Supplementary Material for Spin-resolved charge flow through an AC-driven impurity

Daniel Thuberg\(^1\), Enrique Muñoz\(^3\), Sebastian Eggert\(^2\) and Sebastián A. Reyes\(^1\)
\(^1\)Instituto de Física and Centro de Investigación en Nanotecnología y Materiales Avanzados, Pontificia Universidad Católica de Chile, Casilla 306, Santiago 22, Chile and
\(^2\)Physics Department and Research Center OPTIMAS, University of Kaiserslautern, D-67663 Kaiserslautern, Germany

Here we discuss in detail the mathematical formulation and intermediate steps leading to the mean-field theory approximation and corresponding Floquet equations presented in the main body of the article.

PACS numbers: 05.60.-k,

For a system that is periodically driven, periodicity in time allows to express the solutions to the dynamical problem in terms of a set of eigenfunctions \( |\Psi(t)\rangle = e^{-i\omega t} |\Phi(t)\rangle \), with \( \omega \) a Floquet eigenvalue, and an associated periodic eigenfunction \( |\Phi(t + T)\rangle = |\Phi(t)\rangle \). If one restricts the non-equivalent values of \( \omega \) to a first Brillouin zone \( \epsilon \in [-\pi/T, \pi/T] \), then the periodic eigenfunction can be expanded as

\[
|\Phi(t)\rangle = \sum_{n \in Z} e^{-i\omega t}|\Phi_n\rangle,
\]

where each stationary Floquet mode \( |\Phi_n\rangle \) is associated to an eigenvalue \( \epsilon_n = \epsilon + n\hbar\omega \) outside the first Brillouin zone.

Let us consider now the Hamiltonian described in the main body of the article,

\[
\hat{H} = -J \sum_{j,\sigma} \left( \hat{c}_{j+1,\sigma}^\dagger \hat{c}_{j,\sigma} + \text{h.c.} \right) + U \hat{n}_{0,\downarrow} \hat{n}_{0,\uparrow} + (\epsilon_d - \sigma b - \mu \cos(\omega t)) \sum_{\sigma} \hat{n}_{0,\sigma}
\]

The exact treatment of the interaction would require a two-particle eigenbasis. Here, in order to obtain a simpler physical interpretation of the transport properties, we decide to remain in the single-particle eigenbasis \( |j,\sigma\rangle = \hat{c}_{j,\sigma}^\dagger |0\rangle \), for \( \{ \hat{c}_{j,\sigma}, \hat{c}_{j',\sigma'}^\dagger \} = \delta_{\sigma \sigma'} \delta_{j, j'} \) Fermionic operators. Therefore, each stationary Floquet component in the periodic function defined by Eq.(1) is expressed by a linear combination of the form

\[
|\Phi_n\rangle = \sum_j \phi_{j,n}^\sigma |j,\sigma\rangle
\]

Therefore, we treat the Coulomb interaction in a mean-field theory (MFT) approximation, using the standard decoupling of the number operators as follows

\[
U \hat{n}_{0,\uparrow} \hat{n}_{0,\downarrow} \sim U \langle \hat{n}_{0,\uparrow}(t) \rangle \hat{n}_{0,\downarrow} + U \langle \hat{n}_{0,\downarrow}(t) \rangle \hat{n}_{0,\uparrow} - U \langle \hat{n}_{0,\uparrow}(t) \rangle \langle \hat{n}_{0,\downarrow}(t) \rangle
\]

In Eq.(4), we have introduced the definition of the time-dependent expectation value of the number operators in the Floquet eigenstate \( |\Phi(t)\rangle \)

\[
\langle \hat{n}_{0\sigma}\rangle(t) = \langle \Phi(t)|\hat{n}_{0,\sigma}|\Phi(t)\rangle = \sum_{n_1, n_2 \in Z} e^{-i(n_1 - n_2)\omega t} \langle \Phi_{n_2}|\hat{n}_{0,\sigma}|\Phi_{n_1}\rangle
\]

