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ELECTRONIC SPECTRUM OF THE THREE-DIMENSIONAL PENROSE LATTICE

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Electronic spectrum of the three-dimensional Penrose lattice with «central» decoration by atoms is investigated using the tight binding model with the nearest-neighbor interaction. Inverse participation ratios, higher moments of density probabilities, and fractal dimensions of the system are determined. The wave functions are critical (have a power-law dependence on the distance) at all energies in the band and are multifractal measures leading to the entire spectrum of the exponents. The results show that the system is in the critical state of the metal–insulator transition. On critical wave functions, the cubic root temperature dependence of the conductivity is obtained.

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1. INTRODUCTION

Measurements of conductivity show that at low temperatures, perfect quasicrystals (QC) behave similarly to the conventional disordered conductors (disordered metals and heavily doped semiconductors in the vicinity of the metal–insulator transition (MIT)), and the possibility of the electron localization–delocalization (LD) in QCs now is actively discussed. It is known that in disordered conductors, the electrons can undergo a transition to the insulating state (Anderson localization) with the increasing degree of disorder. The electron diffusion coefficient takes a finite value in the conducting phase and vanishes in the insulating phase, which is revealed by crossing of the Fermi level at a certain energy value called the mobility edge. Localization occurs for a sufficiently strong disorder because of quantum interference effects brought about by randomness of the disorder. At finite temperature, according to the scaling theory of the Anderson transition with interacting electrons [1], the correction to the conductivity in the region $L < L_T$ and $\xi < L_T$ (where L is the sample size, $L_T = \sqrt{D\hbar/T}$ is the interaction length, and D is the diffusion coefficient) is proportional to $\sqrt{T}$. In the region where $\xi \gg L_T > L$, $\sigma \sim T^{1/3}$. Sufficiently far on the insulating side, the conductivity follows the Mott law for a variable range hopping (VRH) conductivity, $\sigma = \sigma_0 e^{-(T_0/T)^{1/4}}$.

Quasicrystals have an extremly high resistivity value with a pronounced negative temperature coefficient and a finite small electronic contribution to the specific heat. In contrast to the conventional disordered conductors, QCs become more insulating with increasing the sample quality and annealing of defects. The quality measure of a QC is the resistivity ratio $\mathcal{R} = \rho(4.2\ \mathrm{K})/\rho(300\ \mathrm{K})$. More perfect samples have higher $\mathcal{R}$, and $\mathcal{R}$ ranges from several units to two hundreds and even higher depending on the object and sample quality.

Empirically, R can therefore serve as a parameter to control the MIT. The highest resistivity of all the known quasicrystals occurs in the icosahedral i-Al-Pd-Re QC, where the value of resistivity at 4.2 K exceeds 1 Om · cm. Recent experiments for i-Al-Pd-Re [2, 3] show that for samples with all different ratios $\mathcal{R}$, a square root temperature dependence of conductivity $\sigma \sim \sqrt{T}$ is ordinarily observed at $T < 20$ K. For samples with $\mathcal{R}$ of the order 20 and higher, this dependence is replaced by the $\sigma \sim T^{1/3}$ law at $T < 5$ K. For samples with high $\mathcal{R}$ (~ 45 and higher), a variable range hopping conductivity obeying the Mott law $\sigma = \sigma_0 \exp(-(T_0/T)^{1/4})$ or even the Efros–Shklowski law $\sigma = \sigma_0 \exp(-(T_0{}'/T)^{1/2})$ is observed. (The same

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temperature dependences of σ were obtained by other authors for samples with slightly different values of $\mathcal{R}$ [4, 5].) We thus see that the obvious analogy exists in the behavior of low-temperature conductivity in perfect QC and in disordered conductors near the MIT, although the reasons for the electron localization in these objects are different. This analogy is also valid at the microscopic level.

In the theory of Anderson localization in disordered conductors, one is interested in the effect of a random potential on quantum-mechanical wave functions (WF). When the randomness is weak, the WFs are extended throughout the entire system (metallic side of the MIT), whereas at sufficiently high disorder, all WFs become localized (insulator side of the MIT). In the vicinity of the critical point of the MIT, the WFs are neither extended nor exponentially decaying; as numerical calculations show, they display a scaling behavior and decrease with the distance following a power law («critical» WFs) [6–8].

