Correlation Functions I

1 Introduction

This Lecture provides a comprehensive overview of correlation functions in many-body quantum systems. It begins with basic definitions for expectation values and correlation functions and then distinguishes between static (equal-time) and dynamic (unequal-time) correlations. The discussion moves on to describe one-particle properties and two-particle correlations (including the structure factor), introduces response functions and the fluctuation–dissipation theorem, and finally develops the one-particle and two-particle Green's functions. These tools form the backbone for many-body perturbation theory and are linked directly to measurable physical quantities.

2 Expectation Values and Correlation Functions

The expectation value of an operator $\hat{O}$ is defined by

$$\langle \hat{O} \rangle = \sum_{\alpha} w_{\alpha} \langle \alpha | \hat{O} | \alpha \rangle, \tag{1}$$

with the weights w_{α} chosen appropriately. At zero temperature the ground-state expectation value is

$$\langle \hat{O} \rangle = \langle 0 | \hat{O} | 0 \rangle.$$

For a system in the grand-canonical ensemble one has

$$\langle \hat{O} \rangle = \frac{1}{Z} \mathrm{Tr}\left[e^{-\beta(\hat{H}-\mu\hat{N})} \hat{O} \right], \quad Z = \mathrm{Tr}\left[e^{-\beta(\hat{H}-\mu\hat{N})} \right]. \tag{2}$$

Correlation functions are defined through the deviation from the product of individual expectation values. For example, for two operators,

$$C_{AB}(1,2) = \langle \hat{A}(1)\hat{B}(2) \rangle - \langle \hat{A}(1) \rangle \langle \hat{B}(2) \rangle. \tag{3}$$

3 Static One-Electron Properties

The electron density is defined as

$$n(x) = \langle \hat{n}(x) \rangle = \langle \psi^\dagger(x)\psi(x) \rangle, \tag{4}$$

where x denotes both the spatial and spin coordinates.

The one-body density matrix is given by

$$\rho(x, x') = \langle \psi^\dagger(x)\psi(x') \rangle. \tag{5}$$

Its diagonal gives the density: $\rho(x, x) = n(x)$. The momentum distribution is the Fourier transform of $\rho(x, x')$.

4 Static Two-Particle Correlations: Density Correlations and the Structure Factor

Summary: The pair correlation function quantifies the probability of finding two particles a given distance apart relative to the uncorrelated case. Its Fourier transform is the static structure factor, which is directly measurable by scattering experiments.

The pair correlation function is defined by

$$g(x, x') = \frac{n(x, x')}{n(x)n(x')}, \tag{6}$$

where $n(x, x')$ is the probability of finding one particle at x and another at x'.

The static structure factor is defined by

$$S_{\sigma,\sigma'}(k, k') = \frac{1}{N} \int d\mathbf{r}\, d\mathbf{r}'\, n(x, x')\, e^{i(k\cdot r - k'\cdot r')} + \frac{\delta_{\sigma,\sigma'}}{N} \int d\mathbf{r}\, n(x) e^{i(k-k')\cdot r}. \tag{7}$$

For non-interacting spin-$\frac{1}{2}$ fermions at zero temperature (and in the absence of an external potential) the structure factor is found to be

$$S(k) = \begin{cases} \frac{N}{2}, & k = 0, \\ \frac{k}{4k_F}\left(3 - \left(\frac{k}{2k_F}\right)^2\right), & 0 < k \le 2k_F, \\ 1, & k > 2k_F, \end{cases} \tag{8}$$

where k_F is the Fermi momentum.

For a charged system, however, long-wavelength fluctuations are suppressed by Coulomb interactions. Using sum rules and fluctuation–dissipation arguments, one obtains the bound

$$S(k) \le \frac{k^2}{2\omega_p}\left(1 - \frac{1}{\epsilon_k}\right)^{1/2}, \tag{9}$$

where ω_p is the plasma frequency and ϵ_k the static dielectric susceptibility.

5 Dynamic Correlation Functions

The static correlation functions can be generalized to the dynamic case (unequal times), these are time-dependent correlation functions. Their Fourier transforms (yielding frequency-dependent spectra), and are observed in different spectroscopies. Central to this is the spectral function which encapsulates the system's excitations.

