FIG. 9: (Color online) Equilibrium off-resonant spectral functions calculated with the MCIST technique and NEGF-SCBA for the off-resonant regime. The upper panel shows results for weak electron-vibron coupling ($\gamma_0/\omega_0 = 0.5$), while the lower panel shows results for strong electron-vibron coupling ($\gamma_0/\omega_0 = 0.8$). MCIST calculations give exact results in this case, and can also be performed at the same level of approximation as SCBA (see main text for details). MCIST-SCBA and NEGF-SCBA are virtually identical, but show large discrepancies for the peak positions (main peak and more especially for the vibron side-band peaks) in comparison to the exact results. The parameters are $\varepsilon_0 = +0.5$ (electron transport), $\gamma_0 = 0.2$ (upper panel) and $\gamma_0 = 0.32$ (lower panel), $\omega_0 = 0.4$, $t_{0L,R} = 0.15$.

of the resonant transport regime (i.e. vibron side-band peaks on both sides of the main peak). This is essentially due to the fact that in MCIST, one does not take properly into account the statistics of the Fermi seas of the left and right leads. See for example Eqs. (28) and (29), there are no leads' Fermi distributions in the retarded component of the leads' self-energies $\Sigma_{L,R}^r$.

Now, comparing BA-based calculations with the exact MCIST calculations, one can see from figure 9 that the BA-based calculations give the wrong polaron shift, i.e. the normalized position of the main peak ε_0, especially in the strong electron-vibron coupling regime. Furthermore BA-based calculations also give the wrong energy separation between the main peak and the first vibron

side-band peak. This energy difference should be equal to the vibron energy ω_0, as it is given by exact MCIST calculations. Note that the limits of BA-based calculations were also been studied by Lee *et al.* in a somewhat different context in Ref. [60].

In conclusion, this means that Hartree-Fock (or BA) based calculations for electron-vibron interaction are only valid for weak coupling, as can be expected from a perturbation-expansion based theory. Hence one needs to include higher-order diagrams in the electron-vibron self-energies to go beyond the commonly-used self-consistent Born approximation (Hartree-Fock) in order to obtain correct results for a wide range of parameters. The effects of the higher-order diagrams (here second-order-DX and DPH diagrams) are explored in detail in the following sections.

Additionally, although MCIST calculations are only valid in the off-resonant transport regime at and near equilibrium, they include all possible higher-order diagrams (with bare vibron propagator) and hence can be used as a reference for any perturbation-expansion-based NEGF calculations performed at equilibrium or in the quasi-equilibrium regime.

D. Vertex corrections and polarization effects to the spectral functions

In this section, we present results for the spectral functions when the second-order diagrams (see Figure 3) are included in the calculations of the Green's functions. The reader can find more information about the mathematical expressions for the self-energies corresponding to the second-order diagrams in Appendix A.

These diagrams fall into two types—the double-exchange DX diagram, corresponding to vertex corrections, and the dressed vibron diagram, which includes a single electron-hole bubble, renormalizing the vibron propagator and hence giving rise to polarization effects.

We have used three different levels of approximation to calculate these Green's functions: Firstly, calculations with no self-consistency—the Green's functions are simply calculated using the diagrams in Figure 2 and Figure 3 using the bare propagator G_0 as the electron Green's function. In our model, G_0 is the Green's function of the central region connected to the leads with no electron-vibron interactions. This is a first-order perturbation expansion for which $\Sigma_{e\text{-vib}}^{H,F,DX, \text{ and/or } DP}[G_0]$. We use the abbreviations BA (Born approximation for non self-consistent Hartree and Fock diagrams) and BA+DX (DX for double exchange) and BA+DX+DPH (DPH for dressed vibron, for the GW-like diagram) in the following.

Secondly, we perform partly self-consistent calculations, where the Green's functions are calculated with the first loop of self-consistent calculations with the Hartree and Fock diagrams. We use these Green's functions as a starting point to calculate new, corrected, Green's func-