THÉORIE DE CHAMPS QUANTIQUES
ET MÉTHODES À N CORPS

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Chapter 1

The single–particle Green’s function

Green’s functions are very useful for solving certain partial differential equations, for instance the inhomogeneous wave equations in electrodynamics (see J.D. Jackson, Classical Electrodynamics, Section 6.6). In many-body physics a generalized version of Green’s functions turns out not only to be extremely helpful for analysing certain problems, but also to contain itself a wealth of information about the dynamics of the many-particle system. In this chapter we limit ourselves on the single-particle Green’s function; two-particle Green’s functions, which are related to various response functions or susceptibilities, will be considered later. Furthermore, we consider only Green’s functions at zero temperature. Green’s functions at finite temperatures, especially the so-called Matsubara Green’s functions, do not present additional complications. Essentially, the ground state expectation values are replaced by averages with respect to the grand-canonical ensemble.

1.1 Basic Definitions

We consider a many-body system described by a Hamiltonian $H$, for instance a system of fermions or bosons with short-range interactions. In the Heisenberg picture the time-evolution is given by the time-dependence of creation and annihilation operators

$$
\Psi_\sigma(r, t) = e^{\frac{i}{\hbar}Ht} \Psi_\sigma(r) e^{-\frac{i}{\hbar}Ht},
$$

$$
a_{k\sigma}(t) = e^{\frac{i}{\hbar}Ht} a_{k\sigma} e^{-\frac{i}{\hbar}Ht}.
$$

We define the time-ordering symbol $T$ as an operator which orders a product of time-dependent operators in such a way that the early times are to the right and later times to the left, i.e.

$$
T \left[ \Psi_\sigma(r_1, t_1) \Psi_\sigma^\dagger(r_2, t_2) \right] = \begin{cases} 
\Psi_\sigma(r_1, t_1) \Psi_\sigma^\dagger(r_2, t_2), & t_1 > t_2, \\
\pm \Psi_\sigma^\dagger(r_2, t_2) \Psi_\sigma(r_1, t_1), & t_1 < t_2,
\end{cases}
$$

(1.2)

where the plus and minus signs stand for bosons and fermions, respectively. Let $|\Psi_0>$ describe the exact ground state of $N$ particles. The single-particle Green’s
function is then defined as
\[
G_\sigma(r_1, t_1; r_2, t_2) = -i \left\langle \Psi_0 \left| T \left[ \Psi_\sigma(r_1, t_1) \Psi_\sigma^\dagger(r_2, t_2) \right] \right| \Psi_0 \right\rangle .
\] (1.3)

Here we have implicitly assumed that there are no spin-dependent interactions (such as spin-orbit interactions which would require matrix Green’s functions \(G_{\sigma\sigma'}\)). If the Hamiltonian is time-independent, the Green’s function depends only on \(t := t_1 - t_2\). Moreover, if the system is translationally invariant, \(G\) depends only on \(r := r_1 - r_2\) (this is not true for electrons in a periodic lattice potential). In this case we can introduce the Fourier transform,
\[
G_\sigma(r, t) = \int \frac{d\omega}{2\pi} \int \frac{d^3k}{(2\pi)^3} e^{i(k \cdot r - \omega t)} G_\sigma(k, \omega),
\]
\[
G_\sigma(k, \omega) = \int dt \int d^3r \ e^{-i(k \cdot r - \omega t)} G_\sigma(r, t) .
\] (1.4)

In view of Eq. (1.3) it is easy to see that \(G_\sigma(k, \omega)\) is the (time) Fourier transform of
\[
G_\sigma(k, t) = -i \left\langle \Psi_0 \left| T \left[ a_{k\sigma}(t) a_{k\sigma}^\dagger \right] \right| \Psi_0 \right\rangle .
\] (1.5)

The Green’s function (1.3) can be interpreted as follows. Let us consider the case \(t_1 > t_2\) first where
\[
G_\sigma(r_1, t_1; r_2, t_2) = -i \left\langle \Psi_0 | e^{\frac{i}{\hbar} \hat{H} t_1} \Psi_\sigma(r_1) e^{-\frac{i}{\hbar} \hat{H}(t_1 - t_2)} \Psi_\sigma^\dagger(r_2) e^{-\frac{i}{\hbar} \hat{H} t_2} | \Psi_0 \right\rangle .
\]

We first let evolve the exact ground state until the time \(t_2\) where we add a particle at \(r_2\), then the system evolves further during the time interval \(t_1 - t_2\). The scalar product between the resulting state and a state where at time \(t_1\) a particle has been added at \(r_1\) is then given by the Green’s function. Similarly for \(t_1 < t_2\) we seek the overlap between a state obtained by removing at time \(t_1\) a particle at \(r_1\), with a subsequent evolution until \(t_2\), and a state where at time \(t_2\) a particle is removed at \(r_2\).