Notice that Eq.(5) shows that the interaction couples different Floquet modes \( |\Phi_n\rangle \) through the dynamical expectation value of the local number operators. Let us now calculate the matrix elements involved, using the single-particle representation of the Floquet basis Eq.(3)

\[
\langle \Phi_{n_2}|\hat{n}_{0,\sigma}|\Phi_{n_1}\rangle = \sum_{j_1, j_2, \sigma_1, \sigma_2} (\phi_{j_2, n_2})^\sigma \phi_{j_1, n_1} \times \langle j_2, \sigma_2|\hat{n}_{0,\sigma}|j_1, \sigma_1\rangle = (\phi_{0, n_2}^\sigma)^* \phi_{0, n_1}^\sigma
\]

where we used the identity \( \langle j_2, \sigma_2|\hat{c}_{0,\sigma}^\dagger \hat{c}_{0,\sigma}|j_1, \sigma_1\rangle = \delta_{j_1,0} \delta_{j_2,0} \delta_{\sigma_1, \sigma} \delta_{\sigma_2, \sigma} \). Substituting Eq.(6) into Eq.(5), reduces to the simpler expression

\[
\langle \hat{n}_{0\sigma}\rangle(t) = \sum_{n \in Z} e^{-i\omega t}\nu_{0,n}^\sigma = \nu_{0,n}
\]

where we have defined the parameters

\[
\nu_{0,n}^\sigma = \sum_{m \in Z} (\phi_{0,m}^\sigma)^* \phi_{0,n+m}^\sigma
\]

Using Eq.(7), we can express the product of occupation numbers that appears in Eq.(4) as

\[
\langle \hat{n}_{0,\uparrow}(t) \rangle \langle \hat{n}_{0,\downarrow}(t) \rangle = \sum_{n_1, n_2 \in Z} e^{-i(n_1 + n_2)\omega t}\nu_{0,n_1}^\uparrow \nu_{0,n_2}^\downarrow
\]

Here, we have defined

\[
\beta_n = \sum_{m \in Z} \nu_{0,n}^\uparrow \nu_{0,n-m}^\downarrow
\]

Inserting the MFT terms into the Hamiltonian Eq.(2),
we obtain the effective single-particle MFT Hamiltonian
\[ \hat{H}_{MFT}(t) = -J \sum_{j,\sigma} \left( \hat{c}^\dagger_{j+1,\sigma} \hat{c}_{j,\sigma} + \text{h.c.} \right) \]
\[ + \sum_{\sigma} \left[ \epsilon_d - \sigma b - \mu \cos \omega t + U \sum_{n \in \mathbb{Z}} e^{-in\omega t} \nu_0^\sigma \right] \hat{n}_{0,\sigma} \]
\[ - \sum_{n \in \mathbb{Z}} e^{-in\omega t} \beta_n(t) \]

(11)

The eigenvalue equation for this MFT effective Hamiltonian is
\[ \hat{H}_{MFT}(t) \Phi(t) = (\epsilon + n\hbar\omega) \Phi(t) \]

(12)

Projecting this equation onto a single-particle state of the basis \( \langle i, \sigma' | \), we have
\[ \sum_{n \in \mathbb{Z}} e^{-in\omega t} \sum_{j,\sigma} \phi^\sigma_{j,n} \]
\[ \times \left( \langle i, \sigma' | \hat{H}_{MFT}(t) | j, \sigma \rangle - (\epsilon + n\hbar\omega) \delta_{ij} \delta_{\sigma\sigma'} \right) = 0 \]

(13)

From the orthogonality of the set \( \{ e^{-in\omega t} \}_{n \in \mathbb{Z}} \), we finally obtain the set of finite-differences equations
\[ -J \left( \phi^\sigma_{i+1,n} + \phi^\sigma_{i-1,n} \right) - (\epsilon + n\hbar\omega + \beta_n) \phi^\sigma_{i,n} \]
\[ - \delta_{i,0} \left[ (\epsilon_d + \sigma b) \phi^\sigma_{0,n} + \frac{\mu}{2} \left( \phi^\sigma_{0,n+1} + \phi^\sigma_{0,n-1} \right) \right] \]
\[ + \delta_{i,0} U \sum_{m \in \mathbb{Z}} \nu^\sigma_{0,m} \phi^\sigma_{0,n-m} = 0 \]

(14)

whose numerical and analytical solution is developed and discussed for different physical scenarios in the main body of the article.