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Anharmonic effects in the Fibonacci-chain quasicrystals

V. I. Zubov* and J. N. Teixeira Rabelo
Departamento de Física, Universidade Federal de Goiás, Caixa Postal 131, 74001-970, Goiânia, Goiás, Brazil

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Structural and dynamical properties of the anharmonic Fibonacci-chain quasicrystal have been studied using the unsymmetrized self-consistent-field method. Nonlinear integral equations forming the basis of this method are reduced to a set of transcendental or algebraic equations for the moments of one-particle functions. In the lowest orders of anharmonicity, these equations have been solved for an arbitrary one-dimensional model of various atoms interacting with the nearest neighbors. Herewith, the thermal expansion, the variances of the atomic positions, and high-order moments have been expressed in terms of the second, third, and fourth derivatives of the interatomic potentials. Quantum corrections have been calculated as well. The general results have been applied to the system with two kinds of atoms alternating with each other in a Fibonacci sequence. The interatomic distances, thermal expansions, and effective amplitudes of anharmonic atomic vibrations are calculated versus the temperature. The influence of anharmonicity on the thermodynamic functions of the Fibonacci chain is also discussed as well as possible applications to some real solids.

I. INTRODUCTION

During the last decade, it had been ascertained that, along with crystalline and amorphous solids, there exist quasicrystals.[1,2] They constitute a different kind of solids, which have long-range order but do not possess exact translational symmetry.[1-4] Owing to an aperiodicity, the Bloch theorem is not fulfilled, making the theoretical study of electronic and atomic properties of quasicrystals very complicated. That is why one-dimensional models of quasicrystals are currently drawing considerable attention. In general, one-dimensional models are of great importance in solid-state physics.[5-8] Among atomic properties of such models of quasicrystals, various characteristics of vibrational spectra[9-15] and the dynamical structural factor[16] have been studied for Fibonacci chains. However, on account of the above-mentioned difficulties only the harmonic approximation has been utilized and hence anharmonic effects have not been investigated. At the same time, research into anharmonic effects is of topical interest, since they cause such important phenomena as thermal expansion, deviation from the Dulong and Petit law at high temperatures, etc.

In this work we present a calculation of the influence of anharmonicity of the atomic vibrations on the properties of the Fibonacci chain. For this purpose we use the unsymmetrized self-consistent-field method,[17-21] extending it to arbitrary arrangements of various atoms interacting with nearest neighbors in one dimension.

II. GENERAL APPROACH

In the most general case, the unsymmetrized self-consistent-field method is based on nonlinear integrodifferential equations for the one-particle density matrices and the self-consistent potentials of atoms.[21] These equations satisfy the Bogoliubov statistical variational principle. In the present paper we use the quasiclassical approach; in the coordinate representation the diagonal elements of the one-particle density matrix of the ith atom are then of the form

$$\rho_i(\mathbf{r}_i,\mathbf{r}_i)\approx w_i(\mathbf{r}_i)\left\{1-\frac{\hbar^2}{12m_i\theta^2}[\xi_i(\mathbf{r}_i)-\bar{\xi}_i]\right\} . \tag{1}$$

Here $\theta=kT$, m_i is the atomic mass,

$$w_i(\mathbf{r}_i)=\exp\left[-\frac{u_i(\mathbf{r}_i)}{\theta}\right]\Big/\int\exp\left[-\frac{u_i(\mathbf{r}_i)}{\theta}\right]d\mathbf{r}_i \tag{2}$$

is its classical one-particle probability density, $u_i(r_i)$ its classical self-consistent potential, $\xi_i(r_i)$ the quantum correction to them, and

$$\bar{\xi}_i=\int\xi_i(\mathbf{r}_i)w_i(\mathbf{r}_i)d\mathbf{r}_i . \tag{3}$$

For the arbitrary one-dimensional ($\mathbf{r}_i\to x_i$) system of various atoms interacting with nearest neighbors is shown in Fig. 1, these functions obey the following equations

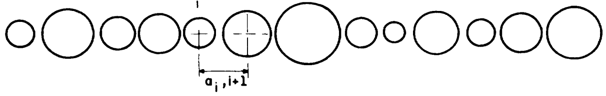

FIG. 1. One-dimensional model with an arbitrary composition of various atoms.

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$$u_i(x_i)=\sum_{j=i\pm1} u_{ij}(x_i)=\sum_{j=\pm1}\left[\int \Phi_{ij}(|x_i-x_j|)w_j(x_j)dx_j-\frac{1}{2}\int \Phi_{ij}(|x_i-x_j|)w_i(x_i)w_j(x_j)dx_i dx_j\right] ; \tag{4}$$

$$\xi_i(x_i)=\xi_i^0(x_i)+\frac{1}{2\theta}(\overline{u_i\xi_i}-\bar{u}_i\bar{\xi}_i)+\frac{1}{\theta}\sum_{j=\pm1}\frac{m_i}{m_j}\left[\bar{\xi}_j u_{ij}(x_i)-\int \Phi_{ij}\xi_j w_j dx_j+\frac{1}{2}\int \Phi_{ij}\xi_j w_i w_j dx_i dx_j\right] , \tag{5}$$

where Φ_{ij} are the interaction potentials, and

$$\xi_i^0(x_i)=\frac{\partial^2 u_i}{\partial x_i^2}-\frac{1}{2\theta}\left[\frac{\partial u_i}{\partial x_i}\right]^2 . \tag{6}$$

It should be noted that the functions ξ_i contain corrections to the one-particle probability densities (2) defined by the classical self-consistent potentials u_i (6) and to these potentials themselves.

