Influence of phason flips, magnetic field, and chemical disorder on the localization of electronic states in an icosahedral quasicrystal

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The influence of phasons, magnetic field, and substitutional chemical disorder on the electronic spectrum and wave functions of icosahedral quasicrystals is investigated by means of tight-binding approximation and level statistic method. The localization of the wave functions has been studied and we show that they are ''critical.'' Phasons smear the electronic spectrum and reduce localization of the critical wave functions. A magnetic field shifts the boundaries of the spectrum, smears it, and lifts its degeneracy. At small magnetic fields (<10 T) the wave functions also become less localized. The small degree of chemical substitutional disorder delocalizes the wave functions, but at greater degree the disorder leads to the Anderson type localization. The results show that the localization of electronic states in an ideal quasicrystal exists due to their coherent interference at the Fermi level which is caused by the specific symmetry and aperiodic long-range order.

I. INTRODUCTION

Quasicrystals are objects that have noncrystallographic symmetry and coordinational atomic long-range order. Quasicrystals are intermetallic alloys, but their electronic and other physical properties are different from those of crystalline and amorphous metallic phases. Like metals, quasicrystals have a nonzero electronic contribution to the specific heat which is smaller than the value calculated within the free-electron model. At the same time, the electrical resistivity of quasicrystals is anomalously high. The highest resistivity of all known quasicrystals displays icosahedral (i)−Al-Pd-Re quasicrystal with values of resistivity at 4.2 K in excess of 1 Ωcm. Recent measurements of the conductivity of pure, perfect $Al_{70.5}Pd_{21}Re_{8.5}$ have shown that the Mott law for the variable range hopping (VRH) conductivity $\sigma = \sigma_0 \exp(-T_0/T)^{1/4}$ is fulfilled at very low temperatures.[1,2] In $Al_{70.5}Pd_{21}Re_{8.5-x}Mn_x$ it was found that VRH including Coulomb interactions $\sigma = \sigma_0 \exp(-T_0/T)^{1/2}$ could describe the experimental data for $x \leqslant 2$ at temperatures between 0.45 and 10 K.[1] The results show that in an ''ideal'' perfect quasicrystal the electronic states at the Fermi level are localized in the Fermi-glass regime, i.e., the density of states at the Fermi-level is nonzero, and the Fermi level is located below the mobility edge. This localization is caused by constructive interference of electronic states as a result of the symmetry characteristics and structure of the quasicrystal.[3–7]

A qualitative information about the nature and characteristic features of such localization can be obtained from theoretical analysis of electronic spectra of quasicrystals. In a one-dimensional quasicrystal (Fibonacci chain) the density of states is highly singular. It is the Cantor set of gaps and the measure of the allowed states (Lebesgue measure) is zero.[3,4] In two-dimensional quasicrystals (Penrose tiling,[8,9] two-dimensional Fibonacci lattice[10]) and three-dimensional (Amman-MacKay network[7]) quasicrystals the spectrum is also singular. It has a very complicated spiky structure which persists even in the pseudogap area[11] but it does not contain a hierarchical gap structure and has a nonzero Lebesgue measure. In all cases the most of the wave functions are ''critical,'' i.e., they are not localized, they are not delocalized, and they decay with increasing distance according to a power law.

The localization of electrons in quasicrystals differs from the Anderson localization. For the Anderson localization which is due to incoherent scattering by the atomic disorder introduced into the system, the electronic states are localized, their spectrum is continuous and the localization is stable against small perturbations (the mobility threshold is shifted continuously with the external perturbation). On the contrary the localization of electronic states in quasicrystals must be unstable with respect to small perturbations that destroy the symmetry of the system. Moreover, one can expect the different behavior of the wave functions at the boundaries and at the center of the band. Therefore the interesting and important problem is to investigate the effect of small perturbations, effect like, for instance, intrinsic defects (phasons) and weak magnetic field, on the electronic spectrum of quasicrystals. It is also interesting to study the influence of chemical substitutional disorder on the properties of quasicrystalline alloy, because this can introduce the effect of Anderson localization.

The influence of phasons on the electronic spectrum was studied mainly for the two-dimensional quasicrystals.[10,12] A model calculation for the two-dimensional Penrose lattice (PL) with random phason strains have shown that its conductance increases compared with the perfect PL.[12] At the same time phason flips in two-dimensional PL (Ref. 13) and two-dimensional Fibonacci lattice[10] smear out the density of states and lead to very strong fluctuations of conductance. The first preliminary results for a three-dimensional model quasicrystal also show that phasons smear the singularities of the spectrum and make the critical wave functions more extended.[14] The investigation of magnetic field effect on the electronic spectrum of two-dimensional PL has shown that the magnetic field leads to a more uniform distribution of the states.[15]

In this paper we present the results of investigations of the influence of phason flips, magnetic field, and chemical substitutional disorder on the electronic spectrum and wave functions of the model three dimensional quasicrystal. The most common model of the quasicrystal is based on the quasiperiodic packing of two structural units. We used the Amman-Kramer tiling composed of prolate and oblate rhombohedrons. Since quasicrystals do not have translational long range order, traditional techniques for calculations of electronic structure in solids based on Bloch's theorem cannot be applied. Thus the quasicrystal has been considered as the structural limit of the sequence of rational approximants with increasing lattice period. The calculations have been done in the framework of tight-binding (TB) approximation, and the level statistic method (LS) was used for the analysis of the electronic spectrum.

The paper is organized as follows. In Sec. II the method of calculation and ways to introduce the phason flips, the chemical disorder and the magnetic field are described. In Sec. III the results of the investigation are presented. In conclusion we discuss the nature of electron localization in quasicrystals.

II. METHOD OF INVESTIGATION

A tight-binding Hamiltonian with constant hopping integrals t_{ij} between nearest neighbors was used. As follows from the results for one-, two-, and three-dimensional quasicrystals such Hamiltonian allows one to analyze qualitatively the effect of quasiperiodicity on electronic spectrum.[3,4,7–9,12] We used the periodic boundary conditions and considered ''central'' and ''vertex'' decorations of rhombohedrons by atoms with one *s*-like orbital per the atom.

