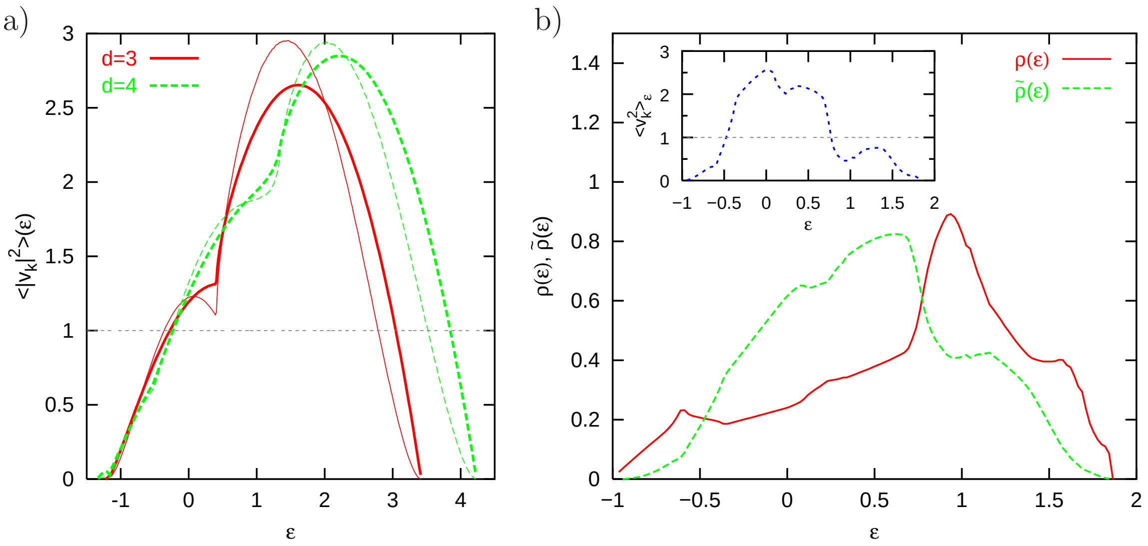

Figure 5.15: a) Exact $\langle|\boldsymbol{v_k}|^2\rangle(\epsilon)$ of the $t-t'$ lattice with $a^* = -0.3333$ (thick lines) in comparison with a computation via (2.62) from the DOS (thin lines). **b)** LDA t_{2g} DOS $\rho(\epsilon)$ (solid line) for $La_{1\text{-}x}Sr_xTiO_3$, derived energy-dependent $d=\infty$ expectation value of the squared Fermi velocity $\langle|\boldsymbol{v_k}|^2\rangle(\epsilon)$ (inset), and $\tilde{\rho}(\epsilon) = \langle|\boldsymbol{v_k}|^2\rangle(\epsilon)\,\rho(\epsilon)$ (dashed line in main figure). The average squared hopping distance is 1.10.

be less pronounced in finite dimensions. Assuming that the LDA spectrum used throughout this chapter is correct, we would therefore expect the true curve for $\tilde{\rho}(\epsilon)$ to lie between both curves shown in the main part of Fig. 5.15 b. Thus, we will for comparison also compute $\sigma(\omega)$ for constant $\langle|\boldsymbol{v_k}|^2\rangle$ and regard the deviations as an upper bound to intrinsic errors.

As a set of intermediate results, we show estimates for the imaginary part of the self-energy on the real axis, $\mathrm{Im}\,\Sigma(\omega)$ in Fig. 5.16. These were calculated by numerical inversion of the lattice Dyson equation (1.30) using a program written as part of this thesis. Our algorithm (see also subsection 4.6.1) implements a modified Newton search with underrelaxation, i.e., the step width is reduced by a factor of 0.5 compared to the usual Newton method.[26] Note that the Dyson equation is local[27] in ω and that the Jacobian needed for the Newton method (with 2 dimensions corresponding to the real and imaginary parts, respectively) can easily be computed numerically. When no causal solution exists for $\Sigma(\omega_0)$ given $G(\omega)$ at an isolated frequency point ω_0, the program issues a warning and interpolates the solution using the adjacent grid points: $\Sigma(\omega_0) = \big(\Sigma(\omega_0-\Delta\omega)+\Sigma(\omega_0+\Delta\omega)\big)/2$.

[26] Analogous to the procedure used in Sec. 4.4, the MEM spectra (with a frequency resolution of $\Delta\omega = 0.1$) have been interpolated (here to $\Delta\omega = 0.02$) before performing the Kramers-Kronig transformation and inverting the Dyson equation.

[27] By "local" we here mean that $\Sigma(\omega_0)$ is for fixed noninteracting DOS only a function of ω_0 and the complex quantity $G(\omega_0)$. Therefore, the inversion of the Dyson equation can be done independently for different frequencies ω_0. The relation between $\Sigma(\omega)$ and $A(\omega) = -\frac{1}{\pi}\mathrm{Im}\,G(\omega)$ is not local, however, since the Kramers-Kronig transform relates $\mathrm{Re}\,G(\omega_0)$ to $\mathrm{Im}\,G(\omega)$ for all ω.