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Electronic stability of disordered systems: application to quasicrystals

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Abstract. This paper is devoted to the study of energetic stability of disordered binary alloys in which atoms are interacting via a tight-binding Hamiltonian. In 1D, for a weak potential, the gain in energy compared to the periodic linear chain is derived as a function of the electronic filling factor and the disorder. Very precise results are given in the case of a quasiperiodic arrangement. This kind of phase plays a very particular role since it is shown that for a given filling factor ν (or Fermi level position), the most stable structure is a quasiperiodic one associated to ν . Moreover, for this structure the fluctuations of the density are unbounded if ν and the stoichiometric coefficients do not fulfil an arithmetical condition. Different features are observed for rational and irrational values of ν . These results which are exact for any concentration and filling factor are illustrated on the quasiperiodic Fibonacci chain. The 2D case is also studied by means of a solvable quasiperiodic Hamiltonian on a subtiling of the octagonal tiling. Numerically, one finds that for a weak potential the crystalline phase is more stable than the quasicrystalline one. The opposite situation is obtained by increasing the potential.

1. Introduction

The study of the stability of 1D chains is an old problem in solid state physics. For instance, one can compare the cohesive energy of the 1D periodic chain to that of the dimerized chain. For a half-filled band it is well known that the latter is more stable. Indeed, a gap appears in the middle of the spectrum which shifts to lower energy the levels near the Fermi level. This is related to the so-called Peierls instability (Peierls 1955). More recently, Kennedy and Lieb (1987) have shown that under simple assumptions, the most stable structure at half-filled band is exactly the dimerized chain.

After the discovery of quasicrystals (Schechtman *et al* 1984), the relevance of a quite similar phenomenon called the Hume-Rothery stability condition (Hume-Rothery 1926) has been discussed by Friedel and Denoyer (1987) in order to explain the stability of quasicrystals. The measurements of a low density of states at the Fermi level in AlLiCu (Wang *et al* 1988) is consistent with this kind of explanation. This also can be an explanation of the high resistivity of these phases compared to their amorphous or crystalline equivalent. In order to study this problem in a quantitative way, Makler and Gaspard (1990) have computed the cohesive energy of the quasiperiodic Fibonacci

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chain with respect to the electronic filling factor. As a generalization of the dimerized chain result, they find that the Fibonacci chain is more stable than the periodic chain for a filling factor near $(3 - \sqrt{5})/2$.

In what follows, a systematic approach of the stability of 1D systems is introduced. The main goal is to extend the theoretical result of Kennedy and Lieb and the numerical work by Makler and Gaspard for any filling factor and atom concentration.

I shall first define a tight-binding Hamiltonian. Then, a general perturbative formula for the energy gain is written when the Fermi level lies in a gap. More complete results are given for 1D quasicrystals, since it will be shown that among all the 1D chains, the quasiperiodic ones play a particular role regarding stability.

In the last part of the paper we study numerically the case of a 2D quasiperiodic tiling which is compared to the square lattice.

2. Hamiltonian for 1D chains

In the part of the paper devoted to the 1D case, one considers an infinite chain S_n built in the following way. We consider a word of length n made with p letters A and q letters B ($p \leq q$). S_n is obtained by gluing an infinite number of identical words of this kind. Sometimes, we shall consider the limit $p \rightarrow +\infty$, $q \rightarrow +\infty$ and $p/n \rightarrow \theta$. The associated chain will be called S_∞ (random, quasiperiodic, ...). We consider then the linear chain built by associating a bond of length l to a letter A and l' to a B.

Given the sequence of A and B, one can define a first neighbour tight-binding Hamiltonian

$$\mathcal{H}_{\text{el}} = - \sum_{i \in \mathbb{Z}} t_i (|i\rangle\langle i+1| + |i+1\rangle\langle i|) \quad t_i \in \{\rho, \rho'\}. \quad (1)$$

The sequence of hopping parameters $-\rho$ and $-\rho'$ is taken to follow exactly the one of A and B (or l and l'). We have chosen negative parameters for the effective potential induced by the electrons to be attractive. In addition, we add to the electronic Hamiltonian a phenomenological repulsive atomic Hamiltonian, in order to prevent the system from collapsing. This classical Hamiltonian is a sum of two-body short-range potentials

$$\mathcal{H}_{\text{at}} = \lim_{m \rightarrow +\infty} \frac{1}{2m} \sum_{i=-m}^m V(r_i) \quad r_i \in \{l, l'\} \quad (2)$$

where r_i is the length of the bond between atoms i and $i+1$.

The hopping parameter is a decreasing function of the distance between atoms since it measures the overlapping between the real atomic potential and the Wannier functions localized at two nearest neighbour sites. This can be written

$$\rho = f(l) \quad \rho' = f(l') \quad (3)$$

where f is a strictly decreasing function of the interatomic distance which is invertible. Thus, $V(r_i)$ is an increasing function of t_i since one can write

$$V(l) = g(\rho) \quad V(l') = g(\rho') \quad g = V \circ f^{-1} \quad (4)$$

g is an increasing function which verifies $g(0) = 0$ since when $l \rightarrow +\infty$ the potential must go to 0 as well as the hopping parameter ρ . These manipulations allow us to eliminate the spatial variables.

Even if the following results in 1D will not depend on the precise form of g in the limit of weak potential, we shall consider

$$g(\rho) = \frac{1}{2\varepsilon} \rho^2 \tag{5}$$

which leads to quite simple calculations. We can justify such a choice. Indeed, in numerical simulations one often takes parameters as exponentially decreasing functions of the distance between atoms:

$$\rho(r) = V \exp(-r/r_0) \quad V(r) = \hat{V} \exp(-\beta r/r_0) \quad \beta > 1 \tag{6}$$

so

$$g(\rho) = \hat{V} \left(\frac{\rho}{V} \right)^\beta.$$

The condition $\beta > 1$ implies that the repulsive potential vanishes at a lower scale than the attractive interaction. If not, the ground state would be the set of isolated atoms. Moreover, the numerical values are often close to 2. For instance, the study of silicon aggregates by Mosseri and Gaspard (1981) uses $\beta = 1.893$. In the following, we strictly take $\beta = 2$. By changing \mathcal{H} by \mathcal{H}/ε and t_i by t_i/ε , we can restrain ourselves to the case $\varepsilon = 1$. The concentration of bonds ρ being $\theta = p/n$, we shall finally study the Hamiltonian

$$\begin{aligned} \mathcal{H}(\rho, \rho', \theta) &= - \sum_{i \in \mathbb{Z}} t_i (|i\rangle\langle i+1| + |i+1\rangle\langle i|) + \frac{1}{2}(\theta\rho^2 + (1-\theta)\rho'^2) \\ t_i &\in \{\rho, \rho'\}. \end{aligned} \tag{7}$$

