Quantum interferences in quasicrystals

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Abstract. – Contributions of quantum interference effects occurring in quasicrystals are reported. First conversely to metallic systems, quasiperiodic ones are shown to enclose original alterations of their conductive properties while downgrading long range order. Besides, origin of localization mechanism are outlined within the context of the original metal-insulator transition (MIT) found in these materials.

Introduction. –

Despite sustained effort and concern, today’s understanding of exotic electronic properties of quasicrystals remains unsatisfactory although quasicrystalline materials have already been implemented to miscellaneous concrete applications. In particular, the role of quasiperiodic order on electronic localization and transport is believed to genuinely entail the most unexpected experimental features whereas so far, no coherent theoretical framework has been successfully ascertained. As a matter of fact, one of the unprecedented tendency of quasicrystals is the enhancement of their conductive ability upon increasing contribution of static (structural disorder) or dynamical excitations (phonons). This has been strongly supported by many experimental evidences and is often referred as an original property in the litterature. Notwithstanding theoretically, given heuristical arguments and numerical investigations (e.g. the Landauer conductance for quasiperiodic Penrose lattices or Kubo formula for 3D-quasiperiodic models) yield to incomplete understanding of the observed properties which range from anomalously metallic behaviors to insulating ones. It is generally assumed that a specific “geometrical localization process” takes place in quasicrystals (sustained by critical states) and that local disruptions of corresponding mesoscopic order reduce quantum interferences, resulting in an increase of conductivity. To tackle this issue on 1D quasiperiodic potential, tight-binding (TBM) as well as continuous Kronig-Penney models have been considered, and phason-type disorder were shown to disclose manifestations of quantum interferences in quasiperiodic order. Here we will show that alteration of critical states may under certain circumstances entail alteration of their propagating ability. Besides, the role of quantum interferences on both sides of the quasicrystalline MIT for higher
dimensional materials is outlined.

Anomalous electronic conductance in 1D-quasicrystals.

For 1D-quasiperiodic systems, we define phasons [14] that keep the essential characteristic of real systems, in the sense that they are a generic form of disorder which has no equivalent in usual metallic and periodic systems. Introducing random disorder into the 1D quasicrystal yield to Anderson localization in the infinite limit. For finite systems, localization lengths may be much larger than the characteristic size so that conductance fluctuations as a function of energy of tunneling electrons (from the leads to the system) keep its self-similar nature and still follow power law behavior [15]. It is thus difficult to relate localization and transport in such situations. On the other hand, tight-binding models (TBM) of perfect quasiperiodic chains have been intensively worked out both analytically and numerically only for some given energies, but the results are supposed to have provided typical features of localization in quasiperiodic structures, such as power-law decrease of wavefunctions or power-law bounded resistances [12]. Let us investigate the role of phasons in TBM.

Hamiltonian is

\[ H = \sum_n t_n (|n\rangle\langle n+1| + |n+1\rangle\langle n|) \]

\( (\gamma = t_A/t_B \) will stand for intensity of quasiperiodic potential, following a Fibonacci sequence ABAABABAABABAAB...) whereas site energies are kept constant) and the Schrödinger equation on a localized basis gives

\[
\begin{pmatrix}
\psi_{n+1} \\
\psi_n
\end{pmatrix} = M_n \begin{pmatrix} \psi_n \\ \psi_{n-1} \end{pmatrix} = M_n M_{n-1} \ldots M_1 \begin{pmatrix} \psi_1 \\ \psi_0 \end{pmatrix} = P_n \begin{pmatrix} \psi_1 \\ \psi_0 \end{pmatrix}
\]

with \( \psi_n \) the component of wavefunction for energy E at site n

\[
M_n = \begin{pmatrix} 0 & -t_{n-1} \\ 1 & -t_n \end{pmatrix} \quad \text{and} \quad P(n) = \prod_{i=1}^{n} M_i
\]

Connecting the system with external perfect metallic leads, one undertakes a transmission study that give access to the Landauer resistance \( \rho_N = \frac{h}{e^2} R/T \) where \( T \) is the fraction of tunneling electrons transmitted from the system to the leads, and \( R \) is the reflected one. It is directly related with the total transfer matrix elements, \( \rho_N = \frac{1}{4}(P_N^2(1,1) + P_N^2(1,2) + P_N^2(2,1) + P_N^2(2,2) - 2) \) and in quasiperiodic Fibonacci chains, resistance can be written down in a closed form at energy E=0.