More important than this interpretation is the use of the single-particle Green’s function for calculating observable quantities. Thus the occupation number of the single-particle state \(k\sigma\) is
\[
\left\langle \Psi_0 \left| a_{k\sigma}^\dagger a_{k\sigma} \right| \Psi_0 \right\rangle = \pm i \lim_{t \uparrow 0} G_\sigma(k, t) .
\] (1.6)

### 1.2 The one-phonon Green’s function

The dynamics of atoms (or ions) around the equilibrium configuration of a periodic crystal can be described by expanding the energy in powers of atomic (ionic) displacement vectors \(\delta \mathbf{R}_i, \ i = 1, \ldots, N\), as described in section 1.6. To simplify the notations, we limit ourselves to the case of one atom (ion) per unit cell. The displacements are expressed in terms of phonon creation and annihilation operators,
\[
\delta \mathbf{R}_i = \frac{1}{\sqrt{NM}} \sum_{q, \lambda} \left( \frac{\hbar}{2\omega_{q\lambda}} \right)^{\frac{1}{2}} \varepsilon_\lambda(q) \left( b_{q\lambda} + b_{-q\lambda}^\dagger \right) e^{iq \cdot \mathbf{R}_i} ,
\] (1.7)
where \( M \) is the atomic (ionic) mass and \( \lambda \) is the branch index (there are just three acoustic modes in the present case). The polarization vectors \( \varepsilon_\lambda (\mathbf{q}) \) are the orthonormal eigenvectors of the harmonic part of the Hamiltonian

\[
M \omega_{\alpha \lambda}^2 \varepsilon_\lambda (\mathbf{q}) = D(\mathbf{q}) \varepsilon_\lambda (\mathbf{q}), \tag{1.8}
\]

\[
\varepsilon_\lambda^* (\mathbf{q}) \cdot \varepsilon_\lambda (\mathbf{q}) = \delta_{\lambda, \lambda'}. \tag{1.9}
\]

Here the dynamical matrix \( D(\mathbf{q}) \) is the Fourier transform of the second derivative in Eq. (??).

We introduce the operators

\[
\varphi_\lambda (\mathbf{R}_i^0) = \frac{1}{\sqrt{V}} \sum_\mathbf{q} \left( b_{\mathbf{q} \lambda} + b_{-\mathbf{q} \lambda}^\dagger \right) e^{i \mathbf{q} \cdot \mathbf{R}_i^0}, \tag{1.10}
\]

which become field operators \( \varphi_\lambda (\mathbf{r}) \) in continuum elasticity theory. The phonon Green’s function is defined as

\[
D_{\lambda \lambda'} (\mathbf{R}_i^0, t_1; \mathbf{R}_j^0, t_2) := -i \langle \Phi_0 | T \left[ \varphi_\lambda (\mathbf{R}_i^0, t_1) \varphi_{\lambda'} (\mathbf{R}_j^0, t_2) \right] | \Phi_0 \rangle, \tag{1.11}
\]

where \( | \Phi_0 > \) is the ground state (the phonon vacuum for a harmonic crystal). Translational symmetry in space and time allows us to write

\[
D_{\lambda \lambda'} (\mathbf{R}_i^0, t_1; \mathbf{R}_j^0, t_2) = D_{\lambda \lambda'} (\mathbf{R}_i^0 - \mathbf{R}_j^0, t_1 - t_2)
\]

\[
= \int \frac{d\omega}{2\pi} \int_{BZ} \frac{d^3 q}{(2\pi)^3} e^{i (\mathbf{q} \cdot \mathbf{r} - \omega t)} D_{\lambda \lambda'} (\mathbf{q}, \omega), \tag{1.12}
\]

where the integration is restricted to the first Brillouin zone. One verifies that \( D_{\lambda \lambda'} (\mathbf{q}, \omega) \) is the Fourier transform of

\[
D_{\lambda \lambda'} (\mathbf{q}, t) = -i \langle \Phi_0 | T \left[ (b_{\mathbf{q} \lambda} + b_{-\mathbf{q} \lambda}^\dagger) (t) (b_{-\mathbf{q} \lambda'} + b_{\mathbf{q} \lambda'}^\dagger) \right] | \Phi_0 \rangle. \tag{1.13}
\]

