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Novel recurrent approach to the generalized Su-Schrieffer-Heeger Hamiltonians

Miloslav Znojil
Institute of Nuclear Physics, Czechoslovak Academy of Sciences, 250 68 Rez near Prague, Czechoslovakia

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The molecule of polyacetylene is contemplated as a typical quantum many-body system with quasi-one-dimensional structure. Its description is usually accompanied by a puzzling yet quite generally accepted belief that there is a significant formal (but practically no physical) difference between the molecules with the linear and cyclic (closed-loop) shapes. Here we shall show that the formal differences are also insignificant, provided only that we search for the respective electronic bound states and energies within the framework of the new recurrent technique. Even in the infinite-molecule limit, the method remains very efficient—its effective Hamiltonians and/or Green's functions remain simple and become expressed in terms of the analytic continued fractions. We also extend the formalism to refined distant-neighbor-interaction models. Numerically our approach proves very reliable—this is illustrated in detail on the simple exactly solvable Hückel Hamiltonians.

I. INTRODUCTION

The one-dimensional and pseudo-one-dimensional solids attract theoreticians by their simplicity as well as by their interdisciplinary aspects relating quantum chemistry to field theory.[1] Their typical and comparatively easily measurable example is the polyacetylene or polyyne molecule.[2] Due to its possible large length, such a system is even of a purely mathematical interest: It may be analyzed in the continuum limit,[3] it exhibits a broad spectrum of the self-localized nonlinear (solitonic and polaronic) nonlinear excitations,[4] etc.

For the finite number N_A of the chained components ("sites" or "acetylenes"), the numerical studies may trace the various deviations from the continuum-limit predictions (cf. Ref. 1 or the recent references as quoted, e.g., in Refs. 4 or 5). Some of them even follow from the "simplest nontrivial" Hückel Hamiltonian

$$H=\left[\begin{array}{ccccc} a_1 & b_1 & \cdots & & \\ b_1 & a_2 & b_2 & & \\ \vdots & \ddots & \ddots & \ddots & \\ & & b_{N-2} & a_{N-1} & b_{N-1} \\ & & & b_{N-1} & a_N \end{array}\right] \tag{1.1}$$

with $a_i=0$ and $b_i=1$, which may be diagonalized exactly.[6]

Of course, a more realistic form of the matrix elements in (1.1) is usually needed in practice. Then, Eq. (1.1) may be interpreted as the Su-Schrieffer-Heeger[7] (SSH) Hamiltonian for the electronic states, and it still remains tractable by the efficient numerical techniques.[8,9]

A number of very interesting problems arises in connection with the possible solitonic excitations of long molecules of the SSH type.[4] This is closely related to their topology, e.g., the parity of N plays then a role. In the latter context, a highly relevant situation is represented by a molecule which forms a closed loop. Unfortunately, the corresponding periodic or cyclic version of the model,

$$H=\left[\begin{array}{ccccc} a_0 & b_0 & \cdots & & b_M \\ b_0 & a_1 & b_1 & & \\ \vdots & \ddots & \ddots & \ddots & \\ & & b_{M-2} & a_{M-1} & b_{M-1} \\ b_M & & & b_{M-1} & a_M \end{array}\right] \tag{1.2}$$

(with an "additional" molecule which "glues" both ends together, i.e., with $N_A=M+1$), ceases to be simple from the purely numerical point of view. In the computations,[5] its eigenstates and energies are usually constructed by a general-matrix diagonalization[9] or by some more complicated algebra (see, e.g., Ref. 10 and references given therein).

Obviously, the new matrix H, (1.2), remains "very sparse" and simple. In our notation, we may see that the new cyclic Hamiltonian describes the linear molecule simply as one of its possible subsystems. Hence, the numerical complexity of the cyclic problems seems quite unsatisfactory and forms one of the main motivations of the present paper.

Indeed, the formal importance of the matrix elements b_M in (1.2) contrasts sharply with their widely accepted physical irrelevance.[5] Thus, in what follows, we intend to show that also the formal difference between the structure of matrices (1.1) and (1.2) need not be considered essential. We shall propose (and verify the reliability of) a method which is recurrent and similar to the Haydock technique.[8] At the same time, in contrast to the assumptions of Ref. 10, we shall be able to treat both linear and cyclic cases (1.1) and (1.2) simultaneously. Moreover, we shall also be able to extend the applicability of the underlying factorization idea immediately to Hamiltonians of the generalized SSH type. This will be our main result.

