Acoustic and electronic properties of one-dimensional quasicrystals

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We study the acoustic and electronic properties of one-dimensional quasicrystals. Both numerical (nonperturbative) and analytical (perturbative) results are shown. The phonon and electronic spectra exhibit a self-similar hierarchy of gaps and many localized states in the gaps. We study quasiperiodic structures with any number of layers and several types of boundary conditions. We discuss the connection between our phonon model and recent experiments on quasiperiodic GaAs-AlAs superlattices. We predict the existence of many gap states localized at the surfaces.

Schechtman *et al.*[1] obtained the electron-diffraction pattern of Al_6Mn and other metallic alloys which show the unusual property of extended icosahedral near-neighbor bond orientational order. However, sharp diffraction peaks can be obtained not only from periodicity but from more general quasiperiodic (QP) structures which can have any type of point symmetry including fivefold.[2-4] In this paper we report nonperturbative numerically exact results concerning acoustic and electronic spectra, specific heat, and the behavior of normal modes for a one-dimensional[5] (1D) quasicrystal (QC). Standard descriptions in the theory of excitations of ordered and disordered systems are used, i.e., the harmonic lattice and a tight-binding model. Also, an alternative analytical perturbative approach is outlined and its consistency with the results obtained using the previous straightforward method is shown. Moreover, we point out the relation between our lattice dynamics model and the remarkable recent experiments, by Merlin *et al.*, on QP GaAs-AlAs superlattices.[6]

The system studied here is the 1D analog[7] of the Penrose lattice and the icosahedral QC. The positions[8] of the atoms in a 1D QP chain are given by $x_n = n + [n/\tau_1 + \phi_1]/\tau_2 + \phi_2$, where ϕ_1 and ϕ_2 are real and $[y]$ denotes the greatest integer less than y. Choosing $\tau_1 = \tau_2 = \tau = (1+\sqrt{5})/2 = 2\cos(\pi/5)$ we get[7] the 1D analog of the Penrose lattice and the icosahedral QC, i.e., a QP sequence of long (L) and short (S) spacings (Fibonacci lattice). This definition is equivalent to prescriptions based on a substitution law[7] and projection techniques.[3,7]

A standard way to study the acoustic properties of a lattice is to consider a nearest-neighbor harmonic chain. This model is represented by an equation of motion

$$\frac{d^2u_n}{dt^2} = k_{n,n+1}u_{n+1} + k_{n,n-1}u_{n-1} - (k_{n,n+1} + k_{n,n-1})u_n \ , \quad (1)$$

where u_n is the displacement of the nth atom ($n = 1, \ldots, N$) from its equilibrium position x_n, and $k_{n,n\pm1}$ are the strengths of the harmonic couplings to the neighboring atoms. All masses are assumed to be identical and their value is absorbed in the definition of the strength constants. The QP sequence of two different distances between atoms includes a QP sequence of two different coupling constants K_L and K_S. We have arbitrarily chosen $K_L = 1$ and $K_S = 1.6180$ for Figs. 1 and 2. The qualitative results obtained do not depend on this choice. In order to complete the specification of the model, fixed-end boundary conditions are imposed, i.e., $u_0 = u_{N+1} = 0$. Other types of boundary conditions will be discussed below.

Assuming a monochromatic time dependence, $u_n \propto \exp(-i\omega t)$, in Eq. (1), the stationary equation of motion is obtained. By diagonalizing it, we obtained the eigenfrequencies and normal modes[9] with N as large as 10946. Figure 1 shows the N frequencies ω_n as a function of n, the mode number. A hierarchy of gaps can readily be seen. We have found[10] that the states in the bands exhibit a power law decay over the length of the system and that there are many isolated *states in the gaps* corresponding to phonons exponentially localized at the surfaces (see Fig. 2). The phonon spectrum in Fig. 1 has a Cantor-set-like structure in the short-wavelength regime.[10] There, every band has two gaps giving rise to three subbands, each one of them having two gaps and so on. In the long-wavelength case, the number of gaps and their size tends to zero, and we recover the standard results for periodic lattices. This is not surprising since long-wavelength phonons (acoustic Goldstone modes) are not sensitive to the detailed structure of the lattice. The specific heat obtained in the present study does not differ qualitatively from the periodic case. Let us recall that for disordered systems (unlike QP systems which are not random) the general conclusion of localization theory is that acoustic waves are always localized in $d \leq 2$, regardless of

