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Eigenenergies of linear systems with periodic structures

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Using a new technique of amplitude analysis, the eigenvalues and eigenenergies are analyzed for finite and infinite linear harmonic chains with any periodic structures of two species. A new phase function which is "additive" for each unit cell can be constructed. In terms of this phase function, the eigenvalue equation is reduced to a low-order algebraic equation specified completely by the unit cell. Symmetry properties among the "cyclicly" permuted unit cells, analytic properties, vertex classification, diagram expansions, leading behavior, and reduction constraints (relating structure of more complicated unit cell to less complicated ones) are developed. For infinite systems, the density of states can be expressed in closed form as a single term. Eigenvectors also demonstrate collective behavior throughout the whole system.

I. INTRODUCTION

In recent years, considerable attention has been focused on the excitation of linear systems composed of two types of species (the binary linear systems).[1,2] Properties of these systems have been analyzed both analytically and numerically. These results are then compared with computer experiments or experimentally measured quantities of pseudolinear physical systems.

In one extreme of an amorphous system, two species of atoms may be distributed randomly among each other. After the classical computer study of Dean,[3] vast amounts of information are now available for the density of states of a randomly disordered chain.[1-8] In general the theoretical studies and computer experiments are in excellent agreement with each other. Starting from the earlier work of Mott and Twose,[4] and Borland[5] most theoretical work indicated that the eigenvectors in such systems are essentially localized at least for regions near the tail of the main energy band.[1-8] However eigenvectors are extremely difficult to calculate for a large disordered system. Characteristics of eigenvectors are therefore less well established than the characteristics of eigenenergies.[9]

In the other extreme, a binary linear system may be completely ordered. For simple mixed linear systems, the properties of both the eigenenergies and eigenvectors are simple and well known.[7,10-16] They are often used as elementary examples in the literature.[16] However limited generalization can be obtained for the general properties of binary systems.

In this paper, we attempt to analyze the binary linear systems from a different approach. We shall study finite and infinite systems with periodic structures. The structures of the unit cell are allowed to be progressively more complicated.

Since the eigenvalue problem is intrinsicly a boundary value problem, in our opinion it is most desirable to start with finite systems where the boundary can be explicitly constructed. The characteristics of the eigenvectors can then be analyzed without possible ambiguities arising from taking asymptotic limits. Examples we worked out explicitly in this paper are finite systems with quite complicated unit-cell structures. Fortunately many analytic properties can be obtained for such systems. Limiting behavior can then be obtained for properties of infinite systems. Results obtained in this paper may be directly usable for pseudolinear physical systems of complicated periodic structures.[16] Also by increasing the size of the unit cell progressively, one may eventually use this method for a complicated linear system as a single cell.

In order to study our systems, a new technique is introduced which allows us to examine analytically many features of a finite periodic system. We shall construct explicitly a "phase function" which is an "additive" quantity for each unit cell. In terms of this phase function, the eigenvalue problem of a finite system is reduced to finding the roots of a low-order polynomial. The structure of the polynomial is completely specified by the structure of the unit cell, and is essentially independent of the size of the system. Thus the explicit evaluation of the secular equation for the eigenenergy is avoided.[17] The phase function constructed here is also the most natural quantity for the density of states of an infinitely long periodic system. There the density of states can be expressed analytically in closed form as a single term relating simply to the phase function. Extensive usage of this phase function allows one to discuss the symmetry in eigenenergy of "cyclicly" permuted linear chains. Simple constraints can also be derived relating higher-order cyclic chains (here we mean chains with more complicated unit-cell structure) to lower-order cyclic chains. A diagrammatic expansion can be derived for the evaluation of this phase function for an arbitrary structured unit cell. Eigenvectors associated with the eigenvalues also demonstrate collective behavior reflecting the unit-cell structure throughout the whole chain.

The phase function discussed here possesses features similar to the phase functions used by Borland in the solutions of the one-dimensional Schrödinger equations,[4] and the phases of the state vectors first introduced by Schmidt.[18] They are however very different physical quantities. Since this phase function is related to the overall phase change of the "standing wave" over the entire unit cell, one may loosely conceive it as complementary to the phase functions of the state functions. However the characteristics of the phase function is closely related to the classical wave aspects of the system, and is difficult to interpret in terms of particle aspects in a quantum-mechanical system. From now on, we shall give it a name, and refer to it as the phase function of the unit cell.

In Sec. II we discuss the Hamiltonian and formulation of the eigenvalue equations suitable for the construction of the phase function. In Sec. III, we discuss the definition of the phase function in connection with the eigenvalue equations. In Sec. IV, detailed construction of the phase function of the unit cell are presented. In Sec. V important properties of the phase function are summarized. These properties not only lead to explicit evaluation of the phase function, but also provide insights to the physical properties of the finite cyclic systems. In Sec. VI, we demonstrate the evaluation of the phase function for lower-order cyclic chains. Expressions for higher-order chains (up to 6th order) are also summarized. In Sec. VII, density of states of infinitely long cyclic chains are worked out that can be compared analytically with the formulation obtained from other existing methods.[11] In Sec. VIII the phase function is applied to a binary system with 5% impurity. In Sec. IX eigenvalues and eigenvectors corresponding to complicated unit-cell structures are studied. Several numerical examples are presented to demonstrate the collective behavior of the eigenvectors in a linear period system.

II. FORMULATION OF EIGENVALUE EQUATIONS

In many linear systems with nearest-neighbor interactions the eigenvalue equations are equivalent in formulation. We shall consider, as an example, only a linear chain of particles of species A and B interacting with their nearest neighbors through ideal springs of identical strength. Consider an eigenfrequency w. The amplitudes u_n satisfy

$$(m_n w^2 - 2k)u_n + k(u_{n-1} + u_{n+1}) = 0, \quad 0 \leq n \leq N+1 \ , \tag{1}$$

where $m = m_A$ or m_B depending on whether the site n is occupied by the species A or B. Corresponding to fixed-ends boundary conditions

$$u_0 = u_{N+1} = 0 \tag{2}$$

Eq. (1) can easily be rewritten as

$$a_n u_n = u_{n+1} + u_{n-1}, \quad 0 \leq n \leq N+1 \ , \tag{3}$$

where

$$a_n = 2 - w^2/w_n^2, \quad w_n^2 = k/m_n \ .$$

Thus a_n can be $a_A = 2 - w^2/w_A^2$ or $a_B = 2 - w^2/w_B^2$ depending on whether the nth site is A or B. In the following we shall always refer to the species with heavier mass as the host atoms (H) and the species with lighter mass as the impurity atoms (I). This is mainly for the convenience of identifying the main energy band. The system we are considering are really mixed crystals where either species may be treated as the host atoms.

