

One-Dimensional Model of the Quasicrystalline Alloy

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A one-dimensional chain of atoms of two types is investigated. It is proven exactly for the model of attracting hard spheres that if the ratio of the numbers of atoms of the two types is irrational, then the state of absolutely minimal energy is quasicrystalline. The quasicrystalline state is also investigated in the case of the Lennard-Jones interatomic potential. All the microscopic values (interatomic spacing, electronic density, etc.) are shown to be quasiperiodic functions varying on Cantor sets. Diffraction patterns, electronic properties, and vibrational spectra are also discussed.

KEY WORDS: Quasicrystals; incommensurability; localization, ground state.

1. INTRODUCTION

Recently systems with quasicrystalline order have become the object of keen interest. This interest has arisen from the experimental observation that the Al-Mn alloy possesses icosahedral symmetry.⁽¹⁾ The icosahedral point group is known to be incompatible with crystalline order, but, as shown by Kalugin *et al.*⁽²⁾ and Levine and Steinhardt,⁽³⁾ it is quite compatible with quasicrystalline order. In the quasicrystalline phase, atoms are positioned quasiperiodically with six independent (incommensurate) periods. Despite the lack of crystal structure, a quasicrystal scatters waves coherently. According to the KKL theory,⁽²⁾ a three-dimensional quasicrystal is a projection of the six-dimensional cubic crystal onto our 3D space. The projector should be chosen so that it projects a 6D cube onto a 3D icosahedron. Below we shall briefly review the main features of the KKL theory, but since in this paper we restrict ourselves to the 1D model, we consider a one-dimensional version of the KKL theory.

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Consider a 2D space \mathbb{R}^2 and a simple square lattice in it (the lattice constant is unity). Present \mathbb{R}^2 as $\mathbb{R}_1 \otimes \mathbb{R}_1^*$, where \mathbb{R}^1 is a physical space (the x axis in Fig. 1) and \mathbb{R}_1^* is an auxiliary nonphysical space (the y axis). Note that the y coordinate has no physical meaning. The slope w of the x axis with respect to the x_1 axis is equal to the golden mean:

$$w = (\sqrt{5} - 1)/2$$

Consider a “tube” in \mathbb{R}^2 of the width D (Fig. 1) and then project all the points of the square lattice belonging to the tube onto the x axis. This procedure creates a sequence $\{x_n\}$ of real numbers ($x_{n-1} < x_n < x_{n+1}$). Put the atoms just at the points x_n . This atomic configuration is not periodic (because w is irrational), but, as shown in Ref. 2, it gives rise to δ -function diffraction spots.

The KKL theory works so well that we are not questioning its utility. But questions inevitably arise:

1. If one constructs the quasicrystalline state of an alloy, it is not sufficient to know the sequence $\{x_n\}$. One must know what sort of atom is situated at the point x_n . The above procedure does not provide this information. Moreover, this procedure also seems to be applicable to pure substances. So, is the KKL theory the theory of an alloy, and if so, then what sorts of atoms should be placed at the points x_n ?

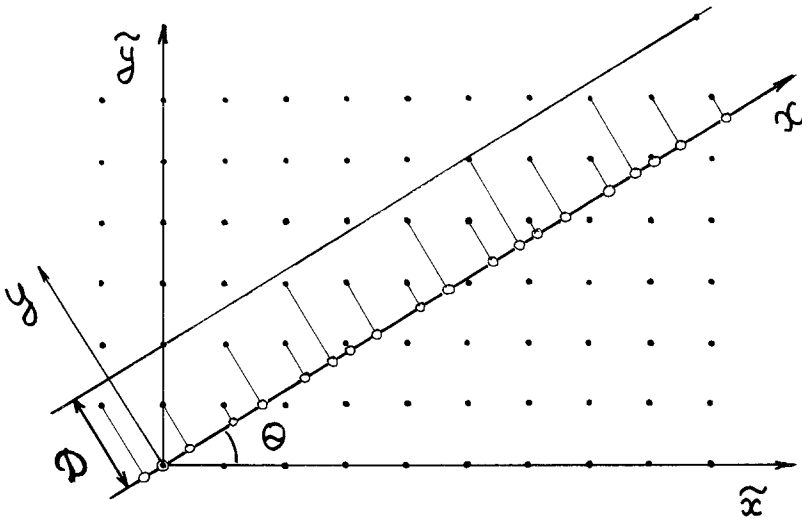


Fig. 1. “Tube rule” of the original 1D KKL theory. Circles on the x axis indicate atomic positions $\{x_n\}$ [$\text{tg } \theta = (\sqrt{5} - 1)/2$].

2. Why do atoms prefer to be just at the points x_n ? Is this configuration stable? Is it a local minimum of the free energy or is it a ground state?

3. Note that the tube width D is not specified. The theory does not give not a unique sequence $\{x_n\}$, but a family of nonequivalent sequences $\{x_n^D\}$ parametrized by D . Do all these sequences represent quasicrystalline states of real substances? This is not so. The width D should be specified. This can be done by using some "common sense" speculations, but this choice is beyond the framework of the KKL theory. For instance, one can require the KKL sequence to be identical to the Penrose tiling.⁽⁴⁾ This is so if and only if

$$D = (1 + w)/(1 + w^2)^{1/2} \quad (1)$$

So, if we *trust* the harmony of nature, we must put D equal to $(w + 1)/(w^2 + 1)^{1/2}$. But is it possible to *prove* Eq. (1)?

4. The KKL theory predicts two Goldstone modes. The second, phason mode is due to the shift of the tube in the y direction. What type of atomic displacement is associated with this shift?

5. The configuration of atoms located at the points $\{x_n\}$ is irregular. It is likely to be unstable because the net force acting on some atom from all neighbors is not zero. Thus, there must be at least small deviations of atoms from the points x_n . What are they equal to? Do they affect the diffraction patterns, electronic density, and phonon spectrum calculated in the framework of the KKL theory?

The aim of this paper is to answer these questions. However, we have done so in the one-dimensional case only. The above five questions are answered as follows.

1. The KKL theory predicts correctly the atomic coordinates of an alloy consisting of hard spheres of two types A and B. The long-range interatomic interactions are indispensable. The theory cannot be applied to pure substances.

2, 3. Under some constraints the ground state of a hard-sphere chain is the state obtained by means of the KKL tube of width D given by formula (1). A tube shift along the y axis does not change the energy.

4. The tube shift corresponds to permutations $A \leftrightarrow B$ in some AB or BA pairs of neighboring atoms (e.g., BABAAB \leftrightarrow BAABAB). Phasons are pinned due to the discreteness of the chain (as in the Frenkel–Kontorova model^(5,6)).

5. Small deviations from the points take place. They are due to the fact that real atoms are not hard spheres. They do not affect diffraction

spectra, but they are likely to change drastically localization properties of electron wave functions and the phonon spectrum.

Now we introduce the 1D model and formulate the problem. Consider a chain of atoms of two types: A and B. The concentrations of atoms are supposed to be fixed:

$$\begin{aligned}\omega &= \lim_{N \rightarrow \infty} (N_A/N), & N &= N_A + N_B \\ w &= \lim_{N \rightarrow \infty} (N_A/N_B), & \omega &= 1/(1+w)\end{aligned}\quad (2)$$

where N_A and N_B are the numbers of atoms A and B in the chain; we put $N_A \geq N_B$. The temperature is put equal to zero. Since we neglect the kinetic energy and all types of fluctuations, the state is characterized by atomic coordinates and by the potential energy of interatomic interactions. Along with atomic coordinates $\{x_n\}$ one must specify what sorts of atoms (A or B) are situated at the points $\{x_n\}$. It is convenient to do this by introducing two types of variables σ_n and x_n . The former are symbolic and take two values: A and B. A sequence of symbols $\{\sigma_n\}$ (e.g., ...ABAABABAA...) gives the order of alternation of atoms A and B in the chain. The sequence $\{x_n\}$ gives the coordinates of the centers of atoms ($x_{n-1} < x_n < x_{n+1}$). The energy is

$$\mathcal{H} = \frac{1}{2} \sum_{i,j=1}^N U_{\sigma_i \sigma_j}(x_i - x_j) \quad (3)$$

where the three functions $U_{AA}(x)$, $U_{BB}(x)$, and $U_{AB}(x)$ are long-range interatomic potentials (Fig. 2). We want to find the states ($\{\sigma_n\}; \{x_n\}$) providing local and absolute minima of the energy (3) for the limit $N \rightarrow \infty$ under the constraint of fixed concentration ω [Eq. (2)]. To find the ground state we shall use a two-stage procedure. First, we fix an arbitrary sequence of symbols $\{\sigma_n\}$ and find the coordinates $\{x_n\}$ by minimizing the energy (3) for given $\{\sigma_n\}$. Along with $\{x_n\}$ one finds the energy

$$\mathcal{H}(\{\sigma_n\}) = \min_{\{x_n\}} \mathcal{H}(\{\sigma_n\}; \{x_n\})$$

Second, one must find an absolute minimum of $\mathcal{H}(\{\sigma_n\})$.