In the case of an infinite system, $-\infty < i < \infty$. For a semi-infinite chain, Eqs. (4) and (5) are valid at $i \geq 2$, while

$$u_1(x_1)=\int \Phi_{12}(x_2-x_1)w_2(x_2)dx_2 -\frac{1}{2}\int \Phi_{12}w_1 w_2 dx_1 dx_2 ; \tag{7}$$

$$\xi_1(x_1)=\xi_1^0(x_1)+\tfrac{1}{2}(\overline{u_1\xi_1}-\bar{u}_1\bar{\xi}_1) +\frac{m_1}{m_2\theta}\left[\bar{\xi}_2 u_1(x_1)-\int \Phi_{12}\xi_2 w_2 dx_2 +\frac{1}{2}\int \Phi_{12}\xi_2 w_1 w_2 dx_1 dx_2\right] . \tag{8}$$

In Eqs. (4) and (5) for a system of N atoms, $2 \leq i \leq N-1$, and equations similar to (7) and (8) can be written for the Nth atom.

The solution of (4), (5), (7), and (8) enables one to calculate the statistical averages of various functions of atomic coordinates

$$\langle \varphi_i \rangle=\bar{\varphi}_i-\frac{\hbar^2}{12 m_i\theta^2}(\overline{\varphi_i\xi_i}-\bar{\varphi}_i\bar{\xi}_i) . \tag{9}$$

In particular, (9) gives the average interatomic distances

$$a_{i,i+1}=\langle x_{i+1}-x_i \rangle \tag{10}$$

and the variances of the atomic positions

$$D_i=\langle (x_i-\langle x_i \rangle)^2 \rangle , \tag{11}$$

which express the effective amplitudes of the atomic vibrations.

One can see that the solution of (5) and (8) possesses the property

$$\sum_i \frac{1}{m_i}\bar{\xi}_i=\sum_i \frac{1}{m_i}\bar{\xi}_i^0=\frac{1}{2}\sum_i \frac{1}{m_i}\overline{\frac{\partial^2 u_i}{\partial x_i^2}} . \tag{12}$$

Because of this and also owing to the second terms in the right sides of (4) and (7), the Helmholtz free energy is determined by the usual formula

$$F=\sum_i\left\{-\theta \ln\left[\left[\frac{m_i\theta}{2\pi\hbar^2}\right]^{1/2}\int e^{-u_i/\theta}dx_i\right] +\frac{\hbar^2}{24 m_i\theta}\overline{\frac{\partial^2 u_i}{\partial x_i^2}}\right\} . \tag{13}$$

Differentiating it gives the internal energy

$$E=\sum_i\left[\frac{\theta}{2}+\bar{u}_i+\frac{\hbar^2}{12 m_i\theta}\left[\overline{\frac{\partial^2 u_i}{\partial x_i^2}}-\frac{\theta}{2}\frac{\partial}{\partial\theta}\overline{\frac{\partial^2 u_i}{\partial x_i^2}}\right]\right] \tag{14}$$

and other thermodynamic functions. Corrections to them can be calculated using statistical perturbation theory. It should be noted that the main anharmonic terms are included in (4)–(14).

III. CLASSICAL APPROXIMATION

In (4) and (7) we change the independent variables

$$x_{i+1}-x_i=a_{i,i+1}+q_{i+1}-q_i , \tag{15}$$

considering that

$$a_{i,i+1}=r_{i,i+1}^0+\Delta a_{i,i+1}(\theta) , \tag{16}$$

where $r_{i,i+1}^0$ is the minimum point of the interatomic potential $\Phi_{i,i+1}$ (i.e., static equilibrium spacing).

Expanding the interaction potentials in a power series of the relative atomic displacements $q_{i+1}-q_i$, (4) takes the form

$$u_i(q_i)=u_{i0}+\sum_{l\geq1}\frac{1}{l!}\mathcal{F}_l^i q_i^l , \tag{17}$$

where

$$u_{i0}=\frac{1}{2}\left[\mathcal{F}_0^i-\sum_{l\geq1}\frac{1}{l!}\mathcal{F}_l^i\overline{q_i^l}\right] ; \tag{18}$$

$$\mathcal{F}_l^i=\sum_{k\geq0}\frac{1}{k!}\left[(-1)^l\Phi_{i,i+1}^{(l+k)}(a_{i,i+1})\overline{q_{i+1}^k} +(-1)^k\Phi_{i-1,i}^{(l+k)}(a_{i-1,i})\overline{q_{i-1}^k}\right], \quad l\geq0 . \tag{19}$$

Relations (17) and (19) together with (2) and

$$\overline{q_i^k}=\int q_i^k w_i(q_i)dq_i, \quad k\geq1; \quad \bar{q}_i=0 \tag{20}$$

constitute a set of transcendental equations for the average interatomic distances (10) and the moments (20) of the one-particle functions in the classical approximation (2).

