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Conductivity of a quasiperiodic system in two and three dimensions

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A generalization of the Aubry-André model in two and three dimensions is introduced which allows for quasiperiodic hopping terms in addition to the quasiperiodic site potentials. This corresponds to an array of interstitial impurities within the periodic host crystal. The resulting model is exactly solvable and I compute the density of states and the ac conductivity. There is no mobility edge as in completely disordered systems but the regular ac conductivity and the strongly reduced Drude weight indicate a precursor of the Anderson transition as the Fermi energy goes from the center to the band edges.

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The description of electron motion in a nonperiodic potential within the single-particle approximation is an elementary problem in solid state physics and still unsolved for the case of a macroscopic number of impurities which break discrete translational invariance. Especially the phenomenon of Anderson localization in a tight-binding model with uncorrelated random site potentials defies exact analytical treatment up to now. Therefore, several attempts have been undertaken to study models with quasiperiodic potential, which constitute a case intermediate between the perfect crystal and a fully disordered system. The simplest realization of this situation is a tight-binding Hamiltonian H_1 where the site energies vary in a quasiperiodic fashion:

$$H_1 = H_0 + \sum_{\mathbf{m},\mathbf{n}} g_{\mathbf{m}} \delta_{\mathbf{nm}} |\mathbf{n}\rangle\langle\mathbf{n}|. \tag{1}$$

The $|\mathbf{n}\rangle$ are local orbitals at site $\mathbf{n}$ of a d-dimensional hypercubic lattice, H_0 describes the Hamiltonian of the periodic lattice and $g_{\mathbf{m}}$ is a quasiperiodic function of $\mathbf{m}$.

A possible choice for $g_{\mathbf{m}}$ is

$$g_{\mathbf{m}} = 2g \cos(\mathbf{Q}\cdot\mathbf{m}), \tag{2}$$

with a vector $\mathbf{Q}$ whose components Q_j are incommensurable with π. This is the d-dimensional Aubry-André model and unsolvable for $d>1$ despite its simplicity. Even in $d=1$ only very limited results can be obtained exactly, e.g., the localization property of the eigenstates if $g>1$.[1]

A general criticism applies to all models of type (1): The doping of the periodic host lattice with impurities is usually not of the substitutional type but the additional atoms sit at interstitial positions. They modify not only the site energies but change locally the orbitals and in turn the overlap integrals defining the hopping matrix elements. Furthermore, an empty impurity orbital may serve as intermediate state for a hopping process connecting distant sites of the host lattice. These effects may be phenomenologically taken into account by the following generalization of Eq. (1):

$$H = H_1 + \sum_{\mathbf{m}} \left(\sum_{\mathbf{n},\mathbf{n}'} g'_{\mathbf{m}}(\mathbf{n}-\mathbf{m},\mathbf{n}'-\mathbf{m}) |\mathbf{n}\rangle\langle\mathbf{n}'| \right). \tag{3}$$

The function $g'_{\mathbf{m}}(\mathbf{n}-\mathbf{m},\mathbf{n}'-\mathbf{m})$ depends on the position of the impurity $\mathbf{m}$ and decays with growing distance of the sites $\mathbf{n},\mathbf{n}'$ from $\mathbf{m}$. This generalization of Eq. (1) seems to be more complicated than the Aubry-André model if both the $g_{\mathbf{m}}$ and the $g'_{\mathbf{m}}$ vary quasiperiodically with $\mathbf{m}$. It is therefore surprising that one may construct such a model which is completely analytically solvable and has a solution in arbitrary dimensions. "Complete solution" means here that the Hamiltonian is diagonalizable and computation of the transport properties can be done analytically. As in most nontrivial soluble models, the solvability rests here on a relation between the quasiperiodic functions $g_{\mathbf{m}}$ and $g'_{\mathbf{m}}$. The starting point is the periodic Hamiltonian

