is too coarse for the numerical integrations which will be performed according to the lowest-order approximation

$$\int_{x_0}^{x_n} dx\, f(x) \approx \Delta x \sum_{l=0}^{n-1} \frac{f(x_l) + f(x_{l+1})}{2}\,, \tag{4.156}$$

where $x_i = i\Delta x$. Therefore, $\mathrm{Im}\, G$ is first interpolated[50] and evaluated on a finer grid with the resolution $\Delta\omega = 0.005$ (dashed line in Fig. 4.27). The Kramers-Kronig transformation is then performed using (4.156) which yields $\mathrm{Re}\, G$ on the same fine grid (solid line). In order to demonstrate the importance of the interpolation procedure, the result of a direct Kramers-Kronig transformation is also shown in Fig. 4.27 (small crosses). The difference between both estimates for G are relatively small, but clearly visible.

The next step, the numerical inversion of the $\boldsymbol{k}$ integrated Dyson equation (on the fine grid) falls into the class of complex root-finding problems (plus a trivial integration). Such problems are less trivial than real-valued one-dimensional root-finding problems since the solution cannot be bracketed. We have accomplished the solution using an adapted two-dimensional (in the Gaussian plane) Newton scheme; its Jacobian is specified by

$$\frac{\partial \mathrm{Im}\, G}{\partial \mathrm{Im}\, \Sigma} = \frac{\partial \mathrm{Re}\, G}{\partial \mathrm{Re}\, \Sigma} = \int_{-\infty}^{\infty} \mathrm{d}\epsilon\, \rho(\epsilon) \frac{(\omega - \epsilon - \mathrm{Re}\, \Sigma)^2 - (\mathrm{Im}\, \Sigma)^2}{\left[(\omega - \epsilon - \mathrm{Re}\, \Sigma)^2 + (\mathrm{Im}\, \Sigma)^2\right]^2}\,, \tag{4.157}$$

where we have suppressed the ω-dependence of G and Σ for notational convenience (since Dyson equation is local in ω anyway), and

$$\frac{\partial \mathrm{Im}\, G}{\partial \mathrm{Re}\, \Sigma} = -\frac{\partial \mathrm{Re}\, G}{\partial \mathrm{Im}\, \Sigma} = \int_{-\infty}^{\infty} \mathrm{d}\epsilon\, \rho(\epsilon) \frac{2\,(\omega - \epsilon - \mathrm{Re}\, \Sigma)\, \mathrm{Im}\, \Sigma}{\left[(\omega - \epsilon - \mathrm{Re}\, \Sigma)^2 + (\mathrm{Im}\, \Sigma)^2\right]^2}\,. \tag{4.158}$$

In our program, the iterative search can be stabilized by underrelaxation (typically using a factor of 0.5). Note that the existence of an analytical solution $\Sigma(\omega)$ (with $\mathrm{Im}\, \Sigma(\omega) < 0$) of the inverse Dyson equation is by no means guaranteed for an arbitrary spectral function $A(\omega)$. For example, the maximum value of the spectral function must not exceed the maximum of the noninteracting DOS in the homogeneous case. On the other hand, numerical errors can easily produce such unphysical spectra since the (unrestricted) MEM does not incorporate model specific physical information. Then, the root-finding algorithm will fail to converge at least for some isolated frequencies ω. In our implementation of the algorithm, such isolated failures can be fixed by linear interpolation of the solutions at adjacent grid points. The fact that this was necessary only for the strongest interaction $U = 5.5$ is a further

[50] We have chosen linear interpolation not only for sake of simplicity, but also for robustness. While for the metallic case a cubic spline interpolation might yield a better approximation of the smooth spectrum, such a higher order scheme is dangerous in general since it may lead to ringing (oscillations) and to nonanalytic solutions (i.e., solutions of the wrong sign) near band edges.