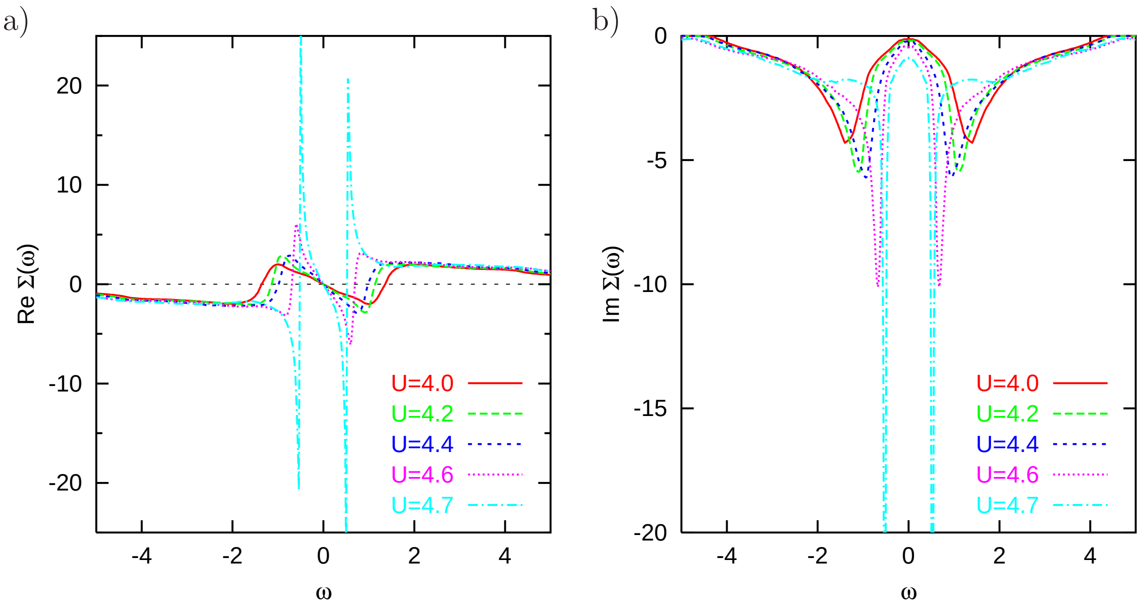

Figure 4.30: QMC results for $T = 0.05$: Self-energy in the metallic phase near the MIT. **a)** The width of the central linear region of $\mathrm{Re}\,\Sigma(\omega)$ decreases with increasing U while the absolute slope near $\omega = 0$ increases. **b)** $\mathrm{Im}\,\Sigma(\omega)$ is nearly quadratic at small $|\omega|$. The very sharp features for $U = 4.7$ might be exaggerated due to numerical errors.

frequencies $|\omega|$. On the other hand, the result for $U = 4.7$ (as well as for all other values of the interaction) is robust numerically, i.e., is nearly invariant under the choice of a default model (within the MEM procedure).

Results for the insulating phase are displayed in Fig. 4.31. Here, $\mathrm{Im}\,\Sigma$ shows a single peak at $\omega = 0$ which narrows with increasing U. While this peak is part of a continuous spectrum [of $\Sigma(\omega)$] for $U \leq 5.0$, it appears δ-function like and surrounded by a full gap for $U = 5.5$. Corresponding to the single-peak structure of $\mathrm{Im}\,\Sigma(\omega)$, the derivative of the real part $\mathrm{Re}\,\Sigma(\omega)$ at $\omega = 0$ is positive (and of large absolute value) which implies that the quasiparticle weight Z as defined in (3.5) is negative.

Before turning to results for the optical conductivity, let us perform some additional checks of the results obtained so far. Since $\Sigma(\omega)$ is a retarded function which is analytic in the upper half plane, it can be expressed in terms of its positive semidefinite spectral function $A_\Sigma(\omega) := -\frac{1}{\pi}\mathrm{Im}\,\Sigma(\omega)$. The norm of this spectral function gives some measure of the total influence of the interaction on the single-particle properties. A priori, one would expect this norm to be a smooth function of U, except possibly for kinks or jumps at phase transitions. Thus, an evaluation of this norm can be useful for identifying outliers caused by numerical errors. This expectation is indeed correct as seen in Fig. 4.32, where circles indicate the numerical estimates based on the self energies shown in Fig. 4.30 and Fig. 4.31. In fact, all results are nearly on a straight line, even across the phase transition at $U \approx 4.7$. Under the assumption that this behavior is universal, i.e., that the true norm does not depend on the temperature and on the model DOS, the total self-energy spectral weight must be proportional