This paper is organized as follows. Section 2 is a survey of mathematical properties of a “tube” atomic configuration (Fig. 1). Most of the results have been obtained previously by different authors in different papers in connection with different physical problems. Here we bring them together and reformulate them in terms of a quasicrystalline alloy. Section 3 is devoted to the exact solution of a particular version of the

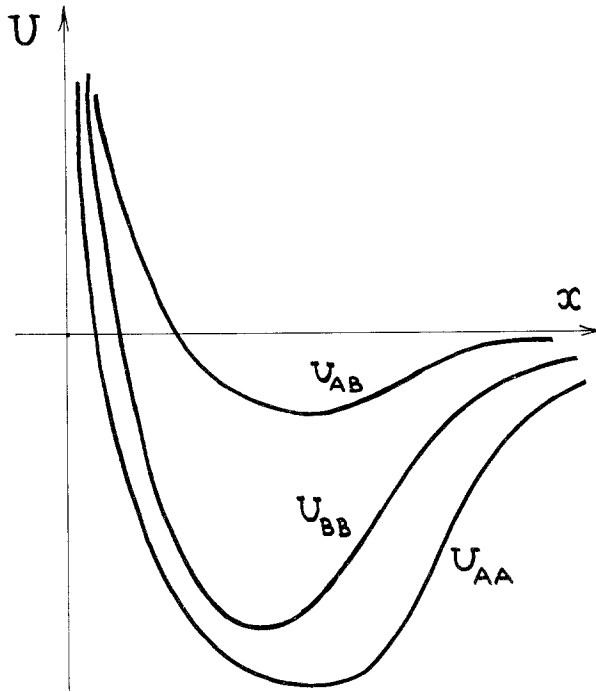


Fig. 2. Interatomic potentials for an alloy of A and B atoms.

present model, namely, atoms are supposed to be attracting hard spheres. We prove a theorem stating that under some conditions a quasicrystalline state is a ground state. Some physical quantities are calculated in the framework of the hard-sphere model. Section 4 describes the general case. Some physical quantities are calculated for the quasicrystalline state, and are shown to be quasiperiodic. The quasicrystalline state gives at least a local energy minimum. We cannot answer the question of whether the quasicrystal is a ground state. Nevertheless, we conjecture that under some conditions the quasicrystal may be a ground state. Some physical arguments for this conjecture are given. Illustrative computer calculations have been carried out (the interatomic potential is taken in the Lennard-Jones form). Adequate agreement with analytical predictions is achieved.

2. "TUBE" CONFIGURATION

In this section we deal only with symbolic sequences $\{\sigma_n\}$. To distinguish between the two sorts of variables, we shall use the term "configuration of atoms" to mean a sequence $\{\sigma_n\}$ (e.g., ...ABBABAB...).

The term "state" will be used in connection with a pair of sequences $(\{\sigma_n\}; \{x_n\})$. It is convenient to represent sequences $\{\sigma_n\}$ by broken lines in the plane (Fig. 3). A horizontal unit interval represents an A atom, a vertical one a B atom. So, each symbolic sequence $\{\sigma_n\}$ is represented by an upward-right-directed path in \mathbb{Z}^2 . In this language the condition of fixed concentration is the condition of fixed average slope: $\text{tg } \theta = w$. Note that a square lattice is used here only to find an order of alternation of A and B atoms, but not the atomic coordinates x_n (as in the KKL theory). Besides, in this scheme an atom is represented by a bond of the lattice, whereas in the KKL procedure it corresponds to a site.

We fix the concentration w and introduce a new frame reference so that the x axis has the slope $\text{th } \theta = w$ (Fig. 4). Consider an arbitrary straight line with the same slope: $y = y_*$. Now we introduce a broken line closest to the straight line $y = y_*$ (Fig. 4). More exactly, we define two modifications of the closest broken lines. The broken line of the type "+" is a path on the square lattice connecting the sites satisfying the condition $y \geq y_*$, i.e., if a site lies on the line $y = y_*$, the "+" broken line passes through this site. The "-" broken line is generated by the condition $y > y_*$, i.e., it does not have common points with the straight line $y = y_*$ (Fig. 5).

Definition 1. A "tube configuration" (of concentration w) is an atomic configuration $\{\sigma_n\}$ represented by the "+" or "-" broken line closest to the line $y = y_*$.

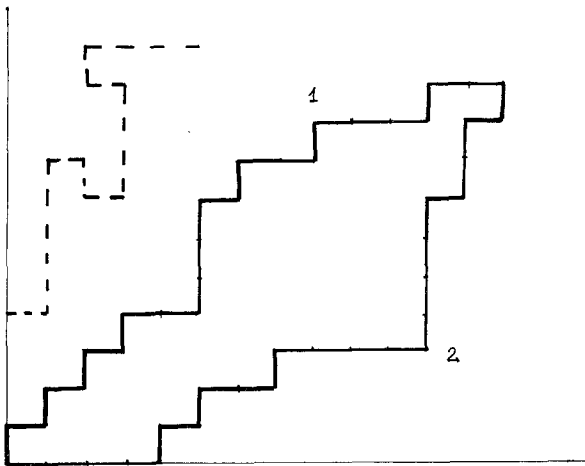


Fig. 3. Correspondence between atomic configurations $\{\sigma_n\}$ and path on a square lattice: path 1 \leftrightarrow BABABABA...; path 2 \leftrightarrow AAAABABA...; $w = \text{th } \theta = 10/13$. The path shown by the dashed line is illegal.

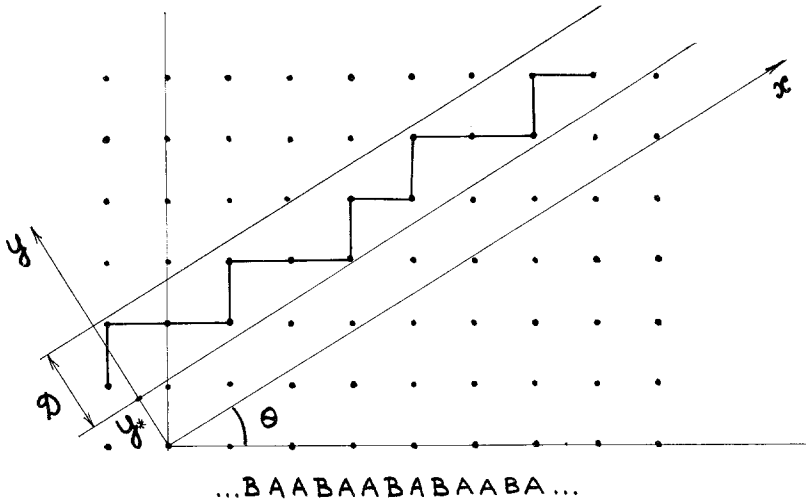


Fig. 4. Tubular atomic configuration. The path in \mathbb{Z}^2 indicates only the order of alternation of A and B atoms.

Assertion 1. A “+” broken line closest to the straight line $y = y_*$ lies in the “tube”

$$y_* \leq y < y + D \tag{4}$$

where the tube width D is given by Eq. (1). In addition, every site of the square lattice belonging to the tube (4) lies on the above closest straight line. In the case of the “-” broken line, Eq. (4) should be slightly modified.

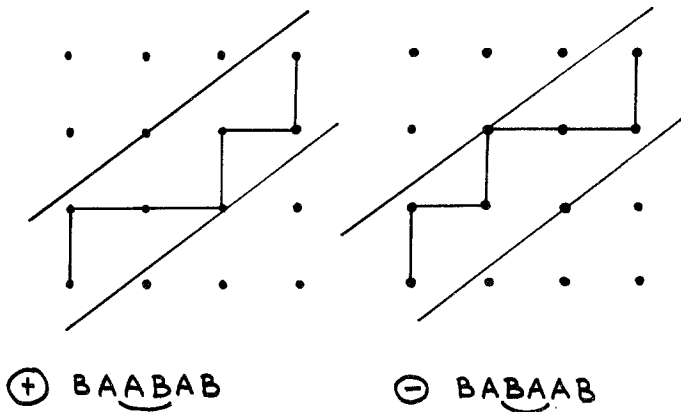


Fig. 5. Localized region where “+” and “-” tubular configurations do not coincide.

Assertion 1 explains the use of the term “tube configuration.” The proof is rather trivial.^(1,8,9) Note that $D = (w + 1)/(w^2 + 1)^{1/2} = \sin \theta + \cos \theta$, where $\text{tg } \theta = w$. This means that a tube of this width can be obtained if a unit square is pulled along the line $y = y_*$. Since an arbitrary unit square on the plane contains a unique point of \mathbb{Z}^2 , all the \mathbb{Z}^2 points of the tube give rise to an upward-right-directed path lying in the tube. And this path is obviously the closest one to the line $y = y_*$.

There are many tube configurations even at the fixed slope w ; they are represented by tubes with different y_* . A given straight line $y = y_*$ generates a unique “+” broken line and a unique “-” one. So, every y_* gives rise to one or two tube configurations (“+” and “-” broken lines may coincide). But a given tube configuration (TC) can be generated by an infinite number of lines $y = y_*$. Actually, the change $y_* \rightarrow y_* + D$ does not affect the atomic configuration $\{\sigma_n\}$. This means that all the TCs can be generated by the lines $y = y_*$, where $y_* \in [0, D)$. For this reason we introduce a parameter

$$\alpha = -\left\{ \frac{y_*}{D} \right\} = -\left[\frac{y_*}{D} - \text{Int} \left(\frac{y_*}{D} \right) \right], \quad \alpha \in S^1 \quad (6)$$

(the points 0 and 1 of the circle of unit length S^1 are set to be identical).