Consider now a unit cell of the cyclic chain with s impurity atoms. (Hereafter, we shall call it cyclic chain of order s.) The unit cell is naturally separated by the impurity atom into s intervals (see Fig. 1). Let the segment length of the intervals be m_1, $m_2, \ldots, m_s$. The general expression for the amplitudes within each interval can be easily derived. Starting from the 0th site at one end, the amplitude in the first interval is simply[4,9,19]

$$u_k = u_k^{(1)} = c_1 \sin(k\phi + \Phi_1), \quad 0 \leq k \leq m_1 \ , \tag{4}$$

where

$$\begin{aligned} &\phi = \cos^{-1}(\tfrac{1}{2}a_H) \ , \\ &\Phi_1 = 0 \ , \end{aligned} \tag{5}$$

and c_1 is an arbitrary normalization factor. Since the site m_1 is occupied by an impurity atom, both the amplitude c_1 and the phase Φ_1 suffers a discontinuous change in extending into the second interval. This can be easily seen as follows

$$\begin{aligned} u_{m_1+1} &= (a_I - a_H)u_{m_1} + (a_H u_{m_1} - u_{m_1-1}) \\ &= c_1\beta \sin(m_1\phi)\sin\phi + c_1 \sin(m_1+1)\phi \ , \end{aligned} \tag{6}$$

where

$$\beta = (a_I - a_H)/\sin\phi \ . \tag{7}$$

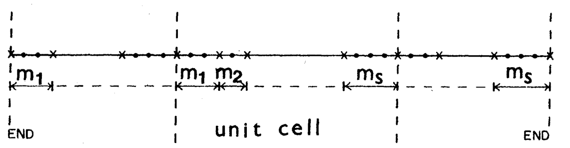

FIG. 1. Unit-cell structure of an s-order cyclic chain.

Comparing with

$$u_{m_1}=c_1\beta\sin(m_1\phi)\sin(0\phi)+c_1\sin(m_1\phi)\ , \tag{4'}$$

it is obvious that the amplitudes in the second interval is the interference between the original wave and a new wave generated by the discontinuity in the mass. Thus

$$u_{m_1+k}\equiv u_k^{(2)}=c_1\beta\sin(m_1\phi)\sin(k\phi)+c_1\sin(m_1+k)\phi\ ,\quad 0\leqslant k\leqslant m_2\ . \tag{8}$$

The above equation can be rewritten as

$$u_k^{(2)}=c_2\sin(k\phi+\Phi_2),\quad 0\leqslant k\leqslant m_2\ , \tag{9}$$

where

$$\tan\Phi_2=\frac{\tan(m_1\phi+\Phi_1)}{1+\beta\tan(m_1\phi+\Phi_1)} \tag{10}$$

and

$$\frac{c_2}{c_1}=\frac{\sin(m_1\phi+\Phi_1)}{\sin(\Phi_2)}\ . \tag{11}$$

Equation (11) is equivalent to

$$\left(\frac{c_2}{c_1}\right)^2=1+2\beta\sin(m_1\phi+\Phi_1)\cos(m_1\phi+\Phi_1)+\beta^2\sin^2(m_1\phi+\Phi_1)\ . \tag{11'}$$

This procedure can be generalized into the jth interval. Defining the amplitude there to be

$$u_k^{(j)}=c_j\sin(k\phi+\Phi_j),\quad 0\leqslant k\leqslant m_j\ , \tag{12}$$

we can easily show that

$$\tan\Phi_{j+1}=\frac{\tan(m_j\phi+\Phi_j)}{1+\beta\tan(m_j\phi+\Phi_j)},\quad 0\leqslant j\leqslant s \tag{13}$$

and

$$c_{j+1}\sin(\Phi_{j+1})=c_j\sin(m_j\phi+\Phi_j)\ , \tag{14}$$

$$\left(\frac{c_{j+1}}{c_j}\right)^2=1+2\beta\sin(m_j\phi+\Phi_j)\cos(m_j\phi+\Phi_j)+\beta^2\sin^2(m_j\phi+\Phi_j)\ . \tag{14'}$$

From the definition of cyclic chain of order s, ϕ_{s+1} is actually the starting phase of the first interval of the second unit cell. The above procedure may therefore be continued. For a finite cyclic chain of N cycles, the displacement vector of the last atom of the last interval of the last unit cell is zero. We shall then consider Eq. (13) with $j=s$ as a formal definition of ϕ_{s+1}. The fixed-end boundary condition is simply

$$\Phi_{s+1}(\text{last unit cell})=0\ . \tag{15}$$

III. PHASE FUNCTION IN EIGENVALUE EQUATION

As a first step toward solving the eigenvalue problem formulated above, we shall relate the initial phase Φ_1 of a unit cell k, with the initial phase Φ_1 of the adjacent unit cell $k+1$. Let

$$y_j=\tan\Phi_j \tag{16}$$

for the Φ_j of the kth cell, Eq. (13) is rewritten as

$$y_{j+1}=\frac{\alpha_j+y_j}{(1+\alpha_j\beta)+(\beta-\alpha_j)y_j},\quad 1\leqslant j\leqslant s\ , \tag{17}$$

where $\alpha_j=\tan(m_j\phi)$. By repeating Eq. (17) s times, we can get, in a straightforward (but tedious) manner,

$$y_{s+1}=\frac{C+Dy_1}{A+By_1}\ , \tag{18}$$

where A,B,C,D are exceedingly clumsy functions of $\alpha_1,\alpha_2,\ldots,\alpha_s$ and β. Instead of evaluating these functions directly, we shall only extract useful information out of these functions (information that is relevant to the eigenvalue conditions).

As we have indicated before, y_{s+1} is actually the initial phase of the $(k+1)$th unit cell. At this point, it is necessary to label explicitly the cells. Let

$$X_k=y_1(\text{of the } k\text{th cell})\ . \tag{19}$$

Equation (18) becomes more transparent as

$$X_{k+1}=\frac{C+DX_k}{A+BX_k},\quad 0\leqslant k\leqslant N\ , \tag{20}$$

where N is the total number of cells in the system. In terms of X_k, the boundary conditions are

$$X_1=X_{N+1}=0\ . \tag{21}$$

In order to analyze Eqs. (20) and (21), we shall now construct the phase function of the unit cell. The phase function we are constructing here should be an additive function of the cell, so that boundary condition Eq. (21) can be imposed easily. It also turns out to be an extremely interesting and useful function in analyzing the properties of the eigenvalues.

Notice that Eq. (20) is a bilinear transformation similar to those of the addition of the tangent functions. We shall first introduce several transformation of variables. Let

$$Z_k=\frac{(DX_k-B)}{(BC-AD)^{1/2}}\ . \tag{22}$$

Equation (20) is translated into

$$Z_{K+1}=\frac{1}{\mu_s-Z_k}\ ,$$

where

$$\mu_s = \frac{-(B+C)}{(BC-AD)^{1/2}} \ . \tag{23}$$

Here μ_s is again a rather complicated function (although not as complicated as A,B,C,D, individually) of β and $\alpha_1, \ldots, \alpha_s$. It is, however, independent of the cell index k. Let

$$\mu_s = 2\cos\theta_s \tag{24}$$

and

$$Z_K = \cos\theta_s + \sin\theta_s \tan\delta_K \ . \tag{25}$$

Equation (23) is finally reduced to the desired form

$$\tan\delta_{K+1} = \tan(\delta_k + \theta_s) \ . \tag{26}$$

The boundary condition of Eq. (21) is now simply

$$\tan N\theta_s = 0 \ . \tag{27}$$

The eigenvalues of Φ are now grouped naturally as solutions of the equations

$$\theta_s = \vartheta_p = p\pi/N, \quad p = 0, 1, 2, \ldots, N-1 \ . \tag{28}$$

with possible values of θ_s all equally spaced. In the following sections, we shall discuss the properties of θ_s and μ_s, and how to evaluate them explicitly.

IV. FORMAL SOLUTIONS OF THE PHASE FUNCTION

The phase function θ_s defined above is a rather complicated function of ϕ. This is only natural, since Eq. (28) implicitly contains all the solutions of the eigenvalues. Instead of evaluating θ_s immediately, we shall first discuss several important properties of θ_s, which lead us to nontrivial insights of the eigenvalue equations. These properties constrain the possible form of μ_s and θ_s so severely, that expressions of θ_s can often be written down without ever evaluating the cumbersome transformations of Eq. (17).