The TB Hamiltonian of the system in the site representation is written as

$$H=\sum_i |i\rangle \epsilon_i \langle i| + \sum_{i,j\neq i} |i\rangle t_{ij} \langle j|, \tag{1}$$

where ϵ_i is one site energies and $|i\rangle, |j\rangle$ are *s*-like wave functions. If atoms only of one type are present, the diagonal elements ϵ_i can be equated to zero. In this case the Schrödinger equation in the tight-binding approximation can be written in the form

$$\sum_j t_{ij}\Psi_i = E\Psi_i, \tag{2}$$

where the transfer integrals are equated to a nonzero constant ($t_{ij}=-1$) in the case of nearest neighbors, and are zero otherwise. We regarded the nearest neighbors as atoms belonging to adjacent rhombohedrons in the ''central'' model and as atoms connected by bonds in the ''vertex'' model.

To characterize the smoothness of the energy spectrum the LS method was used.[7–9,12] It is based on two key equations. The first equation gives the relative number of gaps between levels with widths $\triangle E \leqslant BN^{\beta}$:

$$D(\beta)=\frac{1}{N-1}\sum_{j=1}^{N-1}\theta\left(\beta-\log_N\frac{\epsilon_{j+1}-\epsilon_j}{B}\right), \tag{3}$$

where N is the number of atoms in the approximant basis, $B=\epsilon_N-\epsilon_1$ is the total bandwidth, and θ is the Heaviside function. The second equation yields the band fraction occupied by gaps between levels with widths $\triangle E \leqslant BN^{\beta}$:

$$F(\beta)=\frac{1}{B}\sum_{j=1}^{N-1}(\epsilon_{j+1}-\epsilon_j)\theta\left(\beta-\log_N\frac{\epsilon_{j+1}-\epsilon_j}{B}\right). \tag{4}$$

For the constant B these functions should satisfy the following condition in the thermodynamic limit, irrespective of the smoothness of the spectrum:[8,9,12] $D(\beta)=1$ for $\beta>-1$ and $F(\beta)=0$ for $\beta<-1$. In crystalline and amorphous systems (with smooth spectrum) the curves of $D(\beta)$ and $F(\beta)$ jump from zero to one at $\beta=-1$ in the thermodynamic limit. Therefore an electron spectrum is considered as singular if width of the gaps between levels as a function of the system size do not behave as a 1/N in the thermodynamic limit.

Localization of wave functions have been studied using the statistics of $2p$ norms (moments) of wave functions,[8,9] which are defined as

$$\|\Psi\|_{2p}=\frac{\sum_n |\psi_n|^{2p}}{\left(\sum_n |\psi_n|^2\right)^p}, \tag{5}$$

where ψ_n are the expansion coefficients of the wave function in the tight-binding basis set. The statistical analysis of the distribution of $2p$ norms of wave functions is based on the function $I_{2p}(\gamma)$,[10,11] which yields the relative number of states with $2p$ norms $\|\Psi\|_{2p}\leqslant N^{\gamma}$, i.e.,

$$I_{2p}(\gamma)=\frac{1}{N}\sum_{n=1}^{N}\theta(\gamma-\log_N\|\Psi\|_{2p}). \tag{6}$$

The wave functions were classified in accordance with their normalization integrals. They are delocalized if $\int_{|\vec{r}|<R}|\Psi(\vec{r})|^2 d\vec{r}\sim R^d$, where d is the space dimensionality, and they are localized when their norm $\int|\Psi(\vec{r})|^2 d\vec{r}$ is finite. Wave functions which cannot be normalized in an infinite space but are not delocalized are defined as ''critical.'' For delocalized states, the $2p$ norm of the wave functions depends on the system size as $\|\Psi\|_{2p}^{\text{ext}}\sim N^{1-p}$, as follows from Eq. (5), while exponentially decaying functions have the $2p$ norm $\|\Psi\|_{2p}^{\text{exp.loc.}}\sim 1$. It is known, nevertheless, that the dependence of the $2p$ norm of the wave functions on the system size described by the function $N^{\gamma(p,\alpha)}$ applies to the wave functions whose squared amplitudes decay as power-law functions[10,11] (α is the localization or criticality index; $\alpha=0$ and $\alpha\to\infty$ characterize delocalized and exponentially localized states respectively). So it was assumed that $|\Psi|^2 \sim |r|^{-2\alpha}$. The wave functions with such behavior can be normalized in the three-dimensional case only if $\alpha>3/2$.

Phasons are introduced as follows. For the central decoration of rhombohedra a configuration consisting of two oblate and two prolate rhombohedra is often encountered (the same is for the vertex decoration). In a certain combination these rhombohedra form a rhombic dodecahedron. Phasons were introduced by flipping of rhombohedra which form rhombododecahedron in the real space so that the shape and

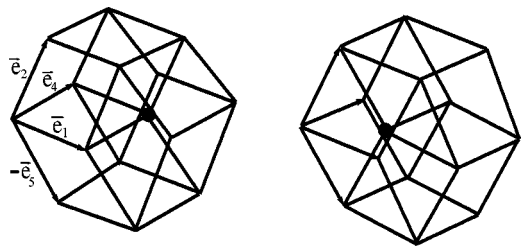

FIG. 1. Flipping of rhombohedra inside of the rhombododecahedron (see text).

orientation of the latter are unchanged (Fig. 1). In doing so, the atoms inside the rhombohedra were transferred into new positions which are inversely to the old ones with respect to the geometric center of the rhombododecahedron, and the number of nearest neighbors remained the same. The analogy of such transformation in the projection technique is a fluctuation of the projection tube. The ratio of the number of prolate rhombohedra to the number of oblate rhombohedra remains unchanged and the average slope of the projection tube in the hyperlattice is constant. When phasons are introduced, the coordination environment for atoms at the centers of rhombohedra is changed, and as a result of it the positions of the nonzero elements of the Hamiltonian matrix are changed.

The magnetic field was introduced in the usual way. We substitute $H(\vec{p})$ by $H(\vec{p}-e\vec{A})$ with vector potential corresponding to the magnetic field $\vec{B}=B\vec{e}_z$. The transfer integral in the presence of the magnetic field gets the form

$$t_{ij}(B)\approx e^{i(e/\hbar)\vec{A}(\vec{R}_i+\vec{R}_j)(\vec{R}_j-\vec{R}_i)}.$$

The Landau gauge $\vec{A}(\vec{r})=-yB\vec{e}_z$ was used. The measure of the field was a ratio of magnetic flux through an area πa_0^2 with a_0—the lattice constant of a cubic approximant to the flux quanta $b=\Phi/\Phi_0$ $(\Phi=\pi a_0^2 B, \Phi_0=h/2e)$.