In general, “+” and “-” broken lines do not coincide, generating two different TCs. We want to find all α giving rise to two different TCs. Bearing in mind Eq. (6), we shall search for y_* of this type [$y_* \in [0, D)$]. It is easy to see that two TCs do not coincide if and only if the line $y = y_*$ contains at least one site of the square lattice (Fig. 5). Therefore we must find all $y_* \in [0, D)$ that are projected from lattice sites. They can be represented as

$$y_* = -n_1 \sin \theta + n_2 \cos \theta, \quad \text{tg } \theta = w$$

where $(n_1; n_2) \in \mathbb{Z}^2$ lies in the tube $0 \leq y_* < D$. This formula is not too useful because of the two nonindependent integers n_1 and n_2 . Introducing a number $n = n_1 + n_2$, we see that when n_2 changes by 1, n also changes by 1 and y_* changes by $\cos \theta$. When n_1 changes by 1, y_* changes by $-\sin \theta$. Substituting $D = \sin \theta + \cos \theta$ into Eq. (6), we see that a change of n_2 by 1 gives rise to the change $\alpha \rightarrow \alpha + \cos \theta / (\sin \theta + \cos \theta)$, and a change of n_1 yields $\alpha \rightarrow \alpha - \sin \theta / (\sin \theta + \cos \theta)$. Note that

$$\cos \theta / (\sin \theta + \cos \theta) = -\sin \theta / (\sin \theta + \cos \theta) \pmod{1}$$

So,

$$\alpha' = \alpha + \cos \theta / (\sin \theta + \cos \theta) \pmod{1}$$

for $n' = n + 1$. Substituting $\operatorname{tg} \theta = w$ into this formula, we have finally the following assertion:

The parameter α gives rise to two different tube configurations (“+” and “-”) if and only if

$$\alpha = n\omega \pmod{1}, \quad \omega = 1/(1+w), \quad n \in \mathbb{Z} \quad (7)$$

If α does not belong to the set (7), a tube configuration is unique.

Now consider how variation of α affects the atomic configuration. First consider the case of rational $w = p/q$. The atomic configuration is periodic; a unit cell contains $p + q$ atoms. The lattice sites $(n_1; n_2)$ and $(n_1 + q; n_2 + p)$ are projected onto the same point of the y axis, so the set (7) consists of $p + q$ points only; they are situated on the circle S^1 equidistantly. When α varies between two neighboring points (7), the tube boundaries are shifted in the y direction, but they do not intersect any lattice site, and therefore the configuration is unchanged. When α passes through one of the points (7), the TC varies abruptly from “-” to “+” type. These two TCs differ only by one permutation $A \leftrightarrow B$ per period (Figs. 4 and 5). Thus, there are only $p + q$ tube configurations $\{\sigma_n\}$. If w is irrational, the set (7) is everywhere dense in S^1 . The points (7) are in some sense discontinuity points of the mapping $\alpha \rightarrow \operatorname{TC}(\alpha)$. When α passes through them, the TC varies abruptly from “-” to “+” type. The “+” and “-” TCs differ by one $A \leftrightarrow B$ permutation only. In general, the change $\alpha \rightarrow \alpha + \delta\alpha$ generates an infinite number of permutations $A \leftrightarrow B$. The distances between permuted pairs AB tends to infinity when $\delta\alpha \rightarrow 0$. So, an infinitesimal change of α generates a chain of distantly spaced local defects (permutations in AB pairs). Thus, in the irrational case there is a continuum of tube configurations $\{\sigma_n\}$ parametrized by α .

Although the sequences $\{\sigma_n\}$ obtained by different α are different, some of them differ from each other only by renumbering $n \rightarrow n + m$. Such atomic configurations are physically equivalent. In fact

$$\{\sigma_{n+m}^x\} = \{\sigma_n^{x'}\}, \quad \alpha' = \alpha + m\omega \pmod{1} \quad (8)$$

In the case of rational w we have immediately that all $p + q$ TCs are physically equivalent. In the case of irrational w the $\operatorname{TC}(\alpha)$ is equivalent to the $\operatorname{TC}(\alpha')$ only if $\alpha' = \alpha + m\omega \pmod{1}$. So, there is a continuum of physically different tube configurations.

Definition 1 and Assertion 1 give two equivalent ways to describe a TC. There are other ways. The lattice sites in the tube (4) or (5) can be numbered by two nonindependent integers $(n_1; n_2)$ or by one integer $n = n_1 + n_2$. The relation between n and $(n_1; n_2)$ is given by the following result:

Assertion 2. Consider a broken line in the tube (4). For any $(n_1; n_2) \in \mathbb{Z}^2$ belonging to the tube, put

$$n = n_1 + n_2$$

Then

$$n_1 = \text{Int}(\omega n + \alpha), \quad n_2 = n - \text{Int}(\omega n + \alpha) \tag{9}$$

For the tube (5), $\text{Int}(x)$ in Eq. (9) should be substituted by $-\text{Int}(-x) - 1$.

Although a lattice site corresponds to a bond between two neighboring atoms, we can number atoms by the same integer $n = n_1 + n_2$. We put that the n th bond connects the n th and the $(n + 1)$ th atoms. In this way the atoms may be numbered by two integers n_1 and n_2 as well as by $n = n_1 + n_2$ [Eq. (9)].

Assertion 3. Consider a broken line in the tube (4). Then:

1. $\sigma_n = A$ iff $(n_1, n_2) \in \mathbb{Z}^2$ corresponds to the subtube

$$y_* \leq y < y_* + \omega D$$

and $\sigma_n = B$ iff $(n_1, n_2) \in \mathbb{Z}^2$ corresponds to the subtube

$$y_* + \omega D \leq y < y_* + D$$

where (n_1, n_2) is connected with n by Eq. (9).

2. $\sigma_n = \sigma(n\omega + \alpha)$

where

$$\sigma(t) = \begin{cases} A, & t \in [0, \omega) \\ B, & t \in [\omega, 1) \end{cases} \tag{10}$$

A fourth method⁽¹⁰⁻¹²⁾ exploits the continued fraction expansion of the concentration ω :

$$\omega = \frac{1}{1 + \frac{1}{S_1 + \frac{1}{S_2 + \frac{1}{\ddots + \frac{1}{S_n + \dots}}}}} = \{1, S_1, S_2, \dots, S_n, \dots\} \tag{11}$$

The continued fraction is finite if ω is rational; it is infinite if ω is irrational.⁽¹³⁾ To obtain the $\text{TC}(\omega, \alpha)$ by this method, we first need to

represent the parameter α as some series analogous to the usual decimal fraction, but ω should be used instead of $1/10$. Define

$$\sigma_n = \{S_n, S_{n+1}, \dots\}, \quad \lambda_n = \prod_{j=0}^n \sigma_j \tag{12}$$

where σ_n is a continued fraction obtained by deleting $S_0, S_1, S_2, \dots, S_{n-1}$ in Eq. (11) {e.g., $\sigma_0 = \omega, \sigma_1 = w, \sigma_2 = 1/[S_2 + 1/(S_3 + \dots)], \dots$ }. Since $0 < \sigma_n < 1$ for all n , $\lambda_n \rightarrow 0$ as $n \rightarrow \infty$. The numbers λ_n describe the accuracy of the approximation of ω by truncated continued fractions $\omega_n = P_n/Q_n$,⁽¹³⁾

$$P_n - \omega Q_n = (-1)^n \lambda_{n+1}$$

It follows directly from the definition (12) that

$$\sigma_{n+1} = \sigma_n^{-1} - S_n, \quad \lambda_{n+1} = \lambda_{n-1} - S_n \lambda_n \tag{13}$$

The representation of a parameter α is:

1. If ω is rational and $\alpha = m\omega \pmod{1}$, $m \in \mathbb{Z}$, then

$$\alpha = \sum_{n=0}^k (-1)^n C_n \lambda_n \tag{14}$$

where λ_n is given by Eq. (12), k is the number of stories of the continued fraction (14), and the C_n are nonnegative integers:

$$\begin{aligned} C_0 &= 1, & 0 &\leq C_1 \leq S_1 \\ 0 &\leq C_n \leq S_n & \text{if } C_{n-1} &= 0 \\ 0 &\leq C_n \leq S_n - 1 & \text{if } C_{n-1} &> 0 \end{aligned} \tag{15}$$

for $n \geq 2$. We write

$$\alpha = 1C_1C_2 \cdots C_k 000\dots$$

2. If ω is irrational, then for any $\alpha \in S^1$

$$\begin{aligned} \alpha &= \sum_{n=0}^{\infty} (-1)^n C_n \lambda_n \\ \alpha &= 1C_1C_2 \cdots C_n C_{n+1} \cdots \end{aligned} \tag{16}$$

where C_n may take values in the set defined by (15).

3. If ω is irrational, then:

(i) If $\alpha = m\omega \pmod{1}$, $m \in \mathbb{Z}$, $m > 0$, then

$$\alpha = 1C_1C_2 \cdots C_j000\dots \tag{17}$$

where C_1, C_2, \dots, C_j are unique.

(ii) If $\alpha = m\omega \pmod{1}$, $m \in \mathbb{Z}$, $m \leq 0$, then there are two sequences $\{C_n^+\}$ and $\{C_n^-\}$ such that

$$\alpha = \sum_{n=0}^{\infty} (-1)^n C_n^+ \lambda_n = \sum_{n=0}^{\infty} (-1)^n C_n^- \lambda_n \tag{18}$$

where

$$\begin{aligned} \{C_n^+\} &= \{1, C_1, \dots, C_{2k}, (S_{2k+1} - 1), 0, S_{2k+3}, 0, \dots\} \\ \{C_n^-\} &= \{1, C_1, \dots, (C_{2k} + 1), 0, S_{2k+2}, 0, S_{2k+4}, \dots\} \end{aligned}$$

or

$$\begin{aligned} \{C_n^+\} &= \{1, C_1, \dots, C_{2k}, C_{2k+1}, 0, S_{2k+3}, 0, \dots\} \\ \{C_n^-\} &= \{1, C_1, \dots, C_{2k}, (C_{2k} - 1), (S_{2k+2} - 1), 0, S_{2k+4}, \dots\} \end{aligned}$$

[Equation (18) is an analogue of the equality $0.9999\dots = 1.000\dots$ for decimal fractions.]

(iii) If $\alpha \neq m\omega \pmod{1}$, $m \in \mathbb{Z}$, then

$$\alpha = 1C_1C_2 \cdots C_nC_{n+1}\dots$$

where the sequence $\{C_n\}$ is unique and consists of an infinite number of terms.