In order to examine the properties of θ_s, it is sufficient to inspect closely the nature of the transformation in Eq. (17) for two successive transformations. With $j=1$

$$y_2 = \frac{\alpha_1 + y_1}{(1+\beta\alpha_1) + (\beta - \alpha_1) y_1} \equiv \frac{c_1 + d_1 y_1}{a_1 + b_1 y_1} \ , \tag{29}$$

where we formally define a 2×2 matrix $\underline{U}_1$:

$$\underline{U}_1 = \begin{pmatrix} 1+\beta\alpha_1 & \beta-\alpha_1 \\ \alpha_1 & 1 \end{pmatrix} \tag{30}$$

as the matrix supporting the transformation $y_1 \rightarrow y_2$. Similarly

$$\underline{U}_k = \begin{pmatrix} 1+\beta\alpha_k & \beta-\alpha_k \\ \alpha_k & 1 \end{pmatrix} \tag{31}$$

is the matrix supporting the transformation $y_k \rightarrow y_{k+1}$. We shall further define matrix $\underline{A}_k$ as the supporting matrix for the transformation $y_1 \rightarrow y_k$

$$\underline{A}_k = \begin{pmatrix} c_k & d_k \\ a_k & b_k \end{pmatrix} \ , \quad y_k = \frac{c_k + d_k y_1}{a_k + b_k y_1} \ . \tag{32}$$

Notice that the quantities (a_k, b_k, c_k, d_k) are unique up to an overall multiplying factor. This ambiguity is removed by requiring

$$\begin{aligned} a_{k+1} &= \alpha_k c_k + a_k \ , \\ b_{k+1} &= \alpha_k d_k + b_k \ , \\ c_{k+1} &= (1+\alpha_k\beta) c_k + (\beta - \alpha_k) a_k \ , \\ d_{k+1} &= (1+\alpha_k\beta) d_k + (\beta - \alpha_k) b_k \ . \end{aligned} \tag{33}$$

Equation (33) is summarized in matrix form as

$$\underline{A}_{k+1} = \underline{U}_k \underline{A}_k \ . \tag{33$'$}$$

As a consequence

$$\underline{A}_{s+1} = \underline{U}_s \underline{U}_{s-1}, \ldots, \underline{U}_1 \ , \tag{34}$$

since $\underline{A}_1 = \underline{U}_1$. Comparing Eq. (34) with Eq. (18), the previous A,B,C,D are just the matrix elements of $\underline{A}_{s+1}$. Thus

$$\begin{aligned} \mu_s = 2\cos\theta_s &= -\mathrm{Tr}(\underline{A}_{s+1}) / (\mathrm{Det}\underline{A}_{s+1})^{1/2} \\ &= -\mathrm{Tr}(\underline{U}_s \underline{U}_{s-1}, \ldots, \underline{U}_1) \Bigg/ \left[\prod_{k=1}^{s} \mathrm{Det}(\underline{U}_k) \right]^{1/2} \ . \end{aligned} \tag{35}$$

Equation (35) is the formal solution of the phase function θ_s. Notice that although the supporting matrix defined in Eq. (32) is ambiguous up to an overall factor, the final result of μ_s is independent of this ambiguity. The transformation relationship (33) is, however, the most useful expression, since the coefficients multiplying β and $\alpha_1, \ldots, \alpha_s$ are always integers in the final expansion of the $\mathrm{Tr}(\underline{U}_s, \ldots, \underline{U}_1)$. From this expression, solutions of μ_s corresponding to lower-order cyclic chains can be written down through inspection. We get, for example,

$$\mu_1 = -(2+\alpha_1\beta)/(1+\alpha_1^2)^{1/2} \tag{36}$$

and

$$\mu_2 = \frac{[2 - 2\alpha_1\alpha_2 + 2(\alpha_1+\alpha_2)\beta + \alpha_1\alpha_2\beta^2]}{[(1+\alpha_1^2)(1+\alpha_2^2)]^{1/2}} \ . \tag{37}$$

As for the higher-order cyclic chains, the explicit expression for μ_s are still nontrivial, since no simple mechanism is available for calculating the trace of product of matrices. It is therefore necessary to examine more closely properties of μ_s utilizing specific properties of the matrices of Eq. (31).

V. PROPERTIES OF THE PHASE FUNCTION

Although it is quite straightforward to evaluate explicitly the expression of μ_s through Eq. (33), it is quite tedious and not inspiring. After all, we are not interested in the full supporting matrix, but only in its traces and its determinants. We shall therefore discuss briefly various properties of μ_s which lead to deeper insight of the contents of Eq. (35) and the physical properties of the eigenvalue equations.

A. Symmetry properties

A symmetry property of the eigenvalue equation is directly revealed by taking the trace of the matrix product. As is well known, both the trace and the determinant are independent of any cyclic permutation of $\underline{U}_s, \underline{U}_{s-1}, \ldots, \underline{U}_1$. μ_s is therefore the same for s different kind of unit-cell structures obtained through cyclic permutation of the segments within the unit cell. In other words the eigenvalues obtained for these systems are identical if a whole segment is moved from one end of a long chain to the other end (see Fig. 2). Notice that the cyclic permutation referred to here are applied to a whole segment and not to the individual host atoms.

B. Reduction of higher-order cyclic chains

Consider an s-order cyclic chain with N unit cycles. Segments of the intervals $m_1, \ldots, m_s$ may be arbitrarily specified. The configurations of the unit cell include special circumstances when the unit cell itself possess cyclic properties. For example, if

$$s = 2q$$

we may choose

$$m_j = m_{q+j}, \quad j = 1, \ldots, q \quad . \tag{38}$$

The s-order cyclic chain of N cycles is now reduced to a $(s/2)$th order cyclic chain of $2N$ cycles. Since the same eigenvalue equations should emerge from either formulation of the phase function, it is necessary that

$$\cos\theta_s = \cos(2\theta_{s/2}) \tag{39}$$

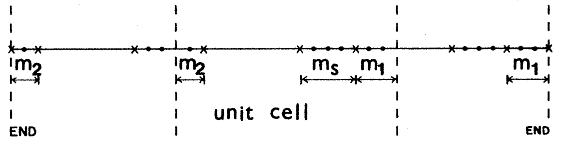

FIG. 2. "Cyclic" permutation of cyclic chain in Fig. 1.

so that

$$\mu_s(\text{reduced}) = 2\mu_q^2 - 1 \quad .$$

In general if $s = pq$ where p and q are integers, a N-cycle sth order cyclic chain may be reduced to pth order cyclic chain with gN cycles, by setting

$$m_j = m_{q+j} = m_{2q+j} = \cdots \quad . \tag{40}$$

Thus

$$\cos\theta_s(\text{reduced}) = \cos(q\,\theta_{s/q}) \quad . \tag{41}$$

Equation (41) is a rather strong consistency relationship between cyclic chains of different orders. It can be an effective tool in building up a higher-order chain out of a given lower-order expression. We shall utilize this to obtain explicit expressions of higher-order chains in the following section.

