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# Electronic transport in quasicrystals: An approach to scattering with fractional multicomponent Fermi surfaces

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The model for electronic transport in quasicrystals is proposed. Unlike all previous attempts to explain unusual electronic properties of quasicrystals by impending localization due to the lack of periodicity in defectless quasiperiodic lattices, the current theory is focused on phonon and impurity scattering in real, ''dirty'' quasicrystals. The standard scattering theory cannot be applied to quasicrystals, due to their unusual band structure, namely the fact that the Fermi surface is nearly obliterated. To solve the problem a fractional multicomponent Fermi-surface model has been introduced: the Fermi surface has been viewed as consisting of relatively large number of residual tiny electron and hole pockets, with impurity random potential scattering electrons between different components. Leaving quasiperiodicity aside, the Dyson equations for the scattering time, dc conductivity and thermopower have been solved analytically. The theory explains the nearly vanishing conductivity, as well as strong temperature dependence of thermopower and related transport properties.

## I. INTRODUCTION

The electronic transport in quasicrystals is one of the puzzling problems of the modern condensed-matter physics and attracts a close attention of both theoreticians and experimentalists (for an extensive review see Ref. 1). The fractal nature of Fermi surface and interplay between localization and delocalization of electronic states proposed by several authors,[2–4] the extremely short mean free path of the electron scattering, low carrier concentration and density of states at the Fermi level, and strong structural and phase disorder lead to the variety of speculations concerning the transport properties. Among them are semimetallic or semiconductor behavior, analogies with metallic glasses, approaching the metal-insulator transition.[1] However, since the electronic properties of quasicrystals exhibit still the metallic character (although with the features mentioned above), any model of electronic transport should be based on a model of the metal-like electron spectrum with well-defined Fermi surface. The main problem arising here is the effect of quasiperiodicity on the Fermi-liquid parameters. In the present paper we propose a simple model of electronic structure which accounts for transport properties largely consistent with those observed experimentally.

So far, there have been two rival theories of electronic properties in quasicrystals. One approach is focused on the effects of quasiperiodicity, namely the failure of Bloch theorem in the absence of periodicity and possible localization.[2–5] The other, called band-structure hypothesis,[6,7,1,8] leaves localization aside but exploits high symmetry of quasicrystals that allows for an extremely tight matching of the Fermi surface with the Brillouin-zone boundary. By placing the Fermi surface at the band gap the cohesion energy is lowered thus improving stability of the alloy, the effect analogous to Peirles mechanism responsible for the formation of charge-density waves. In other words, the band-structure hypothesis views quasicrystals as the most rectified Hume-Rothery alloys. In the course of this paper we will adopt the band-structure hypothesis, without arguing whether or not it is a valid approach.

The band-structure hypothesis assumes that although, technically, the reciprocal space is everywhere densely filled with the Bragg planes only a few, associated with the few strongest Fourier components of the pseudopotential, should be taken into consideration, at least in the first approximation. Because of the high multiplicity of the Bragg planes resulting from high symmetry of quasicrystals the quasi-Brillouin-zone boundary would have some 40 or even 90-something facets, even when only two or three largest terms in the Fourier series for the pseudopotential are taken into account. The exact number of the facets as long their shape and size vary from one particular quasicrytalline alloy to another, but one thing remains in common: the quasi-Brillouin-zone boundary is a very good approximation of a sphere, somewhat resembling a soccer ball (for particular shapes, see Poon's review[1]).

In the simplest Harrison approach to the construction of the Fermi surface this first approximation quasi-Brillouin-zone boundary overlaps the Harrison sphere. As a result, most of the Fermi surface is obliterated, leaving only tiny electron and hole pockets at the face centers and corners, respectively. The number of these pockets, being denoted below as $N$, is merely the number of facets plus the number of corners of the quasi-Brillouin-zone boundary, and varies from 42 to 96 for most known icosahedral quasicrystals. The size and shape of the pockets are determined not only by the reciprocal-space geometry, but also by the strength of the pseudopotential and the position of the Harrison sphere regarding the quasi-Brillouin-zone boundary. The latter, in turn, changes when the alloy composition is varied, resulting in experimentally observed strong dependence of electronic properties on composition. The aim of this article is not to calculate the transport properties of all 200 or so known icosahedral quasicrystalline alloys, but rather provide a general tool. Accordingly, we will consider a model Fermi surface consisting of $N$ components (some of whom are electron- and some holelike in character), each component being a tiny sphere of radius $k_F^{(i)}$. It is worth keeping in mind that for a given quasicrystalline alloy $k_F^{(i)}$ could change with the composition and could even turn zero. Technically, there might exist quasicrystalline alloys where all the $k_F^{(i)}$ turn zero simultaneously, thus making the quasicrystal a multivalley semiconductor. There are experimental indications that such quasicrystals do exist.[9] In this paper we will focus on quasicrystals that are still on the metallic side of the metal-semiconductor transition, though very close to the transition point.

