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To cite this article: M Puviani and F Manghi 2017 *J. Phys.: Conf. Ser.* **841** 012021

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Theory of photon-driven correlated electrons in one dimension

M Puviani¹ and F Manghi^{1,2}

¹ Dipartimento di Scienze Fisiche, Informatiche e Matematiche, Università degli Studi di Modena e Reggio Emilia, Via Campi 213/A, I-41125 Modena, Italy

² CNR-Institute of NanoSciences S3, Via Campi 213/A, I-41125 Modena, Italy

E-mail: matteo.puviani@unimore.it

Abstract. In this paper we present a general theoretical framework to study interacting electrons under the influence of an external time-periodic driving, such as a homogeneous laser field. This is performed through a true many-body calculation and the use of Floquet theory. In particular, we consider a linear atomic chain using the Hubbard model to describe the short-ranged Coulomb interactions between electrons, plus Cluster Perturbation Theory to embed the many-body exact solution for a finite system into both an extended and an infinite lattice. Due to the presence of the external time-periodic perturbation, the electronic problem can be mapped into the study of photon-dressed quasiparticles thanks to Floquet theorem, keeping into account of all the virtual processes (absorption and emission of photons by electrons) with the laser field. This leads to an extension of the many-body static theories to out-of-equilibrium systems. This theoretical approach allowed us to show how the electronic properties of the system can be controlled and tuned varying the laser parameters. Above all, an inverse insulator-to-metal transition can be obtained for the one dimensional infinite lattice, and edge localized states appear as a finite size effect in an extended truncated chain.

1. Introduction

The possibility of driving materials out of equilibrium with the application of a homogeneous laser field has been recently widely studied for simple non-interacting systems but with meaningful results [1,2]. In addition, these problems have become of greater interest thanks to the experimental advances in time- and angle-resolved photoemission spectroscopy (Tr-ARPES) [3] and the possibility of using cold atoms in optical lattices in presence of periodic drivings. In these conditions, the electrons of the material interact with the monochromatic electromagnetic field reaching a nonequilibrium steady state to form “photon-dressed quasiparticles”. These are a combination of electrons from the material and photons from the driving field: therefore they can be treated as free as a whole, replacing the concept of bare electrons interacting with an external field. This scheme allows us to study the problem using the Floquet theory, mapping the original out-of-equilibrium time-periodic problem into an effective steady time-independent one [4,5]. On the other hand, correlated static systems have always been fascinating due to their wide range of properties and applications, as well as for the possibility to induce and control phase transitions.

Therefore, the study of correlated systems with a true many-body approach in out-of-equilibrium conditions is at the same time challenging and interesting for the possibility to



control the new degrees of freedom due to the driving to obtain new properties and reach conditions otherwise not accessible in static conditions. Indeed, the presence of correlation between electrons is affected by the photon-dressing induced by the external time-periodic field, emerging in a competing effect between the local e - e repulsion and the absorption or emission of photons which leads to a renormalization of the kinetic energy of the electrons.

In this paper we considered the prototype system of a one dimensional atomic chain at half filling, described in static conditions by the Hubbard Hamiltonian and predicted to be insulating. Then, we included Floquet theory (section 2) to describe the exact interaction with an external laser field using an effectively time-independent scheme: to do this, the problem must be reformulated using the Green's function formalism. First, we calculate the one-particle Floquet-Green's function in the interacting framework for a finite size atomic cell (section 3). After that, this exact solution is embedded into the extended or infinite lattice with a Cluster Perturbation Theory (CPT) method [6–10], here applied to non-equilibrium conditions, in order to get the spectral functions and densities of states which describe the system (section 4). Eventually, our results are focused on the quasienergy band dispersion of the infinite chain and the comparison with the truncated chain, with highlight to finite-size effects (section 5).

2. The Floquet-Hubbard model

The problem of a lattice with a time-periodic external perturbation is characterized by an electronic time-periodic Hamiltonian $\hat{H}(t) = \hat{H}(t + T)$ ($T = \frac{2\pi}{\Omega}$ being the period of the external perturbation, Ω its frequency). Therefore, the time-dependent Schrödinger equation reads

$$\hat{H}(t)\Psi(\mathbf{x}, t) = i \partial_t \Psi(\mathbf{x}, t) , \quad (1)$$

where $\Psi(\mathbf{x}, t) = \Psi(x^{(1)}, x^{(2)}, \dots, x^{(N)}, t)$ is the many-body wave function for N particles. According to Floquet theorem, which can be interpreted as Bloch theorem in time domain, the solution can be written as a factorization of a quasiparticle wave function periodic in time and a complex exponential playing the role of the time-evolution of the quasiparticle:

