Correlated Fermions in a One-Dimensional Quasiperiodic Potential

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We study analytically one-dimensional interacting spinless fermions in a Fibonacci potential. We show that the effects of the quasiperiodic modulation are intermediate between those of a commensurate potential and a disordered one. The system exhibits a metal-insulator transition whose position depends both on the strength of the correlations and on the position of the Fermi level. Consequently, the conductivity displays a power-law-like size and frequency behavior characterized by a nontrivial exponent.

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Since the discovery of quasicrystals in 1984 by Shechtman *et al.* [1], the electronic properties of quasiperiodic systems have been intensively studied. These metallic alloys are notably characterized by a low electrical conductivity σ which increases when either temperature or disorder increases [2]. The very low temperature behavior of σ is still an open question and depends on the materials. For example, in AlCuFe [3] and AlCuRu [4], a finite conductivity at zero temperature is expected, whereas recent results [5] seem to confirm a Mott's variable range hopping mechanism for *i*-AlPdRe down to 20 mK.

Many theoretical works have attempted to understand how the quasiperiodic order could induce such exotic behaviors. In particular, the case of independent electrons in one-dimensional (1D) systems has been deeply investigated for different structures (Harper model, Fibonacci chain, ... [6,7]), giving rise to singular continuous spectra with an infinite number of gaps. Moreover, the corresponding eigenstates are neither extended nor localized but critical, and are known to be responsible of anomalous diffusion [8,9]. For higher dimensional systems, similar studies had also displayed complex and intricated spectra, with analogous characteristics of the electronic states [10–13]. However, given the complexity of these problems due to the geometry alone, the interactions between electrons have often been neglected. Even in 1D incommensurate structures, few results have been obtained [14–18].

In this Letter, we investigate the effect of the interactions considering a Hubbard-like model for spinless fermions embedded in a Fibonacci potential. We take the correlations into account using a bosonization technique whereas the quasiperiodicity is treated perturbatively. Using a renormalization group approach, we show that the quasicrystalline system displays a metal-insulator transition (MIT) induced by the interactions. The corresponding critical MIT point is found to be strongly dependent on the Fermi level. In marked contrast with the simple cases of disordered or commensurate potentials, the quasiperiodicity leads to a power-law-like dependence of the conductivity either in size or frequency with an exponent depending both on the interactions and on the position of the Fermi level. Though our analysis is performed for a Fibonacci potential, we stress that these results can be extended to any potential having a nonflat dense Fourier spectrum.

Let us consider a model of interacting spinless fermions on a quasiperiodic lattice described by the following Hamiltonian:

$$H = -t \sum_{\langle i,j \rangle} c_i^\dagger c_j + V \sum_i n_i n_{i+1} + \sum_i W_i n_i \,, \quad (1)$$

where $c_i^\dagger$ (respectively, c_i) denotes the creation (respectively, annihilation) fermion operator, $n_i = c_i^\dagger c_i$ represents the fermion density on site i, and $\langle \cdots \rangle$ stands for nearest neighbors pairs. The quasiperiodicity is provided by the W_i's that take two discrete values $W_A = +\lambda/2$ or $W_B = -\lambda/2$ given by the spatial modulation of the Fibonacci chain. In fact, we consider a periodic approximant of this structure with F_l sites per unit cell that can be obtained by l iterations of the substitution rules: $A \to AB$, $B \to A$, where F_l is the lth element of the Fibonacci sequence defined by

$$\begin{aligned} F_1 &= F_2 = 1 \,, \\ F_{l+1} &= F_l + F_{l-1} \,. \end{aligned} \quad (2)$$

We denote $p = F_{l-2}, s = F_{l-1}, n = F_l$, and $n' = s$ (respectively, $n' = p$) if l is even (respectively, odd). In the quasiperiodic limit ($l \to \infty$), the ratio s/p converges toward the golden mean $\tau = (1 + \sqrt{5})/2$. It is also useful to compute the Fourier transform of the potential W. This can be done via the conumbering scheme [19]:

$$\hat{W}\left(q = \frac{2\pi m}{na}\right) = \frac{\lambda e^{i[\pi m n'(s-1)]/n} \sin(\frac{\pi m n' s}{n})}{n \sin(\frac{\pi m n'}{n})} \,, \quad (3)$$

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for $m = 1$ to $n - 1$ (a is the lattice spacing). A global shift of the W_i allows us to deal with a zero-averaged potential so that we can set $\hat{W}(0) = 0$. The interest of this potential lies in the fact that it is perturbatively nontrivial (the Fourier transform is dense in $[0, 2\pi]$, in the quasiperiodic limit). Moreover, the underlying substitution rule provides a self-similar structure that can be readily seen in Fig. 1.