In a few final and very simple tests of the related numerical-precision features, the well-known exact values of the Hückel spectra will be reproduced.

In detail, the material will be separated into the discussion of the linear (Sec. II) and cyclic (Sec. III) cases, and the numerical tests and related considerations will be presented in Sec. IV. Section V is a summary.

II. LINEAR CHAINS

A. The notation

The simple SSH Hamiltonians[7] define the energies and wave functions $|\psi\rangle$ of electrons in the polyacetylene as solutions of the Schrödinger equation

$$H|\psi\rangle = E|\psi\rangle \tag{2.1}$$

with the self-consistently specified matrix elements of H. We may also interpret the wave function $|\psi\rangle$ as pertinent to a single difference equation

$$c_n\langle n-1|\psi\rangle + (a_n - E)\langle n|\psi\rangle + b_n\langle n+1|\psi\rangle = 0\ , \quad c_n = b_{n-1} \tag{2.2}$$

accompanied by the two alternative sets of the related boundary conditions

$$\langle 0|\psi\rangle = 0,\quad \langle N+1|\psi\rangle = 0 \tag{2.3}$$

and

$$\langle 0|\psi\rangle = \langle M+1|\psi\rangle,\quad \langle M|\psi\rangle = \langle -1|\psi\rangle\ , \tag{2.4}$$

respectively. In such a formulation, it is easier to discuss and understand the nature of the most important corrections to the simple SSH model.

For the sake of definiteness, let us pick up just the class of generalizations which takes into account the long-range-hopping corrections (next-neighbor or, in general, *p*th-neighbor interactions—see, e.g., Ref. 11). This corresponds to the $(2p+1)$-term generalization of our difference Schrödinger equation (2.2),

$$\begin{gathered} c_n^{(p)}\langle n-p|\psi\rangle + \cdots + c_n^{(1)}\langle n-1|\psi\rangle + (a_n - E)\langle n|\psi\rangle \\ + b_n^{(1)}\langle n+1|\psi\rangle + \cdots + b_n^{(p)}\langle n+p|\psi\rangle = 0\ , \\ c_n^{(1)} = b_{n-1}^{(1)},\quad c_n^{(2)} = b_{n-2}^{(2)},\quad \ldots,\quad c_n^{(p)} = b_{n-p}^{(p)} \end{gathered} \tag{2.5}$$

and also of the boundary conditions (2.3) or (2.4).

In the first step, for the sake of simplicity of the notation, let us reinterpret the set of the components or projections of the wave function $\langle n|\psi\rangle$ as a partitioned column vector

$$\begin{bmatrix} \vdots \\ (Z_k)_1 \\ (Z_k)_2 \\ \vdots \\ (Z_k)_p \\ (Z_{k+1})_1 \\ \vdots \end{bmatrix} \tag{2.6}$$

and let us start our discussion from the linear molecules, with the boundary conditions of the type (2.3),

$$(Z_0)_j = 0,\quad (Z_{N+1})_j = 0,\quad j = 1, 2, \ldots, p\ . \tag{2.7}$$

Whenever N_A differs from an integral multiple of p, we may still set $N_A = (N-1)p + q$ (with $0 < q < p$) and reinterpret simply Z_1 as a subvector

$$\begin{bmatrix} (Z_1)_1 \\ (Z_1)_2 \\ \vdots \\ (Z_1)_q \end{bmatrix} \tag{2.8}$$

of a smaller dimension. This enables us to rewrite our difference Schrödinger equation (2.5) in the partitioned ("vectorial" or "matrix") three-term form,

$$C_n Z_{n-1} + A_n Z_n + B_n Z_{n+1} = 0,\quad A_n = A_n^T,\ C_n = B_{n-1}^T \tag{2.9}$$

with $C_1 = B_0 = 0$, $B_N = C_{N+1} = 0$, and $n = 1, 2, \ldots, N$. The capital-letter coefficients B, C, and A [notice that $A = A(E)$ in the new notation] coincide with the submatrices of the $(N_A \times N_A)$-dimensional matrix

$$H - EI = \begin{bmatrix} A_1 & B_1 & \cdots & & \\ C_2 & A_2 & B_2 & & \\ \vdots & \ddots & \ddots & \ddots & \\ & & C_{N-1} & A_{N-1} & B_{N-1} \\ & & & C_N & A_N \end{bmatrix} \tag{2.10}$$

entering our Schrödinger equation in its form (2.1).

