Ulmke's Smoothing Trick

A completely different approach was taken by Ulmke (1995). Here, the number of Matsubara frequencies is chosen equal to the number of time slices. In order to enforce the correct analytical behavior of the Fourier transforms, a "smoothing" trick is employed: the naive Fourier transform is combined with an approximate correcting transformation which approaches the identity for $\Delta\tau \to 0$. The algorithm consists of the following two steps:

1. Asymmetric naive Fourier transform $\tilde{G}(i\omega_n) = \Delta\tau \sum_{l=0}^{\Lambda-1} \mathrm{e}^{i\omega_n \tau_l}\, G(\tau_l)$. The difference to the symmetric transform (3.14) is a constant finite real term $\Delta\tau/2$.

2. Smoothing transformation

$$G(i\omega_n) = \frac{\Delta\tau}{\ln(1 + \Delta\tau/\tilde{G}(i\omega_n))}\,. \tag{3.16}$$

This corrected Green function fulfills $\mathrm{Re}\, G(\omega) = 0$ (for half filling and symmetric DOS) and (approximately) $G(i\omega_n) \propto 1/(i\omega_n)$ for $\omega \to \pm\omega_{\max}$. By using the inverse correction transform $\tilde{G}(\omega) = \Delta\tau/(\exp(\Delta\tau/G(\omega) - 1))$ before the inverse Fourier transform, also the artifacts in $G(\tau)$ (or $\mathcal{G}(\tau)$) are removed. Ulmke's (1995) claim that the transformation scheme would be exact in the noninteracting and in the atomic limit is, however, incorrect. The assumed asymptotic form $G(i\omega_n) = 1/(i\omega_n)$ for hopping $t = 0$ applies only to the degenerate $U = 0$ case. Otherwise, $G(i\omega_n)$ is linear for small frequencies in the insulating regime. This misconception already points towards the main deficiency of the scheme: in order to cure a problem at high frequencies, a transformation is applied which changes G irrespective of the frequency. In fact, all values of G are modified significantly which are not large compared to $\Delta\tau$. Among this group, however, are not only points near the Nyquist frequency, but also those with small $i\omega_n$ (in the insulator). Consequently, Ulmke's approach treats insulating solutions much worse than metallic solutions.

In order to illustrate this effect and for a general quantitative comparison, we used the insulating solution $G(\tau)$ for $\beta = 32$, $U = 4.92$, and $\Delta\tau = 0.25$ as provided by Rozenberg as input for the various Fourier transformation schemes. Each output $G(i\omega_n)$ was then transformed to the corresponding self-energy $\Sigma(i\omega_n)$ via the inverted Bethe lattice Dyson equation. As shown in Fig. 3.11, only Jarrell's algorithm yields a self-energy with the correct analytic form, i.e., with negative imaginary part for all positive ω_n.[15] While Ulmke's algorithm just stops at the Nyquist frequency $\pi/\Delta\tau$, Krauth's code overshoots substantially (see also right inset).[16] At small frequencies, the results of Krauth's method and of Jarrell's method agree very well (left inset),

[15] Slight deviations from the quantitatively correct asymptotic form for very large frequencies (not shown) could have been avoided by using the exact asymptotic expression $\Sigma(i\omega_n) \to U^2/(4i\omega_n)$ in this regime; cf. App. C.

[16] This overshooting can be attributed to the use of natural splines; it might have been overlooked since the original code does not output frequency information. The origin of slight deviations for intermediate frequencies $\omega_n \approx 1$ (in comparison with the curves for Jarrell's method and the modified Ulmke method) is unclear.