Tubular configurations should be constructed of clusters of finite size. The smallest one consists of one A atom. We denote it as ϕ_0 . The next cluster ϕ_1 consists of one B atom and S_1 A atoms. ϕ_2 is constructed of one cluster ϕ_0 and S_2 clusters ϕ_1 , etc. Generally, ϕ_n is constructed of one ϕ_{n-2} and S_n clusters ϕ_{n-1} (Fig. 6). ϕ_n consists of p_n B atoms and q_n A atoms, where

$$p_n/(p_n + q_n) = P_n/Q_n = \omega_n = \{1, S_1, \dots, S_n\}$$

is a truncated continued fraction (11). The infinite sequence $\{\sigma_n\}$ of finite clusters ϕ_n is obtained as $n \rightarrow \infty$. We construct the left- and the right-hand parts of $\{\sigma_n\}$ separately. Denote a sequence $\{\sigma_n | n > 0\}$ as $\text{TC}(\omega; \alpha; f, R)$ and $\{\sigma_n | n \leq 0\}$ as $\text{TC}(\omega; \alpha; f, L)$, where $f = \pm 1$ labels “+” or “-” TC (Definition 1).

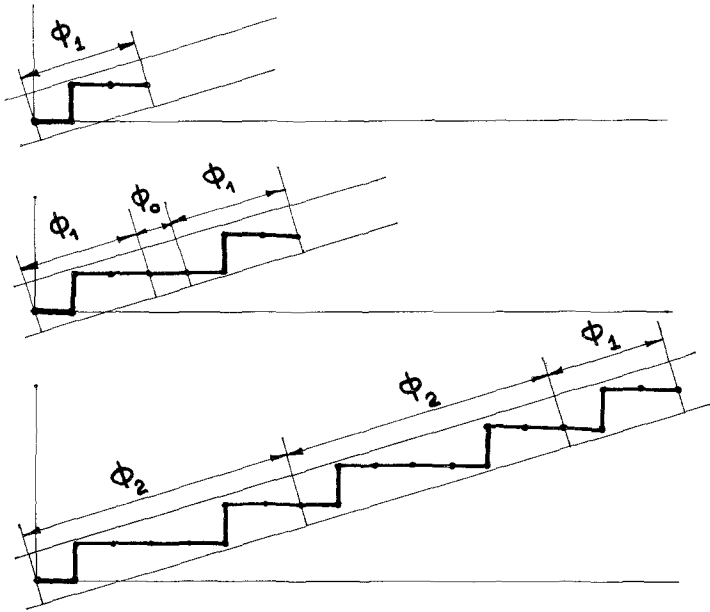


Fig. 6. Three steps of the recurrence procedure (19) for $\omega = (17\sqrt{2} + 7)/(22\sqrt{2} + 9) = \{1, 3, 2, 2, \dots\}$, $\alpha = (9\sqrt{2} + 4)/(22\sqrt{2} + 9) = 1210\dots$

Assertion 4. (i) If ω is rational and $\alpha = m\omega \pmod{1}$, $m \in \mathbb{Z}$, is represented by Eqs. (14) and (15), then TC is periodic:

$$TC(\omega; \alpha; (-1)^{k+1}; R) = \phi_k \phi_k \phi_k \dots$$

$$TC(\omega; \alpha; (-1)^k; R) = TC(\omega; \alpha + (-1)^k \lambda_k; (-1)^{k+1}; R)$$

where ϕ_k is given by the following recurrence procedure:

$$\phi_0 = A, \quad \phi_1 = \underset{S_1 - C_1}{AA \cdots A} \underset{C_1}{B AA \cdots A}$$

$$\phi_n = \underset{S_n - C_n}{\phi_{n-1} \phi_{n-1} \cdots \phi_{n-1}} \underset{C_n}{\phi_{n-2} \phi_{n-1} \phi_{n-1} \cdots \phi_{n-1}}; \quad 2 \leq n \leq k \tag{19}$$

If $\alpha \in (m\omega; m\omega + \lambda_k)$, $m \in \mathbb{Z}$, then

$$TC(\omega; \alpha; +1; R) = TC(\omega; \alpha; -1, R) = TC(\omega; m\omega; +1; R)$$

The left-hand $TC(\omega; \alpha; f; L)$ is given by

$$TC(\omega; \alpha; f; L) = TC(\omega; 1 - \alpha; -f; R)$$

(ii) If ω is irrational, then:

(a) If $\alpha \neq m\omega \pmod{1}$, $m \in \mathbb{Z}$, is represented by Eqs. (15) and (16), then

$$TC(\omega; \alpha; +1; R) = TC(\omega; \alpha; -1; R) = \phi_\infty$$

where ϕ_n are given by the recurrence procedure (19). The left-hand part is

$$\begin{aligned} TC(\omega; \alpha; +1; L) &= TC(\omega; \alpha; -1; L) \\ &= TC(\omega; 1 - \alpha; +1; R) = TC(\omega; 1 - \alpha; -1; R) \end{aligned}$$

(b) If $\alpha = m\omega \pmod{1}$, $m \in \mathbb{Z}$, $m \leq 0$, is represented by Eq. (18), then $TC(\omega; \alpha; +1; R)$ is given by (19) with $C_n = C_n^+$; $TC(\omega; \alpha; -1; R)$ is given by (19) with $C_n = C_n^-$. The representation of $1 - \alpha$ is unique [Eq. (17)] and the left-hand part of the TC is given by

$$\begin{aligned} TC(\omega; \alpha; +1; L) &= TC(\omega; \alpha; -1; L) \\ &= TC(\omega; 1 - \alpha; +1; R) = TC(\omega; 1 - \alpha; -1; R) \end{aligned}$$

(c) If $\alpha = m\omega \pmod{1}$, $m \in \mathbb{Z}$, $m > 0$, is represented by Eq. (17), then

$$\begin{aligned} TC(\omega; \alpha; +1; R) &= TC(\omega; \alpha; -1; R) = \phi_\infty \\ TC(\omega; \alpha; f; L) &= TC(\omega; 1 - \alpha; -f; R) \end{aligned}$$

where

$$1 - \alpha = -m\omega \pmod{1} = m'\omega \pmod{1}, \quad m' < 0$$

Corollary 1. If $\omega = (\sqrt{5} - 1)/2 = \{1, 1, 1, 1, \dots\}$, then TC is given by the recurrence procedure (19) where all $S_n = 1$ and

$$\alpha = 1C_1C_2 \cdots C_nC_{n+1}\dots, \quad C_n = 0; 1$$

is the Fibonacci code,⁽¹³⁾

$$\alpha = \sum_{n=0}^{\infty} (-1)^n C_n \omega^{n+1}$$

Corollary 2. If $\omega = (\sqrt{5} - 1)/2$ and $\alpha = \omega$, then $TC(\omega; \omega; +1; R) = TC(\omega; \omega; -1; R)$ is a Penrose sequence⁽⁴⁾

$$ABAABABAABAAB.. \tag{20}$$

A tubular configuration has one more interesting property, namely, it is a configuration where A and B atoms are mixed as homogeneously as possible⁽¹⁴⁾:

Assertion 5. For any tubular configuration the number of A atoms between every two successive B atoms is only $\text{Int}(1/w)$ or $\text{Int}(1/w) + 1$. Moreover, the number of A atoms between the n_2 th B atom and the $(n_2 + m)$ th B atom is only $\text{Int}(m/w)$ or $\text{Int}(m/w) + 1$.

So, we have described four methods to find a tubular configuration [the closest broken line; broken line in a tube; a quasiperiodic sequence $\sigma_n = \sigma(n\omega + \alpha)$; and a recurrence procedure exploiting the continued fraction expansion of ω]. Although all these methods give the same configuration, it is worth studying them all because the four methods are used in different applications.

3. ATTRACTING HARD SPHERES

Let A and B atoms be hard spheres of diameter a and b , respectively. The interatomic potentials $U_{AA}(x)$, $U_{BB}(x)$, and $U_{AB}(x)$ are shown in Fig. 7. We search for ground states by a two-stage energy minimization:

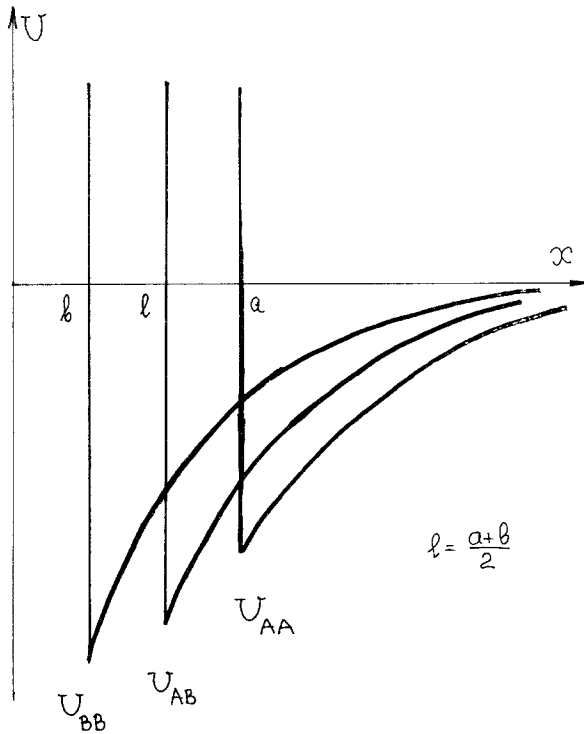


Fig. 7. Interatomic potential for the hard-sphere model.

first we find $\{x_n\}$ for the given order of alternation of A and B atoms $\{\sigma_n\}$, and second we find $\{\sigma_n\}$ minimizing the energy (3) when the concentration ω is fixed. The first stage is trivial:

Assertion 6. For any given configuration of hard spheres the energy (3) takes its minimal value when there are no empty spaces between neighboring atoms. Thus, the distances between atoms are, for AA, a ; for BB, b ; and for AB, $(a+b)/2$.

