

Real Frequency IPT Solver

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Analytical Formulation

The IPT solver is based on the use of only one of the second order skeleton diagrams of the self-energy. This diagram is the same for the single band case as for the Dimer, what is relevant to keep track is how each interaction vertex is composed so to construct the correct form of the Self-Energy when convoluting the Green's functions. As described in the next formula:

$$\Sigma(i\omega_n) = -\frac{U^2}{\beta^2} \sum_{\omega'_n, \Omega_m} \mathbf{G}^0(i\omega_n + i\Omega_m) \mathbf{G}^0(i\omega'_n + i\Omega_m) \mathbf{G}^0(i\omega'_n) \quad (1)$$

where \mathbf{G}^0 is the Free propagator, in the DMFT context is the Weiss field, and Σ is the Self-Energy. Both functions are block matrices. In the paramagnetic case spin label is irrelevant. For the single band case this matrices reduce to scalar functions and for the dimer case they are 2×2 matrices, but they are not multiplied as matrices but **element wise**. Keeping this fact in mind the following derivation will continue ignoring the label indexes of the Greens functions as they are irrelevant for the derivation. $\omega_n^{(f)}$ are fermionic Matsubara frequencies and Ω_m is a bosonic Matsubara frequency, U is the contact Coulomb interaction and β the inverse temperature.

The key idea to analytically continue from the Matsubara imaginary axis into the real frequency axis is through the following relation between the spectral function A and the Matsubara Green function:

$$\mathbf{G}(i\omega_n) = \int \frac{\mathbf{A}(\omega) d\omega}{i\omega_n - w} \quad (2)$$

valid for each entry of the matrix Green function. Let's start focusing on the fermionic bubble while inserting this identity.

$$\Pi(i\Omega_m) = \frac{1}{\beta} \sum_{\omega_n} \mathbf{G}^0(i\omega_n + i\Omega_m) \mathbf{G}^0(i\omega_n) \quad (3)$$

$$= \int dw dw' A(w) A(w') \frac{1}{\beta} \sum_{\omega_n} \frac{1}{i\omega_n - w} \frac{1}{i\omega_n + i\Omega_m - w'} \quad (4)$$

$$= \int dw dw' A(w) A(w') \frac{f(w) - f(w')}{i\omega_n + w - w'} \quad (5)$$

where $f(w)$ is the Fermi-Dirac function. The IPT Self-Energy (12) can be written as:

$$\Sigma(i\omega_n) = -\frac{U^2}{\beta} \sum_{\Omega_m} \mathbf{G}^0(i\omega_n + i\Omega_m) \mathbf{\Pi}(i\Omega_m) \quad (6)$$

$$= -U^2 \int dw dw' dw'' A(w) A(w') A(w'') \frac{[f(w) - f(w')][b(w' - w) + f(w'')]}{i\omega_n - w + w' - w''} \quad (7)$$

here $b(w)$ is the Bose-Einstein distribution. Numerically to calculate this function requires 4 nested loops to evaluate, and is computationally inefficient. In the search of extra improvement the following steps.

$$\Sigma(i\omega_n) = -U^2 \int dw dw' dw'' A(w) A(w') A(w'') \frac{f(-w)f(w')f(-w'') + f(w)f(-w')f(w'')}{i\omega_n - w + w' - w''} \quad (8)$$

Introducing the new notation

$$A^+(w) = f(w)A(w) \quad (9)$$

$$A^-(w) = f(-w)A(w) \quad (10)$$

and doing an analytical continuation $i\omega_n \rightarrow \nu + i\eta$

$$\Sigma(\nu) = -U^2 \int \frac{dw dw' dw'' [A^-(w)A^+(w')A^-(w'') + A^+(w)A^-(w')A^+(w'')]}{\nu + i\eta - w + w' - w''} \quad (11)$$

Taking only the imaginary part, and integrating over w''

$$\Im m \Sigma(\nu) = -\pi U^2 \int dw dw' [A^-(w)A^+(w')A^-(\nu - w + w') + A^+(w)A^-(w')A^+(\nu - w + w')] \quad (12)$$