For example, the dynamic correlation function is defined by

$$C_{AB}(1,2) = \langle \hat{A}(1)\hat{B}(2)\rangle, \tag{10}$$

with various decompositions into retarded, advanced, and time-ordered forms. The retarded function is given by

$$C^R(1,2) = \Theta(t_1 - t_2)[C(1,2) - \tilde{C}(1,2)], \tag{11}$$

and the advanced function by

$$C^A(1,2) = -\Theta(t_2 - t_1)[\tilde{C}(1,2) - C(1,2)], \tag{12}$$

with the time-ordered function

$$C^T(1,2) = \Theta(t_1 - t_2)C(1,2) + \Theta(t_2 - t_1)\tilde{C}(1,2). \tag{13}$$

The spectral function is defined as

$$2\pi A(\omega) = C(\omega) - \tilde{C}(\omega), \tag{14}$$

and the retarded function can be written in its spectral representation as

$$C^R(\omega) = i \lim_{\eta\to 0^+} \left[\mathcal{P} \int d\omega' \, \frac{A(\omega')}{\omega - \omega' + i\eta} \right]. \tag{15}$$

Finally, the Kramers–Kronig relations that link the real and imaginary parts of response functions are given by

$$\operatorname{Re}\chi(\omega) = -\frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty} \frac{\operatorname{Im}\chi(\omega')}{\omega - \omega'} d\omega', \quad \operatorname{Im}\chi(\omega) = \frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty} \frac{\operatorname{Re}\chi(\omega')}{\omega - \omega'} d\omega'. \tag{16}$$

6 Response Functions

Response functions describe how a many-body system reacts to an external perturbation. In this section we extend the discussion to cover several interrelated topics:

1. **Fluctuation–Dissipation Theorem:** This theorem establishes a direct connection between the intrinsic fluctuations in a system (as described by equilibrium correlation functions) and its linear response to an external field. In mathematical terms, if one considers a perturbation coupling to an operator $\hat{A}$ (with its conjugate operator $\hat{B} = \hat{A}^\dagger$), the imaginary part of the response function is related to the spectral density of the fluctuations. For example, one finds

$$\operatorname{Im}\chi(\omega) = \pi\,(1 - e^{-\beta\omega}) \sum_{\alpha,\lambda} w_\alpha\,|A_{\alpha\lambda}|^2\,\delta\Big(\omega + E_\alpha - E_\lambda\Big), \tag{17}$$

   which can also be expressed as

$$\operatorname{Im}\chi(\omega) = \frac{1 - e^{-\beta\omega}}{2} \int dt\,\langle \hat{A}^\dagger(0)\hat{A}(t)\rangle\,e^{i\omega t}. \tag{18}$$

   This relation shows that the response (dissipation) of the system when it is excited is completely determined by its equilibrium fluctuations. Such links lead directly to Kubo formulas, which are central in transport theory.

2. **Density–Density Response:** A particularly important example is the density–density response function. When the external perturbation is an electrostatic potential $v_{\text{ext}}(x,t)$ that couples to the electron density $\hat{n}(x)$, the change in the density is given to first order by

$$\delta n(1) = \int d2\,\chi(1,2)\,v_{\text{ext}}(2), \tag{19}$$

   where the linear response function is defined as

$$\chi(1,2) = -i\,\Theta(t_1 - t_2)\,\langle[\hat{n}(1), \hat{n}(2)]\rangle. \tag{20}$$

   In practice, the density response is often recast in terms of the dielectric function. The induced potential is not only the external one, but also includes the potential arising from the induced charge distribution:

$$\delta v_{\text{tot}}(1) = v_{\text{ext}}(1) + \int d3\,v(1,3)\,\delta n(3). \tag{21}$$

   In Fourier space, this relationship is written via the inverse dielectric function ϵ^{-1}:

$$\delta v_{\text{tot}}(\mathbf{q},\omega) = \epsilon^{-1}(\mathbf{q},\omega)\,v_{\text{ext}}(\mathbf{q},\omega). \tag{22}$$

   Hence, the density–density response function χ is directly related to the measured screening properties of the material.

3. **Dynamic Structure Factor:** The dynamic structure factor $S(\mathbf{Q},\omega)$ characterizes the spectrum of equilibrium fluctuations and is directly accessible through scattering experiments. It is defined as the Fourier transform (in both space and time) of the

pair correlation function. More precisely, for the diagonal elements (after summing over spins) one obtains

$$S(\mathbf{Q},\omega) = \sum_{\sigma,\sigma'} S_{\sigma,\sigma'}(\mathbf{Q},\omega) = \frac{-1}{\pi}(1-e^{-\beta\omega})^{-1}\,\mathrm{Im}\,\chi_{\mathbf{G}=0,\mathbf{G}'=0}(\mathbf{q},\omega), \tag{23}$$

where $\mathbf{Q} = \mathbf{q} + \mathbf{G}$ is the momentum transfer and $\chi_{\mathbf{G}=0,\mathbf{G}'=0}$ is the density response function in a periodic system. The dynamic structure factor gives the probability of exciting modes with energy ω and momentum $\mathbf{Q}$.