In order to analyze the effect of the chemical disorder (disorder due to substitutional impurities[7]) on the electronic spectrum and wave functions, the atoms of a different elements were randomly distributed over the unit sell of rational cubic approximants. A two-component model of a random alloy was employed.[16] In this case in Eq. (1) the diagonal elements ϵ_i can take two possible values, namely ϵ^a and ϵ^b depending on whether atom A or B is at the site i. The difference between the two types of atoms can be characterized by the energy parameter $\delta=\epsilon^a-\epsilon^b$ which is a measure of diagonal disorder. The transfer integrals for nearest neighbors are t^{aa} or t^{bb} depending on which atoms occupy sites i and j. The difference between the transfer integrals for the different types of atoms can be characterized by the energy parameter δ_1, $\delta_1=t^{aa}-t^{bb}$. For the t^{ab} we used the additive limit $t^{ab}=(t^{aa}+t^{bb})/2$. The both kinds of disorder, diagonal and offdiagonal, were investigated.

The density of states (DOS), the integrated density of states (IDOS), the Lebesgue measures, $2p$ norms and the coordination dependence of wave functions were calculated.

We investigated four rational cubic approximants of the icosahedral quasicrystal: 1/1, 2/1, 3/2, 5/3. The unit cells of these approximants contain 32, 136, 576, and 2440 atoms respectively, with one s orbital per atom. The number of atoms/unit cell in the same approximants is strongly increased for the real objects (for example, the 3/2 approximant of i–Al-Pd-Re contains 2292 atoms per unit cell with s, p, and d orbitals and sharply is increased for the approximants of higher order[17]). However we have decided to make use of the model system because it was not only simplified the calculations and gave the possibility to use the LS method in the full volume, but helped to study the influence of quasicrystalline symmetry on the electron localization independently of the atomic nature of the object. Besides, the preliminary results[7] have shown that the four approximants are sufficient to observe the tendency to the localization. Since an increase in the approximant order by one (the order of the 1/1 approximant is one, that of the 2/1 approximant is two, etc.) leads to a decrease in the Brillouin zone volume by a considerable factor ($\sim\tau^{-3}$, where τ is the golden mean), the singular point of the icosahedral quasicrystal is $k=0$. Therefore for the studying of the statistics of levels and calculating the integrated density of states the distribution of energy levels was calculated at $k=0$. The density of states for the three lowest approximants 1/1, 2/1 and 3/2 were calculated by the tetrahedron method using energy levels at 40 k-points in the irreducible part of the Brillouin zone (BZ) of the corresponding approximant. Due to the relatively small volume of the BZ of the 5/3 approximant (as compared to the BZ volume for the first approximant), the reduction in the number of k-points had a little effect on the resulting density of states.

III. RESULTS OF CALCULATIONS

The results for the ideal perfect model i quasicrystal were presented earlier in the Ref. 7. It was shown that the energy spectrum does not contain a hierarchical gap structure typical of the Cantor set of measure zero in a spectrum of a one-dimensional quasicrystal (but there are much common with the two- dimensional case[8]). The spectrum contains a singular part and the thermodynamically large number $(N\rightarrow\infty)$ of gaps between levels are narrower than in traditional systems. The curves of the density of electron states for approximants of higher order are less smooth and more ''spiky'' (Fig. 2). The spectrum is smoother at low energies while strong oscillations are mainly seen at higher energies. The width of the smooth section decreases with increasing approximant order. In the thermodynamic limit strong oscillations in the DOS occur throughout the whole energy range, which means that the bands of the energy spectrum are flat, dispersionless, and the group velocities of electrons are very low. The Lebesgue measures of the energy spectrum are non zero and depend weakly on approximant size, unlike the case of a one-dimensional quasicrystal. Now we present the results of investigation of influence of phasons, magnetic field and chemical disorder.

A. Influence of phasons

Phason flips create the configurations, topologically forbidden for quasicrystalline structure and this influences the electronic system. Phasons smear the electron spectrum, some gaps disappear and new peaks are created. On the other hand, peaks become smaller and even disappear. At the same time at certain higher energies the peaks appear. LS analysis

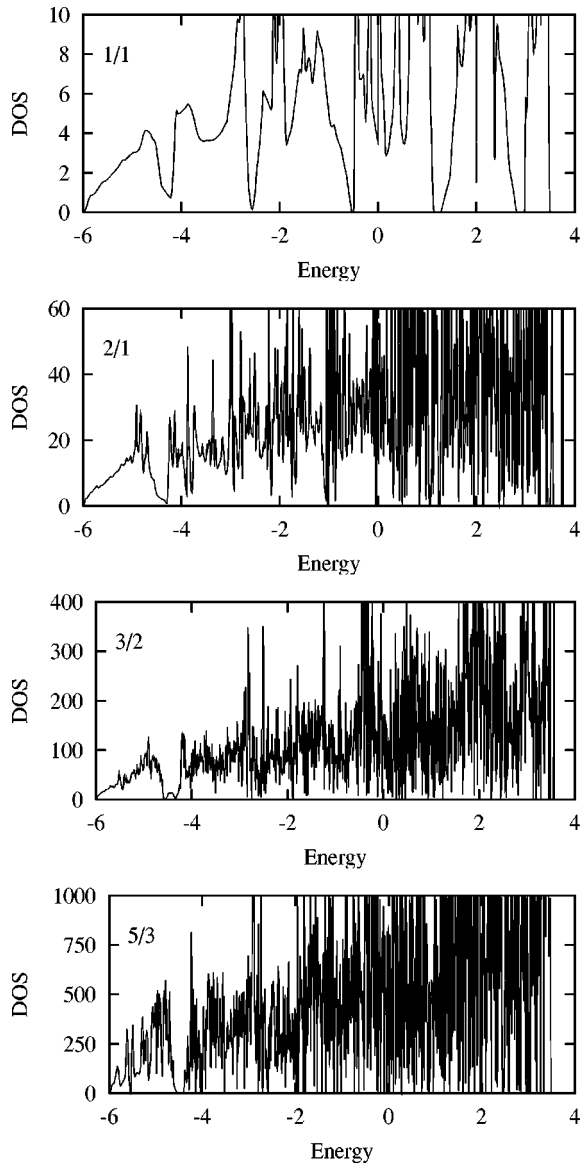

FIG. 2. The DOS for the first four periodic approximants of an icosahedral quasicrystal. The units are arbitrary.