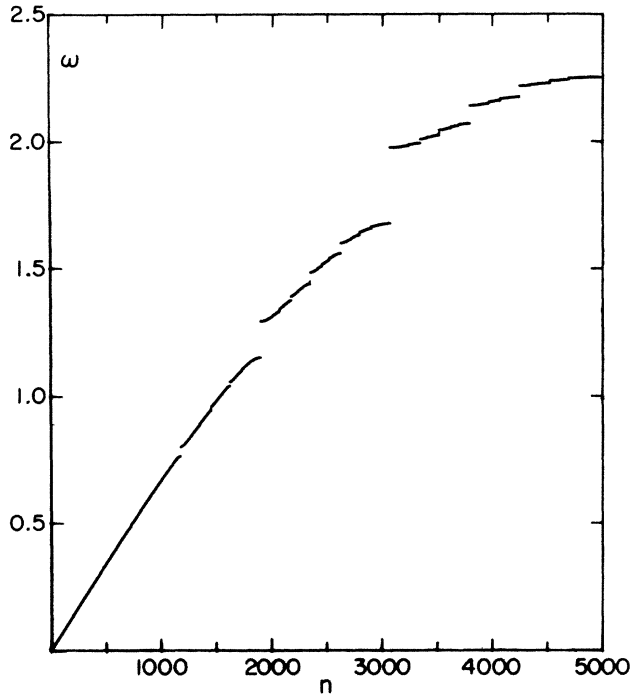

FIG. 1. Phonon spectrum, ω_n versus mode number n, for a harmonic 1D QP chain of 5000 atoms. Each dot (normal mode frequency) corresponds to a possible level for a single phonon. The short-wavelength regime is self similar: every band is divided in three subbands and so on in a Cantor-set—like fashion. Only few gaps and isolated states in the gaps (represented by dots) can be noticed here and in Fig. 3. A detailed and magnified version of these figures show a large number of gaps and isolated states in the gaps.

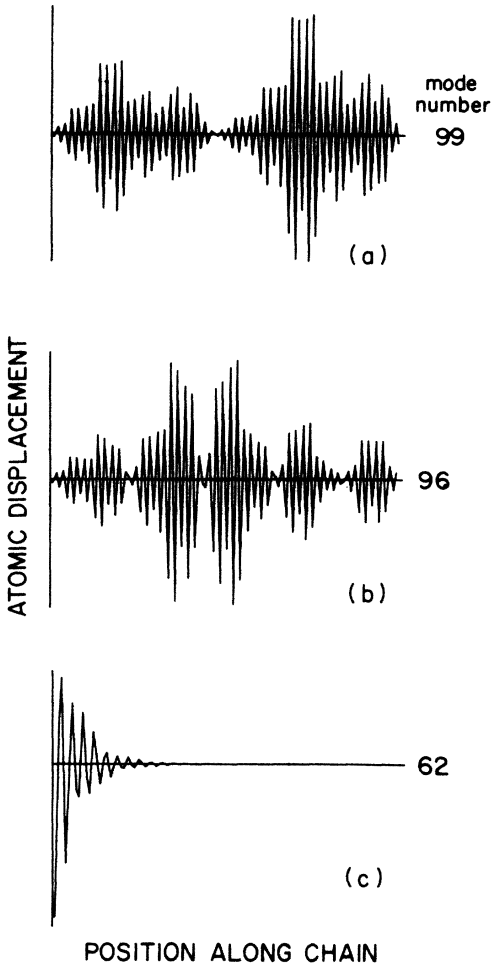

FIG. 2. A few normal modes for a harmonic 1D QP array of 100 atoms: (a) mode in which the two wave packets are equal up to a scale factor, (b) extended state which exhibits three local mirror symmetries, and (c) a localized phonon corresponding to a state in a gap. The same kind of behavior is also obtained for longer chains. For clarity, only results for small N are shown.

the amount of disorder or the impurity concentration.