Further, we consider the case of weak anharmonicity restricting ourselves to its lowest orders; then the equations are linearized and we get their solution

$$\begin{aligned}
\Delta a_{12}&=-\frac{g_{12}\theta}{2f_{12}}\left[\frac{1}{f_{12}}+\frac{1}{f_{12}+f_{23}}\right];\\
\Delta a_{i,i+1}&=-\frac{g_{i,i+1}\theta}{2f_{i,i+1}}\left[\frac{1}{f_{i-1,i}+f_{i,i+1}}+\frac{1}{f_{i,i+1}+f_{i+1,i+2}}\right],\quad i\geq 2\\
D_1&=\frac{\theta}{f_{12}}\left\{1+\frac{\theta}{2f_{12}}\left[\frac{1}{f_{12}}\left[\frac{2g_{12}^2}{f_{12}}-h_{12}\right]+\frac{1}{f_{12}+f_{23}}\left[\frac{g_{12}^2}{f_{12}}-h_{12}\right]\right]\right\}\\
D_2&=\frac{\theta}{f_{12}+f_{23}}\left\{1+\frac{\theta}{2(f_{12}+f_{23})}\left[\frac{g_{12}^2}{f_{12}}\left[\frac{1}{f_{12}}+\frac{1}{f_{12}+f_{23}}\right]+\left[\frac{g_{12}-g_{23}}{f_{12}+f_{23}}\right]^2\right.\right.\\
&\quad\left.\left.+\frac{g_{23}^2}{f_{23}}\left[\frac{1}{f_{12}+f_{23}}+\frac{1}{f_{23}+f_{34}}\right]-\frac{h_{12}}{f_{12}}-\frac{h_{12}+h_{23}}{f_{12}+f_{23}}-\frac{h_{23}}{f_{23}+f_{34}}\right]\right\};
\end{aligned}\tag{21}$$

$$\begin{aligned}
D_i&=\frac{\theta}{f_{i-1,i}+f_{i,i+1}}\left\{1-\frac{\theta}{2(f_{i-1,i}+f_{i,i+1})}\left[\frac{g_{i-1,i}^2}{f_{i-1,i}}\left[\frac{1}{f_{i-2,i-1}+f_{i-1,i}}+\frac{1}{f_{i-1,i}+f_{i,i+1}}\right]\right.\right.\\
&\quad+\left[\frac{g_{i-1,i}-g_{i,i+1}}{f_{i-1,i}+f_{i,i+1}}\right]^2+\frac{g_{i,i+1}^2}{f_{i,i+1}}\left[\frac{1}{f_{i-1,i}+f_{i,i+1}}+\frac{1}{f_{i,i+1}+f_{i+1,i+2}}\right]\\
&\quad\left.\left.-\frac{h_{i-1,i}}{f_{i-2,i-1}+f_{i-1,i}}-\frac{h_{i-1,i}+h_{i,i+1}}{f_{i-1,i}+f_{i,i+1}}-\frac{h_{i,i+1}}{f_{i,i+1}+f_{i+1,i+2}}\right]\right\},\quad i\geq 3\,,
\end{aligned}\tag{22}$$

$$\overline{q_1^3}=\frac{g_{12}\theta^2}{f_{12}^3};\quad \overline{q_i^3}=\frac{(g_{i,i+1}-g_{i-1,i})\theta^2}{(f_{i-1,i}+f_{i,i+1})^3},\quad i\geq 2\,;\tag{23}$$

$$\overline{q_1^4}=\frac{3\theta^2}{f_{12}^2};\quad \overline{q_i^4}=\frac{3\theta^2}{(f_{i-1,i}+f_{i,i+1})^2},\quad i\geq 2\,.\tag{24}$$

Here

$$f_{ij}=\Phi^{\mathrm{II}}(r_{ij}^0),\quad g_{ij}=\Phi^{\mathrm{III}}(r_{ij}^0),\quad h_{ij}=\Phi^{\mathrm{IV}}(r_{ij}^0)\,.\tag{25}$$

One can see from (21) that the thermal average of the distance between two neighboring atoms depends not only on the interaction between them but also on the interaction of each of these atoms with its other neighbor. It follows from (22) that in the harmonic approximation, the effective amplitude of the thermal vibrations of an atom in the model considered is determined only by its interactions with the nearest neighbors. The anharmonic renormalization brings about the dependence of this amplitude on the interactions between its nearest and next-nearest neighbors as well. Inserting (17) and (18) into (13) and (14) we obtain the classical zeroth-order approximation

$$F_0=\frac{1}{2}\sum_i\left[\mathcal{F}_0^i-\theta\ln\frac{m_i\theta^2}{\hbar^2\mathcal{F}_2^i}-\tfrac{1}{2}\mathcal{F}_2^i\overline{q_i^2}+\frac{1}{24}\mathcal{F}_4^i\overline{q_i^4}\right];\tag{26}$$

$$E_0=\frac{1}{2}\sum_i\left[\theta+\sum_{l=0}^{4}\frac{1}{l!}\mathcal{F}_l^i\overline{q_i^l}\right],\tag{27}$$

with the interatomic distances and moments being determined by (21)–(24).

One can deduce from the general expressions derived here the following special cases: the infinite and semi-infinite monatomic (as well as diatomic) linear chains, the semi-infinite chain with adsorbed atoms, and the chain with substitutional impurities, which have been studied in the past[20,22] using special forms of equations for those cases. Below we shall apply the equations derived to the anharmonic Fibonacci chain.