$$\Psi(\mathbf{x}, t) = e^{-iEt} \Phi(\mathbf{x}, t) . \quad (2)$$

We have named E the quasiparticle energy and $\Phi(\mathbf{x}, t)$ the quasiparticle wave function, which can be rewritten according to Fourier expansion as

$$\Phi(\mathbf{x}, t) = \sum_{n=-\infty}^{+\infty} e^{-in\Omega t} \phi_n(\mathbf{x}) . \quad (3)$$

Substituting in (1) the form of the solution provided in (2) we get, after some algebra, the following equation:

$$\left(\hat{H}(t) - i \partial_t \right) \Phi(\mathbf{x}, t) = E \Phi(\mathbf{x}, t) . \quad (4)$$

Defining the Floquet operator as $\hat{H}_F \equiv \hat{H}(t) - i \partial_t$, playing the role of an effective Hamiltonian, equation (4) is mapped into a time-independent eigenvalue problem as follows:

$$\hat{H}_F \Phi_\alpha(\mathbf{x}, t) = E_\alpha \Phi_\alpha(\mathbf{x}, t) , \quad (5)$$

where α are the labels for Floquet eigenstates and their corresponding quasi-energies. Moreover, it's important to notice that, according to Floquet theorem and the expansion in (3), if E_α is a solution, then $E_\alpha + n\Omega$ (with n any integer number) is a solution, too. This means that

there are infinite replicas of Floquet quasienergies (or, equivalently, that they're defined up to multiples of the photon energy, Ω), which physically correspond to the exchange (either emission or absorption) of photons of the electrons with the applied electromagnetic field. Eventually, it's noticeable that while the expectation values of the Hamiltonian calculated for Floquet states are time-dependent (they are not conserved), namely $\langle \Psi_\alpha(t) | \hat{H}(t) | \Psi_\alpha(t) \rangle = \varepsilon_\alpha(t)$; Floquet quasienergies are not, and they are therefore conserved.

Now, in order to study a one-dimensional insulating chain as a true many-body problem, we can use the Hubbard Hamiltonian with one-orbital per atom, nearest-neighbor hopping and on-site Coulomb interaction. In static conditions it is written in the second quantized form as

$$\hat{H} = - \sum_{\langle i,j \rangle} \sum_{\sigma=\uparrow,\downarrow} J_{i,j} \hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + U \sum_i \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow}, \quad (6)$$

J describing the unperturbed hopping (non-local), while U is the repulsive Hubbard term (local). We can now describe the external driving by the vector potential in one dimension $A(t) = A_0 \sin(\Omega t)$: according to Peierls' substitution [11, 12] it can be included in the hopping term of the Hubbard Hamiltonian provided that $J_{i,j} \rightarrow J e^{iA(t)\cdot(x_i-x_j)}$. It can also be rewritten in an expanded form as follows:

$$J e^{iA(t)\cdot(x_i-x_j)} = \sum_{p=-\infty}^{+\infty} J_p(A_0(x_i-x_j)) e^{ip\Omega t}, \quad (7)$$

where $J_p(z)$ is the Bessel function of first kind and order p , with argument z . Moreover, for the driven system we can expand the time-dependent creation and annihilation operators similarly to (3), as follows:

$$\hat{c}_{i,\sigma}^\dagger(t) = \sum_{n=-\infty}^{+\infty} e^{-in\Omega t} \hat{c}_{i,\sigma,n}^\dagger, \quad \hat{c}_{i,\sigma}(t) = \sum_{n=-\infty}^{+\infty} e^{in\Omega t} \hat{c}_{i,\sigma,n}. \quad (8)$$

The time-independent operators appearing in the expansion act both on electrons (creating or annihilating one with spin σ on site i) and on the photons of the driving field, absorbing or emitting n of them (attention must be paid since the sign of n is physically meaningful). With the forementioned Peierls' substitution and the time-dependent creation/annihilation operators defined in (8), starting from (6), we can write the Floquet-Hubbard effective Hamiltonian as

$$\hat{H}_{FH} = -J \sum_{\langle i,j \rangle} \sum_{\sigma=\uparrow,\downarrow} \sum_{n,m=-\infty}^{+\infty} e^{iA(t)\cdot(x_i-x_j)} \hat{c}_{i,n,\sigma}^\dagger \hat{c}_{j,m,\sigma} e^{i(n-m)\Omega t} + U \sum_i \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow} - i\partial_t. \quad (9)$$

Here we have put $J_{i,j} = J$, with the summation performed over i, j neighboring sites. Its solution can be written in the form provided in (3), where the spatial many-body wave function $\phi_n(\mathbf{x})$ can be expanded in a complete set of localized non-interacting N -particle states. However, this can be done via exact diagonalization only for a finite and small number of electrons.