For a harmonic crystal with a Hamiltonian

\[
H = \sum_{\mathbf{q}, \lambda} \hbar \omega_{\mathbf{q} \lambda} \left( b_{\mathbf{q} \lambda}^\dagger b_{\mathbf{q} \lambda} + \frac{1}{2} \right)
\]

the one-phonon Green’s function is easily calculated, using the relations \( | \Phi_0 > = | 0 >, b_{\mathbf{q} \lambda} (t) = e^{-i \omega_{\mathbf{q} \lambda} t} b_{\mathbf{q} \lambda} \). We find

\[
D_{\lambda \lambda'} (\mathbf{q}, t) = \begin{cases} 
- i \delta_{\lambda \lambda'} e^{-i \omega_{\mathbf{q} \lambda} t}, & t > 0, \\
- i \delta_{\lambda \lambda'} e^{i \omega_{\mathbf{q} \lambda} t}, & t < 0.
\end{cases} \tag{1.14}
\]

The Fourier transform of \( e^{-\eta |t|} D_{\lambda \lambda'} (\mathbf{q}, t) \) is \( (\eta > 0, \text{ infinitesimal}) \)

\[
D_{\lambda \lambda'} (\mathbf{q}, \omega) = \delta_{\lambda \lambda'} \frac{2 \omega_{\mathbf{q} \lambda}}{\omega^2 - \omega_{\mathbf{q} \lambda}^2 + i \eta'}, \tag{1.15}
\]

where \( \eta' = 2 \omega_{\mathbf{q} \lambda} \eta > 0 \).
1.3 Spectral representation

We turn now to an interacting many-fermion system with translational symmetry and spin-independent forces between the particles and thus consider the Green’s function (1.5). Using the completeness relation in Fock space

\[ 1 = |0\rangle\langle 0| + \sum_n |\Psi_n^{(1)}\rangle\langle \Psi_n^{(1)}| + \sum_n |\Psi_n^{(2)}\rangle\langle \Psi_n^{(2)}| + \ldots, \]

where \(|0\rangle\) is the vacuum state and \(|\Psi_n^{(1)}\rangle\) is the \(n\)th eigenstate of the Hamiltonian with \(i\) particles, we can write the Green’s function as

\[
G_\sigma(k, t) = -i \left\{ \vartheta(t) \sum_n \langle \Psi_0| a_{k\sigma}(t)|\Psi_n^{(N+1)}\rangle \langle \Psi_n^{(N+1)}| a_{k\sigma}^\dagger |\Psi_0\rangle - \vartheta(-t) \sum_n <\Psi_0| a_{k\sigma}^\dagger |\Psi_n^{(N-1)}\rangle \langle \Psi_n^{(N-1)}| a_{k\sigma}(t)|\Psi_0\rangle \right\},
\]

where \(|\Psi_0\rangle\) is the \(N\)-particle ground state. The relations

\[
\langle \Psi_0| a_{k\sigma}(t)|\Psi_n^{(N-1)}\rangle = e^{i(E_0^{(N)} - E_n^{(N-1)})t} \langle \Psi_0| a_{k\sigma} |\Psi_n^{(N-1)}\rangle,
\]

\[
\langle \Psi_n^{(N-1)}| a_{k\sigma}(t)|\Psi_0\rangle = e^{i(E_n^{(N-1)} - E_0^{(N)})t} \langle \Psi_n^{(N-1)}| a_{k\sigma} |\Psi_0\rangle,
\]

allow us to calculate explicitly the Fourier transform of \(G_\sigma(k, t)e^{-\eta|t|}\),

\[
G_\sigma(k, \omega) = -i \sum_n \int_0^{\infty} dt e^{i \left[ \omega + i\eta + \frac{E_0^{(N)} - E_n^{(N+1)}}{\hbar} \right] t} \left| \langle \Psi_n^{(N+1)}| a_{k\sigma}^\dagger |\Psi_0\rangle \right|^2
\]