IV. QUANTUM CORRECTIONS

Now we proceed to solving Eqs. (5) and (8) and calculating the quantum corrections to the nearest-neighbor distances and variances of the atomic positions. In the lowest order of anharmonicity, (6) is equal to

$$\xi_i^0(q_i)=\mathcal{F}_2^i+\left[\mathcal{F}_3^i-\frac{\mathcal{F}_1^i\mathcal{F}_2^i}{\theta}\right]q_i-\frac{1}{2\theta}(\mathcal{F}_2^i)^2q_i^2-\frac{\mathcal{F}_2^i\mathcal{F}_3^i}{2\theta}q_i^3\,.\tag{28}$$

We try the solution of (5) and (9) in a similar form:

$$\begin{aligned}\xi_i(q_i)&=\xi_i^0(q_i)+\xi_i'(q_i)\\&=\xi_{i0}+k_1^iq_i+\tfrac{1}{2}k_2^iq_i^2+\tfrac{1}{6}k_3^iq_i^3\,.\end{aligned}\tag{29}$$

Then, the correlation moments in (11) are written as

$$\overline{\varphi_i\xi_i}-\overline{\varphi}_i\overline{\xi}_i=\overline{\varphi_i\xi_i^0}-\overline{\varphi}_i\overline{\xi_i^0}+\overline{\varphi_i\xi_i'}-\overline{\varphi}_i\overline{\xi_i'}\,,\tag{30}$$

with correlations between ξ_i^0 and necessary values being

$$\overline{q_1\xi_i^0}=-\frac{g_{12}\theta}{2f_{12}};\quad \overline{q_i\xi_i^0}=\frac{(g_{i-1,i}-g_{i,i+1})\theta}{2(f_{i-1,i}+f_{i,i+1})},\quad i\geq 2\,;\tag{31}$$

$$\overline{q_i^2\xi_i^0}-\overline{q_i^2}\,\overline{\xi_i^0}=-\theta\,.\tag{32}$$

Here we taken into account that $\overline{q_i}=0$ (20).

Inserting (28) and (29) together with (17) and a power series for $\xi(q)$ into (5) and (9) we see that

$$\xi_{i0}\approx\mathcal{F}_2^i;\quad k_2^i\approx-(\mathcal{F}_2^i)^2/\theta;\quad k_3^i\approx-3\mathcal{F}_2^i\mathcal{F}_3^i/\theta \tag{33}$$

and

$$k_1^i=\mathcal{F}_3^i-\frac{\mathcal{F}_1^i\mathcal{F}_2^i}{\theta}+\Delta k^i\ , \tag{34}$$

with Δk^i obeying the following equations,

$$\begin{aligned}
\Delta k^1&=\frac{m_1}{m_2(f_{12}+f_{23})}\left[f_{12}\Delta k^2-\frac{f_{12}g_{23}+f_{23}g_{12}}{2}\right],\\
\Delta k^2&=\frac{m_2}{m_1}\Delta k^1+\frac{m_2}{m_3(f_{23}+f_{34})}\left[f_{23}\Delta k^3-\frac{f_{23}g_{34}+f_{34}g_{23}}{2}\right],\\
\Delta k^i&=\frac{m_i}{m_{i-1}(f_{i,i-1}+f_{i-1,i-2})}\left[f_{i,i-1}\Delta k^{i-1}+\frac{f_{i,i-1}g_{i-1,i-2}+f_{i-1,i-2}g_{i,i-1}}{2}\right]\\
&\quad+\frac{m_i}{m_{i+1}(f_{i,i+1}+f_{i+1,i+2})}\left[f_{i,i+1}\Delta k^{i+1}-\frac{f_{i,i+1}g_{i+1,i+2}+f_{i+1,i+2}g_{i,i+1}}{2}\right],\quad i\geq 3\ .
\end{aligned} \tag{35}$$

Consequently, one can see that the first quantum corrections to the variances of the atomic coordinates are

$$\Delta D_i^Q=\frac{\hbar^2}{12m_i\theta}\ . \tag{36}$$

Corrections to the interatomic distances are defined by

$$\begin{aligned}
\Delta a_{i,i+1}^Q&=\langle q_{i+1}-q_i\rangle\\
&=-\frac{\hbar^2}{12\theta^2}\left[\frac{1}{m_{i+1}}\left(\overline{q_{i+1}\xi_{i+1}^0}+\Delta k^{i+1}\overline{q_{i+1}^2}\right)\right.\\
&\qquad\left.-\frac{1}{m_i}\left(\overline{q_i\xi_i^0}+\Delta k^i\overline{q_i^2}\right)\right]\ .
\end{aligned} \tag{37}$$

Elimination of Δk^i and Δk^{i+1} in (37) with the help of (35) gives

$$\Delta a_{i,i+1}^Q=-\frac{\hbar^2(m_i+m_{i+1})g_{i,i+1}}{24m_im_{i+1}f_{i,i+1}\theta}\ . \tag{38}$$

The quantum correction to the Helmholtz free energy of a chain (per N atoms) is of the form

$$F_Q=\frac{\hbar^2}{24\theta}\sum_{i=1}^{N}\frac{f_{i,i+1}(m_i+m_{i+1})}{m_im_{i+1}}\ . \tag{39}$$

