$\beta\}$ and $\{\boldsymbol{\tau};\boldsymbol{\tau}=\pm 2\boldsymbol{e}_\alpha\}$. Consequently, one may expect the corresponding hopping amplitudes to be different. We will choose to neglect all hopping vectors with $|\boldsymbol{\tau}\cdot\boldsymbol{e}_\alpha|>1$ for any direction α, i.e., only consider vectors of the form $\boldsymbol{\tau}=\sum_{i=1}^{D}\boldsymbol{e}_{\alpha_i}$ with pairwise different directions α_i. This selection can be justified by the following observations:

- For fixed $|\boldsymbol{\tau}|$, the vectors considered are of minimal Euclidean length $|\boldsymbol{\tau}|$ hinting at maximal overlap, i.e., largest $|t_{\boldsymbol{\tau}}|$.
- The fraction of neglected vectors is $\mathcal{O}(1/d)$ in high dimensions (as long as $d\gg D$, cf. footnote 5 on page 30).

For real (and therefore symmetric) hopping amplitudes[22] and in the isotropic case, the amplitudes $t_{\boldsymbol{\tau}}$ are functions of $D=\|\boldsymbol{\tau}\|$ alone, $\epsilon_D(\boldsymbol{k})=t_D\sum_{\|\boldsymbol{\tau}\|=D}\mathrm{e}^{i\boldsymbol{\tau}\cdot\boldsymbol{k}}$. As in the case of t-t' hopping (which corresponds to $D=1,2$ in the present scheme), there are no cross terms in the variance

$$\langle\epsilon^2(\boldsymbol{k})\rangle=\sum_{\boldsymbol{\tau},\boldsymbol{\tau}'}t_{\boldsymbol{\tau}}t_{\boldsymbol{\tau}'}\langle\mathrm{e}^{i(\boldsymbol{\tau}-\boldsymbol{\tau}')\cdot\boldsymbol{k}}\rangle=\sum_{\boldsymbol{\tau}}|t_{\boldsymbol{\tau}}|^2=\sum_{D}\langle\epsilon_D^2(\boldsymbol{k})\rangle \tag{2.43}$$

$$\langle\epsilon_D^2(\boldsymbol{k})\rangle=t_D^2N_D;\quad N_D=2^D\binom{d}{D}\approx\frac{(2d)^D}{D!}\,. \tag{2.44}$$

Here, N_D is the number of hopping terms in shell D and the approximation in (2.44) is valid for $d\gg D$. In order for the total variance to remain finite, the amplitudes t_D must be scaled as $t_D=t_D^*/\sqrt{N_D}$, which is consistent with (2.10) and leads to

$$\langle\epsilon^2(\boldsymbol{k})\rangle=\sum_{D=1}^{\infty}\langle\epsilon_D^2(\boldsymbol{k})\rangle=\sum_{D=1}^{\infty}{t_D^*}^2\,. \tag{2.45}$$

Hopping Matrix Elements and Dispersion; Transformation Function $\mathcal{F}(\tilde{\epsilon})$

Now we have

$$\begin{aligned}\epsilon_D(\boldsymbol{k}) &= t_D 2^D\sum_{\alpha_D>\alpha_{D-1}>\cdots>\alpha_1}\cos(k_{\alpha_D})\cos(k_{\alpha_{D-1}})\ldots\cos(k_{\alpha_1}) && (2.46)\\ &= t_D\frac{2^D}{D!}\left(\frac{d}{2}\right)^{D/2}B_D(\boldsymbol{k}), && (2.47)\end{aligned}$$

where the functions

$$B_D(\boldsymbol{k})=\left(\frac{2}{d}\right)^{D/2}\sum_{\alpha_D\neq\alpha_{D-1}\neq\cdots\neq\alpha_1}\cos(k_{\alpha_D})\cos(k_{\alpha_{D-1}})\ldots\cos(k_{\alpha_1}) \tag{2.48}$$

[22] Note that while Eqn. (1.10) always yields real t_{ij} for atomic orbitals, this is not generally true for Wannier orbitals where phase factors may arise. In a single-band description, however, a restriction to the s-band case of real and isotropic hopping amplitudes is natural since the full Hamiltonian should have the symmetry of the lattice.