$$H_0 = -t \sum_{(\mathbf{n},\mathbf{n}')} |\mathbf{n}\rangle\langle\mathbf{n}'| + \text{H.c.}, \tag{4}$$

where $(\mathbf{n},\mathbf{n}')$ denotes a pair of next neighbors on the d-dimensional hypercubic lattice $\Lambda=\mathbb{Z}^d$ with lattice constant $a=1$. Its matrix elements read in momentum space

$$H_0(\mathbf{p},\mathbf{p}') = -2t \sum_{j=1}^{d} \cos(p_j)\delta(\mathbf{p}-\mathbf{p}'). \tag{5}$$

with $\mathbf{p},\mathbf{p}' \in [-\pi,\pi]^d$.

We introduce two types of potentials related to the site $\mathbf{m}$.

(I) A local potential term with matrix element $V_{\mathbf{m}}(\mathbf{n},\mathbf{n}')$ in position space:

$$V_{\mathbf{m}}(\mathbf{n},\mathbf{n}') = g_{\mathbf{m}}(2\pi)^d \prod_{j=1}^{d} \delta(n_j - n'_j)\delta(n_j - m_j). \tag{6}$$

(II) A nonlocal term

$$V'_{\mathbf{m}}(\mathbf{n},\mathbf{n}') = g'_{\mathbf{m}} \left(\frac{2}{\pi}\right)^d \prod_{j=1}^{d} \frac{(-1)^{n_j+n'_j}}{(n_j - m_j - 1/2)(n'_j - m_j - 1/2)}. \tag{7}$$

The functional form of Eq. (7) agrees with the general expression in Eq. (3) and can be interpreted as perturbative description of a hopping process, where the electron goes from site $\mathbf{n}$ first to the impurity site $\mathbf{m}+1/2$ on the dual lattice and from there to the site $\mathbf{n}'$. The technical reason for this choice of the non-local term is the fact that now both potentials have the same form in momentum space:

$$V_{\mathbf{m}}(\mathbf{p},\mathbf{p}') = g_{\mathbf{m}} \exp[i\mathbf{m}\cdot(\mathbf{p}'-\mathbf{p})], \tag{8}$$

$$V'_{\mathbf{m}}(\mathbf{p},\mathbf{p}') = g'_{\mathbf{m}} \exp[i\tilde{\mathbf{m}} \cdot (\mathbf{p}' - \mathbf{p})] \tag{9}$$

with $\tilde{m}_j = m_j + 1/2$. Because both forms of the potential factorize with respect to the dimension index j, also a mixed type is possible, which is for some j of type I and for the rest of type II. All of these possibilities can be parametrized through a vector $\mathbf{m}$ with integer and/or half-integer components, i.e. $\mathbf{m} \in \Lambda' = (\mathbb{Z}/2)^d$ and we may drop the primes in Eq. (9). The generalization of the Aubry-André model in d dimensions then reads

$$H = H_0 + \frac{1}{(2\pi)^d} \sum_{\mathbf{m} \in \Lambda'} V_{\mathbf{m}} \tag{10}$$

and

$$g_{\mathbf{m}} = \begin{cases} 2g_{\mathrm{loc}} \cos(\mathbf{Q} \cdot \mathbf{m}), & \mathbf{m} \in \Lambda, \\ 2g_{\mathrm{nloc}} \cos(\mathbf{Q} \cdot \mathbf{m}), & \mathbf{m} \in \Lambda' \setminus \Lambda. \end{cases} \tag{11}$$

