results of X-ray absorption spectroscopy (XAS) measurements. In this technique, incident X-ray photons excite core electrons which, in a crude approximation, give rise to the inverse photo effect.[24] In Fig. 5.14, we have adjusted the intensity scale of the experimental curves (Abbate et al., 1991) to be of the order of magnitude of the theoretical curves and have matched the (experimental) absorption edge with the (calculated) Fermi energy. While the XAS peak observed at 2 eV $\lesssim \omega \lesssim$ 5 eV is in good correspondence with the combined contributions of the upper Hubbard band and the uncorrelated e_g band, the low intensity at the Fermi energy seems incompatible with the theory. Here, the situation is similar to PES, where the theory also predicts more weight near the Fermi level than is seen experimentally.

5.4.3 Optical Conductivity

Another interesting spectral property is the optical conductivity $\sigma(\omega)$ which can be determined experimentally via measurements of the reflectivity and a Kramers-Kronig transformation or, more directly, by transmission experiments (see Sec. 4.1). Within the DMFT, the diagrammatic expression for $\sigma(\omega)$ reduces to a bubble diagram which can be evaluated given the local self-energy and the quantity $\tilde{\rho}(\epsilon)$ defined in (2.2). The latter deviates from the noninteracting DOS $\rho(\epsilon)$ by a factor $\langle|\boldsymbol{v_k}|^2\rangle(\epsilon)$ which takes the nonconstant Fermi velocity within the Brillouin zone into account (see chapter 4). While it should be possible to compute $\tilde{\rho}(\epsilon)$ within LDA, this important ingredient for computations of $\sigma(\omega)$ has not (yet) been obtained within our collaboration. In this situation, the general formalism developed in Sec. 2.3 provides for a reasonable starting point by interpreting the LDA DOS $\rho^{\text{LDA}}(\epsilon)$ as the defining property of an isotropic tight-binding model in $d = \infty$. For this model, one can then compute $\tilde{\rho}(\epsilon)$ and thereby $\sigma(\omega)$ on the basis of estimates for $\Sigma(\omega)$ derived from the QMC/MEM spectra. For the original three-dimensional cubic model, this method introduces an additional approximation which (like the DMFT) also becomes exact in high dimensions. This is illustrated in Fig. 5.15 a for the $t-t'$ lattice with $a^* = -0.3333$ (cf. Fig. 2.5 and subsection 4.5.3). Here, the exact evaluation of $\langle|\boldsymbol{v_k}|^2\rangle(\epsilon)$ in three and four dimensions (thick lines) is seen to agree well with the result of an application of (2.62) to the exact finite-dimensional DOS (thin lines), in particular in the region $\epsilon \lesssim 2$ which comprises about 95% of the DOS. The application of this $d = \infty$ approach is also far more accurate than assuming a constant $\langle|\boldsymbol{v_k}|^2\rangle(\epsilon) \equiv 1$ (which would not be correct for any finite-dimensional lattice).

In Fig. 5.15 b we can see that our formalism, i.e., the application of (2.62) to the LDA DOS indeed yields an estimate for $\langle|\boldsymbol{v_k}|^2\rangle(\epsilon)$ which vanishes at the band edges as required physically.[25] Consequently, $\tilde{\rho}(\epsilon)$ is suppressed at the band edges compared to $\rho^{\text{LDA}}(\epsilon)$. The suppression of peaks is also a realistic effect which, however, might

[24] Clearly, matrix elements and selection rules become even more important for this second order process (in the number of electron-photon vertices) than for the regular PES discussed in subsection 5.4.1.

[25] In order to correct for the bandwidth of 0.65 (square-root of the variance of the LDA energy distribution) instead of unity, the expressions for $\langle|\boldsymbol{v_k}|^2\rangle(\epsilon)$ and $\tilde{\rho}(\epsilon)$ stated in Sec. 2.3 have to be multiplied by the squared inverse bandwidth. Only then is the average hopping distance given by the norm of $\tilde{\rho}(\epsilon)$.