Discussions of the problem of localization of electronic states in QCs began immediately after their discovery (see, e.g., [9]). High-resistive QCs are usually attributed to the existence of a deep pseudogap in the density of electronic states (DOS) at the Fermi level (DOS at the Fermi level in QC is low but finite) and to the tendency of the electrons at the Fermi level to be localized. But the presence of a pseudogap is not sufficient to explain the high value of resistivity; its main reasons are seen in the low electron mobility, which is obviously caused by the specific symmetry of QC. From the general standpoint, one can conclude that due to self-invariant structure of QCs, the WFs must be critical. The critical behavior of the wave functions in QCs has been well established in the cases of one- and two-dimensional QCs [10, 11–13]. But for three-dimensional systems (icosahedral quasicrystals), the first publications were controversial [14–16], and even some recent publications contain the claim that in the three-dimensional case, the critical nature of wave functions may be lost to some extent [17, 18]. At the same time, other numerical investigations of the electron spectra of low-order periodic approximants of icosahedral QCs show that most of the WFs are still critical, although the electron spectrum does not contain a hierarchical gap structure typical of the Cantor set of measure zero in one-dimensional QCs [19–21]. Thus, the problem exists and more information on the electron spectra and WFs is required in order to judge about the electron localization in three-dimensional (icosahedral) QCs.

In this paper, we present the results of a numerical investigation of the scaling behavior of the electron spectrum and WFs of the three-dimensional Penrose lattice. The main information needed to characterize the LD transition in QCs is obtained. The inverse participation numbers (the second moments of the density probabilities) and the generalized inverse participation numbers (higher moments) are obtained. Fractal dimensions of the spectrum are obtained and critical behavior of the WFs is studied. The results are important for understanding the electron localization–delocalization transition in icosahedral QCs. This work is a continuation of the previous ones [19, 20], where the singularities of the electron spectrum of icosahedral QCs and the effect of small perturbations on it have been studied using tight-binding and level-statistic methods. In [19], singularities of the electron spectrum were analized, and it was shown that the spectrum is not Cantorian, but contains a singular part. In [20], we studied the influence of chemical disorder and phasons on the electron spectrum by changing on-site energies and transfer integrals.

This paper is organized as follows. In Sec. 2, we consider the main model approximations and calculation technique. In Sec. 3, the results of investigation of the scaling behavior of the electron spectrum are discussed. Section 4 contains conclusions.

2. MODEL APPROXIMATIONS AND CALCULATION TECHNIQUES

The electronic spectrum of the three-dimensional Penrose lattice (the Amman–Kramer network) treated as a structural limit of a sequence of periodic cubic approximants with increasing period has been studied in the framework of the tight-binding approximation (TBA). The first five cubic approximants to the icosahedral QCs (1/1, 2/1, 3/2, 5/3, and 8/5) were investigated. We considered the central decoration of approximants with «atoms» of one type, namely atoms with one s-orbital per atom located at rombohedral centers. The unit cells of these approximants contained 32, 136, 576, 2440, and 10330 atoms respectively. The projection technique for construction of approximants was described previously [19]. To minimize the number of adjustable parameters of the model, we used a Hamiltonian with constant hopping integrals between nearest neighbors (atoms).

The Hamiltonian was expressed as

$$H = \sum_i |i\rangle \varepsilon_i \langle i| + \sum_{i \neq j} |i\rangle t_{ij} \langle j|. \qquad (1)$$

If atoms of only one type are present, the diagonal elements ε_i can be omitted. In this case, the Schrödinger

equation in the tight-binding approximation can be written as

$$\sum_{ij} t_{ij}\Psi_j = E_i\Psi_i, \tag{2}$$

where the transfer integrals are set equal to a nonzero constant $t_{ij} = -1$ only in the case of the nearest-neighbor atoms. The periodic boundary conditions have been used to help reduce the size-dependence effects.

We study the localization problem in the TBA by calculating the inverse participation numbers (moments or $2q$-norms of the wave function) defined by the relation

$$P^{-1} = ||\Psi||_{2q} = \frac{\sum_j |\Psi_j|^{2q}}{(\sum_j |\Psi_j|^2)^q}, \tag{3}$$

from which «participation ratios» and fractal dimensions D_q can be determined. P is called the participation number because it is the measure of the number of sites that contribute to a state of a given energy E_i. The corresponding fraction $p = P/N$ of all the sites is called the participation ratio. The value of p for $q = 2$ is frequently used in the problem of electron localization.