(Fig. 3 and Fig. 4) shows that a singular component of the spectrum decreases with increasing number of the phason flips; the D(β) and F(β) curves become steeper at $\beta=-1$ and approach a crystalline step. So the presence of phasons makes the distribution of interlevel gaps and filling of the band by gaps more uniform. Phasons delocalize wave functions. The localization (or criticality) index α averaged over all band states is diminished with increasing number of the phason flips (Fig. 5). But the influence of phasons is different for different wave functions (see Fig. 6 and Fig. 7). With increasing number of the phason flips the states near the bottom of the band and near the Fermi level became delocalized. New states at high energies which appear when phasons are introduced in the system are more localized than the states near E_F, but they do not contribute to the conductivity of the quasicrystal. So phasons delocalize the electronic states, and therefore the conductivity of the quasicrystal must increase.

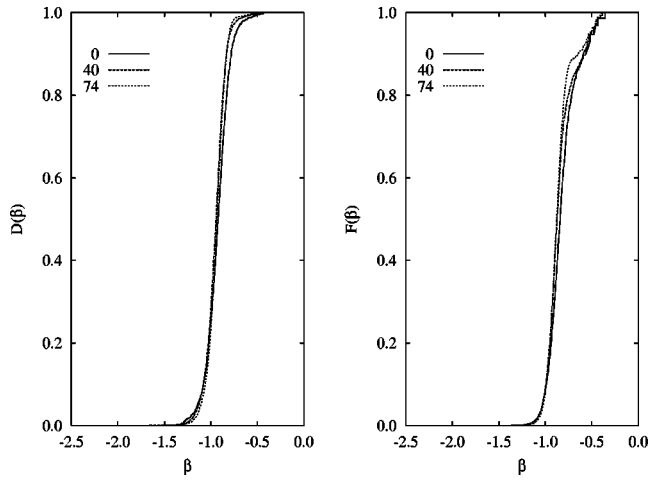

FIG. 3. Influence of phasons on the relative number of gaps $D(\beta)$ and the band fraction occupied by gaps $F(\beta)$ between levels with width $\triangle E \leqslant BN^{\beta}$ (''central'' decoration).

B. Influence of chemical disorder

Chemical disorder was characterized by the three factors, namely the atomic concentration C_b of second component, the difference of on-site energies δ and by the value of δ_1 which defines the difference of transfer integrals. On Fig. 8 the functions $D(\beta)$ and $F(\beta)$ for 3/2 approximant are shown for different degrees of substitutional disorder ($C_b=0.3$). The presence of disorder smears the energy spectrum; the $D(\beta)$ and $F(\beta)$ approach the step function at $\beta=-1$. The dependence of the average localization index α on the degree of disorder is shown for central and vertex decorations on Figs. 9 and 10. The wave functions at low degree of disorder ($\delta=\delta_{\text{crit}}<0.1$) become less localized (Fig. 9). But at $\delta > \delta_{\text{crit}} \sim 0.1$ the tendency to the localization increases again. The results of calculations show that with increasing C_b the tendency to the localization appears at smaller δ_{crit}. The influence of the chemical disorder is different for different electronic states of the band (Fig. 11). Only the wave functions near the bottom of the band and near the Fermi level are affected by disorder. The same is also true for off-diagonal disorder which is characterized by the parameter δ_1

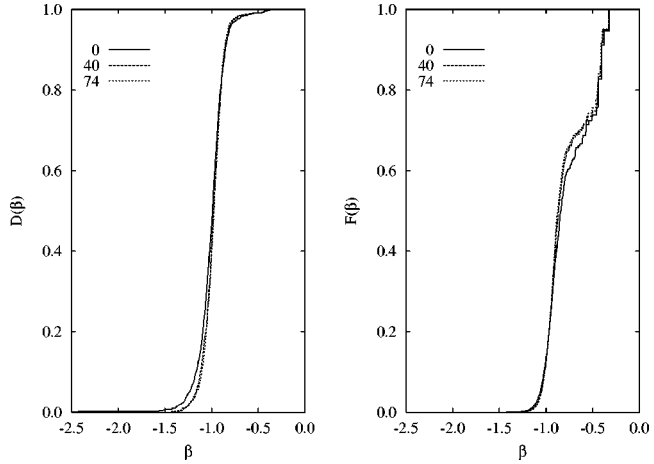

FIG. 4. Influence of phasons on the relative number of gaps $D(\beta)$ and the band fraction occupied by gaps $F(\beta)$ between levels with width $\triangle E \leqslant BN^{\beta}$ (''vertex'' decoration).

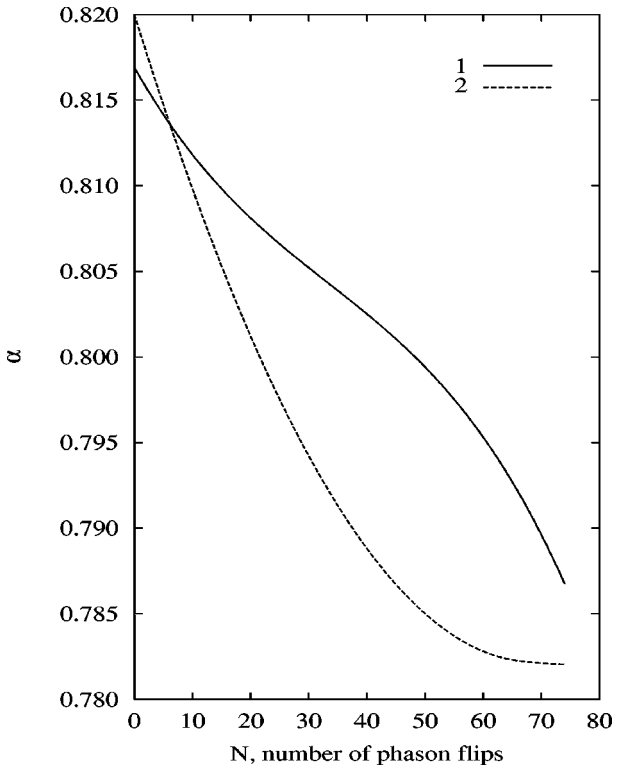

FIG. 5. The localization index α (averaged over all band states) for different number of phason flips 1: ''central'' decoration; 2: ''vertex decoration).