\[
+ i \sum_n \int_0^{\infty} dt e^{i \left[ \omega - i\eta + E_n^{(N-1)} - \frac{E_0^{(N)}}{\hbar} \right] t} \left| \langle \Psi_n^{(N-1)}| a_{k\sigma} |\Psi_0\rangle \right|^2
\]

\[
= \sum_n \left\{ \frac{\left| \langle \Psi_n^{(N+1)}| a_{k\sigma}^\dagger |\Psi_0\rangle \right|^2}{\omega + \frac{E_0^{(N)} - E_n^{(N+1)}}{\hbar} + i\eta} + \frac{\left| \langle \Psi_n^{(N-1)}| a_{k\sigma} |\Psi_0\rangle \right|^2}{\omega + E_n^{(N-1)} - \frac{E_0^{(N)}}{\hbar} - i\eta} \right\}. (1.16)
\]

The operator \(a_{k\sigma}^\dagger\) in the first term increases the momentum by \(\hbar k\) and the energy by

\[
E_n^{(N+1)} - E_0^{(N)} = \varepsilon_n^{(N+1)} + \mu_N
\]

where \(\varepsilon_n^{(N+1)} := E_n^{(N+1)} - E_0^{(N+1)}\) is the excitation energy and \(\mu_n := E_0^{(N+1)} - E_0^{(N)}\) is the chemical potential. Correspondingly, the operator \(a_{k\sigma}\) in the second term removes a momentum \(\hbar k\) and an energy

\[
E_0^{(N)} - E_n^{(N-1)} = \mu_{N-1} - \varepsilon_n^{(N-1)}.
\]

We assume that the differences between the chemical potentials \(\mu_N\) and \(\mu_{N-1}\) and between the excitation energies \(\varepsilon_n^{(N\pm 1)}\) are of order \(\frac{1}{N}\) and can be neglected. (There are cases where this is not always true, for instance a semiconductor with
an energy gap between valence and conduction band.) We define the spectral densities \( A(k, \omega) \) and \( B(k, \omega) \) by the relations

\[
A(k, \omega) := \sum_n \left| \langle \Psi_n^{(N+1)} | a_{k0}^\dagger | \Psi_0 \rangle \right|^2 \delta \left( \omega - \frac{\varepsilon_n}{\hbar} \right),
\]
\[
B(k, \omega) := \sum_n \left| \langle \Psi_n^{(N-1)} | a_{k\sigma} | \Psi_0 \rangle \right|^2 \delta \left( \omega - \frac{\varepsilon_n}{\hbar} \right).
\]

(1.17)

Both functions vanish for \( \omega < 0 \) and we can write \( G_\sigma(k, \omega) \) as an integral

\[
G_\sigma(k, \omega) = \int_0^\infty d\omega' \left\{ \frac{A(k, \omega')}{\omega - \omega' - \frac{\mu}{\hbar} + i\eta} + \frac{B(k, \omega')}{\omega + \omega' - \frac{\mu}{\hbar} - i\eta} \right\}.
\]

(1.18)

In the large volume limit the excitation energies \( \varepsilon_n \) are expected to be dense so that the spectral densities become smooth (real and positive) functions of \( \omega \). Then the integration in Eq. (1.18) can be separated into real and imaginary parts,

\[
ReG_\sigma(k, \omega) = \oint_0^\infty d\omega' \left\{ \frac{A(k, \omega')}{\omega - \omega' - \frac{\mu}{\hbar}} + \frac{B(k, \omega')}{\omega + \omega' - \frac{\mu}{\hbar}} \right\},
\]

(1.19)

\[
ImG_\sigma(k, \omega) = \left\{ \begin{array}{ll} -\pi A(k, \omega - \frac{\mu}{\hbar}) & \omega > \frac{\mu}{\hbar}, \\ \pi B(k, -\omega + \frac{\mu}{\hbar}) & \omega < \frac{\mu}{\hbar}. \end{array} \right.
\]

(1.20)