3. Cluster Floquet-Green's Function

It is convenient for our theoretical development to use the Green's function formalism, here extended to correlated driven systems treated with Floquet approach. In particular, we can write the Floquet-Green's function in the Lehmann representation as follows:

$$G_{ij, nm}(\omega) = \lim_{\eta \rightarrow 0^+} \sum_{n', n'', m', m''} \sum_{\xi} \left(\frac{\langle \Phi_{0,m'}^N | \hat{c}_{j,m}^\dagger | \Phi_{\xi, m''}^{N-1} \rangle \langle \Phi_{\xi, n'}^{N-1} | \hat{c}_{i,n} | \Phi_{0, n''}^N \rangle}{\omega - E_0^N + E_{\xi}^{N-1} - i\eta} \delta_{m''+m, m'} \delta_{n''-n, n'} \right. \\ \left. + \frac{\langle \Phi_{0,m'}^N | \hat{c}_{i,n} | \Phi_{\xi, m''}^{N+1} \rangle \langle \Phi_{\xi, n'}^{N+1} | \hat{c}_{j,m}^\dagger | \Phi_{0, n''}^N \rangle}{\omega + E_0^N - E_{\xi}^{N+1} + i\eta} \delta_{m''-n, m'} \delta_{n''+m, n'} \right). \quad (10)$$

In order to compute it, we need to know all the interacting $(N + 1)$ - and $(N - 1)$ -particles eigenstates and eigenvalues, plus the ground state of N particles and its energy. Actually, this last step requires us to define an interacting many-body ground state for a system in non-equilibrium conditions, whose energy is given up to multiples of the photon energy of the driving. Indeed, even though the result is independent on which replica of the ground state level is chosen, still the states of a Floquet mode are mixed with other replicas of different modes. This means that excited states of a given mode can have lower energies of the ground state of a higher mode (i.e.: if $E_{1,n} - E_{0,n} < \Omega$, then $E_{1,n-1} = E_1 + (n - 1)\Omega < E_{0,n} = E_0 + n\Omega$). In order to solve this intrinsic ambiguity and make a meaningful physical choice, we have adopted an adiabatic criterion: once the ground state for the static condition (represented by a null vector potential $A_0 = 0$) is found (the problem can be solved in this limit even without Floquet approach), we switch the perturbation on increasing the vector potential and we calculate the energy levels for the different values of A_0 . The ground state energy at each value of the external field is then obtained continuously and smoothly following the ground state level through the increasing of the driving, from $A_0 = 0$ up to the desired value.

4. CPT and Lattice Floquet-Green's Function

Once we have obtained the Floquet-Green's function to describe a small cluster of atoms in the presence of correlation and a time-periodic driving, the extension to a larger or infinite system can be performed through Cluster Perturbation Theory. In an operatorial form the following Dyson-like expression holds:

$$\hat{G}^{\text{lat}}(\omega) = \hat{G}^{\text{cl}}(\omega) + \hat{G}^{\text{cl}}(\omega) \hat{T} \hat{G}^{\text{lat}}(\omega) . \quad (11)$$

$\hat{G}^{\text{cl}}(\omega)$ and $\hat{G}^{\text{lat}}(\omega)$ are the cluster and the lattice Floquet-Green's functions respectively, and \hat{T} represents the interaction between clusters. The latter contains solely the hopping term, which is the factor allowing for tunneling of electrons between the atomic sites of the lattice, and is the only non-local term in the Floquet-Hubbard Hamiltonian connecting neighboring clusters. Translated into the Floquet-Hubbard formalism, this becomes

$$G_{ij, nm}^{\text{lat}}(\omega) = G_{ij, nm}^{\text{cl}}(\omega) + \sum_{\langle i', j' \rangle} \sum_{n', m'} G_{i' i', n n'}^{\text{cl}}(\omega) T_{i' j', n' m'}(k, \omega) G_{j' j', m' m}^{\text{lat}}(\omega) , \quad (12)$$

