How to Calculate Energies from $G_\sigma(k, i\omega_n)$ and $\Sigma_\sigma(k, i\omega_n)$

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1 Brief

The outputs of DMFT are generally greens functions, $G_\sigma(k, i\omega_n)$, and self-energies, $\Sigma_\sigma(k, i\omega_n)$, in momentum and Matsubara space. From these outputs, we would like to be able to calculate various observables, the most obvious being the energy of the system. This document presents a derivation of the formulas used to calculate the energy used by the ALPSCore based program *energy-alpscore*.

2 Formula Derivation

The energy per site is given by the expectation value of the Hamiltonian, which in our case is given by the Hubbard Hamiltonian.

$$E = \langle H \rangle$$

$$H = \sum_{k\sigma} \left(\epsilon(k) - \mu\right) c^\dagger_{k\sigma} c_{k\sigma} + U \sum_i \left(n_{i\uparrow} - \frac{1}{2}\right)\left(n_{i\downarrow} - \frac{1}{2}\right)$$

We can split the total energy into kinetic and potential energies as follows.

$$E = E_K + E_V$$

$$E_K = \left\langle \sum_{k\sigma} \left(\epsilon(k) - \mu\right) c^\dagger_{k\sigma} c_{k\sigma} \right\rangle$$

$$E_V = \left\langle U \sum_i \left(n_{i\uparrow} - \frac{1}{2}\right)\left(n_{i\downarrow} - \frac{1}{2}\right) \right\rangle$$

We would like to write these formulas in terms of $G_\sigma(k, i\omega_n)$ and $\Sigma_\sigma(k, i\omega_n)$. Begin by rearranging the expressions, noting that $G^{-1}_\sigma(k, i\omega_n) = i\omega_n - \epsilon(k) + \mu - \Sigma_\sigma(k, i\omega_n)$, and using translational invariance.

$$\begin{aligned} E_K &= \sum_{k\sigma} \left(\epsilon(k) - \mu\right) \left\langle c^\dagger_{k\sigma} c_{k\sigma} \right\rangle \\ &= \sum_{k\sigma} \left(\epsilon(k) - \mu\right) \langle n_{k\sigma} \rangle \\ &= \sum_{k\sigma} \left(i\omega_n - \Sigma_\sigma(k, i\omega_n) - G^{-1}_\sigma(k, i\omega_n)\right) \langle n_{k\sigma} \rangle \end{aligned}$$

$$\begin{aligned} E_V &= \left\langle U \sum_i \left(n_{i\uparrow} n_{i\downarrow} - \frac{1}{2} n_{i\uparrow} - \frac{1}{2} n_{i\downarrow} + \frac{1}{4}\right) \right\rangle \\ &= \frac{UN}{4} - \frac{U}{2} \sum_{i\sigma} \langle n_{i\sigma} \rangle + U \sum_i \langle n_{i\uparrow} n_{i\downarrow} \rangle \\ &= \frac{UN}{4} - \frac{U}{2} \sum_{k\sigma} \langle n_{k\sigma} \rangle + U \sum_i \langle n_{i\uparrow} n_{i\downarrow} \rangle \end{aligned}$$

So we really just need to express $\langle n_{k\sigma} \rangle$ and $\langle n_{i\uparrow} n_{i\downarrow} \rangle$ in terms of $G_\sigma(k, i\omega_n)$ and $\Sigma_\sigma(k, i\omega_n)$. The expectation value of the density is the easier value to calculate. Starting with the definition of the Greens function in imaginary time,

$$\begin{aligned} G_\sigma(k, \tau) &= -\left\langle T_\tau c_{k\sigma}(\tau) c^\dagger_{k\sigma}(0) \right\rangle \\ G_\sigma(k, \tau + \beta) &= -G_\sigma(k, \tau) \\ G_\sigma(k, \tau) &= \frac{1}{\beta} \sum_n G_\sigma(k, i\omega_n) e^{-i\omega_n \tau} \end{aligned}$$