The second stage can be carried out by introducing an effective interaction of steps in the broken lines in Fig. 3 and reducing the problem to the 1D lattice gas of steps. The lattice gas problem has been solved previously.^(10,14-17)

Proposition 7. Denote

$$\begin{aligned}
 J(n_1; n_2) = & U_{\text{BB}}(n_1 a + n_2 b) \\
 & + 2 \sum_{n=0}^{\infty} [U_{\text{AB}}(n_1 a + n_2 b + l + na) \\
 & - U_{\text{AB}}(n_1 a + n_2 b + l - b + na)] \\
 & + \sum_{n=1}^{\infty} n [U_{\text{AA}}(n_1 a + n_2 b + b + na) - 2U_{\text{AA}}(n_1 a + n_2 b + na) \\
 & + U_{\text{AA}}(n_1 a + n_2 b - b + na)] \quad (21)
 \end{aligned}$$

$$n_1, n_2, n \in \mathbb{Z}, \quad n_1 \geq 0, \quad n_2 \geq 1, \quad l = (a+b)/2$$

If $J(n_1; n_2)$ satisfies the conditions

$$0 < J(n_1; n_2) < C/n_1^\gamma \quad (22a)$$

for $n_1 \rightarrow \infty$, $c > 0$, $\gamma > 1$; and

$$\begin{aligned}
 & J(n_1 + 1; n_2) - 2J(n_1; n_2) + J(n_2 - 1; n_2) \\
 & = U_{\text{BB}}(n_1 a + n_2 b + a) - 2U_{\text{BB}}(n_1 a + n_2 b) + U_{\text{BB}}(n_1 a + n_2 b - a) \\
 & \quad + 2[U_{\text{AB}}(n_1 a + n_2 b + l - a) - U_{\text{AB}}(n_1 a + n_2 b + l) \\
 & \quad + U_{\text{AB}}(n_1 a + n_2 b - b + l) - U_{\text{AB}}(n_1 a + n_2 b - b + l - a)] \\
 & \quad + U_{\text{AA}}(n_1 a + n_2 b + b) - 2U_{\text{AA}}(n_1 a + n_2 b) + U_{\text{AA}}(n_1 a + n_2 b - b) > 0 \quad (22b)
 \end{aligned}$$

$$n_1 \geq 1, \quad n_2 \geq 1$$

then all tubular configurations (with the same concentration ω) have the same energy and this value of the energy is an absolute minimum of \mathcal{H} [Eq. (31)] under the constraint of fixed concentration ω .

It should be noted that if

$$U_{AA}(x) \approx -\frac{C_{AA}}{x^\gamma}; \quad U_{BB}(x) \approx -\frac{C_{BB}}{x^\gamma}; \quad U_{AB}(x) \approx -\frac{C_{AB}}{x^\gamma}$$

as $x \rightarrow \infty$, then

$$J(n_1; n_2) \approx \frac{C}{a^2} \frac{1}{(n_1 a)^\gamma}, \quad n_1 \rightarrow \infty$$

$$C = -(a^2 C_{BB} - 2ab C_{AB} + b^2 C_{AA})$$

So, in the case of large n_1 , condition (22b) is reduced to

$$a^2 C_{BB} - 2ab C_{AB} + b^2 C_{AA} < 0$$

The function $J(n_1; n_2)$ is an effective potential describing the repulsion of two steps of the broken line (Fig. 3) separated by n_1 horizontal and n_2 vertical intervals. The condition (22b) is a well-known convexity condition for the lattice gas. Note that $J(n_1; n_2)$ must be strictly convex, and if $U(x) = 0$ for $x > x_*$, then condition (22b) is not fulfilled. So, a tubular configuration becomes a ground state in the case of a long-range interaction only. From Assertions 6 and 7, we have complete information about ground states:

Assertion 8. If (22) is fulfilled, then the ground state of the chain is described by the two sequences $\{\sigma_n\}$, $\{x_n\}$:

- (i) $\{\sigma_n\}$ is a tubular configuration $TC(\omega; \alpha)$, and (ii)

$$x_n = n_1 a + n_2 b + \frac{1}{2} h_n + \beta \tag{23}$$

$$n_1 = \text{Int}(\omega n + \alpha), \quad n_2 = n - \text{Int}(\omega n + \alpha)$$

$$h_n = h(\omega n + \alpha), \quad h(t) = \begin{cases} a, & t \in [0; \omega) \\ b, & t \in [\omega; 1) \end{cases}$$

The integers n_1 and n_2 in Eq. (23) are coordinates of the sites of the square lattice lying on the broken line representing a tubular configuration (Fig. 4). In Eq. (23) we have used Assertion 2 to obtain $(n_1; n_2)$ and Assertion 3 to obtain h_n . One can use the other three methods of Section 2 as well. Assertion 8 states that the ground states are parametrized by two real numbers α and β . The former describes local rearrangements of atoms, and the latter describes the translation of the chain as a whole. If we deal with a

crystal (ω is rational), then the ground state is once continuously degenerate (parameter β). A change of α results in renumbering only. So, the ground states with different α are physically equivalent. If we deal with a quasicrystal (ω is irrational), the ground state is twice continuously degenerate (parameters α and β).

The diffraction pattern is described by a formfactor

$$S(q) = \int_{-\infty}^{+\infty} \rho(x) e^{-iqx} dx = \sum_n S_{\sigma_n} e^{-iqx_n} \quad (24)$$

where $\rho(x)$ is the electronic density, and S_{σ_n} takes three values only:

$$\begin{aligned} S_0 &= \int_{-a/2}^{+a/2} \rho(x) e^{-iqx} dx \\ S_+ &= \int_{-b/2}^{+a/2} \rho(x) e^{-iqx} dx \\ S_- &= \int_{-a/2}^{+b/2} \rho(x) e^{-iqx} dx \end{aligned}$$

$S(q)$ can be calculated as in the KKL theory⁽²⁾

$$\begin{aligned} S(q) &= \sum_{n_1, n_2 \in \mathbb{Z}} I_{n_1, n_2} \delta(q - q_1 n_1 - q_2 n_2) \\ q_1 n_1 + q_2 n_2 &= 2\pi \frac{h_1 + w n_2}{a + w b} = Q_{\parallel} \\ Q_{\perp} &= \frac{2\pi}{(vw)^{1/2} + 1/(vw)^{1/2}} \left(-\frac{h_1}{a} + \frac{h_2}{b} \right), \quad v = \frac{b}{a} \\ I_{n_1, n_2} &= I(Q_{\perp}) \end{aligned} \quad (25)$$

Note that Eq. (25) differs slightly from the result given in Ref. 2. In the KKL theory the atomic coordinates x_n are obtained by projecting the sites of the square lattice onto the x axis:

$$x_n = h_1 \cos \theta + n_2 \sin \theta + \text{const} \quad (\text{tg } \theta = w)$$

This expression coincides with Eq. (23) only if $b/a = w$. In the present model the parameters $v = b/a$ and $w = N_B/N_A$ are independent, whereas in the KKL theory $v = w$. Despite the second parameter, the diffraction pattern remains qualitatively the same. Namely, if w is irrational, the spectrum consists of the δ -function Bragg peaks, which fill the q axis everywhere

densely. Note that this property emerges only to the irrationality of the concentration w ; the parameter $v = b/a$ may be either rational or irrational.

Consider the Schrödinger equation for a wave function $\psi(x)$ of an electron moving in a quasiperiodic potential $V(x)$ created by a chain of hard spheres:

$$-d^2\psi/dx^2 + V(x)\psi(x) = E\psi(x) \tag{26}$$

Since A and B atoms are undeformable, the potential $V(x)$ is constructed by matching two potentials $V_A(x)$, $x \in [0; a]$, and $V_B(x)$, $x \in [0; b]$. The order of alternation of V_A and V_B is the same as the order of alternation of A and B. It is useful to introduce two monodromy matrices T_A and T_B [they belong to $SL(2; \mathbb{R})$]:

$$\begin{pmatrix} \psi(a) \\ \psi'(a) \end{pmatrix} = T_A \begin{pmatrix} \psi(0) \\ \psi'(0) \end{pmatrix}, \quad \begin{pmatrix} \psi(b) \\ \psi'(b) \end{pmatrix} = T_B \begin{pmatrix} \psi(0) \\ \psi'(0) \end{pmatrix} \tag{27}$$

$\{T_A$ can be obtained by solving Eq. (26) with $V(x) = V_A(x)$ on $[0; a]$; in the case of T_B ; $V(x) = V_B(x)$, $x \in [0; b]$. The localization properties of $\psi(x)$ are governed by infinite products

$$T_{\pm} = \prod_{m=0}^{+\infty} T_{\sigma_m}$$

where $\{\sigma_m\}$ describes a tubular configuration. For this problem it is useful to take $\{\sigma_m\}$ in the form given by Assertion 4. Denote

$$T^{(n)} = \prod_{m=0}^{(p_n + q_n)} T_{\sigma_m}$$

where $q_n/(p_n + q_n) = \omega_n$ is the n th truncated continued fraction (11). Equation (19) gives rise to the following recurrence rule:

$$\begin{aligned} T^{(0)} &= T_A, & T^{(1)} &= T_A^{C_1} T_B T_A^{S_1 - C_1} \\ T^{(n)} &= (T^{(n-1)})^{C_n} T^{(n-2)} (T^{(n-1)})^{S_n - C_n} \end{aligned} \tag{28}$$

where C_n are defined in Eq. (16). This problem remains unsolved. The particular case of Eq. (28), namely, $\omega = (\sqrt{5} - 1)/2$, $\alpha = \omega$, has been extensively studied.^(9,18,19) In this case Eq. (28), according to Corollary 2, reduces to

$$T^{(n)} = T^{(n-2)} T^{(n-1)} \tag{29}$$

According to Refs. 9, 18, and 19, the wave function obtained by Eq. (29) is critical: it is neither localized nor extended. The spectrum of Eq. (26) is singular continuous; allowed energies form a Cantor set of zero measure.

