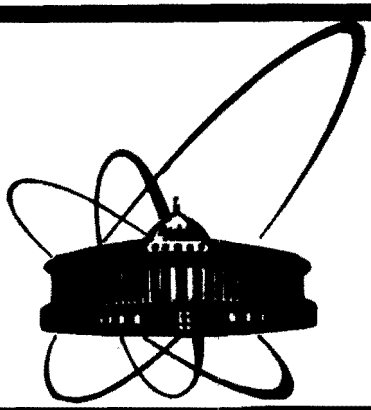

сообщения
объединенного
института
ядерных
исследований
дубна

E17-87-681

M.Znojil

CHAIN MODELS WITH THE PERIODIC BOUNDARY CONDITIONS

1987

1. INTRODUCTION

For a number of systems ranging from the quasilinear molecules /1/ up to the metallic lattices /2/ and chain models /3/, Schroedinger equation has a simple "strong-coupling" form

$$c_n z_{n-1} + a_n z_n + b_n z_{n+1} = 0 , \tag{1.1}$$

where z_n denotes the wavefunction components and coefficients a_n, b_n and c_n correspond to the matrix elements of the Hamiltonian. The boundary conditions pertaining to (1.1) may have a form

$$z_0 = 0 , \quad z_{N+1} = 0 \tag{1.2}$$

or

$$z_0 = z_{N+1}, \quad z_N = z_{-1} \tag{1.3}$$

(cf., e.q., /1/ for details).

In the models of the type (1.1), a number of properties and qualitative features of the system in question may be described numerically in an extremely efficient manner. Formally, we may treat an imposition of the boundary conditions (1.3) as a reformulation and conversion of (1.1) into an $N+1$ — dimensional matrix equation $(H - E)\, z = 0$, i.e.,

$$\begin{pmatrix} a_0 & b_0 & & & & c_0 \\ c_1 & a_1 & b_1 & & & \\ & c_2 & a_2 & b_2 & & \\ & & \cdots & & & \\ & & & c_{N-1} & a_{N-1} & b_{N-1} \\ b_N & & & & c_N & a_N \end{pmatrix} \begin{pmatrix} z_0 \\ z_1 \\ z_2 \\ \cdots \\ z_{N-1} \\ z_N \end{pmatrix} = 0 . \tag{1.4}$$

Such a linear equation is usually solved on the computer.

The trivial boundary conditions (1.2) may be reflected in the same way, giving the matrix equation

$$\begin{bmatrix} a_1 & b_1 & & & \\ c_2 & a_2 & b_2 & & \\ & \cdots & & & \\ & & c_{N-1} & a_{N-1} & b_{N-1} \\ & & & c_N & a_N \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \\ \cdots \\ z_{N-1} \\ z_N \end{bmatrix} = 0 . \qquad (1.5)$$

This equation has a simpler structure and differs from (1.4) formally by the additional requirements $z_0 = b_0 = c_0 = 0$. Moreover, its tridiagonality implies a possibility of using the special recurrent diagonalisation algorithms [4]. They may save significantly both the computer time and storage.

In some cases, a physical interpretation as well as a structure of the results happen to be more transparent for the periodic boundary conditions (1.4) [5]. This inspired the present considerations — we intend to show that the periodic chains of the type (1.4) admit also a use of the recurrent and very simple recurrent computational techniques.

The three-term recurrent structure of the Schroedinger equation (e.g., eq. (1.1)) is not always sufficient in practice. A deeper theoretical analysis of the strong-coupling systems as well as an interpretation of the measurements may necessitate a transition to the more complex Hamiltonians. Hence, we shall extend our attention immediately to the general multicomponent recurrences.

2. SCHROEDINGER EQUATIONS

In the first step, let us introduce an adequate notation. After a partitioning of the wavefunction components into p-plets $Z_m^{[k]}$, $k = 1,2,..,p$, $m = 0,1,...$, we shall postulate the Schroedinger equation as recurrences

$$C_n Z_{n-1} + A_n Z_n + B_n Z_{n+1} = 0 , \qquad (2.1.)$$

where C_n, A_n and B_n are the $p \times p$ —dimensional matrices now.

