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**A NEW ALGEBRAIC
MAJORIZATION-MINORIZATION EIGENVALUE
METHOD**

1986

Perturbation theory starts usually with a decomposition of the Hamiltonian ^{/1/},

$$H = \text{diagonal } H_0 + \text{a small remainder } H_1. \quad (1)$$

Similarly, most of the practical variational algorithms may be characterized by an assumption ^{/2/}

$$H = \text{finite-dimensional } H_0 + \text{an irrelevant } H_1. \quad (2)$$

Here, we intend to describe a novel approach to the Schrödinger eigenvalue problem based on the third alternative ansatz

$$H = \text{special band matrix } H_0 + \text{a small or irrelevant } H_1. \quad (3)$$

In essence, we shall indicate how to construct the special (= diagonalizable) approximate and/or majorizing and minorizing operators H_0 from H , and illustrate the related technicalities for a broad class of the one-body Hamiltonians H .

To begin with, anharmonic oscillator $H = H^{(\text{osc})} + ar^{2t}$, $t = 2, 3, \dots$, whose perturbative interpretation (1) may lead to divergences ^{/3/}, may be considered as an example of (3). Indeed, in the oscillator basis $|n\rangle$ ($H^{(\text{osc})}|n\rangle = (4n+2t+3)|n\rangle$, $n=0, 1, \dots$), the anharmonic eigenvalue problem acquires the algebraic infinite-dimensional $2t+1$ -diagonal form

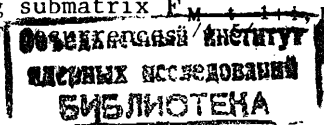
$$Hz = 0, \quad H_{mn} = \langle m | (H^{(\text{osc})} + ar^{2t} - E) | n \rangle, \quad z_n = \langle n | \psi \rangle, \quad m, n = 0, 1, \dots \quad (4)$$

In the purely numerical context, we may preserve simply $H \equiv H_0$ and $H_1 \equiv 0$ in eq. (3) and solve eq. (4) in terms of the matrix continued fractions ^{/4/} (MCF), i.e., essentially, as an infinite-dimensional limit of (2) (cf. § 1 below). In brief, our present intention is just to eliminate (or at least accelerate) algebraically the latter, numerically difficult limiting transition, via a replacement of eq. (2) ($\dim H_0 = N < \infty$) by eq. (3) ($N = \infty$).

1. MCF method ^{/4/}. In the standard Feshbach ^{/5/} model-space form of (4)

$$\sum_{n=0}^{M-1} F_{mn} z_n = 0, \quad 0 \leq m \leq M-1, \quad F_{mn} = H_{mn} \quad \text{for } m \text{ or } n \leq M-t-1, \quad (5)$$

we may define the missing submatrix $F_{m+t-1+j, n-t-1+j} = G_{ij}$, $i, j = 1, 2, \dots, t$ by the MCF



$$G = A_0 - B_0 G_1^{-1} C_1, \quad (6)$$

$$G_k = A_k - B_k G_{k+1}^{-1} C_{k+1}, \quad k = 1, 2, \dots, N_0 - 1,$$

where $G_{N_0} = A_{N_0}$, $N_0 \gg 1$ and

$$(A_k)_{mn} = \mathcal{H}_{M-t-1+tk+m, M-t-1+tk+n}, \quad (7)$$

$$(B_k)_{mn} = \mathcal{H}_{M-t-1+tk+m, M+1+tk+n},$$

$$(C_{k+1})_{mn} = \mathcal{H}_{M-1+tk+m, M-t-1+tk+n}, \quad 0 < m, n \leq t.$$

This enables us to compute G and solve eq.(5) \equiv eq.(4) numerically.