C. Analytic properties

Notice that from Eq. (31)

$$(\det\underline{U}_j)^{-1/2} = (1+\alpha_j^2)^{-1/2} = \cos(m_j\phi) \quad . \tag{42}$$

It immediately follows that μ_s is a polynomial of $\cos m_j\phi$ and $\sin(m_j\phi)$ of degree s. It is also easy to see from Eq. (33) that μ_s is a polynomial of degree s in β. However from the definition, β behaves as a simple pole at $\phi = 0$, while μ_s should not diverge. A power of β is therefore always accompanied by $\sin(m_j\phi)$ to a sufficient power to maintain the proper behavior of μ_s at $\phi = 0$. Under these constraints the allowed expressions of the various terms in Eqs. (35) and (36) are essentially unique. Only the constant coefficients need to be determined. Equation (33) can indeed be expressed as a polynomial of $\cos\phi$ of order $(m_1 + \cdots + m_s)$. Detailed evaluations shall be discussed in the following section.

D. Vertex classification

When the cyclic symmetry of V A is combined with the polynomial properties of V C, a classification of possible expressions contributing to Eq. (35) is possible. This classification is best illustrated in vertex diagrams. Corresponding to a s-order chain, the trace in Eq. (35),

$$T_s = \text{Tr}(\underline{U}_s, \ldots, \underline{U}_1) \quad , \tag{43}$$

can be expressed in terms of polynomials in α_j's (with integer coefficients). In order to accomodate the cyclic properties, we shall first draw a diagram with all possible vertices. (There are altogether s vertices.) Any specific polynomial of $\alpha_1, \ldots, \alpha_s$ is represented by the corresponding selection of ver-

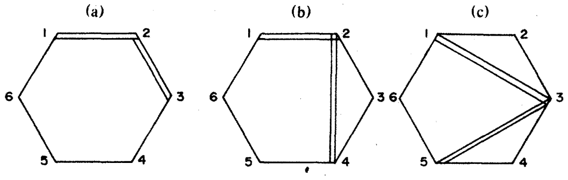

FIG. 3. Typical vertex diagrams of a sixth-order chain.

tices. For example, the diagram illustrated in Fig. 3(a) corresponds to the polynomial $\alpha_1\alpha_2\alpha_3$ of Eq. (43) for a 6th-order cyclic chain. Since Eq. (43) is cyclic with respect to the matrices $\underline{U}_s, \ldots, \underline{U}_1$, $\alpha_1\alpha_2\alpha_3$ term is always accompanied by $\alpha_2\alpha_3\alpha_4$ term. The vertex diagram of Fig. 3(a) really corresponds to

$$\Pi_{123} \equiv \alpha_1\alpha_2\alpha_3 + \alpha_2\alpha_3\alpha_4 + \alpha_3\alpha_4\alpha_5 + \alpha_4\alpha_5\alpha_6 + \alpha_5\alpha_6\alpha_1 \ . \tag{44}$$

Thus all the third-order polynomials of α_j's contributing to T_6 can be grouped into several terms

$$T_6 = \cdots + \nu_1\Pi_{123} + \nu_2\Pi_{124} + \nu_3\Pi_{135} \ , \tag{45}$$

where

$$\Pi_{124} = \alpha_1\alpha_2\alpha_3 + \alpha_2\alpha_3\alpha_5 + \alpha_3\alpha_4\alpha_6 + \cdots \ (12 \text{ terms}) \ ,$$

$$\Pi_{135} = \alpha_1\alpha_3\alpha_5 + \alpha_2\alpha_4\alpha_6 \ ,$$

corresponding to Figs. 3(b) and 3(c), respectively. Furthermore T_6 is a polynomial in β. The most general expression third-order polynomial of α_j' is in the form

$$T_6 = \cdots + \sum_{k=0}^{3} \beta^k (\nu_{k,1} T_{123} + \nu_{k,2} T_{124} + \nu_{k,3} T_{135}) \ , \tag{46}$$

where ν_{kj} are all integers. Notice that higher-order polynomials in β are not allowed, since otherwise the analytic property at $\phi = 0$ is not satisfied.

E. Matrix representation and diagram expansions

Alternatively Eq. (35) may be treated through Pauli matrices, i.e.,

$$\underline{U}_j = (1 + \tfrac{1}{2}\alpha_j\beta)\underline{1} + \tfrac{1}{2}\beta\underline{\sigma}_x + (\alpha_j - \tfrac{1}{2}\beta) i \underline{\sigma}_y \ . \tag{47}$$

Firstly for $\beta = 0$

$$\underline{U}_j = \underline{1} + \alpha_j i \underline{\sigma}_y \ ,$$

$$(\underline{U}_s, \ldots, \underline{U}_1)_{\beta=0} = (1 - \Sigma\alpha_1\alpha_2 + \Sigma\alpha_1\alpha_2\alpha_3\alpha_4 \pm \cdots)\underline{1} + i(\Sigma\alpha_1 + \cdots)\underline{\sigma}_y \ , \tag{48}$$

and

$$T_s(\beta = 0) = 2(1 - \Sigma\alpha_1\alpha_2 + \Sigma\alpha_1\alpha_2\alpha_3\alpha_4 \pm \cdots) \ . \tag{49}$$

For $\beta \neq 0$ we may continue our analysis by introducing

$$\underline{V}_j = \underline{U}_j / (\det \underline{U}_j)^{1/2} \ . \tag{50}$$

One can then rewrite

$$\underline{V}_j = \underline{V}_{j_1} + \underline{V}_{j_2} + \underline{V}_{j_3} \ , \tag{51}$$

where

$$\underline{V}_{j_1} = \exp(i m_j \phi \underline{\sigma}_y) \ , \tag{52a}$$

$$\underline{V}_{j_2} = \tfrac{1}{2}\beta \exp[i m_j (\phi - \tfrac{1}{2}\pi)\underline{\sigma}_y] \ , \tag{52b}$$

$$\underline{V}_{j_3} = \tfrac{1}{2}\beta \exp(i m_j \phi \underline{\sigma}_y)\underline{\sigma}_x \ . \tag{52c}$$

Notice however

$$\exp(i m \phi \underline{\sigma}_y)\underline{\sigma}_x = \underline{\sigma}_x \exp(-i m \phi \underline{\sigma}_y) \ . \tag{52d}$$

In the full expansion of μ_s,

$$\mu_s = \mathrm{Tr}[(\underline{V}_{s_1} + \underline{V}_{s_2} + \underline{V}_{s_3}) \cdots (\underline{V}_{11} + \underline{V}_{12} + \underline{V}_{13})] \ , \tag{53}$$

the $\underline{\sigma}_x$ terms of $\underline{V}_{j_3}$ may be permuted repeatedly and eventually canceled in pairs, leaving only a sequential reverse of signs of the exponents in the process. All the other factors in Eq. (53) are exponents in $\underline{\sigma}_y$. The phases are then simply added together as a single term, and the trace can be taken. In order to keep track of the expansion in Eq. (53), a diagrammatic expansion can be used. A typical diagram corresponding to a term of sixth-order cyclic chain is shown in Fig. 4. There —·—, —×—, —◀— indicate contribution from $\underline{V}_{j_1}$, $\underline{V}_{j_2}$, and $\underline{V}_{j_3}$, respectively. Diagram in Fig. 4 therefore leads to a contribution to μ_6:

$$\begin{aligned} \mu_6 &= \cdots + (\tfrac{1}{2}\beta)^3 \mathrm{Tr} \exp[i\underline{\sigma}_y \phi (m_6 + m_5 - m_4 - m_3 - m_2 + m_1) + I \underline{\sigma}_y \tfrac{1}{2}\pi] \\ &= \cdots (\tfrac{1}{2}\beta)^3 2 \sin[\phi (m_6 + m_5 - m_4 - m_3 - m_2 + m_1)] \ . \end{aligned} \tag{54}$$

Another example is for the β^0 term. There

$$\mu_s = T_v[\exp(i\underline{\sigma}_y \phi \sum_1^s m_j)] = 2\cos\left(\sum_1^s m_j \phi\right)\beta^0 + \cdots \ . \tag{49'}$$

FIG. 4. A typical term in the diagram expansion of a sixth-order chain.