The Fibonacci superlattice,[6] a heterostructure with QP ordering of layers, is an experimental realization of the lattice dynamics model proposed here, i.e., a QP sequence of piecewise constant *(not* sine-like modulated) spring strengths. The 1D QP sequence of AlAs and GaAs (L and S in our notation) has a phonon-level density of states, obtained through Raman scattering of longitudinal acoustic phonons, which exhibits a hierarchy of gaps as predicted by our calculations. The locations of the main gaps in the experimental results[6] and in our calculations occur in a geometric progression with τ as the common ratio. Furthermore, and after our theoretical prediction, Merlin *et al.*[11] have recently found *many isolated states in gaps corresponding to surface phonons.*

For the study of the electronic properties, a stationary tight-binding electron model was used. The basic equation is

$$E\psi_n=\varepsilon_n\psi_n+t_{n,n+1}\psi_{n+1}+t_{n,n-1}\psi_{n-1}\,,$$

$$n=1,2,\ldots,N \quad (2)$$

where ε_n and ψ_n are, respectively, the site energy and the probability amplitude of an electron being at the nth site, while the hopping transition amplitudes, $t_{n,n+1}$, form a QP sequence of two transfer energies T_L and T_S. Fixed-end boundary conditions are imposed at both ends, i.e., $\psi_0=\psi_{N+1}=0$. Several values for ε_n were studied.[10] Here, we will consider the simplest case where $\varepsilon_n=0$ for all n. Figure 3 shows the electron energy spectrum obtained by diagonalizing[9] Eq. (2). A self-similar hierarchy of gaps is present. This property follows from the nonperiodic self-similarity of the lattice.[3,7] The stationary states and their participation ratio (which indicates the degree of localization of each state) were obtained[10] and their behavior is somewhat similar to the normal modes shown in Fig. 2. Isolated states in the gaps are exponentially localized; meanwhile, the rest extend over the length of the system decaying as a power law. The latter ones are not conven-

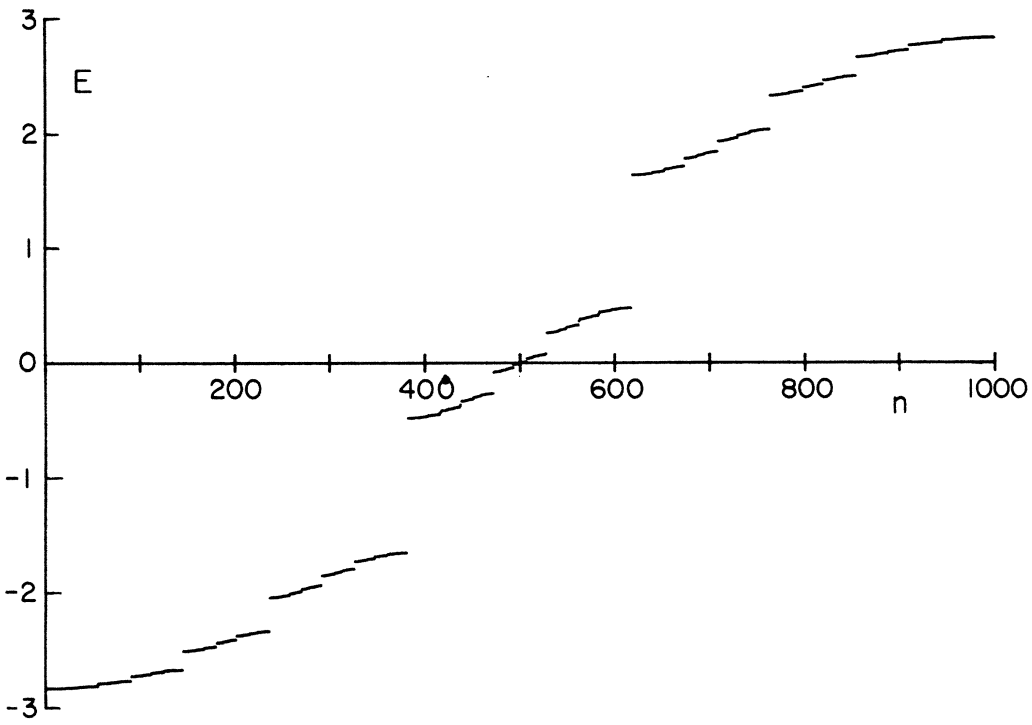

FIG. 3. Electron energy spectrum for a tight-binding model with a QP sequence of two hopping transition amplitudes, $T_L=1$ and $T_S=2$, for a chain with 1000 sites; n labels the stationary state with energy E_n.