B. The factorization and solution of the Schrödinger equation

Let us consider large (finite) or infinite dimensions N_A and small q (not necessarily equal to p). Then, a new and appropriate method of solving our Schrödinger equation may be obtained as a suitable generalization or modification of the construction described in Ref. 12. Its basic idea lies in a factorization of $H - EI$ of the special type,

$$H - EI = U \begin{bmatrix} 1/F_1 & & & \\ & 1/F_2 & & \\ & & \ddots & \\ & & & 1/F_N \end{bmatrix} U^T\ . \tag{2.11}$$

Here, the partitioned factor matrices U are postulated to have a simple form with two nonzero diagonals,

$$U = \begin{bmatrix} 1 & B_1F_2 & 0 & \cdots & 0 \\ \vdots & 1 & B_2F_3 & 0 & \cdots \\ & & \ddots & \ddots & \\ & & & 1 & B_{N-1}F_N \\ & & & & 1 \end{bmatrix}\ . \tag{2.12}$$

A brief inspection of these formulas, where

$$1/F_i = A_i - B_i F_{i+1} C_{i+1}, \quad i=1,2,\ldots,N \tag{2.13}$$

and $B_N=0$ by definition, shows that we must assume an existence of the $(p \times p)$-dimensional inversions,

$$\det(1/F_{i+1}) \neq 0, \quad i=N-1,N-2,\ldots,1 \ . \tag{2.14}$$

Vice versa, once our assumption (2.14) is satisfied in a vicinity of some eigenvalue, we may immediately conclude that the simple equation

$$\det[1/F_1(E)]=0 \tag{2.15}$$

defines the values of the binding energies numerically.

The numerical location of an arbitrary root of the secular equation (2.15) generates also the whole sequence F_n at the same energy as a by-product. This is very important—we may then divide the whole equation (2.1) by the (by definition, regular) matrix U from the left and get

$$\begin{bmatrix} 1/F_1 & & & \\ C_2 & 1/F_2 & & \\ & \ddots & \ddots & \\ & & C_N & 1/F_N \end{bmatrix} \begin{bmatrix} Z_1 \\ Z_2 \\ \vdots \\ Z_N \end{bmatrix} \ . \tag{2.16}$$

The first q rows of the new equation will read $(1/F_1)Z_1=0$, i.e.,

$$(A_1 - B_1 F_2 C_2) Z_1 = 0 \tag{2.17}$$

and determine Z_1 up to an arbitrary normalization $(Z_1)_1 \neq 0$.

From the rest of Eq. (2.16), the remaining components Z_{n+1} of the wave function may immediately be obtained in a recurrent manner. Indeed, the q-dimensional input set Z_1 enables us to define the p quantities

$$Z_2 = -F_2 B_1^T Z_1 \ , \tag{2.18}$$

etc.

As long as we keep the dimension p of the $k>1$ partitions (2.6) constant, it may happen that also the square matrices $B_2, B_3, \ldots$ remain regular. In such a case, Eq. (2.9) may serve directly as an alternative and simpler recurrent definition of the remaining Z's.

C. Repartitioning

In a "subset of measure zero" in the space of coupling constants (which may still be of interest, of course), it may happen that just for our choice of the dimension N and energy E, the decomposition (2.11) of our Hamiltonian ceases to exist, i.e., the determinant of $1/F_{N+1-k}$ becomes zero at some $k<N$ and our requirement (2.14) becomes violated at $i=N-k$.

Such a phenomenon has a simple interpretation. The corresponding $(kN \times kN)$-dimensional submatrix of H becomes singular and we may find the nontrivial eigenstates of H with

$$Z_1 = 0, \ldots, Z_{N-k} = 0 \ , \tag{2.19}$$

and with the given parameter E determining the energy.