(Fig. 12). The narrowing of delocalization interval of wave functions with increasing concentration of the second component C_b shows that the scattering processes on impurities become important. Decreasing α at small δ and δ_1 confirms the destruction of coherent interference of electronic states in quasicrystals, but the subsequent increase of α with increasing δ and δ_1 is a common effect of localization due to disorder in the system (Anderson localization).

C. Influence of magnetic field

It is well known that electronic spectrum in a magnetic field has a complex structure. Hofstadter[18] has shown that the electronic spectrum of square lattice in the magnetic field depends on the rationality or irrationality of number of flux quanta penetrating the area of unit cell. In ''rational'' magnetic field the energy spectrum consists of a finite number of Landau levels, but in the case of the irrational ratio the spectrum is the Cantor set of levels and the field dependence of the spectrum contour has a butterfly shape. In the case of the three- dimensional quasicrystal the ratio of areas of prolate and oblate rhombohedra is an irrational number τ (the ratio of number of prolate rhombohedra to the number of oblate rhombohedra also is irrational). In a magnetic field all wave functions gain a complementary phase depending on the number of the flux quanta (b) penetrating the surface of rhombohedra which is perpendicular to the magnetic field. For the prolate and oblate rhombohedra they are different, and the wave functions gain the different phases. Note, that for $b=1$ the magnetic field is equal to 10^5 T (quasilattice parameter is of the order of several angstrom). This is unrealistically large field. At the same time, the small fields are

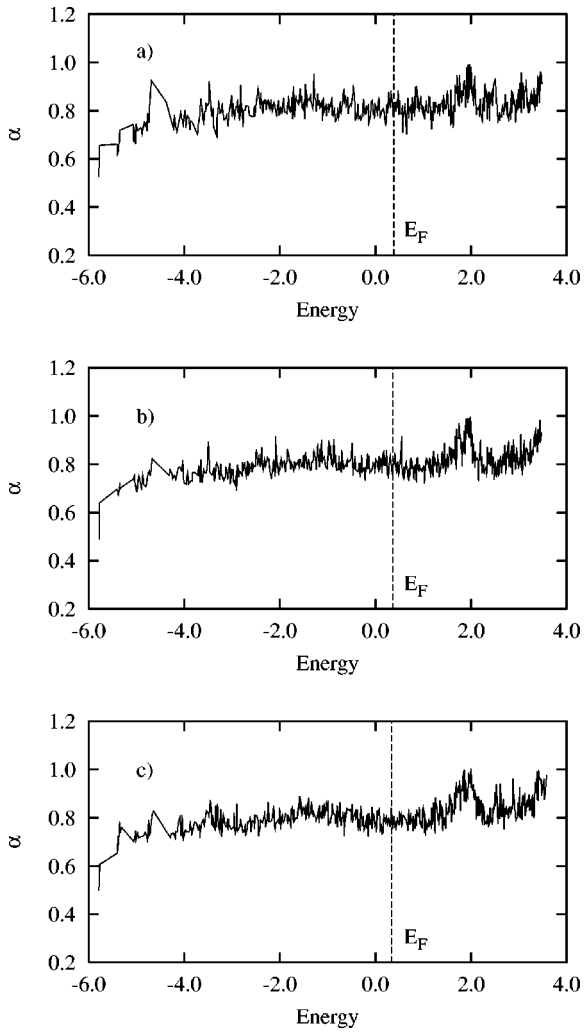

FIG. 6. Distribution of the localization index α on energy band for different number of phason flips (''central'' decoration). (a) 0; (b) 40; (c) 74.

those for which the magnetic length is larger or equal to the quasilattice parameter ($b=10^{-4}$).

The functions $D(\beta)$ and $F(\beta)$ in magnetic field of different strength, for 3/2 approximant (''central'' decoration) are shown on Fig. 13. The $D(\beta)$ and $F(\beta)$ dependencies approach to a step function at $\beta=-1$ in small fields, which shows that interlevel intervals become more uniform and the band fraction occupied by gaps between levels is increased. This is a result of repulsion of levels in a magnetic field. Besides it is seen from the DOS curves that the magnetic field redistributes the levels in groups and in each group the levels are aligned in a quasiperiodic sequence of long and short intervals, which reflects the specific symmetry of the quasicrystal (Fig. 14). The magnetic field also moves quasiperiodically the boundaries of the spectrum.

The influence of magnetic field on the localization of the wave functions is shown on Fig. 15. It is seen that the localization (or criticality) index α decreases in small magnetic field ($H \leqslant 10$ T) which shows that the weak magnetic field destroys the phase coherency of the wave functions. Obviously at the higher fields their shrinkage takes place. However the effect of the strong magnetic field is more complicated and its study is beyond the scope of the present paper.