3. The cohesive energy of 1D chains

For given ρ, ρ' and θ , we define $n(\rho, \rho', \theta, E)$ as the electronic density of states (DOS) and $N(\rho, \rho', \theta, E)$ as the integrated density of states (IDOS). Then, the cohesive energy of the considered chain and the filling factor are defined by

$$\begin{aligned} E(\rho, \rho', \theta, E_F) &= \int_{-\infty}^{E_F} x n(\rho, \rho', \theta, x) dx + \frac{1}{2}(\theta\rho^2 + (1-\theta)\rho'^2) \\ \nu &= N(\rho, \rho', \theta, E_F) \end{aligned} \tag{8}$$

where E_F is the Fermi level and ν is the electronic filling factor, which is the integrated density of states at the Fermi level. Now, we introduce some useful notations:

$$\begin{aligned} \bar{\rho} &= \rho\theta + \rho'(1-\theta) \\ \delta &= \frac{\rho' - \rho}{\bar{\rho}} \quad a(\theta) = \theta(1-\theta) \quad \delta' = a(\theta)\delta \\ \rho &= \bar{\rho}(1 - (1-\theta)\delta) \quad \rho' = \bar{\rho}(1 + \theta\delta) \\ n(\rho, \rho', \theta, E) &= n(\rho/\bar{\rho}, \rho'/\bar{\rho}, \theta, E/\bar{\rho}) = n(\delta, \theta, E/\bar{\rho}). \end{aligned} \tag{9}$$

$\bar{\rho}$ is the average hopping parameter and δ measures the strength of the disordered potential since $\delta = 0$ corresponds to a periodic Hamiltonian. The last line of (9) is a consequence of the linearity of the electronic Hamiltonian with respect to the hopping

parameters ρ and ρ' . It allows us to compute the cohesive energy by means of the DOS for $\bar{\rho} = 1$. Preferring the filling factor to the Fermi level, the cohesive energy can be written in the new variables

$$E(\bar{\rho}, \delta, \theta, \nu) = \bar{\rho} \int_{-\infty}^{E(\nu)} xn(\delta, \theta, x) dx + \frac{1}{2} \bar{\rho}^2 (1 + a(\theta) \delta^2). \quad (10)$$

In (10), we have inversed locally the expression $\nu = N(\delta, \theta, E_F/\bar{\rho})$ and we have defined $E(\nu) = E_F/\bar{\rho}$. This operation must be done carefully. Indeed, in general the filling factor is not a strictly increasing function of the Fermi level since it is constant in a gap. So, we have to define $E(\nu)$ for values of ν for which a gap exists. For these filling factors, $E(\nu)$ will be taken to be the lowest edge of the gap. One can check easily that any other choice in the gap gives the same value for the cohesive energy since the DOS is zero in a gap.

Now, we have to minimize the energy given by (10) with respect to both parameters $\bar{\rho}$ and δ which can be treated as independent ones. We first optimize the energy with respect to $\bar{\rho}$. The energy being a quadratic and linear function of $\bar{\rho}$, this procedure is particularly simple and leads to

$$\bar{\rho}_{\text{opt}} = - \frac{\int_{-\infty}^{E(\nu)} xn(\delta, \theta, x) dx}{1 + a(\theta) \delta^2}. \quad (11)$$

We use this value to finally find a cohesive energy $E(\nu, \theta, \delta)$ which depends on the filling factor, the disordered sequence of A and B and the strength of the potential:

$$E(\nu, \theta, \delta) = - \frac{(\int_{-\infty}^{E(\nu)} xn(\delta, \theta, x) dx)^2}{2(1 + a(\theta) \delta^2)}. \quad (12)$$

The effect of the repulsive potential (on the denominator) is quadratic in δ . This is a very general feature which is verified for any smooth enough function g , at least to the leading order in δ . We are left with the energy function (12) to minimize with respect to δ . This is a very complicated task since the density of states in (12) depends on δ and is not known for a general disordered chain and for any δ . Thus, we shall compare the cohesive energy of the periodic linear chain ($\delta = 0$) to the one obtained for a weak potential ($|\delta| \ll 1$) on a disordered chain. We shall study this chain by means of perturbation theory.

First of all, we give the cohesive energy of the periodic chain. This structure is obtained by setting $\theta = 0$ (only one kind of hopping parameter) or $\delta = 0$ ($\rho = \rho'$). The spectrum (as well as the DOS and IDOS) can be exactly computed by means of the Bloch-Floquet theory:

$$\begin{aligned} \hat{N}(E) &= 1 - \frac{1}{\pi} \arccos\left(\frac{E}{2}\right) & E \in [-2, 2] \\ E(\nu) &= -2 \cos(\pi\nu) & \nu \in [0, 1] \\ \hat{n}(E) &= \frac{1}{\pi\sqrt{4-E^2}}. \end{aligned} \quad (13)$$

Then, the integral (12) can be easily calculated. One finds

$$\hat{E}(\nu) = E(\nu, \theta = 0, \delta) = E(\nu, \theta, \delta = 0) = -2 \left(\frac{\sin \pi\nu}{\pi} \right)^2. \quad (14)$$

In the following, we study the difference between (14) and the cohesive energy of a disordered chain.

4. Stability of 1D disordered chains

We recall that we consider an infinite periodic chain with an elementary cell of n atoms. In this cell, there are p bonds of type ρ and q of type ρ' ($p+q=n$). We can apply the Bloch theorem to such an Hamiltonian by introducing a Bloch vector k . Then, the electronic Hamiltonian can be written

$$\mathcal{H} = - \begin{pmatrix} 0 & t_1 & 0 & t_n e^{ik} \\ t_1 & \ddots & \ddots & 0 \\ 0 & \ddots & \ddots & t_{n-1} \\ t_n e^{-ik} & 0 & t_{n-1} & 0 \end{pmatrix} \quad t_i \in \{\rho, \rho'\}. \tag{15}$$

Generically, the spectrum of \mathcal{H} consists in n bands. Their edges are given by the $2n$ states associated to $k=0$ and $k=\pi$ and the 1DOS in a gap is a multiple of $1/n$. For a weak potential the centre E_j and the half-width δ_j of a gap are given by perturbation theory. If the 1DOS in the considered gap is j/n the first-order perturbation theory gives (we recall that $\bar{\rho} = 1$)

$$E_j = -2 \cos(j\pi/n) + O(\delta^2)$$

$$\delta_j = \frac{\delta}{n} \left| \sum_{i=1}^n \varepsilon_i \exp\left(\frac{2ij\pi}{n}\right) \right| + O(\delta^2) \tag{16}$$

where $\varepsilon_i = -1$ if $t_i = \rho$ and $\varepsilon_i = +1$ if $t_i = \rho'$. Indeed, δ_j is given by $|\langle j+|\mathcal{H}|j-\rangle|$ where $|j\pm\rangle$ are the two degenerated states of the periodic Hamiltonian ($t_i = 1$) corresponding to the filling factor j/n . We shall use these expression further when we will look for the most stable structure. We forget about the exact value of δ_j and define the edges of the gaps and of the spectrum

$$E_j^\pm = E_j \pm \delta_j \quad E^\pm = \pm 2 + O(\delta^2). \tag{17}$$

Each gap in the spectrum induces a local modification of the DOS of the periodic linear chain \hat{n} . Thus, we shall write

$$n(\delta, \theta, E) = \hat{n}(E) + \sum_{j=1}^{n-1} n_j(E)$$

$$\int_{E^-}^{E^+} n_j(x) dx = 0 \tag{18}$$

since generically, we expect the presence of $n-1$ gaps. The second line ensures that the integrated density of states remains normalized to 1. Moreover, the 1DOS in the j th

