I. SUPPLEMENTARY MATERIAL (1) – DECOUPLING SCHEMES

A. Spectral function of the correlated-hopping model

Here we present and solve the equations for the spectral function \( \langle \langle d_\sigma d_\sigma^\dagger \rangle \rangle \) of the full model including correlated hopping. The following commutator will be needed:

\[
[d_\sigma, H] = \varepsilon_\sigma d_\sigma + Un_\sigma d_\sigma - x \sum_{\lambda k} V_{\lambda k\varphi} c_{\lambda k\varphi}^\dagger d_\sigma d_\sigma + \sum_{\lambda k} V_{\lambda k\varphi}^* c_{\lambda k\varphi} - x \sum_{\lambda k} V_{\lambda k\varphi}^* n_\varphi c_{\lambda k\varphi} - x \sum_{\lambda k} V_{\lambda k\varphi}^* d_\sigma^\dagger c_{\lambda k\varphi} d_\sigma.
\]  

The spectral function is found to fulfil the equation

\[
[\omega - \varepsilon_\sigma] \langle \langle d_\sigma d_\sigma^\dagger \rangle \rangle_\omega = 1 + \sum_{\lambda k} V_{\lambda k\varphi}^* \langle \langle c_{\lambda k\varphi} d_\sigma^\dagger \rangle \rangle_\omega - x \sum_{\lambda k} V_{\lambda k\varphi}^* \langle \langle n_\varphi c_{\lambda k\varphi} d_\sigma^\dagger \rangle \rangle_\omega.
\]

\[
- x \sum_{\lambda k} \left[ V_{\lambda k\varphi} \langle \langle c_{\lambda k\varphi}^\dagger d_\sigma d_\sigma^\dagger \rangle \rangle_\omega + V_{\lambda k\varphi}^* \langle \langle d_\sigma^\dagger c_{\lambda k\varphi} d_\sigma^\dagger \rangle \rangle_\omega \right] + U \langle \langle n_\varphi d_\sigma d_\sigma^\dagger \rangle \rangle_\omega.
\]  

Fife new GFs have appeared on the rhs of the last equation. In turn we calculate all of them, again using the equation of motion (B5) of the main text. The simplest one is given by

\[
(\omega - \varepsilon_\lambda k) \langle \langle c_{\lambda k\varphi} d_\sigma^\dagger \rangle \rangle_\omega = V_{\lambda k\varphi} \langle \langle D_\sigma d_\sigma^\dagger \rangle \rangle_\omega = V_{\lambda k\varphi} \langle \langle d_\sigma d_\sigma^\dagger \rangle \rangle_\omega - x V_{\lambda k\varphi} \langle \langle n_\varphi d_\sigma d_\sigma^\dagger \rangle \rangle_\omega.
\]  

The next GF, which plays an as important role as the spectral one, is that multiplied by \( U \). For future reference, the required commutator is given as follows:

\[
[n_\varphi d_\sigma, H] = (\varepsilon_\sigma + U)n_\varphi d_\sigma - \sum_{\lambda k} V_{\lambda k\varphi} c_{\lambda k\varphi}^\dagger d_\sigma d_\sigma + (1 - x) \sum_{\lambda k} V_{\lambda k\varphi}^* n_\varphi c_{\lambda k\varphi} + V_{\lambda k\varphi}^* d_\sigma^\dagger c_{\lambda k\varphi} d_\sigma.
\]

Its use immediately leads to the following equation:

\[
[\omega - \varepsilon_\sigma - U] \langle \langle n_\varphi d_\sigma d_\sigma^\dagger \rangle \rangle_\omega = \langle \langle n_\varphi \rangle \rangle - \sum_{\lambda k} V_{\lambda k\varphi} \langle \langle c_{\lambda k\varphi}^\dagger d_\sigma d_\sigma^\dagger \rangle \rangle_\omega
\]

\[
+(1 - x) \sum_{\lambda k} \left[ V_{\lambda k\varphi}^* \langle \langle n_\varphi c_{\lambda k\varphi} d_\sigma^\dagger \rangle \rangle_\omega + V_{\lambda k\varphi}^* \langle \langle d_\sigma^\dagger c_{\lambda k\varphi} d_\sigma^\dagger \rangle \rangle_\omega \right].
\]
With the notation analogous to that introduced previously:

\[ S_{n}^{sp} = \sum_{\lambda k} V_{\lambda k} \langle \langle n_{\sigma} c_{\lambda k \sigma} | d_{\sigma}^{\dagger} \rangle \rangle_\omega, \quad (6) \]

\[ S_{d}^{sp} = \sum_{\lambda k} V_{\lambda k}^{*} \langle \langle d_{\sigma}^{\dagger} c_{\lambda k \sigma} | d_{\sigma} \rangle \rangle_\omega, \quad (7) \]

\[ S_{c}^{sp} = \sum_{\lambda k} V_{\lambda k}^{*} \langle \langle c_{\lambda k \sigma} d_{\sigma} | d_{\sigma}^{\dagger} \rangle \rangle_\omega, \quad (8) \]

where ‘sp’ refers to the spectral GF, we rewrite Eqs. (2) and (5) in the more convenient form

\[
[\omega - \varepsilon_{\sigma} - \Sigma_{\sigma}](\langle \langle d_{\sigma} | d_{\sigma}^{\dagger} \rangle \rangle_\omega = 1 - x(S_{n}^{sp} + S_{d}^{sp} + S_{c}^{sp}) + (U - x\Sigma_{\sigma})(\langle \langle n_{\sigma} d_{\sigma} | d_{\sigma}^{\dagger} \rangle \rangle_\omega, \quad (9) \]

\[
[\omega - \varepsilon_{\sigma} - U](\langle \langle n_{\sigma} d_{\sigma} | d_{\sigma}^{\dagger} \rangle \rangle_\omega = (\langle \langle \sigma \rangle \rangle - S_{n}^{sp} + (1 - x)(S_{d}^{sp} + S_{c}^{sp}). \quad (10) \]