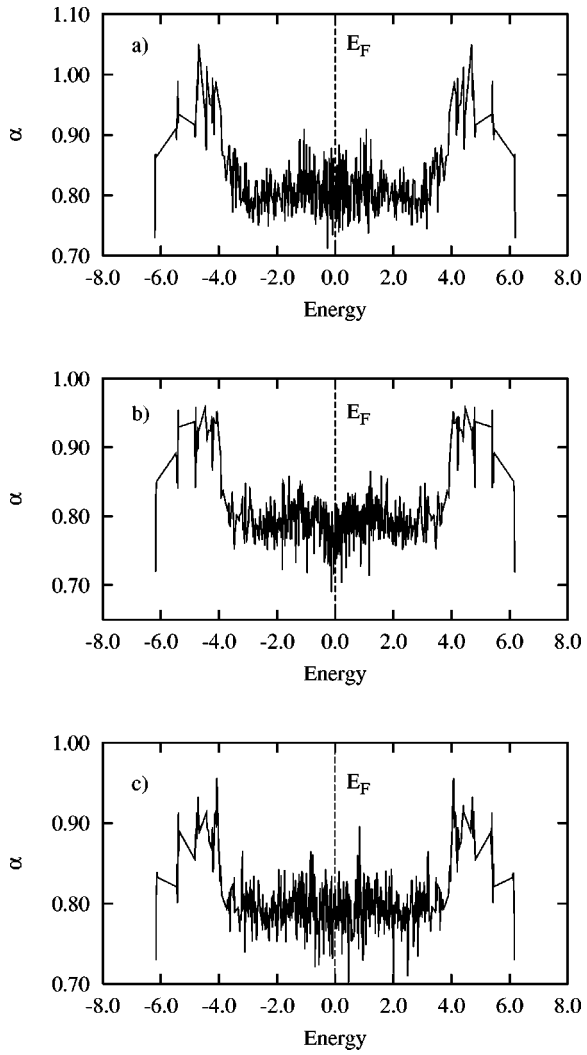

FIG. 7. Distribution of the localization index α on energy band for different number of phason flips (''vertex'' decoration). (a) 0; (b) 40; (c) 74.

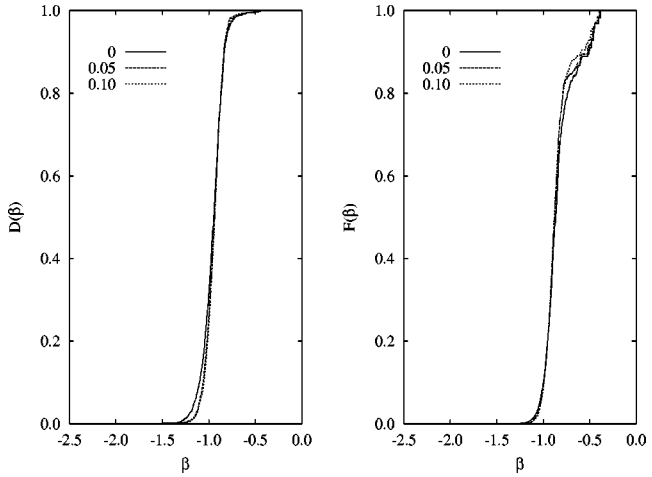

FIG. 8. Influence of substitutional chemical disorder on the relative number of gaps $D(\beta)$ and the band fraction occupied by gaps $F(\beta)$ between levels with width $\triangle E \leqslant BN^{\beta}$ (''central'' decoration).

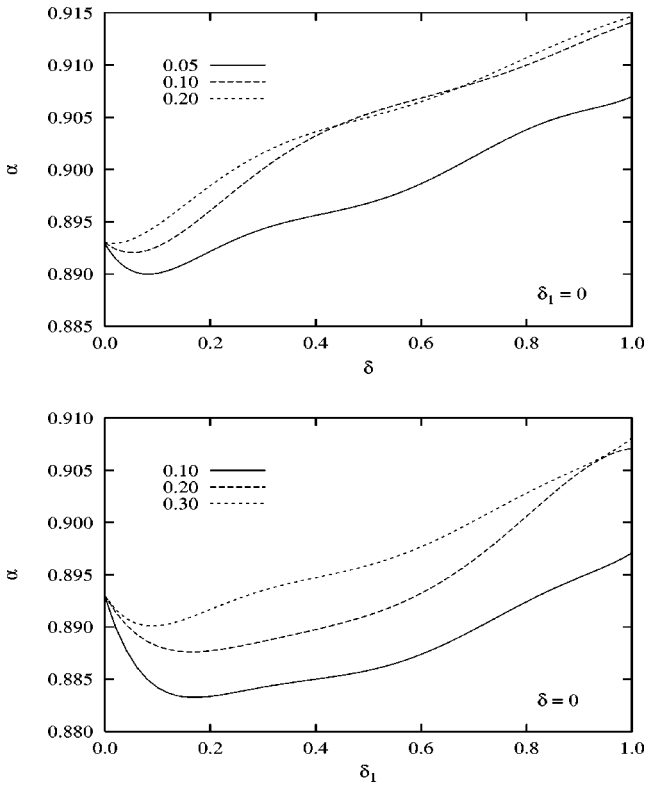

FIG. 9. Dependence of the localization index α (averaged over all bands) at different degrees of the chemical disorder C_b (''central'' decoration).

IV. CONCLUSION

It has been demonstrated that the electron spectrum of the model perfect icosahedral quasicrystal contains a singular

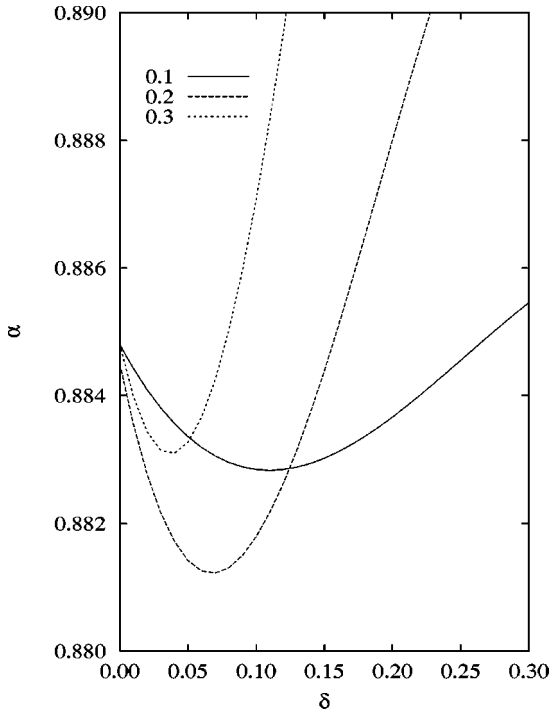

FIG. 10. Dependence of the localization index α (averaged over all bands) at different degrees of the chemical disorder C_b (''vertex'' decoration). $\delta_1 = 0$.

