Effect of Zener oscillations on the electronic properties of quasicrystals

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(Submitted 19 July 1995)
Pis'ma Zh. Éksp. Teor. Fiz. **62**, No. 4, 349–351 (25 August 1995)

The electronic properties of quasicrystals are studied in a model which assumes that all electronic states at the Fermi level undergo Bragg reflection and are localized. The properties of the quasicrystals are determined by Zener (Bloch) oscillations. © *1995 American Institute of Physics.*

In Ref. 1 Zener (Bloch) oscillations arising in an electric field as a result of the reflection of electrons at the boundaries of the Brillouin zone were used to explain the transverse conductivity of a layered metal containing impurities. In the present paper this idea is used to describe the electronic properties of quasicrystals.

The electronic properties of quasicrystals are different from those of other metallic objects. The resistivity of quasicrystals is anomalously high (it reaches 2 $\Omega \cdot$cm in the stable icosahedral phase of the system AlPdRe (Ref. 2)), and it decreases with increasing temperature and increases with increasing structural order and annealing of defects.[3,4]

Decagonal quasicrystalline alloys are characterized by conductivity anisotropy: The conductivity along the packing axis of the quasicrystalline planes with a finite period (tenfold axis) behaves as in a normal metal, whereas in the planes themselves the conductivity behaves in the manner described above.[5] Another specific feature is that the electron contribution to the heat capacity is lower than in a normal metal, the Hall constant is large and is strongly temperature dependent, and the optical conductivity does not follow Drude's law.[3,5] Virtually all quasicrystalline phases, including alloys with transition elements, are weakly diamagnetic in a wide temperature range (Mn-containing alloys, which are paramagnetic, are exceptions).[5]

Of the different reasons considered for this behavior of the properties, we note the following:

a) the existence of a pseudogap at the Fermi level; this gap is obtained in calculations of the electronic spectrum for the approximant,[3] but it is not always observed experimentally;[5]

b) the specific nature of the behavior of the wave functions, which in one- and two-dimensional crystals oscillate on all scales, and are neither localized nor extended states: the spectrum has zero measure[6,7] and, consequently, the resistance is a power-law function of the size of the object; in three-dimensional problems contradictory results are obtained in the weak-coupling approximation: According to Ref. 8, the conductivity must be finite and according to Ref. 9 (perturbation theory), it must be infinite;

c) the role of localization effects has also been discussed.[3]

All of these factors are important, but they are not sufficient to describe systematically the electronic properties of quasicrystals.

In the present paper we propose a model which can apparently explain the basic features of the electronic properties of quasicrystals. The model is based on a band theory, which takes into account the specific nature of the quasicrystalline state and the effect of Zener (Bloch) oscillations.

A quasicrystal can be regarded as the limit of a sequence of approximants whose lattice constant $a \to \infty$. The reciprocal lattice of a quasicrystal consists of a collection of reciprocal-lattice vectors which densely fill the reciprocal space everywhere. All electronic states at the Fermi level undergo Bragg reflection (each scattering wave vector is a reciprocal-lattice vector). A perfect quasicrystal is thus a "Bragg" insulator with zero electron group velocity and, correspondingly, zero conductivity at zero absolute temperature.

In such a system electronic oscillations (Zener or Bloch) appear when an electric field E is applied. The probability of Zener breakdown is small, since the lattice constant is infinite and the states at the Fermi level lie in close proximity to the gap at the boundary of a Jones pseudoband. The spatial scale of the Zener oscillations is of the order of the characteristic size a_R of a structural unit (the edge length of a rhombohedron).

Oscillations occur with a high frequency $\hbar\omega = eEa$ (the lattice constant a is infinite) and, correspondingly, with period T less than all characteristic scattering times in the system. In this case $\tau > T$ always ("pure" limit in the Varlamov problem), where τ is the characteristic scattering time determined by some elastic or inelastic collisions, the Zener oscillations are stable, and the standard Drude law does not hold.

We shall express the conductivity in terms of the diffusion coefficient: $\sigma = \rho(E_F)e^2D$ (Einstein's relation), where $\rho(E_F)$ is the single-particle density of states. In the "pure" limit[1] ($\tau > T$) $D \approx a_R^2/\tau$. Therefore, $\sigma \sim \tau^{-1}$. In an ideal quasicrystal at zero temperature, $\tau \to \infty$ and $\sigma \to 0$. As the temperature increases and phonons and other scattering processes come into play, σ will increase. As long as the quasicrystalline state is not destroyed, the Zener oscillations are stable and the condition $\sigma \sim \tau^{-1}$ holds in a wide temperature range and even with large structural distortions.

In layered quasicrystals $\sigma_\parallel \sim \tau^{-1}$ in the quasicrystalline planes, and the "dirty" limit with normal-metal conductivity described by Drude's formula, $\sigma_\perp \sim \tau$, is realized along the packing axis [in the "dirty" limit, $\tau < T$, the standard diffusion anistropy is present instead of stable Zener oscillations; $D_\perp = v_\perp^2(p_\perp)\tau$, $\sigma_\perp \sim \tau$ (Ref. 1)].

The "Bragg" insulator state can obviously explain the finite but low electronic contribution to the heat capacity, the absence of paramagnetism of the electron gas, and the weak diamagnetic response of quasibound electrons (the paramagnetism of alloys with manganese is probably attributed to the large local moment of manganese).

We wish to thank A. A. Varlamov for a helpful discussion and for his interest in this study. We also thank D. V. Livanov for reading the manuscript and for a number of valuable remarks.

This work was performed as part of the program of the International Center for

Fundamental Physics in Moscow, with financial support from INTAS (Grant 93-2492) and the International Science Foundation (Grant MQQ000).

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Translated by M. E. Alferieff