The remaining GFs appearing on the rhs of Eq. (5) are calculated in a similar way. In order to obtain the following equations of motion:

\[
[\omega - \varepsilon_{\lambda k}](\langle \langle n_{\sigma} c_{\lambda k \sigma} | d_{\sigma}^{\dagger} \rangle \rangle_\omega = (1 - x)V_{\lambda k \sigma}(\langle \langle n_{\sigma} d_{\sigma} | d_{\sigma}^{\dagger} \rangle \rangle_\omega - \sum_{\lambda' k'} V_{\lambda' k' \sigma}^{*} \langle \langle c_{\lambda' k' \sigma}^{\dagger} D_{\sigma} c_{\lambda k \sigma} | d_{\sigma}^{\dagger} \rangle \rangle_\omega + \sum_{\lambda' k'} V_{\lambda' k' \sigma}^{*} \langle \langle D_{\sigma}^{\dagger} c_{\lambda' k' \sigma} c_{\lambda k \sigma} | d_{\sigma}^{\dagger} \rangle \rangle_\omega, \quad (11) \]

\[
[\omega - \varepsilon_{\lambda k} - \varepsilon_{\sigma} + \varepsilon_{\sigma}](\langle \langle d_{\sigma}^{\dagger} c_{\lambda k \sigma} n_{\sigma} | d_{\sigma}^{\dagger} \rangle \rangle_\omega - \sum_{\lambda' k'} V_{\lambda' k' \sigma}^{*} \langle \langle c_{\lambda' k' \sigma}^{\dagger} n_{\sigma} c_{\lambda k \sigma} | d_{\sigma}^{\dagger} \rangle \rangle_\omega + \sum_{\lambda' k'} V_{\lambda' k' \sigma}^{*} \langle \langle c_{\lambda' k' \sigma}^{\dagger} D_{\sigma} c_{\lambda k \sigma} | d_{\sigma}^{\dagger} \rangle \rangle_\omega, \quad (12) \]

\[
[\omega + \varepsilon_{\lambda k} - \varepsilon_{\sigma} - U](\langle \langle c_{\lambda k \sigma}^{\dagger} d_{\sigma} | d_{\sigma}^{\dagger} \rangle \rangle_\omega = \langle \langle c_{\lambda k \sigma}^{\dagger} d_{\sigma} \rangle \rangle_\omega - V_{\lambda k \sigma}^{*}(\langle \langle n_{\sigma} d_{\sigma} | d_{\sigma}^{\dagger} \rangle \rangle_\omega + (1 - x) \sum_{\lambda' k'} V_{\lambda' k' \sigma}^{*} \langle \langle c_{\lambda' k' \sigma}^{\dagger} n_{\sigma} c_{\lambda k \sigma} | d_{\sigma}^{\dagger} \rangle \rangle_\omega + x \sum_{\lambda' k'} V_{\lambda' k' \sigma}^{*} \langle \langle c_{\lambda' k' \sigma}^{\dagger} D_{\sigma} c_{\lambda k \sigma} | d_{\sigma}^{\dagger} \rangle \rangle_\omega, \quad (13) \]

we have used the commutators

\[
[\langle \langle n_{\sigma} c_{\lambda k \sigma} | H \rangle \rangle = \varepsilon_{\lambda k} n_{\sigma} c_{\lambda k \sigma} + (1 + x)V_{\lambda k \sigma} n_{\sigma} d_{\sigma} - \sum_{\lambda k} (V_{\lambda k \sigma} c_{\lambda k \sigma}^{\dagger} D_{\sigma} c_{\lambda k \sigma} + V_{\lambda k \sigma}^{*} D_{\sigma}^{\dagger} c_{\lambda k \sigma} c_{\lambda k \sigma}), \quad (14) \]

\[
[c_{\lambda k \sigma}^{\dagger} d_{\sigma}, H] = (-\varepsilon_{\lambda k} + U + \varepsilon_{\sigma} + \varepsilon_{\sigma}) c_{\lambda k \sigma}^{\dagger} D_{\sigma} d_{\sigma} + (1 - x) \sum_{\lambda' k'} (V_{\lambda k \sigma} c_{\lambda k \sigma}^{\dagger} D_{\sigma} c_{\lambda' k' \sigma} + V_{\lambda k \sigma}^{*} D_{\sigma}^{\dagger} c_{\lambda k \sigma} c_{\lambda' k' \sigma}) + x \sum_{\lambda' k'} (V_{\lambda k \sigma}^{*} c_{\lambda' k' \sigma}^{\dagger} n_{\sigma} c_{\lambda k \sigma} + V_{\lambda k \sigma}^{*} c_{\lambda k \sigma}^{\dagger} n_{\sigma}^{\dagger} d_{\sigma}^{\dagger}). \quad (15) \]

\[
[d_{\sigma}^{\dagger} c_{\lambda k \sigma}, H] = (\varepsilon_{\lambda k} + \varepsilon_{\sigma} - \varepsilon_{\sigma}) d_{\sigma}^{\dagger} c_{\lambda k \sigma} d_{\sigma} + (1 - x)V_{\lambda k \sigma} n_{\sigma} d_{\sigma} - \sum_{\lambda' k'} V_{\lambda' k' \sigma}^{*} c_{\lambda' k' \sigma}^{\dagger} D_{\sigma} c_{\lambda k \sigma} + \sum_{\lambda' k'} V_{\lambda' k' \sigma}^{*} D_{\sigma}^{\dagger} c_{\lambda k \sigma} c_{\lambda' k' \sigma}. \quad (16) \]

The above EOM for the GFs are used to find the sums $S_{n}^{sp}$, $S_{d}^{sp}$, and $S_{c}^{sp}$. However, we note that more complicated GFs have appeared on the rhs of each of the GFs defining these parameters. To close the system of equations, one needs to project those higher-order GFs onto the lower ones. This projection or decoupling is the subject of the next few subsections.
B. Decoupling scheme I

Naturally there are a several ways of approximating equations for higher-order GFs. The simplest one, which we shall call decoupling I, consists in an approximation analogous to the one used to calculate the transport GFs, i.e., to project them onto \( \langle \langle d_\sigma | d_\sigma^\dagger \rangle \rangle \) and \( \langle \langle n_\sigma d_\sigma | d_\sigma^\dagger \rangle \rangle \) only. Such a decoupling leads to very simple formulae for the parameters \( S_{n,d,c}^{\alpha} \):

\[
S_{n}^{\alpha} = (1 - x) \Sigma_{0\sigma} \langle \langle n_\sigma d_\sigma | d_\sigma^\dagger \rangle \rangle \omega \\
S_{d}^{\alpha} = b_{1\sigma} + (1 - x) \Sigma_{\sigma}^{(1)} \langle \langle n_\sigma d_\sigma | d_\sigma^\dagger \rangle \rangle \omega + (b_{1\sigma} \Sigma_{0\sigma} - \Sigma_{0\sigma}^{T}) \langle \langle D_\sigma | d_\sigma^\dagger \rangle \rangle \omega, \\
S_{c}^{\alpha} = b_{2\sigma} + [(1 - x) \Sigma_{2\sigma}^{T} + b_{2\sigma} \Sigma_{0\sigma}] \langle \langle d_\sigma | d_\sigma^\dagger \rangle \rangle + \{x \Sigma_{2\sigma}^{T} - \Sigma_{\sigma}^{(2)} - x b_{2\sigma} \Sigma_{0\sigma} \langle \langle n_\sigma d_\sigma | d_\sigma^\dagger \rangle \rangle \omega. 
\]