Here \( \oint \) indicates the principal part

\[
P \int_{x_1}^{x_2} dx \frac{f(x)}{x - x_0} = \lim_{\varepsilon \to 0} \left\{ \int_{x_1}^{x_0-\varepsilon} dx \frac{f(x)}{x - x_0} + \int_{x_0+\varepsilon}^{x_2} dx \frac{f(x)}{x - x_0} \right\},
\]

if \( x_1 < x_0 < x_2 \), and the imaginary part comes from the semi-circles around the simple poles. Sometimes one writes symbolically

\[
\lim_{\eta \to 0} \frac{1}{x - x_0 \pm i\eta} = P \frac{1}{x - x_0} \mp i\pi \delta(x - x_0).
\]

(1.21)

Eq. (1.20) implies that the imaginary part of \( G(k, \omega) \) changes sign for \( \omega = \mu \). Inserting Eq. (1.20) into (1.19) we obtain the dispersion relation

\[
ReG_\sigma(k, \omega) = \frac{1}{\pi} \oint_0^\infty d\omega' \left\{ -\frac{ImG_\sigma(k, \omega' + \frac{\mu}{\hbar})}{\omega - \omega' - \frac{\mu}{\hbar}} + \frac{ImG_\sigma(k, -\omega' + \frac{\mu}{\hbar})}{\omega + \omega' - \frac{\mu}{\hbar}} \right\}
\]

\[
= \frac{1}{\pi} \oint_{-\infty}^\infty d\omega' \frac{ImG_\sigma(k, \omega')}{\omega' - \omega} \text{sign} (\omega' - \mu).
\]

(1.22)

1.4 Analytic properties

Eq. (1.17) implies a useful sum rule,

\[
\int_0^\infty d\omega \ [A(k, \omega) + B(k, \omega)] = \langle \Psi_0 | \{ a_{k\sigma}, a_{k\sigma}^\dagger \} | \Psi_0 \rangle = 1.
\]

(1.23)
It allows us to obtain the large $\omega$ behavior of $G_{\sigma}(k, \omega)$,
\[
G_{\sigma}(k, \omega) \sim \frac{1}{|\omega|} \int_0^\infty d\omega' \left[ A(k, \omega') + B(k, \omega') \right] = \frac{1}{\omega}.
\] (1.24)

We investigate now the analytic properties of $G_{\sigma}(k, \omega)$ by considering $\omega$ as a complex variable. Eq. (1.22) immediately implies that $G_{\sigma}(k, \omega)$ is not analytic. If sign $(\omega' - \mu)$ would be replaced by 1 then we could write
\[
\int_{-\infty}^{\infty} d\omega' \frac{\text{Im} G_{\sigma}(k, \omega')}{\omega' - \omega} = \int d\zeta \frac{\text{Im} G_{\sigma}(k, \zeta)}{\zeta - \omega}.
\]

(the integral over the half circle vanishes in view of Eq. (1.24)), which corresponds to the Cauchy formula for an analytic function in the upper half plane. Similarly we can show that by replacing sign $(\omega' - \mu)$ by -1 we obtain a function which is analytic in the lower half plane, since
\[
-\int_{-\infty}^{\infty} d\omega' \frac{\text{Im} G_{\sigma}(k, \omega')}{\omega' - \omega} = \int d\zeta \frac{\text{Im} G_{\sigma}(k, \zeta)}{\zeta - \omega}.
\]

We now define “advanced” and “retarded” Green’s functions $G_A$ and $G_R$ which are analytic in the lower and upper half-planes, respectively,
\[
\begin{align*}
\text{Re}G_A &= \text{Re}G_R = \text{Re}G, \\
\text{Im}G_A &= -\text{Im}G \text{ sign } (\omega - \mu), \\
\text{Im}G_R &= \text{Im}G \text{ sign } (\omega - \mu).
\end{align*}

(1.25)

On the real line we have
\[
G_A(k, \omega) = \begin{cases} 
G_{\sigma}(k, \omega) & \text{for } \omega < \mu, \\
G_{\sigma}^*(k, \omega) & \text{for } \omega > \mu,
\end{cases}
\]
\[
G_R(k, \omega) = \begin{cases} 
G_{\sigma}(k, \omega) & \text{for } \omega > \mu, \\
G_{\sigma}^*(k, \omega) & \text{for } \omega < \mu.
\end{cases}
\]