In the computations, the appearance of a singularity in the inversion $1/F \rightarrow F$ may prove to be a nuisance even for $p=1$.[9] In the $p>1$ cases, we may get rid of it very easily, via a rearrangement of the matrix H. One of the simplest possibilities lies in mere repartitioning of the vectors Z—it preserves both the existence and form of our factorization (2.11). For the sake of definiteness, we shall diminish the dimension of Z_N to some integer $r<p$,

$$\begin{bmatrix} (Z_N)_1 \\ (Z_N)_2 \\ \vdots \\ (Z_N)_r \end{bmatrix} \ . \tag{2.20}$$

This leaves all the preceding formulas unchanged. We must only keep in mind that the former parameters N and q have also changed, reproducing the original total length

$$N_A = (N-2)p + q + r \tag{2.21}$$

of the molecule.

The broader partitioning freedom (2.21) may prove useful even in the nonsingular cases. In particular, we would recommend a choice of $q=1$ [with variable $r=r(N_A)$]. Indeed, our secular equation (2.14) acquires then the explicit scalar form

$$E = \langle 1|H|1 \rangle - \sum_{m,n=1}^{p} (B_1)_{1n} [F_2(E)]_{nm} (C_2)_{m1} \ . \tag{2.22}$$

This leads to a very natural Green's-function interpretation of our auxiliary quantity $1/F_1$ and, in an implicit manner, defines the binding energies as mean values of a continued-fractional "effective Hamiltonian" $H^{\text{eff}} = H - B_1 F_2 C_2$.

III. CYCLIC CHAINS

A. The nearest-neighbor interactions

In the cyclic SSH model (1.2), the tridiagonal Hamiltonian (1.1) becomes complemented by the additional nonzero matrix elements in the corners. However trivial such a change may seem, it forces us to treat H as a general matrix[5] or, in an algebraic setting, to switch to a complicated algebra.[10] Here, we intend to show how the recurrent factorization applies to both Eqs. (1.1) and (1.2) without any difficulties.

In the first step, we shall deal with $p=1$. Then, the decomposition of the type (2.11) will only slightly be modified. In its scalar form,

$$H - EI = U \begin{bmatrix} 1/f_0 & & & \\ & 1/f_1 & & \\ & & \ddots & \\ & & & 1/f_M \end{bmatrix} U^T \ , \tag{3.1}$$

the enriched structure (1.2) of the matrix H demands the new structure of the matrix factors, e.g.,

$$U=\begin{bmatrix} 1 & d_1f_1 & d_2f_2 & d_3f_3 & \cdots & d_Mf_M \\ \vdots & 1 & b_1f_2 & 0 & \cdots & 0 \\ & & 1 & b_2f_3 & & \\ & & & \ddots & \ddots & \\ & & & & 1 & b_{M-1}f_M \\ & & & & & 1 \end{bmatrix} . \quad (3.2)$$

They have the two (scalar) diagonals of preceding section complemented by the nonzero elements in their zeroth row.

When comparing Eq. (3.1) with its linear-molecule $p=1$ analogue, we may immediately see that the recurrent specification of the auxiliary sequence f_i remains unchanged for the positive subscripts $i>0$. Thus, it remains for us to guarantee that the factorization (3.1) reproduces also the matrix elements of H with the zero subscripts (provided that we rename also b_M as c_0). This is done easily—we set $d_M=b_M$ and define

$$d_k=-b_kf_{k+1}d_{k+1},\quad k=M-1,M-2,\ldots,2 . \quad (3.3)$$

The simplicity of this formula (which defines d's as products of b's and f's) is a consequence of the fact that most matrix elements in the first row of H vanish. Vice versa, the nonzero values of b_0 and a_0 imply that we must require that

$$d_1=-b_1f_2d_2+b_0 \quad (3.4)$$

and, finally,

$$1/f_0=a_0-E-\sum_{j=1}^{M} d_j^2f_j . \quad (3.5)$$

To summarize, in the cyclic $p=1$ case, Eqs. (2.13) may be complemented by the definitions (3.3)–(3.5), and all of the formalism (based on the factorization of $H-EI$) remains essentially the same. In particular, the energies follow again from the transcendental equation of the type (2.15),

$$1/f_0=0 . \quad (3.6)$$

The components of the wave functions are to be generated from the difference Schrödinger equation (2.9). This will be discussed in the following subsection.

