Correlation Functions II

One-Particle Green's Function: Overview

The one-particle Green's function is defined as

$$G(x_1, t_1; x_2, t_2) = -i \langle T\{\psi(x_1, t_1)\psi^\dagger(x_2, t_2)\}\rangle.$$

It encodes the propagation of single particles and serves as the foundation for many-body techniques.

Greater and Lesser Propagators

Greater Propagator:

$$G^{>}(x_1, t_1; x_2, t_2) = -i \langle \psi(x_1, t_1)\psi^{\dagger}(x_2, t_2) \rangle.$$

Represents the amplitude for particle addition (creation at x_2, t_2 and annihilation at x_1, t_1).

Lesser Propagator:

$$G^{<}(x_1, t_1; x_2, t_2) = i \langle \psi^{\dagger}(x_2, t_2)\psi(x_1, t_1) \rangle.$$

Describes the amplitude for particle removal (or hole propagation).

In equilibrium, these are related by:

$$G^{<}(\omega) = -e^{-\beta(\omega-\mu)} G^{>}(\omega).$$

Constructing Causal and Time-Ordered Green's Functions

From the greater and lesser functions, we build:

- **Retarded:**

$$G_R(x_1, t_1; x_2, t_2) = \theta(t_1 - t_2)\Big[G^>(x_1, t_1; x_2, t_2) - G^<(x_1, t_1; x_2, t_2)\Big].$$

- **Advanced:**

$$G_A(x_1, t_1; x_2, t_2) = -\theta(t_2 - t_1)\Big[G^>(x_1, t_1; x_2, t_2) - G^<(x_1, t_1; x_2, t_2)\Big].$$

- **Time-Ordered:**

$$G_T(x_1, t_1; x_2, t_2) = \theta(t_1 - t_2)G^>(x_1, t_1; x_2, t_2)$$

$$+\theta(t_2 - t_1)G^<(x_1, t_1; x_2, t_2).$$

Green's Function in Frequency Space

Starting with the spectral (Lehmann) representation:

$$G(z) = i \int_{-\infty}^{\infty} \frac{d\omega' \, A(\omega')}{z - \omega'},$$

where $A(\omega')$ is the spectral function.

Analytic continuation yields:

$$G_R(\omega) = \lim_{\eta \to 0^+} G(\omega + i\eta), \quad G_A(\omega) = \lim_{\eta \to 0^+} G(\omega - i\eta).$$

Moreover,

$$A(x_1, x_2, \omega) = -\frac{1}{\pi} \, \mathrm{Im} \; G_R(x_1, x_2, \omega).$$

Diagonal Green's Functions for Independent Particles

For a non-interacting system with eigenfunctions $\psi_k(x)$ and eigenvalues ϵ_k:

$$\psi(x) = \sum_k \psi_k(x) c_k,$$

the retarded Green's function in the eigenbasis is:

$$G_{0,R}(k,\omega) = \frac{1}{\omega - \epsilon_k + i\eta},$$

and hence the spectral function is:

$$A_{kk}(\omega) = -\frac{1}{\pi} \text{Im } G_{0,R}(k,\omega) = \delta(\omega - \epsilon_k).$$

Spectral Function for Interacting Systems

For an interacting many-body system, using the Lehmann representation:

$$G^{>}(x_1, t_1; x_2, t_2) = -i \langle \psi(x_1, t_1) \psi^{\dagger}(x_2, t_2) \rangle,$$

one inserts a complete set of eigenstates. Define the Dyson amplitudes:

$$f_{\alpha\lambda}(x) = \langle \alpha | \psi(x) | \lambda \rangle.$$

After Fourier transformation, one finds:

$$G^{>}(x_1, x_2, \omega) = -2\pi i \sum_{\alpha,\lambda} w_\alpha \, f_{\alpha\lambda}(x_1) f^*_{\alpha\lambda}(x_2) \, \delta(\omega + E_\alpha - E_\lambda),$$

$$G^{<}(x_1, x_2, \omega) = +2\pi i \sum_{\alpha,\lambda} w_\lambda \, f_{\alpha\lambda}(x_1) f^*_{\alpha\lambda}(x_2) \, \delta(\omega + E_\alpha - E_\lambda).$$

Then the spectral function is given by:

$$A(x_1, x_2, \omega) = \frac{i}{2\pi} \Big[G^{>}(x_1, x_2, \omega) - G^{<}(x_1, x_2, \omega) \Big],$$

or explicitly,

$$A(x_1, x_2, \omega) = \sum_{\alpha,\lambda} f_{\alpha\lambda}(x_1) f^*_{\alpha\lambda}(x_2) \, \delta(\omega + E_\alpha - E_\lambda) \, [w_\alpha + w_\lambda].$$