The WFs were classified in accordance with their normalization integrals. They are considered delocalized if

$$\int_{|r|<R} |\Psi(r)|^2 dr \sim R^d,$$

where d is the space dimensionality. They are assumed localized when their finite norms exist, and are defined as «critical», $\Psi \sim r^\alpha$, when they cannot be normalized in an infinite space and are not delocalized. Strongly localized WFs correspond to the case where $\alpha = \infty$ and freely extended wave functions correspond to the case where $\alpha = 0$; Ψ can be normalized in three-dimensional case only for $\alpha \geq 3/2$. For extended states, the moments of the WF depend on the system size as $||\Psi||_{2q}^{extended} \sim N^{1-q}$, as follows from Eq. (3). For exponentially decaying localized functions, we have $||\Psi||_{2q}^{exp.loc} \approx N^0$. We can therefore obtain the exponent of the wave functions by analyzing the system size dependence of the moments calculated in the system of a sufficient size. For the relative number of states with moments $||\Psi||_{2q} \leq N^\gamma$, the integrated distribution function defined as

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

gives the integrated distribution of the exponents of a power-law decay for a specified system if the finite-size correction is negligible. The procedure of finding the exponent α has been described in [19] (also see [13] for two-dimensional Penrose lattice), and we here note that the behavior of the function $\gamma(q, \alpha)$ was analyzed for the first five approximants, and as a result, the «localization» exponent α was found for each approximant under investigation.

From the relation $P_q \sim N^{-D_q(q-1)}$, which is applied near the «critical» point, we obtained the fractal dimensions D_q of the system (here, N is the number of atoms in the unit cell of an approximant).

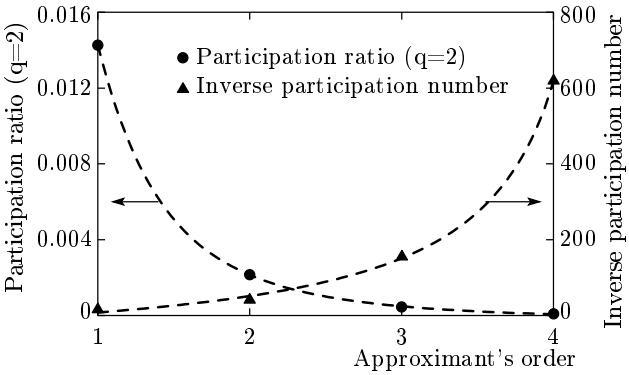

Fig. 1. Inverse participation numbers P^{-1} and the participation ratio ($q = 2$) for the first five rational approximants

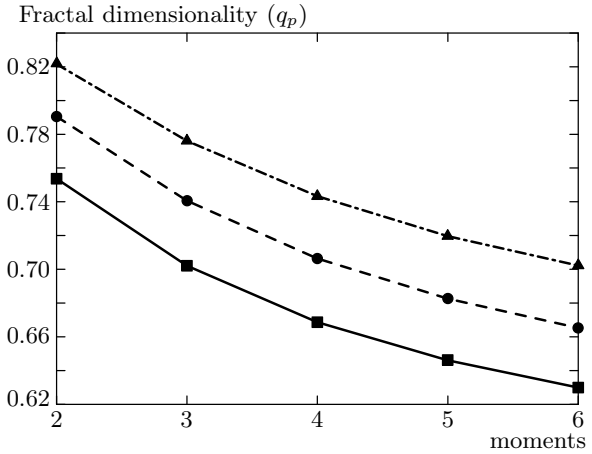

Fig. 2. Fractal dimensionality (q_p) for different moments ($2q$-norms) of the spectrum ($D_{p=0} = 3$ for all approximants)

3. RESULTS AND DISCUSSIONS

The results of calculations are presented in Figs. 1–4. The behavior of the inverse participation numbers,

