Dimer IPT in the atomic limit

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In the dimer-Hubbard model, working in the orbital basis, the $'11'$ (local) component of the second order IPT reads

$$\Sigma_{U11}^{\alpha\beta}(\tau) = -\alpha\beta U^2 \mathcal{G}_{011}^{\alpha\beta}(\tau)^2 \mathcal{G}_{011}^{\beta\alpha}(-\tau), \tag{1}$$

where the indices $\alpha, \beta = +, -$ denote the forward and backward branches in the Keldysh contour. Rotating this expression into Keldysh basis, and going into Fourier space, we can write the following expression for the retarded component,

$$\begin{split}\Sigma_{U11}^{R}(\omega) = -\left(\frac{U}{2}\right)^2 [\mathcal{G}_{011}^{R}(-\omega)^* \circ \big(\mathcal{G}_{011}^{K}(\omega) \circ \mathcal{G}_{011}^{K}(\omega) + \mathcal{G}_{011}^{R}(\omega) \circ \mathcal{G}_{011}^{R}(\omega)\big) + \\ +2\mathcal{G}_{011}^{K}(-\omega) \circ \mathcal{G}_{011}^{R}(\omega) \circ \mathcal{G}_{011}^{K}(\omega)],\end{split} \tag{2}$$

We concentrate on the imaginary part, since the real part can be recovered via the Kramers-Kronig relations. The expression can be further simplified using

- again, the Kramers-Kronig relations
- the fact that we work with the convention $\mathrm{Re}G^K = 0$
- the fact that at half-filling we have $\mathrm{Im}G^R(-\omega) = \mathrm{Im}G^R(\omega)$ and $\mathrm{Im}G^K(-\omega) = -\mathrm{Im}G^K(\omega)$

This yields the expression that we work with,

$$\begin{split}\mathrm{Im}\Sigma_{U11}^{R}(\omega) = -\left(\frac{U}{2}\right)^2 [2\mathrm{Im}\mathcal{G}_{011}^{K}(\omega) \circ \mathrm{Im}\mathcal{G}_{011}^{K}(\omega) \circ \mathrm{Im}\mathcal{G}_{011}^{R}(\omega) + \\ + \mathrm{Im}\mathcal{G}_{011}^{R}(\omega) \circ \big(\mathrm{Im}\mathcal{G}_{011}^{K}(\omega) \circ \mathrm{Im}\mathcal{G}_{011}^{K}(\omega) + 4\mathrm{Im}\mathcal{G}_{011}^{R}(\omega) \circ \mathrm{Im}\mathcal{G}_{011}^{R}(\omega)\big)].\end{split} \tag{3}$$

In the case of the atomic limit in equilibrium, we have

$$\mathrm{Im}\mathcal{G}_{011}^{R}(\omega) = -\frac{\pi}{2}\left(\delta(\omega - t) + \delta(\omega + t)\right), \tag{4}$$

and via FDT,

$$
\begin{aligned}
\mathrm{Im}\mathcal{G}^K_{011}(\omega) =& 2\tanh\left(\frac{\beta\omega}{2}\right)\mathrm{Im}\mathcal{G}^R_{011}(\omega) \\
=& -\pi\tanh\left(\frac{\beta\omega}{2}\right)\left(\delta(\omega-t)+\delta(\omega+t)\right).
\end{aligned} \tag{5}
$$

After doing the convolutions, we obtain

$$
\begin{aligned}
\mathrm{Im}\Sigma^R_{U11}(\omega) = -\pi\frac{U^2}{32}(& \left[1+3\tanh^2\left(\frac{\beta t}{2}\right)\right]\left[\delta(\omega-3t)+\delta(\omega+3t)\right]+ \\
& +3\left[1-\tanh^2\left(\frac{\beta t}{2}\right)\right]\left[\delta(\omega-t)+\delta(\omega+t)\right]).
\end{aligned} \tag{6}
$$