Spectral Function and Analytic Continuation at $T = 0$

At zero temperature and fixed particle number:

$$G(z) = i \int_{-\infty}^{\infty} \frac{d\omega' \, A(x_1, x_2, \omega')}{z - \omega'}.$$

The retarded Green's function is

$$G_R(\omega) = \lim_{\eta \to 0^+} G(\omega + i\eta),$$

so that

$$A(x_1, x_2, \omega) = -\frac{1}{\pi} \text{Im } G_R(x_1, x_2, \omega).$$

For the time-ordered Green's function:

$$G_T(\omega) = \begin{cases} G_R(\omega) & \omega > \mu, \\ G_A(\omega) & \omega < \mu, \end{cases}$$

which implies

$$A(x_1, x_2, \omega) = \frac{1}{\pi} \begin{cases} +\text{Im}[i \, G_T(x_1, x_2, \omega)] & \omega > \mu, \\ -\text{Im}[i \, G_T(x_1, x_2, \omega)] & \omega < \mu. \end{cases}$$

Why Use the Time-Ordered Green's Function?

The time-ordered (Feynman) Green's function G_T is crucial because:

1. It appears naturally in perturbation theory and allows the use of Wick's theorem.
2. It is the standard object in the Matsubara formalism for finite temperature.
3. It is computationally convenient; analytic continuation then gives G_R or G_A.
4. Many-body techniques such as the Dyson equation are formulated in terms of G_T.

Electron Density from G_T

The electron density at x is:

$$n(x) = \langle \psi^\dagger(x,t)\psi(x,t)\rangle = -i\, G_T(x,t;x,t^+),$$

with t^+ an infinitesimally later time.

At $T = 0$, using the Lehmann representation,

$$n(x) = \int_{-\infty}^{\infty} d\omega\, A(x,x,\omega) f(\omega),$$

with $f(\omega) = \theta(\mu - \omega)$, so that

$$n(x) = \sum_\lambda |f_\lambda(x)|^2\, \theta(\mu - \epsilon_\lambda).$$

One-Particle Density Matrix and Momentum Distribution

The one-particle density matrix is defined by

$$\rho(x, x') = \langle \psi^\dagger(x', t)\psi(x, t)\rangle = -i\, G_T(x, t; x', t^+).$$

At $T = 0$,

$$\rho(x, x') = \sum_\lambda \theta(\mu - \epsilon_\lambda)\, f_\lambda(x) f_\lambda^*(x').$$

Projecting onto plane-wave states yields the momentum distribution:

$$\rho(k) = \sum_\lambda \theta(\mu - \epsilon_\lambda) |\langle k | f_\lambda \rangle|^2.$$

Kinetic Energy from G_T

The kinetic energy operator is

$$\hat{T} = -\frac{1}{2}\nabla^2.$$

Its expectation value can be written as:

$$\langle T \rangle = -\frac{1}{2}\int d^3x \lim_{x' \to x} \nabla_x^2 \rho(x, x').$$

Substituting the Lehmann representation,

$$\langle T \rangle = -\frac{1}{2}\sum_\lambda \theta(\mu - \epsilon_\lambda) \int d^3x\, f_\lambda^*(x)\, \nabla^2 f_\lambda(x).$$

Relating G_T to the Coulomb Energy

The Coulomb (electron–electron) interaction energy is given by:

$$\langle V_{ee} \rangle = \frac{1}{2} \int d^3x \, d^3x' \, v(x - x') \, n(x, x'),$$

with the pair correlation function

$$n(x, x') = \langle \psi^\dagger(x) \psi^\dagger(x') \psi(x') \psi(x) \rangle.$$

Even though V_{ee} is a two-body operator, the equation of motion for the field operator relates its effects to the one-particle Green's function. For example, via the Galitskii–Migdal formula one obtains:

$$E = \frac{1}{2} \int d^3x \lim_{x' \to x} \left[\frac{\partial}{\partial t} - h(x) \right] G(x, t; x', t^+),$$

where $h(x) = -\frac{1}{2}\nabla^2 + v_{\text{ext}}(x)$.

Summary and Conclusions

- We defined expectation values, static and dynamic correlation functions.
- Static one-electron properties (density, density matrix, momentum distribution) and two-particle correlations (pair correlation function, structure factor) were discussed.
- Dynamic correlations lead to spectral functions and are linked via Kramers–Kronig relations.
- Response functions and the fluctuation–dissipation theorem connect microscopic fluctuations to macroscopic observables.
- The one-particle Green's function, built from greater and lesser propagators, provides the foundation for describing particle propagation, and its spectral representation encodes excitation spectra.
- Derived quantities such as electron density, kinetic energy, and even Coulomb energy can be expressed in terms of the one-particle Green's function.