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A NEW PERTURBATIVE TREATMENT OF PENTADIAGONAL HAMILTONIANS

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1. INTRODUCTION

In the various physical models [1], the tridiagonal Hamiltonians are quite common, and their numerical diagonalisation is also a standard and well understood procedure [2]. Unfortunately, this situation changes after a transition to the pentadiagonal case. For example, an anharmonic oscillator

$$H = p^2 + \tilde{g}_1 r^2 + \tilde{g}_2 r^4, \qquad \tilde{g}_2 > 0, \tag{1.1}$$

may be recalled as a classical "homework" pentadiagonal matrix in the harmonic oscillator basis $|n\rangle$: Its computer diagonalisation must proceed via a preliminary tridiagonalisation [2], its alternative perturbation treatment is known to lead to the divergent Rayleigh-Schroedinger (RS) perturbation series [3], etc.

A unified treatment of the pentadiagonal and, say, real and symmetric Hamiltonians

$$H = \begin{pmatrix} \alpha_0 & \beta_0 & \gamma_0 & & & & \\ \beta_0 & \alpha_1 & \beta_1 & \gamma_1 & & & \\ & \cdots & \gamma_{k-2} & \beta_{k-1} & \alpha_k & \beta_k & \gamma_k \\ & & & \cdots & & & \end{pmatrix} \tag{1.2}$$

has also the obvious physical reasons since most of the abovementioned tridiagonal models necessitate often an improvement represented just by an inclusion of another diagonal.

In our preceding papers [4], we have considered the general band-matrix Hamiltonians. For their diagonalisation, we have proposed and described an "inversion-perturbation" modification of the RS theory. In a way, this formalism may be understood as a perturbation counterpart to the recurrent numerical method of Graffi and Grecchi [5] based on a use of the auxiliary generalised continued fractions.

In the present paper, we intend to describe an improvement of the method of [4], getting rid of any use of recurrences. In Sect. 2, we start from a slight "vectorial continued fractional" (VCF, [6]) modification of the numerical algorithm of Ref. /5/ . Then, we relate this technique to the classical method of Feshbach /7/ in Sect. 3. We recall also a recent algebraic "fixed-point" construction of the VCF asymptotics /8/ and arrive at a rigorous power-series representation of the effective Hamiltonians.

In Sect. 4, we return to a more detailed description of our modified RS (MRS) perturbation theory and incorporate the VCF techniques into its formalism. This enables us to describe a final synthesis of our considerations in Sect. 5. The "capped", algebraically specified VCF approximants are interpreted there as a MRS input, and the resulting "capped MRS" (CRS) perturbation theory is described in detail. The numerical anharmonic-oscillator illustration of convergence is also added.

Sect. 6 is a summary.

2. THE VECTORIAL CONTINUED FRACTIONS

In the standard vatiational framework, we consider usually a finite-dimensional truncation of the Schroediner equation

$$H^{[N]}\,\psi^{[N]} = E^{[N]}\,\psi^{[N]}, \qquad N \gg 1 \tag{2.1}$$

where

$$H^{[N]} = \begin{pmatrix} \alpha_0 & \beta_0 & \gamma_0 & & \\ & \cdots & & & \\ & \gamma_{N-3} & \beta_{N-2} & \alpha_{N-1} & \beta_{N-1} \\ & & \gamma_{N-2} & \beta_{N-1} & \alpha_N \end{pmatrix} \qquad \psi^{[N]} = \begin{pmatrix} \langle 0|\psi^{[N]}\rangle \\ \cdots \\ \langle N-1|\psi^{[N]}\rangle \\ \langle N|\psi^{[N]}\rangle \end{pmatrix} \tag{2.2}$$

For the sake of definitness, we may recall here the anharmonic oscillator (1.1) since it is one of the most popular "homework" pentadiagonal matrices in the standard harmonic oscillator basis $|n\rangle$, $n = 0,1,\ldots$. Its matrix elements read

$$\begin{aligned} \alpha_n &= (\tilde g_1 + 1)x_n + \tilde g_2(y_{n-1}^2 + x_n^2 + y_n^2) \\ x_n &= \langle n|r^2|n\rangle = 2n + \ell + 3/2, \quad \ell = 0,1,\ldots \\ y_n &= \langle n|r^2|n+1\rangle = (n+1)^{1/2}(n+\ell+3/2)^{1/2}, \\ \beta_n &= (\tilde g_1 - 1)y_n + \tilde g_2 y_n(x_n + x_{n+1}), \quad \gamma_n = \tilde g_2 y_n y_{n+1}, \end{aligned} \tag{2.3}$$

$n = 0,1,\ldots$ /5/ and are simple functions of parameters.