The subsequent Harrison approximations lead to the subsequent splitting of these pockets into smaller ones and so on. Because of icosahedrical symmetry and quasiperiodicity of the lattice this splitting procedure continues indefinitely. As a result the volume of quasi-Brillouin zone as well as the size of each pocket tend to zero, while the number of pockets goes to infinity. In the limit the fractal structure appears and the notion of the density of states in the rigorous understanding loses its sense. This situation takes place in an ideal quasicrystal, namely with no electron scattering processes and at zero temperature. In real quasicrystal one has to take into account smearing of the electron states in momentum space. Since the energy of quasiparticle is defined with in accuracy of its uncertainity $\delta\epsilon\sim\max\{T,\tau^{-1}\}$ ($T$ is temperature, $\tau$ is the electron relaxation time), the splitting of Fermi surface within Harrison procedure makes sense as long as the characteristic size of pockets is greater that $\delta\epsilon$. As a result, we argue, that electronic structure of a quasicrystal can be modeled by a set of electron and hole pockets (or valleys) with the characteristic size of order of $\delta\epsilon$. Within this model both the number of valleys $N$ and the stage at which the Harrison procedure should be stopped are defined by either temperature or inverse electronic relaxation time. The symmetry of such multipocket electronic structure reflects the quasicrystal symmetry, but it is unimportant for transport properties which are integral characteristics.

In this paper we show that the electronic structure determines the main features of transport in quasicrystals. In the model of the many-valley Fermi surface, two kinds of electronic elementary scattering processes are possible. The first kind is the intravalley process which begins and ends in the same valley. The second kind are intervalley processes during which electron is scattered from one valley to another. We find that due to different momentum transfer involved in intra- and intervalley scattering, different types of conductivity are realized. Namely, intravalley processes result in a nonmetallic character of conductivity reminiscent of one observed in the vicinity of metal-insulator transition, while intervalley scattering can be described within the Drude model. Notice, that the importance of both elastic and inelastic scattering for intervalley transitions between tiny electron and hole pockets was mentioned in Ref. 10 in the context of first-principals calculations of electronic properties of model quasicrystals.

The paper is organized as follows. In Sec. II, we examine the electron relaxation time in quasicrystal and discuss different scattering mechanisms. In Sec. III, we consider the nature of electrical conductivity, within our model. In Sec. IV, we evaluate thermopower in a quasicrystal taking into account both electron-impurity and electron-phonon scattering processes. Finally, in Sec. V, we summarize and discuss our results comparing them with the experimental data. We use units whereby $\hbar=k_B=c=1$.

## II. RELAXATION TIMES IN QUASICRYSTALS

In our model of the many-pocket Fermi surface, we consider the set of $N$ electron and hole pockets distributed within the Brillouin zone. At zero temperature the finite relaxation time is solely due to structural or chemical disorder while with temperature increase the scattering on the quasilattice vibrations contributes to the electron relaxation. Introduce the effective chemical potential in each pocket:

$$\mu_i=\frac{k_F^{(i)2}}{2m}, \tag{1}$$

where $i=1...N$ is the pocket number, $k_F^{(i)}$ is the radius of a corresponding pocket and $m$ is the effective mass of a charge carrier. Since the distance between the pockets in the momentum space is of the order of reciprocal Angstrom and the pockets are rather small, we may assume that the distance between the pockets is much greater than pocket radii as well as the broadening of Fermi surface due to both temperature and scattering.

First, consider the scattering of electron on structural imperfections. One can define the electron Green function as a $N\times N$ matrix:

$$G_{ij}(\mathbf{r},\mathbf{r}',t,t')=-\langle T(\psi_i(\mathbf{r},t)\psi_j^\dagger(\mathbf{r}',t'))\rangle, \tag{2}$$

where $\psi_i$ and $\psi_j^\dagger$ are electron field operators for the $i$th and $j$th valleys. In the absence of scattering the $\hat{\mathbf{G}}$ matrix is diagonal with

$$G_{ii}^{(0)}(\mathbf{k},\omega_n)=\frac{1}{i\omega_n+\mu_i-(k^2/2m)}. \tag{3}$$

Scattering of electrons by structural imperfections results in both the renormalization of diagonal elements and the appearance of nonzero nondiagonal elements of the $\hat{\mathbf{G}}$ matrix.[11] We consider the scattering to be isotropic and the corresponding amplitude $\hat{\mathbf{U}}$ (which also is presented by $N\times N$ matrix) to be independent of the transfer momentum. Under these assumptions, the amplitudes of electron scattering between different valleys are the same, so $\hat{\mathbf{U}}=U_0\hat{\mathbf{K}}$, where $U_0$ is the amplitude for Born scattering of electron by impurity center and $K_{ij}=1$ for all $i$ and $j$.