where the summation is performed over neighboring sites. $T_{i' j', n' m'}(k, \omega) = \sum_l J_{n' - m'}(A_0(x_{i'} - x_{j'})) e^{ikR_l}$ is the effective time-independent hopping as appearing in expression (7) with the periodicity of the cluster. The lattice Floquet-Green's function can be computed numerically by equation (12): it is valid both for an infinite lattice and for an extended finite one. In the former case periodicity is included in the hopping term of interactions between clusters, while in the latter one a Floquet-Green's function for M -sites (M large) can be computed starting from a few-sites function explicitly including the interactions (which are here a finite number) between neighboring clusters (in this case the k -dependence in it vanishes). For an infinite lattice we can compute the spectral functions of the photon-dressed quasiparticles as

$$D(k, \omega) = -\frac{1}{\pi} \sum_b \text{Im} \{ G_b^{\text{lat}}(k, \omega) \} , \quad (13)$$

where the summation is intended over all the bands, and with

$$G_b^{\text{lat}}(k, \omega) = \sum_{ij, nm} e^{-ik(x_i - x_j)} c_{i, n}^b(k)^* c_{j, m}^b(k) G_{ij, nm}^{\text{lat}}(k, \omega) . \quad (14)$$

The coefficients $c_{i,n}^b(k)$ and $c_{j,m}^b(k)$ are obtained from the solution of the Floquet problem without interactions (single-particle). On the other hand, for a finite chain the local and the total density of states are given respectively by

$$n_i(\omega) = -\frac{1}{\pi} \sum_b \sum_{n,m} \text{Im}\{(c_{i,n}^b)^* c_{i,m}^b G_{ii,nm}^{\text{lat}}(\omega)\}, \quad n(\omega) = \sum_i n_i(\omega). \quad (15)$$

5. Results

Using this theoretical approach, we firstly computed the exact diagonalization for a cluster formed by two sites at half occupation, then we calculated the infinite lattice Floquet-Green's function and the corresponding spectral function. We performed a systematic calculation of the Floquet quasienergy bands for different values of the correlation ($0 < U < 4$) and the external field parameters ($0 < A_0 < 5$ and $1 < \Omega < 10$), analyzing their features: in particular, as pointed out in [13], an insulator-to-metal transition can be driven by the external field at low frequencies ($\Omega \lesssim J$) and values of A_0 non-trivially depending on these parameters. However,

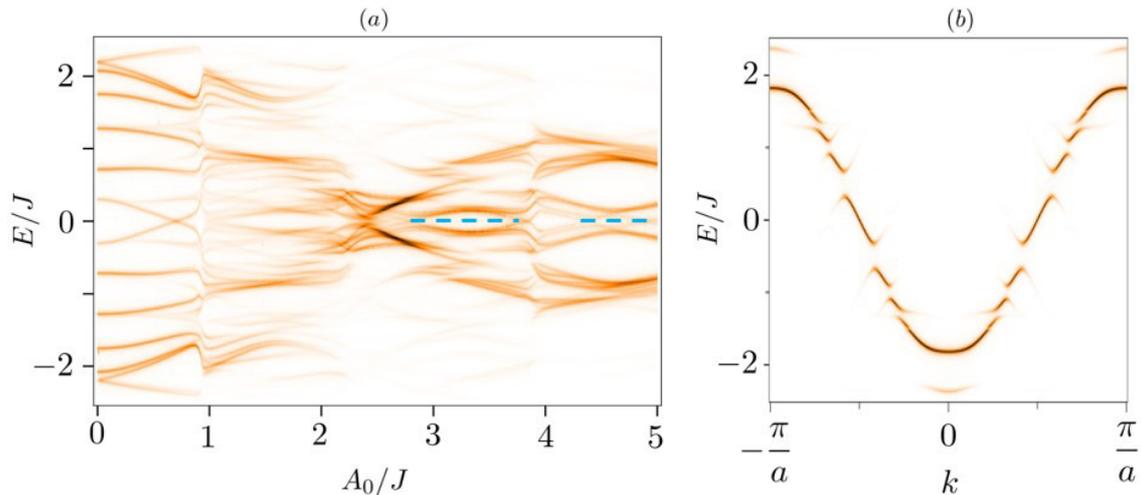


Figure 1. (a) Zero-mode Floquet quasienergy band dispersion for an infinite 1D chain calculated for $U/J = 2.0$ and $\Omega = 1.0 J$ in 11 k-points in the FBZ, as a function of the field intensity A_0/J . Dashed blue lines are drawn in correspondence of the zero-energy states of the finite chain lying in the bulk gap (see Fig. 2(a)). (b) Zero-mode quasienergy band dispersion for $U/J = 2.0$, $\Omega = 1.0 J$ and $A_0/J = 0.7$ within the FBZ.

