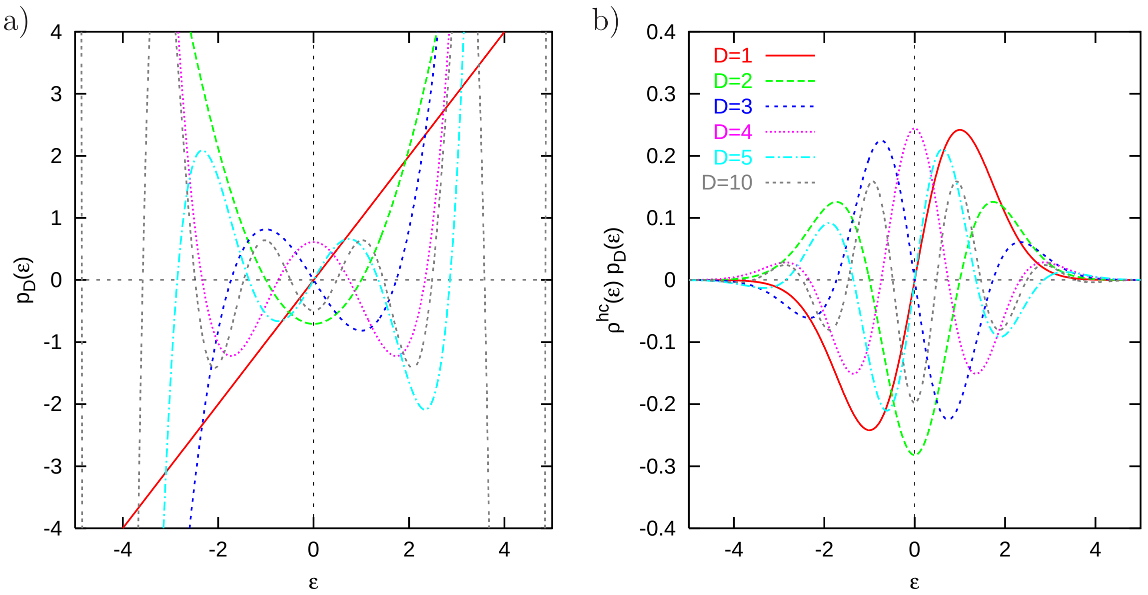

Figure 2.14: a) Rescaled Hermite polynomials $p_D(x) = \mathrm{He}_D(x)/\sqrt{D!}$ forming the basis set in expansion (2.52) of the generalized dispersion for small order D. **b)** Dual basis, i.e., same curves multiplied by ρ^{hc} as in (2.55). The legend in b) applies to both graphs.

The evaluation of the hopping matrix elements

$$t_D^* = \frac{1}{\sqrt{2\pi D!}} \int_{-\infty}^{\infty} \mathrm{d}\epsilon\, \mathcal{F}(\epsilon)\, \mathrm{He}_D(\epsilon)\, \mathrm{e}^{-\epsilon^2/2} = \int_{-\infty}^{\infty} \mathrm{d}\epsilon\, \mathcal{F}(\epsilon)\, p_D(\epsilon)\, \rho^{\mathrm{hc}}(\epsilon)\,, \tag{2.55}$$

where $\mathcal{F}(x)$ is yet unknown [to be obtained by numerical inversion of (2.61)], generically requires numerical integration. As shown in Fig. 2.14b, the kernel $p_D(\epsilon)\rho^{\mathrm{hc}}(\epsilon)$ falls off exponentially with increasing $|\epsilon|$ for fixed hopping range D. Due to this fact and due to the increasingly oscillatory behavior, the matrix elements t^* can be expected to fall off rapidly with $D \to \infty$ for any monotonic (or, weaker, a reasonably smooth) transformation function $\mathcal{F}$.

Transformation Function $\mathcal{F}(\epsilon)$, DOS, and Fermi Velocity

For a given transformation function $\mathcal{F}(x)$, we can obtain the DOS by transforming the corresponding δ-functions in (2.1),

$$\rho(\epsilon) = \sum_{\substack{i=1 \\ \mathcal{F}(\tilde{\epsilon}_i)=\epsilon}}^{N(\epsilon)} \frac{1}{\mathcal{F}'(\tilde{\epsilon}_i)} \rho^{\mathrm{hc}}(\tilde{\epsilon}_i)\,, \tag{2.56}$$

($N(\epsilon)$ is the multiplicity of solutions of the equation $\mathcal{F}(\tilde{\epsilon}) = \epsilon$) which simplifies to

$$\rho(\epsilon) = \frac{1}{\mathcal{F}'(\mathcal{F}^{-1}(\epsilon))} \rho^{\mathrm{hc}}(\mathcal{F}^{-1}(\epsilon)) \tag{2.57}$$