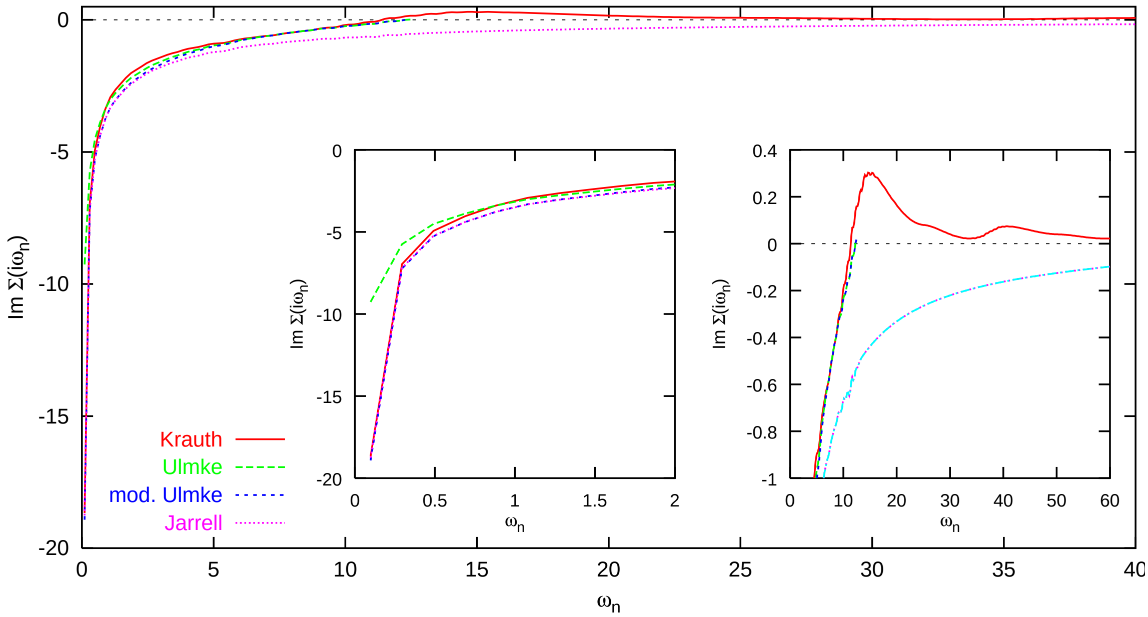

Figure 3.11: Comparison of Fourier-transform schemes for the step $G(\tau) \longrightarrow G(i\omega_n)$; here represented as $\Sigma(\omega) = \omega - G^{-1}(\omega) - (W/4)^2 G(\omega)$ for better resolution of the differences. For all methods, the imaginary-time solution $G(\tau)$ for the insulating phase at $\beta = 32$, $U = 4.92$, and $\Delta\tau = 0.25$ provided by Rozenberg (see text) was used as input. The left inset concentrates on low frequencies where the smoothing artifact of Ulmke's original method (long-dashed line) is seen clearly; the modified version does not show this artifact. At high frequencies (right inset), Krauth's curves overshoot substantially while Jarrell's method yields $1/\omega$ decay; Ulmke's method (both versions) makes no predictions beyond the Nyquist frequency.

while Ulmke's code is off by a factor of about 2. As we will check below, this striking disagreement completely destabilizes any insulating solution (for $\Delta\tau = 0.25$).

Improved Smoothing Method

In order to further isolate the inaccurate treatment of $G(i\omega_n)$ at small frequencies as the cause of this problem, we searched for a specific cure within the general framework of the smoothing trick. Obviously, the smoothing transformation (3.16) has to be replaced by an explicitly frequency-dependent formulation. While interpolation (using the result of the "naive" transform at small frequencies) is in principle possible, our choice is better controlled: we replaced $\Delta\tau$ in (3.16) by $\big(1 - (\omega_n \Delta\tau/\pi - 1)^8\big)\Delta\tau$. The additional factor fulfills two requirements: it is very close to the value 1 when ω_n is of the order of the Nyquist frequency $\pi/\Delta\tau$ and of the order $\Delta\tau$ for $\omega_n \to 0$ (while always being smaller than 1). Therefore, the smoothing trick can still work for large frequencies while the error at low frequencies is now $\mathcal{O}(\Delta\tau^2)$ instead of $\mathcal{O}(\Delta\tau)$. The dramatic improvement is apparent in Fig. 3.11: the short-dashed line ("mod. Ulmke") is indistinguishable from the result of Jarrell's method for small frequencies