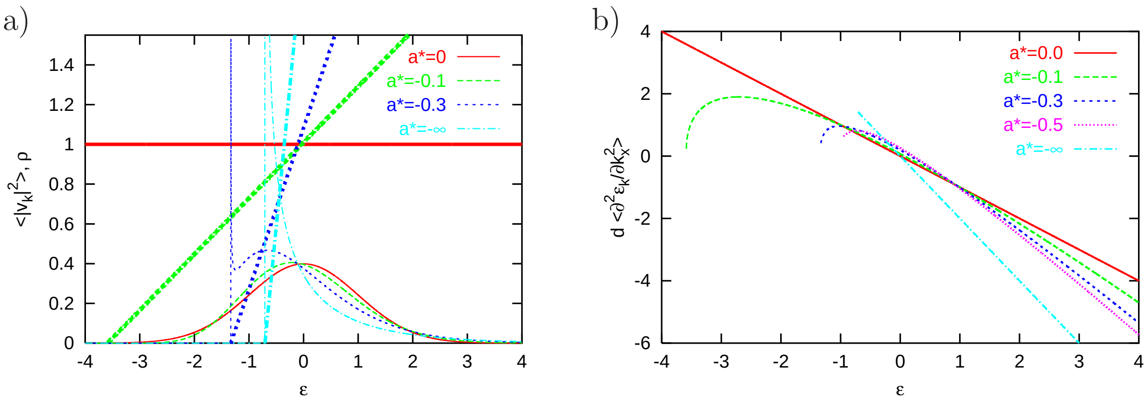

Figure 4.24: DMFT transport characteristics of the $t-t'$ lattice: **a)** For finite frustration, the squared Fermi velocity $\langle|v_{\boldsymbol{k}}|^2\rangle(\epsilon)$ (thick lines) is not constant, but vanishes linearly at the band edge of the noninteracting DOS (thin lines). **b)** $d\langle\frac{\partial^2\epsilon_{\boldsymbol{k}}}{\partial k_x^2}\rangle(\epsilon) = \tilde{\rho}'(\epsilon)/\rho(\epsilon)$ needed for computing the Hall conductivity and the f-sum. Deviations from the linear hc form ($a^*=0$) are most significant near the band edge.

In (4.147) we have already set $t^* = \sqrt{1/(1+a^{*2})}$ in order to guarantee unit variance of the corresponding DOS. Note that the inverse transformation function $\mathcal{F}^{-1}$ is not unique for the $t-t'$ lattice; this didn't matter here because both roots corresponding to the same $\epsilon_{\boldsymbol{k}}$ also yield the same $v^2_{\boldsymbol{k},x}$. As expected on physical grounds, the Fermi velocity vanishes at the band edge. In fact, $\langle v^2_{\boldsymbol{k},x}\rangle(\epsilon)$ is proportional the distance from the band edge as illustrated in Fig. 4.24 (thick lines). Evidently, the assumption of $\langle v^2_{\boldsymbol{k},x}\rangle(\epsilon)$ being constant (as implied by the formulas derived for the hc lattice) is bad already for $|a^*| = 0.1$ and fails completely for stronger frustration $|a^*| = 0.3$ and beyond. In particular, the dependence of transport properties on the degree of frustration may even be dominated by the change in $\langle v^2_{\boldsymbol{k},x}\rangle(\epsilon)$.

The evaluation of the second derivative is a bit more complicated since here both roots of $\mathcal{F}(\tilde{\epsilon}) = \epsilon$ contribute differently. Therefore, we split the total DOS of the $t-t'$ lattice

$$\rho(\epsilon, a^*) = \begin{cases} \sqrt{\frac{2}{\pi}\frac{1+a^{*2}}{r(\epsilon,a^*)}}\exp\left(-\frac{1+r^2(\epsilon,a^*)}{4a^{*2}}\right)\cosh\left(\frac{r(\epsilon,a^*)}{2a^{*2}}\right) & \text{for } \operatorname{sign}(a^*)\epsilon < r_0 \\ 0 & \text{otherwise}\,, \end{cases} \tag{4.148}$$

where $r(\epsilon, a^*) = \sqrt{1+2a^*(a^*-\sqrt{2}\epsilon\sqrt{1+a^{*2}})}$ and where the band edge is given by $r_0 = (a^* + 1/(2a^*))/\sqrt{2}$, into two contributions (with the same boundaries):

$$\rho^{\pm}(\epsilon, a^*) = \sqrt{\frac{1}{2\pi}\frac{1+a^{*2}}{r(\epsilon,a^*)}}\exp\left(-\frac{\left(1\pm r(\epsilon,a^*)\right)^2}{4a^{*2}}\right). \tag{4.149}$$

Using the notation

$$h_0(\epsilon, a^*) = \frac{1}{2a^{*2}} - \sqrt{2}(a^* + \frac{1}{a^*}); \quad h^{\pm}(\epsilon, a^*) = \frac{\sqrt{2}a^* h_0(\epsilon,a^*) \pm \sqrt{1+h_0(\epsilon,a^*)}}{1+a^{*2}} \tag{4.150}$$