\[
(\rho_N)_{\text{Fibonacci}} = \frac{1}{4} (\gamma^{2s(N)} + \gamma^{-2s(N)}) - \frac{1}{2} = \left( \frac{\gamma^{s(N)} - \gamma^{-s(N)}}{2} \right)^2
\]

coefficients \( s(N) \) following a quasiperiodic pattern (Fig.1). Phason disorder is introduced via -BB- units, resulting from of a transition between two isomorphic Fibonacci chains [13]. One shows that for one phason, whatever its position, Landauer resistance for the N-th chain is exactly [14]

\[
(\rho_N)_{\text{one-phason}} = \left( \frac{\gamma^{s(N)} - \gamma^{-s(N)+1}}{2} \right)^2
\]

whereas in the highest density case corresponding to chains of typical form (BB)-ABBABBAABBBABBAA-(BB) (where the external units are associated with constant hopping integrals) calculations lead to [13]
\[
\left(\rho_N\right)_{\text{multiple-phason}} = \left(\frac{\gamma_{\tilde{s}(N)} - \gamma^{-\tilde{s}(N)}}{2}\right)^2
\]

with \(\tilde{s}(N)\) a new complex function of \(N\) calculated iteratively which manifest self-similar fluctuations with respect to \(s(N)\). From such studies one finds that phason disruptions of quasiperiodic order are not able to alter the localization mechanism which do remain basically the same in the limit \(N \to \infty\). To unveil interesting aspects of quantum interferences one has to start from a continuous approach of the Schrödinger equation in Kronig-Penney models in which the potential describing the interaction of the electron with the lattice is represented by a sum of Dirac distributions with intensity \(V_n\) localized at \(x_n\). Following the works and discussions of Kollar and Siito\cite{17}, and M. Baake et al.\cite{18}, we focus our attention around so-called conducting points \((k = k_s)\), that correspond to the commutations of transfer matrix, and which are worked out analytically

\[
\rho_N|_{k = k_s} = \left(\frac{\lambda}{2k_s}\right)^2 \frac{\sin^2 N\varphi}{\sin^2 \varphi}
\]

with \(\varphi\), depending on \(k_s^2\) and \(\lambda\), and is defined by \(\cos \varphi = \cos k_s a + \lambda/2k_s \sin k_s a\). The analytical form of \(\rho_N|_{k = k_s}\) indicates that when \(N \to \infty\), the Landauer resistance oscillates but remains bounded, so that the energies \(k_s^2\) correspond to states that lead to best transmission, reminding that localized states will display exponential increase of resistance. For energies in the vicinity of \(k_s^2 = (k_s + \varepsilon)^2\) (taking \(\lambda = 2k_s(\cos \varphi_s - \cos k_s)/\sin k_s\) and \(\varphi_s = (m\pi)/N\) with \(m=1,...,N-1\), one finds self similar patterns for values of the scattering potential around \(\varphi \sim \frac{\pi}{2}\). This suggests that \(\rho_N|_{\text{one-phason}} (x_P)\) reveal critical states which are robust against phason disorder as found in the TBM for \(E=0\) case. The typical patterns represented on Fig.2 actually encloses oscillations of resistance which smaller oscillations are described by some coefficients \(s(n)\) previously introduced.

Second, two symmetric zones corresponding to \(m < N - 4P\), and \(m > 4P\) are such that \(\rho_N|_{\text{Fibonacci}} (x_P, m, \varepsilon) > \rho_N|_{\text{one-phason}} (x_P, m, \varepsilon)\) in the strict sense \((x_P\) a degree of freedom related with the position of phason defects, \(P\) the total number of available positions for a given \(N)\). A simple pattern of \(\rho_N|_{\text{one-phason}} (k, m, x_P) \sim \alpha(m/P) \sin\left(\frac{2m\pi}{P} x_P\right)\) is found with eigenfrequency of \(m/P = 5/472 = 0.0106\) as revealed by the power spectrum of \(m=5\) curve is given on Fig.3. Superimposed small oscillations are an unphysical effect due to a Fourier transform of a finite signal.

The different behaviors found in this study suggest that in some case local disruption of long range quasiperiodic order has improved the conductive ability of the chain in a systematic manner, which is consistent with the abovementioned remarkable feature of quasicrystalline materials. Analyzing the interference pattern of the Landauer resistance as a function of phason defect suggest that extendedness (as a localization properties of available states at such energies) has also been jointly improved. This is shown by a bounded and simple oscillatory pattern for the resistance, common to what is found for extended eigenstates in a periodic systems. Some affected states (by phasons) may remain self-similar with same transmission ability as in the Fibonacci case whereas others will manifest an improved transmission ability.

Quantum interference mechanisms in high-dimensionnal quasicrystals.