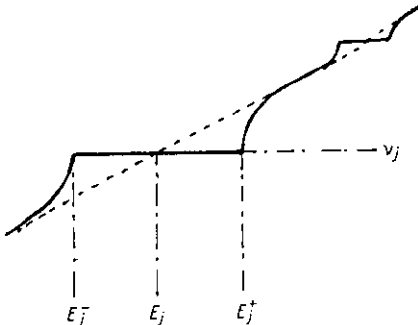


Figure 1. Schematic behaviour of the 1DOS near a gap where Van Hove singularities prevail.

gap is exactly j/n , so that we have the following normalization conditions which can be easily interpreted on figure 1.

$$\begin{aligned}
 N(\delta, \theta, E_j^-) - \hat{N}(E_j^-) &= \hat{N}(E_j^+) - N(\delta, \theta, E_j^+) \\
 &= \int_0^{E_j^-} n_j(x) dx + O(\delta^2) = \int_{E_j^+}^{E^+} n_j(x) dx + O(\delta^2) \\
 &= \frac{1}{\pi} \left[\cos^{-1}\left(\frac{E_j^-}{2}\right) - \cos^{-1}\left(\frac{E_j^+}{2}\right) \right] + O(\delta^2) \\
 &= \frac{1}{\pi} \left[\cos^{-1}\left(\frac{E_j}{2}\right) - \cos^{-1}\left(\frac{E_j^+}{2}\right) \right] + O(\delta^2) \\
 &= \frac{\delta_j}{\pi\sqrt{4 - E_j^2}} + O(\delta^2).
 \end{aligned}
 \tag{19}$$

In the second line of (19), we have neglected up to an order $O(\delta^2)$ the contribution of all functions n_k for $k \neq j$. This is justified below.

Around the gap centred at E_j the density of states is dominated by the strong 1D Van Hove singularities (figure 1):

$$\begin{aligned}
 n_j(E) &\propto \frac{1}{\sqrt{(E - E_j^+)(E - E_j^-)}} \\
 &\propto \frac{1}{\sqrt{(E - E_j)^2 - \delta_j^2}}.
 \end{aligned}
 \tag{20}$$

When $|E - E_j| \gg \delta_j$, n_j goes to zero, which leads to the following expression for the DOS:

$$\begin{aligned}
 n_j(E) &= \alpha_j \left[\frac{|E - E_j|}{\sqrt{(E - E_j)^2 - \delta_j^2}} - 1 \right] + O(\delta_j^2) \\
 &= -\hat{n}(E) \quad \text{for } E \in [E_j^-, E_j^+].
 \end{aligned}
 \tag{21}$$

This expression is obtained by imposing that $n_j(E)$ is at least an order $O(\delta^2)$ when E goes to infinity. α_j can be computed from the condition (17). One easily finds

$$\begin{aligned}
 n_j(E) &= \frac{1}{\pi\sqrt{4 - E_j^2}} \left[\frac{|E - E_j|}{\sqrt{(E - E_j)^2 - \delta_j^2}} - 1 \right] + O(\delta_j^2) \\
 &= -\hat{n}(E) = -\frac{1}{\pi\sqrt{4 - E_j^2}} + O(\delta_j) \quad \text{for } E \in [E_j^-, E_j^+].
 \end{aligned}
 \tag{22}$$

We have replaced $\hat{n}(E)$ in the gap by its value at the centre E_j up to order $O(\delta_j)$. By integrating on the gap of width $2\delta_j$, the contribution of this term will be a $O(\delta_j^2)$. So, one can see that in (17), the contributions of other gaps than gap j to the first integral is of order $O(\sum \delta_k^2) = O(\delta^2)$.

Now, we assume that the Fermi level lies in the gap indexed by j . We then compute the cohesive energy of the chain. First of all, we have

$$\begin{aligned}
 \int_{E_j^+}^{E^+} xn_j(x) dx &= E_j \int_{E_j^+}^{E^+} n_j(x) dx + \int_{E_j^+}^{E^+} (x - E_j)n_j(x) dx \\
 &= \frac{\delta}{\pi\sqrt{4 - E_j^2}} \left[E_j + \delta_j \int_1^{u_1} u \left(\frac{u}{\sqrt{u^2 - 1}} - 1 \right) du \right] + O(\delta^2)
 \end{aligned}
 \tag{23}$$

where we have performed the change of variable $u = (E - E_j) / \delta_j$. This last integral can be exactly computed. Since we only need the leading terms, we finally obtain:

$$\int_{E^-}^{E_j^-} x n_j(x) dx = \frac{\delta_j}{\pi \sqrt{4 - E_j^2}} \left[E_j + \frac{1}{2} \delta_j \ln \left(\frac{1}{\delta_j} \right) \right] + O(\delta^2)$$

$$\int_{E_j^+}^{E^+} x n_j(x) dx = \frac{\delta_j}{\pi \sqrt{4 - E_j^2}} \left[E_j - \frac{1}{2} \delta_j \ln \left(\frac{1}{\delta_j} \right) \right] + O(\delta^2).$$
(24)

On this expression (24), we easily check that condition (18) is fulfilled. Now, we subtract to (12) the cohesive energy of the periodic chain. Thus, the difference of both energies is given by

$$\Delta E(\nu_j, \theta, \delta) = - \frac{(\int_{-\infty}^{E_j^-} x n(\delta, \theta, x) dx)^2}{2(1 + a(\theta)\delta^2)} + \frac{1}{2} \left(\int_{-\infty}^{E_j} x \hat{n}(x) dx \right)^2$$

$$= 2 \frac{|\sin(\pi \nu_j)|}{\pi} \left[\int_{E^-}^{E_j^-} x n_j(x) dx - \int_{E_j^+}^{E^+} x \hat{n}(x) dx \right] + O(\delta^2).$$
(25)

The first integral of the second line has already been computed in (24), whereas the second one can be exactly performed. It cancels exactly the linear term of (24) so that the final result reads:

$$\Delta E(\nu_j, \theta, \delta) = - \frac{\delta_j^2}{2\pi^2} \ln \left(\frac{1}{\delta_j} \right) + O(\delta^2).$$
(26)

If δ_j behaves linearly in δ , (26) shows that for sufficiently small δ , the disordered chain will be more stable than the periodic one, at least for $\nu = \nu_j$, or close enough to ν_j . This result does not depend on the repulsive potential, provided that it is sufficiently smooth (say \mathcal{C}^2).