The multiterm analogues of the boundary conditions (1.2) and (1.3) read

$$Z_0^{[k]} = 0 , \quad Z_{N+1}^{[k]} = 0 , \qquad k = 1,2,...,p \qquad (2.2)$$

and

$$Z_0^{[k]} = Z_{N+1}^{[k]} , \quad Z_N^{[k]} = Z_{-1}^{[k]} , \quad k = 1,2,...,p \qquad (2.3)$$

respectively.

Of course, the partitioned-matrix generalisation of the Schroedinger eq. (1.4),

$$\begin{bmatrix} A_0 & B_0 & & & & C_0 \\ C_1 & A_1 & B_1 & & & \\ & C_2 & A_2 & B_2 & & \\ & & \cdots & & & \\ & & & C_{N-1} & A_{N-1} & B_{N-1} \\ B_N & & & & C_N & A_N \end{bmatrix} \begin{bmatrix} Z_0 \\ Z_1 \\ Z_2 \\ \cdots \\ Z_{N-1} \\ Z_N \end{bmatrix} = 0 . \qquad (2.4)$$

as well as the analogous generalisation of (1.5)

$$\begin{bmatrix} A_1 & B_1 & & & \\ C_2 & A_2 & B_2 & & \\ & \cdots & & & \\ & & C_{N-1} & A_{N-1} & B_{N-1} \\ & & & C_N & A_N \end{bmatrix} \begin{bmatrix} Z_1 \\ Z_2 \\ \cdots \\ Z_{N-1} \\ Z_N \end{bmatrix} = 0 . \qquad (2.5)$$

are to be analysed numerically. In this formulation, our main task may be characterised briefly as an extension of the more or less standard recurrent band-matrix methods [6,7] to the more complicated periodic-boundary-condition case (2.4).

3. THE RECURRENT FACTORISATION

The Hamiltonian entering the Schroedinger eq. (2.4),

$$H - E = \begin{bmatrix} A_0 & B_0 & & & & C_0 \\ C_1 & A_1 & B_1 & & & \\ & C_2 & A_2 & B_2 & & \\ & & & & C_{N-1} & A_{N-1} & B_{N-1} \\ B_N & & & & & C_N & A_N \end{bmatrix} \qquad (3.1)$$

is to be decomposed now, in the spirit of [6], into a product of matrices $H - E = U \times L$, where U and L have a simpler structure.

For the sake of definitness, let us postulate that

$$U = \begin{bmatrix} I & X_1 \cdot F_1 & X_2 \cdot F_2 & & \cdots & & X_N \cdot F_N \\ & I & B_1 \cdot F_2 & 0 & \cdots & & 0 \\ & & I & B_2 \cdot F_3 & \cdots & & 0 \\ & & & \cdots & & I & B_{N-1} \cdot F_N \\ & & & & & & I \end{bmatrix} \qquad (3.2)$$

and

$$L = \begin{bmatrix} 1/F_0 & & & & & \\ Y_1 & 1/F_1 & & & & \\ Y_2 & C_2 & 1/F_2 & & & \\ Y_3 & 0 & C_3 & 1/F_3 & & \\ \cdots & & & \cdots & & \\ Y_N & 0 & \cdots & 0 & C_N & 1/F_N \end{bmatrix} \tag{3.3}$$

and notice that the decomposition $H - E = UL$ represents in fact the direct generalisation of the continued-fractional formulas /6/.

Due to the regularity of the first factor U, our Schroedinger equation (2.4) may be re-written as a simpler matrix requirement

$$L Z = 0 . \tag{3.4}$$

The explicit specification of its matrix elements is a recurrent procedure. With the initial values

$$F_N = 1/A_N , \quad X_N = C_0 , \quad Y_N = B_N \tag{3.5}$$

it may be characterised as a recurrent definition of the auxiliary sequence of matrices

$$F_k = 1/(A_k - B_k F_{k+1} C_{k+1}) , \quad k = N-1 , N-2 , \ldots , 1 \tag{3.6}$$