2. Modified MCF method^{5,6/}. The MCF method acquires the partially non-numerical features whenever the MCF $N \rightarrow \infty$ convergences may be reinterpreted as a fixed-point (FP) asymptotic property of (6),

$$G_k = G_k^{(0)} + \text{small corrections} \quad (8)$$

$$G_k^{(0)} = A_k - B_k G_{k+1}^{(0)-1} C_{k+1}.$$

Indeed, an algebraic and compact solution of the basic FP quadratic $t \times t$ equation (8) exists and has been used to accelerate the MCF convergence for various particular (nonpolynomial, singular and p -dependent) anharmonicities^{6/}. In our example (4) we may renormalize z and \mathcal{H} in (4),

$$z_n \rightarrow \text{constant}(n) \times z_n$$

$$\mathcal{H}_{M+m, M+n} \rightarrow \text{constant}(m) \times \mathcal{H}_{M+m, M+n} \times \text{constant}(n) \quad (9)$$

$$\mathcal{H}_{M+n, M+n} = \binom{2t}{t+m-n} + O(1/n), \quad n \gg 1,$$

and arrive at a closed leading-order FP formula

$$G_k^{(0)} \approx G^{(0)} = SS^T, \quad S_{mn} = \binom{t}{n-m}, \quad m, n = 1, 2, \dots, t. \quad (10)$$

In the present paper this is our starting point.

3. Perturbative FP method^{5/}. Let us introduce the modification $\mathcal{H}^{(0)}$ of \mathcal{H} that will be constant asymptotically

$$\mathcal{H} = \begin{pmatrix} \dots & & & \\ \dots & C_N A_N B_N & \dots & \\ \dots & & & \end{pmatrix} \rightarrow \mathcal{H}^{(0)} = \begin{pmatrix} \dots & & & \\ \dots & C^{(0)} A^{(0)} B^{(0)} & \dots & \\ \dots & & & \end{pmatrix}, \quad (11)$$

where $A^{(0)} = SS^T + S^T S$, $B^{(0)} = C^{(0)T} = S^T S^T$, $N \gg 1$ while $\mathcal{H}_{mn}^{(0)} \equiv \mathcal{H}_{mn}$ for $m, n \leq M_1 = M - 1 + Nt$, i.e. within a finite "extended model space". Due to the algebraic identity

$$G^{(0)} = A^{(0)} - B^{(0)} G^{(0)-1} C^{(0)} \quad (12)$$

this gives precisely $G_N \equiv G^{(0)}$ for $N_0 = \infty$ used in (6), and our approximate Hamiltonian $\mathcal{H}^{(0)}$ may be interpreted now as diagonalizable exactly via eq.(5).

We may introduce also the corrections $\mathcal{H}^{(1)} = \mathcal{H} - \mathcal{H}^{(0)}$ and apply the ordinary perturbation theory. This is an important observation related to eqs.(1)+(3). Now, let us combine eqs.(3)+(2).

4. Majorization-minorization (MM) idea. We may notice that the asymptotic part

$$D_{mn}(t) = \mathcal{H}_{M_1+m, M_1+n}^{(0)} \binom{2t}{t+m-n}$$

of $\mathcal{H}^{(0)}$ is a positively semi-definite matrix, $D(t) \geq 0$ which is zero within the "extended model space". Obviously, by a multiple of this matrix, $gD(t)$, we may try to majorize the whole perturbation $\mathcal{H}^{(1)} = \mathcal{H} - \mathcal{H}^{(0)}$. A modification of (11),

$$\mathcal{H}^{(0)} \rightarrow \mathcal{H}^{(g)} = \begin{pmatrix} \dots & & & \\ \dots & C^{(g)} A^{(g)} B^{(g)} & \dots & \\ \dots & & & \end{pmatrix}$$

$$A^{(g)} = (1+g)A^{(0)}, \quad B^{(g)} = (1+g)B^{(0)}, \quad C^{(g)} = (1+g)C^{(0)}$$

will majorize then the original matrix \mathcal{H} . Similarly, we may try to use a negative g and re-interpret eq.(13) as a definition of the matrix which minorizes \mathcal{H} . In this way, the minimax property^{2/} of the sum of matrices $\mathcal{H}^{(g)} + (\mathcal{H} - \mathcal{H}^{(g)})$ will imply that the precise energies E become sandwiched between the pair of spectra $E^{(g)}$ of eq.(5) whenever we use the pair of initial values $G_N = (1+g)G_N^{(0)}$, $N = N_0 < \infty$ in (6). This is our main idea.