B. The generalized cyclic model with $p>1$

In the case of the generalized SSH Schrödinger difference equation (2.5), the periodicity requirements read

$$\langle m|\psi\rangle=\langle m+N_A|\psi\rangle . \quad (3.7)$$

In the partitioned notation, such a condition induces again the nonzero $(p\times p)$-dimensional submatrices into the corners of H. As a consequence, we recommend the "maximal" partitioning with $q=p$ and with $r=r(N_A)$.

Having in mind the results of the preceding subsection, it is sufficient again to return to the partitioned (capital-letter) denotation in the Hamiltonian

$$H=EI=\begin{bmatrix} A_0 & B_0 & \cdots & & C_0 \\ C_1 & A_1 & B_1 & & \\ \vdots & \ddots & \ddots & \ddots & \\ & & C_{M-1} & A_{M-1} & B_{M-1} \\ B_M & & & C_M & A_M \end{bmatrix} , \quad (3.8)$$

where $A_n=A_n^T$ and $C_n=B_{n-1}^T$. Also, we may change the uppermost-row indices in the other formulas of the preceding section and, in particular, in the factorization requirement (2.11),

$$H-EI=U\begin{bmatrix} 1/F_0 & & & \\ & 1/F_1 & & \\ & & \ddots & \\ & & & 1/F_M \end{bmatrix}U^T \quad (3.9)$$

with the new factor matrices

$$U=\begin{bmatrix} 1 & D_1F_1 & D_2F_2 & D_3F_3 & \cdots & D_MF_M \\ \vdots & 1 & B_1F_2 & 0 & \cdots & 0 \\ & & 1 & B_2F_3 & & \\ & & & \ddots & \ddots & \\ & & & & 1 & B_{M-1}F_M \\ & & & & & 1 \end{bmatrix} . \quad (3.10)$$

Obviously, we reobtain recurrences (2.13) complemented by the supplementary initialization

$$D_M=C_0 \quad (3.11)$$

and by the further recurrent formulas

$$D_k=-D_{k+1}F_{k+1}C_{k+1},\quad k=M-1,M-2,\ldots,2 \quad (3.12)$$

and

$$D_1=-D_2F_2C_2+B_0 . \quad (3.13)$$

At $p=1$, they degenerate to the scalar equations of the preceding subsection.

The slightly modified expression now defines the quantity F_0, of course,

$$1/F_0=A_0-\sum_{j=1}^{M} D_jF_jD_j^T . \quad (3.14)$$

In comparison with Sec. II, the latter equation represents the only significant complication appearing in our formalism after the imposition of the periodic boundary conditions. The new definition of the p-dimensional "model-space" wave-function components becomes more complicated than Eq. (2.17),

$$\left[A_0-\sum_{j=1}^{M} D_jF_jD_j^T\right]Z_0=0 . \quad (3.15)$$

As an explicit model-space restriction of the full Schrödinger equation, it displays also the change in the effective-interaction interpretation of the matrices F in the cyclic case.

We are coming to the climax of our construction: As long as each row of our partitioned recurrences (2.9) contains three terms and there is no truncation similar to (2.7) anymore, we must proceed in full analogy with the linear molecule again. We divide our Schrödinger equation (2.1) by U from the left,

$$U^{-1}(H-EI)Z=\begin{bmatrix} 1/F_0 & & & \\ & 1/F_1 & & \\ & & \ddots & \\ & & & 1/F_M \end{bmatrix} U^T Z=0 \ , \tag{3.16}$$

and identify the first p rows of this new equation with the model-space equation (3.15). The second p rows read

$$Z_1=-F_1 D_1^T Z_0 \tag{3.17}$$

and defines the second set of Z's. Of course, the rest of Eq. (3.16),

$$Z_k=-F_k D_k^T Z_0 - F_k C_k Z_{k-1}, \quad k=2,3,\ldots,M \tag{3.18}$$

makes the construction complete. Alternatively, under the same assumptions as made in Sec. II, Eq. (2.9) could also be employed for the same purpose.