4. **Link to Experiment:** All the above quantities are not only theoretically significant but also measurable. For example:

   - *Loss Function:* In momentum-resolved electron energy-loss spectroscopy (EELS), one measures the loss function

     $$-\mathrm{Im}\,\epsilon^{-1}(\mathbf{Q},\omega) = \mathrm{Im}\,\epsilon_M(\mathbf{Q},\omega)\Big/\Big[\big(\mathrm{Re}\,\epsilon_M(\mathbf{Q},\omega)\big)^2 + \big(\mathrm{Im}\,\epsilon_M(\mathbf{Q},\omega)\big)^2\Big], \tag{24}$$

     where ϵ_M is the macroscopic dielectric function. Plasmon peaks, for example, are identified by zeros in $\mathrm{Re}\,\epsilon_M$ and corresponding peaks in the loss function.
   - *Inelastic X-ray Scattering (IXS):* IXS directly measures the dynamic structure factor $S(\mathbf{Q},\omega)$, revealing details about collective excitations (phonons, plasmons, etc.) in the material.
   - *Optical Absorption:* For vanishing momentum transfer ($\mathbf{q} \to 0$), the imaginary part of the macroscopic dielectric function, $\mathrm{Im}\,\epsilon_M(0,\omega)$, is directly related to the absorption spectrum. Differences between absorption and loss spectra can be understood in terms of the role of screening at different momentum transfers.

   Thus, the theoretical framework developed here connects microscopic many-body physics to experimental observables.

Detailed Discussion:

The starting point is the linear response of the expectation value of an operator $\hat{A}$ due to a perturbation that couples to $\hat{B}$:

$$\delta\langle\hat{A}(1)\rangle = i\int_{t_0}^{t_1} dt_2 \int d2\,\phi(2)\,\langle[\hat{B}(2),\hat{A}(1)]\rangle, \tag{25}$$

which immediately suggests the definition of the response function $\chi_{AB}(1,2)$ above.

The fluctuation–dissipation theorem (FDT) is then derived by comparing the response of the system to a weak perturbation with the intrinsic fluctuations that occur at equilibrium. Essentially, FDT tells us that the same processes responsible for dissipation (as encoded in $\mathrm{Im}\,\chi(\omega)$) are also responsible for spontaneous fluctuations (given by the time-dependent correlation functions).

When the perturbation couples to the charge density, the resulting density–density response function $\chi(1,2)$ leads directly to the dielectric function via the relation (24) for the inverse dielectric function ϵ^{-1}. In a periodic solid, these relations are expressed in reciprocal space , connecting microscopic fluctuations to the macroscopic screening properties.

The dynamic structure factor serves as a bridge between theory and experiment. In scattering experiments, one measures how incident particles (photons, electrons, or neutrons) exchange energy and momentum with the system. The measured intensity is directly proportional to $S(\mathbf{Q},\omega)$, which in turn is connected via the FDT to $\operatorname{Im}\chi(\omega)$. This allows one to infer the energy spectrum of collective excitations, such as plasmons and phonons.

One particle Greens Function

Greater and Lesser Propagators

The greater and lesser propagators are the fundamental building blocks that distinguish between processes of particle addition and removal.

- **Greater Propagator:**

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

  This function represents the amplitude for creating (or adding) a particle at the point x_2 and time t_2 and then later annihilating (or removing) that same particle at the point x_1 and time t_1. In physical terms, it describes the propagation of an extra particle (for example, an electron) through the system.

- **Lesser Propagator:**

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

  This function corresponds to the amplitude for removing a particle (or, equivalently, creating a hole) at x_1 and time t_1 and then reintroducing that particle at x_2 and time t_2. It thus captures the dynamics of hole propagation.

In equilibrium these two functions are not independent—they are related by a thermal factor. For example, one often finds a relation such as

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

which reflects that, at finite temperature, the relative probability of particle addition versus removal is governed by Fermi-Dirac statistics.

In summary:

- $G^{>}(x_1,t_1;x_2,t_2)$ provides information about the propagation of an extra electron (particle addition) through the system.

- $G^<(x_1, t_1; x_2, t_2)$ describes the propagation of a hole (particle removal).

These functions are essential for understanding experiments such as photoemission (which probes electron removal) and inverse photoemission (which probes electron addition). Moreover, they form the basis for constructing the retarded and advanced Green's functions via analytic continuation.

Constructing Green's Functions from Greater and Lesser Propagators

From the propagators described above, one can build the causal (retarded and advanced) and time-ordered Green's functions.

The retarded Green's function is given by:

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

and the advanced Green's function is

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

The time-ordered Green's function is defined as

$$G_T(t_1, t_2) = \theta(t_1 - t_2)G^>(t_1, t_2) + \theta(t_2 - t_1)G^<(t_1, t_2)\,.$$

6.1 Green's function in frequency space

In frequency space we start from the spectral (or Lehmann) representation of the Green's function, writing the Green's function as an integral over its spectral function $A(\omega')$:

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

where z is a complex frequency variable. This representation shows that $G(z)$ is analytic everywhere except along the real axis (where the spectral weight $A(\omega')$ is nonzero).

