1971; Georges et al., 1996)

$$E = \lim_{\eta \to 0^+} T \sum_{n,\sigma} \int_{-\infty}^{\infty} \mathrm{d}\epsilon \frac{\mathrm{e}^{i\omega_n \eta}\, \epsilon\rho(\epsilon)}{i\omega_n - \epsilon - \Sigma(i\omega_n)} + \frac{1}{2} T \sum_{n,\sigma} \Sigma_\sigma(i\omega_n) G_\sigma(i\omega_n)\,. \tag{3.7}$$

Note the convergence factor $\mathrm{e}^{i\omega_n\eta}$ which is essential in order to get the correct result. Obviously, such a term is difficult to handle numerically; in practice, η may be replaced, e.g., by the time discretization parameter $\Delta\tau$, which also determines the cutoff frequency in the infinite sum. This approximation can be avoided by evaluating the noninteracting part separately. For the kinetic energy, this implies

$$\begin{aligned} E_{\text{kin}} &= \lim_{\eta \to 0^+} 2T \sum_{n=-\infty}^{\infty} \mathrm{e}^{i\omega_n\eta} \int_{-\infty}^{\infty} d\epsilon\, \epsilon\rho(\epsilon)\, \frac{1}{i\omega_n - \epsilon - \mu - \Sigma(i\omega_n)} && (3.8)\\ &= 2\int_{-\infty}^{\infty} d\epsilon \frac{\epsilon\rho(\epsilon)}{\mathrm{e}^{\beta\epsilon}+1} + 2T \sum_{n=-\infty}^{\infty} \int_{-\infty}^{\infty} d\epsilon\, \epsilon\rho(\epsilon) \left(G_\epsilon(i\omega_n) - G^0_\epsilon(i\omega_n)\right) && (3.9)\\ &\approx 2\int_{-\infty}^{\infty} d\epsilon \frac{\epsilon\rho(\epsilon)}{\mathrm{e}^{\beta\epsilon}+1} + 2T \sum_{n=-L/2+1}^{L/2} \int_{-\infty}^{\infty} d\epsilon\, \epsilon\rho(\epsilon) \left(G_\epsilon(i\omega_n) - G^0_\epsilon(i\omega_n)\right)\,, && (3.10) \end{aligned}$$

where we have assumed the paramagnetic case and $\mu = 0$. Here, the interacting and noninteracting "momentum-dependent" Green functions read

$$G_\epsilon(i\omega_n) = \frac{1}{i\omega_n - \epsilon - \mu - \Sigma(i\omega_n)}\,; \qquad G^0_\epsilon(i\omega_n) = \frac{1}{i\omega_n - \epsilon - \mu}\,. \tag{3.11}$$

In (3.10), the terms in the Matsubara sum fall off at least as $1/\omega^2$, which makes it well-defined also without convergence factor. At the same time, the truncation error is reduced significantly. This is particularly important for our code, where the number of Matsubara frequencies is comparatively small since it equals the number of time slices L (see Sec. 3.4). The complementary ingredient to the energy is the double occupancy D with $E = E_{\text{kin}} + UD$. In the context of QMC calculations, this observable is best calculated directly from Wick's theorem when sampling over the auxiliary field. The overall behavior of D and E in the Hubbard model can be read off (for $T = 0.1$) from the middle and lower parts of Fig. 3.6, respectively. For small U, the kinetic energy increases quadratically while D and, consequently, E_{pot} and E increase linearly. The potential energy reaches a maximum below $U = 3$. A region of strong curvature of D, E_{pot}, and E_{kin} near $U = 4.6$ gives a rough indication of the metal-insulator crossover. The total energy E, however, hardly shows any anomalies at this scale. Note also that the solutions for D and E are quite close to the results of plain zero-temperature second-order perturbation theory. We will see later that the agreement actually becomes better for low-temperature QMC data, extrapolated to $T \to 0$. The offset of the curves for E gives (for not too large U) an indication of the specific heat $c_V = \mathrm{d}E/\mathrm{d}T$ which is linear within the Fermi-liquid phase and is, in general, best evaluated by fitting the temperature dependence of E.