If the quasiperiodic perturbation is small enough, we can focus on the low energy properties around the Fermi level. To treat the interactions, it is convenient to use a bosonic representation of the fermion operators. In this representation, the Hamiltonian (1) becomes

$$H = H_0 + H_W , \tag{4}$$

where H_0 stems from the periodic part ($\lambda = 0$) of (1) and reads in the continuum limit [20]:

$$H_0 = \frac{1}{2\pi} \int dx \left[(uK)(\pi \Pi)^2 + \left(\frac{u}{K}\right)(\partial_x \phi)^2 \right]. \tag{5}$$

In (5), ϕ is a boson field related to the long wavelength part of the fermionic density by $\rho(x) = -\nabla\phi(x)/\pi$, and Π is its canonically conjugate field. All the interactions are absorbed in the two constants u and K, where u is the renormalized Fermi velocity [in the noninteracting case ($K = 1$), $u = v_F = 2ta \sin(k_F a)$], and K is the parameter controlling the decay of various correlation functions. For weak interactions, u and K can be perturbatively expressed in terms of the microscopic parameters t and V:

$$uK = v_F, \qquad \frac{u}{K} = v_F + \frac{V}{\pi}[2 - 2\cos(2k_F a)]. \tag{6}$$

Actually, the representation (5) is more general [21,22] and gives the correct low energy description of the system, even when the interactions are strong provided the exact u and K parameters are used. The quasiperiodic part H_W can also be written in terms of the boson fields [23]:

$$H_W = \frac{1}{\pi\alpha} \int dx\, W(x) \cos[2k_F x - 2\phi(x)], \tag{7}$$

where k_F is the Fermi wave vector and α is a short distance cutoff of the order of the lattice constant a.

The effect of the quasiperiodic potential is computed using a perturbative renormalization group (RG) approach, similar to the one for a single harmonic [24]. The RG equations for the potential and the interaction parameter read

$$\frac{dK}{dl} = -\frac{K^2}{2} G(l), \tag{8}$$

$$\frac{dy_q}{dl} = (2 - K) y_q , \tag{9}$$

$$G(l) = \sum_{\varepsilon = \pm 1} \sum_q y_q^2 J[(q + \varepsilon 2k_F)\alpha(l)], \tag{10}$$

where $y_q = \alpha \hat{W}(q)/u$ is the dimensionless Fourier components of W, and $\alpha(l) = \alpha(0)e^l$ is the renormalized short distance cutoff. In (10), the sum over q is performed for $q = 2\pi m/n$ with $m \in [1, n - 1]$, and J is an ultraviolet regulator whose precise form depends on the cutoff procedure. For convenience, we choose a Gaussian form $J(x) = e^{-x^2}$ but, as discussed in Refs. [25,26], the physical properties are independent of this choice provided J decreases sufficiently rapidly. Note that the renormalization of the velocity u is neglected since it is of higher order in the potential amplitude λ.

The physical properties of the system are determined by the long distance behavior of K. If K converges toward a fixed point, the system remains metallic but with the renormalized parameter (K^*, u^*). Otherwise, the solution flows to a strong coupling regime whose physics depends on the precise nature of the potential W. Note that expression (7) is valid for any lattice potential perturbatively treated. For a single harmonic [$\hat{W}(q) = \lambda \delta_{q,q_0}$] two situations occur. If $q_0 \neq 2k_F$, R stops the renormalization of K at large enough length scale and the potential is irrelevant. On the contrary, if $q_0 = 2k_F$, one recovers the usual metal-insulator transition at $K_c = 2$. In the disordered case, the $\hat{W}(q)$'s are given by a uniform averaged distribution: $\overline{\hat{W}^*(q)\hat{W}(q')} = y\delta_{qq'}$. In the limit of weak disorder, (9) can be integrated neglecting the renormalization of K: $y(l) = y(0)e^{(2-K)l}$. Then, Eq. (8) simply becomes

$$\frac{dK}{dl} = -K^2 C e^{(3-2K)l}, \tag{11}$$

where C is a constant. Equation (11) defines a critical value $K_c = 3/2$, separating an insulating phase ($K < K_c$) from a metallic state ($K > K_c$) [27].