For future reference we write the above equations in the form

\[
S_{i}^{\alpha} = S_{i}^{(0)} + S_{i}^{(0)} \langle \langle d_\sigma | d_\sigma^\dagger \rangle \rangle \omega + S_{i}^{(2)} \langle \langle n_\sigma d_\sigma | d_\sigma^\dagger \rangle \rangle \omega, 
\]

with \( i = n,d,c \), and the following expressions for \( S_{i}^{(0,1,2)} \):

\[
S_{n}^{(0)} = S_{n}^{(1)} = 0, \quad S_{n}^{(2)} = (1 - x) \Sigma_{0\sigma}, \\
S_{d}^{(0)} = b_{1\sigma}, \quad S_{d}^{(1)} = b_{1\sigma} \Sigma_{0\sigma} - \Sigma_{1\sigma}^{T}, \quad S_{d}^{(2)} = (1 - x) \Sigma_{\sigma}^{(1)} - x (b_{1\sigma} \Sigma_{0\sigma} - \Sigma_{1\sigma}^{T}), \\
S_{c}^{(0)} = b_{2\sigma}, \quad S_{c}^{(1)} = (1 - x) \Sigma_{2\sigma}^{T} + b_{2\sigma} \Sigma_{0\sigma}, \quad S_{c}^{(2)} = x \Sigma_{2\sigma}^{T} - \Sigma_{\sigma}^{(2)} - x b_{2\sigma} \Sigma_{0\sigma}.
\]

With the help of these “expansion” parameters, one finds

\[
\langle \langle d_\sigma | d_\sigma^\dagger \rangle \rangle \omega = \frac{1 - x (S_{n}^{(0)} + S_{d}^{(0)} + S_{c}^{(0)}) + n_{\text{eff}} I_{d}(x)}{\omega - \varepsilon_{\sigma} - \Sigma_{0\sigma} + x \Sigma_{2\sigma} - I_{d}(x) B_{d}(x)},
\]

where

\[
n_{\text{eff}} = \langle n_\sigma \rangle - S_{c}^{(0)} + (1 - x) (S_{n}^{(0)} + S_{d}^{(0)}),
\]

and

\[
\Sigma_{d} = S_{n}^{(1)} + S_{d}^{(1)} + S_{c}^{(1)}, \quad B_{d}(x) = (1 - x) (S_{n}^{(1)} + S_{d}^{(1)}) - S_{c}^{(1)}. 
\]

Here we introduced \( I_{d}(x) \):

\[
I_{d}(x) = \frac{U - x (\Sigma_{0\sigma} + S_{c}^{(2)} + S_{d}^{(2)} + S_{n}^{(2)})}{\omega - \varepsilon_{\sigma} - U - \Sigma_{nd}},
\]

where the new symbol reads

\[
\Sigma_{nd} = (1 - x) (S_{n}^{(2)} + S_{d}^{(2)}) - S_{c}^{(2)}. 
\]

It has to be stressed that the coefficients \( S_{n,d,c}^{(\alpha)} \) are projections of the corresponding terms \( S_{n,d,c}^{\alpha} \) in Eqs. (6)–(7) onto the functions \( \langle \langle d_\sigma | d_\sigma^\dagger \rangle \rangle \) and \( \langle \langle n_\sigma d_\sigma | d_\sigma^\dagger \rangle \rangle \). This means that as long as one projects onto this set of functions the general formula Eq. (24) is valid independent of the particular decoupling. In practice the decouplings we try require projections onto a slightly different set of functions, but the general scheme remains unchanged and will be used in the following.
C. Decoupling scheme II

Next we proceed somewhat differently, which we call scheme II. The functions containing on the lhs three operators, two of which with the spin label $\bar{\sigma}$ and one with the label $\sigma$, are decoupled by projecting them onto a single GF with operator labelled by $\sigma$, with the coefficients depending on $\bar{\sigma}$. This decoupling takes care of the spin-$\bar{\sigma}$ fluctuations. The GFs with five operators on the lhs are decoupled as follows:

\[ \langle \epsilon_\bar{\sigma}^\dagger c_{\lambda k\bar{\sigma}} d_\sigma n_\bar{\sigma} | d_\sigma^\dagger \rangle \omega \approx \langle \epsilon_\bar{\sigma}^\dagger c_{\lambda k\bar{\sigma}} d_\sigma n_\bar{\sigma} | d_\sigma^\dagger \rangle \omega - \langle \epsilon_\bar{\sigma}^\dagger c_{\lambda k\bar{\sigma}} d_\sigma n_\bar{\sigma} | d_\sigma^\dagger \rangle \omega \\
- \langle \epsilon_\bar{\sigma}^\dagger c_{\lambda k\bar{\sigma}} (c_{\lambda k\bar{\sigma}} \dagger) | d_\sigma^\dagger \rangle \omega + \langle \epsilon_\bar{\sigma}^\dagger c_{\lambda k\bar{\sigma}} (c_{\lambda k\bar{\sigma}} \dagger) | d_\sigma^\dagger \rangle \omega \]

(30)

and

\[ \langle \epsilon_\bar{\sigma}^\dagger c_{\lambda k\bar{\sigma}} d_\sigma n_\bar{\sigma} | d_\sigma^\dagger \rangle \omega \approx \langle \epsilon_\bar{\sigma}^\dagger c_{\lambda k\bar{\sigma}} d_\sigma n_\bar{\sigma} | d_\sigma^\dagger \rangle \omega - \langle \epsilon_\bar{\sigma}^\dagger c_{\lambda k\bar{\sigma}} d_\sigma n_\bar{\sigma} | d_\sigma^\dagger \rangle \omega \\
- \langle \epsilon_\bar{\sigma}^\dagger c_{\lambda k\bar{\sigma}} (c_{\lambda k\bar{\sigma}} \dagger) | d_\sigma^\dagger \rangle \omega + \langle \epsilon_\bar{\sigma}^\dagger c_{\lambda k\bar{\sigma}} (c_{\lambda k\bar{\sigma}} \dagger) | d_\sigma^\dagger \rangle \omega \]

(31)

where the last terms have been added to correct for the double counting from two previous terms. These decouplings introduce GFs which enter the definitions of the parameters $S^{\text{ep}}_\sigma$. The following decouplings are performed for GFs with other spin structures:

\[ \langle \epsilon_\bar{\sigma}^\dagger c_{\lambda k\bar{\sigma}} d_\sigma n_\bar{\sigma} | d_\sigma^\dagger \rangle \omega \approx \langle \epsilon_\bar{\sigma}^\dagger c_{\lambda k\bar{\sigma}} d_\sigma n_\bar{\sigma} | d_\sigma^\dagger \rangle \omega - \langle \epsilon_\bar{\sigma}^\dagger c_{\lambda k\bar{\sigma}} d_\sigma n_\bar{\sigma} | d_\sigma^\dagger \rangle \omega \\
- \langle \epsilon_\bar{\sigma}^\dagger c_{\lambda k\bar{\sigma}} (c_{\lambda k\bar{\sigma}} \dagger) | d_\sigma^\dagger \rangle \omega + \langle \epsilon_\bar{\sigma}^\dagger c_{\lambda k\bar{\sigma}} (c_{\lambda k\bar{\sigma}} \dagger) | d_\sigma^\dagger \rangle \omega \]