4. GENERAL CASE

In this section we study states $(\{\sigma_n\}; \{x_n\})$ of a chain that minimizes the energy (3) with interatomic potentials $U_{AA}(x)$, $U_{BB}(x)$, and $U_{AB}(x)$ shown in Fig. 2. In the framework of the two-stage minimization, we should take an arbitrary configuration $\{\sigma_n\}$ and then find corresponding $\{x_n\}$ and $\mathcal{H}(\{\sigma_n\})$. Unfortunately, we cannot carry out this scheme completely. We have found $\{x_n(\{\sigma_n\})\}$ and $\mathcal{H}(\{\sigma_n\})$ not for all $\{\sigma_n\}$, but only for tubular configurations. The TCs are parametrized by α (Section 2), so we obtain $\{x_n(\alpha)\}$, $\mathcal{H}(\alpha)$, $\alpha \in S^1$. Formulas for $\{x_n(\alpha)\}$ will be given below. Now the energy:

Assertion 9. Denote

$$\mathcal{H}(\omega; \alpha) = \min_{\{x_n\}} \mathcal{H}(\{\sigma_n\}; \{x_n\}), \quad \{\sigma_n\} = \text{TC}(\omega; \alpha)$$

Then, for any ω , α_1 , α_2 , we have $\mathcal{H}(\omega; \alpha_1) = \mathcal{H}(\omega; \alpha_2)$.

Thus, we shall investigate a family of states $(\{\sigma_n(\alpha)\}, \{x_n(\alpha; \beta)\})$, where α varies in S^1 and ω is fixed. The states have the same energy and they are at least metastable. The second parameter β describes simply chain translation, $x_n \rightarrow x_n + \beta$. We cannot find out whether or not these states are ground states [because we do not know $\mathcal{H}(\{\sigma_n\})$ for all $\{\sigma_n\}$], but we believe that the both alternatives are possible:

Conjecture. If some conditions imposed on the interatomic potentials $U_{AA}(x)$, $U_{BB}(x)$, and $U_{AB}(x)$ are satisfied, then the states $(\{\sigma_n\}; \{x_n\})$, where $\{\sigma_n\}$ are tubular configurations, are ground states.

We can give two arguments for this conjecture. First, if the atoms are almost hard spheres, the elasticity is a small correction. So the energy of almost hard spheres is close to the energy of hard spheres. The latter takes its absolutely minimal value on tubular configurations (Assertion 7). It is reasonable to believe that a small correction does not change the situation drastically. Second, there is an analogy with the Frenkel-Kontorova model, where there is also two-stage minimization and some limit case ($V \rightarrow \infty$) reduced to a 1D lattice gas. In that model Aubry^(5,6) has proven a theorem which states that if one compares the ‘‘lattice gas’’ limit case (described by $\{\sigma_n\}$ only) and the general case (described by $(\{\sigma_n\}, \{x_n\})$), then both $\{\sigma_n\}$ coincide. The present model is not equivalent to the FK model, but a qualitative analogy holds.

If the concentration ω is irrational and $\{\sigma_n\} = \text{TC}(\omega; \alpha)$, we call the state of a chain (characterized by $\{\sigma_n\}, \{x_n\}$) a quasicrystalline state. The main property of this state is that all the physical values depending on the

x coordinate (or equivalently on the number n) are quasiperiodic functions of n :

$$A_n = A(n\omega + \alpha)$$

As an example, consider interatomic spacings

$$d_n = x_{n+1} - x_n \tag{30}$$

The quasiperiodicity can be described by two equivalent methods. The first way is

$$d_n = d(n\omega + \alpha), \quad d(t): S^1 \rightarrow \mathbb{R}^1 \tag{31}$$

The second one is geometrical. Consider the broken line in the tube (Fig. 4) and change one integer n by two (nonindependent) integers n_1, n_2 (Assertion 2): $d_n = d_{n_1, n_2} = d(\mathbf{r}), \mathbf{r} \in \mathbb{Z}^2$. The quasiperiodicity implies that $d(\mathbf{r})$ depends on the perpendicular coordinate $y + \alpha D$ only. The function $d(y + \alpha D)$ differs from $d(t)$ in Eq. (31) only by the dilation of the argument by D times. Below we try to explain why $d(\mathbf{r})$ depends on y only. If we take into consideration only nearest neighbors, we must conclude that all AA bonds are equivalent. The same property holds for AB bonds. Thus, in this approximation d takes two values only: d_{AA} and d_{AB} . It is clear from Fig. 8 that the tube can be divided into three subtubes. The sites in the inner tube correspond to AA bonds, those in the upper tube to BA bonds, and those in the lower tube to AB bonds. Thus, in this approximation $d(\mathbf{r})$ depends

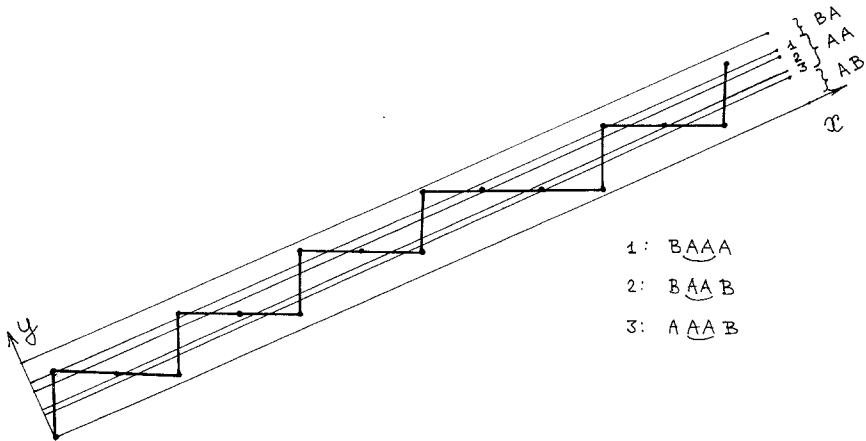


Fig. 8. Fractalization of the tube giving rise to quasiperiodicity. The upper subtube contains BA bonds, the lower one contains AB bonds, and the inner subtube contains AA bonds. The latter subtube is subdivided by the three smaller subtubes 1, 2, 3.

on y only (Fig. 9). Then consider next nearest neighbors. Now not all AA bonds are equivalent; there are BAAB, AAAB, BAAA. So, d_{AA} splits into two values d_{BAAB} and $d_{AAAB} = d_{BAAA}$. The inner tube (yielding d_{AA}) can be divided in three subtubes. The sites in the inner part of the inner tube correspond to AA bonds of the BAAB type. The two other subtubes of the inner tubes correspond to AA bonds of the AAAB and BAAA types. Thus, in this approximation $d(\mathbf{r})$ depends on y only and takes three values d_{AAAB} , d_{BAAB} , d_{AABA} . Then we should consider further splitting of AA bonds into bonds of, say, the $AB \cdots AAAB \cdots B$ type. This results in fractalization of the tube (in the y direction). Thus, $d(\mathbf{r})$ depends on y only and $d(y)$ has discontinuities at points y that are the boundaries of the subtubes. It can be easily shown that corresponding discontinuity points t are $t = m\omega \pmod{1}$, $m \in \mathbb{Z}$ [cf. Eq. (7)]. The symmetry between, e.g., AAAB and BAAA results in the property

$$d(t) = d(-t)$$

If $\omega = q/(p+q)$ is rational, $d(t)$ takes $p+q$ values only. It changes abruptly when t passes through one of $p+q$ points, $t = m\omega \pmod{1}$, and it is constant when t varies between these points (Fig. 10). If ω is irrational, $d_n = d(n\omega + \alpha)$ is quasiperiodic. The function $d(t): S^1 \rightarrow \mathbb{R}^1$ has discontinuities at the points $t = m\omega \pmod{1}$, which fill the circle S^1 everywhere densely. This means that the image of the circle S^1 is a Cantor set in \mathbb{R}^1 . It is also possible to establish a hierarchy of the discontinuities: the greater is

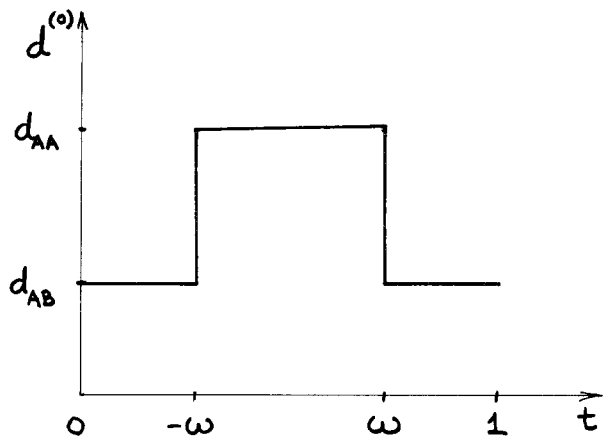


Fig. 9. The function $d^{(0)}(t)$ describing interatomic distances $d_n = d(n\omega + \alpha)$ in the hard-sphere approximation.

