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

Daniel Thuberg[1], Enrique Muñoz[1], 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.

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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 $|\Psi(t)\rangle = e^{-i\hbar^{-1}\epsilon t}|\Phi(t)\rangle$, with ϵ a Floquet eigenvalue, and an associated periodic eigenfunction $|\Phi(t+T)\rangle = |\Phi(t)\rangle$. If one restricts the non-equivalent values of ϵ to a first Brillouin zone $\epsilon \in [-\pi\hbar/T, \pi\hbar/T]$, then the periodic eigenfunction can be expanded as

$$|\Phi(t)\rangle = \sum_{n\in Z} e^{-in\omega t}|\Phi_n\rangle, \tag{1}$$

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,

$$\begin{aligned}\hat{H} &= -J\sum_{j,\sigma}\left(\hat{c}^\dagger_{j+1,\sigma}\hat{c}_{j,\sigma} + h.c.\right) + U\hat{n}_{0,\uparrow}\hat{n}_{0,\downarrow} \\ &+ (\epsilon_d - \sigma b - \mu\cos(\omega t))\sum_\sigma \hat{n}_{0,\sigma}\end{aligned} \tag{2}$$

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 $|j,\sigma\rangle = \hat{c}^\dagger_{j\sigma}|0\rangle$, for $\{\hat{c}_{j\sigma}, \hat{c}^\dagger_{j'\sigma'}\} = \delta_{\sigma\sigma'}\delta_{j,j'}$ Fermonic operators. Therefore, each stationary Floquet component in the periodic function defined by Eq.(1) is expressed by a linear combination of the form

$$|\Phi^\sigma_n\rangle = \sum_j \phi^\sigma_{j,n}|j,\sigma\rangle \tag{3}$$

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

$$\begin{aligned}U\hat{n}_{0,\uparrow}\hat{n}_{0,\downarrow} &\sim U\langle\hat{n}_{0,\uparrow}\rangle_{(t)}\hat{n}_{0,\downarrow} + U\langle\hat{n}_{0,\downarrow}\rangle_{(t)}\hat{n}_{0,\uparrow} \\ &\quad -U\langle\hat{n}_{0,\uparrow}\rangle_{(t)}\langle\hat{n}_{0,\downarrow}\rangle_{(t)}\end{aligned} \tag{4}$$

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

$$\begin{aligned}\langle\hat{n}_{0\sigma}\rangle_{(t)} &= \langle\Phi(t)|\hat{n}_{0,\sigma}|\Phi(t)\rangle \\ &= \sum_{n_1,n_2\in Z} e^{-i(n_1-n_2)\omega t}\langle\Phi_{n_2}|\hat{n}_{0,\sigma}|\Phi_{n_1}\rangle\end{aligned} \tag{5}$$

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)

$$\begin{aligned}\langle\Phi_{n_2}|\hat{n}_{0,\sigma}|\Phi_{n_1}\rangle &= \sum_{j_1,j_2,\sigma_1,\sigma_2}\left(\phi^{\sigma_2}_{j_2,n_2}\right)^*\phi^{\sigma_1}_{j_1,n_1} \\ &\quad\times\langle j_2,\sigma_2|\hat{n}_{0,\sigma}|j_1,\sigma_1\rangle \\ &= \left(\phi^\sigma_{0,n_2}\right)^*\phi^\sigma_{0,n_1}\end{aligned} \tag{6}$$

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

$$\langle\hat{n}_{0\sigma}\rangle_{(t)} = \sum_{n\in Z} e^{-in\omega t}\nu^\sigma_{0,n} \tag{7}$$

where we have defined the parameters

$$\nu^\sigma_{0,n} = \sum_{m\in Z}\left(\phi^\sigma_{0,m}\right)^*\phi^\sigma_{0,n+m} \tag{8}$$

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

$$\begin{aligned}\langle\hat{n}_{0,\uparrow}\rangle_{(t)}\langle\hat{n}_{0,\downarrow}\rangle_{(t)} &= \sum_{n_1,n_2\in Z} e^{-i(n_1+n_2)\omega}\nu^\uparrow_{0,n_1}\nu^\downarrow_{0,n_2} \\ &= \sum_{n\in Z} e^{-in\omega t}\beta_n\end{aligned} \tag{9}$$

Here, we have defined

$$\beta_n = \sum_{m\in Z}\nu^\uparrow_{0,n}\nu^\downarrow_{0,n-m} \tag{10}$$

Inserting the MFT terms into the Hamiltonian Eq.(2), we obtain the effective single-particle MFT Hamiltonian

$$\begin{aligned}\hat{H}_{MFT}(t) &= -J\sum_{j,\sigma}\left(\hat{c}^{\dagger}_{j+1,\sigma}\hat{c}_{j,\sigma}+h.c.\right)\\ &+\sum_{\sigma}\left[\epsilon_d-\sigma b-\mu\cos\omega t+U\sum_{n\in Z}e^{-in\omega t}\nu^{\bar{\sigma}}_{0,n}\right]\hat{n}_{0,\sigma}\\ &-\sum_{n\in Z}e^{-in\omega t}\beta_n(t)\end{aligned} \tag{11}$$

The eigenvalue equation for this MFT effective Hamiltonian is

$$\hat{H}_{MFT}(t)|\Phi(t)\rangle = (\epsilon+n\hbar\omega)\,|\Phi(t)\rangle \tag{12}$$

Projecting this equation onto a single-particle state of the basis $\langle i,\sigma'|$, we have

$$\begin{aligned}&\sum_{n\in Z}e^{-in\omega t}\sum_{j,\sigma}\phi^{\sigma}_{j,n} \qquad (13)\\ &\times\left(\langle i,\sigma'|\hat{H}_{MF}(t)|j,\sigma\rangle-(\epsilon+n\hbar\omega)\delta_{ij}\delta_{\sigma',\sigma}\right)=0\end{aligned}$$

From the orthogonality of the set $\left\{e^{-in\omega t}\right\}_{n\in Z}$, we finally obtain the set of finite-differences equations

$$\begin{aligned}&-J\left(\phi^{\sigma}_{i+1,n}+\phi^{\sigma}_{i-1,n}\right)-\left(\epsilon+n\hbar\omega+\beta_n\right)\phi^{\sigma}_{i,n}\\ &-\;\delta_{i,0}\left[\left(\epsilon_d+\sigma b\right)\phi^{\sigma}_{0,n}+\frac{\mu}{2}\left(\phi^{\sigma}_{0,n+1}+\phi^{\sigma}_{0,n-1}\right)\right]\\ &+\;\delta_{i,0}U\sum_{m\in Z}\nu^{\bar{\sigma}}_{0,m}\phi^{\sigma}_{0,n-m}=0\end{aligned} \tag{14}$$

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