How to compute free energy in LDA+DMFT?

We print $F+TS_{imp}$, where S_{imp} is the entropy of the impurity model. To get free energy, we need to do

$$F = (F+TS_{imp}) - TS_{imp}$$

How to compute S_{imp}?

If T is large enough, so that probability for no kinks (histogram for $n=0$) is finite (maybe $>10^{-5}$), we can compute Z_{imp} from the following relation:

$$P_0 = \frac{Z_{atom}}{Z_{imp}}$$

where P_0 is probability for no kinks, Z_{atom} is partition function of the atom, printed in "nohup_imp.out"

We thus have $e^{-\beta F_{imp}} = Z_{imp} = \frac{Z_{atom}}{P_0}$ or $F_{imp} = -T\ln\left(\frac{Z_{atom}}{P_0}\right)$

Energy of the impurity is

$$E_{imp} = Tr\left(\left[\varepsilon_{imp} + \Delta - \omega_n \frac{d\Delta}{d\omega_n}\right] G_{imp}\right) + \frac{1}{2} Tr\left(\Sigma_{imp} G_{imp}\right)$$

and is printed in "info.out"

To get entropy, we just calculate $TS_{imp} = E_{imp} - F_{imp}$

At lower T, P_0 becomes too small to be useful. We have to integrate energy from desired temperature to T_∞, where T_∞ is high enough that P_0 becomes finite.

How to integrate impurity energy? First, we fix Δ and ε_{imp} to it's DMFT converged value. We just change T and compute E_{imp}. We can use the following formula: $S = S_{T_\infty} - \int_T^{T_\infty} \frac{1}{T}\frac{dE_{imp}}{dT}\,dT$ but it is better to use $E_{imp}(\beta)$ formula, which avoids differentiation:

$$S = S_{T_\infty} - \frac{E_{T_\infty}}{T_\infty} + \frac{E_T}{T} - \int_{\frac{1}{T_\infty}}^{\frac{1}{T}} E(\beta)\,d\beta, \quad \text{where } \beta = \frac{1}{T}.$$