The above diagrammatic evaluation is particularly suitable for computer analysis.

F. Leading behavior

Another nontrivial property of μ_s deals with the leading expansions of Eq. (35). We shall first construct from Eq. (33)

$$t_k = b_k + c_k \tag{55a}$$

and

$$r_k = d_k + \beta c_k - a_k \ . \tag{55b}$$

Equations (33) then leads to

$$t_{k+1} = \alpha_k r_k + (\text{terms independent of } \alpha_k) \ ,$$

$$r_{k+1} = \alpha_k \beta r_k - \alpha_k t_k + (\text{terms independent of } \alpha_k) \ .$$

To the leading order of α_k, we therefore obtain an identity

$$r_{k+1} - z t_{k+1} = \alpha_k (\beta - z) \left(r_k - \frac{1}{(\beta - z)} t_k \right)$$

for any z. If we choose in particular $z = 1/(\beta - z)$, i.e.,

$$z = z_0 = \tfrac{1}{2}[\beta \pm (\beta^2 - 4)^{1/2}] \ , \tag{56}$$

a recursive relationship is obtained in the form

$$r_{k+1} - z_0 t_{k+1} = \frac{\alpha_k}{z_0}(r_k - z_0 t_k) \ . \tag{57}$$

Repeated use of Eq. (57) may lead to

$$(r_n - z_0 t_n) = \frac{\alpha_n, \ldots, \alpha_k}{(z_0)^{n-k}}(r_k - z_0 t_k) \ . \tag{58}$$

To take advantage of Eqs. (57) and (58), we may analytically continue β to $|\beta| < 2$. With

$$\beta = 2\cos\eta \tag{59}$$

the value of $z_0 = e^{\pm i\eta}$ is now complex. However other terms in Eqs. (57) and (58) are still real. We may now extract the trace t_s as

$$t_s \equiv b_s + c_k = (\alpha_s, \ldots, \alpha_k) \left(t_k \frac{\sin(s-k)\eta}{\sin\eta} - r_k \frac{\sin(s-k+1)\eta}{\sin\eta} \right) \ . \tag{60}$$

Since t_k, r_k may be calculated easily for small k, the leading terms of t_s may be easily calculated through Eq. (60).

VI. EXPLICIT EXPRESSIONS

In this section, we shall present explicit expressions for the lower-order chains. These expressions already correspond to rather complicated mixed linear crystals. The solution for first-order and second-order cyclic chains are already given in Eqs. (36) and (37):

$$\mu_1 = -(2 + \alpha_1 \beta)/(1 + \alpha_1^2)^{1/2} \ , \tag{36'}$$

$$\mu_2 = 2\frac{[1 - \alpha_1\alpha_2 + (\alpha_1 + \alpha_2)\beta + \frac{1}{2}\alpha_1\alpha_2\beta^2]}{[(1+\alpha_1^2)^{1/2}(1+\alpha_1^2)^{1/2}]} \ . \tag{37'}$$

We shall first consider the third-order chain. Starting from the reduction technique of Sec. V B,

$$\cos\theta_3(\text{reduced}) = \cos 3\theta_1 \ ,$$

$$= \frac{-1 + \frac{3}{2}\alpha_1\beta - 3\alpha_1^2\beta^2 - \frac{1}{2}\alpha_1^3\beta^3}{(1+\alpha_1^3)^{3/2}} \ . \tag{61}$$

From the symmetry property of Sec. V C, the only generalization available for Eq. (61) is

$$3\alpha_1 \rightarrow \Pi_1 = \alpha_1 + \alpha_2 + \alpha_3 \ , \tag{62a}$$

$$3\alpha_1^2 \rightarrow \Pi_{12} = \alpha_1\alpha_2 + \alpha_2\alpha_3 + \alpha_3\alpha_4 \ , \tag{62b}$$

$$\alpha_1^3 \rightarrow \Pi_{123} = \alpha_1\alpha_2\alpha_3 \ . \tag{62c}$$

Thus

$$\mu_3 = 2\cos\theta_3$$

$$= \frac{-2 + 2\Pi_{12} + 3\beta\Pi_1 + 3\beta\Pi_{123} - 2\beta^2\Pi_{12} - \beta^3\Pi_{123}}{[(1+\alpha_1^2)(1+\alpha_2^2)(1+\alpha_3^2)]^{1/2}} \ . \tag{63}$$

Even with the techniques summarized in Sec. V, the algebraic procedure becomes somewhat too lengthy to be presented in detail, we shall therefore work out the fourth-order chain explicitly in Appendix B and only list the results up to sixth-order chain in Table I. These results suggest, that perhaps it might not be too optimistic, that an explicit expression of the phase function would be obtainable for cyclic chain of any order.

TABLE I. Expressions for μ_s.

		s					
k[a]	Π/Σ[b]	1	2	3	4	5	6
0	1	2	2	2	2	2	2
	Σ_{12}	−2	−2	−2	−2	−2	−2
	Σ_{1234}				2	2	2
	Σ_{123456}					−2	−2
1	Σ_1	1	2	3	4	5	6
	Σ_{123}			−3	−4	−5	−6
	Σ_{12345}					5	6
2	Σ_{12}		1	2	3	4	5
	Π_{13}				1	2	3
	Π_{14}						4
	Σ_{1234}				−4	−6	−8
	Σ_{1235}						1
	Σ_{1234}						0
	Σ_{123456}						8
3	Σ_{123}			1	2	3	4
	Π_{124}					1	2
	Π_{135}						4
	Σ_{12345}					−5	−8
4	Σ_{1234}				1	2	3
	Π_{1235}						1
	Π_{1234}						1
	Π_{123456}						−6
5	Σ_{12345}					1	2
6	Σ_{123456}						1

[a] k is the power of β associated with the Π or Σ terms.

[b] $\Sigma_{12}=\sum_{j=1}^{3}\sum_{k=1}^{3}\alpha_j\alpha_k$, $\Pi_{12}=\sum_{j=1}\alpha_j\alpha_{j+1}$, where $\alpha_{s+1}=\alpha_1$.

VII. DENSITY OF STATES OF INFINITELY CYCLIC CHAINS

Consider the limiting situation when the number of cycle N becomes large, eigenvalues ϑ_p's also become dense over the whole region from 0 to π. Since ϑ_p are equally spaced, the number of states in a given interval is just

$$G(\vartheta_p)\Delta\vartheta_p=\Delta p/N$$

so that

$$G(\vartheta_p)=1/\pi \quad . \tag{64}$$

Transforming back to the original variable ϕ, we get

$$G(w^2)=g(\vartheta_p)\frac{d\theta}{d\cos\theta}\frac{d\cos\phi}{dw^2}=f(w^2)G_0(w^2) \quad , \tag{65}$$

where

$$f(w^2)=\frac{d\cos\theta}{d\cos\phi}\frac{1}{\sin\theta} \quad , \quad G_0(w^2)=\frac{1}{\pi}\frac{d(\cos\phi)}{dw^2} \quad .$$

In the above equation $G_0(w^2)$ is the density of states of the homogeneous chain (in the absence of the impurity atoms) and $f(w^2)$ is the form factor associated with the cyclic structure.

Since θ_s is an explicit function of $\cos\phi$, the form factor may be calculated in a straightforward manner, and the density of states can be expressed in a closed form.