V. THE FIBONACCI CHAIN

Equations derived in the preceding sections are applicable to any one-dimensional atomic model in which the nearest neighbors interact. Consequently, to study anharmonic effects in the Fibonacci chain we only have to choose a special alternation of atoms of two kinds. It is well known[16] that the Fibonacci chain can be generated using the following inflation rule

$$A_n\rightarrow A_{n+1}B_{n+1},\quad B_n\rightarrow A_{n+1}\ , \tag{40}$$

where A and B are the kinds of atoms or interatomic couplings. In any generation, the numbers of the elements of such a system are equal to the Fibonacci numbers. For the sixth nontrivial generation, the sequence is represented in Fig. 2. In the limit $n\rightarrow\infty$ the fractions of the A and B elements form the golden section, i.e., their ratio tends to

$$\tau=\frac{\sqrt{5}+1}{2}\ . \tag{41}$$

Formulas (23)–(27), (38), and (39) show that calculations of integrated properties of any one-dimensional model with nearest-neighbor interactions need the partial values related to various clusters, up to six-atom clusters. These partial values are necessary to compute the mean-square relative atomic displacements, which in the approximation used are

$$D_{ij}=D_i+D_j\ . \tag{42}$$

In the Fibonacci chain, the number of different k-atomic clusters is[15]

$$C(k)=k+1,\quad k=1,2,3,\ldots\ , \tag{43}$$

with "monatomic clusters" being the atoms A and B themselves, whose fractions come to τ_1 and τ_2, respectively, where

$$\tau_1=\tau-1=\frac{\sqrt{5}-1}{2};\quad \tau_i=\tau_1^i,\quad i=2,3,\ldots\ . \tag{44}$$

Let us enumerate all necessary clusters and their fractions:

(a) $k=2$: AB,BA τ_2; AA τ_3;

(b) $k=3$: ABA τ_2; AAB,BAA τ_3; BAB τ_4;

(c) $k=4$: $BAAB,AABA,ABAA$ τ_3; $ABAB,BABA$ τ_4;

(d) $k=5$: $ABAAB,BAABA$ τ_3; $ABABA,AABAB,BABAA$ τ_4; $AABAA$ τ_5;

(e) $k=6$: $ABAABA$ τ_3; $AABABA,ABABAA,BAABAB,BABAAB$ τ_4; $AABAAB,BAABAA$ τ_5.

ABAABABAABAABABAABABA...

FIG. 2. Sixth generation, Eq. (40), for the Fibonacci chain.

TABLE I. Numbers τ_i, the fractions of various clusters.

i	1	2	3	4	5
τ_i	$\frac{\sqrt{5}-1}{2}$	$\frac{3-\sqrt{5}}{2}$	$\sqrt{5}-2$	$\frac{7-3\sqrt{5}}{2}$	$\frac{5\sqrt{5}-11}{2}$

The corresponding numbers τ_i are given in Table I. It is easy to see that

$$\begin{aligned}\tau_1+\tau_2=2\tau_2+\tau_3=\tau_2+2\tau_3+\tau_4=3\tau_3+2\tau_4\\ =2\tau_3+3\tau_4+\tau_5\\ =\tau_3+4\tau_4+2\tau_5\\ =\cdots=1\ . \end{aligned} \tag{45}$$

In the static state, the length and internal energy of the Fibonacci chain containing $N \gg 1$ atoms are

$$L_0=N(\tau_3 r_0+2\tau_2 r_0')\,;\quad U_0=-N(\tau_3\varepsilon+2\tau_2\varepsilon')\ . \tag{46}$$

[For shortness we use $r_{AA}^0=r_0$, $r_{AB}^0=r_0'$, $\varepsilon=-\Phi_{AA}(r_{AA}^0)$, $\varepsilon'=-\Phi_{AB}(r_{AB}^0)$, and similar symbols are used for the force constants (25).]

We consider the infinite Fibonacci chain. Then, according to (21) we get the thermal expansion of the average distance between two A atoms

$$\Delta a_{AA}=-\frac{g\theta}{f(f+f')}\ . \tag{47}$$

Such an expansion between AB atoms depends on their other neighbors:

$$\Delta a_{AB}^a=-\frac{(f+3f')g'\theta}{4f'^2(f+f')}\quad \text{for } AABA \text{ and } ABAA\ ; \tag{48a}$$

$$\Delta a_{AB}^b=-\frac{g'\theta}{2f'^2}\quad \text{for } ABAB \text{ and } BABA\ . \tag{48b}$$

The quantum correction to the distance between two neighbors (38) depends only on their kinds,

$$\Delta a_{AA}^Q=-\frac{\hbar^2 g}{12m_A f\theta}\,;\quad \Delta a_{AB}^Q=-\frac{\hbar^2(m_A+m_B)g'}{24m_A m_B f'\theta}\ . \tag{49}$$