Now, let us study the infinite limit, that is, when $n \rightarrow +\infty$. The density of states of the infinite structure S_∞ has a countable set of gaps that can be finite or even zero. We call $\mathcal{N} = \{\nu_j\}$ the set of the values of the IDOS in these gaps. Hence, each gap is labelled by the value taken by the IDOS inside it (for recent results concerning this gap labelling see Bellissard (1991)). If the gap does not scale linearly with δ , (26) shows that the effect of the opening gap is (less than) an order $O(\delta^2)$. The effect of the repulsive interatomic potential can make this term positive, provided it is strong enough (β large enough). Thus, even if the Fermi level stands in this gap, the periodic chain is still more stable. Conversely, if the gap at ν_j still opens linearly, then the first-order perturbation term induces the stabilization of the disordered structure:

$$g_j = \lim_{n \rightarrow +\infty} \frac{1}{n} \left| \sum_{l=1}^n \varepsilon_l \exp(2i\pi l \nu_j) \right|$$

$$\Delta E(\nu_j, \theta, \delta) = - \frac{1}{2} \left(\frac{\delta g_j}{\pi} \right)^2 \ln \left(\frac{1}{\delta g_j} \right) + O(\delta^2).$$
(27)

Here, we have kept the g_j in the logarithmic term (although it contributes to an order δ^2) in order to have a function of the single variable δg_j . Moreover, one can see that g_j is not zero if and only if the Fourier transform of the sequence $\{\varepsilon_l\}$ contains a Dirac peak for a wavevector equal to $2\pi \nu_j$. This is a typical feature of a relatively well ordered structure. As an example and a possible test of (27), we apply the preceding formalism to the quasicrystalline case.

5. Stability of 1D quasicrystals

As mentioned in the introduction, quasicrystals are good candidates in order to illustrate the stabilization of a structure by the opening of a gap at the Fermi level. Quasicrystals are quite well ordered structure in the sense that they can be arbitrarily well approximated by periodic crystals.

In 1D, this can be seen by the following construction called the cut and projection method (Duneau and Katz 1985, Kalugin *et al* 1985, Elser 1985). Consider the semi-opened strip \mathcal{S} built by translating the unit square of a 2D square lattice along a line of slope τ . As can be proved and as can be seen in figure 2, there exists only one path included in \mathcal{S} , along the bonds of the square lattice, provided τ is irrational. The sequence of vertical and horizontal bonds is quasiperiodic for an irrational slope, whereas it is periodic of unit cell $n = p + q$ when $\tau = p/q$. We now consider the tight-binding Hamiltonian built by associating letter A to a vertical bond and letter B to an horizontal one. Then, we proceed exactly like in section 2.

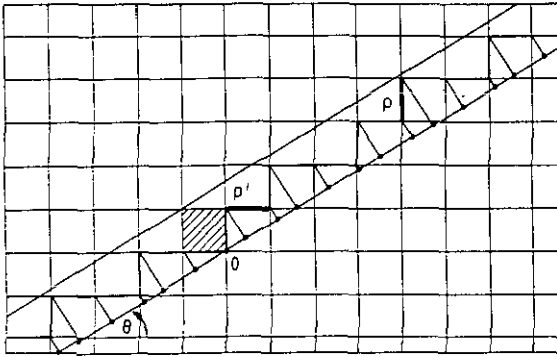


Figure 2. The cut and projection method.

This kind of Hamiltonian has been introduced in a different context by Kohmoto *et al* (1983) and Ostlund *et al* (1983). They find a renormalization group procedure allowing numerical computation of the spectrum for $\tau = (\sqrt{5} - 1)/2$ (the Fibonacci chain) in a very efficient way. In the following, we shall compare the theoretical results for quasicrystals to numerical studies performed on the Fibonacci chain.

First of all, we recall the result for the gaps opening in 1D quasicrystals of irrational slope τ (Sire and Mosseri 1989):

$$\mathcal{N} = \{ \nu_j^\pm = \pm j\theta[1], j \in \mathbb{N} \} \quad \theta = \frac{\tau}{1 + \tau}$$

$$g_j = \frac{2}{\pi j} |\sin(\pi j \theta)| \quad (28)$$

where θ is as previously the concentration of ρ and $[]$ denotes the modulo operator. This shows that all the gaps of quasicrystals open linearly with δ . This can be related to the fact that the Fourier spectrum of a quasiperiodic sequence $\{\epsilon_i\}$ consists in a dense set of Dirac peaks. Indeed, recently Luck has related singularities in the Fourier spectrum to the opening of gaps (Luck 1989).

Finally, the difference between the cohesive energy of the quasicrystal and the periodic chain reads

$$\Delta E(\nu_j^\pm, \theta, \delta) = \hat{E}(\nu_j^\pm) \left[\frac{1}{\pi^2} \left(\frac{\delta}{j} \right)^2 \ln \left(\frac{j}{\delta} \right) + O(\delta^2) \right] \tag{29}$$

where we recall that \hat{E} is given by (14). We find that for any j , the quasicrystal with filling factor $\nu_j^\pm = \pm j\theta$ [1] is more stable than the linear chain, at least for sufficiently small modulation δ . We can estimate the critical value of δ under which this situation occurs. If we assume that the $O(\delta^2)$ roughly does not depend on j or at least does not go to zero when j tends to infinity, this critical value $\delta_c(j)$ is reached when both terms in (29) are of the same magnitude. This implies

$$\delta_c(j) \sim j \exp(-Cj^2) \tag{30}$$

which goes to zero very rapidly. Thus, for large j (that is for small gap) the gain in energy below $\delta_c(j)$ will be very small (of order δ_c^2). In the case of quasicrystals, the $O(\delta^2)$ is found to be a smooth slowly varying function of ν so that this argument is valid in this case.

In order to verify these results, we show in figure 3, $\Delta E/\delta^2 \hat{E}$ as a function of ν . The curve has a set of minima (cusps) which are found to hold for ν belonging to \mathcal{N} . As δ is decreasing, we find that these minima are also slowly decreasing, whereas new domains of stability appear.

We have also checked the validity of (29) for $j = 1$ and $j = 2$. For different values of δ , we have plotted $\Delta E/\delta^2 \hat{E}(\nu_j)$ as a function of $\ln \delta$. We find perfect lines, as

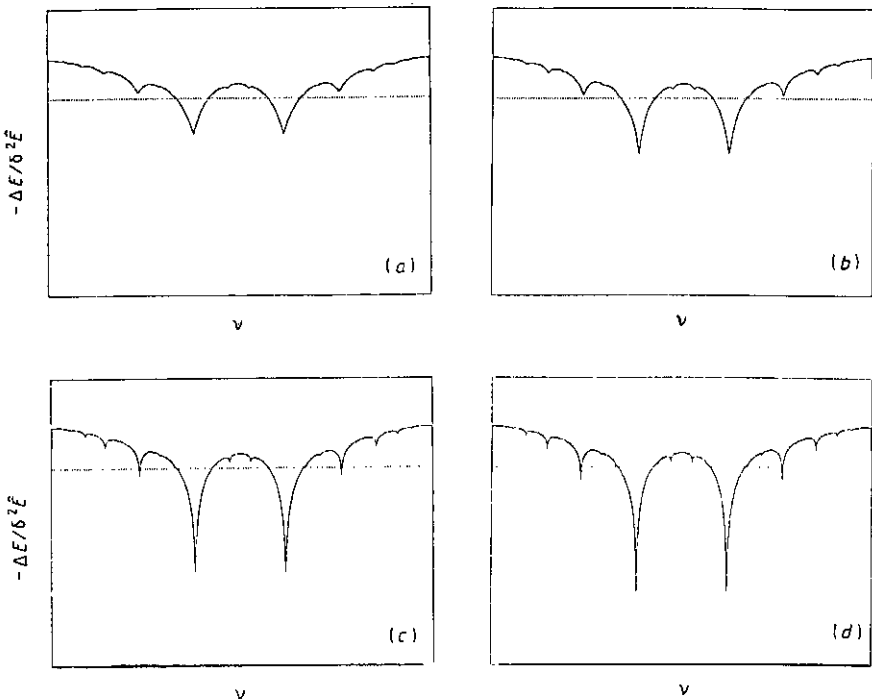


Figure 3. $-\Delta E/\delta^2 \hat{E}$ as a function of $\nu \in [0, 1]$ for: (a) $\delta' = 0.1$; (b) $\delta' = 0.01$; (c) $\delta' = 0.001$; (d) $\delta' = 0.005$. The dotted line corresponds to energy 0.