and of their products

$$X_k = -X_{k+1} F_{k+1} C_{k+1} , \quad k = N-1, N-2, \ldots, 2 \tag{3.7}$$

and

$$Y_k = -B_k F_{k+1} Y_{k+1} , \quad k = N-1 , N-2, \ldots, 2 . \tag{3.8}$$

The remaining items must be computed separately, with

$$X_1 = -X_2 F_2 C_2 + B_0 \tag{3.9}$$

and

$$Y_1 = -B_1 F_2 Y_2 + C_1 \tag{3.10}$$

and, finally, by the formula

$$1/F_0 = A_0 - X_1 F_1 Y_1 - X_2 F_2 Y_2 - \ldots - X_N F_N Y_N . \tag{3.11}$$

The latter matrix differs from its continued fractional predecessors encountered in the block-wise tridiagonal case (2.5) /6/, but an overall structure of the formulas remains only slightly modified.

4. THE SOLUTIONS FOR THE PERIODIC BOUNDARY CONDITIONS

In the light of eq. (3.4), the secular equation $\det (H - E) = 0$ acquires here the simple form $\det L = 0$. Moreover, when we assume that the recurrences (3.6) remain non-singular in a vicinity of an eigenvalue E, this zero E of our pN — dimensional secular determinant $\det L$ will coincide precisely with the zero E of determinant of our only remaining and not necessarily regular diagonal submatrix of L,

$$\det 1/F_0 = 0 . \tag{4.1}$$

Due to the validity of eq. (4.1) at each eigenvalue E, we may also find the corresponding p — dimensional vector L_0 which satisfies the related p — dimensional homogeneous equation,

$$\sum_{k=1}^{p} (1/F_0)^{[i,k]} Z_0^{[k]} = 0 . \tag{4.2}$$

Up to an overall normalisation, it will coincide with the first p components of the wavefunction Z in (3.4).

The rest of our Schroedinger equation (3.4) acquires the recurrent form again, with the second initial vector

$$Z_1 = -F_1 Y_1 Z_0 \tag{4.3}$$

and with the subsequent sequence of definitions

$$Z_k = -F_k Y_k Z_0 - F_k C_k Z_{k-1} , \quad k = 2, 3, \ldots, N \tag{4.4}$$

this is our final formula.

We may summarise that the recurrences (4.3) — (4,4) and (3.5) — (3.11) enable us to extend an arbitrary auxiliary solution of equations (4.1) and

(4.2) to a full solution of our Schroedinger equation (2.4) related to the periodic choice of the boundary conditions (2.3).

In the computations, we may also recommend taking the final $k=N$ result of eq. (4.4) and using its backward insertion in the first row of eq. (2.4) as a selfconsistency check

$$C_0 Z_N + A_0 Z_0 + B_0 Z_1 = 0 . \tag{4.5}$$

In the case of stability of the employed recurrences, a numerical investigation of the $N \to \infty$ limit becomes then feasible in the full analogy with the purely tridiagonal case [7].

5. A REMARK ON APPLICABILITY OF THE PERTURBATION TECHNIQUES

In practice, an approximation of some $p > 1$ chain models by the simpler Hamiltonians H' with $p' < p$ is usually very natural [1,5]. In such a setting, we may treat the general Hamiltonian as a superposition of H' with some small perturbation and, in accord with our preceding methodical paper [8], employ simply a suitable form of the standard Rayleigh-Schroedinger perturbation theory [9]. A necessary and sufficient condition of applicability is merely an availability of inverse of the matrix $H'-E$.

In this context, our present factorisation of sect. 3 may immediately be recalled as a suitable technical background of the formalism, with the binding energies and wavefunctions given in the quoted paper [8]. The input "unperturbed" propagator

$$R = 1/(E-H) = -(1/L) \times (1/U) \tag{5.1}$$

(with the simplified $H=H'$) may easily be constructed in terms of the inverse

$$U^{-1} = \begin{bmatrix} I & -D_{01} & D_{02} & -D_{03} & D_{04} & \cdots \\ & I & -D_{12} & D_{13} & -D_{14} & \cdots \\ & & \cdots & & & \cdots \\ & & & & I & -D_{N-1N} \\ & & & & & I \end{bmatrix} , \tag{5.2}$$

where

$$D_{01} = X_1 F_1 , \quad D_{0k} = D_{0k-1} B_{k-1} F_k + (-1)^{k+1} X_k F_k , \quad k = 2, 3, \ldots, N . \tag{5.3}$$

The two-term recurrences should be used again as definitions of the necessary matrix elements

$$D_{jj} = 1 , \quad D_{jk} = D_{jk-1} B_{k-1} F_k , \quad k = j+1, j+2, \ldots, N \tag{5.4}$$
$$j = 1, 2, \ldots, N-1 ,$$

The derivation of these formulas as well as their modification for the lower triangular matrix L is entirely straightforward.