For a numerical solution of (2.1), let us postulate now first that the $N+1$ - dimensional Hamiltonian is factorised in accord with the prescription

$$E^{[N]}I - H^{[N]} = UDU^T. \tag{2.4}$$

Here, D is a diagonal matrix

$$D_{nn} = g_n^{-1}, \quad n = 0,1,\ldots,N \tag{2.5}$$

and U is an upper triangular and tridiagonal factor

$$U = \begin{pmatrix} 1 & -h_0 g_1 & -\gamma_0 g_2 & \\ & 1 & -h_1 g_2 & -\gamma_1 g_3 \\ & & \cdots & \end{pmatrix}. \tag{2.6}$$

The decomposition (2.4) - (2.6) becomes an algebraic identity, provided only that the relations

$$\begin{aligned} g_n &= (E - \alpha_n - h_n^2 g_{n+1} - \gamma_n^2 g_{n+2})^{-1}, \quad E = E^{[N]} \\ h_n &= \beta_n + \gamma_n g_{n+2} h_{n+1}, \quad n = 0,1,\ldots,N \end{aligned} \tag{2.7}$$

hold. They must be complemented by the regularity conditions and initial values,

$$1/g_k \neq 0, \quad k = 1,2,\ldots,N \qquad g_{N+1} = g_{N+2} = 0, \tag{2.8}$$

and define in fact just the above mentioned vectorial continued fractions in the limit $N \to \infty$ /6/ .

A use of decomposition (2.4) converts our truncated Schoedinger equation into an equivalent form

$$DU^T\psi^{[N]} = 0 \tag{2.9}$$

since det U = 1. Moreover, due to the recurrent character of the factorisation (2.4), the regularity assumption (2.8) implies that the solution of (2.9) becomes almost trivial,

$$1/g_0 = 0 \qquad \langle k|\psi^{[N]}\rangle = \langle 0|\psi^{[N]}\rangle (U^T)^{-1}_{ko}, \quad k = 1,2,\ldots,N. \tag{2.10}$$

In particular, an evaluation of energies becomes practically reduced to mere localisation of poles of our VCF "Green's function" g_0.

In what follows, we shall work in a purely non-numerical spirit - the cut-off parameter N will be considered infinite. We shall also drop the redundant square-bracketed superscripts$^{[\infty]}$.

3. THE FIXED-POINT VCF EXPANSIONS

3.1. The Zero-Order Fixed-Point Approximation

As a consequence of the $n \gg 1$ asymptotically smooth character of our example (2.3), we may try to interpret recurrences (2.7) as an iterated mapping with almost constant coefficients. This may inspire us to a use of a zero-order estimate

$$g_n \approx g_{n+1} \approx g_{n+2} \approx \hat{g} = \hat{g}(n), \quad h_n \approx h_{n+1} \approx \hat{h} = \hat{h}(n), \quad n \gg 1. \qquad (3.1)$$

An insertion of this assumption in eq. (2.7) is a definition of a fixed-point of the mapping

$$\hat{g} = (E - \alpha_n - \hat{h}^2 \hat{g} - \gamma_n^2 \hat{g})^{-1}, \quad \hat{h} = \beta_n + \gamma_n \hat{g} \hat{h} \qquad n \gg 1. \qquad (3.2)$$

An algebraic treatment of these equations is straightforward. With an abbreviation

$$\hat{h} = \hat{h}(n) = \beta_n / (1 - \gamma_n \hat{g}) \qquad (3.3)$$

they degenerate to a pair of quadratic equations

$$\gamma_n^2 \hat{g}^2 - \hat{X}\hat{g} + 1 = 0 \qquad \hat{X} = E - \alpha_n - \beta_n^2/(\hat{X} - 2\gamma_n), \quad n \gg 1 \qquad (3.4)$$

with the closed solution.