For the Green function averaged over the configuration of scattering centers we can write down the matrix Dyson equation:

$$\hat{\mathbf{G}}^{-1}=[\hat{\mathbf{G}}^{(0)}]^{-1}-\hat{\mathbf{\Sigma}} \tag{4}$$

with $\hat{\mathbf{\Sigma}}$ being the matrix self-energy. The matrix equation for the self-energy is

$$\hat{\mathbf{\Sigma}}(\mathbf{k},\omega)=n_{\mathrm{imp}}\int\frac{d^3k'}{(2\pi)^3}\hat{\mathbf{U}}(\mathbf{k},\mathbf{k}')\hat{\mathbf{G}}(\mathbf{k}',\omega)\hat{\mathbf{U}}(\mathbf{k}',\mathbf{k}). \tag{5}$$

Here $n_{\mathrm{imp}}$ is the concentration of scattering centers. Substituting Eq. (4) in Eq. (5) after straightforward algebra one obtains that $\hat{\mathbf{\Sigma}}$ has the same matrix structure as $\hat{\mathbf{U}}$: $\hat{\mathbf{\Sigma}}=\Sigma_0\hat{\mathbf{K}}$. In evaluating $\Sigma_0$ we take into account that the ratios $G_{ii}^{(0)}/G_{jj}^{(0)}$ for $i\neq j$ are of order $T/\mu$ and could be neglected. Finally, we obtain

$$\begin{aligned}\Sigma_0=&\sum_{i=1}^{N}n_{\mathrm{imp}}|U_0|^2\\&\times\int\frac{d^3k}{(2\pi)^3}\frac{1}{G_{ii}^{(0)-1}-\Sigma_0(1-\Sigma_{j\neq i}(G_{jj}^{(0)}/G_{ii}^{(0)}))},\\\simeq&\sum_{i=1}^{N}n_{\mathrm{imp}}|U_0|^2\int\frac{d^3k}{(2\pi)^3}\frac{1}{i\omega_n+\mu_i-k^2/2m-\Sigma_0}.\end{aligned} \tag{6}$$

The electron relaxation time is conditioned by the imaginary part of the self-energy. Integrating over $\mathbf{k}$ we obtain an analytic solution for the Dyson equation, in a form of a simple algebraic equation for the imaginary part:

$$\mathrm{Im}\Sigma_0=-\frac{\pi}{2^{3/2}m^{3/2}n_{\mathrm{imp}}|U_0|^2}\sum_{i=1}^{N}\frac{\mathrm{Re}\sqrt{\mu_i+\omega-i\mathrm{Im}\Sigma_0}}{\mu_i}. \tag{7}$$

If all valleys had the same size: $\mu_i=\mu_0$ for all $i$, the solution further simplifies:

$$\frac{1}{\tau(\omega)}=\frac{N}{\tau_0}\left[1+\frac{\omega}{\mu_0}+\left(\frac{N}{4\mu_0\tau_0}\right)^2\right]^{1/2}. \tag{8}$$

In the last equation we introduced time $\tau_0^{-1}=n_{\mathrm{imp}}|U_0|^2m^{3/2}(2\mu_0)^{1/2}/\pi=n_{\mathrm{imp}}|U_0|^2\nu(\mu_0)/2\pi$, where $\nu(\mu_0)$ is the density of states at the Fermi level. If the metal had only one tiny valley $\tau_0$ would be its relaxation time.

For most quasicrystals one should not expect too close a proximity to the metal-semiconductor transition, i.e., though $\mu_0$ is much smaller than in most normal metals it is still far from being vanishingly small. In that case, Eq. (8) becomes simply

$$\tau=\frac{\tau_0}{N}, \tag{9}$$

where time $\tau_0$ refers to intravalley scattering. The effective time given by Eqs. (8,9) governs the electronic transport at low temperatures, i.e., in the region of residual resistivity.

As temperature increases, the number of electrons scattered by quasilattice vibrations increases with the corresponding reduction in total relaxation time. Below we study the effect of phonon scattering on the electron relaxation time. For simplicity we present only the semiquantitative consideration assuming the validity of the Mattisen rule, which implies that the total relaxation rate is a sum of the relaxation rates due to different contributing scattering mechanisms. In doing so, we will avoid a narrow temperature interval where the interference of electron-impurity and electron-phonon interactions occurs.