5. General potential as an example. The above MM "principle" may be both refined and extended. In the one-body problem and example

$$\left[-\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + V(r) \right] \psi(r) = E \psi(r), \quad \ell = 0, 1, \dots \quad (14)$$

it becomes applicable, e.g., after a replacement of $V(r)$ by its arbitrary Padé approximant $V = V_{pq}$,

$$V(r) = V^{(1)}(r) + \frac{V^{(2)}(r)}{V^{(3)}(r)}, \quad V^{(i)}(r) = \sum_{j=0}^{n^{(i)}} a_j^{(i)} r^{2j}, \quad i=1,2,3, \quad (15)$$

$$a_q^{(1)} > 0, \quad n^{(1)} = q \geq 1, \quad n^{(2)} + 1 = n^{(3)} = p > 0, \quad V^{(3)} > 0,$$

where, in accordance with the analytic structure of the input interaction, we may achieve an arbitrary pre-determined precision [7].

The essential technicality is to rewrite eqs.(14)+(15) as eq.(4) with the nonsymmetric $2t+1$ -diagonal matrix

$$H_{mn} = \text{const}(m) \langle m | V^{(3)} (-D^2 + V^{(1)} - E) + V^{(2)} | n \rangle \text{const}(n), \quad (16)$$

where $t=p$ for $q=1$ and $t=p+q$ for $q>1$. Its peculiarity lies in its asymptotic form

$$H = H[\gamma] (1 + O(1/M^2)), \quad \gamma = \frac{a_{p-1}^{(3)}}{a_p^{(3)}} + \frac{a_{q-1}^{(1)}}{a_q^{(1)}}, \quad q > 2, \quad (17)$$

$$H_{mn}^{[\gamma]} = \begin{pmatrix} 2t & & \\ & \ddots & \\ & & 2t-2 \end{pmatrix} + \frac{\gamma}{M} \begin{pmatrix} 2t-2 & & \\ & \ddots & \\ & & 2t-2 \end{pmatrix}, \quad m, n \geq M$$

compatible with (9) in the leading-order approximation (for the sake of brevity, we omit the similar $q=1$ and $q=2$ formulas here). Hence, we may recall the preceding results and use eqs.(5)-(13) with the following modifications.

6. The second-order FP approximation. By means of the ansatz

$$G_{N_0-k} = SS^T + S^T |\beta\rangle \rho_k \langle \beta| S, \quad \langle \beta| = (1, -1, 1, \dots, (-1)^{t+1}) \quad (18)$$

we may convert our MCF recurrences (with the second-order asymptotics (17) of H) into a one-dimensional mapping $\rho_{k+1} \rightarrow \rho_k$,

$$\rho_k = (\rho_{k+1} + \gamma M^{-1}) / (1 + t\rho_{k+1}), \quad (19)$$

where the higher-order corrections may be neglected for $M \gg 1$ and $\gamma > 0$. The quadratic eq.(8) for matrices degenerates then into an ordinary scalar one, so that an improvement of (10) reads

$$G_k \approx G^{[\gamma]} = SS^T + S^T |\beta\rangle \lambda \langle \beta| S, \quad \lambda = (\gamma/Mt)^{1/2}. \quad (20)$$