From (22) and (42) we obtain the mean-square relative displacements (MSRD) of atoms in the classical approximation

$$D_{AA}=\frac{2\theta}{f+f'}\left\{1+\frac{\theta}{2(f+f')}\left[\frac{2}{f+f'}\left[\frac{g^2}{f}-h\right]+\left[\frac{g-g'}{f+f'}\right]^2+\frac{3f+f'}{f(f+f')}\left[\frac{g'^2}{f'}-h'\right]\right]\right\}\ ; \tag{50}$$

$$D_{AB}^a=\frac{\theta}{f'}\left[1+\frac{(7f+9f')\theta}{16f'^2(f+f')}\left[\frac{g'^2}{f'}-h'\right]\right]\quad \text{for } ABABAA \text{ and } AABABA\ ; \tag{51a}$$

$$\begin{aligned}D_{AB}^b=\frac{\theta}{2(f+f')}\left\{\frac{f+3f'}{f'}+\frac{\theta}{f+f'}\left[\frac{2}{f+f'}\left[\frac{g^2}{f}-h\right]+\left[\frac{g-g'}{f+f'}\right]^2\right.\right.\\ \left.\left.+\frac{f+f'}{2}\left[\frac{3f+f'}{f(f+f')^2}+\frac{3f+5f'}{4f'^3}\right]\left[\frac{g'^2}{f'}-h'\right]\right]\right\}\quad \text{for } BAABAB \text{ and } BABAAB\ ;\end{aligned} \tag{51b}$$

$$\begin{aligned}D_{AB}^c=\frac{\theta}{2(f+f')}\left\{\frac{f+3f'}{f'}+\frac{\theta}{f+f'}\left[\frac{2}{f+f'}\left[\frac{g^2}{f}-h\right]+\left[\frac{g-g'}{f+f'}\right]^2\right.\right.\\ \left.\left.+\frac{f+f'}{2}\left[\frac{3f+f'}{f(f+f')^2}+\frac{f+3f'}{2f'^3}\right]\left[\frac{g'^2}{f'}-h'\right]\right]\right\}\\ \text{for } AABAAB \text{ and } BAABAA\ .\end{aligned} \tag{51c}$$

The quantum corrections to MSRD

$$D_{AA}^Q=\frac{\hbar^2}{6m_A\theta}\,;\quad D_{AB}^Q=\frac{\hbar^2(m_A+m_B)}{12m_A m_B\theta} \tag{52}$$

as well as those to the interatomic distances (49) depend on the reduced masses of the neighbors.

VI. NUMERICAL RESULTS AND DISCUSSION

To perform numerical calculations we utilize the interatomic potentials in the standard Lennard-Jones form

$$\begin{aligned}\Phi_{AA}(r)=\Phi(r;r_0,\varepsilon)=\epsilon\left[\left[\frac{r_0}{r}\right]^{12}-2\left[\frac{r_0}{r}\right]^6\right]\ ;\\ \Phi_{AB}(r)=\Phi(r;r_0',\varepsilon')\ .\end{aligned} \tag{53}$$

At that, it is convenient to express the quantum corrections (49) and (52) as

$$\begin{aligned}\Delta a_{AB}^Q=-\left[\frac{\Lambda'}{4\pi}\right]^2\frac{r_0'g'^*}{3f'^*\theta^*}\ ;\\ \Delta a_{AA}^Q=-\left[\frac{\Lambda}{4\pi}\right]^2\frac{r_0^2\varepsilon g^*}{3r_0'\varepsilon' f^*\theta^*}\ ;\end{aligned} \tag{54}$$

$$D_{AB}^Q=\left[\frac{\Lambda'}{2\pi}\right]^2\frac{r_0'^2}{6\theta^*}\,;\quad D_{AA}^Q=\left[\frac{\Lambda}{2\pi}\right]^2\frac{r_0^2\varepsilon}{6\varepsilon'\theta}\ . \tag{55}$$

Here

$$\Lambda=\frac{2\pi\hbar}{r_0\sqrt{m_A\varepsilon}},\quad \Lambda'=\frac{2\pi\hbar}{r_0'\sqrt{2\varepsilon' m_A m_B/(m_A+m_B)}} \tag{56}$$

are the de Boer parameters[23] for the AA and AB pairs of atoms, and

$$\theta^*=\frac{\theta}{\varepsilon'};\quad f^*=\frac{r_0'^2 f}{\varepsilon'},\quad f'^*=\frac{r_0'^2 f'}{\varepsilon'},$$
$$g^*=\frac{r_0'^3 g}{\varepsilon'},\quad g'^*=\frac{r_0'^3 g'}{\varepsilon'}. \tag{57}$$

Note that we reduce all force constants to the parameters of the interatomic potential Φ_{AB} but not to those of Φ_{AA} since the AB bonds predominate.

The classical parts of the expansions (47) and (48) and MSRD (50) and (51) can be expressed in terms of dimensionless parameters (57) as well. Then, the relative thermal expansions and MSRD are functions of the dimensionless temperature and depend on r_0'/r_0, ε'/ε, Λ, and Λ'.

We have studied two cases: (1) small A atoms and large B atoms; (2) large A atoms and small B atoms. In the first case (Fig. 3), we adopt

$$r_0'/r_0=1.08,\quad \varepsilon'/\varepsilon=1.39,\quad \Lambda=0.17,\quad \Lambda'=0.99\ . \tag{58}$$

These parameters correspond to Ar and Xe, using the known rule

$$r_0'=r_{AB}^0=(r_{AA}^0+r_{BB}^0)/2,\quad \varepsilon'=\varepsilon_{AB}=\sqrt{\varepsilon_{AA}\varepsilon_{BB}}\ . \tag{59}$$

In Fig. 4 we show the relative expansions of the interatomic distances $\Delta a_{AA}/r_0$, $\Delta a_{AB}^a/r_0'$, and $\Delta a_{AB}^b/r_0'$ and that of the length of the Fibonacci chain

$$\Delta L/L_0=N[\tau_3(\Delta a_{AA}+2\Delta a_{AB}^a)+2\tau_4\Delta a_{AB}^b]/L_0\ . \tag{60}$$

(It is known[5] that in the harmonic approximation there is no thermal expansion.) The MSRD in this model are plotted in Fig. 5. Here we represent also D_{AA} in the harmonic approximation to demonstrate the harmonic effects.