The terms in the integral are convolutions with the particularity that when integrating over w' this convolutions runs over the array backwards. Convolutions can be calculated at a cost of $\mathcal{O}(N \log N)$ operations using the FFT. Then to recover the real part of the Self-Energy through the Kramers-Kronig relation(KK), which is only valid for casual functions. In the case of the single band one applies KK directly. Nevertheless in the Dimer case one has first to rotate Σ to the diagonal basis where it is casual and negative $\forall \nu$. In the same diagonal basis one performs the Hilbert transform over the density of states to recover G_{loc} and evaluate the self-consistency condition to update G^0 . Then one has to rotate back to the local basis and extract A^0 .

Single band

Further simplifying expression 13, using the definition of convolution for the integral in w . Because of particle-hole symmetry and a half-filled system $A^+(w) = A^*(-w)$

$$\begin{aligned} \Im m \Sigma(\nu) &= -\pi U^2 \int dw' [A^+(w')[A^- * A^-](\nu + w') + A^-(w')[A^+ * A^+](\nu + w')] \\ &= -\pi U^2 ([A^+ * [A^+ * A^+]](\nu) + [A^+ * [A^+ * A^+]](-\nu)) \end{aligned} \quad (13)$$

In this case I'll study the Metallic solution, where the know 3 peak structure appears, also there is a lot of states in the preformed gap. As can be seen in figure 1, where temperature is $\beta = 100$ and $U = 2.8$

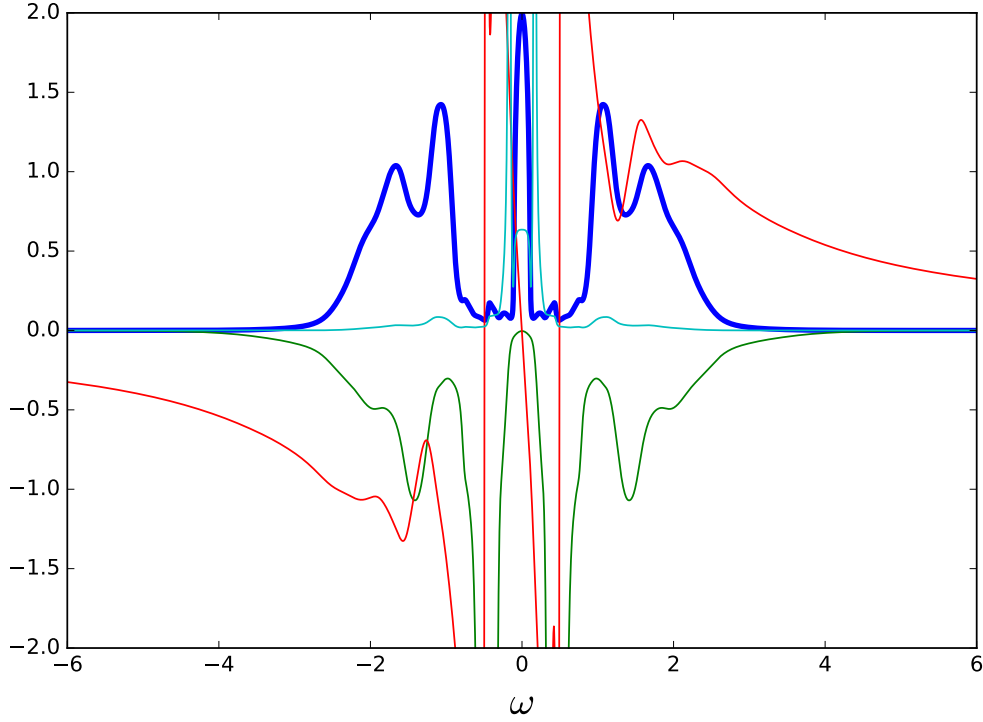


Figure 1: Green functions for the single band DMFT real frequency IPT solution. Thick blue is $-\Im m G(\omega)$, green $\Im m \Sigma(\omega)$, red $\Re e \Sigma(\omega)$, cyan $-\Im m G^0(\omega)$