(32)

and

\[ \langle \epsilon_\bar{\sigma}^\dagger c_{\lambda k\bar{\sigma}} d_\sigma n_\bar{\sigma} | d_\sigma^\dagger \rangle \omega \approx \langle \epsilon_\bar{\sigma}^\dagger c_{\lambda k\bar{\sigma}} d_\sigma n_\bar{\sigma} | d_\sigma^\dagger \rangle \omega - \langle \epsilon_\bar{\sigma}^\dagger c_{\lambda k\bar{\sigma}} d_\sigma n_\bar{\sigma} | d_\sigma^\dagger \rangle \omega \\
- \langle \epsilon_\bar{\sigma}^\dagger c_{\lambda k\bar{\sigma}} (c_{\lambda k\bar{\sigma}} \dagger) | d_\sigma^\dagger \rangle \omega + \langle \epsilon_\bar{\sigma}^\dagger c_{\lambda k\bar{\sigma}} (c_{\lambda k\bar{\sigma}} \dagger) | d_\sigma^\dagger \rangle \omega \]

(33)

With this decoupling scheme, we find the system of equations for the sums $S^{\text{ep}}_n$, $S^{\text{ep}}_d$, and $S^{\text{ep}}_\sigma$. The equation for $S^{\text{ep}}_n$ reads

\[ S^{\text{ep}}_n = (1 - x) \Sigma_{\bar{\sigma}0}(n_\bar{\sigma} d_\sigma^\dagger) + x b_{0\bar{\sigma}}(S^{\text{ep}}_d - S^{\text{ep}}_\sigma), \]

(34)

and depends on the two remaining parameters $S^{\text{ep}}_d$ and $S^{\text{ep}}_\sigma$. Scheme II also introduces the new self-energy

\[ b_{0\bar{\sigma}}(\omega) = \sum_{\lambda k} V^*_{\lambda k\bar{\sigma}} \langle d_\sigma^\dagger c_{\lambda k\bar{\sigma}} \rangle \omega, \]

(35)

The other two parameters are found to read

\[ S^{\text{ep}}_d = b_{1\bar{\sigma}} + (b_{1\bar{\sigma}} \Sigma_{0\bar{\sigma}} - \Sigma^T_{1\bar{\sigma}} + x s_{1\bar{\sigma}} b_{1\bar{\sigma}}) \langle d_\sigma^\dagger \rangle \omega \]

\[ + \left[ (1 - x) \Sigma^{(1)}_{\bar{\sigma}} - x (b_{1\bar{\sigma}} \Sigma_{0\bar{\sigma}} - \Sigma^T_{1\bar{\sigma}}) \right] \langle n_\bar{\sigma} d_\sigma^\dagger \rangle \omega - x b_{1\bar{\sigma}} S^{\text{ep}}_n, \]

\[ S^{\text{ep}}_\sigma = b_{2\bar{\sigma}} + \left[ (1 - x) \Sigma^T_{2\bar{\sigma}} + b_{2\bar{\sigma}} \Sigma_{0\sigma} + x s_{2\bar{\sigma}} b_{2\bar{\sigma}} \right] \langle d_\sigma^\dagger \rangle \omega \]

\[ + \left[ x \Sigma^T_{2\bar{\sigma}} - \Sigma^{(2)}_{\bar{\sigma}} - x b_{2\bar{\sigma}} \Sigma_{0\sigma} \right] \langle n_\bar{\sigma} d_\sigma^\dagger \rangle \omega - x b_{2\bar{\sigma}} S^{\text{ep}}_n. \]

(37)

Here we encounter spin-dependent shifts,

\[ s_{\sigma} = \sum_{\lambda k} V^*_{\lambda k\sigma} \langle d_\sigma^\dagger c_{\lambda k\sigma} \rangle, \]

(38)

and other self-energies, which have definitions similar to those found earlier in the process of calculating the transport GF, except for the energies in the denominators where $\varepsilon_1$ is replaced by $\varepsilon_{1\bar{\sigma}}$ and $\varepsilon_2$ is replaced by $\varepsilon_{2\bar{\sigma}}$. In particular, $b_{1\bar{\sigma}}(\omega)$ reads

\[ b_{1\bar{\sigma}}(\omega) = \sum_{\lambda k} V^*_{\lambda k\bar{\sigma}} \langle d_\sigma^\dagger c_{\lambda k\bar{\sigma}} \rangle \omega - \varepsilon_{1\bar{\sigma}} + i \gamma_{1\bar{\sigma}}, \]

(39)

where

\[ \varepsilon_{1\bar{\sigma}} = \varepsilon_{\sigma} - \varepsilon_{\bar{\sigma}} + x (s_{\sigma} - s_{\bar{\sigma}}), \]

(40)

\[ \varepsilon_{2\bar{\sigma}} = \varepsilon_{\sigma} + \varepsilon_{\bar{\sigma}} + U - x (s_{\sigma} + s_{\bar{\sigma}}). \]
The structure of the equations requires first the solutions for $S^{\text{sp}}_d$ and $S^{\text{sp}}$, later the spectral GF $\langle\langle d_{\sigma}|d_{\sigma}^\dagger\rangle\rangle_\omega$ can be computed. It is convenient to introduce the following notation:

\begin{align}
C_0 &= b_{2x\sigma}, \\
C_1 &= (1-x)\Sigma^T_{2x\sigma} + \tilde{b}_{2x\sigma} \Sigma_{0\sigma} + x s_{\sigma} b_{2x\sigma}, \\
C_2 &= x \Sigma^T_{2x\sigma} - \Sigma^T_{2\sigma} - x b_{2\sigma} \Sigma_{0\sigma}, \\
D_0 &= b_{1x\sigma}, \\
D_1 &= \tilde{b}_{1x\sigma} \Sigma_{0\sigma} - \Sigma^T_{1x\sigma} + x s_{\sigma} b_{1x\sigma}, \\
D_2 &= (1-x)\Sigma^T_{2\sigma} - x (\tilde{b}_{1x\sigma} \Sigma_{0\sigma} - \Sigma^T_{1x\sigma}),
\end{align}

and solve the following matrix equation:

\begin{equation}
\begin{pmatrix}
xb_{0\sigma} & -xb_{0\sigma} & 1 \\
xb_{1x\sigma} & 1 & 0 \\
1 & xb_{2x\sigma} & 0
\end{pmatrix}
\begin{pmatrix}
S^{\text{sp}}_d \\
S^{\text{sp}} \\
S^{\text{sp}}_n
\end{pmatrix}
= \begin{pmatrix}
0 \\
0 \\
C_0
\end{pmatrix} + \begin{pmatrix}
D_0 \\
D_1 \\
C_1
\end{pmatrix}\langle\langle d_{\sigma}|d_{\sigma}^\dagger\rangle\rangle_\omega + \begin{pmatrix}
(1-x)\Sigma_{0\sigma} \\
D_2 \\
C_2
\end{pmatrix}\langle\langle n_{\sigma}d_{\sigma}|d_{\sigma}^\dagger\rangle\rangle_\omega.
\end{equation}