To demonstrate, we shall work out two simple examples, where the analytic solutions may also be obtained relatively easily from another independent method (sequential Green's function).[14] In example one, equal concentrations of the two species are considered. This corresponds to $s=1$, $m_1=2$, as shown

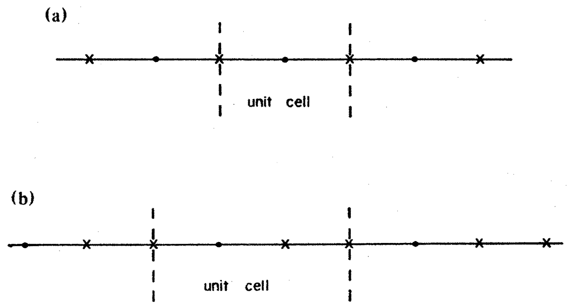

FIG. 5. (a) Alternative chain with concentration ratio 1:1. (b) Second-order cyclic chain with concentration ratio 2:1.

in Fig. 5(a). We get from Eq. (35)

$$\cos\theta_1 = \cos 2\phi + (a_l - a_H)\cos\phi = \tfrac{1}{2} a_H a_l - 1$$

and

$$\frac{d\cos\theta_1}{d\cos\phi} = a_l + a_H \ .$$

Thus

$$G(w^2) = \frac{1}{\pi}\frac{a_l + a_H}{a_l a_H}\left[1 - \frac{4}{a_l a_H}\right]^{-1/2} \tag{66}$$

in agreement with the results [Eq. (B7)] obtained by the sequential method (see Appendix B).

The second nontrival example corresponds to a mixed crystal with concentration ratio 2:1. The unit-cell structure is therefore $s=2$, $m_1=2$, and $m_2=1$ as shown in Fig. 5(b):

$$\begin{aligned}\cos\theta_2 &= \cos 3\phi + \beta \sin 3\phi + \tfrac{1}{2}\beta^2 \sin 2\phi \sin\phi \\ &= \tfrac{1}{2}(a_l^2 a_H - 2a_l - a_H) \ .\end{aligned} \tag{67}$$

As a consequence

$$\frac{d\cos\theta_2}{d\cos\phi} = a_l^2 + 2a_l a_H - 3 \tag{68}$$

and

$$G(w^2) = \frac{1}{\pi}\frac{1}{2\cos\theta_2}(a_l^2 + 2a_l a_H - 3) \ , \tag{69}$$

in agreement with the results [Eq. (B12)].

VIII. FREQUENCY SPECTRUM OF CHAIN OF 40 ATOMS WITH A 5% CONCENTRATION OF LIGHT ATOMS

In practical applications, a binary system with dilute impurities is sometimes studied with periodical-boundary conditions. This is equivalent to an infinite cyclic system with fairly complicated unit-cell structures. Numerical analysis is often necessary in order to carry out the details of the frequency spectrum.

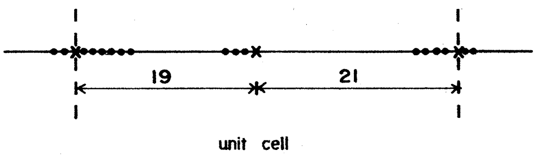

FIG. 6. A unit structure with impurity concentration of 5%, impurity site at 19 and 21.

To demonstrate our method, we shall select an example that has been reported in the literature.[14] This sytem consists of 38 heavy atoms (H) and two light atoms (l) at sites 12 and 31. This corresponds to $s=2$, $m_1=19$, $m_2=21$ (see Fig. 6), and

$$\begin{aligned}\cos\theta_2 = {} & \cos(40\phi) + \beta\sin(40\phi) \\ & + \tfrac{1}{2}\beta^2 \sin(21\phi)\sin(19\phi) \ ,\end{aligned} \tag{70}$$

with

$$\beta = \left[\frac{1}{W_H^2} - \frac{1}{W_l^2}\right]\frac{W^2}{\sin\phi} = 2\left[\frac{1}{W_H^2} - \frac{1}{W_l^2}\right]\tan\tfrac{1}{2}\phi \ . \tag{71}$$

In general when the mass ratio is close to 1, β is small, $\theta_2 \sim 40\phi$. And the frequency spectrum of the system is almost the same as that of the homogeneous chain. When the mass ratio $M_H/M_l >> 1$, β can be large. In a large region of ϕ, $\cos\theta_2$ varies rapidly beyond the region (0,1) and band gaps develop. Only at the long-wavelength limit, both ϕ and β tend to zero. Figure 7 corresponds to a choice of $M_l/M_H = 3$. In order to compare the molecular dynamics with electronic states, we have also calculated, in Fig. 8, the density of states of 40 atoms with $a_H = 1 - E$, and $a_l = 2 - E$.

The same results can also be obtained through the Green's-function technique of Ref. 20. It is interesting to observe that various seemingly independent

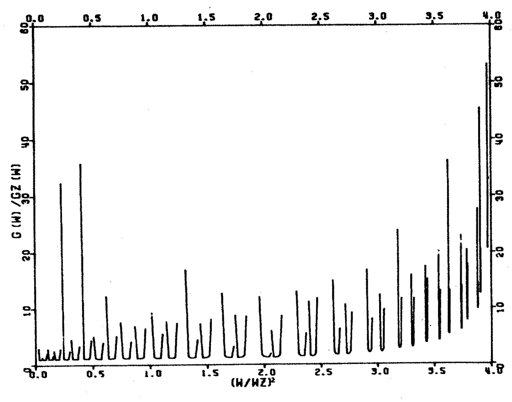

FIG. 7. The relative density of state $G(w^2)/G_0(w^2)$. $G_0(w^2)$ is the density of states of the corresponding homogeneous chain. Here $m_H = 3.0\ m_l$, with configuration of Fig. 6.

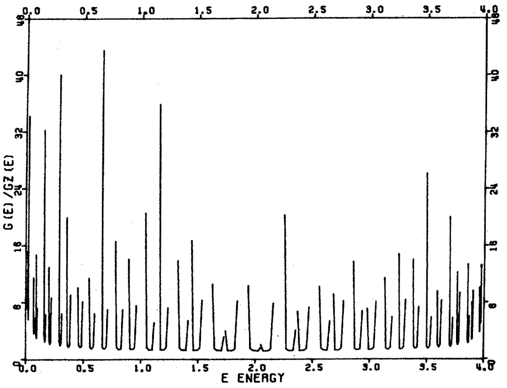

FIG. 8. The relative density of state $G(E)/G_0(E)$. $G_0(E)$ is the density of states of the corresponding homogeneous chain. Here $a_H = 1 - E$, $a_I = 2 - E$, with configuration of Fig. 6.

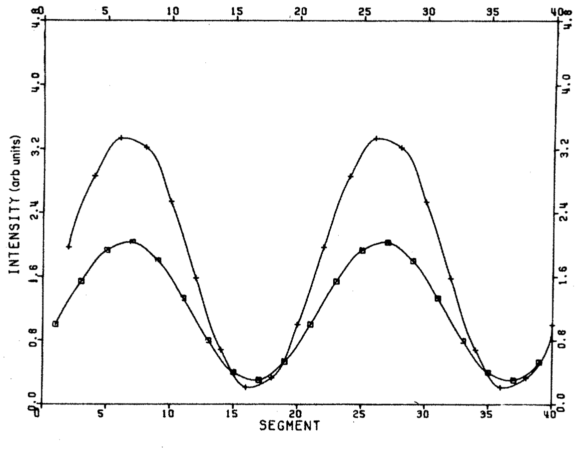

FIG. 9. The intensity $I_j = C_j^2$ for a chain of 40 segments, with $s = 2$, $m_1 = 3$, $m_2 = 5$ and $\beta = 1/\cos\phi$, $\phi = 0.800\,17$.

terms of E in the Green's-function technique can indeed be summed to a closed analytic form expressible as Eq. (65).