The difference between scattering by impurities and phonons lies in the fact that electron-phonon interaction is able to change the electron momentum only by a small amount, of the order of $T/u$, where $u$ is the velocity of sound, while scattering on the structural disorder provides the transfer momentum of the order of the reciprocal Angstrom. Note, that the momentum transfer that large is necessary for intervalley scattering. In this manner there exists a characteristic temperature: $T^*\sim u/a$ ($a$ is the average interatomic distance) below which the phonons are unable to scatter electrons from one pocket to another, thus permitting only intravalley processes. Accordingly, for temperatures $T<T^*$ the effective relaxation time is given by

$$\frac{1}{\tau_{\mathrm{tot}}}=\frac{N}{\tau_0}+\frac{1}{\tau_{\mathrm{ph}}(T)}, \tag{10}$$

with $\tau_{\mathrm{ph}}(T)$ being the electron relaxation time due to electron-phonon scattering. We believe that in this temperature range the total electron relaxation is dominated by scattering on impurities even in pure samples, due to large value of $N$. On the other hand, if the temperature exceeds $T^*$ the scattering by phonons provides the effective intervalley electron processes with the essential shortening of electron-phonon time. As a result, for $T>T^*$ we have

$$\frac{1}{\tau_{\mathrm{tot}}}=\frac{N}{\tau_0}+\frac{N}{\tau_{\mathrm{ph}}(T)}. \tag{11}$$

It is important that at $T\sim T^*$ the sharp decrease of the electron-phonon scattering time should be observed with the corresponding change in the character of conductivity. The interplay between impurity and phonon scattering mechanisms is governed by the purity of a sample. In sufficiently clean samples electron-phonon scattering would dominate over impurity scattering in the entire temperature range above $T^*$.

## III. MECHANISMS OF ELECTRICAL CONDUCTIVITY

A successful model of electronic transport in quasicrystals should be able to find a reasonable explanation for the main features in the conductive properties of these materials. The distinctive transport features of quasicrystals are (1) The extremely low values of electrical conductivity at zero temperature; (2) the increase of conductivity with temperature; and (3) unusually strong thermopower temperature dependence sometimes leading to a sign change. In the beginning of this section we present the quantitative analisys of the mechanisms of electrical conductivity based on the model introduced above and then perform some calculations. As it was mentioned above one has to distinguish between the transport properties associated with the intravalley and intervalley processes whose competition results in a number of interesting issues.

Consider the case of icosahedral phase with weak structural disorder at low temperature thus ignoring scattering by phonons. To understand the character of electrical conductivity one has to consider the parameter $k_F^{(0)}l \sim \mu_0 \tau$ in comparison with unity ($l$ is the electron mean free path). The value of this parameter governs whether the conductivity has metallic or nonmetallic character. One has

$$k_F^{(0)}l \sim \frac{k_F^{(0)}}{m^2 n_{\mathrm{imp}} |U_0|^2}. \tag{12}$$

It is seen from this estimation, which because of the fractional nature of the Fermi surface $k_F^{(0)}$ could be extremely small, that implies $k_F^{(0)}l \leqslant 1$, at least in the case of not too low concentration of scattering centers. The case of the highly ordered phase with the very weak structural disorder ($\tau_0 \rightarrow \infty$, $n_{\mathrm{imp}} \rightarrow 0$) requires a more detailed consideration. At a first glance, in this limit the parameter (12) rises and the condition of localization $\mu_0 \tau \sim 1$ is no longer valid. Closer examinations, however, shows that, as was mentioned earlier, the size of the pocket is defined by the uncertainity of the electron energy, that is $\tau^{-1}$ at zero temperature. It means that the condition of strong localization is fulfilled independently upon the disorder strength. This leads to the nonmetallic (localization) regime of conductivity conditioned by intravalley scattering even in the case of weak disorder. Let us note, that the physical reason for this phenomenon is the small momentum transfer $k_F^{(0)}$ involved in intravalley processes.