3.2. The $n \gg 1$ Asymptotic Fixed-Point Series

In accord with Feshbach /7/ , the $N = \infty$ limit of (2.1) is equivalent to the finite-dimensional equation

$$(E - H^{eff})|\phi\rangle = 0, \qquad |\phi\rangle = \sum_{m=o}^{M} |m\rangle\langle m|\psi\rangle \qquad (3.5)$$

provided only that the so-called "effective Hamiltonian" is introduced as an $M + 1$ - dimensional matrix

$$H^{eff} = P(H + HRH)P, \quad P = \sum_{m=o}^{M} |m\rangle\langle m|, \quad R = Q \frac{1}{EI - QHQ} Q, \quad Q = I - P. \qquad (3.6)$$

Most of the matrix elements of H^{eff} coincide with the original H. This follows from the insertion of (2.4) (with $N = \infty$) in (3.6),

$$H^{eff} = EI - PUPDPU^T P. \qquad (3.7)$$

The only exception are the four lowest rightmost elements which have a different though simple explicit VCF form

$$\alpha_M^{eff} = E - g_M^{-1} \neq \alpha_M \qquad \beta_{M-1}^{eff} = h_{M-1} \neq \beta_{M-1}$$
$$\alpha_{M-1}^{eff} = E - g_{M-1}^{-1} - h_{M-1}^2 g_M \neq \alpha_{M-1} \qquad (3.8)$$

in accord with our formula (3.7). We may conclude that by means of our replacement (3.1) of the exact VCF quantities by their fixed-point approximants, we may accelerate the convergence of the numerical solution of eq. (2.1).

In the latter context, we may return to our anharmonic oscillator example and recall an existence of the explicit systematic corrections to the zero-order estimates (3.1) /8/ . The corresponding constructions may be given very easily the form of asymptotic expansions of our effective matrix elements (3.8). For the sake of definitness, the third-order formula

$$\hat{g}(n) = (-1 + 2\rho - 2\rho^2 + \frac{3}{2}\rho^3)/\gamma_n, \quad \rho = \rho(n) = n^{-1/4}$$
$$\hat{h}(n) = (2 + 2\rho - \frac{1}{2}\rho^3)\gamma_n, \qquad n \geq N_{FP} \gg 1 \qquad (3.9)$$

will be used in the numerical tests below.

4. THE MODIFIED RS PERTURBATION THEORY

4.1. The Separable Selfconsistency

An ansatz $H = H_o + \lambda H_1$ and

$$|\psi\rangle = |\psi^{(N)}\rangle + O(\lambda^{N+1}) \qquad |\psi^{(N)}\rangle = \sum_{m=o}^{N} |\psi_m\rangle \lambda^m,$$
$$E = E^{(N)} + O(\lambda^{N+1}), \quad E^{(N)} = \sum_{m=o}^{N} E_m \lambda^m, \qquad |\lambda| \ll 1 \qquad (4.1)$$

converts any Schroedinger bound-state problem of the form (3.1) into the well known RS set of equations

$$H_o |\psi_o\rangle = E_o |\psi_o\rangle \tag{4.2}$$

(the so-called unperturbed problem) and

$$(E_o I - H_o)|\psi_k\rangle = H_1|\psi_{k-1}\rangle - \sum_{m=1}^{k} E_m |\psi_{k-m}\rangle, \quad k=1,2,\ldots \tag{4.3}$$

(the recurrent definition of corrections [9]).

Recently, we have considered relations (4.2) - (4.3) as a rigorous re-formulation of the Schroedinger eigenvalue problem and tried to weaken the usual assumption of a complete solvability of the unperturbed problem. In a resulting MRS perturbation theory with non-diagonal propagators [4] , the unperturbed equation (4.2) has been made satisfied identically via a separable re-definition of H. Thus, we may put

$$H_o = H + G|0\rangle\langle 0| \qquad \lambda H_1 = -G|0\rangle\langle 0| \tag{4.4}$$

and apply simply the MRS technique [4] to any pentadiagonal H.

Let us notice that a use of some suitable separable mean-field correction of the type (4.4) is quite common in the standard RS context where $|0\rangle = |\psi_o\rangle$ and $G \neq 0$ corresponds merely to a trivial "selfconsistent" modification of E_o. Here, it becomes more essential since the unperturbed problem is not assumed to be exactly solvable anymore.

4.2. The MRS Perturbation Theory

In accord with Ref. [4] , an essential MRS input is an available M = 1 unperturbed propagator

$$R = Q\frac{1}{E_o I - QHQ}Q, \quad Q = 1 - |0\rangle\langle 0| \tag{4.5}$$

which enters both the closed solution

$$|\psi_o\rangle = |0\rangle + RH|0\rangle \tag{4.6}$$

of (4.2) and the higher-order wavefunction corrections

$$|\psi_k\rangle = RH_1|\psi_{k-1}\rangle - \sum_{m=1}^{k} E_m \cdot R|\psi_{k-m}\rangle, \quad k = 1,2,\ldots \tag{4.7}$$

(with the standard normalisation $\langle 0|\psi_k\rangle = 0$, k = 1,2,...).