We can calculate

$$\begin{aligned} \langle n_{k\sigma} \rangle &= \left\langle c^\dagger_{k\sigma} c_{k\sigma} \right\rangle \\ &= \left\langle c^\dagger_{k\sigma}(0) c_{k\sigma}(\tau = 0^-) \right\rangle \\ &= -\left\langle T_\tau c_{k\sigma}(\tau = 0^-) c^\dagger_{k\sigma}(0) \right\rangle \\ &= G_\sigma(k, \tau \to 0^-) \\ &= \frac{1}{\beta} \sum_n G_\sigma(k, i\omega_n) e^{i\omega_n 0^+} \\ &= \frac{1}{\beta} \sum_n G_\sigma(k, i\omega_n) \end{aligned}$$

In order to write $\langle n_{i\uparrow} n_{i\downarrow} \rangle$ in terms of $G_\sigma(k, i\omega_n)$ and $\Sigma_\sigma(k, i\omega_n)$, we make use of two identities (that you can find in Coleman),

$$\sum_{k\sigma} c^\dagger_{k\sigma} \left[H_0, c_{k\sigma}\right] = -H_0$$

$$-2V = \sum_{k\sigma} c^\dagger_{k\sigma} \left[V, c_{k\sigma}\right]$$

Where H_0 is the non-interacting part of the Hamiltonian and V is a general interaction of the form

$$V = \sum_{k_1 k_2 k_3 k_4} V(k_1, k_2, k_3, k_4) c^\dagger_{k_1} c^\dagger_{k_2} c_{k_3} c_{k_4}$$

where the k_i indices stand for all relevant state indices, ie momentum and spin. We also use the equation of motion for an operator O,

$$\frac{\partial O}{\partial \tau} = [H, O]$$

In our case,

$$V = \sum_i n_{i\uparrow} n_{i\downarrow} = H - H_0 - \frac{UN}{4} + \frac{U}{2} \sum_{k\sigma} n_{k\sigma}$$

$$\begin{aligned} H_0 &= \sum_{k\sigma} \left(i\omega_n - \Sigma_\sigma(k, i\omega_n) - G^{-1}_\sigma(k, i\omega_n) \right) n_{k\sigma} \\ &= \frac{1}{\beta} \sum_{nk\sigma} \left[-1 e^{i\omega_n 0^+} + (i\omega_n - \Sigma_\sigma(k, i\omega_n)) G_\sigma(k, i\omega_n) e^{i\omega_n 0^+} \right] \end{aligned}$$

So,

$$\begin{aligned} \left\langle \sum_i n_{i\uparrow} n_{i\downarrow} \right\rangle &= \langle V \rangle \\ &= \left\langle -\frac{1}{2} \sum_{k\sigma} c^\dagger_{k\sigma} \left[\sum_i n_{i\uparrow} n_{i\downarrow}, c_{k\sigma} \right] \right\rangle \\ &= \frac{-1}{2} \sum_{k\sigma} \left\langle c^\dagger_{k\sigma} \left[H - H_0 - \frac{UN}{4} + \frac{U}{2} \sum_{k\sigma} n_{k\sigma}, c_{k\sigma} \right] \right\rangle \\ &= \frac{-1}{2} \sum_{k\sigma} \left\langle c^\dagger_{k\sigma} [H, c_{k\sigma}] \right\rangle - \left\langle c^\dagger_{k\sigma} [H_0, c_{k\sigma}] \right\rangle \\ &+ \frac{U}{2} \left\langle c^\dagger_{k\sigma} \left[\sum_{k\sigma} n_{k\sigma}, c_{k\sigma} \right] \right\rangle \\ &= -\frac{1}{2} \left(\sum_{k\sigma} \left[\left(\frac{\partial G_\sigma(k,\tau)}{\partial \tau} \right)_{\tau \to 0^-} - \frac{U}{2} \langle n_{k\sigma} \rangle \right] + H_0 \right) \\ &= -\frac{1}{2} \sum_{nk\sigma} \left[\frac{-i\omega_n}{\beta} G_\sigma(k, i\omega_n) e^{i\omega_n 0^+} - \frac{U}{2\beta} G_\sigma(k, i\omega_n) e^{i\omega_n 0^+} \right] \\ &+ -\frac{1}{2\beta} \sum_{nk\sigma} \left[-1 e^{i\omega_n 0^+} + (i\omega_n - \Sigma_\sigma(k, i\omega_n)) G_\sigma(k, i\omega_n) e^{i\omega_n 0^+} \right] \\ &= \frac{1}{2\beta} \sum_{nk\sigma} \Sigma_\sigma(k, i\omega_n) G_\sigma(k, i\omega_n) + \frac{U}{4\beta} \sum_{nk\sigma} G_\sigma(k, i\omega_n) \end{aligned}$$