Here, $\mathbf{Q}$ denotes some vector in $\mathbb{R}^d$ such that Q_j/π are irrational. We may further assume that the numbers Q_j/π are linearly independent over $\mathbb{Z}$. In this case, no point of the lattice is equivalent to another. The original Aubry-André model is recovered for $g_{\mathrm{nloc}} = 0$. We set in the following $g_{\mathrm{loc}} = g_{\mathrm{nloc}} = g$. The potential term $V_{\mathbf{Q}} = (2\pi)^{-d} \Sigma_{\mathbf{m} \in \Lambda'} V_{\mathbf{m}}$ can be rewritten in momentum space:

$$V_{\mathbf{Q}}(\mathbf{p},\mathbf{p}') = g[\delta_{4\pi}(\mathbf{p}' - \mathbf{p} + \mathbf{Q}) + \delta_{4\pi}(\mathbf{p}' - \mathbf{p} - \mathbf{Q})]. \tag{12}$$

Here, $\delta_{4\pi}(x)$ denotes the delta-function with fundamental period 4π: $\delta_{4\pi}(x + 4n\pi) = \delta_{4\pi}(x)$ for $n \in \mathbb{Z}$. The quasiperiodic potential translates in momentum space to displaced delta functions, which, however, do not have 2π periodicity but 4π periodicity due to the addition of the nonlocal terms of type II. As a result, only finitely many points in momentum space are connected through the potential term, even if $\mathbf{Q}/\pi$ is irrational.

The simplest case is realized if just two sites in momentum space are connected. This happens if one of the Q_j lies in the interval $[\pi, 2\pi]$. The other components of $\mathbf{Q}$ can be chosen at will. The Brillouin zone splits into three regions R_0, R_1 and R_2, where R_0 contains points, which are not affected by the potential (12) at all, whereas R_1 and R_2 are mutually connected through the potential:

$$R_1 = \prod_{j=1}^{d} [-\pi, \pi - Q_j],$$

$$R_2 = \prod_{j=1}^{d} [-\pi + Q_j, \pi],$$

$$R_0 = \prod_{j=1}^{d} [-\pi, \pi] \setminus (R_1 \cup R_2) \tag{13}$$

(see Fig. 1 for the case $d=2$).

It has to be emphasized that this splitting is equivalent to a reduction of the Brillouin zone and concomitant generation of subbands only if $\mathbf{Q}/\pi$ is a rational vector. In the general case the model does not have a band structure.

Nevertheless, vectors $\mathbf{p}$ from R_1 can be used to label the two-dimensional invariant subspaces $\mathcal{H}_{\mathbf{p}}$, which are spanned by $|\mathbf{p}\rangle$ and $|\mathbf{p}+\mathbf{Q}\rangle$. On these subspaces, the Hamiltonian can be easily diagonalized:

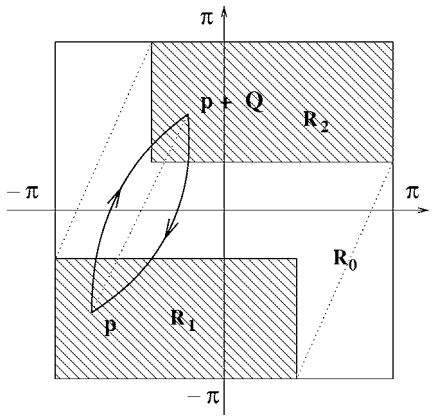

FIG. 1. The three regions R_0, R_1, R_2 for $d=2$.

$$H|_{\mathcal{H}_{\mathbf{p}}} = \begin{pmatrix} -2t \sum_j \cos(p_j) & g \\ g & -2t \sum_j \cos(p_j + Q_j) \end{pmatrix}. \tag{14}$$

In the following we have set for simplicity $t = 1/2$. Figures 2 and 3 give the density of states in two and three dimensions, respectively. The total DoS is composed from two "bands," where the p band stems from the region R_0, which is unaffected by the quasiperiodic potential and the eigenstates of Eq. (10) are the pure momentum eigenstates $|\mathbf{p}\rangle$ for $\mathbf{p} \in R_0$. These are located in a region around $E=0$, the band center. The q band is gapped and contains the eigenstates $|\psi^{\pm}_{\mathbf{p}}\rangle$ in $\mathcal{H}_{\mathbf{p}}$ for each $\mathbf{p} \in R_1$ and energy eigenvalues $E^{\pm}_{\mathbf{p}}$. It is located predominantly at the band edges.