Now we turn to intervalley processes. Here the momentum transfer $\Delta k$ is of order of $a^{-1}$, where $a$ is the average interatomic distance. In this case $\Delta k l \gg 1$. Turning on intervalley scattering processes eliminates the localization situation and provides for the metallic character of conductivity. At zero temperature, the nonzero contribution to conductivity appears as a result of intervalley processes only while the intravalley contribution is zero. The detailed theory which allows us to evaluate the intervalley conductivity within Kubo formalism is given in the Appendix. To estimate the residual conductivity one can use the Drude model with the effective relaxation time in the form of Eq. (9):

$$\sigma(T=0) = \sum_{i=1}^{N} \sigma_i \sim N e^2 v_F^{(0)2} \nu \frac{\tau_0}{N} \sim \frac{e^2 v_F^{(0)2}}{n_{\mathrm{imp}} |U_0|^2}. \tag{13}$$

The magnitude of conductivity is extremely small due to its proportionality to $v_F^{(0)2}$. It is worth discussing the variation of $\sigma(T=0)$ with changing the strength of structural disorder. If the disorder is negligible conductivity tends to zero, because neither intervalley nor intravalley processes are possible. With the rise of $n_{\mathrm{imp}}$, the nonzero $\sigma(T=0)$ appears, those magnitude could be calculated through Eq. (13). Thus, residual conductivity should rise with the structural and phase disorder, as it is seen in experiments. The reason for this effect is the possibility for electron to be scattered from one valley to another with the large momentum transfer of order of $a^{-1}$. In this context Eq. (13) should be considered only at a fixed strength of disorder (at given $n_{\mathrm{imp}}$), because $v_F^{(0)}$ in Eq. (13) is ruled by $n_{\mathrm{imp}}$. To gain greater insight into why the above statement is valid, we write at zero temperature: $m v_F^{(0)2} \sim \delta\epsilon \sim \tau^{-1} \sim N/\tau_0$, which implies $v_F^{(0)} \sim N m n_{\mathrm{imp}} |U_0|^2$. Substituting this estimate in Eq. (13) one gets

$$\sigma(T=0) \sim e^2 N^2 m^2 n_{\mathrm{imp}} |U_0|^2, \tag{14}$$

what describes the variation of residual conductivity with the disorder strength.

Now let us discuss the nonzero, but still low temperatures. In this case the intervalley scattering contribution is given by the same temperature-independent Eq. (13). Intravalley processes, however, will contribute to conductivity in the same manner as temperature-dependent conductivity in the vicinity of metal-insulator transition. It is well established,[12] that near metal-insulator transition conductivity goes to zero according with $T^{1/2}$ law. Considering this contribution as a small correction to temperature-independent conductivity from intervalley processes, at low temperatures, we can write

$$\sigma(T) = \sigma(0) + \alpha\sqrt{T}, \tag{15}$$

with $\alpha$ being the temperature-independent factor. When the temperature further increases, the electron relaxation time will decrease due to scattering by phonons according to Eqs. (10) and (11). In this temperature range the contribution from intervalley processes begins to depend upon temperature, and total conductivity will be dominated by this contribution. In this case Eq. (13) can be rewritten as

$$\sigma(T) \sim N e^2 \sqrt{\frac{m}{\tau_{\mathrm{tot}}(T)}}, \tag{16}$$

where we have again used the relation $m v_F^{(0)2} \sim \tau_{\mathrm{tot}}^{-1}$ assuminq $\tau_{\mathrm{tot}}^{-1} > T$. It is seen that conductivity increases with the rise of temperature due to scattering by quasilattice vibrations. Note that then temperature exceeds $\tau_{\mathrm{tot}}^{-1}$ the $v_F^{(0)}$ in Eq. (13) will be defined as $m v_F^{(0)2} \sim T$. The intervalley contribution to conductivity in this case is $\sigma(T) \sim N e^2 m^{1/2} T^{3/2} \tau_{\mathrm{tot}}(T)$.

The phonon-induced crossover in relaxation time at temperature $T^*$ results in the corresponding changes in conductivity behavior. Note, that unlike ordinary metallic systems, in quasicrystals this phonon crossover temperature is less than Debye temperature.

## IV. FEATURES IN THERMOPOWER

The thermoelectric coefficient $\beta(T)$ of a quasicrystal can be calculated by analogy with Eq. (13). In this consideration we restrict ourselves for the case of not too low temperature, where the thermoelectric coefficient quickly tends to zero. So, we consider only intervalley scattering:

$$\beta = \sum_{i=1}^{N} \beta_i, \quad \beta_i = -\frac{1}{9}\pi^2 e T \frac{d}{d\mu_i}\left( v_i^{(0)2} \nu(\mu_i) \frac{\tau_0}{N} \right). \tag{17}$$