Therefore $G_A$ is the analytic continuation of $G$ from $\omega < \mu$ to $\omega > \mu$, while $G_R$ is the analytic continuation of $G$ from $\omega > \mu$ to $\omega < \mu$. The spectral representation which corresponds to Eq. (1.18) is
\[
\begin{align*}
G_R(k, \omega) &= \int_0^\infty d\omega' \left\{ \frac{A(k, \omega')}{\omega - \omega' - \frac{\mu}{h} + i\eta} + \frac{B(k, \omega')}{\omega + \omega' - \frac{\mu}{h} + i\eta} \right\}, \\
G_A(k, \omega) &= G_R^*(k, \omega).
\end{align*}
\] (1.26)

One readily verifies that in coordinate representation these functions are given by
\[
\begin{align*}
G_A(r_1, t_1; r_2, t_2) &= i\delta(t_2 - t_1) \langle \Psi_0 \left\{ \Psi_{\sigma}(r_1, t_1), \Psi_{\sigma}^*(r_2, t_2) \right\} | \Psi_0 \rangle, \\
G_R(r_1, t_1; r_2, t_2) &= -i\delta(t_1 - t_2) \langle \Psi_0 \left\{ \Psi_{\sigma}(r_1, t_1), \Psi_{\sigma}^*(r_2, t_2) \right\} | \Psi_0 \rangle.
\end{align*}
\]
\] (1.27)
1.5 Quasi-particle poles

For independent fermions the Green’s function $G_\sigma(k,t)$ is given by Eq. (??), i.e., for $t > 0$

$$G_\sigma(k,t) = -i\theta(\varepsilon_k - \mu)e^{-\frac{i}{\hbar}\mathbf{kk}^t}. \quad (1.28)$$

$G_\sigma(k,\omega)$ has a simple pole at $\frac{\varepsilon_k}{\hbar} - i\eta$ for $\varepsilon_k > \mu$ (cf. Eq. (??)). We now discuss the Green’s function for interacting fermions

$$G_\sigma(k,\omega) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega t} G_\sigma(k,\omega).$$

For $\omega < \mu$ $G_\sigma(k,\omega)$ is equal to $G_A(k,\omega)$; therefore it is analytic in the lower half-plane. For $\omega > \mu$ $G_\sigma(k,\omega)$ is equal to $G_R(k,\omega)$, which is expected to have singularities in the lower half-plane. We assume that there is a simple pole at $\varepsilon_k - i\gamma_k$. We can then deform the integration contour as follows:

Here $G_\sigma$ is replaced by $G_A$ to the left of $\omega = \mu$ and by $G_R$ at the right-hand side. The integral over the horizontal line is very small if $t$ is sufficiently large. One can also show that the integrals over $\gamma_1$ and $\gamma_2$ can be neglected if $\frac{\hbar}{\varepsilon_k - \mu} \ll t \ll \frac{\hbar}{\gamma_k}$ (see Abrikosov et al., Section 7.2). This is only possible if $\gamma_k \ll (\varepsilon_k - \mu)$. In this case the only contribution arises from the circle surrounding the pole, i.e.

$$G_\sigma(k, t) \approx -ia e^{-\frac{i}{\hbar}\varepsilon_k t} e^{-\frac{i}{\hbar}\gamma_k t}, \quad (1.29)$$

where $a$ is the residue of $G_R$ at the pole. Thus the time dependence (1.28), which is just that of a single particle, is replaced by that of a quasi-particle with a renormalized energy $\varepsilon_k$ and a finite lifetime $\frac{\hbar}{\gamma_k}$. Due to the Pauli principle scattering processes close to the Fermi surface are strongly reduced so that the inequality $\gamma_k \ll (\varepsilon_k - \mu)$ appears to be very reasonable in this region. On the other hand the assumption of a simple pole is not always justified. In one dimension branch cuts can occur instead.

1.6 Photoemission

The single-electron Green’s function can be investigated experimentally by angular resolved photoelectron spectroscopy (ARPES), provided that a few simplifying assumptions are valid. We choose the Coulomb gauge for the electromagnetic
field, $\nabla \cdot \mathbf{A}(\mathbf{r}, t) = 0$, and set the electrostatic potential equal to zero, $\Phi(\mathbf{r}, t) = 0$. Then the linear coupling of the electrons to the electromagnetic field is given by

$$V(t) = \frac{e}{m} \sum_i \mathbf{A}(\mathbf{r}_i, t) \cdot \mathbf{p}_i.$$  \hfill (1.30)

