for a monotonic (i.e., invertible) function[24] $\mathcal{F}(x)$. In order to solve for $\mathcal{F}(x)$ we form the integral

$$\int_{-\infty}^{\epsilon} \mathrm{d}\epsilon' \rho(\epsilon') = \int_{-\infty}^{\tilde{\epsilon}} \mathrm{d}\tilde{\epsilon}' \rho^{\mathrm{hc}}(\tilde{\epsilon}'); \quad \epsilon = \mathcal{F}(\tilde{\epsilon}) , \tag{2.58}$$

which leads to

$$R(\mathcal{F}(\tilde{\epsilon})) = \mathrm{erf}(\tilde{\epsilon}/\sqrt{2}), \quad R(\epsilon) := 2 \int_{-\infty}^{\epsilon} \mathrm{d}\epsilon' \rho(\epsilon') - 1 . \tag{2.59}$$

We obtain

$$\mathcal{F}(\tilde{\epsilon}) = R^{-1}(\mathrm{erf}(\tilde{\epsilon}/\sqrt{2})) \quad \Leftrightarrow \quad \mathcal{F}^{-1}(\epsilon) = \sqrt{2}\, \mathrm{erf}^{-1}(R(\epsilon)) \tag{2.60}$$

or, summarizing,

$$\boxed{\mathcal{F}^{-1}(\epsilon) = \sqrt{2}\, \mathrm{erf}^{-1}\Bigg(2 \int_{-\infty}^{\epsilon} \mathrm{d}\epsilon' \rho(\epsilon') - 1\Bigg) .} \tag{2.61}$$

This concludes our presentation of the general algorithm for constructing a tight-binding Hamiltonian, i.e., hopping matrix elements, from a given DOS in $d = \infty$ based on ideas developed by van Dongen (2001).

For later use we also evaluate the Fermi velocity, $\boldsymbol{v_k}$. From (2.57) and (2.60) we have

$$\mathcal{F}'(\mathcal{F}^{-1}(\epsilon)) = \frac{\rho^{\mathrm{hc}}(\sqrt{2}\, \mathrm{erf}^{-1}(R(\epsilon)))}{\rho(\epsilon)} \tag{2.62}$$

which we can use for computing

$$\boldsymbol{v_k} \;\; = \;\; \nabla \mathcal{F}(\epsilon_{\boldsymbol{k}}^{\mathrm{hc}}) = \mathcal{F}'(\mathcal{F}^{-1}(\epsilon)) \boldsymbol{v}_{\boldsymbol{k}}^{\mathrm{hc}} \tag{2.63}$$

by numerical integration and application of the inverse error function. As will be discussed in detail in subsection 2.4.1 and chapter 4, the behavior of the squared Fermi velocity $\langle |\boldsymbol{v_k}|^2 \rangle(\epsilon) := \tilde{\rho}(\epsilon)/\rho(\epsilon)$ [cf. definitions (2.1) and (2.2)] dramatically changes from that observed in the hc lattice: for any nontrivial transformation it is no longer effectively constant but depends strongly on energy. In particular, the Fermi velocity vanishes at the band edges as physically required in any dimension.

A practical application of the general dispersion formalism proceeds as follows from a given target DOS $\rho(\epsilon)$:

1. compute $\mathcal{F}^{-1}(\epsilon)$ using (2.61)

2. invert numerically or analytically to obtain $\mathcal{F}(\epsilon)$

3. evaluate transport properties, e.g., $\langle |\boldsymbol{v_k}|^2 \rangle(\epsilon)$ or $\tilde{\rho}(\epsilon)$ using (2.62) and (2.63)

[24] Here and in the following, $\mathcal{F}^{-1}$ denotes the functional inverse, not the fraction $1/\mathcal{F}$.