IV. A TEST OF THE METHOD ON THE HÜCKEL MODEL OF POLYACETYLENE

In accord with our preceding constructions, a formal similarity between the linear and cyclic molecules emerges only after we use the different dimension N_A in the two cases. The details may also numerically be illustrated on the simple Hückel example.

A. The exact solvability

The simplest Hückel N-dimensional Hamiltonian is given by Eq. (1.1) with $b_0=1$ and $a_0=\text{const}$ (say, zero).[6] The corresponding difference Schrödinger equation (2.2) has the form

$$z_n-2yz_{n+1}+z_{n+2}=0 \tag{4.1}$$

[with $E=2y$ in (2.1)] and may easily be recognized as recurrences satisfied by the Tchebyshev polynomials $T_n(y)$ and $U_n(y)$ of the first or second kind, respectively.[13] As a consequence, we just have to match the general solution

$$z_n=aU_n(y)+bT_n(y) \tag{4.2}$$

to the boundary conditions (2.3). Since $T_0=U_0=1$, we get $a+b=0$, i.e.,

$$z_n=a[U_n(y)-T_n(y)]=-byU_{n-1}(y) \tag{4.3}$$

for $y\neq 0$. The second boundary condition $z_{N+1}=0$ implies then simply the following explicit formula:

$$E=E_j=2y_j=2\cos[j\pi/(N+1)], \quad j=1,2,\ldots,N \ . \tag{4.4}$$

This formula describes the whole exact and complete spectrum of energies. In what follows, we shall use it in our numerical tests.

B. Periodic boundary conditions in the same example

The closed-chain analogue of the preceding tridiagonal (in fact, two-diagonal) exactly solvable Hückel model of the polyacetylene satisfies just the different boundary conditions. We employ an alternative form of the general solution

$$z_n=cU_n(y)-dU_{n-1}(y) \tag{4.5}$$

and postulate (2.4), i.e.,

$$z_{M+1}=z_0, \quad z_M=z_{-1} \ . \tag{4.6}$$

As long as $U_{-1}(x)=0$ and $U_{-2}(x)=U_0(x)=1$, we may write immediately

$$\begin{aligned} c&=cU_{M+1}(y)-dU_M(y) \ , \\ d&=cU_M(y)-dU_{M-1}(y) \ . \end{aligned} \tag{4.7}$$

The ratio of these equations implies that

$$U_M^2=(U_{M+1}-1)(U_{M-1}+1) \ , \tag{4.8}$$

while the rest defines simply the value of c as a function of d.

After an elementary trigonometric representation of Eq. (4.8),

$$\sin^2 s=\sin^2 s\cos^2 t-\sin^2 t(1-\cos s)^2 \ , \tag{4.9}$$

with $y=\cos t$ and $s=(M+1)t$, we obtain our final explicit spectral formula similar to (4.4),

$$E_j=2y_j=2\cos[2j\pi/(M+1)] \ , \quad j=0,1,\ldots,N_C, \ N_C=\lfloor (M+1)/2 \rfloor \ . \tag{4.10}$$

It is necessary to notice that the latter formula defines the doubly degenerate energies unless $j=0$ or $j=N_C$. A part of the spectrum coincides with the even energy levels (4.4), of course.

C. The numerical tests—energies

The exactly solvable examples always provide a suitable testing ground for the new methods. In the present context and notation, the linear molecules represent merely a "subsystem" of the cyclic ones (with $Z_0=0$). Of course, as a special case, they need not be considered separately. Moreover, their studies are already available—Sec. II describes just a generalization of the method of Ref. 12 after all. Moreover, a diagonalization of the $p=1$ version of the SSH model [tridiagonal Hamiltonian (1.1)] represents already a very standard numerical task.[9] Thus, we shall restrict our tests and attention to the less standard problem of Sec. III.

An evaluation of the nondegenerate ground-state energy [$j=0$ in (4.10)] remains standard; we search for the eigenvalue pertinent to our model-space Schrödinger equation (3.15). For the sake of simplicity, we shall use $p=1$:

TABLE I. The numerical confirmation of validity of our secular equation (3.6) in the vicinity of the exact ground-state energy.