IX. EIGENFREQUENCY AND EIGENVECTORS OF FINITE SYSTEMS

For finite systems, one may either solve Eq. (28) analytically or numerically. Since Eqs. (28) and (35) contain all the information of the eigenfrequencies, the solutions can be expected to be rather complicated. Nevertheless one important feature of the solution may still be studied. We shall first introduce

$$\cos\phi = \tfrac{1}{2}(Z + 1/Z) \ . \tag{72}$$

It follows from Eq. (49'), that

$$\mu_s = (Z^M + 1/Z^M)\beta^0 + (\text{higher-order polynomial in } \beta) \ , \tag{73}$$

where $M = m_1 + m_2 + \cdots + m_s$. But all other terms in β are in the form

$$\frac{\sin m\phi}{\sin\phi} = (Z^m - Z^{-m})/(Z - Z^{-1}) = Z^{m-1} + Z^{m-2} + \cdots + Z^{-(m-1)} \ . \tag{74}$$

Thus the explicit form of Eq. (28) is

$$Z^{2M} + \cdots + 1 = 0 \ . \tag{75}$$

We can therefore find M pairs of solutions

$$Z_j = e^{\pm i\phi_j}, \quad \phi_j = \text{real}, \quad j = 1, \ldots, M' \tag{76a}$$

or

$$Z_j = P_j, 1/P_j, \quad P_j = \text{real}, \quad j = M' + 1, \ldots, M \ . \tag{76b}$$

Solution in the form of Eq. (76a) leads to

$$\cos\phi = \cos\phi_j, \quad |\cos\phi| \leq 1$$

and the corresponding W^2 is in the main band of the host atoms. Solution in the form Eq. (76b) corresponds to

$$\cos\phi = \tfrac{1}{2}(P_j + 1/P_j), \quad |\cos\phi| > 1$$

and the corresponding W^2 being outside the main band, is usually referred to as localized states. Since ϑ_p may possess N values, all $N \times M$ states are accounted for.

In Figs. 9–11, several typical solutions are plotted.[21] As we can see eigenvectors of the second-order cyclic chain are naturally separated into two en-

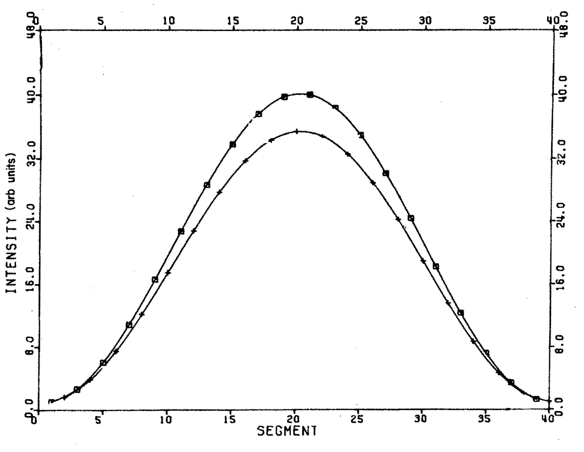

FIG. 10. The intensity $I_j = C_j^2$ for a chain of 40 segments, with $s = 2$, $m_1 = 6$, $m_2 = 2$ and $\beta = 1/\cos\phi$, $\phi = 1.695\,33$.

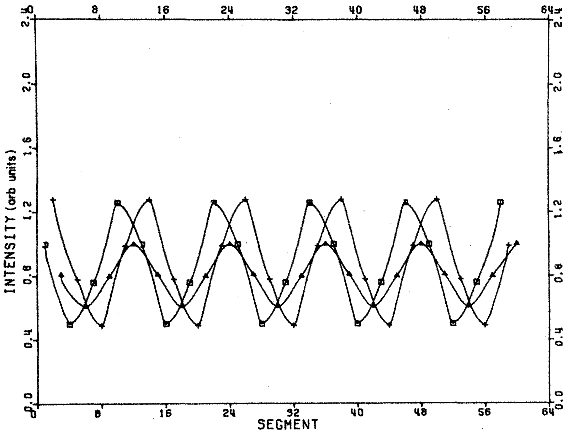

FIG. 11. The intensity $I_j = C_j^2$ for a chain of 60 segments. with $s=3$, $m_1=5$, $m_2=3$, $m_3=2$, and $\beta = 1/\cos\phi$, $\phi = 1.565\,16$.

velopes, while the third-order chain in general reveals a threefold envelope. Detailed study of the eigenvectors shall be reported elsewhere in a separate paper.

X. CONCLUSION

In this work we have analyzed the eigenvalues and eigenvectors of a finite and infinite linear cyclic systems. By constructing a phase function of the unit cell, the nature of the eigenvalues of the system can be analyzed without explicitly solving the secular equations. The phase function also allows us to discuss the symmetry of the eigenvalue equation as well as the reduction of a higher-order cyclic chain to lower order. The density of states of an infinitely cyclic chain may also be expressed in close forms. In general a diagram expansion can be constructed which leads to the new lower-order eigenvalue equation for an arbitrary periodic chain without using the traditional secular equations. Eigenvectors corresponding to a finite system demonstrate interesting collective (global) properties. The above formulation can be generalized to more than one dimensional and with more than two atomic species with short-range orderings (interaction in tridiagonal block forms). It can be adopted for the electronic states of a system as well as eigenvalues of Schrödinger equations in a quantum-mechanical system. These aspects are to be reported separately.

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APPENDIX A

Using the reduction technique, the phase function of a fourth-order cyclic chain can be reduced to

$$\cos 4\theta_1 = 8\cos^4\theta_1 - 8\cos^2\theta_1 + 1 = [(1-6\alpha_1^2+\alpha_1^4) + (8\alpha_1 - 8 - \alpha_1^3)\beta_1 + (10\alpha_1^2 - 2\alpha_1^4)\beta^2 + 4\alpha_1^3\beta^3 + \tfrac{1}{2}\alpha_1^4\beta^4]/(1+\alpha_1^2)^2 \; . \tag{A1}$$

Using the properties of Sec. V D, the general expression of $\cos\theta_4$ is

$$\mu_4 = 2\cos\theta_4 = \sum_{n=\text{even},k}^{4} A_{n,k}\Sigma(\alpha_1, \ldots, \alpha_k)\beta^n + \sum_{n=\text{even}}^{4} B_n(\alpha_1\alpha_3 + \alpha_2\alpha_4)\beta^n \; , \tag{A2}$$

where all the $A_{n,k}$ and β_n are integers. It is clear that we need to replace

$$(8\alpha_1 - 8\alpha_1^3)\beta \leftrightarrow 2\beta \sum \alpha_1 - 2\beta \sum \alpha_1\alpha_2\alpha_3 \; , \tag{A3}$$

$$4\alpha_1^3\beta^3 \leftrightarrow \beta^3 \sum \alpha_1\alpha_2\alpha_3 \; , \tag{A4}$$

$$\tfrac{1}{2}\alpha_1^4\beta^4 \leftrightarrow \tfrac{1}{2}\beta^4\alpha_1\alpha_2\alpha_3\alpha_4 \; , \tag{A5}$$

$$(10\alpha_1^2 - 2\alpha_1^4)\beta^2 \leftrightarrow (3A_{2,2} + B_2\alpha^2 - \alpha_1\alpha_2\alpha_3\alpha_4)\beta^2 \; , \tag{A6}$$

$$(1 - 6\alpha_1^2 + \alpha_1^4)\beta^0 \leftrightarrow 1 + (3A_{0,2} + B_0)\alpha^2 + \alpha_1\alpha_2\alpha_3\alpha_4 \; . \tag{A7}$$