Dimer lattice

The dimer lattice requires to use equation 13 for both local and intersite Weiss field propagators. Then the solution is straight forward and stable. Figure 2 shows the metallic solution, whereas figure 3 is for the insulator. The main features to highlight is that in the diagonal basis one finds on each a quasiparticle. Both of these are wider than their equivalent in the single band case, also the preformed gap is smooth with an apparent flat density of states, unlike the single band case where there is some ringing of the states. For the insulator, there is a very complex structure. There is more than just Hubbard bands. The poles of the Self-Energy are not at the Fermi level, but at the band edge of their corresponding band. The Hubbard bands have a large structure. Figure 4 presents the spectral function of the dimer at this coexistence point.

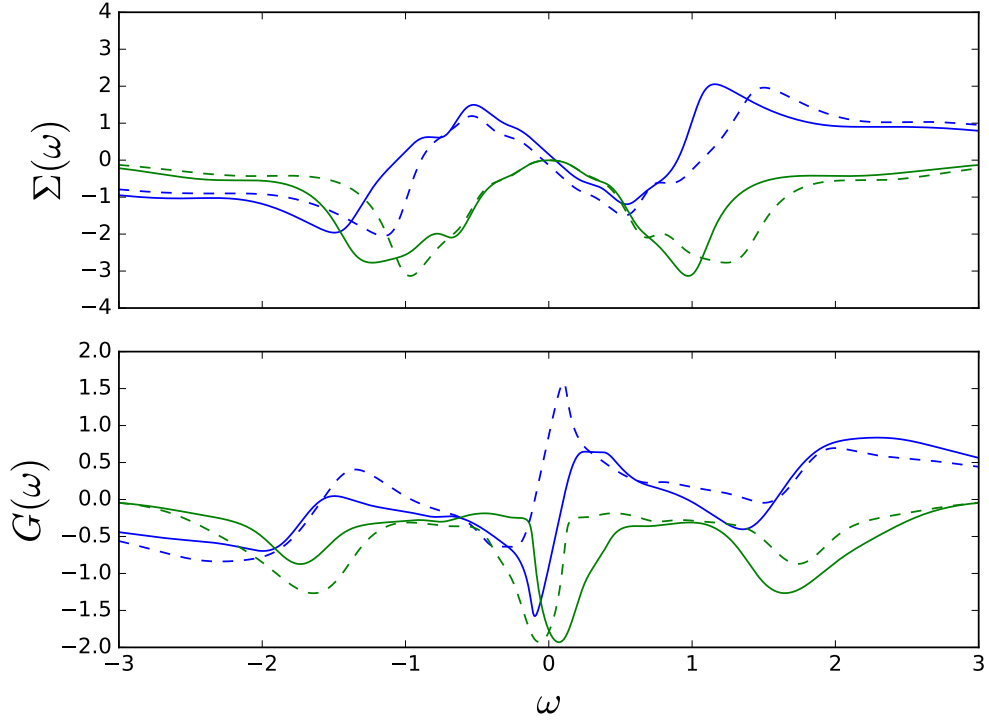


Figure 2: Metallic Self-energy (top) and Green Function (bottom) for the interacting dimer. Blue corresponds to real part and Green is Imaginary part. Full line is the symmetric sum of local and intersite functions, dashed is the difference.

