contact with a related approach.

2.4.1 Model in $d = \infty$

A practical application of the theory outlined in Sec. 2.3 always proceeds in two steps: first, one has to find the energy transformation function $\mathcal{F}$ which relates the "target" DOS to the DOS of the hypercubic lattice [cf. (2.57)] and suffices for the computation of all transport related properties discussed in this work. In a second step one may fully determine the underlying microscopic tight-binding model by computing the corresponding scaled hopping matrix elements.

In order to determine the inverse of the transformation function via (2.60), we need to compute the function R defined in (2.59) in terms of an integral over the DOS.[26] Using (2.24) for unit variance, R can be obtained in closed form,

$$\begin{aligned} R(\epsilon) &= -1 + \frac{2}{\pi} \int_{-2}^{\epsilon} \mathrm{d}\epsilon' \sqrt{1 - \epsilon'^2/4} \\ &= \frac{1}{\pi} \left(\epsilon \sqrt{1 - \epsilon^2/4} + 2 \sin^{-1}(\epsilon/2) \right) . \end{aligned} \tag{2.68}$$

Since we defined the function $\mathcal{F}$ to be smooth and monotonic, it can easily be obtained from $\mathcal{F}^{-1}(\epsilon) = \sqrt{2}\ \mathrm{erf}^{-1}(R(\epsilon))$ using numerical root-finding algorithms. The transformation function shown as solid line in Fig. 2.16 a is monotonic, antisymmetric, and smoothly approaches an asymptotic value of $+2$ (-2) for very high (low) energies $\tilde{\epsilon}$. Keeping in mind that $\mathcal{F}$ was defined as a mapping function which when applied to the hc DOS (i.e., energy levels with a Gaussian distribution function) yields the target DOS, we see that the boundedness of $\mathcal{F}$ guarantees sharp band edges, while the linearity at small energies with a slope greater than one flattens out the central part of the DOS compared to the hc case [cf. (2.71)]. Slight variations of the transformation functions only lead to a slight redistribution of spectral weight. This can be illustrated by replacing the (analytically inaccessible) transformation function $\mathcal{F}$ by a hyperbolic tangent,

$$\mathcal{F}(\tilde{\epsilon}) \approx a \tanh\left(\sqrt{\frac{\pi}{2a}}\, \tilde{\epsilon} \right); \quad a \approx 2.176, \tag{2.69}$$

where the coefficients were chosen subject to the requirements that the corresponding DOS has unit variance and that it agrees with the Bethe DOS for $|\epsilon| \to 0$. Due to the boundedness we again obtain sharp band edges, now with finite slopes; otherwise the "tanh" DOS is hardly distinguishable from the semi-elliptic Bethe DOS, as seen in Fig. 2.16 b.

In order to determine the microscopic model, we have to apply (2.55) to the numerically evaluated transformation function $\mathcal{F}$. As shown in Table 2.1, the scaled hopping matrix elements fall off exponentially fast – only a fraction 10^{-3} of the total energy variance arises from hopping amplitudes beyond 3rd-nearest neighbors and

[26] Note that $R(\mu) = 2n(\mu) - 1$ when n is the electron filling for a chemical potential μ at $T = 0$.