Electronic properties of a 3D quasicrystal with a weak potential

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The motion of an electron in a 3D icosahedral quasicrystal is analyzed in the weak-coupling approximation. Even an ideal quasicrystal has a finite conductivity. The mean free time is estimated to be $\tau \sim V_0^{-1} \exp((V_0/E_F)^{-1/4})$, where V_0 is the effective atomic potential.

The motion of an electron in a 1D quasiperiodic potential was analyzed in Refs. 1–3. Regardless of the potential force, the spectrum has a zero measure; the wave functions oscillate at all scales; and the resistance is a power-law function of the length. In the present letter we show (in the weak-coupling approximation) that in the 3D case an electron is scattered by weak harmonics of the potential in the same way that it would be scattered by impurities. This result contradicts the results of Ref. 4, reached by perturbation theory.

1. We start with the one-electron Hamiltonian $\mathscr{H} = \epsilon(p) + V(x)$, where $V(\mathbf{x}) \ll E_F$ (weak coupling). This approximation can be expected to be valid for the Al_6CuLi_3 quasicrystal, since all the components of this compound are good metals. In the k representation the quasicrystal potential V is written in the form[5]

$$V(\mathbf{k}) = \sum_{m_1, \ldots, m_6} V_{m_1, \ldots, m_6} \delta[\mathbf{k} - \mathbf{k}_{m_1, \ldots, m_6}], \tag{1}$$

where $V_{\mathbf{m}} = V_0 F(\mathbf{k}^*_{\mathbf{m}})$. Here $\mathbf{k}_{\mathbf{m}}$ and $\mathbf{k}^*_{\mathbf{m}}$ are the projections of the 6D reciprocal-lattice vector onto the real (R^3) and dual (R^{3*}) subspaces, and $F(\mathbf{k}^*)$ is the form factor of the tube. For simplicity, we are ignoring the atomic form factor. In the weak-coupling approximation we have $V_0 \ll E_F$.

Important to our problem of determining whether the quasicrystal has a finite conductivity is the asymptotic behavior of the function $F(\mathbf{k}^*)$ as $|\mathbf{k}^*| \to \infty$. For an ideal quasicrystal, the cross section of a tube is a polyhedron T in R^{3*}; in the simplest model, it would be a triacontrahedron.[6] The asymptotic behavior of $F(\mathbf{k}^*)$ is dominated by the vertices of polyhedron T. The contribution of one vertex is

$$F(\mathbf{k}^*) \sim |(c_1, \mathbf{k}^*)(c_2, \mathbf{k}^*)(c_3, \mathbf{k}^*)|^{-1} \tag{2}$$

where $|(c_1 \mathbf{k}^*)| \gg 1, |(c_2 \mathbf{k}^*)| \gg$, and $|(c_3 \mathbf{k}^*)| \gg 1$, where c_1, c_2, and c_3 are the edges of polyhedron T which emerge from the given vertex.

2. We begin the analysis with a perturbation theory in k space. To each state with a momentum $\mathbf{p}$ we add an admixture of states with momenta of the type $\mathbf{p} + \mathbf{k}_{\mathbf{m}}$, where $\mathbf{k}_{\mathbf{m}}$ is a quasicrystal vector. This admixture is a large fraction only if the states $\mathbf{p}$ and $\mathbf{p} + \mathbf{k}_{\mathbf{m}}$ are at resonance, i.e., only if $|\epsilon(\mathbf{p}) - \epsilon(\mathbf{p} + \mathbf{k}_{\mathbf{m}})| < |V_{\mathbf{m}}|$.

For given $\mathbf{p}$ ($|\mathbf{p}| \sim p_F$) and $V < V_0$, we denote by $n(V)$ the density along the energy scale of the quantities $\epsilon(\mathbf{p} + \mathbf{k}_{\mathbf{m}})$ such that $|V_{\mathbf{m}}| > V$. In other words, the probability that there exists a state with momentum $\mathbf{p} + \mathbf{k}_{\mathbf{m}}$ such that $|V_{\mathbf{m}}| > V$ and $E_F < \epsilon(\mathbf{p} + \mathbf{k}_{\mathbf{m}}) < E_F + dE$ is $n(V)dE$. For $n(V)$ we find the expression

$$n(V) = b V^{-1} \ln^2 (V_0/V), \text{ where } b \sim V_0/E_F \ll 1. \tag{3}$$

The average number of states which are at resonance with the given state is $N \sim \int V dn(V)$. Instead of analyzing specific expression (3) for $n(V)$, we discuss two cases.

We first assume $N \ll 1$. The electron is then localized in momentum space: Each eigenstate of the Hamiltonian is a superposition of a small number of states with momenta of the type $\mathbf{p} + \mathbf{k}_{\mathbf{m}}$. The effect of the lattice potential reduces to simply a renormalization of the spectrum. There is no scattering, and the conductivity is infinite.