Where we used that

$$\frac{1}{\beta} \sum_n e^{i\omega_n 0^+} = -\frac{1}{2\pi i} \int dz \frac{e^{z0^+}}{e^{\beta z} + 1}$$

By the residue theorem, with a contour that encompasses the poles at $e^{\beta z} = -1$, $\beta z = i(2n+1)\pi$, $z = i(2n+1)/\beta = i\omega_n$, along the imaginary axis. If we reverse the direction of the contour, we would instead pick up the poles outside of this contour, those belonging to e^{z0^+}. But this function has no poles, and thus no residues. So,

$$\frac{1}{\beta} \sum_n e^{i\omega_n 0^+} = 0$$

Our final results for the energy in terms of $G_\sigma(k, i\omega_n)$ and $\Sigma_\sigma(k, i\omega_n)$ are then:

$$E = E_K + E_V$$

$$E_K = \frac{1}{\beta} \sum_{nk\sigma} \left[-1 + (i\omega_n - \Sigma_\sigma(k, i\omega_n)) G_\sigma(k, i\omega_n) \right]$$

$$\begin{aligned} E_V &= \frac{UN}{4} - \frac{U}{2\beta} \sum_{nk\sigma} G_\sigma(k, i\omega_n) \\ &\quad + \frac{1}{2\beta} \sum_{nk\sigma} \Sigma_\sigma(k, i\omega_n) G_\sigma(k, i\omega_n) + \frac{U}{4\beta} \sum_{nk\sigma} G_\sigma(k, i\omega_n) \\ &= \frac{UN}{4} - \frac{U}{4\beta} \sum_{nk\sigma} G_\sigma(k, i\omega_n) \\ &\quad + \frac{1}{2\beta} \sum_{nk\sigma} \Sigma_\sigma(k, i\omega_n) G_\sigma(k, i\omega_n) \end{aligned}$$

The energy should be a real valued quantity, and one can check that the above formulas satisfy this constraint by using that

$$\begin{aligned} G^*(i\omega_n) &= G(-i\omega_n) \\ \Sigma^*(i\omega_n) &= \Sigma(-i\omega_n) \end{aligned}$$

Since the frequency sums kill any terms that have odd frequency parity, only certain combinations of real ($\Re$) and imaginary ($\Im$) parts survive

$$E_K = \frac{2}{\beta} \sum_{n \geq 0, k\sigma} \left[-1 - \Re\Sigma\Re G - \omega_n \Im G + \Im\Sigma\Im G \right]$$

$$E_V = \frac{UN}{4} - \frac{2U}{4\beta} \sum_{n \geq 0, k\sigma} \Re G + \frac{2}{2\beta} \sum_{n \geq 0, k\sigma} (\Re\Sigma\Re G - \Im\Sigma\Im G)$$

So there are really three terms that we need to compute

$$\begin{aligned} I_1 &= 2 \sum_{n \geq 0, k\sigma} \left[-1 - \omega_n \Im G \right] \\ I_2 &= 2 \sum_{n \geq 0, k\sigma} (\Re\Sigma\Re G - \Im\Sigma\Im G) \\ I_3 &= 2 \sum_{n \geq 0, k\sigma} \Re G \end{aligned}$$

So

$$\begin{aligned} E_K &= \frac{I_1}{\beta} - \frac{I_2}{\beta} \\ E_V &= \frac{UN}{4} - \frac{U}{4\beta} I_3 + \frac{1}{2\beta} I_2 \end{aligned}$$

3 High Frequency Tails

The above formulas tell us how to calculate the energy theoretically, but on a computer we cannot actually do the full summation over Matsubara frequencies. The stored greens functions and self-energies are always truncated at some maximum frequency, $i\omega_{n_m}$. We cannot simply truncate the sum, however, because these functions decay slowly as a function of $i\omega_n$ due to the discontinuity in $G_\sigma(k,\tau)$ at $\tau = 0$.