predicted by (29). Moreover, the slopes are very near their theoretical value. For instance for $j = 1$, we find 1.817 ± 2 instead of $(\pi\theta(1 - \theta))^{-2} = 1.81813 \dots$. Finally the ratio between both slopes is found to be 4.015 instead of the exact value $(2/1)^2 = 4$. All these results are shown in figure 4.

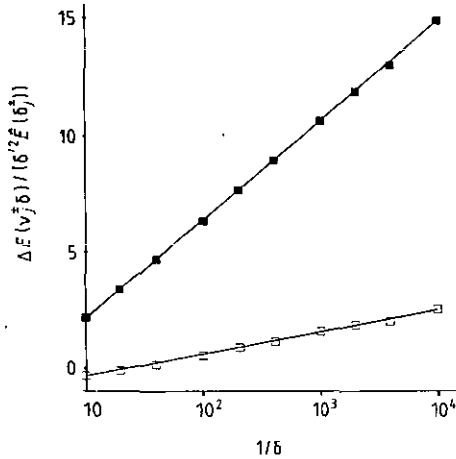


Figure 4. For $j=1$ (full squares) and $j=2$ (open squares) we have plotted $\Delta E(\nu_j^\pm, \delta) / (\delta^2 \dot{E}(\nu_j^\pm))$ as a function of $\ln(1/\delta)$.

As can be seen in figure 3, the minimum of ΔE at ν_j^\pm is a cusp. This is an important feature from a physical point of view. Indeed, if we add a small amount of disorder to the original structure, we expect the effect to be the addition of a small smooth term to the previously computed ΔE . Thus, even if $\Delta E(\nu_j^\pm)$ changes, it remains a strict minimum provided the additional noise is weak enough.

So, in the following we shall study the minimum of ΔE in the vicinity of ν_j , in the general case. In the same spirit as for (25), we obtain for $\nu \geq \nu_j$:

$$\Delta E(\nu, \theta, \delta) = \Delta E(\nu_j, \theta, \delta) + 2 \frac{|\sin(\pi\nu_j)|}{\pi} \times \left[\int_{E_j^+}^{E(\nu)} xn(\delta, \theta, x) dx - \int_{E_j}^{-2\cos(\pi\nu)} x\hat{n}(x) dx \right] + O(\delta^2). \tag{31}$$

Now, we assume $|E(\nu) - E(\nu_j)| \ll \delta_j$. One can easily see that x can be replaced by E_j^+ in the first integral, whereas the second one is easily computed:

$$\begin{aligned} \Delta E(\nu, \theta, \delta) &= \Delta E(\nu_j, \theta, \delta) + 2 \frac{|\sin(\pi\nu_j)|}{\pi} \\ &\times \left[E_j^+ \int_{E_j^+}^{E(\nu)} n(\delta, \theta, x) dx + \frac{2}{\pi} (\sin(\pi\nu_j) - \sin(\pi\nu)) \right] \\ &+ O(\delta^2, (\nu - \nu_j)^2) \\ &= \Delta E(\nu_j, \theta, \delta) + 2\delta_j \frac{|\sin(\pi\nu_j)|}{\pi} (\nu - \nu_j) + O(\delta^2, (\nu - \nu_j)^2). \end{aligned} \tag{32}$$

The derivation for $\nu \leq \nu_j$ is strictly similar to (31), (32) and gives a contribution of the opposite sign so that in (32) one can replace $(\nu - \nu_j)$ by $|\nu - \nu_j|$. In the case of a quasiperiodic chain (29) and (32) give the following expression for ΔE near ν_j^\pm :

$$\Delta E(\nu, \theta, \delta) = \hat{E}(\nu) \left[\frac{1}{\pi^2} \left(\frac{\delta}{j} \right)^2 \ln \left(\frac{j}{\delta} \right) - 2 \frac{\delta}{j} |\nu - \nu_j^\pm| \right] + O(\delta^2, (\nu - \nu_j^\pm)^2). \quad (33)$$

This calculation confirms the presence of symmetric cusps. Numerically, and for small δ , the accuracy of (33) is perfect for the Fibonacci chain (figure 5). The second-order terms in $(\nu - \nu_j^\pm)$ can also be computed from (31). Only the leading term in δ is symmetric.

In the following section, we are looking for the most stable structure for a given sufficiently small δ .

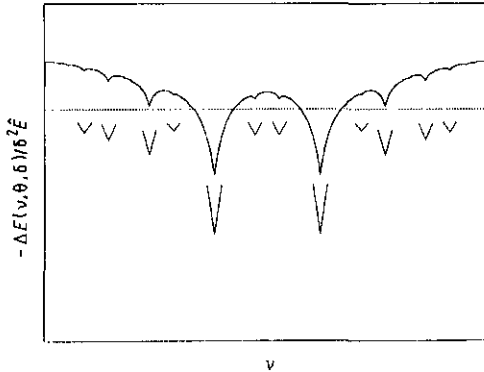


Figure 5. The theoretical cusps (33) are shown below their numerical counterpart.

6. Quasicrystals: an equilibrium state

The title of this section is a partial answer to our problem. In the following, we shall prove that for a given filling factor ν the more stable structure is a quasicrystal.

From the beginning of this paper, we were dealing with chains made of a sequence of bonds A and B. These chains can also be seen as sequences of atoms α and β . We define an atom of kind α to be surrounded by one bond A and one bond B (no matter of the order), whereas an atom of type β is surrounded by two A's or two B's. The α -atoms can be seen as 'anisotropic' while β -atoms are 'isotropic' regarding their orbitals. The concentration of α -atoms is not *a priori* related to θ which is the concentration of bonds of kind A.

The first problem we are interested in is the following. We fix θ and ν and look for the most stable structure at least at sufficiently small potential δ . From (27), at small enough δ , ΔE is an increasing function of the width of the gap at the Fermi level, that is an increasing function of g_j . So, we are left to find the structure which leads to the maximum value of this quantity.