The MRS energies

$$E_k = \frac{1}{\langle\psi_o|\psi_o\rangle}\left[\langle\psi_o|H_1|\psi_{k-1}\rangle - \sum_{m=1}^{k-1}\langle\psi_o|\psi_{k-m}\rangle E_m\right], \quad k=1,2,\ldots \tag{4.8}$$

remain defined by the ordinary RS formula but, for the sake of selfconsistency, we must accept also a restriction

$$G = E_o - \langle 0|H|\psi_o\rangle. \tag{4.9}$$

It specifies the auxiliary coupling $g = g(E_o)$ for an arbitrary choice of the free MRS parameter E_o [4] .

In a more detailed MRS analysis, a similarity between the resolvents in (4.5) and (3.6) enables us to use again a VCF factorisation formula

$$Q(E_o I - H)Q = WDW^T. \tag{4.10}$$

Here, the matrix W differs from the $N = \infty$ matrix U in (2.6) just by an absence of the first row and column. We may also write

$$R = (W^T)^{-1}\begin{pmatrix} g_1 & & \\ & g_2 & \\ & & \ddots \end{pmatrix} W^{-1}. \tag{4.11}$$

For the sake of simplicity, our VCF formulas (4.10) and (4.11) are to be partioned now into the 2x2 - dimensional submatrices.

$$W = \begin{pmatrix} I_1^{(-)} & -\Gamma_2 & & \\ & I_3 & -\Gamma_4 & \\ & & I_5^{(-)} & -\Gamma_6 \\ & & & \ldots \end{pmatrix} \qquad I_k^{(\pm)} = \begin{pmatrix} 1 & \pm h_k g_{k+1} \\ 0 & 1 \end{pmatrix}$$

$$\Gamma_k = \begin{pmatrix} \gamma_{k-1} & 0 \\ h_k & \gamma_k \end{pmatrix}\begin{pmatrix} g_{k+1} & 0 \\ 0 & g_{k+2} \end{pmatrix}. \tag{4.12}$$

This will simplify the inversion since

$$W^{-1} = \begin{pmatrix} I_1^{(+)} & \pi_1^{(3)} & \pi_1^{(5)} & \pi_1^{(7)} & \ldots \\ & I_3^{(+)} & \pi_3^{(5)} & \pi_3^{(7)} & \ldots \\ & & \ldots & & \end{pmatrix}, \tag{4.13}$$

where

$$\pi_k^{(\ell)} = I_k^{(+)}\Gamma_{k+1} I_{k+2}^{(+)}\Gamma_{k+3}\cdots I_{\ell-2}^{(+)}\Gamma_{\ell-1} I_\ell^{(+)}. \tag{4.14}$$

We may summarise that the general pentadiagonal Hamiltonian admits a straightforward MRS treatment, provided only that we start from a recurrent specification of the auxiliary VCF sequence.

5. THE NEW FIXED-POINT VERSION OF THE MRS PERTURBATION THEORY

An essence of the numerical VCF algorithm (cf. Sect. 2) lies in a repeated evaluation of the auxiliary E-dependent VCF sequences (h_n, g_n), $E \to E^{[N]}$, while the perturbative formulas of Sect. 4 contain just a single set of these VCF quantities evaluated at a single value of the energy-guess MRS parameter $E = E_0$.

In what follows, we shall show how to get rid of the numerical ($N \to \infty$) VCF recurrents by means of a replacement of all the VCF quantities h_n and g_n by some a priori chosen "quasi-VCF" or "capped" quantities $\hat{h}(n)$ and $\hat{g}(n)$, $n \geq N \gg 1$.