To compute the conductivity, we first note that the p band is not affected by the potential: The current commutes with the Hamiltonian and we get a diagonal ac conductivity [$\beta = (kT)^{-1}$]:

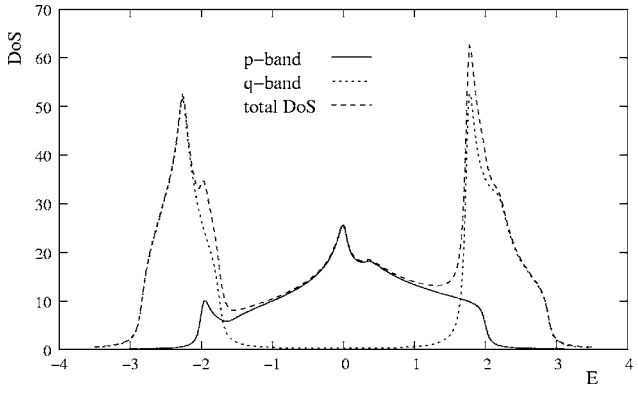

FIG. 2. Density of states for $d=2$. The potential is quasiperiodic with $Q_x = 2\pi - 4$ and $Q_y = 2\pi - 2\sqrt{2}$. The coupling constant is $g=2$.

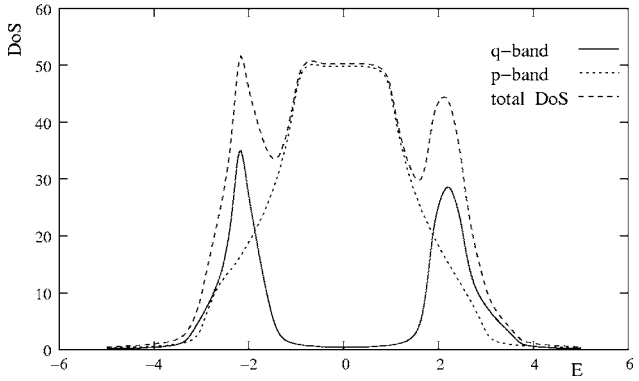

FIG. 3. DoS for $d=3$. Here, $Q_x=2\pi-4$, $Q_y=2\pi-2\sqrt{3}$ and $Q_z=2\pi-\sqrt{5}$ with coupling $g=2$.

$$\mathrm{Re}[\sigma_{kk}(\omega)] = \pi D_0(\beta)\delta(\omega) + \sigma_{kk}^{\mathrm{reg}}(\omega) \tag{15}$$

with vanishing regular part, $\sigma_{kk}^{\mathrm{reg}}(\omega)=0$ and the Drude weight $D_0(\beta)$ of the pure system, which is only reduced because R_0 does not cover the whole Brillouin zone.

In the q band, however, we obtain a nonvanishing $\sigma_{kk}^{\mathrm{reg}}$ because the current $\mathbf{J}$ does not commute with H on the spaces $\mathcal{H}_{\mathbf{p}}$:

$$J_k|_{\mathcal{H}_{\mathbf{p}}} = e\begin{pmatrix} \sin(p_k) & 0 \\ 0 & \sin(p_k+Q_k) \end{pmatrix}. \tag{16}$$

The (anisotropic) Drude weight $D_k^q(\beta)$ of the q band is computed as

$$D_k^q(\beta) = \beta \int_{R_1} d\mathbf{p} n_F(E_{\mathbf{p}}^{\pm}) |\langle \psi_{\mathbf{p}}^{\pm}|J_k|\psi_{\mathbf{p}}^{\pm}\rangle|^2 \tag{17}$$

with the Fermi function $n_F(E)=[1+\exp\beta(E-E_F)]^{-1}$. D_k^q approaches D_0 for $Q_k \to 0, 2\pi$, i.e., when the potential becomes periodic in the k direction. Figure 4 shows D_x^q/β for small temperatures and E_F located in the gap of the q band as function of Q_x and Q_y.