We may summarise that the analogy between eqs. (2.4) and (2.5) is almost complete — both cases admit a use of the recurrent construction of the solutions, by the methods with almost the same structure.

6. AN ILLUSTRATION ON THE EXACTLY SOLVABLE EXAMPLES

6.1. The Exactly Solvable Model with the Trivial Boundary Conditions

Let us recall first a $p=1$ example of eq. (2.5) or (1.5) [10]

$$\begin{bmatrix} -2x & 1 & & & \\ 1 & -2x & 1 & & \\ & 1 & -2x & 1 & \\ & & \cdots & & \\ & & & 1 & -2x \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \\ z_3 \\ \cdots \\ z_N \end{bmatrix} = 0 \tag{6.1}$$

as a methodical inspiration of the present considerations. Without the first and last line (boundary conditions), this is a set of equations satisfied identically by any superposition

$$z_n = a\, U_n(x) + b\, T_n(x) \tag{6.2}$$

of Tchebyshev polynomials U and T of the second and first kind, respectively [11]. Obviously, the boundary conditions ((2.2) or (1.2)) restrict this freedom.

At $n=0$, we may insert the values of polynomials ($T_0 = U_0 = 1$) and get $a+b=0$, i.e.,

$$z_n = b[T_n(x) - U_n(x)] = -bx\, U_{n-1}(x) , \quad bx = 0 . \tag{6.3}$$

At $n = N+1$, we may write $x = \cos t$ and get the complete admissible spectrum of energies in an elementary form

$$x = x_k = \cos[k\pi/(N+1)], \quad k = 1, 2, \ldots, N \tag{6.4}$$

6.2. An Exactly Solvable Model with the Periodic Boundary Conditions

In the spirit of eq. (6.1), let us consider its analogue

$$\begin{bmatrix} -2x & 1 & & & 1 \\ 1 & -2x & 1 & & \\ & 1 & -2x & 1 & \\ & & \ldots & & \\ & & 1 & -2x & 1 \\ 1 & & & 1 & -2x \end{bmatrix} \cdot \begin{bmatrix} z_0 \\ z_1 \\ z_2 \\ \ldots \\ z_{N-1} \\ z_N \end{bmatrix} = 0 \tag{6.5}$$

with the general solution (6.2) re-written in an alternative form

$$z_n = cU_n(x) - dU_{n-1}(x) \tag{6.6}$$

where $c = a + b$ and $d = d(x) = bx$.

The periodic boundary conditions (2.3) or (1.3) acquire here the more complicated character,

$$\begin{aligned} c &= cU_{N+1}(x) - dU_N(x) \\ cU_N(x) &- dU_{N-1}(x) = d. \end{aligned} \tag{6.7}$$

Let us assume that $cd = 0$ and eliminate this product from (6.7),

$$U_N^2 = (U_{N+1} - 1)(U_{N-1} + 1). \tag{6.8}$$

In terms of the trigonometric functions, this equation reads

$$\sin^2 s = \sin^2 s \cos^2 t - \sin^2 t (1 - \cos s)^2, \quad s = (N+1)t \tag{6.9}$$

and leads immediately to the compact and explicit eigenvalue formula again,

$$x = \cos t = \cos[2k\pi/(N+1)], \quad k = 0, 1, \ldots, [(N+1)/2]. \tag{6.10}$$

6.3. The Numerical Tests

In contrast to the simple spectrum (6.4), our periodic solution (6.10) does not possess $N+1$ different energies. The more detailed analysis recovers that unless $k = 0$ or $k = [(N+1)/2]$, the eigenvalues (6.10) are doubly degenerate. We may also see immediately that all the degenerate energies coincide with the even non-degenerate eigenvalues of the subsystem (6.1). Hence, the pairs of the related eigenvectors may still be obtained very easily, namely, from the pair of normalisations $z_0 = 1$ and $z_0 = 0$ and $z_1 = 1$.