We imagine a periodic solid of volume $V$. For periodic boundary conditions the eigenstates of the single-particle Hamiltonian

$$H_0 = \sum_i \left[ \frac{1}{2m} \mathbf{p}_i^2 + U(\mathbf{r}_i) \right]$$  \hfill (1.31)

are Bloch wave functions

$$\Psi_{\nu \mathbf{k}}(\mathbf{r}) = e^{i \mathbf{k} \cdot \mathbf{r}} \psi_{\nu \mathbf{k}}(\mathbf{r})$$  \hfill (1.32)

with band index $\nu$ and $\mathbf{k} \in BZ$. In second quantized representation with respect to the Bloch basis we have

$$H_0 = \sum_{\nu \mathbf{k} \sigma} \varepsilon_{\nu \mathbf{k} \sigma} a_{\nu \mathbf{k} \sigma}^\dagger a_{\nu \mathbf{k} \sigma},$$  \hfill (1.33)

$$V(t) = \sum_{\nu \mathbf{k}, \nu' \mathbf{k}', \sigma} \langle \nu \mathbf{k} | \frac{e}{m} \mathbf{A}(\mathbf{r}, t) \cdot \mathbf{p} | \nu' \mathbf{k}' \rangle \mu_{\mathbf{k}'} a_{\nu' \mathbf{k} \sigma}^\dagger a_{\nu \mathbf{k} \sigma}.$$  \hfill (1.34)

We assume a monochromatic wave

$$\mathbf{A}(\mathbf{r}, t) = a_0 \cos(\mathbf{q} \cdot \mathbf{r} - \omega t).$$  \hfill (1.35)

The discrete translational symmetry implies conservation of crystal momentum (modulo a reciprocal lattice vector). Thus we get

$$\langle \nu \mathbf{k} | \frac{e}{m} \mathbf{A}(\mathbf{r}, t) \cdot \mathbf{p} | \mu \mathbf{k}' \rangle$$

$$= [\Delta(\mathbf{k}' - \mathbf{k} + \mathbf{q}) e^{-i \mathbf{q} \cdot \mathbf{r}} + \Delta(\mathbf{k}' - \mathbf{k} - \mathbf{q}) e^{i \mathbf{q} \cdot \mathbf{r}}] \psi_{\nu \mu}(\mathbf{k}, \mathbf{k}''),$$

where

$$\psi_{\nu \mu}(\mathbf{k}, \mathbf{k}') = \frac{\hbar e}{2m} \int d^3r \psi_{\nu \mathbf{k}}(\mathbf{r}) a_0 \cdot (\mathbf{k}' - i \nabla) \psi_{\mu \mathbf{k}'}(\mathbf{r}).$$  \hfill (1.36)

Restricting ourselves to direct transitions $(\mathbf{k}' = \mathbf{k} \pm \mathbf{q})$, we arrive at

$$V(t) = V(\mathbf{q}) e^{-i \omega t} + V(-\mathbf{q}) e^{i \omega t},$$  \hfill (1.37)

where

$$V(\mathbf{q}) := \sum_{\nu \mathbf{k}, \nu' \mathbf{k}, \sigma} \psi_{\nu \mu}(\mathbf{k}, \mathbf{k} - \mathbf{q}) a_{\nu \mathbf{k} \sigma}^\dagger a_{\nu' \mathbf{k} \sigma}. $$  \hfill (1.38)

The total Hamiltonian of the system is

$$H(t) = H_0 + H_{\text{int}} + V(t),$$

where $H_0$ and $V(t)$ are given, respectively, by Eqs. (1.33) and (1.37) and $H_{\text{int}}$ describes the electron-electron interaction. Let the system initially be in the $N$-
particle ground state \( |\Psi_0^{(N)}\rangle \) of \( H_0 + H_{\text{int}} \) with energy \( E_0^{(N)} \). Then the transition rate due to the absorption of energy \( \hbar \omega \) and momentum \( \hbar \mathbf{q} \) from the electromagnetic field is given by Fermi’s golden rule

\[
 w_{i \rightarrow f} = \frac{2\pi}{\hbar} \sum_n \left| \langle \Psi_n^{(N)} | V(\mathbf{q}) | \Psi_0^{(N)} \rangle \right|^2 \delta \left( \hbar \omega - E_n^{(N)} + E_0^{(N)} \right) . \tag{1.39}
\]

