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**PERTURBATION THEORY  
WITH THE MATRIX CONTINUED FRACTIONS**

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## 1. INTRODUCTION

A typical starting point of the various perturbative computations is a physically motivated decomposition of the Hamiltonian

$$H = T + V. \quad (1.1)$$

The pair of components  $T$  and  $V$  should be such that  $V$  is small, i.e.,  $H = T$  is a good zero-order approximation.

In the various systems exemplified by the chain models in the solid-state physics<sup>/1/</sup>, by the polyacetylene molecules<sup>/2/</sup>, etc., the strong-coupling component  $T$  of the Hamiltonian  $H$  has a form of a band matrix with some  $2s+1$  nonzero diagonals,

$$T = \sum_{\substack{m,n=0 \\ |m-n| \leq s}}^{\infty} |m\rangle T_{mn} \langle n|. \quad (1.2)$$

In the standard Rayleigh-Schroedinger (RS) perturbation theory<sup>/3/</sup>, on the contrary, we have to use a diagonal-matrix approximation with  $s = 0$ . Then, the "strong-coupling structure" (1.1) + (1.2) of the Hamiltonian  $H$  may lead to difficulties.

As a typical example, we may recall the anharmonic oscillator

$$H = p^2 + x^2 + \kappa x^4. \quad (1.3)$$

A divergence of the standard RS expansions takes place here<sup>/4/</sup>. This may be related to an inadequacy of the standard  $s = 0$  RS assumption

$$H = H_0 + \lambda H_1. \quad (1.4)$$

with a formal measure of smallness  $\lambda \approx 0$ .

In our preceding papers<sup>/5/</sup>, the simplest nontrivial weakening of the RS assumption  $s = 0$  has been formulated as a tri-diagonality postulate (Eq. (1.2) with  $s = 1$ ). The numerical

tests confirmed the feasibility and convergence of the resulting modified RS formalism. In the present paper, we shall be interested in an extension of these results to  $s > 1$ .

An essence of any  $s > 0$  generalization lies in fact in an evaluation of the unperturbed propagator. Thus, in analogy to the simple  $s = 0$  RS formula

$$R = \sum_{n=1}^{\infty} |n\rangle \frac{1}{E_0 - T_{nn}} \langle n|, \quad (1.5)$$

the  $s = 1$  construction<sup>/5/</sup> preserves a non-numerical character by means of an introduction of the analytic continued fractions. Here, we shall generalize this procedure and describe an analogous analytic solution of the related technical questions for  $s > 1$ .

In Sect. 2, a straightforward though rather formal generalization is described for an arbitrary matrix form of  $T$ . Then, we point out that the assumption (1.2) with some  $s < \infty$  preserves in fact a full analogy with its  $s = 1$  special case. This in fact is an essence of feasibility of our non-numerical specification of the unperturbed propagator  $R$ .

In Sect. 3, the matrix continued fractional (MCF) technique is introduced and described in detail (Sect. 3.1). An efficiency of the resulting "inversion-perturbation" (IP) theory is tested then numerically on the standard example (1.3) (Sect. 3.2).

Section 4 is a summary.

## 2. THE EXTENDED RS PERTURBATION THEORY

### 2.1. The RS Diagonality Restriction

In the textbook spirit<sup>/3/</sup>, the RS formalism may be derived very easily after an introduction of a small variable  $\lambda$  in the Schroedinger equation

$$H|\psi\rangle = E|\psi\rangle, \quad (2.1)$$

via Eq. (1.4). Indeed, an insertion of the asymptotic-series ansatz

$$|\psi\rangle = \sum_{k=0}^N |\psi_k\rangle \lambda^k + O(\lambda^{N+1}), \quad E = \sum_{k=0}^N E_k \lambda^k + O(\lambda^{N+1}), \quad (2.2)$$

converts then the matrix bound-state problem (2.1) into a hierarchy of relations

$$H_0 |\psi_0\rangle = E_0 |\psi_0\rangle, \quad (2.3)$$

and

$$(H_0 - E_0) |\psi_k\rangle + H_1 |\psi_{k-1}\rangle = \sum_{m=1}^k E_m |\psi_{k-m}\rangle \quad k = 1, 2, \dots \quad (2.4)$$

In the standard  $s = 0$  RS context, we may start now from a knowledge of the complete solution of the unperturbed problem (2.3), specify the unperturbed propagator by the formula (1.5) and treat Eq. (2.4) as a recurrent definition of corrections in the final RS solution (2.2)<sup>/3/</sup>.

