Chapter 4

Optical Conductivity

In this chapter, we will discuss electronic transport, in particular the ($\boldsymbol{q} = 0$) optical conductivity $\sigma(\omega)$. Transport properties are not only very important technologically, but can also be probed accurately by a variety of techniques. As we will see below, measurements, e.g., of reflectivity, electronic energy loss, and of the direct-current (dc) conductivity are, thus, valuable tools for determining the electronic structure of materials. Specifically, a metal-insulator transition as discussed in chapter 3 is signaled by a vanishing Drude weight, i.e., a suppression of $\sigma(\omega)$ at low frequencies (and specifically for $\omega = 0$).[1]

We will here focus on the exact theory of transport strictly in the limit of infinite dimensionality ($d \to \infty$) or, more generally, infinite lattice coordination number ($Z \to \infty$), but also mention implications for an approximate treatment of the finite-dimensional case. Since all directional transport vanishes in infinite dimensions,[2] e.g.,

$$\sigma_{xx}(\omega) \stackrel{d\to\infty}{\longrightarrow} 0 + \mathcal{O}(1/d) \tag{4.1}$$

for the optical conductivity in x direction, we will consider leading corrections, e.g., $d\sigma_{xx}(\omega)$ or $\sum_\alpha \sigma_{\alpha\alpha}(\omega)$. While the fact that most unscaled transport properties vanish in high dimensions might be viewed as a conceptual complication, their computation is much simplified in this limit: due to the effective locality of the vertex function (for $\boldsymbol{q} = \mathbf{0}$), their diagrammatic expressions reduce to the bubble diagram. Consequently, $\sigma(\omega)$ can be evaluated from the full interacting Green function and the unrenormalized current vertex. It is important to note that the current vertex introduces a dependence on lattice structure and hopping parameters beyond the noninteracting DOS so that models which are equivalent in the DMFT with respect to local properties may differ significantly in terms of transport properties. In fact, we will show in this chapter that $\sigma(\omega)$ is not uniquely defined on "the Bethe lattice", i.e., on

[1] In principle, we could have used results for $\sigma(\omega)$ in order to determine the MIT transition lines $U_{\mathrm{c}1}$ and $U_{\mathrm{c}2}$ in chapter 3. The attainable accuracy is, however, much better for the energy E and for the double occupancy D since these observables do not require an analytic continuation via MEM.

[2] Strictly speaking, this statement only applies to total or partial weights, i.e., integrals over finite frequency ranges and only when the lattice is essentially isotropic, i.e., when the kinetic energy is not dominated by a subset of directions. In particular, the limits $\omega \to 0$ and $d \to \infty$ do not necessarily commute.