The solution can be written as

\begin{equation}
\begin{pmatrix}
S^{\text{sp}}_d \\
S^{\text{sp}} \\
S^{\text{sp}}_n
\end{pmatrix} = \begin{pmatrix}
S^{(0)}_d \\
S^{(0)} \\
S^{(0)}_n
\end{pmatrix} + \begin{pmatrix}
S^{(1)}_d \\
S^{(1)} \\
S^{(1)}_n
\end{pmatrix}\langle\langle d_{\sigma}|d_{\sigma}^\dagger\rangle\rangle_\omega + \begin{pmatrix}
S^{(2)}_d \\
S^{(2)} \\
S^{(2)}_n
\end{pmatrix}\langle\langle n_{\sigma}d_{\sigma}|d_{\sigma}^\dagger\rangle\rangle_\omega,
\end{equation}

with an obvious definition of $S^{(\alpha)}$, $\alpha = 0,1,2$ and $i = n,d,c$. We shall not write these parameters here.

With the above formulae for the sums, the solution of the system of equations (9), (10) is an easy task and results in the following spectral GF, which formally is the same as that given in (24), together with (25)–(29):

\begin{equation}
\langle\langle d_{\sigma}|d_{\sigma}^\dagger\rangle\rangle_\omega = \frac{1 - x(S^{(0)}_d + S^{(0)} + S^{(0)}_n) + n_{\text{eff}} I_d(x)}{\omega - \varepsilon_{\sigma} - \Sigma_{0\sigma} + x \Sigma_{d} - I_d(x) B_d(x)}.
\end{equation}

Currently, of course, the parameters $S^{(0,1,2)}$ are given by the solution of the matrix equations (48) and (49), while for decoupling I they are given by the scalar expressions (21)–(23).

We also need the following off-diagonal GF:

\begin{equation}
\langle\langle n_{\sigma}d_{\sigma}|d_{\sigma}^\dagger\rangle\rangle_\omega = \frac{n_{\text{eff}} + B_d\langle\langle d_{\sigma}|d_{\sigma}^\dagger\rangle\rangle_\omega}{\omega - \varepsilon_{\sigma} - U - \Sigma_{nd}}.
\end{equation}

It is still necessary to calculate some of the self-energies. It has to be noted that not all correlations for the correlated-hopping model can be expressed exactly by the appropriate GFs. We have seen one example, namely the average occupation of the dot, $\langle n_d \rangle$; the other one is the shift defined in (38). It is very difficult, albeit in principle possible, to exactly express the shifts in terms of known GFs, except in equilibrium: in the latter case, using the fluctuation-dissipation theorem and real values for the tunneling parameters, $V_{\lambda\kappa\sigma} = V_{\lambda\kappa\sigma}^*$, one can write

\begin{equation}
s_{\sigma} = \sum_{\lambda\kappa} V_{\lambda\kappa\sigma}^* \langle d_{\sigma}^\dagger c_{\lambda\kappa\sigma} \rangle = \int \frac{d\omega}{2\pi} \frac{-2}{\epsilon^2(\omega - \mu) + 1} \text{Im} \left[ \sum_{\lambda\kappa} \frac{|V_{\lambda\kappa\sigma}|^2}{\omega - \varepsilon_{\lambda\kappa} + i0^+} \langle\langle D_{\sigma}|d_{\sigma}^\dagger\rangle\rangle_\omega \right] = \tilde{\Gamma}_{\sigma} \int \frac{d\omega}{2\pi} \frac{1}{\epsilon^2(\omega - \mu) + 1} \text{Re} \langle\langle D_{\sigma}|d_{\sigma}^\dagger\rangle\rangle_\omega,
\end{equation}

where additionally the wide-band approximation (cf. Eq. (B10) in App. B of the main text) was assumed to be valid. As discussed in the main text, the above approximations for the GFs result in a transport GF which to a very good approximation obeys the $x$-symmetry of the model. The spectral GF, however, violates this symmetry. In view of this fact we have tried still another, more complicated decoupling scheme.

\section{Decoupling scheme III}

The above decoupling II projected the higher-order GFs onto the lower ones, but only those which already appeared in the sequence of equations. However, a closer inspection of the equations (30)–(33) shows that the functions on their lhs can also be projected onto
\langle \langle \langle n_{\sigma} c_{\lambda \kappa \sigma} | d_{\sigma}^I \rangle \rangle \rangle^*_\omega, \) which has not appeared hitherto. This function formally is of the same order as \( \langle \langle \langle n_{\sigma} c_{\lambda \kappa \sigma} | d_{\sigma}^I \rangle \rangle \rangle^*_\omega. \) In contrast, however, the spin structure indicates that it might be of special importance for \( n_{\sigma} = 1, \) as changing \( x \) into \((2 - x)\) leaves the hopping term \( V_{\lambda \kappa \sigma} \) unchanged up to an overall sign. This decoupling is denoted as III. It introduces another parameter, which we call \( S^{\text{III}}_\sigma. \) It reads

\[
S^{\text{III}}_\sigma = \sum_{\lambda k} V^*_{\lambda \kappa \sigma} \langle \langle \langle n_{\sigma} c_{\lambda \kappa \sigma} | d_{\sigma}^I \rangle \rangle \rangle^*_\omega
\]  

(53)

We are not presenting the resulting system of equations. It is sufficient to note that the matrices in (48) will have the dimension \( 4 \times 4. \) What is more important: even this decoupling does not lead to a solution for the spectral GF symmetric with respect to the change \( x \leftrightarrow 2 - x. \)

We would like to note that the calculations using decouplings II and III lead to results which are essentially unchanged compared to those presented in the figures, obtained within the decoupling I.

### E. An alternative point of view: matrix formulation

Our methodology in the previous sections has been to obtain the transport, \( \langle \langle D_{\sigma} | D_{\sigma}^I \rangle \rangle^*_\omega, \) and spectral GFs, \( \langle \langle d_{\sigma} | d_{\sigma}^I \rangle \rangle^*_\omega, \) by using the EOM and calculating each of them independently. In fact, the operator relation \( D_{\sigma} = d_{\sigma}^I (1 - x n_{\sigma}) \) allows to write

\[
\langle \langle D_{\sigma} | D_{\sigma}^I \rangle \rangle^*_\omega = \langle \langle d_{\sigma} | d_{\sigma}^I \rangle \rangle^*_\omega - x \langle \langle n_{\sigma} d_{\sigma} | d_{\sigma}^I \rangle \rangle^*_\omega - x \langle \langle d_{\sigma} n_{\sigma} d_{\sigma}^I \rangle \rangle^*_\omega + x^2 \langle \langle n_{\sigma} d_{\sigma} n_{\sigma} d_{\sigma}^I \rangle \rangle^*_\omega,
\]

(54)

which shows that to obtain both GFs one may alternatively consider the matrix GF \( G_{\sigma} = \langle \langle \phi_{\sigma} | \phi_{\sigma}^* \rangle \rangle^*_\omega, \) where \( \phi = \{d_{\sigma}, n_{\sigma} d_{\sigma}^I\}^T, \) and \( T \) denotes the matrix transpose operation.