6.1. Irrational filling factors

We first consider the case $\theta = p/n \leq \frac{1}{2}$ and periodic structures of size n as introduced in section 2, that we shall make go to infinity. Then, as seen in section 4, the filling factor in a gap is of the form $\nu_j = j/n$ and g_j is given by (16). In the following, we assume $\nu_j \leq \frac{1}{2}$ since one can easily see that the properties for ν and $1 - \nu$ are strictly identical. Moreover, we are first interested in the case of irrational ν so that

$$\lim_{n \rightarrow +\infty} \nu_j = \nu \notin \mathbb{Q}. \tag{34}$$

One can always take j and n mutually prime since the limit is irrational. Then, g_j can also be written

$$\begin{aligned} g_j &= \frac{1}{n} \left| \sum_{l=1}^n \varepsilon_l \exp\left(\frac{2i\pi lj}{n}\right) \right| \\ &= \frac{1}{n} \left| \sum_{l=1}^n \eta_l \exp\left(\frac{2i\pi l}{n}\right) \right| \quad \varepsilon_l = \eta_{j[n]}. \end{aligned} \tag{35}$$

The transformation from the ε_l to the η_l bears resemblance to the conumerotation approach (relabelling of sites) used in Sire and Mosseri (1989). In (35), we recall that p of the η_l are equal to -1 , and q to $+1$. Moreover, it is shown in the appendix that up to a global shift the sequence $\{\eta_l\}$ which leads to the maximum value of g_j is the following:

$$\eta_l = \begin{cases} -1 & l \in [1, p] \\ +1 & l \in [p+1, n]. \end{cases} \tag{36}$$

The corresponding sequence of A and B defined from the sequence $\{\varepsilon_l\}$ is quasiperiodic since it can be built by means of a circle mapping. Indeed, from (36) and the definition of the η_l (34), it is easy to show that

$$\varepsilon_l = 1 - 2\chi_\theta(l\nu) \tag{37}$$

where χ_θ is the characteristic function of the window $[0, \theta]$ on the circle (of perimeter 1), whence the name of the sequence. Equation (37) holds for any θ and for irrational ν . One can add in (37) a global phase to $l\nu$. This leads to the same structure up to a (eventually infinite) translation. The circle algorithm is illustrated in figure 6(a).

The circle sequence as an abstract sequence of -1 and 1 can be shown to be always quasiperiodic although the binary structure built by associating a length l to -1 and

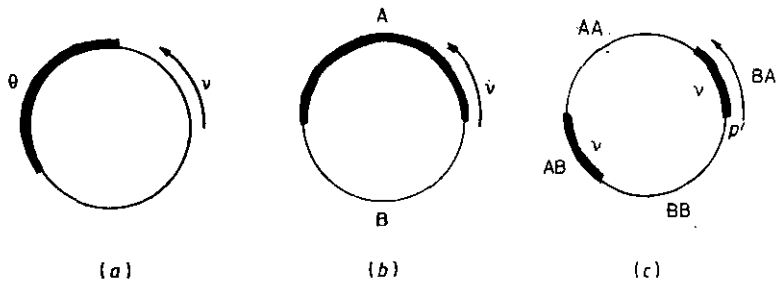


Figure 6. (a) The circle algorithm. (b) If $\theta = \frac{1}{2}$ there are two symmetric windows associated to AB and BA. (c) This is equivalent to a circle mapping with both window and velocity twice larger (equal to 2ν).

l' to 1 has been conjectured to have a singular continuous Fourier spectrum if the following arithmetical 'Kesten condition' is not fulfilled:

$$\exists r \in \mathbb{Z} / \quad \theta = r\nu [1]. \quad (38)$$

General references devoted to the circle sequence and a study of a wide class of disordered sequences can be found in Godrèche and Luck (1990).

We note that this condition (38) is likely to be the physically observed situation. If each atom contributes for a rational number of electrons, the filling factor and the concentration could be related by such a relation. Now, when seen as a sequence of atoms α and β , the abstract chain of atoms is still quasiperiodic. If we associate -1 to an α -atom and since it corresponds to the occurrence of AB or BA in the bond sequence, one can see that the sequence is obtained from a circle mapping with two disconnected windows or only one whether $\nu < \theta$ or not. The associated optimal concentration of α -atoms is 2ν if $\nu < \theta$ and $\theta + \nu$ otherwise.

Now, we are interested in the links between the cut and projection method of section 5 and the circle mapping. If the Kesten condition (38) is fulfilled by ν and θ , then it can be shown that the bond sequence as well as the atomic sequence can be built from a cut and projection-like algorithm (Godrèche and Oguey 1990). For instance, if $\nu = \theta$ the most stable structure is exactly the quasicrystal of slope $\tau = \theta/(1 - \theta)$ which has been described in the beginning of section 5. When θ and ν do not satisfy the Kesten condition, the atomic structure cannot be built from such a method. For instance, if we associate a vertical (resp. horizontal) bond to each A (resp. B) of the sequence, the fluctuations around the line of slope $\theta/(1 - \theta)$ are not bounded but grow logarithmically with the number of bonds.

There is very particular case which corresponds to a physically important situation. Suppose we are now looking for the most stable structure for a given ν but letting θ free. It can be shown by direct computation of g_j given by (36) that the optimum value is $\theta = \frac{1}{2}$. Since $\frac{1}{2}$ cannot satisfy the Kesten condition with irrational ν , the sequence of bonds cannot be built from the cut and projection method with a bounded strip. This is in contrast with the derived abstract sequence of atoms α and β . Indeed, for this particular value of θ , the sequence of atoms can be built from a circle with two windows of size ν which are symmetric with respect to the centre of the circle (figure 6(b)). By identifying points P and P' of figure 6(c), this sequence is exactly the same as the one obtained with only one window of length twice larger (2ν) and the velocity being 2ν . Then, (38) is satisfied with $r = 1$. One can show that the obtained sequence of α and β is exactly similar to the one built from a strip of slope $2\nu/(1 - 2\nu)$ with a proportion 2ν of α -atoms. The fact that the most stable structure has equal proportions of A and B bonds is reminiscent of the dimerized chain case which has been shown to be the most stable structure for $\nu = \frac{1}{2}$. In the following, we study the stability of disordered chains at rational filling factor.

6.2. Rational filling factors

We define $\nu = j/n$. For such a filling factor, the gap width is proportional to

$$g_{j/n} = \lim_{N \rightarrow \infty} \frac{1}{N} \left| \sum_{l=1}^N \varepsilon_l \exp\left(\frac{2i\pi jl}{n}\right) \right| = \frac{1}{n} \left| \sum_{k=1}^n (2\theta^{(k)} - 1) \exp\left(\frac{2i\pi jk}{n}\right) \right| \quad (39)$$

$$\frac{1}{n} \sum_{k=1}^n \theta^{(k)} = \theta$$

where $\theta^{(k)}$ is the probability that $\varepsilon_l = -1$ for indexes of the form $l = jk[n]$. In the same spirit as in the appendix, one can show that up to an irrelevant global shift, the largest value of $g_{j/n}$ under the condition of the last line of (39) is

$$\theta^{(k)} = \begin{cases} 1 & \text{if } jk[n] \in [0, p[\\ 0 & \text{if } jk[n] \in]p, n[\\ n\theta - p & \text{if } jk_0[n] = p \end{cases} \quad (40)$$

where p is the integer part of $n\theta$. We note that for $\theta = p/n$ we recover (36). So, for irrational θ and up to the main order in δ given by (27), there are an uncountable number of evenly stable structures for rational filling factor, since the only requirement is that $\theta^{(k_0)}$ (which is a probability) is $n\theta - p < 1$.