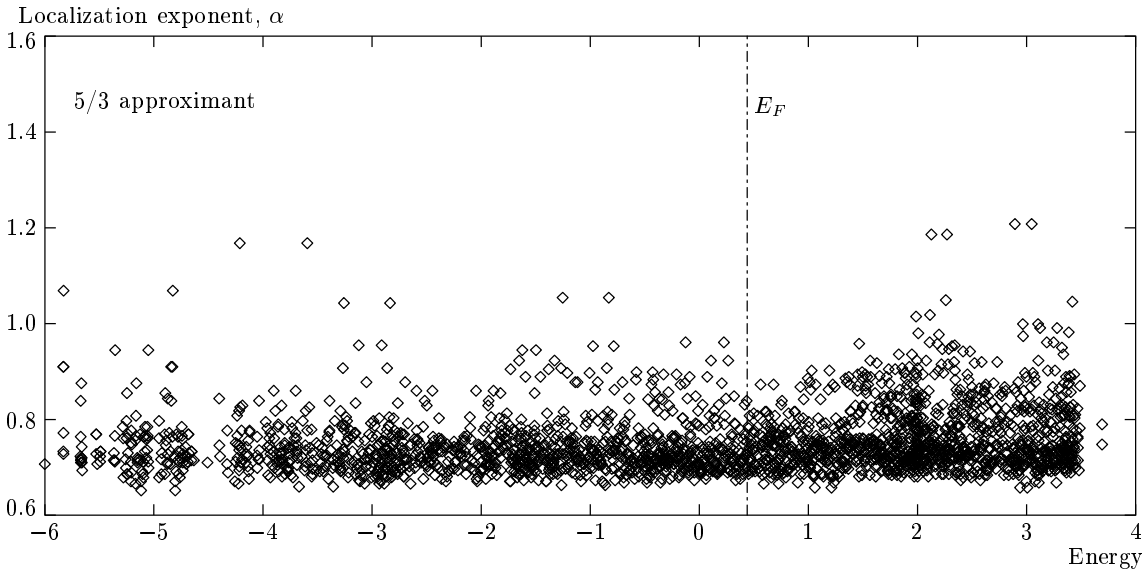

Fig. 3. Distribution of the localization exponent α ($\Psi \sim r^{-\alpha}$) on the energy band. The eigenstates are critical at all energies

participation ratios (Fig. 1), and fractal dimensions (Fig. 2) shows that the electronic states are neither localized nor delocalized in all the considered approximants (the first five approximants were considered). Indeed, the inverse participation numbers P are proportional to N^{γ}, where γ must vanish for localized states because they fit into a sample of a given size, and $\gamma = 1$ for states uniformly extended over the entire sample. Because the calculated value of P does not satisfy both these limits, we can assume that the WF or rather its envelope fall as an inverse power of the distance, $\Psi \sim r^{-\alpha}$. We next see (Fig. 2) that the calculated dimensions D_q of the system satisfy the inequalities $D_0 > D_1 > D_2 > \ldots$, where for all approximants, D_0 is equal to topological dimension (3), and the dimensions are therefore not simple fractal, but multifractal. The multifractality regime means that the system is in the critical state, and the WFs at criticality are multifractal measures leading to the entire spectrum of critical exponents. The spectrum of multifractal dimensions has universal features for states in the vicinity of the MIT. We can therefore conclude that the ground state of the three-dimensional perfect QC is a critical state of the MIT.

The results in Fig. 3 show that the WFs are critical at all energies in the band. The dependence $\Psi \sim r^{-\alpha}$ is typical of the critical state of the system. It is known that systems without characteristic intrinsic length scales obey homogeneity laws under rescaling. The absence of length scales means that some observable F shows a typical homogeneity law $F(sx) = s^k F(x)$, where k is called the homogeneity exponent and s is a real number. This implies that the rescaling of x can be compensated by a rescaling of the observable F. For real-valued functions $F(x)$, the solution of the homogeneity equation is a power-law function $F(x) \sim x^k$. The function $\Psi \sim r^{-\alpha}$ is therefore a solution of the homogeneity equation with the homogeneity exponent $k = \alpha$, and we have a scale-invariant behavior of the system, typical of the critical states. If $F(x)$ is a functional of powers q of those observables that are involved in the definition of $F(x)$ (i.e., moments in our case), $F(x)=F^{[q]}(x)$, then in the simplest situation, $k(q)$ defined by

$$F^{[q]}(sx) = s^{k(q)} F^{[q]}(x)$$

is a linear function of q. If $k(q)$ significantly deviates from linearity, the scaling behavior of $F(x)$ is anomalous, and the system therefore shows the multifractal behavior [22]. Calculations show that the multifractal behavior of the system becomes pronouncedly apparent for higher-order approximants (5/3).