The Drude weight D_k^q approaches a nonzero large coupling limit $g \to \infty$ with the exception of the (rational) value $Q_k/\pi=1$, where the expectation value of J_k in the eigenstates of H goes to zero. This behavior is seen in Fig. 5.

Apart from D_k^q, which is reduced in the q band due to

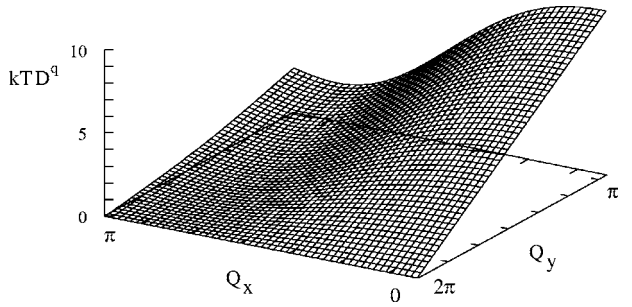

FIG. 4. Drude weight of the q band D_x^q/β for $d=2$. The maximum at $Q_y=\pi$ and $Q_x=0$ corresponds to the Drude weight of the pure system D_0. The minimum along $Q_y=2\pi$ is due to the vanishing area of R_1 in this case.

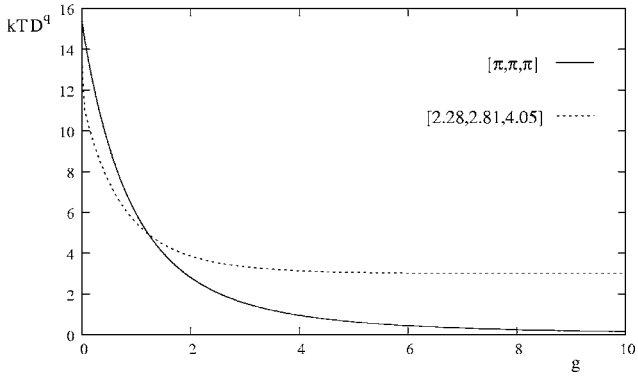

FIG. 5. Drude weight D_x^q/β for $d=3$ and two different vectors $\mathbf{Q}$. The large coupling limit is zero for periodic $\mathbf{Q}=(\pi,\pi,\pi)$ and nonzero for quasiperiodic $\mathbf{Q}=(2\pi-4, 2\pi-2\sqrt{2}, 2\pi-\sqrt{5})$.

scattering from the quasiperiodic potential, the regular part of the ac conductivity does not vanish:

$$\sigma_{kk}^{\mathrm{reg}}(\omega) = \pi \frac{1-e^{-\beta\omega}}{\omega} \int_{R_1} d\mathbf{p} n_F(E_{\mathbf{p}}^-) |\langle \psi_{\mathbf{p}}^-|J_k|\psi_{\mathbf{p}}^+\rangle|^2 \delta(\omega + E_{\mathbf{p}}^- - E_{\mathbf{p}}^+) \tag{18}$$

with $E_F \leqslant 0$. Because $E_{\mathbf{p}}^+ - E_{\mathbf{p}}^-$ is bounded from below by $2g$, the ac conductivity vanishes for frequencies below this threshold. $\sigma_{xx}^{\mathrm{reg}}(\omega)$ is plotted in Fig. 6 for various values of β, g, and $\mathbf{Q}$ in $d=2$. The form of $\sigma^{\mathrm{reg}}(\omega)$ in three dimensions is very similar.