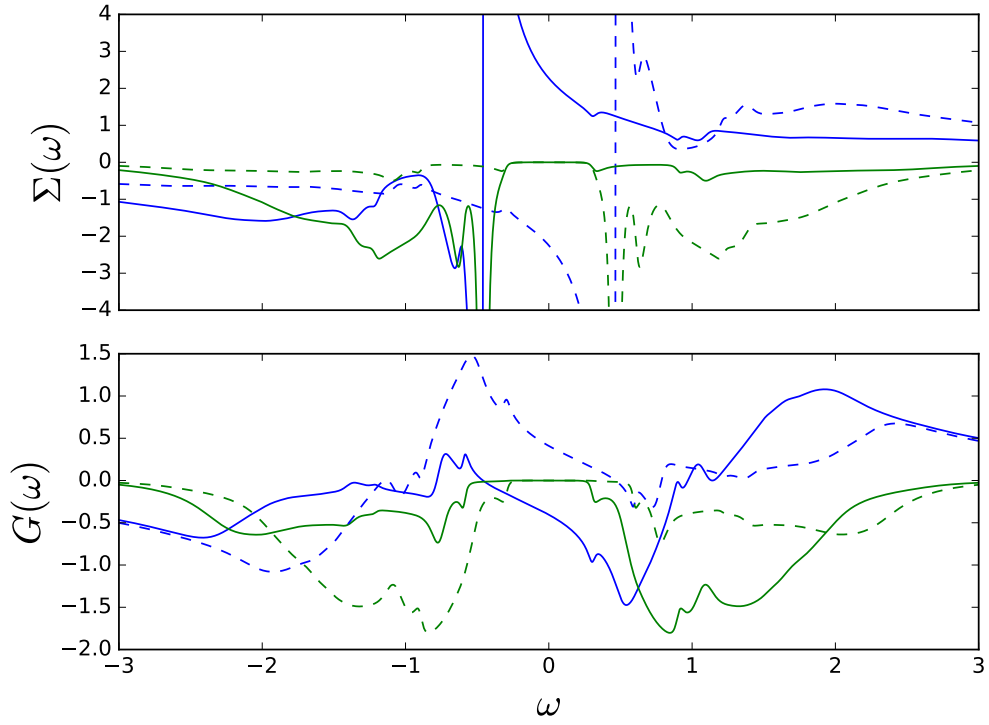


Figure 3: Insulating Self-energy (top) and Green Function (bottom) for the interacting dimer. Blue corresponds to real part and Green is Imaginary part. Full line is the symmetric sum of local and intersite functions, dashed is the difference.

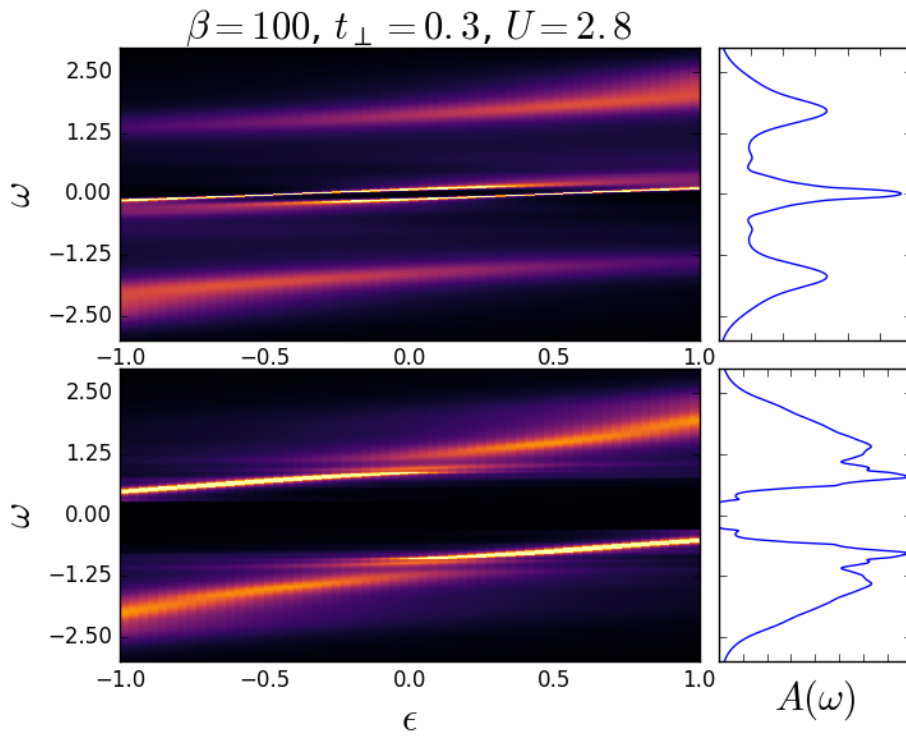


Figure 4: Comparison of the electronic structure. The real frequency solver gives a lot more states around the band edges in the insulator.