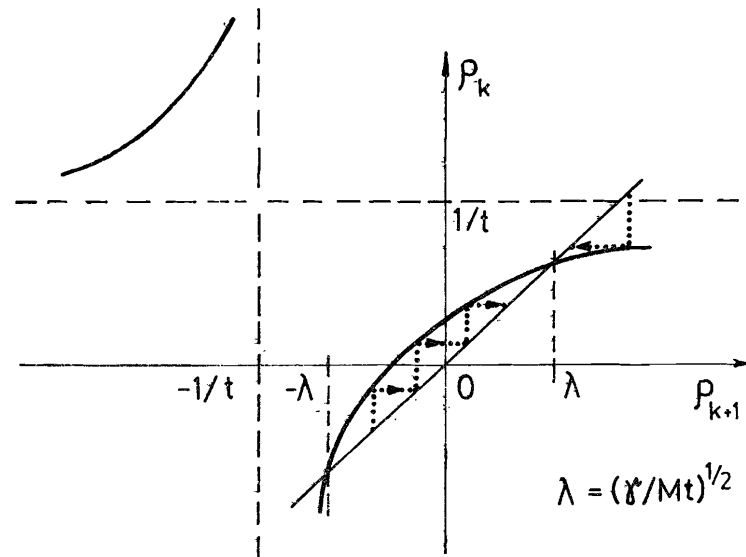


Fig.1. Mapping (19) and a pattern of its iterations (dotted lines).

Here, the plus-sign choice in λ follows from the simple geometric interpretation of the iterated mapping (19) (see fig.1). Thus, whenever we replace $H \rightarrow H[g]$, i.e., $G \rightarrow G[g]$, $g = g(\rho) = Mt\rho^2$ in (5) and choose $\rho \in (\lambda_{(-)}, \lambda_{(+)})$, $\lambda_{(\pm)} = \lambda \pm |\text{const.} M^{-1}|$, we may interpret $E[g]$ as the second-order FP-perturbative energy approximations.

7. The second-order MM method. In the same manner as in § 4, we may achieve a majorization/minorization of the Hamiltonian

$$H[g(\rho_{(-)})] \leq H \leq H[g(\rho_{(+)})] \quad (21)$$

provided that

$$0 \ll \rho_{(-)} < \lambda_{(-)}, \quad \lambda_{(+)} < \rho_{(+)} \ll \infty. \quad (22)$$

The resulting "sandwiching" of binding energies

$$E[g(\rho_{(-)})] < E < E[g(\rho_{(+)})] \quad (23)$$

may be tested on the potentials of § 5.

For simplicity, we have restricted our attention to the simplest non-trivial $t=2$ case ($q=1, p=2$ or $q=2$ and $p=0$) and verified the sandwiching phenomenon (23) for various sets of coup-

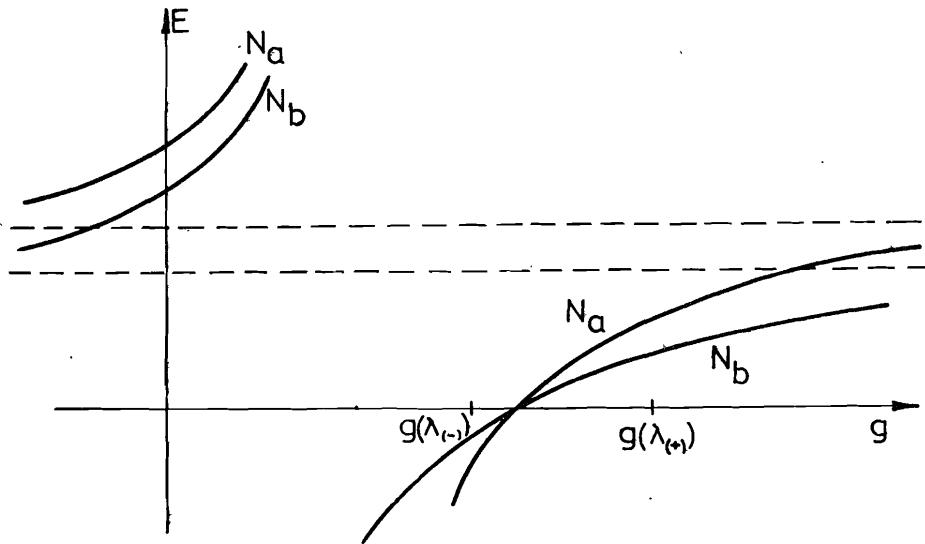


Fig.2. Sandwiching phenomenon as it manifests itself numerically (various $t=2$ potentials, arbitrary units, $g=0$ not fixed, $N_b > N_a > 1$).