In the second case (Fig. 6),

$$r_0'/r_0=0.926,\quad \varepsilon'/\varepsilon=0.719\ ,\quad \Lambda=0.053,\quad \Lambda'=0.099\ . \tag{61}$$

The relative expansions and MSRD of this model are drawn in Figs. 7 and 8, respectively. For comparison we

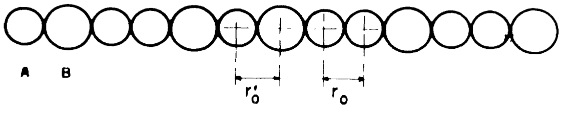

FIG. 3. Fibonacci chain consisting of small A and large B atoms.

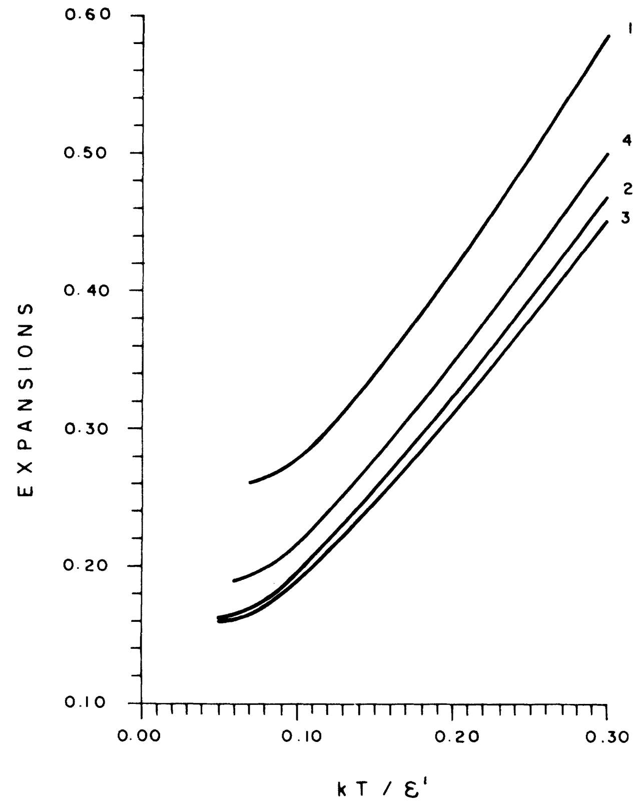

FIG. 4. Thermal expansions of the Fibonacci chain drawn in Fig. 3: (1) $10\Delta a_{AA}/r_0$, (2) $10\Delta a_{AB}^a/r_0'$, (3) $10\Delta a_{AB}^b/r_0'$, (4) $10\Delta L/L_0$.

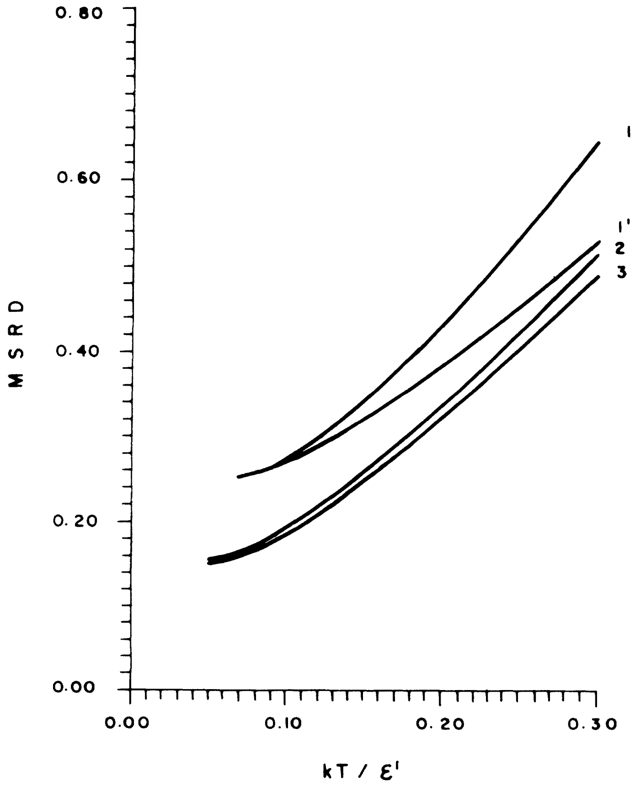

FIG. 5. Mean-square relative displacements of atoms in the Fibonacci chain with small A and large B atoms: (1) $100D_{AA}/r_0$ (1′) the same in the harmonic approximation, (2) $100D_{AB}^b/r_0'\approx 100D_{AB}^c/r_0'$, (3) $100D_{AB}^b/r_0'$.