this is not due to the Floquet quasienergies replicas, but to virtual processes, since it shows up also in the zero Floquet mode where the average number of photons exchanged is zero. In Fig. 1(a) is represented the quasienergy band dispersion for some k-points for different A_0 values in the case of $\Omega = 1.0 J$ and $U/J = 2.0$: the closure of the gap in the Floquet zero-mode around the Fermi level in the quasienergy band dispersion occurs at $A_0/J \approx 0.7$, $A_0/J \approx 2.78$, $A_0/J \approx 3.84$ and higher values. In Fig. 1(b), instead, the band dispersion within the FBZ is reported for the specific value of $A_0/J = 0.7$, for which the gap is closed and the chain has a metal behaviour. With the same parameters of the driving field we calculated the density of states for an extended linear chain of 30 atoms, with the repetition of a 2-sites cluster: the results are shown in Fig. 2(a) as a function of the vector potential A_0 . It can be seen that for this finite system zero-energy levels appear in correspondence of the gap of the infinite lattice band dispersion (reported as dashed blue lines in Fig. 1(a)). Moreover, analyzing for these

parameters the local density of states for each site of the chain as represented in Fig. 2(b), it is clear that these zero-energy states appearing in the finite chain are localized at the edges and exponentially decay in the inside.

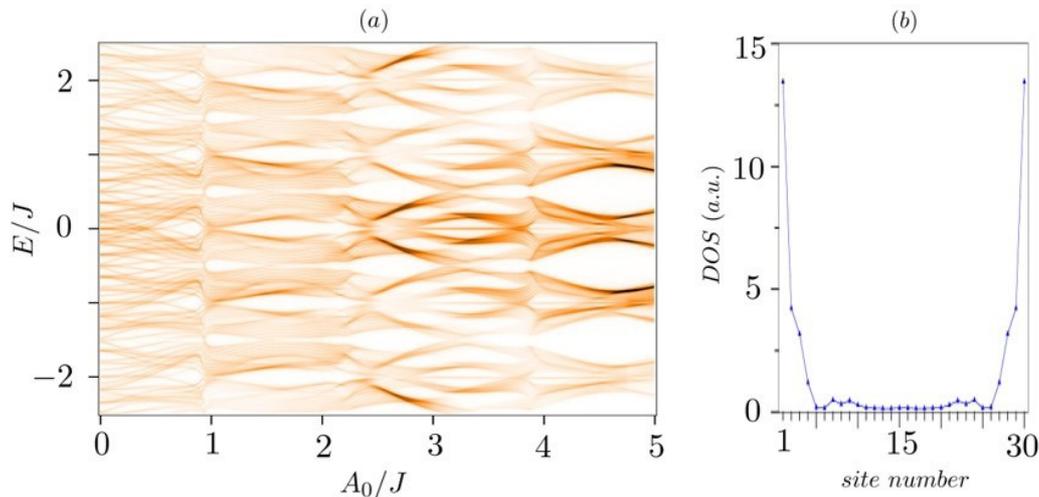


Figure 2. (a) Density of states of an open 1D chain with 30 atoms, calculated for $U/J = 2.0$ and $\Omega = 1.0 J$. In panel (b) the local densities of states for the zero-energy level are reported as a function of the sites positions, for $U/J = 2.0$, $\Omega = 1.0 J$ and $A_0/J = 3.0$.

6. Conclusion

In conclusion, we have developed a theoretical method to calculate Floquet quasienergies for extended correlated systems driven out of equilibrium by a periodic perturbation. In order to treat the many-body problem we used the exact diagonalization of the Hubbard model including Floquet theory for time-periodic systems in it. Moreover, we combined CPT to the Floquet-Green's function formalism in order to describe extended or infinite lattices. In this paper, we applied the theory to a one dimensional chain, comparing the infinite lattice to the truncated chain in order to characterize the finite size effects for this system. In fact, in the periodic lattice insulating and metallic phases can be driven by the external field, while gapless edge states appear in the bulk insulating phase. Since this procedure is fairly general, it can be extended to 2- or 3-dimensional lattices, while the Hubbard model could be also applied to superconductors describing attractive $e - e$ interactions.

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