In a numerical test of properties of our recurrent method, we intend to study the behaviour of the secular equation (say, (4.1)) and "selfconsistency" (condition (4.5)) in a vicinity of the exact "energies" x.

For the different choices of the free parameters N and k, the results are summarised in two tables. Table 1 illustrates a reliability of evaluation of the energies. Under certain restrictions (admitting the degenerate levels at even N only), our sample of results illustrates nicely the stability of roots of the secular equation in our recurrent methodical framework.

It is worth emphasising that near the degenerate energies, we encounter in fact a singularity of our whole decomposition of the Hamiltonian ($1/F_1 \to 0$ in (3.3)). This makes our test very persuading. It is really rather surprising that we obtained the correct energies for the even N's. In the more complicated examples (including the odd N's here), the singularities will not cancel so nicely due to the larger rounding errors.

In fact, a "decay" of the doubly degenerate root into a pair of the simple roots of $1/F_0$ and $1/F_1$ represents an important and rather unexpected merit of the present method. Indeed, the general numerical determination of the doubly degenerate roots of the secular determinant is very difficult. In our approach, functions $1/F_0$ and $1/F_1$ are more easily tractable since their roots are simple.

Table 2 displays the behaviour of the test identity (4.5) after the recurrent evaluation of the wavefunctions. We may notice again a remarkable stability of recurrences for even dimensions N (where the singularities of F_0 and F_1 cancel each other with a very good precision). For odd N, the second wavefunction still remains precise enough, but the first wavefunction may be seen to suffer from the mutual interplay of both the singularities (by chance, both of them are seen at $N = 11$). The exceptions (marked by the asterisk *) appear whenever the energy becomes non-degenerate.

We may summarise that, rather surprisingly, even the degenerate levels may be treated sometimes by the present method. Nevertheless, our main interest concern the simple, non-degenerate roots. There, no problems appear and, by the way, all the values of $1/F$ and Q practically coincide. Hence, also the recurrently evaluated wavefunctions are sufficiently precise and satisfy very well our testing identity (4.5). This confirms our belief in a reliability and numerical stability of the proposed recurrent algorithm when applied to the more realistic physical models in the future [12].

Table 1

Recurrent method for energies — verification of eq. (4.1)

first level (k = 0, exact x = 1)				
dimension	error	y = x − d	y = x	y = x + d
N	d		$10^4/F_0(y)$	
2	9.10^{-4}	55	0.00045	-55
3	5.10^{-4}	41	0.0021	-41
4	3.10^{-4}	33	0.00078	-33
48	3.10^{-6}	3.3	-0.00077	-3.4
49	3.10^{-6}	3.3	-0.00024	-3.3
50	3.10^{-6}	3.2	-0.00027	-3.2

second level (k = 1)				
dimension	energies	y = x − d	y = x	y = x + d
N	x		$10^4/F_0(y)$	
2	-0.500	27	0.088	-27
4	0.309	17	0.098	-16
18	0.946	4.4	0.035	-4.3
20	0.956	3.9	0.028	-3.9

eleventh level (k = 10)				
dimension	energies	y = x − d	y = x	y = x + d
N	x		$10^4/F_0(y)$	
18	-0.986	4.2	- 0.16	-4.5
20	-0.989	4.1	+0.16	-3.8

Table 2

Recurrent method for wavefunctions — verification of eq. (4.5)

normalisation		$z_0 = 1$		$z_0 = 0$, $z_1 = 1$		
deviations		$G(y) = 10^4 x(a_0 z_0 + b_0 z_1 + c_0 z_N)$				
N	x	y = x − d	x	x + d	x − d	x	x + d
2	-0.50	28	0.35	-27	18	0.23	-18
3	1.00	41	0.000	-41	10^4	10^4	10^4
4	0.31	16	-0.39	-17	-5.5	0.13	5.7
5	-0.50	14	6.2	-15	8.9	-0.24	-9.4
6	-0.90	12	-0.18	-12	55	-0,85	-57
7	-1.00 (*)	21	0.000	-21	10^4	10^4	10^4
8	-0,94	9,3	0.14	-9.0	74	1.1	-73
9	-0.81	9.5	-12.0	-8.4	20	0.57	-19
10	-0.65	7.8	0.31	-7.2	8.9	0.35	-8.2
11	-0.50	3.7	0.088	0.094	4.8	0.23	-4.3
12	-0.35	6.7	0.38	-5.9	2.7	0.16	-2.4

