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Electronic conductivity of icosahedral quasi-crystals

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Quasi-crystals are characterized by aperiodical atomic long-range order and the rotation symmetry that is forbidden for periodical structures (the existence of the 5-, 8-, 10-, and 12-fold axes of rotation). The former feature distinguishes quasi-crystals from amorphous objects (glasses), while the latter distinguishes them from crystals and incommensurate structures. Quasi-crystals are usually alloys of metallic elements, but their properties are different from those of crystalline and amorphous metallic phases. Like metals, quasi-crystals bear a finite electron contribution to their heat capacity, but this contribution is approximately one order of magnitude smaller than that defined in the nearly free electron approximation (pseudogap and, accordingly, low density of states $N(E_F)$ at the Fermi level).

However, the low density of states at the Fermi level does not explain the abnormally small low-temperature electric conductivity of quasi-crystals. The electrical resistivity of quasi-crystals decreases with increasing temperature, and it increases with increasing structural order and annealing of defects. The resistivity ratio $\mathcal{R} = \rho(4.2\ \mathrm{K})/\rho(300\ \mathrm{K})$ for the majority of stable quasi-crystals is several units, but for the icosahedral alloy i-Al–Pd–Re, whose perfect samples have $\rho(4.2\ \mathrm{K}) \geqslant 1\ \Omega\ \mathrm{cm}$, the ratio $\mathcal{R}$ may be as high as 200 and even higher, depending on the perfectness of the specimen.

The conductivity of quasi-crystals is represented as $\sigma = \sigma(0) + \Delta\sigma(T)$, where $\sigma(0)$ is the conductivity at zero temperature, which depends on structural disorder, and $\Delta\sigma(T)$ is the temperature-dependent component which may also depend on structural disorder. Almost all quasi-crystals exhibit a power-law temperature dependence $\Delta\sigma(T) \sim T^{\beta}$, where the exponent β usually varies within the interval $1/\sqrt{3} \leqslant \beta \leqslant 1.5$ in the range from ultralow temperatures to 700–1000 K. Linear dependence is usually observed at high temperatures. A reasonable explanation of the power-law temperature dependence of conductivity and its value at $T = 0$ K was proposed by Burkov et al. [1], who used the model of a Fermi surface with a large number of electron and hole pockets.

Recent experiments with perfect quasi-crystals of i-Al–Pd–Re have shown that at $T \leqslant 10$ K the conductivity can obey the Mott law

$$\sigma = \sigma_0 \exp\left[-\left(\frac{T_0}{T}\right)^{1/4}\right],$$

which describes hopping conduction with variable jump length. This implies that the sample occurs in the insulator state (Fermi glass), when the density of states at the Fermi level is finite, but the electron states are localized. Electron localization plays an important role in the low-temperature electron transport in amorphous alloys, granulated metallic films, and doped semiconductors. For these systems, electron localization is the consequence of disorder in the system (the Anderson localization).

Localization of electrons in a quasi-crystal differs in its nature from appropriate localization in standard disordered systems. The alloy i-Al–Pd–Re is a well-ordered quasi-crystal, and the improvement of structural order leads to an increase in its resistivity. Localization in quasi-crystal is a consequence of interference (phase coherence) of the electron states, and thus is associated with the symmetry and structure of the object: the more perfect the material, the more localized its electrons. While in the case of conventional Anderson localization the electron states are localized because the phase coherence of extended wave functions is destroyed by disorder, the main cause of localization in quasi-crystals is the phase coherence of wave functions.

This can be proved by treating the quasi-crystal as the structural limit of the sequential of rational periodical approximants (crystal analogs) with increasing lattice period. The volume of the Brillouin zone decreases with increasing order of the approximant, because the lattice

period increases. Accordingly, in the quasi-crystalline limit the volume of the Brillouin zone becomes infinitesimal. Using the conventional method of the construction of Fermi surface [2], we see that the Fermi surface in the quasi-crystalline limit becomes multiply connected, and has many electron and hole pockets (valleys). Accordingly, in the atomically ordered pure quasi-crystal the electron states become localized, since the condition of strong localization: $k_{\mathrm{F}}^{i} l \sim 1$ is satisfied for the electron in each ith valley. Therefore, each pocket (valley) is the counterpart of the center of localization in the conventional disordered system. This analogy gives a straightforward explanation of the variable hopping conductivity in a perfect quasi-crystal at low temperatures, and allows it to be described in the context of the model of a multivalley Fermi surface.