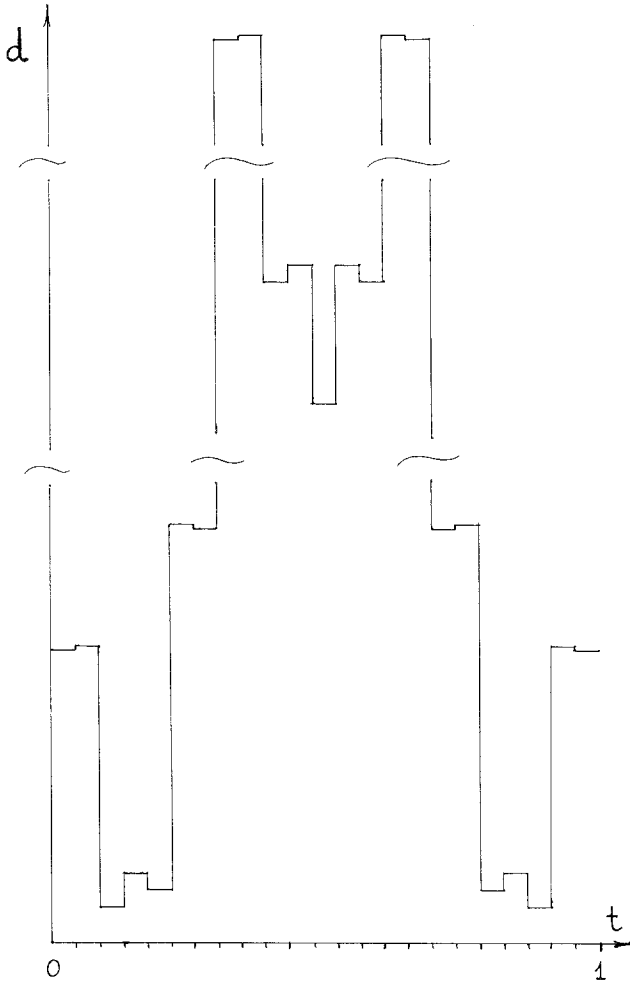


Fig. 10. The function $d(t)$ obtained numerically for $\omega = 16/23$.

m , the smaller the height of the step at the point $t = m\omega(\text{mod } 1)$. For example, if $U(x) \approx \text{const}/x^\gamma$ as $x \rightarrow \infty$, then

$$\Delta d(m\omega) = -\text{sgn}(m) \frac{C(m)}{m^{\gamma+1}}$$

$$C(m) = \begin{cases} C_1, & m = \text{Int}[k/(1-\omega)], \quad k \in \mathbb{Z} \\ C_2, & m = \text{Int}[k/(1-\omega)] + 1, \quad k \in \mathbb{Z} \\ C_3, & \text{else} \end{cases} \quad (32)$$

So far we have not used the special properties of d_n . The same can be said about any other physical value A_n [the monodromy matrix T_n , Eq. (41); the form factor of the diffraction S_n ; etc.].

Now we try to find the function $d(t)$. The coordinates x_n are obtained by the set of nonlinear equations

$$\partial \mathcal{H} / \partial x_n = 0$$

which can be rewritten in the form

$$\begin{aligned} & f_{\sigma_n \sigma_{n+1}}(d_n) \\ & + [f_{\sigma_{n-1} \sigma_{n+1}}(d_{n-1} + d_n) + f_{\sigma_n \sigma_{n+2}}(d_n + d_{n+1})] \\ & + [f_{\sigma_{n-2} \sigma_{n+1}}(d_{n-2} + d_{n-1} + d_n) + f_{\sigma_{n-1} \sigma_{n+2}}(d_{n-1} + d_n + d_{n+1}) \\ & + f_{\sigma_n \sigma_{n+3}}(d_n + d_{n+1} + d_{n+2})] + \dots = 0 \end{aligned} \quad (33)$$

where

$$f(x) = dU/dx$$

We put $d_n = d(n\omega + \alpha)$ [Eq. (31)]:

$$\begin{aligned} & f_{\sigma(t)\sigma(t+\omega)} + [f_{\sigma(t-\omega)\sigma(t+\omega)}(d(t-\omega) + d(t)) \\ & + f_{\sigma(t)\sigma(t+2\omega)}(d(t) + d(t+\omega))] + \dots = 0 \end{aligned} \quad (34)$$

where $\sigma(t)$ is given in Assertion 3. So, a nonlinear functional equation for $d(t)$ is

$$\sum_{m=1}^{\infty} \sum_{k=1}^m f_{\sigma(t+k\omega-m\omega)\sigma(t+k\omega)} \left(\sum_{j=k-m}^{k-1} d(t+j\omega) \right) = 0 \quad (35)$$

Equation (35) is an exact equation. We try to solve it approximately for interatomic potentials with a sharp minimum, namely, $|U_{AA}(a+b)|$ and $|U_{AB}(l+a)|$ are small compared with $|U_{AA}(a)|$ and $|U_{AB}(l)|$ (Fig. 2). In this case the interatomic distance d_n is set basically by the interaction of two nearest neighbors; the influence of the next nearest neighbors can be considered as a perturbation. In the zeroth order in Eq. (34) all terms except the first one should be omitted: $f_{\sigma(t)\sigma(t+\omega)}(d^{(0)}(t)) = 0$, so $d^{(0)}(t)$ takes two values only: a for AA pairs and $l = (a+b)/2$ for AB pairs (Fig. 9). Note that $d^{(0)}(t)$ coincides with $d(t)$ of the hard-sphere approximation (Section 3). The next order of the perturbation theory can be obtained in the usual way: since $d - d^{(0)}$ is small, we expand the first

term of Eq. (34), $f(d) = f(d^{(0)}) + f'(d^{(0)})(d - d^{(0)})$ and substitute $d^{(0)}(t)$ instead of $d(t)$ into other (small) terms:

$$d(t) = d^{(0)}(t) - \sum_{m=2}^{\infty} \sum_{k=1}^m f_{\sigma(t+k\omega-m\omega)\sigma(t+k\omega)} \left(\sum_{j=k-m}^{k-1} d^{(0)}(t+j\omega) \right) \times [f'_{\sigma(t)\sigma(t+\omega)}(d^{(0)}(t))]^{-1} \quad (36)$$

where $d^{(0)}(t)$ is shown in Fig. 9 and $f'_{\sigma(t)\sigma(t+\omega)}(d^{(0)}(t))$ takes two values only: $v_{AA} = \partial^2 U_{AA}(a)/\partial x^2$ if $t \in [1-\omega; \omega)$ and $v_{AB} = \partial^2 U_{AB}(l)/\partial x^2$ if $t \in [0, 1-\omega) \cup [\omega; 1)$. Equation (36) can be simplified if the Hubbard criterion (Assertion 5) is employed:

$$\sum_{j=k-m}^{k-1} d^{(0)}(t+j\omega) = R_m(t) = R_m^+, R_m^-, \text{ or } \frac{R_m^+ + R_m^-}{2}$$

$$R_m^+ = \text{Int}(m\omega) \cdot a + [m - \text{Int}(m\omega)] b$$

$$R_m^- = [\text{Int}(m\omega) + 1] a + [m - \text{Int}(m\omega) - 1] b$$

It is noteworthy that $\sum_{k=1}^m f(R_m(t))$ has discontinuities at the points $t = \pm\omega, \pm 2\omega, \dots, m\omega$. General expressions for the magnitudes of the steps are cumbersome, but for $U(x) \approx C/x^7$ and large m we obtain Eq. (32).

To check Eqs. (31) and (32) we have calculated $\{d_n\}$ numerically. Interatomic potentials have been chosen in the Lennard-Jones form (Fig. 2):

$$U_{AA}(x) = C_{AA} \left(\frac{a^6}{2x^{12}} - \frac{1}{x^6} \right), \quad U_{BB}(x) = C_{BB} \left(\frac{b^6}{2x^{12}} - \frac{1}{x^6} \right)$$

$$U_{AB}(x) = C_{AB} \left(\frac{l^6}{2x^{12}} - \frac{1}{x^6} \right)$$

The symbolic sequence $\{\sigma_n\}$ has been obtained analytically by means of the ‘‘tube rule’’ [Eq. (10)]. This sequence has fixed the order of alternation of A and B atoms. The atomic coordinates x_n have been found by direct numerical solution of the system of nonlinear equations $\partial \mathcal{H} / \partial x_n = 0$ [we have not used Eqs. (35) and (36)]. Interatomic distances $d_n = x_{n+1} - x_n$ appear to be of the form $d_n = d(n\omega + \alpha)$, where $d(t)$ (Fig. 10) possesses all the properties predicted above: it is symmetric, it is close to $d^{(0)}(t)$ (Fig. 9), and it has discontinuities at the points $t = m\omega \pmod{1}$. Moreover, the heights of the steps are proportional to m^{-7} [in agreement with Eq. (32)].

Assuming that we know $d(t)$, we find different physical quantities. First consider the average interatomic spacing

$$L = \lim_{N \rightarrow \infty} \frac{x_{N+1} - x_1}{N} = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N d_n \quad (37)$$

Substituting $d_n = d(n\omega + \alpha)$, we have (due to the ergodicity)

$$L = \int_0^1 d(t) dt \tag{38}$$

In the hard-sphere model $L^{(0)} = (a + bw)/(1 + w)$. In the general case the chain contracts and $L < L^{(0)}$. The average spacing L determines positions of the spots in the diffraction pattern. Unlike the case of hard spheres, the form factor S_n in Eq. (26) takes infinitely many values $S_n = S(n\omega + \alpha)$, where $S(t)$ has steps at the points $t = m\omega \pmod{1}$ (the KKL theory takes into consideration only the two largest steps at the points $t = \pm\omega$). The form factor $S(q)$ can be expressed via the incommensurate modulation $\varphi_n = x_n - nL$, which can be obtained from $d(t)$:

$$\varphi(t + \omega) - \varphi(t) = d(t) - L$$

Substituting $x_n = \varphi_n + nL$ into Eq. (26), we have

$$S(q) = \sum_{n_1, n_2 \in \mathbb{Z}} I_{n_1, n_2} \delta\left(q - \frac{2\pi}{L}(n_1 + \omega n_2)\right) \tag{39}$$

$$I_{n_1, n_2} = \frac{1}{L} \int_0^1 e^{-iq\varphi(t)} \int_0^{d(t)} \rho(x) e^{-iqx} dx e^{-2\pi i n_2 t} dt$$

In the case of a quasicrystal (ω is irrational) the spectrum consists of δ -function peaks filling the reciprocal space everywhere densely. Since $L < L^{(0)}$, the positions of the peaks differ slightly from those given by the hard-sphere approximation [Eq. (25) can be rewritten in the form of Eq. (39), but it contains $L^{(0)}$ instead of L]. Qualitatively, the pattern remains the same as in the KKL theory.

