The One-particle Green's function of an Electron-Summary

The wavefunction of the ground state of a system consisting of N interacting electrons $\rightarrow$ a complicated function of N coordinates in the real and spin space:

$$\Psi_0^{(N)} = \Psi_0(x_1, x_2, \ldots, x_N) \qquad \text{with} \quad x_i = (\mathbf{r}_i; \chi_i)\,.$$

Application of field operators $\hat{\psi}(\mathbf{r})$ or $\hat{\psi}^\dagger(\mathbf{r})$ annihilates or creates an electron with spin α at the point $\mathbf{r}$, respectively:

$$\hat{\psi}_\alpha(\mathbf{r})\Psi_0^{(N)} \rightarrow \Psi^{(N-1)} \qquad \text{bzw.} \quad \hat{\psi}_\alpha^\dagger(\mathbf{r})\Psi_0^{(N)} \rightarrow \Psi^{(N+1)}\,.$$

A transformation of this problem from the real space representation ("first quantization") into the so-called particle number representation ("second quantization"):

$$\Psi_0^{(N)} = |n_1, n_2, \ldots, n_j, \ldots, n_\infty > \qquad \text{mit} \quad \sum_{i=1}^{\infty} n_i = N\,,$$

with $n_i = 0$ or 1 (according to Pauli's principle).

Application of the c operators $\hat{c}_j$ or $\hat{c}_j^\dagger$ annihilates or creates the electronic single-particle quantum state $|j>$:

$$\hat{c}_j\,|\Psi_0^{(N)}> = |\Psi^{(N-1)}> \propto |n_1, n_2, \ldots, n_j - 1, \ldots, n_\infty >$$

or

$$\hat{c}_j^\dagger\,|\Psi_0^{(N)}> = |\Psi^{(N+1)}> \propto |n_1, n_2, \ldots, n_j + 1, \ldots, n_\infty > \;.$$

A connection between the field operators and the $\hat{c}$ operators by the use of the one-particle basis $\psi_i(x)$ is given by

$$\hat{\psi}_\alpha(\mathbf{r}) = \sum_i \psi_i(x)\,\hat{c}_i \qquad \text{bzw.} \qquad \hat{\psi}_\alpha^\dagger(\mathbf{r}) = \sum_i \psi_i^*(x)\,\hat{c}_i^\dagger\,.$$

Definition of a one-particle Green's function for an interacting system of electrons (see Eq. (1.1)):

$$iG_{\alpha,\beta}(\mathbf{r}t,\mathbf{r}'t') =< \Psi_0^{(N)}|\hat{T}\left[\hat{\psi}_{H\alpha}(\mathbf{r}t)\,\hat{\psi}^{\dagger}_{H\beta}(\mathbf{r}'t')\right]|\Psi_0^{(N)} > \ .$$

$\hat{T}$ means the time-ordening operator which guarantees that the time arguments in this equation fulfill the condition $t > t'$. In case of $t < t'$, this operator causes a commutation of the both field operators, leading (in case of electrons) to a negative sign of the matrix element.

The "H" in the field operators means that they are used in the Heisenberg representation instead of the Schrödinger representation.

For $t > t'$ one gets

$$iG_{\alpha,\beta}(\mathbf{r}t,\mathbf{r}'t') = \left(< \Psi_0^{(N)}|\hat{\psi}_{H\alpha}(\mathbf{r}t)\right)\left(\hat{\psi}^{\dagger}_{H\beta}(\mathbf{r}'t')|\Psi_0^{(N)} >\right)$$

and, further,

$$iG_{\alpha,\beta}(\mathbf{r}t,\mathbf{r}'t') = \underbrace{\left(\hat{\psi}^{\dagger}_{H\alpha}(\mathbf{r}t)|\Psi_0^{(N)} >\right)^{\dagger}}_{\left[\Psi_\alpha^{(N+1)}(\mathbf{r}t)\right]^*}\ \underbrace{\left(\hat{\psi}^{\dagger}_{H\beta}(\mathbf{r}'t')|\Psi_0^{(N)} >\right)}_{\Psi_\beta^{(N+1)}(\mathbf{r}'t')}\ .$$

Interpretation of a Green's function:

The Green's function describes the overlap between a multiparticle function of $(N+1)$ electrons, when the additional electron at $(\beta\mathbf{r}'t')$ has propagated to $(\alpha\mathbf{r}t)$,

or, alternatively,

the Green's function gives the probability that an electron of spin β which has been at $\mathbf{r}'$ at time t' appears with spin α at the position $\mathbf{r}$ at the later time t.

What is such a Green's function good for?

As it shall be evident in the following, a Green's function leads us (directly or indirectly) to a great number of - partly measurable! - informations about the physics of electrons in an electron gas.

How do we calculate a Green's function?

In case of a system of mutually interacting electrons, the Green's function $G_{\alpha,\beta}$ cannot be written down by a compact formula, but it can - in principle - be obtained with high accuracy by the use of perturbation theory.

Starting points of a perturbation expansion:

(1) an operator $\hat{H}_1$ that describes the interaction,
(2) the non-interacting Green's function $G^0_{\alpha,\beta}$.

Some details of this perturbation expansion are described in Sec. 1.2.1 of this textbook. The formal connection between the interacting and the non-interacting Green's functions G and G_0 reads as

$$iG_{\alpha,\beta}(\mathbf{r}t,\mathbf{r}'t') =< \Psi_0^{(N)}|\hat{T}\left[\hat{\psi}_{H\alpha}(\mathbf{r}t)\,\hat{\psi}^{\dagger}_{H\beta}(\mathbf{r}'t')\right]|\Psi_0^{(N)}> \ .$$

$$iG^0{}_{\alpha,\beta}(\mathbf{r}t,\mathbf{r}'t') =< \Phi_0^{(N)}|\hat{T}\left[\hat{\psi}_{I\alpha}(\mathbf{r}t)\,\hat{\psi}^{\dagger}_{I\beta}(\mathbf{r}'t')\right]|\Phi_0^{(N)}> \ .$$

In the last expression, $\Phi_0^{(N)}$ means the ground-state wave function of a system of N non-interacting electrons, and $\hat{\psi}_I$ indicates that the field operators have to be taken in the interaction representation [compare with Eqs. (1.10) and (1.11) in this textbook].