Dimension of the model M	Deviation $e=e(M)$	$Q(E)=10^4/f_0(E)$ $E=1-e$	$E=1$	$E=1+e$
2	0.0009	55	0.000 45	-55
3	0.0005	41	0.0021	-41
4	0.0003	33	0.000 78	-33
48	0.000 003	3.3	$-0.000\,77$	-3.4
49	0.000 003	3.3	$-0.000\,24$	-3.3
50	0.000 003	3.2	$-0.000\,27$	-3.2

In contrast to the purely tridiagonal case (to the evaluations encountered within the framework of the so-called Lanczos method[9]), we have a number of terms now which are summed in the formula (3.5) for $1/f_0$. Thus, we have performed the first test, with the results shown in Table I. The quantity $E=1$ represents the exact energy value for all M, and we display the numerically obtained values of the "secular determinant" $Q(E)=10\,000/f_0$ at the exact $E=1$ and at neighboring points. The inspection of our results recovers that $Q(E)$ remains practically linear in the intervals shown in the Table I. The sensitivity to the "errors" in the energy remains very satisfactory for all dimensions M of the model, and the computations also remain extremely quick.

In our model, the excited energies are mostly doubly degenerate. In such a case, the standard numerical algorithms fail, and the matrix $p>1$ forms of the present formalism must *a priori* be recommended even for an analysis of the tridiagonal models.[12] Nevertheless, an interesting phenomenon has been encountered during the corresponding numerical test: In an attempt to demonstrate a failure of the $p=1$ formalism at the degenerate energies, we succeeded at the odd dimensions M only. For the even dimensions M, very surprisingly, the $p=1$ prescription still worked and gave us the pattern of results similar to the nondegenerate situation. The sample of these results may be found in Table II.

An explanation of the above phenomenon is rather straightforward and will be given in the following subsection.

D. The numerical tests — wave functions

A specific feature of the periodic boundary conditions (3.7) lies in a possibility of an arbitrary movement (up and down) along the "infinite" vector (2.6). Once we fix any p "initial" components Z_0 by solving our model-space Schrödinger equation (3.15), we may generate $Z_1, Z_2, \ldots, Z_M$ in a recurrent manner, from Eqs. (3.17) and (3.18). This is a procedure which employs the auxiliary sequence $F_n(E)$ at the numerically determined energy E. The corresponding error in energy will be projected then also into our wave functions. Thus, a nice simultaneous test of precision may be based on a verification of periodicity of the resulting Z_n's, say, via the formula

$$C_0 Z_M + A_0 Z_0 + B_0 Z_1 = 0 \; . \tag{4.11}$$

In the present $p=1$ Hückel example with the variable dimension M, we have computed the numerical value of the right-hand-side zero, i.e., of the three-term sum in (4.11). The $p=1$ results have a structure sampled here in Table III. We may add the following comments.

(a) For the nondegenerate ground states, the recurrent procedure and Eq. (3.15) are stable. Hence, we display just the results obtained for the "questionable" first excit-

TABLE II. The unexpected numerical applicability of our secular equation (3.6) near the excited energy levels (4.10) for even dimensions M.

Dimension of the model M	Exact value of the energy $X=X(M)$	$Q(E)=10^4/f_0(E)$ $E=X-e$	$E=X$	$E=X+e$
		First excited state ($j=1$)		
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
		Tenth excited state ($j=10$)		
18	-0.986	4.2	-0.16	-4.5
20	0.989	4.1	0.16	-3.8

ed states ($j=1$) and variable M.

(b) The change of normalization from (A) to (B),

$$(\mathrm{A})\ z_0=1\ ,$$

$$(\mathrm{B})\ z_1=1 \text{ and } z_0=0\ ,$$

is equivalent to a transition to the linear-molecule subsystem with the dimension $N=M$. It proves impossible whenever the energy ceases to be degenerate. These cases are marked by an asterisk—"large" means $O(10^4)$ in Table III.

(c) As a particular consequence of the above remark, we may interpret also the double degeneracy of energies as a reflection of simultaneous existence of the two possible normalizations. The singularity appears at $k=N-1$ and we get $1/f_1=0$ with $p=1$ at the exact energy. In principle, the factorization must be "regularized" by a repartitioning.

