as a special case of the l-norm $\|\boldsymbol{v}\|_l := (\sum_{\alpha=1}^{d} |v_\alpha|^l)^{1/l}$. Clearly, the shortest lattice vectors are the unit vectors $\pm\boldsymbol{e}_\alpha$ with length 1 which define nearest neighbors (NN) while for $d > 1$ next-nearest neighbors (NNN) are connected by the sum of two different primitive lattice vectors $\pm\boldsymbol{e}_\alpha \pm \boldsymbol{e}_\beta$ with $\alpha \neq \beta$ and length $\sqrt{2}$. For $d \geq 3$, third-nearest neighbors have length $\sqrt{3}$ while among the fourth-nearest neighbors are those connected by extended hopping along the coordinate axis (length 2). While even for a full simple cubic lattice of Wannier orbitals some hopping matrix elements may exactly vanish for symmetry reasons, hopping to, e.g., 4^{th} or 10^{th} nearest neighbors (i.e., a 2-3 fold increase of the Euclidean hopping range compared with NN) is not necessarily negligible.[4]

Scaling and Dispersion

Generically, the number of D^{th}-nearest neighbors in d dimensions is of the order $(2d)^D$, provided[5] that $D \lesssim d$. In order for the variance of the DOS to remain finite the hopping matrix elements then have to be scaled[6] as $t_{ij} = t^*_{ij}(2d)^{-\|\boldsymbol{r}_i-\boldsymbol{r}_j\|/2}$. Here, we used a short notation for the 1-norm, also called "taxi cab metric" or "New York metric",

$$\|\boldsymbol{v}\| := \|\boldsymbol{v}\|_1 = \sum_{\alpha=1}^{d} |v_\alpha| \,. \tag{2.4}$$

For the remainder of this section we restrict the matrix elements to NN and NNN hopping with amplitudes t and t', respectively, as illustrated in Fig. 2.1 for $d = 3$. This corresponds to a dispersion

$$\begin{aligned} \epsilon_{\boldsymbol{k}}^{tt'} &= -\frac{t}{L}\sum_{\langle i,j\rangle} \exp\left[i\boldsymbol{k}(\boldsymbol{R}_i - \boldsymbol{R}_j)\right] - \frac{t'}{L}\sum_{\langle\langle i,j\rangle\rangle} \exp\left[i\boldsymbol{k}(\boldsymbol{R}_i - \boldsymbol{R}_j)\right] && (2.5)\\ &= -2t\sum_{\alpha=1}^{d} \cos(k_\alpha) - 2t'\sum_{\substack{\alpha,\beta=1\\ \alpha\neq\beta}}^{d} \cos(k_\alpha)\cos(k_\beta), && (2.6)\end{aligned}$$

[4] Note that long-range hopping is compatible with a local Coulomb interaction provided the latter is understood as the non-Hartree part of the full interaction (whereas the Hartree part is absorbed into the lattice potential).

[5] This assumption arises in all DMFT calculations and is clearly generically violated in any finite dimension: In the DMFT perturbation expansion[] one assumes that at every vertex $\mathcal{O}(d)$ directions can be chosen independently which is only true if the dimension is larger than the number of vertices, i.e., the order of the diagram. In other words, for a given dimension, higher order diagrams are treated worse within a local approximation than lower order diagrams; the limits of infinite-order perturbation theory and infinite dimensionality do not commute. Physically, this means that there exists no critical dimension above which the DMFT is always qualitatively correct. For consequences of the violation of scaling relations in the context of our construction of general kinetic energies, see Sec. 2.3.

[6] A counter example to this general rule is extended hopping along the axes (Müller-Hartmann, 1989*a*) which only contributes to the energy if scaled as $t_{ij} = t^*_{ij}\,(2d)^{-1/2}$. It leads to a Gaussian DOS although, in general, the lattice is neither bipartite nor shows perfect nesting (cf. subsection 2.1.3).