If we are now looking for the most stable structure, only fixing ν , it is obtained for $\theta = \frac{1}{2}$. The associated structure is now almost surely determined by (40) (consider a unit cell twice larger if n is odd). This is a crystal, the proportion of α -atoms being $\min(2\nu, 2(1-\nu))$. For the special case $\nu = \frac{1}{2}$, there are only α -atoms and we recover the dimerized chain... ABABAB... This exactly the result of Kennedy and Lieb (1987).

The conclusion for the 1D case is that for any filling factor and concentration of the alloy the most stable structure is quasiperiodic when seen as an abstract sequence of bonds or atoms. When the concentration of bonds is free of varying the most stable structure has $\theta = \frac{1}{2}$ and an atomic concentration which is related to the filling factor. As a consequence, the periodic chain is never stable regarding electronic cohesive energy. This is illustrated in figure 7 where we have shown the domain of stability of this chain compared with (quasi-)crystals built from the cut and projection method, with rational slopes whose denominator is bounded by n going from 3 to $+\infty$.

In the following section we study the stability of a 2D quasicrystal (the labyrinth) which is related to the octagonal quasiperiodic tiling.

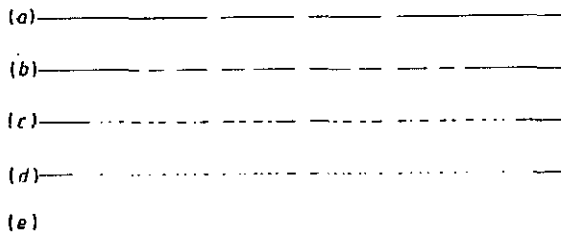


Figure 7. Stability domain (for a given δ) of the periodic chain, compared to approximants of slope with denominator lower than (a) 3, (b) 5, (c) 10, (d) 15 and (e) $+\infty$.

7. Stability of the labyrinth

In this section, we shall try to extend the different results obtained in 1D to higher dimensions. This will be done numerically on a particular example in two dimensions, although one can easily apply such a procedure to similar examples in 3D. The labyrinth which is shown in figure 8 has been introduced as a subtiling of the quasiperiodic

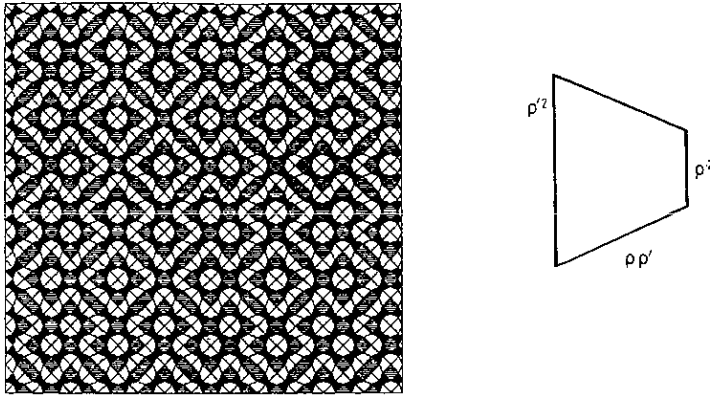


Figure 8. The labyrinth and the three hopping parameters.

octagonal tiling (Sire *et al* 1989). It consists in an assembly of squares, kites and trapezoids. It is a quasiperiodic tiling itself and is topologically equivalent to a square lattice. So, one can see the labyrinth as a modulation of this 2D crystal. This quasiperiodic modulation has something to do with the 'silver mean' $\sqrt{2}-1$ as explained in the reference given above.

We now introduce a tight-binding Hamiltonian on the labyrinth. There are three kinds of bonds on this tiling. We associate to each of them a hopping term respectively equal to $-\rho'^2$, $-\rho\rho'$ and $-\rho^2$ following the decreasing order of the length of these bonds. For $\rho = \rho'$, this Hamiltonian reduces to a periodic one. It has been shown (Sire 1989) that there exists an exact renormalization group for such a Hamiltonian which allows one to compute numerically the spectrum of very large periodic approximants of the labyrinth with a great accuracy. For instance, the spectrum of a sample of 10^8 atoms is calculated in less than one minute on a good PC. Now, we write the cohesive energy of the labyrinth. As in 1D, we add a repulsive interatomic potential which is proportional to the square of the hopping term between each couple of nearest neighbours. Setting $\alpha = \rho/\rho'$, the total Hamiltonian reads

$$\mathcal{H} = -\rho'^2 \sum_{\langle i,j \rangle} t_{ij} |i\rangle\langle j| + \rho'^4((1-p-q) + p\alpha^2 + q\alpha^4)$$

$$t_{ij} \in \{1, \alpha, \alpha^2\} \quad p = \sqrt{2}-1 \quad q = \frac{3}{2}-\sqrt{2} \tag{41}$$

where p and q are the proportions of medium and short bonds in the tiling. We define $n(\alpha, E)$ to be the DOS of the Hamiltonian with hopping parameters 1, α and α^2 . Moreover, ν is the IDOS at the Fermi level and $E(\nu) = E_F/\rho'^2$. Then, the cohesive energy is given by a formula similar to the 1D case:

$$E(\alpha, \nu, \rho') = \rho'^2 \int_{-\infty}^{E(\nu)} xn(\alpha, x) dx + \rho'^4((1-p-q) + p\alpha^2 + q\alpha^4)$$

$$\nu = \int_{-\infty}^{E(\nu)} n(\alpha, x) dx. \tag{42}$$

We consider α and ρ' as independent variables and perform the minimization of this energy with respect to ρ' . One easily finds

$$E(\alpha, \nu) = -\frac{[\int_{-\infty}^{E(\nu)} xn(\alpha, x) dx]^2}{4((1-p-q) + p\alpha^2 + q\alpha^4)}. \tag{43}$$

For $\alpha = 1$, we recall that we obtain the cohesive energy of the periodic square lattice. By means of the exact renormalization group, we have computed $E(\alpha, \nu)$ for different values of α . Compared to the 1D case many interesting features appear. We first recall the different regimes for the spectrum of the labyrinth when α goes from 1 to 0. When α is close enough to 1, the spectrum is made of only one band whereas a finite number of bands appears in a second regime by decreasing α . Then, by further decreasing α , the spectrum consists in an infinite number of gaps, and the Lebesgue measure of the spectrum vanishes. The values of the 1DOS in the gaps can be shown to be integral combinations of 1 and $1/\sqrt{2}$. These results will be related to the ones obtained for $\Delta E/\hat{E}(\alpha, \nu)$ which is the relative difference between the cohesive energy of the labyrinth and that of the square lattice.