We write the full matrix GF in the following form:

\[
G_{\sigma}(\omega) = \begin{pmatrix}
\langle \langle d_{\sigma} | d_{\sigma}^I \rangle \rangle^*_\omega; \\
\langle \langle n_{\sigma} d_{\sigma} | d_{\sigma}^I \rangle \rangle^*_\omega; \\
\langle \langle d_{\sigma} n_{\sigma} d_{\sigma}^I \rangle \rangle^*_\omega; \\
\langle \langle n_{\sigma} d_{\sigma} n_{\sigma} d_{\sigma}^I \rangle \rangle^*_\omega
\end{pmatrix} = \begin{pmatrix}
g^{(11)}(\omega); g^{(12)}(\omega) \\
g^{(21)}(\omega); g^{(22)}(\omega)
\end{pmatrix},
\]

(55)

which clearly shows that its determination requires the known commutators (1) and (4). The easiest way is to use the EOM to get each of the functions \( g^{(ij)}(\omega). \) For the (11) entry of the matrix, one finds

\[
(\omega - \varepsilon_{\sigma} - \Sigma_{0\sigma}) \langle \langle d_{\sigma} | d_{\sigma}^I \rangle \rangle^*_\omega = 1 + (U - x \Sigma_{0\sigma}) \langle \langle n_{\sigma} d_{\sigma} | d_{\sigma}^I \rangle \rangle^*_\omega - x (S^I_n + S^I_d + S^I_c),
\]

(56)

which is formally similar to (9) except that currently the parameters \( S^I_i \) appear (replacing the parameters \( S^{\text{III}}_i \)). The other matrix elements in (55) are found using known commutators:

\[
(\omega - \varepsilon_{\sigma} - \Sigma_{0\sigma}) \langle \langle n_{\sigma} d_{\sigma} | d_{\sigma}^I \rangle \rangle^*_\omega = \langle \langle n_{\sigma} \rangle \rangle + (U - x \Sigma_{0\sigma}) \langle \langle n_{\sigma} d_{\sigma} | d_{\sigma}^I \rangle \rangle^*_\omega - x (S^{II}_n + S^{II}_d + S^{II}_c),
\]

(57)

\[
(\omega - \varepsilon_{\sigma} - U) \langle \langle n_{\sigma} d_{\sigma} | d_{\sigma}^I \rangle \rangle^*_\omega = \langle \langle n_{\sigma} \rangle \rangle - S^I_c + (1 - x) (S^{II}_n + S^{II}_d).
\]

(58)

The last equation is the same as (10). Finally, we have

\[
(\omega - \varepsilon_{\sigma} - U) \langle \langle n_{\sigma} d_{\sigma} | n_{\sigma} d_{\sigma}^I \rangle \rangle^*_\omega = \langle \langle n_{\sigma} \rangle \rangle - S^{III}_c + (1 - x) (S^{II}_n + S^{II}_d).
\]

(59)

In the above, we have introduced the notation

\[
S^I_n = \sum_{\lambda k} V^*_{\lambda \kappa \sigma} \langle \langle n_{\sigma} c_{\lambda \kappa \sigma} | d_{\sigma}^I \rangle \rangle^*_\omega,
\]

(60)

\[
S^{II}_n = \sum_{\lambda k} V^*_{\lambda \kappa \sigma} \langle \langle n_{\sigma} c_{\lambda \kappa \sigma} | n_{\sigma} d_{\sigma}^I \rangle \rangle^*_\omega,
\]

(63)

and analogous expressions for \( S^{II}_d, S^{II}_c, \) and \( S^{III}_c. \)

Note that the equation of motion for the Green functions defining the two sets of parameters \( S^I_i \) and \( S^{II}_i \) will differ from each other by the terms resulting from corresponding anti-commutators in Eq. (B5) of the main text. On the other hand, the novel functions require the previously encountered commutators (14), (15), and (16). The
final result will depend on the decoupling scheme used to calculate higher-order GFs entering the definitions of $S_I^f$. For the sake of completeness, we shall write the full equation for the GF $G(\omega)$ when all higher-order GFs are projected analogously to the decoupling $I$. One finds:

\[
\begin{pmatrix}
\omega - \varepsilon_\sigma - \Sigma_{0\sigma} - \Sigma_1; -U_{\text{eff}} \\
-\Sigma_{21}; -\Sigma_2
\end{pmatrix}
G_\sigma(\omega) = \begin{pmatrix}
1 - x(b_{1\sigma} + b_{2\sigma}); \\
(n_{\sigma}) - x(N_{2\sigma} + N_{1\sigma})
\end{pmatrix}
\begin{pmatrix}
(n_{\sigma}) - b_{2\sigma} + (1 - x)b_{1\sigma}; \\
(n_{\sigma}) - b_{2\sigma} + N_{2\sigma} + (1 - x)N_{1\sigma}
\end{pmatrix},
\]

with the self-energies $b_{i\sigma}$, $N_{i\sigma}$, etc., $i = 1, 2$, defined earlier, and

\[
U_{\text{eff}} = U - x[\Sigma_{0\sigma} + (1 - x)(\Sigma_{0\sigma} + \Sigma^{(1)}_1) + x(\Sigma_{1\sigma} + \Sigma^{(1)}_2 - (\tilde{b}_{1\sigma} + \tilde{b}_{2\sigma})\Sigma_{0\sigma}) - \Sigma^{(2)}_\sigma],
\]

\[
\Sigma_1 = -x[(1 - x)\Sigma^T_{2\sigma} - \Sigma^T_{1\sigma} + (\tilde{b}_{1\sigma} + \tilde{b}_{2\sigma})\Sigma_{0\sigma}],
\]

\[
\Sigma_2 = -x(\Sigma^T_{2\sigma} - \tilde{b}_{2\sigma}\Sigma_{0\sigma}) + \Sigma^{(2)}_1 + (1 - x)^2(\Sigma_{0\sigma} + \Sigma^{(1)}_\sigma) - x(1 + x)(\tilde{b}_{1\sigma}\Sigma_{0\sigma} - \Sigma^T_{1\sigma}),
\]

\[
\Sigma_{21} = -(1 - x)(\Sigma^T_{1\sigma} + \Sigma^T_{2\sigma}) + [(1 - x)\tilde{b}_{1\sigma} - \tilde{b}_{2\sigma}]\Sigma_{0\sigma}.
\]

It is easy to check that for the Hubbard model ($x = 0$) the above equation reduce to the correct expressions. One finds $U_{\text{eff}} = U$, $\Sigma_1 = 0$, and

\[
\Sigma_2 = \Sigma_{0\sigma} + \Sigma^{(1)}_1 + \Sigma^{(2)}_\sigma,
\]

as well as

\[
\Sigma_{12} = (\tilde{b}_{1\sigma} - \tilde{b}_{2\sigma})\Sigma_{0\sigma} - \Sigma^T_{1\sigma} - \Sigma^T_{2\sigma}.
\]

In addition, the expression for $\langle\langle d_\sigma|d_\sigma^\dagger\rangle\rangle_{\omega} = g_{11}^{\omega}$ agrees with Eq. (24) in the main text. Only slightly more complicated formulae are obtained with other decouplings, but we shall not write them down here. It turns out that none of the approaches leads to a spectral GF that fulfils the required $x$-symmetry, $g_{21}^{\omega}(\omega) = g_{21-\omega}(\omega)$. This shows that higher-order functions have to be calculated as discussed in [2]. Note that the symmetry of the transport GF is best fulfilled with the decoupling I, as discussed in the main text.