(d) As a result of a repartitioning of $H-EI$ with $p=2$, our secular equation (2.15) would acquire a (2×2)-dimensional determinantal character. For even dimensions M, the double (numerically difficult) zero of $1/f_0$ "decays" into the two simple zeros in a product representation of the determinant of $1/F_0$ with $p=2$. This is also an explanation of the numerical success of Table II. We may notice also that the pair of wave functions has a good precision for even M.

(e) For the odd dimensions, the "subsystem solution" remains comparatively good, in spite of the bad quality of the "genuine cyclic" one. For a good evaluation of the latter, the $p=2$ formalism seems necessary.

V. SUMMARY

In a methodical setting, our paper presented a $q<p$ and $r<p$ generalization of the factorization method of Ref. 12 and its extension to the nonbanded Hamiltonians of the polyacetylene type. We have shown also a few results of computations, but our numerical results should be read as preliminary: They have to be complemented by the realistic calculations going beyond their purely methodical meaning. Nevertheless, in their spirit, many of the transparent features of the solvable Hückel model may immediately be transferred to the more realistic situations. Thus, in the conclusion, we would like to emphasize a few physical aspects of such a transfer which seem relevant from the entirely pragmatic point of view.

(a) A "natural" formal framework of solving all the polyacetylene-type Schrödinger equations has been found in the factorization method. In this context, a particular

TABLE III. The test of nonperiodicity of the numerical wave functions. See text for significance of asterisk.

Dimension of the model M	Exact value of the energy $X=X(M)$	$10^4(a_0z_0+b_0z_1+b_Mz_M)$ $E=X-e$	 $E=X$	 $E=X+e$
		(A) Normalization $z_0=1$		
2	-0.50	28	0.35	-27
3*	1.00	41	0.000	-41
4	0.31	16	-0.39	-17
5	-0.50	14	6.2	-15
6	-0.90	12	-0.18	-12
7*	-1.00	21	0.000	-21
8	-0.94	9.3	0.14	-9.0
9	-0.81	9.5	-12.0	-8.4
10	-0.65	7.8	0.31	-7.2
11	-0.50	3.7	0.088	0.094
12	-0.35	6.7	0.38	-5.9
		(B) Normalization $z_1=1$ and $z_0=0$		
2	-0.50	18	0.23	-18
3*	1.00	large	large	large
4	0.31	-5.5	0.13	5.7
5	-0.50	8.9	-0.24	-9.4
6	-0.90	55	-0.85	-57
7*	-1.00	large	large	large
8	-0.94	74	1.1	-73
9	-0.81	20	0.57	-19
10	-0.65	8.9	0.35	-8.2
11	-0.50	4.8	0.23	-4.3
12	-0.35	2.7	0.16	-2.4

emphasis may be put upon an easy transition to the infinite-molecule limit and, in particular, upon a possible comparison of results with the predictions of the models solvable in that limit.

(b) The recurrent character of the presented constructions proves extremely suitable for computations with the "realistic" Hamiltonians. We might even consider the unstable systems or systems described by the complex Hamiltonians. A rather trivial change in the notation (e.g., replacing transpositions by the Hermitian conjugation) as well as in the interpretation (e.g., employing also the transposed versions of the formulas) will be sufficient for that purpose.

(c) The more or less standard imposition of the different boundary conditions (i.e., a use of the different Hamiltonian matrices) has been combined with a change of dimensions. In the cyclic case, this helped us to clarify a role which is played by an excitation of a subsystem. In fact, an emergence of the purely computational singularities finds a natural physical counterpart in an interpretation of a part of the spectrum. Such an interplay of the intuitive and computational insight seems quite important for future applications.

(d) Up to now, the simplicity of diagonalization of the linear systems and of the systems without any long-range hopping and/or $p > 1$ interactions unvoluntarily supported their preferred choice in the quantitative studies. Nevertheless, in the computational study of solitons,[14] a little bit simpler construction is characteristic, on the contrary, to the periodic case. We believe that our demonstration of an easy feasibility of calculations for both the linear and periodic systems (as well as for the studies of influence of the $p > 1$ corrections) might encourage the further realistic computations concerning the nontrivial (say, topological, solitonic, etc.) aspects of solid-state physics and quantum chemistry.

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