The replacement violates obviously the VCF recurrences (2.7), so that the capped quantities do not correspond to our original Hamiltonian H anymore. Nevertheless, we may introduce a new, capped analogue of recurrences (2.7),

$$\hat{g}(k) = [E_0 - \hat{\alpha}_k - \hat{h}^2(k)\hat{g}(k+1) - \gamma_k^2 \hat{g}(k+2)]^{-1}$$
$$\hat{h}(k) = \hat{\beta}_k + \hat{\gamma}_k \hat{g}(k+2)\hat{h}(k+1), \quad k \geq N_{FP} \gg 1 \tag{5.1}$$

and treat these new relations as if they were obtained from some other pentadiagonal matrix T with the capped matrix elements.

$$T = \begin{pmatrix} \hat{\alpha}_0 & \hat{\beta}_0 & \hat{\gamma}_0 & \\ \hat{\beta}_0 & \hat{\alpha}_1 & \hat{\beta}_1 & \hat{\gamma}_1 \\ & \dots & & \end{pmatrix}. \tag{5.2}$$

This is our main idea - the new matrix T is to be used now as a new approximate Hamiltonian within the old MRS perturbative framework.

For the sake of definitness (and with the anharmonic oscillator example in mind), we shall restrict our further attention to the fixed-point type of sequences $h(n)$ and $\hat{g}(n)$ (cf. (3.9)). This will guarantee that the capped perturbation

$$V = H - T \tag{5.3}$$

defined by the relations (5.2), (5.3) and

$$\hat{\gamma}_k = \gamma_k \qquad \hat{\beta}_k = \hat{h}(k) - \gamma_k \hat{g}(k+2)\hat{h}(k+1)$$
$$\hat{\alpha}_k = E_0 - \hat{g}^{-1}(k) - \hat{h}^2(k)\hat{g}(k+1) - \gamma_k^2 \hat{g}(k+2), \quad k \geq N_{FP} \gg 1 \tag{5.4}$$

will be small, proportional to the deviations

$$h_k - \hat{h}(k) \qquad g_k - \hat{g}(k). \tag{5.5}$$

Within the framework of the MRS formalism, it remains for us to replace (4.4) by the "capped RS" (CRS) postulate

$$H_0 = T + \hat{G}|0\rangle\langle 0| \qquad \lambda H_1 = V - \hat{G}|0\rangle\langle 0|. \tag{5.6}$$

Then, the CRS propagator becomes defined by the capped analogue

$$\hat{R} = Q \frac{1}{E_0 I - QTQ} Q = (W^T)^{-1} \begin{pmatrix} \hat{g}_1 & & \\ & \hat{g}_2 & \\ & & \ddots \end{pmatrix} \hat{W}^{-1}, \tag{5.7}$$

of the product (4.11), and all the remaining CRS formulas may be also written in their modified capped form.

In particular, the unperturbed equation may be satisfied in accord with the capped MRS prescriptions (4.6) and (4.9),

$$|\hat{\psi}_0\rangle = |0\rangle + \hat{R}T|0\rangle \qquad \hat{G} = E_0 - \langle 0|T|\hat{\psi}_0\rangle, \tag{5.8}$$

so that we end up essentially with the same formulas as before,

$$|\hat{\psi}_1\rangle = \hat{R}(V - \hat{E}_1)|\hat{\psi}_0\rangle$$
$$\lambda\hat{E}_1 = (\langle\hat{\psi}_0|V|\hat{\psi}_0\rangle - \hat{G})/\langle\hat{\psi}_0|\hat{\psi}_0\rangle \tag{5.9}$$
$$\hat{E}_2 = \langle\hat{\psi}_0|(V - \hat{E}_1)\hat{R}(V - \hat{E}_1)|\hat{\psi}_0\rangle/\langle\hat{\psi}_0|\hat{\psi}_0\rangle,$$

etc.

In the Tables 1 - 3, a representative set of the CRS numerical tests is given. The results confirm that the transition $H \to T$ and the whole CRS re-arrangement of the Hamiltonian causes merely an inessential modification of the MRS V=0 results, say, of Ref. [4]. The convergence rate is quick (Table 1) and

Table 1

A sample of convergence of the CRS expansions. For the first excited state energy $E_{exact} = 13.156\ 800$ [10] *of the s-wave Hamiltonian* $H = p^2 + r^2 + r^4$, *we use the* $N_{FP} = 10$ *in (5.4)*

N	E
0	13.2
1	13.155 62
2	13.157 22
3	13.157 027
4	13.156 949
5	13.156 898
6	13.156 863
7	13.156 839
8	13.156 823
9	13.156 812
10	13.156 803

practically independent of the choice of E_0 (Table 2). Moreover, the E_0-dependence weakens in the higher-order approximations, even for the non-negligible magnitude of the errors (5.5) (Table 3). Hence, a use of the fixed-point approximation leads to an efficient algorithm which may be considered one of most adequate techniques for evaluation of the anharmonic-oscillator-like spectra.