tional extended (Bloch) states. The number of eigenstates contained in each band is equal to a Fibonacci number, F_n, i.e., $F_n=F_{n-1}+F_{n-2}$ for $n\geq 2$ with $F_0=F_1=1$. Each band with F_n eigenstates splits in three subbands containing F_{n-2}, F_{n-3}, and F_{n-2} states, respectively. Of course, several of our results obtained in the context of lattice dynamics are encountered again in our electronic study. However, the Goldstone modes present in the phonon case are absent in the electronic study. In both the phonon and electron spectra, the gap locations are labeled by $n=N\ (m\tau \bmod 1)$, where m is any integer. Gap size generally decreases with increasing m. The larger the value of $|T_S-T_L|$ ($|K_S-K_L|$) is, the larger the size of the main gaps become. In general, the results obtained in the present work still remain valid when lattice size is varied. A few of the previous features can be obtained from very different studies (mostly using transfer-matrix techniques) done on Harper's equation[12] and the diagonal QP case.[13] The latter has been studied as a dynamical system map using a recursion relation for transfer matrices.

The scaling index is uniform (nonuniform) for the electron (phonon) spectrum as can easily be appreciated from Fig. 3 (1). The scaling properties of the wave functions, however, constitute a more difficult problem. We have proved,[14,15] based on a novel renormalization-group approach, that the envelope of the wave functions exhibits a power-law decay for all states, except for the isolated states in the gaps, which have an exponentially decaying envelope. For some of the former ones, the wave-function scales as L^{γ}, where L is the length of the system, $\gamma=\ln f/\ln\tau$, and $f=|T_S/T_L|$.

Let us now concentrate on the important effect of surfaces and impurities on the spectra. Let N and F_k be the number of particles in the chain and a Fibonacci number, respectively. The four types of lattices considered in the present work are (1) periodic boundary conditions (PBC) and $N=F_k$, (2) PBC and $N\neq F_k$, (3) fixed ends for *any* value of N, and (4) free ends for *any* value of N. Case (1) does not exhibit any (localized) states in gaps, since it corresponds to a finite lattice without surfaces and with bonds ordered in a QP sequence. The Fibonacci rule, $L\rightarrow LS$ and $S\rightarrow L$, produces QP chains with $N=F_k$ only. Case (2) shows states localized at the joining point of the chain since there the bonds are joined in forbidden ways (e.g., $S-S$ or $L-L-L$) breaking the perfect QP order. A forbidden connection behaves as an impurity and impurities tend to form localized states. Cases (3) and (4) do have surfaces and they effectively act as impurities. The large number of (localized) states in the gaps are surface states, and they have recently been observed experimentally.[11] Superlattices are finite, they do have surfaces and the number of layers is not restricted to be a Fibonacci number. Therefore, the appropriate cases from the experimental point of view are neither (1), studied in Ref. 3,

