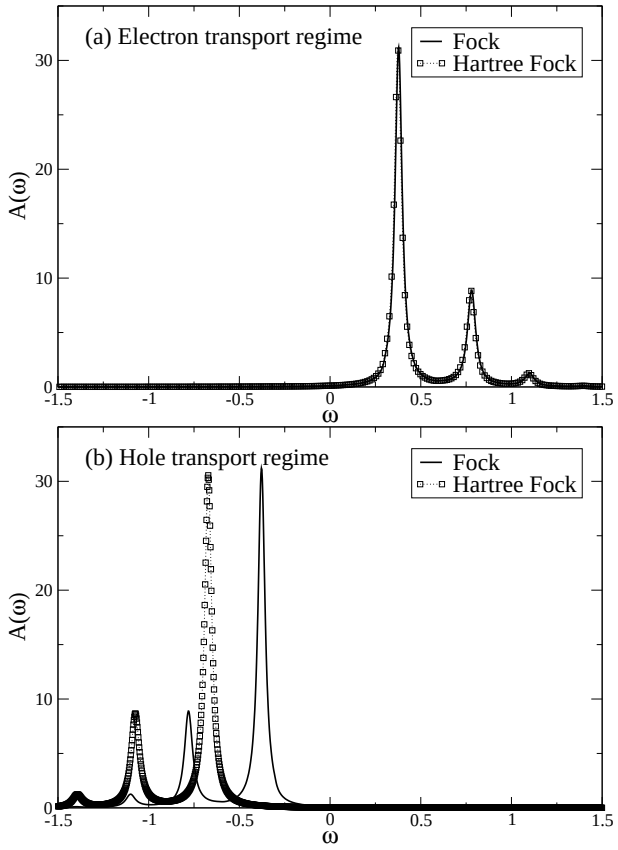

FIG. 4: Equilibrium (zero bias) spectral functions $A(\omega)$ for the off-resonant (a) electron and (b) hole transport regime. Calculations were performed with the Fock-like electron-vibron diagram (solid line) and with both the Hartree and Fock-like diagrams (symbols and dotted line). For the electron transport regime the inclusion of the Hartree self-energy has no effect, but for the hole transport regime it shifts the entire spectral function to lower energies. The parameters are $\varepsilon_0 = +0.5(-0.5)$ for electron (hole) transport $\gamma_0 = 0.21, \omega_0 = 0.3, t_{0L,R} = 0.15, \eta = 0.005$ and $\mu_L = \mu_R = \mu^{\rm eq} = 0$.

A. At equilibrium

We first consider the spectral functions at equilibrium, with no applied bias. Figure 4 shows $A(\omega)$ for the off-resonant regime, and Figure 5 shows the resonant transport regime.

In the equilibrium many-body language, the features in the spectral functions obtained at positive energies ($\omega \geq 0$, above the Fermi level) correspond to electron excitations, while the features at negative energies ($\omega \leq 0$, below the Fermi level) correspond to hole excitations.

1. Off-resonant transport regime

For the off-resonant electron transport regime (Figure 4(a)) all the features in the spectral function are above the Fermi level $\mu^{\rm eq}$ and hence correspond to electron excitations. The main peak corresponds to adding an electron in the single available level. This peak is broadened by the coupling to the leads, and its position in energy $\tilde{\varepsilon}_0$ is renormalised by the electron-vibron interaction, i.e. $\tilde{\varepsilon}_0$ is close to the static the polaron shift $\tilde{\varepsilon}_0 \approx \varepsilon_0 - \gamma_0^2/\omega_0$.

The lesser peaks in the electron-transport spectral function are vibron side-band peaks arising from resonance with $n = 1, 2, 3, ...$ excitations in the vibration mode. These peaks correspond to vibration excitation (vibron emission) only. At zero vibron temperature, these are the only available mechanisms for vibrational excitations. We note, and discuss further in section III C, that these side-band peaks should occur at integer multiples of ω_0 away from the main peak, but that for both our Fock-only and Hartree-Fock SCBA calculations the peak-peak separation is slightly wider than this.

In this regime, the Hartree self-energy is negligible, because most of the spectral weight is above the Fermi level and $\Sigma^H_{e\text{-vib}} \propto \int^{\mu^{\rm eq}} {\rm d}\omega A(\omega) \sim 0$. This implies that the polaron shift is mainly due to the Fock-like self-energy.

For the off-resonant hole-transport regime (Figure 4(b)), all the features in the spectral function occur at $\omega < 0$ and therefore correspond to hole excitations. The vibron side band peaks are at lower frequencies than the main peak because they correspond to the emission of vibrons by holes rather than electrons.

When we include just the Fock-like self-energy, the hole spectral function is symmetric (with respect to the equilibrium Fermi level $\mu^{\rm eq}$) with the electron spectral function, as can be seen clearly in figure 5. Adding the Hartree self-energy, however, breaks this electron-hole symmetry. As most of the spectral weight is below $\mu^{\rm eq}$, the expression for $\Sigma^H_{e\text{-vib}}$ given in equation Eq.(A15) reduces to a constant $2\gamma_0^2/\omega_0$ (i.e. twice the polaron shift) as $\int \frac{d\omega}{2\pi} {\rm i}G^<(\omega) \sim 1$. As a result of this the whole spectral function is shifted to the left by this amount.

2. Resonant transport regime

We now turn to the resonant transport regime, with the spectral function shown in Figure 5. Here our electronic level ε_0 is broadened by the coupling to the leads and is partially filled with electrons. We can see that calculations performed with only the Fock-like self-energy preserve the electron-hole symmetry. The spectral function presents peaks located both at positive and negative energies, which correspond to the emission of vibrons by electrons or holes respectively. As in the previous section, the inclusion of the Hartree self-energy (equation (A15)) breaks down the electron-hole symmetry and the features are shifted to lower energies with a corresponding modification of the spectral weights for each peak.

We note here that the inclusion of the Hartree self-energy thus modifies so drastically the spectral function that it will also strongly affect the I-V characteristics of the junction in comparison to calculations performed