In all the situations where the  $s = 0$  RS series (2.2) fails to converge, we may still start from some  $s \geq 1$  decomposition (1.1) and try to apply the same philosophy<sup>/5/</sup>, with the operator  $T$  treated again as an unperturbed part of the full Hamiltonian  $H$ , and with an arbitrary choice of the "unperturbed" initial state  $|0\rangle \neq |\psi_0\rangle$ .

### 2.2. An Inversion-Perturbation Formalism

In the first step, a projection operator  $Q = 1 - |0\rangle\langle 0|$  is to be introduced. This enables us to define the unperturbed propagator

$$R = Q \frac{1}{E_0 I - QTQ} Q, \quad (2.5)$$

say, as a numerically defined function of some (arbitrary) unperturbed energy parameter  $E_0$ .

In the  $s = 1$  IP formalism as realised in Ref.<sup>/5/</sup>, we replaced the RS identification of  $H_0$  with  $T$  (in (2.3) and (2.4)) by a more flexible specification

$$H_0 = T + g|0\rangle\langle 0|, \quad \lambda H_1 = V - g|0\rangle\langle 0|. \quad (2.6)$$

This contains a new, separable "Hartree-Fock" field  $g|0\rangle\langle 0|$  with some suitable (presumably small but variable) coupling  $g$ . For  $s > 1$ , Eq. (2.6) will be used in the present paper.

The physical value of  $g$  is to be chosen in a way simplify, say, the unperturbed Eq. (2.3)

$$(T + g|0\rangle\langle 0| - E_0) |\psi_0\rangle = 0. \quad (2.7)$$

After an arbitrary normalisation  $\langle 0 | \psi_0 \rangle = 1$ , we obtain the solution

$$|\psi_0\rangle = |0\rangle + RT|0\rangle \equiv |\phi\rangle, \quad (2.8)$$

if and only if

$$g = E_0 - \langle 0 | T | \phi(E_0) \rangle, \quad (2.9)$$

(cf. also <sup>5/</sup>). This fixed  $g = g(E_0)$  uniquely.

The latter pair of definitions of  $|\psi_0\rangle$  and  $g(E_0)$  represents in effect an elimination of the unperturbed problem (2.3) from the whole formalism. Thus, an IP introduction of the parameter  $g$  in (2.6) may be understood as a "selfconsistent" adaptation of the unperturbed Hamiltonian  $T$  to the a priori chosen value  $E_0$  of the trial energy parameter.

In a partial analogy to the RS theory, the IP unperturbed problem Eq. (2.3) is also satisfied identically. The zero-order IP wavefunction (2.8), on the contrary, acquires here already the structure typical for the higher-order RS wavefunctions.

A systematic construction of all the higher-order IP corrections remains the standard recurrent procedure familiar from its RS predecessor. From the subsequent rows of Eq. (2.4), we obtain

$$\lambda |\psi_1\rangle = R |\chi\rangle, \quad |\chi\rangle = \lambda(V - E_1)|\phi\rangle \quad (2.10)$$

$$\lambda E_1 = (\langle \phi | V | \phi \rangle - g) / \langle \phi | \phi \rangle, \quad \lambda^2 E_2 = \langle \chi | R | \chi \rangle / \langle \phi | \phi \rangle,$$

etc.

### 3. AN ELIMINATION OF NUMERICAL INVERSION IN THE IP FORMALISM

#### 3.1. An Introduction of the Matrix Continued Fractions

A numerical inversion defines  $R$  in Eq. (2.5) for an arbitrary non-diagonal matrix  $T$ . Let us recall now our restriction (1.2) and pay our further attention only to the band matrices  $T$ .

After the denotation

$$\begin{aligned} \langle i | T | j \rangle &= (a_k)_{mn} & i &= (k-1)s + m & j &= (k-1)s + n \\ &= (b_k)_{mn} & i &= (k-1)s + m & j &= ks + n \\ &= (c_{k+1})_{mn} & i &= ks + m & j &= (k-1)s + n \\ & & m, n &= 1, 2, \dots, s & k &= 1, 2, \dots \end{aligned} \quad (3.1)$$

i.e.,  $s \times s$  - dimensional partitioning

$$QTQ = \begin{bmatrix} a_1 & b_1 & & & \\ c_2 & a_2 & b_2 & & \\ & & \dots & & \\ & & c_k & a_k & b_k \end{bmatrix} \quad (3.2)$$

we shall be able to construct the unperturbed propagator  $R$  in a purely algebraic manner.

