momentum space.

The second motivation for studying the relation between lattices and corresponding densities of states is that the knowledge of the DOS is not sufficient for the computation of two-particle properties like susceptibilities and, in particular, transport properties. In fact, a large part of chapter 4 is devoted to the question of how the optical conductivity $\sigma(\omega)$ can be defined and computed for the Bethe lattice (or, more generally, for a lattice with a semi-elliptic DOS in the limit $d = \infty$). It would be desirable to find a regular isotropic[3] and translationally invariant lattice (with a well-defined $\boldsymbol{k}$-space) with the same single-particle properties (i.e., the same DOS) as the Bethe lattice. Transport properties could then be computed directly from first principles. As shown in Sec. 2.4 and in subsection 4.4.5, this is indeed possible. Another important application of the new method developed in this work is the computation of the optical conductivity for a given LDA DOS in Sec. 5.4. Although here, in principle, the full dispersion $\epsilon_{\boldsymbol{k}}$ could be calculated, an educated guess for the DMFT estimate of $\sigma(\omega)$ will be obtained without the numerically complicated evaluation of $\nabla\epsilon_{\boldsymbol{k}}$.

A third point relates to the question of how relevant results calculated in $d = \infty$ are to the finite-dimensional systems of the real world. Since the DOS represents the noninteracting limit of the model Hamiltonian in any dimension, it seems questionable to rely on features of the DOS which are not robust under change of dimensions, i.e., cannot be obtained under similar assumptions concerning the hopping matrix elements in at least any dimension $3 \leq d \leq \infty$. One example where a feature is not generic although it occurs in $d = 3$ and $d = \infty$ is the singularity of the fcc DOS at the lower band edge. This feature is not present in any finite dimension $d > 3$ unless NNN hopping is chosen appropriately; see, e.g., Ulmke (1998) and Sec. 2.1. Even more importantly, our study of the paramagnetic Mott metal-insulator transition performed in chapter 3 would not be complete without a discussion of microscopic mechanisms for frustration and their implications for the DOS and for transport properties in infinite and finite dimensions.

The numerically exact studies of tight-binding models in large but finite dimensions presented in this chapter were made possible by the development of a computer program which allows for the computation of the DOS in arbitrary (finite) dimensions given the dispersion $\epsilon_{\boldsymbol{k}}$. This computation is performed by Monte Carlo sampling of the d-dimensional integral (volume V_B of the Brillouin zone)

$$\rho(\epsilon) = \frac{1}{V_B}\int \mathrm{d}\boldsymbol{k}\; \delta(\epsilon - \epsilon_{\boldsymbol{k}}) \tag{2.1}$$

on a discretized energy interval. Originally, the computation of the DOS was only a byproduct (at no additional cost) of computations of

$$\tilde{\rho}(\epsilon) = \frac{1}{V_B}\int \mathrm{d}\boldsymbol{k}\; \delta(\epsilon - \epsilon_{\boldsymbol{k}})|\boldsymbol{v}_{\boldsymbol{k}}|^2 \tag{2.2}$$

[3] Here and in the following, we use the term *isotropic* for a lattice with hypercubic symmetry since in that case the cartesic axes are equivalent and all transport properties are isotropic in the long-wavelength limit.