We solve this problem by utilizing analytic high frequency tails for $G_\sigma(k, i\omega_n)$ and $\Sigma_\sigma(k, i\omega_n)$,

$$\Sigma_\sigma^{tail}(k, i\omega_n) = \Sigma_\sigma^0(k) + \frac{\Sigma_\sigma^0(k)}{i\omega_n} + \mathcal{O}\left(\frac{1}{(i\omega_n)^2}\right)$$

$$G_\sigma^{tail}(k, i\omega_n) = \frac{c_\sigma^1(k)}{i\omega_n} + \frac{c_\sigma^2(k)}{(i\omega_n)^2} + \frac{c_\sigma^3(k)}{(i\omega_n)^3} + \mathcal{O}\left(\frac{1}{(i\omega_n)^4}\right)$$

The coefficients in these expansions can be calculated by hand (though it is tedious, see Emanuel's thesis for details), and are computed during the DMFT program and stored with the GFTools greens functions. In the following, we explicity use that $c_\sigma^1(k) = 1$.

The tails enable us to write the frequency sums as

$$\sum_n f(i\omega_n) = \sum_{n \le n_m} f(i\omega_n) + \sum_{n > n_m} f^{tail}(i\omega_n)$$

The energy terms can now be written as (supressing momentum and spin, and only keeping up to order $1/\omega_n^2$ terms)

$$\begin{aligned} I_1 &= 2\sum_{n_m \ge n \ge 0} [-1 - \omega_n \Im G] + 2\sum_{n > n_m} \left[-1 - \omega_n \Im G^{tail}\right] \\ &= 2\sum_{n_m \ge n \ge 0} [-1 - \omega_n \Im G] - 2\sum_{n > n_m} \frac{c_3}{\omega_n^2} \\ &= 2\sum_{n_m \ge n \ge 0} [-1 - \omega_n \Im G] - 2c_3\Psi \end{aligned}$$

$$\begin{aligned} I_2 &= 2\sum_{n_m \ge n \ge 0} (\Re\Sigma\Re G - \Im\Sigma\Im G) + 2\sum_{n > n_m} \left(\Re\Sigma^{tail}\Re G^{tail} - \Im\Sigma^{tail}\Im G^{tail}\right) \\ &= 2\sum_{n_m \ge n \ge 0} (\Re\Sigma\Re G - \Im\Sigma\Im G) + 2\sum_{n > n_m} \left(\frac{-c^1\Sigma^1}{\omega_n^2} - \frac{\Sigma^0 c^2}{\omega_n^2}\right) \\ &= 2\sum_{n_m \ge n \ge 0} (\Re\Sigma\Re G - \Im\Sigma\Im G) + 2\left(-c^1\Sigma^1 - \Sigma^0 c^2\right)\Psi \end{aligned}$$

$$\begin{aligned} I_3 &= 2\sum_{n_m \ge n \ge 0} \Re G + 2\sum_{n > n_m} \Re G^{tail} \\ &= 2\sum_{n_m \ge n \ge 0} \Re G - 2\sum_{n > n_m} \frac{c_2}{\omega_n^2} \\ &= 2\sum_{n_m \ge n \ge 0} \Re G - 2c_2\Psi \end{aligned}$$

Where

$$\begin{aligned} \Psi &= \sum_{n > n_m} \frac{1}{\omega_n^2} \\ &= \frac{\beta^2}{\pi^2 4}\sum_{k=0}^{\infty} \frac{1}{(n_m + 0.5 + k)^2} \\ &= \frac{\beta^2}{\pi^2 4}\psi^{(1)}(n_m + 0.5) \end{aligned}$$

Where $\psi^{(n)}(x)$ is the digamma function, which can be computed with a GSL function call (gsl_sf_psi_n).