We have introduced and solved a tight-binding model with quasiperiodic local and nonlocal potentials in arbitrary dimension. The eigenstates fall into two groups, where one group (states in the p band around $E=0$) exhibits the properties of the pure system but states at the band edges (q band), although still extended, have different transport properties due to the influence of the quasiperiodic potential: a strongly reduced Drude weight and nonzero regular ac conductivity. This can be interpreted as a precursor of the Anderson transition expected for lattices with uncorrelated site po-

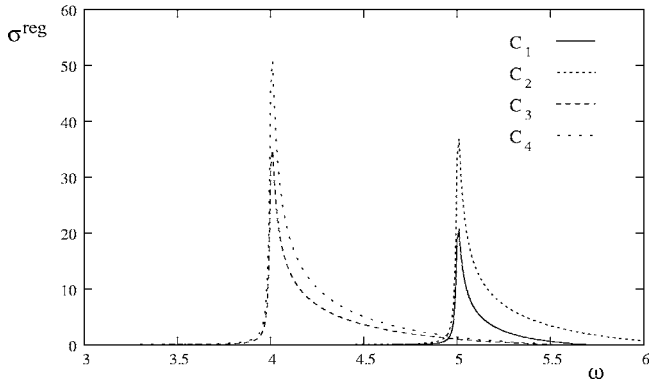

FIG. 6. $\sigma_{xx}^{\mathrm{reg}}(\omega)$ for various parameters: C_3 corresponds to $g=2$, $\beta=1$, $\mathbf{Q}=(2\pi-4, 2\pi-3)$, C_4 has the same g and $\mathbf{Q}$ but $\beta=5$, C_2 and C_1 both have $g=2.5$ and $\beta=1$ but different $\mathbf{Q}$: $(2\pi-4, 2\pi-3)$ and $(2\pi-4.8, 2\pi-2.5)$. Although R_1 has the same area in both cases, the ac conductivity is quite different. $E_F=-2$ in all cases; the Fermi energy lies within the lower q band.

tentials. For irrational values of Q_j/π the system has no band structure in the usual sense. Nevertheless, the density of states is absolute continuous and therefore "bandlike."[2] This feature has been found numerically in the two-dimensional labyrinth tiling,[2] the analogous three-dimensional model[3] and the square Fibonacci tiling[4] for a certain range of parameters. The "bandlike" spectra are *prima facie* closer to the experimentally observed quasiperiodic systems[5] than the models which exhibit a singular continuous spectrum like most of the one-dimensional examples.[6] But this does not mean that the present model is typical for real quasicrystals. The main objection to the physical relevance of the form (7) for the nonlocal term is the following: the hopping matrix elements decay algebraically with distance from the impurity site whereas the decay should be exponential. In this respect the model resembles the Lloyd model, which describes uncorrelated disorder with a broad (Lorentzian) distribution of the site potentials.[7] However, only the disorder-averaged DoS can be analytically calculated in the Lloyd model, not the transport properties. It is therefore only partially solvable. Of course, the "long-range" nature of the quasiperiodic hopping term has a delocalizing effect on the eigenstates and is probably the reason for the absence of a mobility edge in the generalized Aubry-André model.

In addition to the conductivity, one may study the temporal behavior of wave packets initially located at a single site and the associated (anomalous) diffusion of the electrons. This has been done numerically for several quasiperiodic systems in two and three dimensions.[2,3,8] Moreover, some theoretical predictions relating spectral and diffusive properties have been made.[9] These predictions can now be tested analytically in the present model, which will be the subject of a forthcoming paper. A second line of future investigation is a perturbation theory around the exactly solvable point $g_{\mathrm{loc}}=g_{\mathrm{nloc}}$. This introduces a 2π-periodic displaced delta function with a weight proportional to $g_{\mathrm{loc}}-g_{\mathrm{nloc}}$, a quantity which may serve as small parameter of the perturbative expansion. It is possible that localized states appear as soon as $g_{\mathrm{loc}}-g_{\mathrm{nloc}}$ becomes nonzero, in which case the localized regime would be perturbatively accessible.

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