In order to determine separately B_0, B_2, $A_{0,2}$, $A_{2,2}$, we may use the reduction of the fourth-order chain to a second-order chain and compare $\cos\theta_4$ (reduced) to

$$\cos 2\theta = 2\cos^2\theta_2 - 1 = 2[1 - \alpha_1\alpha_2 + (\alpha_1+\alpha_2)\beta + \tfrac{1}{2}\alpha_1\alpha_2\beta^2]^2/[(1+\alpha_1^2)(1+\alpha_2^2)] - 1 \; . \tag{A8}$$

Here the β^0 term is

$$2(1-\alpha_1\alpha_2)^2 - (1+\alpha_1^2) = 1 - 4\alpha_1\alpha_2 + \alpha_1^2\alpha_2^2 \; .$$

Letting $\alpha_3=\alpha_1$, $\alpha_4=\alpha_2$ in Eq. (A2), we get

$$-4\alpha_1\alpha_2-(\alpha_1^2+\alpha_2^2)=\tfrac{1}{2}A_0(\alpha_1^2+\alpha_2^2+4\alpha_1\alpha_2)+\tfrac{1}{2}\beta^0(\alpha_1^2+\alpha_2^2)\ . \tag{A9}$$

Thus

$$A_{0,2}=-2\ ,\quad B_0=0\ . \tag{A10}$$

The β^2 term is

$$3\alpha_1\alpha_2+2(\alpha_1^2+\alpha_2^2)=\tfrac{1}{2}A_{22}(\alpha_1^2+\alpha_2^2+4\alpha_1\alpha_2)+\tfrac{1}{2}B_2(\alpha_1^2+\alpha_2^2)\ .$$

Thus

$$A_{2,2}=3\ , \tag{A11}$$

$$B_2=1\ . \tag{A12}$$

In summary

$$\begin{aligned}\mu_4=&\,2\left(1-\sum\alpha_1\alpha_2+\alpha_1\alpha_2\alpha_3\alpha_4\right)\beta^0\\&+4\left(\sum\alpha_1-\sum\alpha_1\alpha_2\alpha_3\right)\beta^1\\&+\left(3\sum\alpha_1\alpha_2+2(\alpha_1\alpha_2+\alpha_2\alpha_4)\right)\beta^2\\&+\left(2\sum\alpha_1\alpha_2\alpha_3\beta^3+\alpha_1\alpha_2\alpha_3\alpha_4\right)\beta^4\ .\end{aligned} \tag{A13}$$

Explicit expressions of the phase function up to the sixth order are given in Table I.

APPENDIX B

In this appendix we use the Green's-function method to obtain results given in Eqs. (66) and (69). We shall use the notation Ref. 14. Corresponding to the first example in Sec. VII [Fig. 5(a)]

$$x_1=\frac{1}{a_H-x_2}\ , \tag{B1}$$

$$x_2=\frac{1}{a_l-x_1}\ , \tag{B2}$$

so that

$$x_1=\tfrac{1}{2}a_H-\tfrac{1}{2}a_H\left[1-\frac{4}{a_Ha_l}\right]^{1/2} \tag{B3}$$

and

$$x_2=\tfrac{1}{2}a_l-\tfrac{1}{2}a_l\left[1-\frac{4}{a_Ha_l}\right]^{1/2}\ . \tag{B4}$$

We therefore get

$$D_{11}=\frac{1}{a_H-2x_1}=\frac{1}{a_H}\left[1-\frac{4}{a_Ha_l}\right]^{-1/2}\ , \tag{B5}$$

$$D_{22}=\frac{1}{a_H-2x_2}=\frac{1}{a_H}\left[1-\frac{4}{a_Ha_l}\right]^{-1/2}\ , \tag{B6}$$

and

$$G=\frac{1}{\pi}I_m(D_{11}+D_{22})=\frac{1}{\pi}\frac{(a_H+a_l)}{a_Ha_l}\left[1=\frac{4}{a_Ha_l}\right]^{-1/2}\ . \tag{B7}$$

Corresponding to the second example of Section VII [Fig. 5(b)], we get

$$x_n=\frac{1}{a_{n+1}-x_{n+1}},\quad n=1,\ldots,4\ , \tag{B8}$$

$$y_n=\frac{1}{a_{n-1}-y_{n-1}}\ , \tag{B9}$$

with the boundary conditions

$$x_4=x_1\ , \tag{B10}$$

$$y_4=y_1\ . \tag{B11}$$

Using the explicit values of a_{n+1},

$$x_1=\frac{1}{a_H-x_2}\ ,\quad x_2=\frac{1}{a_l-x_3}\ ,\quad x_3=\frac{1}{a_l-x_1}\ . \tag{B12}$$

We may get

$$x_3=\frac{a_l^2a_H-2a_l+a_H}{2(a_la_H-1)}-\frac{\sqrt{\Delta}}{2(a_la_H-1)}\ , \tag{B13}$$

$$x_2=\frac{a_H}{2}-\frac{\sqrt{\Delta}}{2(a_l^2-1)}\ , \tag{B14}$$

and

$$x_1=\frac{a_l^2a_H-a_H}{a(a_la_H-1)}-\frac{\sqrt{\Delta}}{2(a_la_H-1)}\ , \tag{B15}$$

where

$$\Delta=(a_l^2a_H-2a_l-a_H)^2-4\ . \tag{B16}$$

Comparing with Eq. (67), we notice that

$$\Delta=-4\sin^2\theta_2\ .$$

Since

$$y_2=x_2\ ,\quad y_1=x_3\ ,\quad y_3=x_1\ , \tag{B17}$$

we get

$$D_{11}=\frac{1}{a_l-(x_1+y_1)}=\frac{a_la_H-1}{\sqrt{\Delta}}\ , \tag{B18}$$

$$D_{33}=D_{11}\ , \tag{B19}$$

and

$$D_{22}=\frac{1}{a_l-(x_2+y_2)}=\frac{a_l^2-1}{\sqrt{\Delta}}\ . \tag{B20}$$

Thus

$$\begin{aligned}G&=\frac{1}{\pi}I_m(D_{11}+D_{22}+D_{33})\\&=\frac{1}{\pi}\frac{1}{\sqrt{-\Delta}}(a_l^{12}+2a_la_H-3),\quad\text{if }\Delta>0\\&=0,\quad\text{if }\Delta\leqslant 0\ .\end{aligned} \tag{B21}$$

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[17] For large and finite systems, numerical calculations of the eigenenergies become extremely difficult. Not only does the size of the matrices become too large for any computer, propagation of errors also becomes too severe for the determination of the zeros of the secular determinate. The use of negative eigenvalue theorem in Ref. 3 or the techniques in Ref. 9 may delay the difficulty somewhat but would not be able to avoid the above difficult eventually as the systems increase in size. Since the phase function is independent of the size of the system, the above difficulties are completely bypassed.

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[20] Private communication with Professor S. Y. Wu.

[21] The results here are in complete agreement with results obtained through the use of numerical techniques developed in Ref. 9.