A simple estimate shows that

$$\beta \sim -e T k_F^{(0)} \tau_0, \quad S = -\frac{\beta}{\sigma} \sim \frac{T}{e\mu_0}, \tag{18}$$

where $S(T)$ is thermopower (or Seebeck coefficient). With $\mu_0$ much smaller than the typical value of Fermi energies in metals, one concludes that diffusion thermopower in quasicrystals is much larger than in ordinary metals. Apart from the large absolute value of diffusion thermopower, the possible sign change with the temperature is also the characteristic feature of quasicrystals. Note, that similar behavior was observed in a number of metallic systems like metallic glasses, Chevrel phases, and high-temperature superconducting cuprates.[13,14] Usually the thermopower sign change is attributed to the phonon processes (like phonon drag or electron-phonon-impurity interference) which can account for the contributions opposite in sign to the diffusion thermopower.[15] These phonon contributions dominate diffusion thermopower at temperatures $T \ll \Theta$ ($\Theta$ is Debye temperature), but are substantially reduced at $T \geqslant \Theta$ due to phonon-phonon scattering, leaving the diffusion component as the leading contribution. To take into account the influence of electron-phonon interaction on thermopower one has to replace in Eq. (18) $\tau_0$ by $\tau_{\mathrm{tot}}$ given by Eqs. (10) and (11). As the drag effect is concerned, it will affect thermopower at the temperature range between $\Theta^2/\mu_0$ and $\Theta$. In this case,

$$\beta \sim -e\left(\frac{T}{\Theta}\right)^2 \mu_0 k_F^{(0)} \tau_{\mathrm{tot}}, \quad S \sim -\frac{T^2}{e\Theta^2}. \tag{19}$$

Equations (18) and (19) together with Eqs. (10) and (11) provide a quite complex temperature dependence of thermopower in the entire temperature range below $\Theta$. It is important to mention that the phonon-drag contribution can be of any sign depending on whether normal or Umklapp processes dominate.[15] Another interesting feature of the thermopower in the model of fractional Fermi surface is the low value of degeneration temperature of electron gas. Indeed, electron gas could be considered a Fermi gas if the temperature is less than $T_{\mathrm{deg}}$, which is of order of magnitude $\mu_0$ and in result can reach a hundred of Kelvins. It means that at $T > T_{\mathrm{deg}}$ one has to consider electron gas as a Boltzmann gas. In this case thermopower is nearly temperature independent and rather large in magnitude: $S \sim 1/e$.[16] This effect also results in an unusually large absolute value of thermopower at high temperatures. The situation is complicated by the existence of two kinds of charge carriers. If the degeneration temperatures for electrons and holes differ, it is easy to imagine that at some temperature between $T_{\mathrm{deg}}^{(e)}$ and $T_{\mathrm{deg}}^{(h)}$ thermopower would change a sign.

## V. DISCUSSION

Comparing our theory with experiment, it is important to keep two things in mind. Firstly, the existing experimental data are quite controversial, and, secondly, our model is of rather general character, so, it is able to describe only common features of quasicrystals distinctive from properties of usual metallic systems. Thus when discussing experimental data the main problem is to reveal the properties unique to quasicrystals.

Initial experimental studies of electron transport in the icosahedral phase indicated metalliclike behavior with large residual resistivities (of order $100 \mu\Omega$ cm), with the monotonic decrease of resistivity with temperature increasing up to room temperature.[1] Together with the strong temperature dependences of thermopower and Hall coefficient, these observations were reminiscent of metallic-glass behavior.[13] However, further studies of Al-Cu-Fe(Ru) compounds that form stable, nearly defect-free icosahedral phases, showed enormally large resistivity up to $0.1\Omega$ cm (Ref. 17) and even $1\Omega$ cm in system Al-Pd-Re,[18] which increases with increasing strength of structural order. It is quite obvious that these phases cannot be considered by analogy with metallic glasses where structural disorder is the intrinsic property. Behavior of resistivity of highly ordered icosahedrical phases seems to be the inherent feature of these materials.

Different theoretical models have been proposed to account for an unusual electron transport in quasicrystals but all of them considered ideal, defectless quasicrystals with the exception of Ref. 5, which treated the structural disorder in quasicrystals in terms of random phasons. As we pointed out before, in the defectless case the Fermi surface has an infinite number of zero-area pockets. Moreover, because of the special type of order, the electron wave functions cannot be presented in the Bloch form. As a result, these theories[19,20] predict either zero or infinite conductivity at zero temperature. Our model, developed for real, dirty quasicrystals, provides the natural explanation for a low value of conductivity. The reason is the smearing of electronic states by both temperature and scattering which result in the existence of a Fermi surface with a finite number of valleys whose number depends on the strength of disorder. Because the characteristic size of a valley is conditioned by the uncertainity of electron energy, the localization of electronic states occurs in the limit of ordered (defectless) phase resulting in zero conductivity at zero temperature. The deviation from ordering leads to a possibility of intervalley scattering which provides the nonzero, but small value of zero-temperature conductivity.