Considering the behavior of the localization exponent α, we see that α tends to a certain value in the thermodynamic limit ($N \to \infty$). It is known from the theory of Anderson transitions that near the transition into the dielectric (metallic) state, the correlation (localization) length ξ tends to infinity. As mentioned above, the Anderson localization theory for interacting electrons implies that $\sigma \propto T^{1/3}$ at the critical point

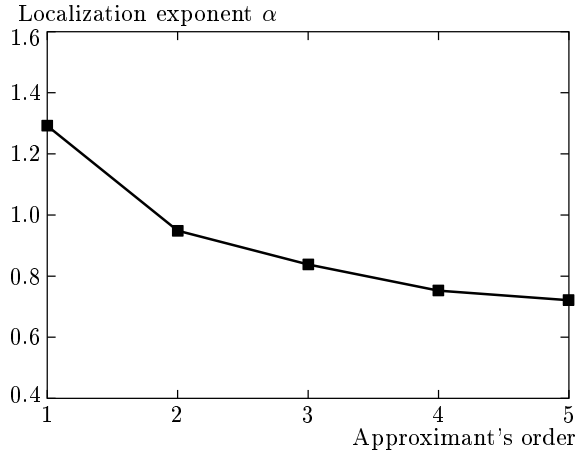

Fig. 4. The localization exponent α (averaged over the band) for different approximants

of the MIT, where $\xi \gg L_T > L$, with $L_T = \sqrt{D\hbar/T}$ being the «interaction» length [3]. For QCs, the conventional picture of the Anderson localization in disordered systems is not relevant. In QCs, the electronic states can be localized by the quasiperiodic potential itself, and as we have shown (Fig. 3), the WFs in the three-dimensional QC behave as in the critical state of the MIT for conventional disordered systems. As shown in [23], it is possible to obtain the $\sigma \propto T^{1/3}$ dependence by considering a variable range hopping conductivity (VRH) on the critical WFs. Following the Mott procedure, we define the tunneling integral on the critical WFs as

$$I \sim |\Psi|^2 \sim |R^{-\alpha}|^2 \equiv \exp(-2\alpha \ln R). \qquad (4)$$

We then define the conductivity

$$\sigma \propto I \exp\left(-\Delta E)/kT\right),$$

where $\Delta E = 3/(4\pi R^3 N(E_F))$ is the minimal activation energy for hopping over the distance R. The expression

$$\exp(-2\alpha \ln R) \exp(-\Delta E/kT) \qquad (5)$$

has a maximum when the exponent $(-2\alpha \ln R - \Delta E/kT)$ has a minimum. Substituting ΔE and finding this minimum, we obtain $\sigma \propto T^{2\alpha/3}$. In order to obtain $\sigma \propto T^{1/3}$, the exponent α must be equal to 0.5. The results of calculations of α (Fig. 4) show that α decreases as the order of the approximant increases. It is difficult to say to what value α tends in the thermodynamic limit, but the tendency is obvious. The results of calculations also show that the value of α depends on the moment number, and the last expression for σ should involve some realization of α. Therefore, the result coincides with the experiment and predictions of the scaling theory of localization for the «critical» region of MIT.

4. CONCLUSION

The result of investigating scaling behavior of the electron spectrum for the first several periodic approximants (1/1, 2/1, 3/2, 5/3, 8/5) of the three-dimensional Penrose lattice with central decoration have been presented. The critical behavior effects are visible even for these low-order approximants. The calculated WFs are «critical» for all energies in the band and are multifractal measures with the entire spectrum of «critical» exponents. The electronic states are more localized at the Fermi level than at the bottom of the band. The results show that the background state of the perfect regular icosahedral QC should be the «critical» state of the localization–delocalization transition. The nature of electron localization in icosahedral quasicrystals has been discussed previously [9, 19, 20], and it was shown that this localization is unstable under small perturbations (phasons, chemical disorder, and the magnetic fields). The «critical» behavior of the WFs can explain the experimentally observed power-law dependence of conductivity, $\sigma \propto T^{1/3}$. Calculating the VRH probability on «critical» WFs, we immediately obtain the $\sigma \propto T^{2\alpha/3}$ law. For coincidence with the experiment, the realization of the exponent α should be equal to 0.5 in the thermodynamic limit. At the same time, it is impossible to obtain the Mott law on «critical» WFs for the VRH conductivity on insulating side of the MIT, and new ideas are necessary.

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