grams and levels of self-consistency. We have considered the case for which real excitations of vibrons are possible $V = 0.45 > \omega_0$.

The interpretation of the results is not as straightforward as in the equilibrium case, because non equilibrium effects are sometimes counter intuitive. However, the overall shapes of spectral functions are quite similar to that obtained within Hartree-Fock based calculations (see Section III B 1) in the sense that they present a central peak with vibron side-band peaks on both sides.

Similarly to the resonant regime at equilibrium, the main effects of the second-order DX diagram is to narrow the width of all peaks, and to shift slightly the side-band peaks towards the main peak.

As mentioned in the previous section, the main effect of the second-order DPH diagram is to broaden the peaks, in opposition to the effects of the DX diagram. However here, the broadening in the non-equilibrium condition appears less important than in the case of the resonant regime at equilibrium. Hence full self-consistent calculations performed with both DX and DPH second-order diagrams give a narrowing of the peaks with a corresponding increase of their amplitude in comparison to SCBA calculations.

Finally, out of equilibrium, it can be seen that the results given by a full self-consistent calculation (curve SC(BA+DX) in Figure 13) are strongly different from a second-order correction to an Hartree-Fock calculation (SCBA+DX curve in 13) which gives an excessively narrowed central peak.

This means that in the weak/intermediate electron-vibron coupling, second-order corrections to a SCBA calculations are only good enough at equilibrium, however at non-equilibrium full self-consistency needs to be performed with all diagrams of the same order.

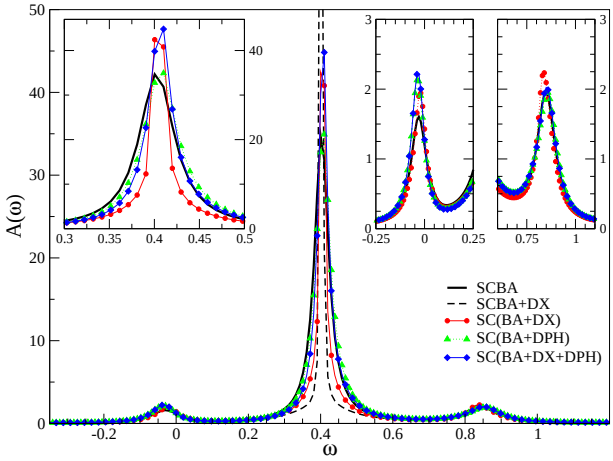

FIG. 13: (color online). Non-equilibrium spectral function (bias $V = 0.45 > \omega_0$) for the off-resonant transport regime for the weak/intermediate electron-vibron coupling. Calculations were performed self-consistently with first-order Hartree and Fock-like diagrams (SCBA curve), and with second-order DX and/or DPH diagrams (SC(BA+DX,+DPH,+DX+DPH) curves). Second-order DX correction to SCBA is also shown (SCBA+DX curve). The top-left inset shows a zoom on the central peak around $\omega \sim 0.4$, and the top-right insets show a zoom on the vibron side-band peaks around $\omega \sim 0.0$ and $\omega \sim 0.8$. The other parameters are $\varepsilon_0 = +0.5$, $\gamma_0 = 0.2, \omega_0 = 0.4, t_{0L,R} = 0.15, \eta = 0.025, \eta_V = 1$. The second-order DX diagram narrows the peaks with a slight shift of the side-band peaks towards the central peak. The narrowing is too strong in the case of partially self-consistent calculations (SCBA+DX). The second-order DPH diagram broadens the peak, but not as much as in the resonant case. Full self-consistent calculations including both second-order diagrams result in an intermediate behaviour for the modifications of the spectral functions.

4. *Resonant regime at finite bias*

As we have already shown in the first-order electron-vibron diagrammatic calculations, the spectral functions for the off-resonant and resonant regime at non-equilibrium are qualitatively similar, in the sense that they present a central peak with vibron side-band peaks on both sides. One can compare for example the spectral functions obtained for Hartree-Fock-like calculations at non-equilibrium shown in Figure 6 and Figure 8.

Hence, and again on a qualitative level, the effects of the second-order DX and DPH diagrams on the resonant case at finite bias are similar to what has been obtained for the off-resonant non-equilibrium case described in the previous section. The effects of these higher-order diagrams on the full non-equilibrium transport properties for the different transport regimes will be presented in a forthcoming paper.

However before turning the discussion to the linear-response properties of the system at and near equilibrium, we would like to comment on a specific aspect of the effects of higher-order diagrams.

The narrowing of the vibron side-band peaks and of the main central peak due to higher-order (DX) diagrams was also obtained by other authors (see for example Ref. [84]). In this paper, a different non-equilibrium approach was used. It consists of starting with an electron dressed by a vibron (a polaron) in the isolated central region, then using perturbation expansion theory (with partial resummation) in terms of the coupling of the central region to the non-equilibrium left and right leads. However, the results for the spectral functions in Ref. [84] were only given for the resonant transport regime at equilibrium and all calculations were performed without the Hartree-like diagram. Though we have already shown that such a diagram plays a crucial role in the spectral properties of the system in the resonant regime at and out of equilibrium.