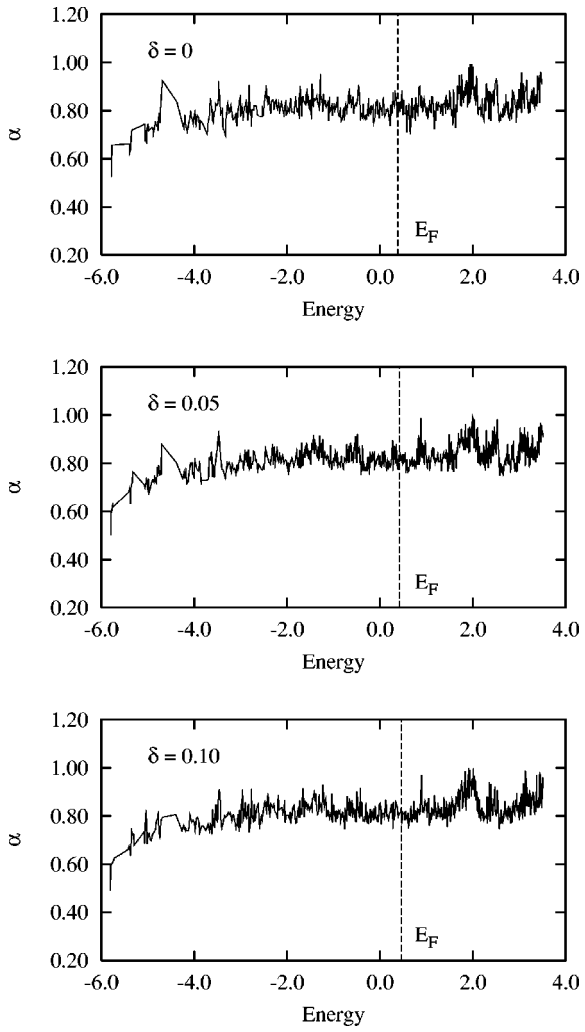

FIG. 11. Distribution of the localization index α on energy band at different degrees of chemical disorder (''central'' decoration). $C=0.1$.

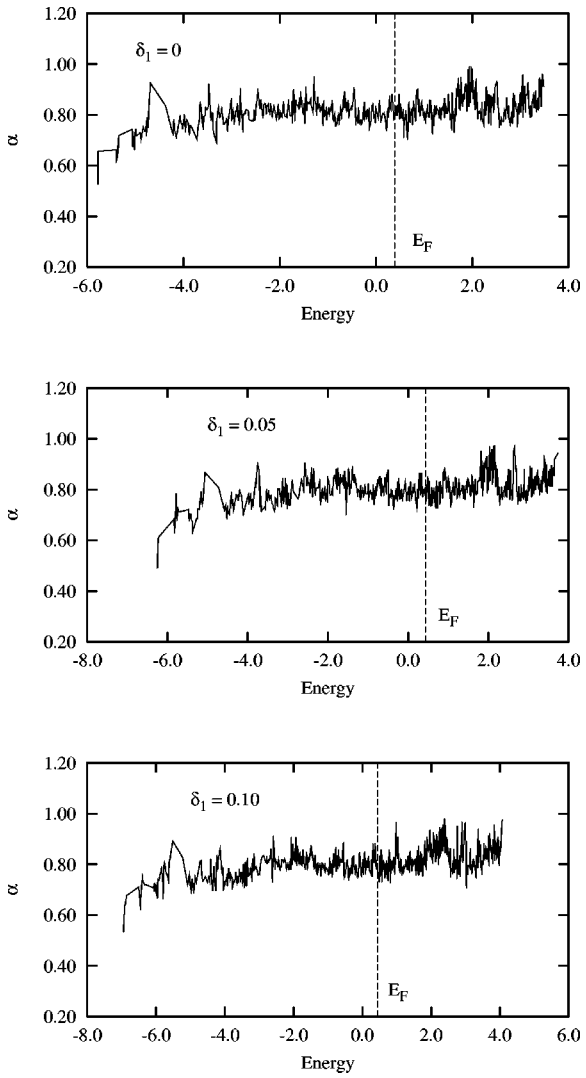

FIG. 12. Distribution of the localization index α on energy band at different degrees of chemical disorder (''central'' decoration). $C=0.1$.

(nonsmooth) component and wave functions are critical.[7] Criticality or localization index is larger for the band center than for the edges. Small perturbations, such as phason flips, a weak magnetic field, a very low degree of the chemical substitutional disorder smear the singularities of the spectrum and make the critical wave functions more extended. The degree of influence is different for the center of the band and for the band edges. This tendency is opposite to well-known case of Anderson localization. The results show that in a pure quasicrystal all electronic states at the Fermi level are localized. This localization is a consequence of coherent interference of electronic states which is caused by the specific symmetry and structure of quasicrystal. Simple considerations can justify this conclusion. Within the six-dimensional periodic description of icosahedral structure it is obvious that each scattering wave vector in a quasicrystal corresponds to a reciprocal wave vector in a periodic structure of higher dimension. Thus a set of reciprocal lattice vectors densely fill the reciprocal space of the quasicrystal, and all electronic states at the Fermi level have zero group velocity due to Bragg reflections (of course, with different intensities). It is convenient to elucidate this picture considering quasicrystal as a limit of a sequence of rational approximants with increasing period. The Brillouin zone volume is diminished with increasing order of the approximant because the lattice period is increased, and becomes infinitely small ($\sim\hbar^3$) in a quasicrystalline limit. Then in the Harrison approach to the construction of the Fermi surface[19] (FS) the FS becomes fractional; that it is multiconnected with a large number of electron and hole ''pockets.'' In a perfect quasicrystal the number of FS ''pockets'' is practically infinite. The condition of strong localization $k_F^i l\sim 1$, where l is mean free path, will be fulfilled for the electrons in each ith FS valley. So conductivity of pure quasicrystals at zero temperature must be zero.

