4.2 Kubo Formalism

In this section, we will discuss the formalism leading to expressions for $\sigma(\omega)$ both in the continuum and on the lattice in enough detail to expose the microscopic origin and ranges of validity of sum rules.

4.2.1 Kubo Formalism in the Continuum

As reviewed in App. D.1, the interaction of a particle at position $\boldsymbol{r}$ with charge q with an external time varying electric field may be fully described in terms of a shift of its momentum by $q\boldsymbol{A}(\boldsymbol{r})/c$, where $\boldsymbol{A}(\boldsymbol{r})$ is the vector potential. Furthermore, within the Coulomb gauge, the electrical interaction between charged particles is instantaneous. In the nonrelativistic limit, we can, thus, assume the following first-quantized electronic Hamiltonian for a number of N_e electrons,[9]

$$H = H_{\text{int}}(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_{N_e}) + \sum_{i=1}^{N_e} \frac{1}{2m} \left(\boldsymbol{p}_i - \frac{e}{c}\boldsymbol{A}(\boldsymbol{r}_i, t)\right)^2 . \tag{4.27}$$

Here, the interaction Hamiltonian H_{int} may contain arbitrary interactions of electrons with a (static) lattice potential as well as electron-electron interactions. This term will enter the results only implicitly via its influence on the eigenstates of the unperturbed system and their occupation in the thermal ensemble. From (4.27) and $\boldsymbol{v}_i = \nabla_{\boldsymbol{p}_i} H$ we can read off the total current,

$$\int \mathrm{d}\boldsymbol{r}\, \boldsymbol{J}(\boldsymbol{r}, t) = \sum_{i=1}^{N_e} e\, \boldsymbol{v}_i = \sum_{i=1}^{N_e} \frac{e}{m} \left(\boldsymbol{p}_i - \frac{e}{c}\boldsymbol{A}(\boldsymbol{r}_i)\right) . \tag{4.28}$$

In (4.28), we may distinguish a diamagnetic contribution $-\sum_{i=1}^{N_e} \frac{e^2}{mc}\boldsymbol{A}(\boldsymbol{r}_i)$ from the paramagnetic current, the density of which reads in symmetrized form,[10]

$$\boldsymbol{j}(\boldsymbol{r}, t) = \frac{e}{2m} \sum_{i=1}^{N_e} \left(\boldsymbol{p}_i \delta(\boldsymbol{r} - \boldsymbol{r}_i) + \delta(\boldsymbol{r} - \boldsymbol{r}_i)\boldsymbol{p}_i\right) . \tag{4.29}$$

Denoting the thermal expectation value[11] of some observable $\mathcal{O}$ in the presence of the vector potential by $\langle \mathcal{O} \rangle_A$, the current density is, thus, exactly given by

$$\langle \boldsymbol{J}(\boldsymbol{r}, t) \rangle_A = \langle \boldsymbol{j}(\boldsymbol{r}, t) \rangle_A - \frac{e^2}{mc}\boldsymbol{A}(\boldsymbol{r}, t) \langle n(\boldsymbol{r}, t) \rangle_A . \tag{4.30}$$

Since we only need the linear response current, i.e., contributions to $\boldsymbol{J}$ which are at most linear in $\boldsymbol{A}$, we can take the density expectation value in (4.30) in zeroth order. In the long-wavelength limit, the diamagnetic contribution is then $-\frac{e^2 n_0}{mc}\boldsymbol{A}(\boldsymbol{r}, t)$,

[9] Note that following the usual convention the electron charge is here denoted as e, not $-e$.

[10] Here and in the following, we use the upper-case symbol $\boldsymbol{J}$ for the total current and the lower-case symbol $\boldsymbol{j}$ for the paramagnetic current or its density.

[11] Due to the explicit time dependence of H, we here have to use a generalized definition of the thermal average in terms of a time-dependent density operator $\hat{\rho}(t)$; see App. D.2.