Apart from conductivity, the thermopower of quasicrystals exhibits enormously large absolute magnitude, which also can be considered as a unique property. Even ignoring possible phonon contributions, the large magnitude of diffusion thermopower has also found explanation within our model due to two possible factors: the small size of the valleys and extremely low degeneration temperature. It is also easy to understand the experimentally observed[1,21] reducing of density of states at the Fermi level with respect to the ordinary metals, which is proportional to the Fermi momentum. The model of fractional Fermi surface also provides the dependence of electronic properties upon the strength of disorder, because the effective Fermi energy is governed by the inverse electron relaxation time.

It is interesting to compare the results of the present paper with first-principals calculations of the band structures[22] and transport properties in a crystalline approximant based on the two-dimensional Penrose lattice.[10] Reference 10 treated the random phasons as centers of elastic scattering providing small value of conductivity at zero temperature. Contrary to this theory, our model exploits only very common features of quasicrystals, but describes three-dimensional systems at finite temperature. Although two-dimensional calculations of Ref. 10 cannot be directly applied to realistic three-dimensional icosahedral phases, both theories demonstrate the remarkable agreement which concerns the effect of randomness on the transport properties of quasicrystalline phases. We notice that although calculations of band structures in the realistic model structures of quasicrystals produce electron and hole pockets not only at the Brillouin-zone surface, but at many other points in the Brillouin zone,[10] it does not essentially affect our model. Really, the only assumption neccessary for the model validity is the separation of pockets in the momentum space on the distances comparable with the $p_F$ or even $p_F/N^{\alpha}$ where $\alpha$ is between 1/2 and 1/3 depending on the surface or volume distribution of the pockets.

In summary, we have proposed a model of multiple-valley fractional Fermi surface for electronic structure of quasicrystals which provides a natural explanation for a number of physical properties of these materials. The Dyson equations for the electron Green function and a couple of vertices have been solved analytically. The interplay between intravalley and intervalley scattering processes in combination with the suggestion about the localization regime in each valley accounts for a small value, of zero-temperature electrical conductivity and square-root temperature dependence at low temperatures, large absolute value, and strong temperature dependence of thermopower. The developed formalism could be used for a detailed calculation of transport properties of particular quasicrystalline alloys.

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## APPENDIX

For rigorous evaluation of kinetic coefficients we have to know not only diaganol but all elements of the matrix $\hat{\mathbf{G}}$. The Dyson equation is

$$\hat{\mathbf{G}}=(\hat{\mathbf{G}}^{(0)^{-1}}-\Sigma_0\hat{\mathbf{K}})^{-1}. \tag{A1}$$

Here $\Sigma_0=-i/2\tau(\omega)$ with $\tau(\omega)$ given by Eq. (8) Taking into account the following property of the $\hat{\mathbf{K}}$ matrix: $\hat{\mathbf{K}}\hat{\mathbf{A}}\hat{\mathbf{K}}=\hat{\mathbf{K}}\Sigma_{i,j}^{N}A_{ij}$, where $\hat{\mathbf{A}}$ is any $N\times N$ matrix, we have

$$\begin{aligned}\hat{\mathbf{G}}=\hat{\mathbf{G}}^{(0)}+\Sigma_0&\left[1+\Sigma_0\sum_{i,j}^{N}G_{ij}^{(0)}+\left(\Sigma_0\sum_{i,j}^{N}G_{ij}^{(0)}\right)^2+\cdots\right]\\&\times\hat{\mathbf{G}}^{(0)}\hat{\mathbf{K}}\hat{\mathbf{G}}^{(0)}\\=\hat{\mathbf{G}}^{(0)}&+\frac{\Sigma_0}{1-\Sigma_0\Sigma_{i,j}^{N}G_{ij}^{(0)}}\hat{\mathbf{G}}^{(0)}\hat{\mathbf{K}}\hat{\mathbf{G}}^{(0)}.\end{aligned} \tag{A2}$$

Finally, we use the fact that $\hat{\mathbf{G}}^{(0)}$ has only diagonal elements: $G_{ij}^{(0)}=G_{ii}^{(0)}\delta_{ij}$ ($\hat{\delta}$ is a unity matrix). As a result, components of the $\hat{\mathbf{G}}$ matrix become

$$G_{ij}=G_{ii}^{(0)}\delta_{ij}+\frac{\Sigma_0}{1-\Sigma_0 Sp\hat{\mathbf{G}}^{(0)}}G_{ii}^{(0)}G_{jj}^{(0)}. \tag{A3}$$

[Note that there is no summation over the repeating indexes in Eq. (A3).]