In the first step, a suitable factorisation of  $E_0 I - QTQ$  into a product of matrices

$$E_0 I - QTQ = UDL, \quad (3.3)$$

will be introduced. Its main aim is to simplify the inversion since  $R = L^{-1} D^{-1} U^{-1}$ .

In terms of elements of the block-diagonal factor

$$D_{ij}^{-1} = (f_k)_{mn} \quad i = (k-1)s + m \quad j = (k-1)s + n \quad m, n = 1, 2, \dots, s \quad k = 1, 2, \dots \quad (3.4)$$

the simple algebra defines already the respective block-two-diagonal upper and lower triangular matrix factors

$$U = \begin{bmatrix} I & -b_1 f_2 & & & \\ & I & -b_2 f_3 & & \\ & & \dots & & \\ & & & I & -b_k f_{k+1} \\ & & & & \dots \end{bmatrix}, \quad L = \begin{bmatrix} I & & & & \\ -f_2 c_2 & I & & & \\ & & \dots & & \\ & & & -f_k c_k & I \\ & & & & \dots \end{bmatrix}. \quad (3.5)$$

The corresponding inversion formula

$$U^{-1} = \begin{bmatrix} I & & & & \\ & b_1 f_2 & & & \\ & & b_1 f_2 & b_2 f_3 & \dots \\ & & & I & \\ & & & & b_2 f_3 & \dots \\ & & & & & I & \dots \end{bmatrix} \quad (3.6)$$

may be, mutatis mutandis, written also for the transposed matrix  $L$ .

Obviously, our assumption (3.3) implies that the submatrices  $f_n$  in (3.4) must satisfy the relations

$$f_n = (E_0 I - a_n - b_n f_{n+1} c_{n+1})^{-1} \quad n = 1, 2, \dots \quad (3.7)$$

with a convenient initial choice of  $f_{N+1} = 0$ . Of course, these relations must be considered in the limit  $N \rightarrow \infty$ . For  $s = 1$ , they define the quantities which are known as the analytic continued fractions<sup>/6/</sup>. For  $s > 1$ , we obtain their MCF generalisation<sup>/7,8/</sup>

$$f_k = \frac{1}{E_0 I - a_k - b_k \frac{1}{E_0 I - a_{k+1} - \dots} c_{k+1}} \quad (3.8)$$

Due to Eq. (3.6), we may summarise that for any  $s \geq 1$ , the whole inversion (2.5) is defined now explicitly in terms of the auxiliary  $s \times s$ -dimensional MCF matrices  $f_n$ . In a way, this array plays now a role (is an IP analogue) of the RS unperturbed energies.

### 3.2. The Anharmonic Oscillator Example

In the standard harmonic oscillator basis  $|n\rangle$ ,  $n = 0, 1, \dots$ , the anharmonic oscillator Hamiltonian (1.3) is represented by a pentadiagonal Hamiltonian matrix<sup>/7/</sup>

$$H = \begin{pmatrix} a_0 & \beta_0 & \gamma_0 & & & & & & & & \\ & \beta_0 & a_1 & \beta_1 & \gamma_1 & & & & & & \\ & & & \dots & & & & & & & \\ & & & & \gamma_{k-2} & \beta_{k-1} & a_k & \beta_k & \gamma_k & & \\ & & & & & & & & & & \end{pmatrix} \quad (3.9)$$

with the simple matrix elements

$$a_n = 6\kappa n^2 + O(n), \quad \beta_n = 4\kappa n^2 + O(n), \quad \gamma_n = \kappa n^2 + O(n). \quad (3.10)$$

In Ref.<sup>/5/</sup>, we have chosen a "maximal" tridiagonal subset of the matrix elements (3.9) as our non-diagonal IP dominant component T of the Hamiltonian, and tested an efficiency of the corresponding  $s = 1$  IP algorithm.

From the purely algebraic point of view, the present  $s > 1$  IP generalisation seems more suitable for a "selfconsistent" incorporation of the large off-diagonal matrix elements of

the pentadiagonal Hamiltonian (3.9) into T. For the sake of brevity, we shall study here an extreme choice only,

$$T = H(V = 0) \quad (3.11)$$

with the well established MCF convergence<sup>/7-8/</sup>.

For the first three energy levels, we have obtained a good convergence (cf. Tables 1 - 3). In comparison with the  $s = 1$  numerical tests of Ref.<sup>/5/</sup>, it proved accelerated, roughly speaking, by a factor of two. Obviously, this reflects a "complete selfconsistency" of T in the present case.