We now investigate the case of the Fibonacci potential. For a given maximum renormalization length scale $l_{\max}$ corresponding to accessible physical range, different cases

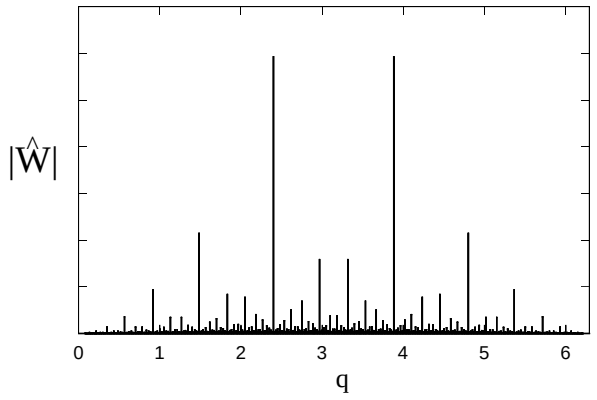

FIG. 1. Fourier transform of the diagonal Fibonacci potential for the 15th approximant with $F_{15} = 610$ sites per cell.

must be distinguished. If the Fermi momentum $2k_F$ is close to a main peak of the Fourier spectrum (3), then, at long distance (i.e., $l \sim l_{\max}$), the flow of K is controlled by this harmonic [see Fig. 2 (upper curve)] and its behavior is similar to the periodic one.

There is a transition at $K_c = 2$, with a metallic phase for $K > 2$ where the quasiperiodic potential is irrelevant. In this phase, the system has gapless excitations whose correlations are given by (5) with renormalized parameters. For $K < 2$, the quasiperiodicity is relevant and the system has a charge gap given by

$$\Delta \sim y_{2k_F}^{1/[2-K(0)]}. \tag{12}$$

Note that, for $K = 1$ (noninteracting case), one obtains a linear scaling of the gap opening. Our methods allow us to recover very simply the perturbative results [28] derived by quite different methods for the particular case of noninteracting electrons. The effect of the interactions is thus essentially to change the scaling of the gaps and to allow a MIT at $K_c = 2$ (attractive interactions).

A more unusual behavior is encountered when the Fermi level is far from a dominant harmonic of the quasiperiodic potential. Indeed, the low energy properties up to $l_{\max}$ are no more dominated by the ultimate presence of a gap or not but by the precise dependence of G with the scale. The specific feature of the quasiperiodic case is that, contrary to the disordered case, *G a priori* depends on the Fermi level. As shown in Fig. 3, it is reasonable to approximate this behavior by an exponential scaling. To know whether such a description is asymptotically correct or not, one would need an analytical calculation of G, a rather complicated task. In this context, the flow of K is given by

$$\frac{dK}{dl} = -K^2 D e^{(4-2K-\mu)l}, \tag{13}$$

where D is a constant.

The position of the MIT point is then given by $K_c = 2 - \mu/2$. In addition, the Fibonacci potential seems to provide a unique value $\mu \simeq 2$ (see Fig. 3) that leads to a transition for the noninteracting point $K_c = 1$. It would be interesting to know if this result remains true beyond the perturbative theory, and if it is a generic property of self-similar potentials. Finally, note that intermediate cases can also occur [see Fig. 2 (lower curve)] for which G cannot be naively approximated by an exponential law. In this context, one cannot simply extract a critical behavior from the RG equations. This deserves further investigations.

So, the quasicrystal differs from a periodic one, for which the gap acts only for a given position of the Fermi level with $K_c = 2$, and a disordered system for which the potential is relevant regardless of the position of the Fermi level, but below a constant critical value $K_c = 3/2$. This important modification of K_c is reminiscent of a correlated disorder with long range correlations in space for which the averaged disorder potential $\overline{\hat{W}^*(q)\hat{W}(q')} = \delta_{qq'}\Delta(q)$ is not constant.

The consequences of the scale dependence of G can be directly seen on transport quantities. In the regime where the RG equations are valid, the conductivity can be computed using a perturbative method. The simplest is to use the so-called memory function formalism [29] where the conductivity is expressed as $\sigma(\omega) = i/[\omega + M(\omega)]$. The memory function M, contrarily to σ, can be computed perturbatively in the scattering potential. We refer the readers to [30] for the technical details and give here only the main results. The high frequency optical conductivity and the dependence of the resistance with respect to the system size $L = e^l$ are given by

$$\sigma(\omega) \propto \mathrm{Im}M(l_\omega)/\omega^2, \tag{14}$$

$$R(L) \propto L\,\mathrm{Im}M(l_L), \tag{15}$$

where in each case the memory function M is computed at a renormalized frequency scale $l_\omega = \log(t/\omega)$ or at a renormalized size scale $l_L = \log[L/\alpha(0)]$. As for the single harmonic case [31], a perturbative calculation of M in power of the scattering potential gives