REFERENCES

1. *Baeriswyl D. In: Theoretical Aspects of Band Structures and Electronic Properties of Pseudo-One-Dimensional Solids, ed. H.Kamimura, D.Reidel.Publ. Comp., Amsterdam, 1985.*
2. *Mach R. JINR Comm. E1.4-86-680, Dubna, 1986.*
3. *Bullett D.W., Haydock R, Heine V., Kelly M.J. Solid State Physics, v.35, ed. H.Ehrenreich et al., Academic, New York, 1980.*
4. *Wilkinson J.H. The Algebraic Eigenvalue Problem, Clarendon, Oxford, 1965.*
5. *Malek J., Drechsler S., Heiner E. – Phys. Stat. Sol., to appear.*
6. *Graffi S., Grecchi V. – Lett. Nuovo Cimento, 1975, 12, p.425.*
   Znojil M. – Phys. Rev., 1981, D24, p.903.
7. *Znojil M. – J. Math. Phys., 1984, 25, p.2579; JINR. Comm. E5-87-634, Dubna, 1987.*
8. *Znojil M. – Phys. Rev., 1987, A35, , p.2448; Phys. Lett., 1987, A120, p.317; JINR Comm. E4-87-655, E4-87-667, Dubna, 1987.*
9. *Morse P.M. Feshbach H. Methods of Theoretical Physics, McGraw-Hill, New York, 1953.*
10. *Znojil M., Flynn M., Bishop R.F. in preparation.*
11. *Korn G.A., Korn T.M. Mathematical Handbook, McGraw-Hill, New York, 1968.*
12. *Malek J. Znojil M. in preparation.*

Received by Publishing Department
on September 10, 1987.

SUBJECT CATEGORIES OF THE JINR PUBLICATIONS

Index	Subject
1.	High energy experimental physics
2.	High energy theoretical physics
3.	Low energy experimental physics
4.	Low energy theoretical physics
5.	Mathematics
6.	Nuclear spectroscopy and radiochemistry
7.	Heavy ion physics
8.	Cryogenics
9.	Accelerators
10.	Automatization of data processing
11.	Computing mathematics and technique
12.	Chemistry
13.	Experimental techniques and methods
14.	Solid state physics. Liquids
15.	Experimental physics of nuclear reactions at low energies
16.	Health physics. Shieldings
17.	Theory of condenced matter
18.	Applied researches
19.	Biophysics

Зноил М. E17-87-681

Модели сильной связи с периодическими граничными условиями

Предлагается новая рекуррентная схема численного решения уравнения Шредингера для систем с сильной связью между близкими состояниями данного базиса. Традиционная теория возмущений расходится и стандартные рекуррентные схемы оказываются не применимы при наличии периодических граничных условий. В статье пополняется этот методический пробел и оба названные подхода усовершенствуются соответствующим способом. Для их иллюстрации описывается также одна точно решаемая простая модель, энергии и состояния которой воспроизводятся почти точно при использовании настоящего метода. Делается заключение, что рекуррентные подходы к стандартным (тривиальным) и периодическим граничным условиям вполне эквивалентны.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Сообщение Объединенного института ядерных исследований. Дубна 1987

Znojil M. E17-87-681

Chain Models with the Periodic Boundary Conditions

The well-know recurrent tractability of the tridiagonal Hamiltonians and their band-matrix generalizations is extended to the similar strong-coupling quantum systems (chain models) with the periodic boundary conditions. Keeping in mind, e.q., the possible applications to the polyacetylene-like quasi-one-dimensional molecules, the recurrent method of diagonalising the resulting more general Hamiltonian matrices is destribed in detail. On a simple exactly solvable example, it is demonstrated that the method may be expected to work well in the realistic applications in the future.

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

Communication of the Joint Institute for Nuclear Research. Dubna 1987