II. SUPPLEMENTARY MATERIAL (2) – CALCULATION OF LESSER GREEN FUNCTIONS AND EXPECTATION VALUES

Above we have shown various formulae for the retarded functions. However, the currents flowing through the system, as well as certain expectation values and various self-energies, are to be determined in terms of the lesser GFs. In equilibrium, the required expectation values can be calculated via the fluctuation-dissipation theorem. For the dot GFs it reads $g^\omega_{2\sigma}(\omega) = f(\omega)A_\sigma(\omega)$, and relates the correlation function $g^\omega(\omega)$ to the dissipative part of the retarded GF, i.e., the spectral function $A(\omega) = i[g^\sigma(\omega) - g^\sigma(\omega)]/2\pi$, with $f(\omega)$ the Fermi-Dirac function.

Out-of-equilibrium the situation is more complicated, and we shall explain the procedure in detail, recalling that the formal structure of the non-equilibrium Green functions for the complex time contour is the same as for double time GFs for real times [3]. Using the EOM for the operator $A(t)$,

\[
i\hbar\frac{\partial A(t)}{\partial t} = [A(t), H],
\]

with $[A, B] = AB - BA$, and Zubarev notation for the time-ordered GF of the operators $A$ and $B$:

\[
\langle\langle A(t)|B(t')\rangle\rangle = -i\langle T_t[A(t)B(t')]\rangle,
\]

where the time ordering operator $T_t$ is defined by

\[
T_t[A(t)B(t')] = \Theta(t - t')A(t)B(t') + \Theta(t' - t)B(t')A(t)
\]

with $\Theta(.)$ the Heaviside step function. The minus sign applies to fermionic operators. For this case, the EOM (using $\hbar = 1$) for the GF (74) reads

\[
i\frac{\partial\langle\langle A(t)|B(t')\rangle\rangle}{\partial t} = \delta(t - t')\langle\langle A, B\rangle\rangle + \langle\langle [A(t), H]|B(t')\rangle\rangle,
\]
where $\{A, B\} = AB + BA$. Sometimes it is useful to differentiate with respect to $t'$, with the result
\[
-i \frac{\partial}{\partial t'} \langle\langle A(t)|B(t')\rangle\rangle = \delta(t-t')\langle\{A, B\} \rangle - \langle\langle A(t)|[B(t'), H]\rangle\rangle. \tag{77}
\]
We find it convenient to use Zubarev’s notation also for contour-ordered functions,
\[
\langle\langle A(t)|B(t')\rangle\rangle_C = -i\langle TC[A(t)B(t')]\rangle.
\tag{78}
\]
This definition encompasses a number of quantities. In particular, it gives the time-ordered GF \((74)\) if both time arguments lie on the upper branch of the contour \(C\), and the lesser function \(\langle\langle A(t)|B(t')\rangle\rangle^<\) if \(t\) lies on the upper and \(t'\) on the lower branch \([3]\); then
\[
\langle\langle A(t)|B(t')\rangle\rangle^< = +i\langle B(t')A(t)\rangle. \tag{79}
\]
The knowledge of the lesser GF (denoted by the superscript \(<\)) allows the calculation of various averages under non-equilibrium conditions, as encountered earlier.

Here we shall illustrate the general procedure by showing how to calculate the correlation function \(\langle D^\dagger_\alpha c_{\lambda k\sigma}\rangle\) entering the definition of the quantity \(\tilde{h}_1(\omega)\). Obviously \([3]\) the aforementioned correlation function is given by the corresponding lesser GF \((79)\) as \(\langle c_{\lambda k\sigma}(t)|D^\dagger_\sigma(t)\rangle^<\). To calculate the latter, let us recall \([3]\) that the adequate contour-ordered GF \(\langle\langle c_{\lambda k\sigma}(t)|D^\dagger_\sigma(t')\rangle\rangle_C\), from which the lesser one can be obtained, \(\langle D^\dagger_\alpha c_{\lambda k\sigma}\rangle = -i\langle c_{\lambda k\sigma}(t)|D^\dagger_\sigma(t)\rangle^<\), \(\tag{80}\)
has the same formal structure and fulfils the same equation as the time-ordered one \((74)\). The lesser GF, in turn, is obtained from the time-ordered one by applying Langreth’s theorem \([4]\). The EOM for the above time-ordered GF reads
\[
i \frac{\partial}{\partial t} \langle\langle c_{\lambda k\sigma}(t)|D^\dagger_\sigma(t')\rangle\rangle = \delta(t-t')\langle\{c_{\lambda k\sigma}(t), D^\dagger_\sigma(t)\}\rangle + \langle\langle [c_{\lambda k\sigma}(t), H]|D^\dagger_\sigma(t')\rangle\rangle. \tag{81}\]
Evaluating the commutator one finds
\[
i \left( i \frac{\partial}{\partial t} - \varepsilon_{\lambda k} \right) \langle\langle c_{\lambda k\sigma}(t)|D^\dagger_\sigma(t')\rangle\rangle = V_{\lambda k\sigma} \langle\langle D_\sigma(t)|D^\dagger_\sigma(t')\rangle\rangle. \tag{82}\]
Considering the last equation as a matrix equation with respect to time variables \([3]\), one defines the diagonal-in-time inverse GF, \(g^{-1}_{0\lambda k\sigma}(t, t'') = (i \frac{\partial}{\partial t} - \varepsilon_{\lambda k})\delta(t-t'')\); the result is
\[
\langle\langle c_{\lambda k\sigma}(t)|D^\dagger_\sigma(t')\rangle\rangle = V_{\lambda k\sigma} \int dt_1 g_{0\lambda k\sigma}(t, t_1) \langle\langle D_\sigma(t_1)|D^\dagger_\sigma(t')\rangle\rangle. \tag{83}\]
Then using Langreth’s theorem \([4]\) the desired (lesser) component of the non-equilibrium function is obtained:
\[
\langle\langle c_{\lambda k\sigma}(t)|D^\dagger_\sigma(t')\rangle\rangle^< = i\langle D^\dagger_\sigma(t')c_{\lambda k\sigma}(t)\rangle \\
eq V_{\lambda k\sigma} \int dt_1 \left[ g_{0\lambda k\sigma}(t_1) \langle\langle D_\sigma(t_1)|D^\dagger_\sigma(t')\rangle\rangle^< + g_{0\lambda k\sigma}^<(t_1) \langle\langle D_\sigma(t_1)|D^\dagger_\sigma(t')\rangle\rangle^a \right], \tag{84}\]
where the subscripts \(r(a)\) denote retarded (advanced) GFs. It is useful to write down the above equation in frequency space:
\[
\langle\langle c_{\lambda k\sigma}|D^\dagger_\sigma\rangle\rangle^< = V_{\lambda k\sigma} g_{0\lambda k\sigma}^r(\omega) \langle\langle D_\sigma|D^\dagger_\sigma\rangle\rangle^< + g_{0\lambda k\sigma}^<(\omega) \langle\langle D_\sigma|D^\dagger_\sigma\rangle\rangle^a, \tag{85}\]
and use the formula
\[
\langle D^\dagger_\sigma(t)c_{\lambda k\sigma}(t)\rangle = \int \frac{d\omega'}{2\pi} \langle D^\dagger_\sigma c_{\lambda k\sigma}\rangle_{\omega'} \tag{86}\]
with positive infinitesimal \(\gamma = 0^+\), and
\[
g_{0\lambda k}^<(\omega) = 2\pi i f_\lambda(\omega) \delta(\omega - \varepsilon_{\lambda k}). \tag{88}\]
and express the averages \( \langle D^\dagger_\sigma c_{\lambda k\sigma} \rangle \) in App. B (main text) of \( \tilde{D}_\sigma \) encountered the term which is exact in the wide-band limit. In the derivation