In the model of a multicomponent Fermi surface with a practically infinite number of valleys, all the electrons in the pure ordered quasi-crystal must be localized at zero temperature. At a finite temperature, the electron scattering from one valley to the next one is possible not only through thermal excitation, but also through tunneling. At low temperatures, the processes with a low transfer of momentum are more likely: in real space this corresponds to jumps to long distances (the feasibility of conduction with a variable jump length). Following the Mott procedure, one can find the optimal jump length R by calculating the maximum probability of the jump: $\exp(-2\alpha R)\exp(-\Delta E/k_{\mathrm{B}}T)$, where $1/\alpha = \xi$ is the localization length of the wave function, and the excitation energy is $\Delta E \sim 1/R^3 N(E_{\mathrm{F}})$. Whence directly follows the Mott law $\sigma = \sigma_0 \exp\left[-(T/T_0)^{1/4}\right]$ with the characteristic temperature $T_0 \sim 1/\xi^3 N(E_{\mathrm{F}})$. The Mott law does not hold when $R < \xi$ and $T_0 < T$. In the case of a quasi-crystal, however, it is always possible to find a state for which $T_0 < T$, although $R > \xi$. Indeed, the object with a multicomponent Fermi surface has a hierarchy of localization lengths ξ. Therefore, T_0 may change from one specimen to another depending on the previous history of the specimen.

Such a mesoscopic situation is typical for both quasi-crystals and for conventional disordered systems near the metal – insulator transition. In the regime of localization the wave functions are exponentially damped, and they are extended from the 'metal' side of the transition. Near the transition point the localization length shows a power-law increase (diverges), and becomes greater than any of the characteristic dimensions of the system, and so the calculated eigenstates do not directly reflect any kind of localization. At the metal – dielectric transition point itself there is no characteristic length scale, the eigenvalues exhibit fractal features, and the wave functions are 'critical' (showing a power-law decrease with the distance).

For the 3D Anderson model it was found that the strong fluctuations of the amplitude of the wave function exhibit the multifractal features at all length scales, and the singularity of the spectrum does not depend on the size of the system [3, 4]. The same is typical of the quasi-crystal. The analysis performed in Refs [5, 6] in the tight-binding approximation using the method of level statistics revealed that the electron spectrum of the 3D icosahedral crystal contains a singular part, has a nonzero measure of allowed gaps, and the majority of wave functions are critical. In contrast to the Anderson localization, the localization of electrons in quasi-crystals is unstable with respect to small perturbations: phasons, substitution disorder, magnetic field; moreover, the states are more strongly localized in the middle of the band rather than on its edges, as is the case with the Anderson localization [6]. Because of this, increasing temperature and introducing defects may induce the transition of a quasi-crystal into metallic state, the object occurs on the 'metallic' side of the metal – insulator transition, the electron states are smeared out due to the inelastic scattering, and the number of pockets on the Fermi surface is effectively reduced. The Fermi surface will contain a finite number of pockets (whose size is determined by the uncertainty relation), and tunneling becomes unlikely. The conductivity with variable hopping conductivity mechanism no longer works, and dominating are the processes of the intervalley and intravalley scattering, which determine the power-law temperature dependence of conductivity, and the value of residual conductivity. At $T > u/a \sim \theta_{\mathrm{D}}$, where u is the sound velocity, and a is the interatomic distance, the intervalley electron – phonon scattering becomes efficient and leads to the linear temperature dependence of conductivity at high temperatures [7].

In this way, even though the Bloch theorem does not apply to quasi-crystals, it is possible to explain their conductivity in the framework of conventional electronic theory of solids using the multivalley Fermi surface mode.

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