Contrary to the 1D case, in the limit $\alpha \rightarrow 1$ (which is the analogue of $\delta \rightarrow 0$), the square lattice is clearly more stable than the labyrinth for any filling factor ν (figure 9(a)). This can be explained by the absence of gaps in the spectrum. By increasing the strength of the quasiperiodic potential, some pseudo-gaps appear in the spectrum and one can observe some local minima for ΔE which remain positive (figure 9(b)). By still decreasing α , the quasicrystal becomes more stable than the square lattice for a certain range of the filling factor (figure 9(c)). We note that in this regime and contrary to the 1D case, the local minima do not have the shape of a cusp and do not seem to hold for particular values of the filling factor. This is due to the fact that even for these values of α , the gaps are still closed. Nevertheless, there are regions in the spectrum where the density of states is very weak. Finally, by further decreasing α ,

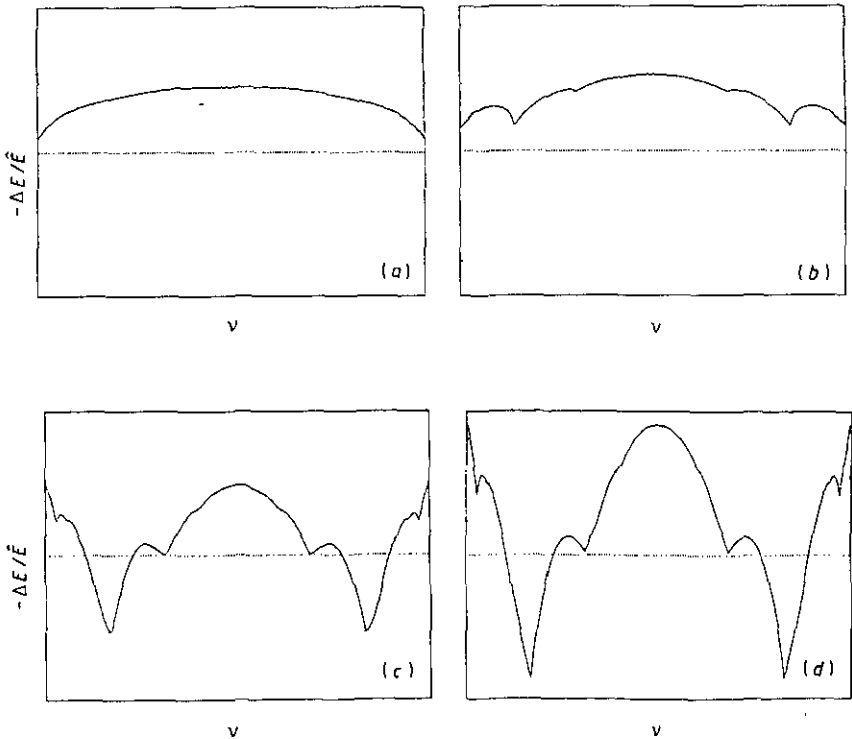


Figure 9. $-\Delta E/\hat{E}$ for (a) $\alpha = 0.99$, (b) $\alpha = 0.9$, (c) $\alpha = 0.7$ and (d) $\alpha = 0.3$. Parts (a) and (b) (resp. (c) and (d)) are at the same scale.

we now see perfect cusps associated to the opening of gaps. For instance, the IDOS corresponding to the deepest minimum of figure 9(d) is numerically found to be very close to $3 - 2\sqrt{2}$ which is the filling factor associated to the largest gap.

These results lead us to make two major comments. First of all, contrary to the 1D case, one can prevent the occurrence of the stabilization by replacing the interatomic repulsive potential by a strongest one. This is due to the absence of a singular behaviour of ΔE as a function of α .

The second remark concerns the fact that one needs a sufficiently strong electronic potential for the quasicrystal to be stabilized. This is a new feature compared to the 1D case for which stabilization occurs surely for weak enough (infinitesimal) modulations. This clearly favours the occurrence of structures with a finite modulation in more than 1D.

8. Conclusion

In this paper, we have studied the stabilization of unidimensional disordered binary alloys by their electronic energy. The main result is that generically the most stable structure for a given filling factor (and eventually for a given concentration) is a quasiperiodic one. The fundamental reason is that such structures lead to the largest gap at the Fermi level, the cohesive energy being an increasing function of the width of this gap. Moreover, we have found that the density fluctuations are unbounded when ν and the bonds concentration cannot be related by the 'Kesten condition'. It would be interesting to know whether these results can be extended to any potential strength.

In two dimensions, the result is qualitatively different for the labyrinth since stability is obtained provided the repulsive energy is not strong enough and for a sufficiently strong modulation. Moreover, contrary to the 1D case, the shape of the minima is not systematically a cusp.

As an application and as was claimed in the literature, this mechanism could explain the stability of quasicrystalline phases. Note finally that our results 1D are profoundly related to the stabilization of uniform flux phases on a square lattice (work in preparation).

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Appendix

In this appendix, it is shown that g_j given in terms of η_l by (35) takes its maximum value when this sequence is given by (36) (up to a cyclic shift of the η_l).

Suppose that the η_l are in a configuration for which g_j is maximal. By a correct cyclic shift of the sequence, one can assume

$$\sum_{l=1}^n \eta_l \exp\left(\frac{2i\pi l}{n}\right) = r \exp(i\phi) \quad |\phi| \leq \frac{\pi}{n}. \quad (44)$$

We assume that ϕ is positive (one treats the other case in the same spirit). Now, suppose that there exists an integer $m_1 \in I =]-q/2, q/2]$ such that $\eta_{m_1} = -1$ (this must be understood modulo n). Then, there exists another integer $m_2 \in]-n/2, n/2]$ outside I such that $\eta_{m_2} = +1$, since there are q numbers of the sequence taking the value $+1$ and I contains exactly q integers. Now, consider the new configuration obtained by exchanging the sign of η_{m_1} and η_{m_2} . Defining $\phi_i = 2\pi m_i/n$ and $r' = 2|\exp(i\phi_1) - \exp(i\phi_2)|$, the modulus of the sum associated to this configuration is

$$\begin{aligned} R^2 &= |r \exp(i\phi) + 2 \exp(i\phi_1) - 2 \exp(i\phi_2)| \\ &= r^2 + r'^2 + 4r[\cos(\phi_1 - \phi) - \cos(\phi_2 - \phi)] \\ &= r^2 + r'^2 + 4rF(\phi, \phi_1, \phi_2). \end{aligned} \quad (45)$$

We have $|\phi_1| \leq |\phi_2|$ and the equality occurs if and only if q is even, $m_1 = q/2$ and $m_2 = -q/2$, so that $0 < \phi_1 = -\phi_2$. Since $\phi \geq 0$, one can easily check that F is then positive.

Now, if the equality is not true we have $|\phi_2| - |\phi_1| \geq 2\pi/n$. If $\phi < \pi/n$, then $|\phi_2 - \phi| > |\phi_1 - \phi|$ and F is strictly positive. Otherwise, F can be zero but cannot vanish simultaneously with r' .

Finally, in each case we found that $R > r$, which is in contradiction with the initial assertion that the sequence $\{\eta_l\}$ leads to the maximal value of g_j (or r). This ensures that the values of l for which $\eta_l = 1$ are the q integers included in I . This solution is exactly the one given by (36) up to a global shift.

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