lings. The results exhibit the same pattern of behaviour (fig.2) and confirm also our expectations that a choice of $g \ll g(\lambda_{(-)})$ makes the estimate $E[g]$ worse than the simple truncation result $\approx E[\infty]$. Thus, for the practical purposes, we may propose the following algorithm:

(a) choose a pair of indices N in (18) ($N_a < N_b$) and compute the two curves $E = E_{a,b}[g]$ as functions of $g = g(\rho)$.

(b) find an intersection $E = E_a[g_0] = E_b[g_0]$ which gives the best energy approximation.

(c) use the deviation $\epsilon = |g_0 - \gamma + O(M^{-1})|$ in our estimate of the upper and lower energy bounds $E_b[g_0 + \epsilon]$, E and $E_a[g_0 - \epsilon] < E$, respectively.

Summarizing our numerical experience, we may notice that

(i) contrary to the variational methods, we obtain roughly the same precision for both the upper and lower energy estimates,

(ii) contrary to the perturbative computations, our "best" approximate energy value is accompanied also by a reliable error estimate.

8. Outlook. Throughout the text, one of our most important mathematical pre-requisites was the semi-definite character of $D(t)$. Its particular and simple combinatorial form as well as the related matrix identities (12), etc., may easily be generalized: We may start from any H_0 equal asymptotically to a semi-definite band matrix (cf. e.g. Ref. ^{75/} for further details). In this way, our MM method and the corresponding nonnumerical results as well as the improved numerical algorithms will be of interest in various physical domains, ranging from the solid-state models (vectorial chains ^{78/}) and nuclear microscopic Hamiltonians (based on the doorway-hallway hypothesis ^{79/}) up to various quantum system represented in the generalized Lanczos basis ^{74-67/}. These applications are under current investigation at present.

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Зноил М.

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Новый алгебраический метод майоризации и миноризации собственных значений

Обсуждается возможность параллельной майоризации и миноризации E -энергий системы для данного Гамильтониана H . Цель работы - улучшить эффективность существующих методов вариационного или возмущительного типа при помощи таких специальных ленточных матриц $H_0^{(1,2)}$, что $H_0^{(1)} \geq H$ и $H_0^{(2)} \leq H$. В таком случае, конструкция Фешбаха /в терминах матричных цепных дробей/ позволит точное построение соответствующих энергий E_0 , что и составляет основу метода. Его применение рассматривается для двух случаев: для ангармонического осциллятора и для любого локального потенциала, представленного при помощи аппроксимации Падэ. Приводим к общему алгоритму: непрерывный переход от $H_0^{(1)}$ к $H_0^{(2)}$, плюс повышение точности даст две энергетические кривые, пересечение которых представляет оптимальный результат.

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Znojil M.

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A New Algebraic Majorization-Minorization Eigenvalue Method

A parallel majorization and minorization of a Hamiltonian H (i.e., its energies E) is proposed as an improvement of the standard variational or perturbative techniques. It employs band matrices H_0 ($H_0^{(1)} \geq H$, $H_0^{(2)} \leq H$) diagonalizable exactly by means of the analytic matrix continued fractions. The application of this general methodical idea to the one-body problem with the anharmonic and Padé potentials is described in detail. A new, "optimal" computational algorithm is suggested whenever a smooth interpolation between $H_0^{(1,2)}$ exists.

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

Communication of the Joint Institute for Nuclear Research. Dubna 1986