In fractional FS model with practically infinite number of valleys all electrons are localized at zero temperature. So there exists an analogy with a heavily doped semiconductor or strongly disordered system. Each valley of FS plays a role of the localization center in a doped semiconductor. At finite temperatures an intervalley scattering will take place. At low temperatures the process with highest probability is the intervalley scattering with a small momentum transfer in a neighboring valley. In the real space this corresponds to

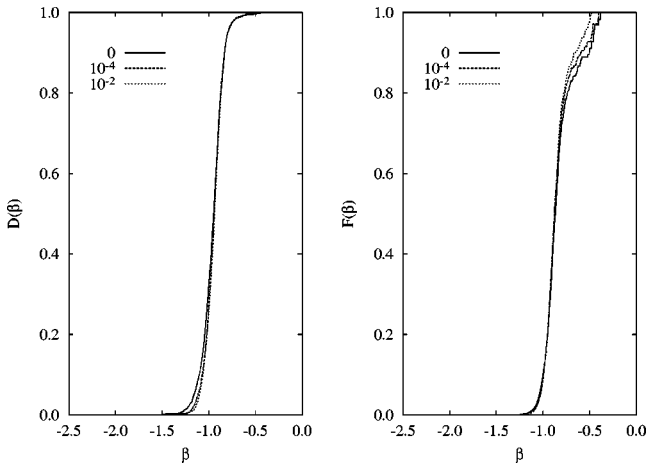

FIG. 13. Influence of magnetic field on the relative number of gaps $D(\beta)$ and the band fraction occupied by gaps $F(\beta)$ between levels with width $\triangle E \leqslant BN^{\beta}$.

hopping on a large distance. Two factors contribute to this. First the thermal excitation with the probability proportional to $\exp(-\triangle E/T)$, where $\triangle E$ is inversely proportional to density of states at the Fermi level, and ξ^3 (ξ is effective hopping distance). Secondly, the tunneling will take place with probability which contains the factor $\exp(-2\alpha r)$ where $1/\alpha$ is the decay length of the wave function. Then following the

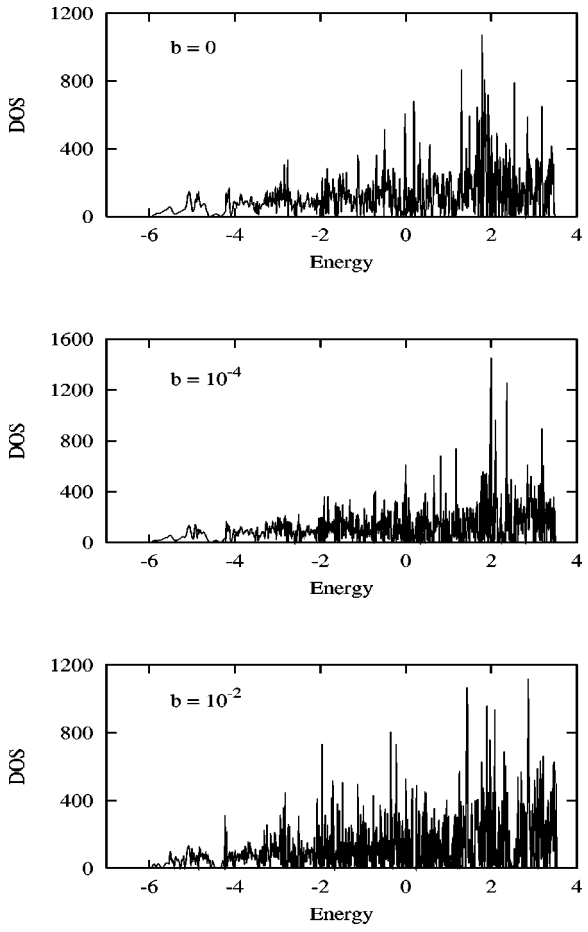

FIG. 14. The DOS for 3/2 approximant in magnetic field (''central'' decoration).

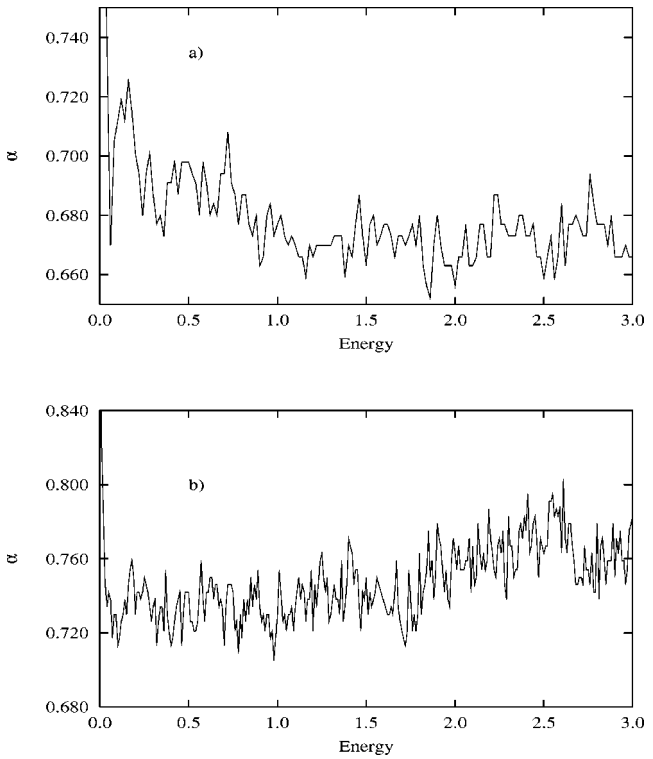

FIG. 15. Influence of magnetic field on the localization index α. (a) ''central'' decoration [$\alpha(0) \approx 0.891$]; (b) ''vertex'' decoration [$\alpha(0) \approx 0.888$].

Mott procedure[20] we can find the optimal ξ and obtain the Mott law for VRH conductivity.

At higher temperatures ($T > 10$ K) the electronic states are smeared by temperature and scattering. This leads to the FS with a finite number of valleys, and this number depends on the character of perturbations.[21] Therefore a crossover from VRH regime to another temperature dependence of the conductivity must occur. Impurities and other structural imperfections (second phases, grain boundaries) can also give the same effect and the finite residual conductivity at $T = 0$ K will appear.

It is interesting to note that according to the results of investigation of localization behavior of the wave functions in a magnetic field one has to expect the negative magnetoresistance in small magnetic fields ($H \leqslant 10$ T). However at higher fields it has to change sign. Recently the experimental proof of such behavior has appeared. According to the experimental data[22] the magnetoresistance of the perfect i–Al-Pd-Re samples [$R = \rho(1.29\ \text{K})/\rho(300\ \text{K}) > 12$] at very low temperatures (~ 0.2 K) is negative in fields $H < 13$ T and changes sign at the higher field.

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