(If we would have quantized the electromagnetic field this would just correspond to the absorption of a single photon with energy \( \hbar \omega \) and momentum \( \hbar \mathbf{q} \). In the case of non-interacting electrons \( (H_{\text{int}} = 0) \) the ground state is a single Slater determinant of Bloch functions \( \Psi_{\mu k} \) with \( \varepsilon_{\mu k} < \varepsilon_F \). The photoemission process can then be simply described in terms of level occupations. Thus, for a given outgoing electron in the level \( \mu \mathbf{k} \) the transition has to occur starting from a level \( \mu \mathbf{k}' \) with energy \( \varepsilon_{\mu k} = \varepsilon_{\nu k} - \hbar \omega \) and crystal momentum \( \mathbf{k}' = \mathbf{k} - \mathbf{q} \) (with \( \omega = c q \)). The determination of labels \( \mu \mathbf{k}' \) where for a given energy \( \varepsilon_{\mu k} \) such a photoemission occurs allows then to map out the band structure of occupied levels.

The energy eigenstates \( |\Psi_n^{(N)}\rangle \) of interacting electrons can not be written as single Slater determinants of one-particle wave functions, but rather as superpositions of Slater determinants. To describe a photoemission process with a high-energy outgoing electron we may limit ourselves to those states where the photoelectron does not scatter from the other electrons before entering the detector, i.e. we assume

\[
 |\Psi_n^{(N)}\rangle \approx a_{\nu k \sigma}^\dagger |\Psi_{n-1}^{(N-1)}\rangle ,
 E_n^{(N)} \approx \varepsilon_{\nu k} + E_{n-1}^{(N-1)} , \tag{1.40}
\]

where \( |\Psi_{n-1}^{(N-1)}\rangle \) are the eigenstates of \( H_0 + H_{\text{int}} \) for \( N - 1 \) electrons. The transition matrix elements in (1.39) are then given by

\[
 \langle \Psi_n^{(N-1)} | V(\mathbf{q}) | \Psi_0^{(N)} \rangle = \sum_{\mu \sigma} v_{\nu \mu}(\mathbf{k}, \mathbf{k} + \mathbf{q}) \langle \Psi_{n-1}^{(N-1)} | a_{\mu k - \nu \sigma} | \Psi_0^{(N)} \rangle .
\]

We suppose that in the ground state all bands are filled except maybe one. In this case there are no contributions to (1.39) originating from two different bands and we get

\[
 w_{i \rightarrow f} = \frac{2\pi}{\hbar} \sum_{n_{\mu \sigma}} |v_{\nu \mu}(\mathbf{k}, \mathbf{k} + \mathbf{q})|^2 \left| \langle \Psi_{n-1}^{(N-1)} | a_{\mu k - \nu \sigma} | \Psi_0^{(N)} \rangle \right|^2 \delta \left( \hbar \omega - \varepsilon_{\nu k} - E_{n-1}^{(N-1)} + E_0^{(N)} \right) . \tag{1.41}
\]

The contribution of a single band \( \lambda \) is simply proportional to

\[
 A_\lambda(\mathbf{k} - \mathbf{q}, \omega') = \sum_n \left| \langle \Psi_{n-1}^{(N-1)} | a_{\lambda k - \omega' \sigma} | \Psi_0^{(N)} \rangle \right|^2 \delta \left( \omega' - \frac{E_{n-1}^{(N-1)} - E_0^{(N)} + \mu}{\hbar} \right) ,
\]

where \( \omega' := \omega - \varepsilon_{\mu k} - \mu \). The comparison with Eq. (1.17) shows that this is indeed the spectral density of the single-particle Green’s function.
The assumption that the interaction between the photoelectron and the other electrons can be neglected is questionable since the mean-free path between collisions is short (typically a few A). Only some electrons, namely those originating from the region close to the surface, have a chance to reach the counter without losses due to scattering. It is this primary contribution which we have expressed in terms of the spectral density of the single-electron Green’s function (fortunately, this is also the most prominent part in actual experiments, the secondary contributions being rather structureless).

At the same time this reduction to the surface region has a drawback. The surface breaks the translational invariance, therefore the selection rule for the momentum components perpendicular to the surface is no longer valid. This leads to broadening of spectral features except if the energy dispersion $\varepsilon_{\mathbf{q}, \mathbf{k}}$ depends little on $k_\perp$, as in layered materials.

**Literature**