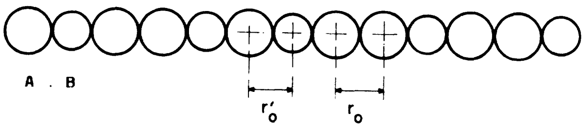

FIG. 6. Fibonacci chain consisting of large A and small B atoms.

show also the harmonic approximation for D_{AA}.

So, we have solved the basic equations of the quasiclassical method of the unsymmetrized self-consistent-field for a one-dimensional model of a solid with an arbitrary composition of various atoms interacting with their nearest neighbors, taking into account weak anharmonicity. After that we have applied these general results to study anharmonic effects in the Fibonacci-chain quasicrystal. Just the anharmonicity is responsible for the thermal expansion of solids, in particular, quasicrystals. Besides, one can see from Figs. 5 and 8, that at constant pressure the effective amplitudes of the thermal atomic vibrations are enhanced as a consequence of the anharmonic effects. Our method enables one also to investigate the influence of the anharmonicity on thermal properties of quasicrystals. For instance, it leads to a deviation from the Dulong and Petit law at high temperatures.

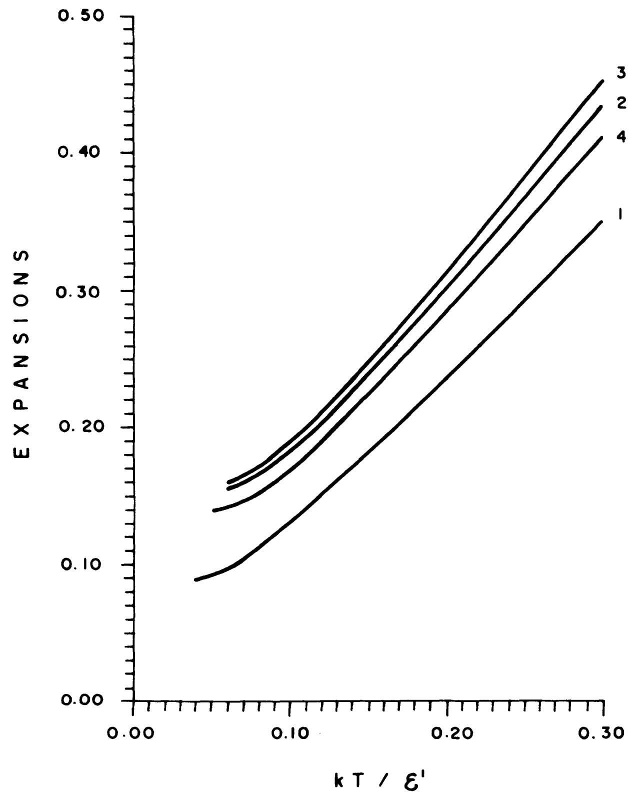

FIG. 7. Thermal expansions of the Fibonacci chain with large A and small B atoms. Designations are the same as in Fig. 4.

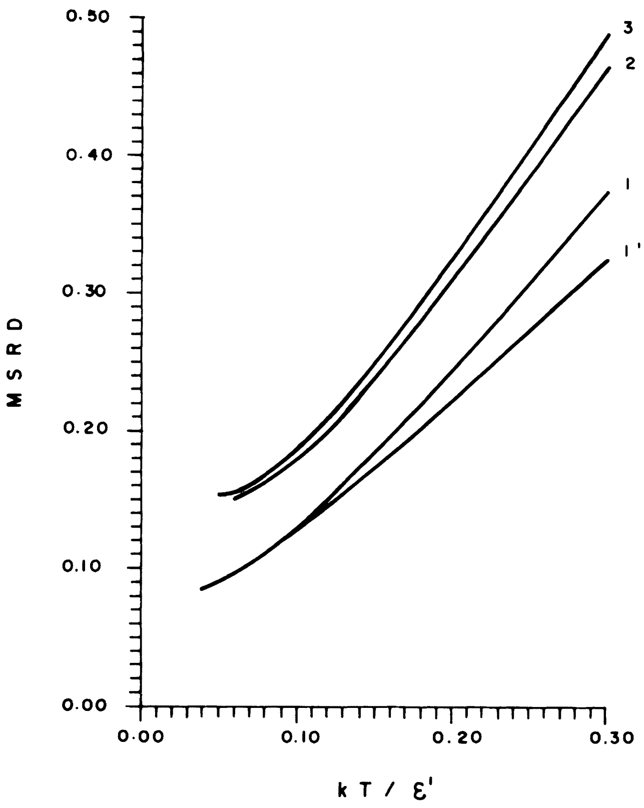

FIG. 8. MSRD in the Fibonacci chain with large A and small B atoms. Designations are the same as in Fig. 5.

In our calculations we have employed the Lennard-Jones potential with parameters which correspond to Ar and Xe, just because the interatomic forces are known better for rare-gas solids.[24] Although derived for one-dimensional models of quasicrystals, our results may be applicable to higher dimensions, since some multicomponent alloys based on Al reveal just the one-dimensional quasicrystal behavior.[25–27] Unfortunately, thermal expansions of their interlayer distances have not been measured. A realization of such measurements and comparison of data with our results will allow one to obtain information about force constants in these substances. In conclusion, we note that the Fibonacci sequence occurs not only for quasicrystals but sometimes also for thermal expansion of the interplanar distances of certain crystals with surfaces.[28]

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*Permanent address: Department of Theoretical Physics, People's Friendship University, 117198, Moscow, Russia.

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