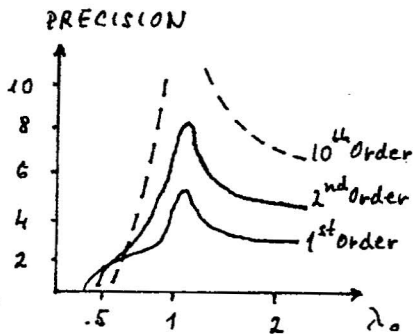


Fig. 2

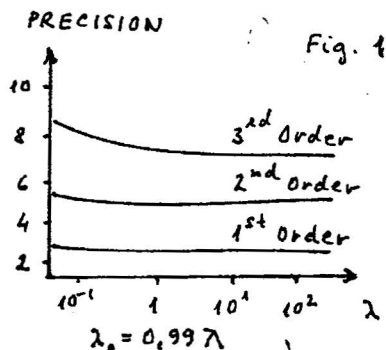


Fig. 1

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 con-

vergence is very good for $\lambda_0 > \lambda^{(\text{inflection})}$ and conjecture that $\lambda_0^{(\text{inflection})} \leq 1$ is a "natural" boundary of the convergence domain, or at least of a domain of a reliable use of the MRS asymptotic series.

Références.

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- /2/ - " - , Dubna, JINR communication E5 - 87 - 634.
- /3/ ibid., E4 - 87 - 655, /4/ ibid., E4 - 87 - 667.