Table 1

A sample of convergence of the ground-state energies, with  $E_{\text{exact}} = 4.648\ 8127$ <sup>/9/</sup>

N	$E^{(N)}$	
0	6.000	7.000
1	4.688	4.803
2	4.644	4.611
3	4.649 4	4.654
4	4.648 805	4.649 2
5	4.648 823	4.648 2

Table 2

The dependence of results on the guess parameter  $E_0 = E^{(0)}$ ; the first-excited-state energies with  $E_{\text{exact}} = 13.156\ 800$ <sup>/9/</sup>

$E^{(0)}$	$E^{(9)}$	$E^{(10)}$
12.8	13.156 709	13.156 706
13.0	13.156 769	13.156 769
13.2	13.156 777	13.156 777
13.4	13.156 793	13.156 793
13.6	13.156 759	13.156 792
13.8	13.156 667	13.156 447

Table 3

An interplay of parameters  $N$  and  $E_0$  for the second excited state with  $E_{\text{exact}} = 23.297442^{19}$ . The deviations  $D = (E^{(N)} - E_{\text{exact}}) \cdot 10$  are tabulated

$E_0$	23.0	23.1	23.2	23.2	23.4	23.5	23.6
N							
1	-155.	-68.	-16.4	-0.046	-17.8	-68.	-149.
2	-81.	-23.	-2.7	-0.046	+2.8	+21.	+67.
3	-41.	-7.6	-0.46	-0.046	-0.55	-6.2	-2.7
4	-21.	-2.5	-0.11	-0.046	-0.16	+1.5	+9.4
5	-10.6	-0.78	-0.061	-0.046	-0.12	-0.44	-2.7
6	-5.3	-0.23	-0.061	-0.046	-0.12	-0.03	+0.18
7	-2.7	-0.06	-0.061	-0.046	-0.14	-0.09	+0.08
8	-1.3	-0.02	-0.061	-0.046	-0.14	-0.11	-0.35
9	-0.69	0.00	-0.061	-0.046	-0.14	-0.11	-0.03
10	-0.37	0.00	-0.061	-0.046	-0.14	-0.12	-0.20

#### 4. SUMMARY

In a methodical context, our results illustrate nicely that the role of a small IP parameter is in fact played by the error  $E_0 - E_{\text{exact}}$  of coupling  $g$ . It is also worth mentioning that a trial and error choice of the best value of  $E_0$  (such that  $g$  becomes equal to zero) may be used as a sort of optimisation of the IP prescription. In fact, this has already been derived from different principles and used in a numerical MCF solution of the problem in question (cf. <sup>17/</sup>).

We may notice that a many-times repeated computation of the auxiliary sequence  $f_n$  is needed to find the  $E_0$  giving  $g = 0$ . In this context, our IP formalism of Sect. 3.1 is more economical - it necessitates an evaluation of merely one set of the MCF auxiliary matrices  $f_n(E_0)$ .

In our sample of applications, an overall pattern of dependence of the results and their precision on our choice of  $E_0$  remains the same as in Ref. <sup>15/</sup> - weak and flat in a sufficiently broad interval of  $E_0$ 's. This is fairly obvious from our numerical results where, for the sake of definiteness, we have chosen  $\kappa = 1$  and restricted our attention to the s-wave only. This proved sufficient for the illustration purposes and enabled us to confirm a good and reliable applicability of the IP formalism to the higher excited states.

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Теория возмущений с матричными цепными дробями

Теория возмущений Рэлея-Шредингера расширяется на случай ленточных матриц  $H_0$ , которые представляют обобщение обыкновенного диагонального приближения. Ожидается улучшение сходимости возмущительных рядов вследствие "самосогласованного" эффективного включения больших недиагональных матричных элементов  $H$  в невозмущенный пропагатор  $R$ . Последний оператор и весь ряд теории возмущений алгебраически удается построить как функции вспомогательных матричных цепных дробей. Сходимость демонстрируется численно на примере ангармонического осциллятора - формализм применим в качестве общей и новой техники пересуммирования.

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Znojil M.

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Perturbation Theory with the Matrix Continued Fractions

An idea of using the nondiagonal unperturbed Hamiltonians is further developed. We admit a band-matrix structure of  $H_0$  and describe how the propagator  $R$  may be constructed in terms of the matrix continued fractions. The new perturbation prescription is then described in more detail. Its numerical test employs the standard anharmonic oscillator example and shows a good applicability of the formalism, presumably to all the systems with a strong coupling between the neighbouring "unperturbed" orbitals.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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