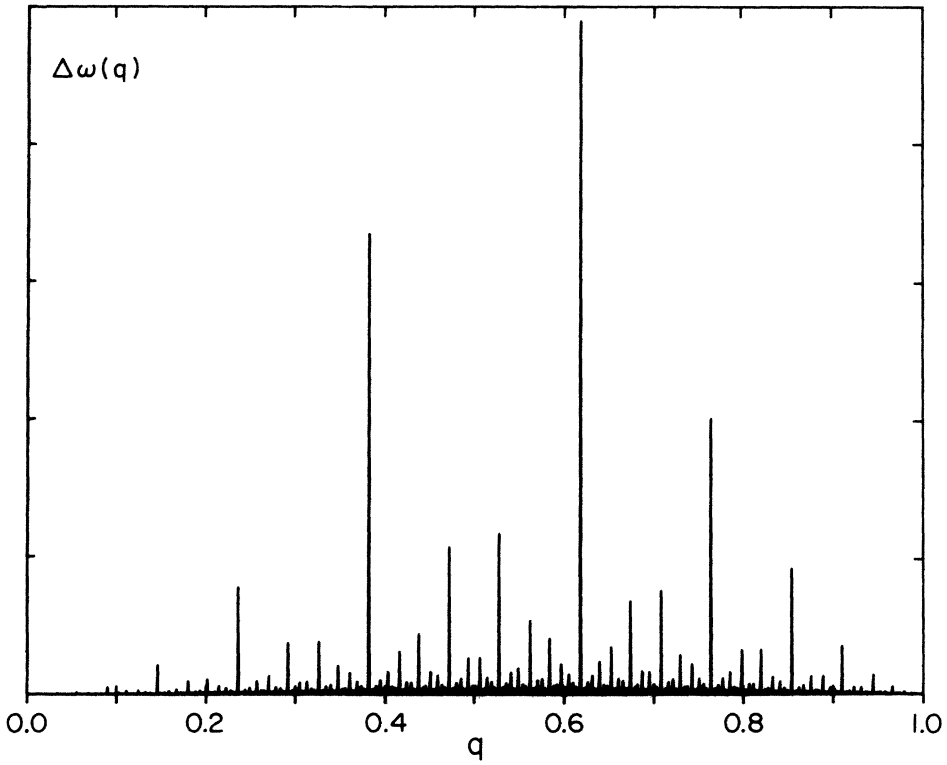

FIG. 4. The frequency shift $\Delta\omega(q)$ displayed in Eq. (3) plotted as a function of the normalized mode number q. The locations and sizes of the *gaps* in the spectrum shown in Fig. 1 correspond to the locations and sizes of the *peaks* in $\Delta\omega(q)$.

nor (2) but (3). Figures 1 through 3 refer to case (3).

The general features of the results obtained above concerning the gap structure of the phonon and electron spectra can also be obtained using perturbation theory, where the small parameter here is $|K_S-K_L|$ ($|T_S-T_L|$) for the phonon (electron) case. For example, in the case of the lattice dynamics described by Eq. (1), it can be shown[10] using degenerate perturbation theory among the time reversed modes that the frequency spectrum is given by $\omega^{\pm}(q)=\omega_0(q)\pm\Delta\omega(q)$, where $\omega_0(q)$ is the unperturbed frequency and where $\Delta\omega(q)$ is given by

$$\Delta\omega(q)\propto\left|\sin(\pi q)N^{-1}\sum_{n=1}^{N}k_{n,n+1}e^{4i\pi nq}\right| . \tag{3}$$

In Fig. 4, $\Delta\omega(q)$ is plotted. The positions and sizes of the *peaks* in $\Delta\omega(q)$ correspond to the positions and sizes of the *gaps* in the spectrum shown in Fig. 1. In particular, the locations of the peaks in Eq. (3) are given by $q=m\tau$ (mod1), where m is any integer.[16] Clearly, this alternative approach is not as general as the previous nonperturbative exact numerical solutions which are valid for any values of the harmonic coupling strengths (K_L,K_S) and hopping transition amplitudes (T_L,T_S). However, in their common region of validity, both are totally consistent.[17]

In conclusion, we have obtained and studied some of the features of the phonon and electron spectra, and normal modes for a finite one-dimensional quasicrystal. The calculations reported here are based on a *realistic* QP system which (like the Fibonacci superlattice) is finite, has a number of layers not restricted to be a Fibonacci number, and has surfaces. This system exhibits an interesting localization problem even in one dimension. We find many isolated states in the gaps corresponding to exponentially localized phonon and electron surface states. A longer discussion will be given in forthcoming publications.[10,14]

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[5]Besides its relevance for the study of the Fibonacci superlattice, an apparent major limitation of this study is the restriction to 1D, but 2D and 3D QC are defined in terms of 1D QP sequences (Ref. 2). Therefore, some of the qualitative pictures of the solution of the 1D model may be carried over to higher-dimensional cases.

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[12]Note that Harper's equation [see, for instance, S. Ostlund and R. Pandit, Phys. Rev. B **29**, 1394 (1984), and references therein] models a (incommensurate) system with (a) two superimposed competing periodicities, and (b) a sine-modulated potential. The systems studied here have neither two periodic structures superimposed (as for incommensurate systems) nor a sine-modulated potential. Furthermore, crucial properties (metal-insulator transition, nature of the electronic wave functions, etc.) in Harper's equation are determined by the strength of the potential. This is not the case in the present study based on the Schrödinger equation (2). Moreover, the self-similarity present in the Fibonacci lattice studied here is completely *nonexistent* in the lattices used in the studies based on Harper's equation. For a review, see J. Sokoloff, Phys. Rep. **126**, 4, 189 (1985).

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