Now consider a localization problem for an electron wave function. The Schrödinger equation with a quasiperiodic potential $V(x)$ can be reduced to an infinite product of the monodromy matrices

$$T = \prod_{n=0}^{\infty} T_n \tag{40}$$

where $T_n \in SL(2; \mathbb{R})$ is obtained by solving Eq. (26) on $[x_n; x_{n+1}]$:

$$\begin{pmatrix} \psi(x_{n+1}) \\ \psi'(x_{n+1}) \end{pmatrix} = T_n \begin{pmatrix} \psi(x_n) \\ \psi'(x_n) \end{pmatrix}$$

Unlike the hard-sphere model, T_n takes, not two values T_A and T_B , but infinitely many values. In fact, the atoms are deformed and different A (or B) atoms are not equivalent. T_n is a quasiperiodic function of n :

$$T_n = T(n\omega + \alpha) \tag{41}$$

where $T(t): S^1 \rightarrow SL(2; \mathbb{R})$ varies on the Cantor-type subset of $SL(2; \mathbb{R})$. The function $T(t)$ has a countable set of discontinuity points $t = m\omega \pmod{1}$ [cf. Eq. (7)].

There is another equation, reduces to Eqs. (40) and (41) with $T(t)$ of this type:

$$-\varphi_{n+1} + 2\varphi_n - \varphi_{n-1} + V(n\omega + \alpha) \varphi_n = E\varphi_n \tag{42}$$

where $V(t)$ has discontinuities at the points $t = m\omega \pmod{1}$ (the larger m , the smaller the step), so $V(t)$ varies on the Cantor set. Peyrard and Aubry⁽²⁰⁾ have investigated numerically a particular case of Eq. (42) when studying the vibrational spectrum of the Frenkel–Kontorova chain in the state discribed by a Cantorus. Unfortunately, even for this case the localization problem remains unsolved. It is worthy to note that Eqs. (40) and (41) can be treated by means of Oseledec’s multiplicative ergodic theorem,⁽²¹⁾ which states that the limit

$$T = \lim_{N \rightarrow \infty} \left[\left(\prod_{n=1}^N T_n \right) \left(\prod_{n=1}^N T_n \right)^\dagger \right]^{1/(2N)}$$

exists for almost all ω and α and it defines Liapunov indices. Unfortunately, we cannot solve the localization problem. We mention it here only to formulate the problem correctly and point out that the recurrence procedures (28) and (29) can be applied to hard spheres only. The fact that $T(t)$ takes only two values T_A and T_B changes the symmetry of Eq. (26); namely, Eqs. (28) and (29) have scaling symmetry, whereas the general version of Eq. (26) does not possess this symmetry. Bearing in mind that the wave function in the hard-sphere approximation is critical (neither localized nor extended),^(9,18,19) we may conjecture that in a general case localization properties of the electron wave function can be very different from those obtained in the hard-sphere approximation [Eqs. (28) and (29)].

It is also interesting to investigate a phonon spectrum:

$$\sum_m U''_{\sigma_n \sigma_m} (x_n - x_m)(u_n - u_m) = m_n \Omega^2 u_n \tag{43}$$

where $m_n = m(n\omega + \alpha)$; $m(t) = m_A$, $t \in [0; \omega)$; $m(t) = m_B$, $t \in [\omega, 1)$. The dynamical matrix

$$\begin{aligned} K_{nm} &= U''_{\sigma_n \sigma_m} (x_n - x_m) \\ &= U''_{\sigma(n\omega + \alpha) \sigma(m\omega + \alpha)} \left(\sum_{j=n}^{m-1} d(j\omega + \alpha) \right) \end{aligned}$$

is quasiperiodic. Consider an approximation of almost hard spheres [in this case the minimum of $U(x)$ is very sharp]. The leading term should be obtained by keeping the nearest neighbors only and by substituting $d^{(0)}(t)$ instead of $d(t)$ in Eq. (93) [i.e., all A (or B) atoms are assumed to be identical]:

$$-v_n u_{n+1} + (v_n + v_{n+1}) u_n - v_{n-1} u_{n-1} = m_n \Omega^2 u_n \tag{44}$$

where $v_n = v(n\omega + \alpha)$, and

$$v(t) = f'_{\sigma(t)\sigma(t+\omega)}(d^{(0)}(t))$$

takes two values only [cf. Eq. (36)]:

$$\begin{aligned} v_{AA} &= \partial^2 U_{AA}(a)/\partial x^2 & \text{if } t \in [1-\omega; \omega) \\ v(t) &= v_{AB} = \partial^2 U_{AB}(l)/\partial x^2 & \text{if } t \in [0; 1-\omega) \cup [\omega; 1) \end{aligned}$$

Equation (44) can be reduced to an equation analogous to Eq. (28). The only difference is that there are four types of T_A : T_{AAA} , T_{BAB} , T_{AAB} , and T_{BAA} . But if we consider two types of clusters:

$$\tilde{A} = \underbrace{AA \cdots A}_{C_1} \underbrace{B AA \cdots A}_{S_1 - C_1}, \quad \tilde{B} = \underbrace{A \cdots A}_{C_1} \underbrace{B AA \cdots A}_{S_1 - C_1 + 1}$$

there will be only two monodromy matrices $T_{\tilde{A}}$ and $T_{\tilde{B}}$ satisfying Eq. (28), where $\sigma_2 = 1/w - S_1$ should be used instead of ω . The formulas for $T_{\tilde{A}}$ and $T_{\tilde{B}}$ are trivial but cumbersome. We give here only the formulas for the particular case of the golden mean $\omega = (\sqrt{5} - 1)/2$, $\alpha = \omega$:

$$\begin{aligned} T^{(n+1)} &= T^{(n-1)} T^{(n)} \\ T_0 &= T_{\tilde{A}}, \quad T_1 = T_{\tilde{B}} T_{\tilde{A}} \\ T_{\tilde{A}} &= T_{BAA} T_{AAB} T_B, \quad T_{\tilde{B}} = T_{BAB} T_B \\ T_{BAA} &= \begin{pmatrix} ((v_{AA} + v_{AB} - m_A \Omega^2)/v_{AA}) & -v_{AB}/v_{AA} \\ 1 & 0 \end{pmatrix} \\ T_{AAB} &= \begin{pmatrix} ((v_{AA} + v_{AB} - m_A \Omega^2)/v_{AB}) & -v_{AA}/v_{AB} \\ 1 & 0 \end{pmatrix} \\ T_{BAB} &= \begin{pmatrix} (2v_{AB} - m_A \Omega^2)/v_{AB} & -1 \\ 1 & 0 \end{pmatrix} \\ T_B &= \begin{pmatrix} (2v_{AB} - m_B \Omega^2)/v_{AB} & -1 \\ 1 & 0 \end{pmatrix} \end{aligned} \tag{45}$$

Thus, in the framework of the almost-hard-sphere approximation according to Refs. 9, 18, and 19, the phonon spectrum is singular continuous, the eigenfrequencies form a Cantor set of zero measure, and U_n is neither localized nor extended. The approximate equation (44) possesses scaling symmetry, while the exact equation (43) does not. In a general case the dynamical matrix cannot be reduced to the product of two 2×2 matrices $T_{\bar{A}}, T_{\bar{B}}$. So, due to different symmetries of Eqs. (43) and (44), the phonon spectrum obtained by the exact equation may be rather different from that obtained by the approximate recurrence procedure (44).

Thus, we see that the KKL theory is in some sense an approximate theory that takes into consideration the nearest neighbors only and considers atoms as undeformable spheres. In the framework of this theory all A atoms are identical, as are all B atoms (actually, the physical properties of an A atom depend on the environment: an A atom in, say, an AAA cluster differs from an A atom in an AAB cluster). In other words, the KKL theory takes into consideration only the largest steps in the graphs of all the quasiperiodic functions $A_n = A(n\omega + \alpha)$, which are situated at the points $t = \pm\omega$ (cf. Figs. 9 and 10). This approximation gives the leading term of the perturbation theory, but we have shown that if one takes into account the small corrections from the distant neighbors and from the deformability of the chain, the situation may change. Namely, the KKL approach is good for the diffraction pattern, but it may be somewhat incorrect when one deals with electronic and phonon spectra. On any account, Eqs. (42) and (43) deserve special attention.

In conclusion, we want to say why we have introduced long-range forces $U(r) \sim 1/r^\nu$. It is known that in two and three dimensions it is possible to give examples of lattice gas models with finite-range interactions [$U(r) = 0$ for $r > r_*$], which have almost periodic ground states.^(23,24) All these models form the class of models based on Berger's theorem.⁽²²⁾ Unfortunately, even 2D and 3D versions of the KKL model do not belong to this class. Moreover, it is easy to show that in one dimension it is impossible to obtain a quasiperiodic ground state if interatomic forces have finite range. So, 1D quasicrystals require infinite-range forces. However the one-dimensional situation may differ strongly from higher dimensional cases, it is worth investigating it because, first, some phenomena that occur in one dimension may also appear in three dimensions and, second, there are alloys (e.g., pyrrhotite, $\text{Fe}_{1-x}\text{S}^{(25)}$) that are quasiperiodic in one direction. On any account, one-dimensional quasicrystals are being extensively investigated.⁽²⁶⁾

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