4. optionally: determine microscopic model parameters, i.e., the hopping matrix elements t^*_D using (2.55)

The only choice inherent in this procedure beyond the usual assumptions for large dimensions is contained in step 1 which by construction produces a monotonic transformation function $\mathcal{F}$.

Example: Flat-band System

One interesting limiting case of a monotonic transformation function which we can treat analytically is the step function $\mathcal{F}(x) = 2\Theta(x) - 1$ corresponding to a flat band DOS, $\rho(\epsilon) = (\delta(\epsilon - 1) + \delta(\epsilon + 1))/2$. Due to the nonanalytic step at $\epsilon = 0$ we expect the decay of the hopping matrix elements t^*_D to be much slower than in generic cases, at least for monotonic $\mathcal{F}$. Using the identity

$$\int_0^x \mathrm{d}y\, \mathrm{e}^{-y^2/2}\mathrm{He}_n(y) = \mathrm{He}_{n-1}(0) - \mathrm{e}^{-x^2/2}\mathrm{He}_{n-1}(x) \tag{2.64}$$

for $x = \infty$ and $\mathrm{He}_{2n}(0) = (-1)^n(2n-1)!!$, $\mathrm{He}_{2n+1}(0) = 0$ we can evaluate (2.55) for the case at hand (trivially, $t^*_{2n} = 0$):

$$t^*_{2n+1} = \frac{2}{\sqrt{2\pi(2n+1)!}} \int_0^\infty \mathrm{d}\epsilon\, \mathrm{He}_{2n+1}(\epsilon)\, \mathrm{e}^{-\epsilon^2/2} \tag{2.65}$$

$$= (-1)^n \sqrt{\frac{2}{\pi}} \frac{(2n-1)!!}{\sqrt{(2n+1)!}} \tag{2.66}$$

$$\stackrel{n\to\infty}{\longrightarrow} (-1)^n (\pi n)^{-3/4}\,. \tag{2.67}$$

The asymptotic form, obtained by applying the Stirling formula and retaining only leading powers of n, is accurate to within 1% for $n > 30$. As expected, t^*_{2n+1} falls off slowly; the power $-3/4$ is only slightly smaller than the threshold value $-1/2$ required for the convergence of the sum $\sum_D {t^*_D}^2$. Correspondingly, the transformation function converges only slowly to its limiting form. Both the hopping matrix elements and the transformation functions, corresponding to truncated series expansions with $D \leq 2N+1$, are shown in Fig. 2.15. We do not attempt to calculate truncation effects for the DOS for this toy model which is complicated due to the many branches formed by the oscillatory truncated transformation functions. Still, the main features of the DOS for a model with truncated hopping range are clear: the two δ-peaks (of the $D_{\max} = \infty$ model) are broadened with a potentially irregular shape, while a finite density of states remains at $\epsilon = 0$ for finite maximal hopping range. Furthermore, we can read off from (2.67) and (2.71) that the gap develops very slowly for $D_{\max} \to \infty$ with $\rho(0) \propto D_{\max}^{-1/2}$.