Now we turn to evaluation of electrical conductivity and thermoelectric coefficient. Within Kubo formalism, kinetic coefficients can be calculated in terms of correlators which refer to fermion loops with the corresponding vector vertices.[11] Namely

$$\begin{aligned}\begin{bmatrix}\sigma_{\alpha\beta}\\ \beta_{\alpha\beta}\end{bmatrix}=\lim_{\Omega\to 0}\frac{1}{-i\Omega}\sum_{\omega_n}\int\frac{d^3k}{(2\pi)^3}Sp\Bigg\{&\hat{\mathbf{\Gamma}}_{\alpha}^{(E)}\hat{\mathbf{G}}(\omega_n+\Omega_k,\mathbf{k})\\&\times\begin{bmatrix}\hat{\mathbf{\Gamma}}_{\beta}^{(E)}\\ \hat{\mathbf{\Gamma}}_{\beta}^{(H)}\end{bmatrix}\hat{\mathbf{G}}(\omega_n,\mathbf{k})\Bigg\}.\end{aligned} \tag{A4}$$

Here $\hat{\mathbf{\Gamma}}_{\alpha}^{(E)}$ and $\hat{\mathbf{\Gamma}}_{\alpha}^{(H)}$ are the vertices associated with the electric and heat current operators, respectively, averaged upon the configuration of scattering centers. Without scattering the corresponding vertices would be $\hat{\gamma}_{\alpha}^{(E)}=ev_{\alpha}\hat{\delta}$, $\hat{\gamma}_{\alpha}^{(H)}=-i\omega_n v_{\alpha}\hat{\delta}$, where $\mathbf{v}$ is the electron velocity (we again consider the model of uniform valleys). The renormalized vertex obeys the equation

$$\hat{\mathbf{\Gamma}}=\hat{\boldsymbol{\gamma}}+n_{\text{imp}}\int\frac{d^3k'}{(2\pi)^3}\hat{\mathbf{U}}(\mathbf{k},\mathbf{k}')\hat{\mathbf{G}}(\mathbf{k}',\omega)\hat{\mathbf{\Gamma}}\hat{\mathbf{G}}(\mathbf{k}',\omega)\hat{\mathbf{U}}(\mathbf{k}',\mathbf{k}). \tag{A5}$$

Straightforward calculations show that renormalization correction to the bare vertex is proportional to the integral containing matrix $\hat{\mathbf{v}}$, which is zero as a result of averaging over angles of vector $\mathbf{k}$. Finally renormalization of the vector vertex $\hat{\boldsymbol{\gamma}}$ is absent as in the case of isotropic metal with a one-valley Fermi surface. Under these conditions Eq. (A4) reduces to

$$\begin{aligned}\begin{bmatrix}\sigma_{\alpha\beta}\\ \beta_{\alpha\beta}\end{bmatrix}=\lim_{\Omega\to 0}\frac{e}{-i\Omega}\sum_{\omega_n}&\begin{bmatrix}e\\ -i\omega_n\end{bmatrix}\\&\times\int\frac{d^3k}{(2\pi)^3}v_{\alpha}v_{\beta}Sp\{\hat{\mathbf{G}}(\omega_n+\Omega_k,\mathbf{k})\hat{\mathbf{G}}(\omega_n,\mathbf{k})\}.\end{aligned} \tag{A6}$$

Then we evaluate the trace over valley indices using Eq. (A3). Here we use the same reasoning for terms like $G_{ii}^{(0)}/G_{jj}^{(0)}$ at $i\neq j$ in denominators as when calculating the relaxation time. Transforming the sum over fermion frequency into contour integral and making analytical continuation $(i\Omega_{\nu}\to\Omega)$ we finally obtain

$$\begin{aligned}\begin{bmatrix}\sigma_{\alpha\beta}\\ \beta_{\alpha\beta}\end{bmatrix}=\frac{e}{4\pi T^2m^2}\sum_{i=1}^{N}&\int_{-\infty}^{\infty}\begin{bmatrix}2eT\\ -\omega\end{bmatrix}\frac{d\omega}{\cosh^2(\omega/2T)}\int\frac{d^3k}{(2\pi)^3}\\&\times\frac{k_{\alpha}k_{\beta}\tau^{-2}(\omega)}{\{[\omega+\mu_i-(k^2/2m)]^2+[1/4\tau^2(\omega)]\}}.\end{aligned} \tag{A7}$$

The last equation results in Eqs. (12) and (17) after integration over $\omega$ and summation over valleys, under the condition of uniformity of valleys.

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