axis, since

$$
\begin{aligned}
-\frac{dn_\epsilon}{d\epsilon} &= \frac{1}{\pi}\int_{-\infty}^{\infty} \mathrm{d}\omega\, \mathrm{Im}\left(G_\epsilon^2(\omega)\right) n_\mathrm{f}(\omega) \;=\; T\sum_n G_\epsilon^2(i\omega_n) \\
&= T\sum_n \frac{(\epsilon+\mathrm{Re}\,\Sigma_n)^2-(\omega_n-\mathrm{Im}\,\Sigma_n)^2}{\left((\epsilon+\mathrm{Re}\,\Sigma_n)^2+(\omega_n-\mathrm{Im}\,\Sigma_n)^2\right)^2}\,. \qquad (4.88)
\end{aligned}
$$

Since the terms in (4.88) decay as $1/\omega_n^2$, the sum over n does not require additional convergence factors. Furthermore, due to the fast convergence, the sum is insensitive to the large-frequency behavior of the self-energy. Since, on the other hand, QMC methods in general and the particular Fourier-transform techniques used in this work do not yield good estimates for Σ_n at large frequencies, the estimate for (4.88) will be even much better conditioned than, e.g., the estimate (3.10) for the kinetic energy. In fact, we found that computing n_ϵ by integrating over $\mathrm{d}n_\epsilon/\mathrm{d}\epsilon$ as given by (4.88) reduces the $\Delta\tau$ error for the kinetic energy considerably when compared with the direct computation (3.10).

4.3.3 f-sum Rule and General Dispersion Formalism

Within the framework of the general dispersion method developed in Sec. 2.3, the full noninteracting dispersion $\epsilon_{\boldsymbol{k}}$ can be written in terms of the transformation function $\mathcal{F}$ and the dispersion $\epsilon_{\boldsymbol{k}}^{\mathrm{hc}}$ of the hypercubic lattice with NN hopping only. Then, the derivatives appearing in (4.47) through (4.50) read

$$
\frac{\partial\epsilon_{\boldsymbol{k}}}{\partial k_x} = \frac{\partial}{\partial k_x}\mathcal{F}(\epsilon_{\boldsymbol{k}}^{\mathrm{hc}}) \;=\; \mathcal{F}'(\epsilon_{\boldsymbol{k}}^{\mathrm{hc}})\frac{\partial\epsilon_{\boldsymbol{k}}^{\mathrm{hc}}}{\partial k_x} \qquad (4.89)
$$

and

$$
\frac{\partial^2\epsilon_{\boldsymbol{k}}}{\partial k_x^2} = \mathcal{F}'(\epsilon_{\boldsymbol{k}}^{\mathrm{hc}})\frac{\partial^2\epsilon_{\boldsymbol{k}}^{\mathrm{hc}}}{\partial k_x^2} + \mathcal{F}''(\epsilon_{\boldsymbol{k}}^{\mathrm{hc}})\left(\frac{\partial\epsilon_{\boldsymbol{k}}^{\mathrm{hc}}}{\partial k_x}\right)^2 . \qquad (4.90)
$$

Using (for $a=1$)

$$
\epsilon_{\boldsymbol{k}}^{\mathrm{hc}} = \sqrt{\frac{2}{d}}\sum_{\alpha=1}^{d}\cos(k_\alpha); \quad \frac{\partial\epsilon_{\boldsymbol{k}}^{\mathrm{hc}}}{\partial k_x} = -\sqrt{\frac{2}{d}}\sin(k_x); \quad \frac{\partial^2\epsilon_{\boldsymbol{k}}^{\mathrm{hc}}}{\partial k_x^2} = -\sqrt{\frac{2}{d}}\cos(k_x) \qquad (4.91)
$$

we can carry out the sum in (4.64)

$$
\begin{aligned}
\tilde\rho(\epsilon) &= \lim_{d\to\infty} d\tilde\rho_{xx}(\epsilon) \\
&= \frac{1}{N}\sum_{\boldsymbol{k}}\lim_{d\to\infty} d\Big(\frac{\partial\epsilon_{\boldsymbol{k}}}{\partial k_x}\Big)^2\delta(\epsilon-\epsilon_{\boldsymbol{k}}) \\
&= \lim_{d\to\infty}\frac{d}{(2\pi)^d}\int\mathrm{d}k_x\int\mathrm{d}\boldsymbol{k}_\perp\big(\mathcal{F}'(\epsilon_\perp^{\mathrm{hc}}(\boldsymbol{k}_\perp)+\epsilon_\parallel(k_x))\big)^2\frac{2}{d}\sin^2(k_x) \\
&\quad\times\delta\left(\epsilon-\mathcal{F}\left(\epsilon_\perp^{\mathrm{hc}}(\boldsymbol{k}_\perp)+\epsilon_\parallel(k_x)\right)\right) \\
&= \left[\lim_{d\to\infty}\frac{1}{(2\pi)^{d-1}}\int\mathrm{d}\boldsymbol{k}_\perp\left(\mathcal{F}'\left(\epsilon_\perp^{\mathrm{hc}}(\boldsymbol{k}_\perp)\right)\right)^2\delta\left(\epsilon-\mathcal{F}\left(\epsilon_\perp^{\mathrm{hc}}\right)\right)\right]\frac{1}{2\pi}\int\mathrm{d}k_x\,2\sin^2(k_x) \\
&= \rho(\epsilon)\left(\mathcal{F}'(\mathcal{F}^{-1}(\epsilon)\right)^2, \qquad (4.92)
\end{aligned}
$$