$$M(l) \propto G(l)e^{-l}. \tag{16}$$

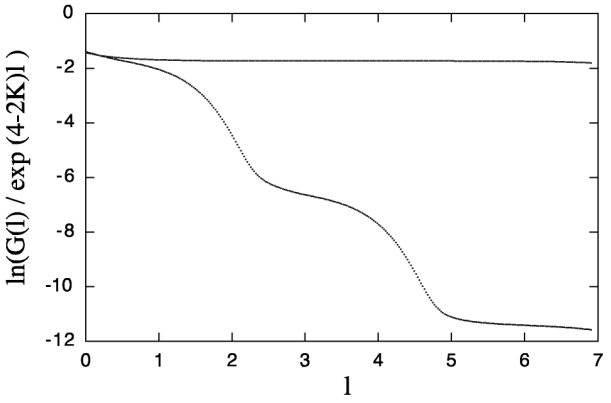

FIG. 2. Behavior of G for $2k_F = 2.63$ (lower curve) and $2k_F = 2.4$ (upper curve).

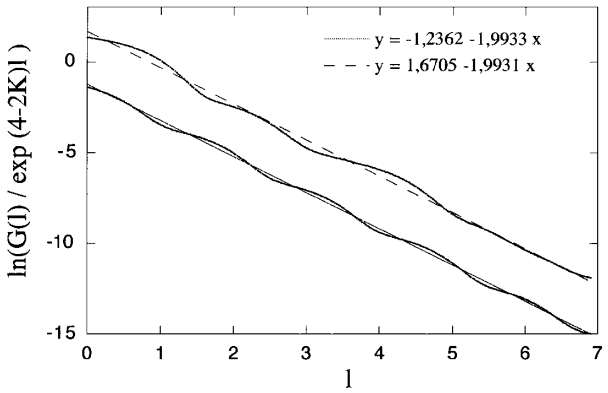

FIG. 3. Behavior of G for $2k_F = \pi$ (lower curve) and $2k_F = 1.95$ (upper curve). Both cases have been offset for clarity.

This expression remains valid as long as one remains in the perturbative regime, i.e., as long as the renormalization of K in (8) remains small. This is true for all length scales in the metallic regime $K > K_c$, where the potential W is irrelevant. For $K < K_c$, this holds until a certain length scale L_{SC} corresponding to the strong coupling limit. Using (15) and (13), one straightforwardly gets the resistance for the quasiperiodic system:

$$R(L) \sim L^{4-2K-\mu}, \tag{17}$$

so that $R(L) \sim L^{4-2K}$, $R(L) \sim L^{3-2K}$ for the commensurate and disordered cases, respectively. As foreseen, in the regime where the scattering potential is relevant the resistance increases with the scale. For noninteracting ($K = 1$) disordered electrons we simply recover the Ohm's law, which is valid below the localization length. For a quasicrystal with a dense Fourier spectrum, we find a nonuniversal power law increase of the resistance, with an exponent depending *both* on the interactions and on the position of the Fermi level. Correspondingly, there is a power law frequency dependence of the optical conductivity $\sigma(\omega) \sim (1/\omega)^{5-2K-\mu}$. The properties of potential W have thus a direct impact on the increase of the resistance. This is in contrast with both the disordered and the commensurate cases where the scaling of the resistance depends only upon the interactions. Such a behavior and the relationship between the conductivity exponent and the spectrum of the quasiperiodic potential should be testable in numerical simulations, or in artificially engineered systems. Note that for the noninteracting case, some numerical observations of a power law behavior for the conductivity have already been reported [32].

For $K < K_c$, the previous perturbative analysis ceases to be valid beyond the length scale L_{SC} for which $G(l_{SC}) \sim 1$. For the commensurate and the disorder case, this defines the correlation length respectively associated to the gap and to the localization length. Above L_{SC}, the resistance grows exponentially with the size of the system $R(L) \sim e^{L/L_{SC}}$. For the quasiperiodic case, our analysis shows that a corresponding typical length exists as well. However, its physical interpretation and the physical behavior above L_{SC} are still to be understood. Since for a noninteracting system the wave functions of a quasiperiodic system exhibit algebraic decay, a reasonable guess is that above L_{SC} the resistance keeps increasing as a power law but very likely with another exponent than $4 - 2K - \mu$. Clearly, the investigation of this strong coupling regime deserves further studies.

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