Some effort to investigate quantum interferences effects in small quasiperiodic penrose approximants have been made \cite{19}. Here we propose how quantum interferences on both
sides of a metal-insulator transition in real materials might be analyzed. Indeed, weak localization regime has been found in experiments for some quasicrystalline materials (AlCuFe,...) whereas other systems such as AlPdRe-quasicrystals behave differently being very close to a metal-insulator transition\[4,30]. Two different focus may be considered for a general understanding of quantum interferences in quasicrystals. First, as there exist approximant phases (periodic) sharing the same behavior, weak localization correction beyond Drude approximation should apply for that systems as well as for corresponding quasicrystals. The only recurrent approximation when solving the cooperon diffusion equation is to assume that scatters are uncorrelated i.e \[\langle \mathcal{U}(r)\mathcal{U}(r') \rangle_{\text{disorder}} = c \delta(r-r')\langle \mathcal{U}(r) \rangle = \sum_{i=1}^{N} U(r - R_i), c\text{ the impurity concentration, } u\text{ typical strength}.\] The calculation of the quantum correction of the conductivity in this regime is enclosed in phase factor interferences of the two-particle Green’s function \(\langle G G^* \rangle\). By performing configuration averaging beyond the mean free path length scale, then \(\langle G G^* \rangle_{\text{disorder}}\) reduces phase interference to the \((k' = -k)\)-Cooperon pole, as a consequence of time reversal symmetry, the possibility to have a coherent distribution of scatters is usually neglected.

However, assuming that the distribution of scatters is constrained to, let’s say for sake of illustration, a mirror-plane symmetry, i.e. \(\forall \alpha \in \{R_\alpha, \alpha = 1, N\}\) there is a site \(R_\beta = -R_\alpha\), then without performing any diagrammatic expansion, we just notice that weak localization related with average of the potential scattering \(\langle \mathcal{U}(r)\mathcal{U}(r') \rangle_{\text{disorder}}\) corresponding to phase factors \(\sum_{\alpha\beta} (\mathcal{U}(r)\mathcal{U}(r'))_{\text{disorder}} = \frac{1}{N^2} \int d^2 r_1 d^2 r_2 \mathcal{U}(r_1)\mathcal{U}(r_2) e^{-i k R_\alpha} e^{-i p R_\beta}\) will display new terms associated to above-mentioned symmetry, \(\langle e^{-i k R_\alpha + p R_\beta} \rangle_{\text{disorder}} = \langle e^{i (p-k) R_\alpha} \rangle_{\text{disorder}} = \delta_{p-k,0}\) that will increase the contribution of phase interferences. Say in another way, if a double symmetrical loop crosses in the mirror plane and in a region with extension less or equal to \(\lambda_F\), then four equivalent pathes will interfere at the returning point instead of the usual two of the weak localization scheme, resulting in a total interference amplitude will be 4 times stronger \(\langle | A_I + A_{II} + A_{I} + A_{IV} |^2 = 16 | A |^2 \rangle\). Similar ideas have already been introduced in context of mesoscopic physics\[24\] but we propose here that they may serve as a path to follow a metal-insulator in quasicrystals in which even disorder may keep some strong correlated properties\[24\].

The second focus is suggested by the close proximity of a metal-insulator transition and gives a very dissimilar weight to quantum interferences. Any critical point of an electronic localisation-delocalisation transition can essentially be described by its anomalous diffusion which means that two-particle Green function reads \(\langle | G^+(r, r'; E) |^2 \rangle \sim \left| r - r' \right|^{-\eta + 2 - D}\) with \(\eta\) a critical exponent (and the propagator represents the transition probability in real space of an electron of \(E\) energy from site \(|r\rangle\) to \(|r'\rangle\)), and which directly affect the conductivity of the system since

\[
\sigma_{DC} = \frac{2e^2}{h} \lim_{\varepsilon \to 0} 4\varepsilon \int d^D r_1 d^D r_2 \langle | G^+(r, r'; E) |^2 \rangle_{\text{disorder}}
\]

Power law behavior have been found analytically in quasiperiodic systems\[21,22\], numerically for quantum Hall systems\[29\] and 3D quasiperiodic systems\[3,10\]. No characteristic length scale can be defined (no more validity of mean free path approximation) and interference effects are intrinsically defining the dominant transport mechanism. This has also been recently discussed on realistic models of 3D-quasicrystals by scaling analysis of the Kubo-formula\[3,10\].

In both cases the presence of phasons as demonstrated in 1D systems may weaken the interference effects while destroying quasiperiodic long range order. Working this out analytically in realistic models remains a great challenge.

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Figure captions:

Fig.1: Multifractal distribution of $|s(N)|$ for the Fibonacci chain of 800 sites.

Fig.2: The power spectrum of a self-similar pattern shown in the inset. The highest frequency is given by $\nu = 0.5$ which is related to the change of $\rho_N(x_P \rightarrow x_P + 1)$. On respective figures five unambiguous frequencies have been located and named $\nu_{n=1,5}$.

Fig.3: Power spectrum of the pattern given in the inset for $m=5$, chain of 2000 sites.
Power spectrum

\[ \nu = \frac{5}{472} = 0.0106 \]

\[ \rho_N \]
Power spectrum

Frequency

$X_p$

$\rho_N$

$\nu_1 = 0.027$

$\nu_2 = 0.117$

$\nu_3$, $\nu_4$,

$\nu_5 = 0.264$