Table 2

The dependence of results on the guess parameter $E_0 = E^{(0)}$

$E^{(0)}$	$E^{(9)}$	$E^{(10)}$
12.8	13.156 789	13.156 777
13.0	13.156 807	13.156 798
13.2	13.156 812	13.156 803
13.4	13.156 816	13.156 809
13.6	13.156 788	13.156 813
13.8	13.156 682	13.156 463

Table 3.

A step-by-step weakening of dependence on the parameter E_0. *We display the "number of correct digits"* $P = -\ln \times |E^{(N)} - E_{exact}|$ *for the ground-state energy and* $N_{FP} = 5$

E_0 \ order N	1	2	3	8
-2.0	0.61	1.02	1.43	2.97
-1.0	0.69	1.15	1.60	2.99
0.0	0.80	1.31	1.80	3.00
1.0	0.95	1.52	2.05	3.00
2.0	1.15	1.80	2.43	2.99
3.0	1.47	2.18	1.59	2.99

6. SUMMARY

In the MRS perturbation formalism with the non-diagonal propagators and with the "optimal" zero-order approximation $T = H$, a CRS re-arrangement (a transition to $T \neq H$) generates only a small perturbation $V = H - T$ for the sufficiently reliable (e.g., fixed-point) quasi-VCF approximation. A priori, we may expect then a good convergence and summarise:

(a) Our old inversion-perturbation algorithm [4] "compresses" the information contained in the five (or 2s+1 in general) diagonals of H into an auxiliary VCF array. This array plays a role of certain "generalised unperturbed energies". Thus, the preparatory numerical recurrent generation of VCF's from H is just a MRS analogue of the RS "preliminary diagonalization" of H_0, which is rarely performed in the actual applications.

(b) In the present paper, we have started the MRS construction of perturbation series directly from an a priori given quasi-VCF generalised spectrum. As a general CRS perturbation theory, this parallels more closely most textbook RS applications where the exact unperturbed spectrum is also known in advance.

(c) Besides the described fixed-point version of the CRS theory, the various other types of the quasi-VCF input (say, the finite, $N < \infty$ VCF approximants) are also possible of course. All of them might provide new ideas for resummations of the divergent RS expansions, especially in all the situations where the divergence has been caused by a strong-coupling character (band-matrix structure) of the Hamiltonian itself.

(d) In comparison with the RS theory with diagonal H_0, our "non-diagonal solvability of T" is a much weaker requirement. More realistic Hamiltonians H may lie close to some capped T, and the convergent CRS expansions should exist for a broader class of Hamiltonians in principle. In the computations, such an expectation seems to be confirmed also by our anharmonic oscillator example.

(e) Even in its present fixed-point version, the whole CRS prescription and, in particular, the $H \to T$ replacement are by far not unique. In general, the closer lies the capped input to the exact VCF image of H itself, the quicker will also be the rate of convergence of the CRS perturbation expansions. In practice, the input or "exactly solvable" models T may be related also to some independent physical information in principle. For a broad class of systems of interest, this opens an entirely new way of their non-RS "selfconsistent" perturbation treatment.

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Новая трактовка 5-диагональных гамильтонианов

Предложена новая формулировка теории возмущений Рэлея - Шредингера. Цель работы - избавиться от проблем с построением невозмущенного пропагатора. Конкретно рассматриваются гамильтонианы с пятью диагоналями, и сначала используются так называемые векторные цепные дроби. Последние вспомогательные величины заменяются их алгебраическими приближениями /типа асимптотического "приближения неподвижной точки"/, которые интерпретируются как вступительные данные /типа обобщенного невозмущенного спектра/. Получается общая новая схема возмутительных вычислений, примененная для иллюстрации к примеру ангармонического осциллятора.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

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A New Preturbative Treatment of Pentadiagonal Hamiltonians

A new formulation of the Rayleigh - Schroedinger perturbation theory is proposed. It is inspired by a recurrent construction of propagators, and its main idea lies in a replacement of the auxiliary matrix elements (generalised continued fractions) by their non-numerical approximants. In a test of convergence (the anharmonic oscillator), the asymptotic fixed-point approximation scheme is used. The results indicate a good applicability of this fixed-point version of our formalism to systems with a band-matrix structure of the Hamiltonian.

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

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