If, on the other hand, the condition $N \gg 1$ holds, we cannot use perturbation theory. The electron may be scattered by harmonics of the lattice potential an unbounded number of times; i.e., the electron will be delocalized in momentum space [a more precise delocalization condition, condition (8), is given below]. The electron spends a certain time τ in each state with a definite momentum, and this time can be identified as the mean free time. The conductivity is determined from the Drude formula. For a quasicrystal, we are dealing with specifically this case.

The motion of the electron in k space is in a set of states with momenta $\mathbf{p} + \mathbf{k}_{\mathbf{m}}$ ($\mathbf{p} = \text{const}$) such that

$$|\epsilon(\mathbf{p}) - \epsilon(\mathbf{p} + \mathbf{k}_{\mathbf{m}})| < \tau^{-1}. \tag{4}$$

If we represent this set in a 6D space, it will be unbounded along R^{3*}. The

probability for a return to the initial state in diffusion in a set of this sort is not unity, so if we are interested in simply orders of magnitude, we can ignore it. We then find the problem of diffusion on a lattice without loops, i.e., on a tree. This approximation is not valid for 1D or 2D quasicrystals, since weak-localization effects (in k space) may prove important.

3. Let us formulate the problem of an electron on a tree and point out a way to solve it. The Hamiltonian includes the potentials at the vertices, E_α, and jumps between neighboring vertices, $V_{\alpha\beta}$, which are random quantities. The potentials E_α are distributed uniformly over a very wide range of energies E_0. The number of branches emerging from a given vertex is not bounded. The probability that a branch with a jump amplitude in the interval $(V,V+dV)$ will emerge from a given vertex and go to a vertex whose potential is in the interval $(E,E+dE)$ is $dn(V)dE$.

We select a certain vertex as a root of the tree, and we place it at the zero level. The vertices with which it is connected are placed at the first level; etc. We select an energy ϵ. We denote by α a vertex of level j. We consider the subtree consisting of vertex α and all branches above it. We denote by G_α the Green's function $G_{\alpha\alpha}(\epsilon)$ on this subtree. We express G_α in terms of the Green's function G_{α_i} of these vertices α_i of level $j+1$ which are connected with vertex α:

$$G_\alpha^{-1} = \epsilon - E_\alpha - \Sigma_\alpha, \quad \Sigma_\alpha = \sum_i |V_{\alpha\alpha_i}|^2 G_{\alpha_i}. \tag{5}$$

Assuming that G_α and Σ_α are random quantities, we can find the relationship between their distribution functions at levels j and $j+1$. In an infinite tree, these distribution functions must be the same, so we find a closed system of equations.

We assume $\Sigma = \beta - i\gamma$ $(\gamma \geqslant 0)$, and we assume that $g(\gamma)$ is the distribution function of γ. In order of magnitude, γ^{-1} is equal to the time spent by the electron at one vertex. In the localization case we would have $g(\gamma) = \delta(\gamma)$, and in the delocalization case $g(\gamma) \neq 0$ at $\gamma > 0$.

Introducing the auxiliary function $\varphi(z) = \langle \exp(-izV^2 \operatorname{Im} G) \rangle_{G,V}$, we find the system of equations

$$\begin{aligned} \varphi(z) &= \int\int\int (e^{i\alpha z} - 1) K_V(\alpha, \gamma) g(\gamma)\, d\alpha\, d\gamma\, dn(V), \\ g(\gamma) &= \frac{1}{2\pi} \int_{-\infty}^{+\infty} \exp(\varphi(z)) e^{-i\gamma z}\, dz, \end{aligned} \tag{6}$$

where

$$K_V(\alpha,\gamma) = \begin{cases} V\gamma^{1/2}\alpha^{-3/2}(1-\alpha\gamma/V^2)^{-1/2}, & \text{for} \quad \alpha\gamma < V^2 \\ 0, & \text{for} \quad \alpha\gamma \geqslant V^2. \end{cases}$$

Allowing for the finite magnitude of the range of energies E_0, we find a cutoff of the function $K_V(\alpha,\gamma)$:

$$(V/E_0)^2 < \alpha/\gamma < (E_0/V)^2. \tag{7}$$

Using the expansion $\exp(\varphi(z)) \approx 1 + \varphi(z)$, we find the delocalization condition:

$$\int V \ln(E_0/V)\, dn\ (V) > \frac{1}{4}\ . \tag{8}$$

This condition holds for $n(V)$ as in (3).

Solving Eqs. (6) with $n(V)$ as in (3), we find a function $g(\gamma)$ with a sharp maximum at the point

$$\gamma_0 \sim V_0 \exp\left(-\lambda b^{-1/4}\right), \tag{9}$$

where λ is a numerical constant. In this manner, we find an estimate of the mean free time of the electron: $\tau \sim \gamma_0^{-1}$.

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