\[
\frac{1}{2\pi i} \int \frac{d\omega}{\omega - \varepsilon_\lambda k + i\gamma} = \frac{1}{2\pi i} \int \frac{d\omega}{\omega - \varepsilon_\lambda k + i\gamma},
\]

using the last formula and introducing (89) into the definition (B33) in App. B (main text) of \( b_{1,\sigma}(\omega) \), one obtains the final expression

\[
\frac{1}{2\pi i} \int \frac{d\omega}{\omega - \varepsilon_\lambda k + i\gamma} = \frac{1}{2\pi i} \int \frac{d\omega}{\omega - \varepsilon_\lambda k + i\gamma},
\]

which is exact in the wide-band limit. In the derivation we encountered the term

\[
- i \sum_{\lambda k} \int d\omega' \left[ |V_{\lambda k\sigma}|^2 \frac{\langle \langle D_{\sigma} | d^\dagger_{\sigma \sigma} \rangle \rangle \langle t' \rangle}{2\pi \omega - \varepsilon_\lambda k + i\gamma} \right],
\]

then perform the analytic continuation, and later find the lesser GF \( \langle \langle D_{\sigma}(t) | c^\dagger_{\lambda k'\sigma}(t') \rangle \rangle \). Hence we first calculate the appropriate time-ordered function, this time differentiating w.r.t. \( t' \), then use that some integrals vanish in the wide-band limit: this leads to considerable simplifications of the formulae, which turn out to be exact [2] even out-of-equilibrium. The application of the above scheme allows the derivation of closed formulae for all self-energies. The results are summarised in App. C.

Finally we derive the sum rule Eq. (A8) in App. A of the main text for the correlated-hopping model, which is exact in the wide-band limit. We start with the EOM for the number operator \( n_\sigma \):

\[
\langle \frac{d n_\sigma}{dt} \rangle = \sum_{\lambda k} \left[ V^*_{\lambda k\sigma} \langle D^\dagger_\sigma c_{\lambda k\sigma} \rangle - V_{\lambda k\sigma} \langle c^\dagger_{\lambda k\sigma} D_\sigma \rangle \right],
\]

and express the averages \( \langle D^\dagger_\sigma c_{\lambda k\sigma} \rangle \) and \( \langle c^\dagger_{\lambda k\sigma} D_\sigma \rangle \) in terms of the corresponding lesser GFs:

\[
\langle \langle c_{\lambda k\sigma} D^\dagger_\sigma \rangle \rangle \Rightarrow V_{\lambda k\sigma} \left[ g_{\lambda k}^g(\omega) \langle \langle D_{\sigma} | D^\dagger_\sigma \rangle \rangle \right] + \left[ g_{\lambda k}^g(\omega) \langle \langle D_{\sigma} D^\dagger_\sigma \rangle \rangle \right],
\]

and

\[
\langle \langle D_{\sigma} c^\dagger_{\lambda k\sigma} \rangle \rangle \Rightarrow V^*_{\lambda k\sigma} \left[ \langle \langle D_{\sigma} | D^\dagger_\sigma \rangle \rangle g_{\lambda k}^g(\omega) \right] + \left[ \langle \langle D_{\sigma} D^\dagger_\sigma \rangle \rangle g_{\lambda k}^g(\omega) \right].
\]

Inserting the last equations into (95), and noting that in the steady state (we are interested in) one has \( \langle dn/dt \rangle = d\langle n \rangle/dt = 0 \), one obtains Eq. (A8). That formula is also valid for the model (5) (see the main text) supplemented with other density-density interactions. For the Hubbard model with \( x = 0 \) it reduces to the formula for the charge density on the dot as derived previously [5]:

\[
\langle n_\sigma \rangle = i \int \frac{dE}{2\pi} \frac{\Gamma^R_{\sigma} f_L(E) + \Gamma^R_{\sigma} f_R(E)}{\Gamma^R_{\sigma} + \Gamma^R_{\sigma}} [g_{\sigma}^0(E) - g_{\sigma}^a(E)],
\]

with \( g_{\sigma}^a(E) = \langle \langle d_{\sigma} | d^\dagger_{\sigma} \rangle \rangle \). The last formula, (98), is exact in the absence of correlated hopping \( x = 0 \), i.e., for the simple Hubbard model.
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[1] U. Eckern and K. I. Wysokiński, Charge and heat transport through quantum dots with local and correlated-hopping interactions, preprint, https://arxiv.org/abs/2104.09507 (revised version).
[2] R. Van Roermund, S. Shiau, and M. Lavagna, Anderson model out of equilibrium: Decoherence effects in transport through a quantum dot, Phys. Rev. B 81, 165115 (2010).
[3] H. Haug and A.-P. Jauho, Quantum Kinetics in Transport and Optics of Semiconductors, Second, Substantially Revised Edition, Springer, Berlin, 2008.
[4] D. C. Langreth, in Linear and Nonlinear Electron Transport in Solids, edited by J. T. Devreese and V. E. Van Daren, Nato ASI Ser. B, Vol. 17, Plenum, New York, 1976.
[5] M. Lavagna, Transport through an interacting quantum dot driven out-of-equilibrium, J. Phys. Conf. Ser. 592, 012141 (2015).