To obtain the retarded and advanced Green's functions, one "approaches" the real frequency axis from different sides:

- The **retarded Green's function** is defined by taking the limit as

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

  Here the infinitesimal positive imaginary part $+i\eta$ shifts the poles slightly below the real axis, ensuring that $G_R(t)$ vanishes for $t < 0$ (the causality condition).

- Similarly, the **advanced Green's function** is obtained by

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

In this case, the poles are shifted slightly above the real axis.

In practice, one first computes (or defines) the Fourier transforms of the greater and lesser propagators, $G^>(\omega)$ and $G^<(\omega)$, which are directly related to the spectral function by

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

Then, using the spectral representation, one performs the analytic continuation to the complex plane. The limits $\omega \pm i\eta$ pick out the correct boundary conditions for the retarded (causal) and advanced (anti-causal) functions.

In summary, the analytic continuation is performed by:

1. Expressing the Green's function in the spectral form

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

2. Evaluating this function on the real axis with an infinitesimal shift, i.e., setting $z = \omega \pm i\eta$.

3. Defining

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

This method ensures that the retarded Green's function is causal (nonzero only for $t > 0$) and the advanced one satisfies the corresponding condition for $t < 0$.

Diagonal Green's Functions for Independent Particles

In the case of independent (non-interacting) particles, the system's Hamiltonian can be diagonalized. Let the single-particle eigenfunctions and eigenvalues be denoted by $\psi_k(x)$ and ϵ_k, respectively. The field operator can then be expanded as:

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

where c_k annihilates a particle in state k.

For independent particles, the greater and lesser propagators in the eigenbasis become:

$$G_0^>(k,t) = -i\, e^{-i\epsilon_k(t-t_0)}\Big[1 - f(\epsilon_k)\Big]\,, \tag{26}$$

$$G_0^<(k,t) = i\, e^{-i\epsilon_k(t-t_0)}\, f(\epsilon_k)\,, \tag{27}$$

with $f(\epsilon_k)$ the Fermi-Dirac distribution. Notice that these expressions depend only on the eigenstate k and its energy ϵ_k; there is no mixing between different k-states. Consequently, the propagators (and hence the constructed Green's functions) are diagonal in this basis.

Upon combining $G_0^>$ and $G_0^<$ to form the retarded Green's function, one obtains:

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

and similarly,

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

The diagonality reflects the fact that in a non-interacting system the eigenstates of the Hamiltonian evolve independently (i.e., the Hamiltonian is already diagonal in the eigenbasis). There is no off-diagonal mixing because there are no interaction terms to couple different states.

In an orthonormal basis (say, the eigenbasis of the non-interacting Hamiltonian), one can write the spectral function as

$$A_{ij}(\omega) = \frac{i}{2\pi}\Big[G_{ij}^>(\omega) - G_{ij}^<(\omega)\Big] \,,$$

where i and j label the basis states. When the spectral function is real, its diagonal elements are related to the retarded Green's function by

$$A_{ii}(\omega) = -\frac{1}{\pi}\,\mathrm{Im}\; G_{R,ii}(\omega) \,.$$

For independent particles the Hamiltonian is diagonal in this basis so that

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

and consequently,

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

indicating that the excitations are sharp and occur exactly at the eigenenergies ϵ_k.

Thus, in an orthonormal basis, the spectral function and the retarded Green's function are directly related via the imaginary part, reflecting the fact that the spectral function contains the full information about the energy distribution of the excitations.

Derivation of the Spectral Function for Interacting Particles

For a many-body system (with interactions), the time-ordered one-particle Green's function is defined as

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

where $\psi(x,t)$ and $\psi^\dagger(x,t)$ are the field operators, and the average is taken over the thermal ensemble (or the ground state at zero temperature).

Step 1: Insertion of a Complete Set of Eigenstates

Assume that the many-body Hamiltonian $\hat{H}$ has eigenstates $\{|\alpha\rangle\}$ with eigenenergies E_α. We can insert a complete set of eigenstates between the field operators. For example, consider the greater propagator:

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

Inserting complete sets yields terms of the form

$$\sum_{\alpha,\lambda} w_\alpha\,\langle\alpha|\psi(x_1,t_1)|\lambda\rangle\langle\lambda|\psi^\dagger(x_2,t_2)|\alpha\rangle\,,$$

where w_α is the statistical weight (for example, $w_\alpha = e^{-\beta(E_\alpha-\mu N_\alpha)}/Z$ at finite temperature).

We introduce the *Dyson amplitudes*

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

Due to the time evolution in the Heisenberg picture, these matrix elements acquire phase factors:

$$\langle\alpha|\psi(x,t)|\lambda\rangle = f_{\alpha\lambda}(x)e^{-iE_\lambda t}\,,$$

and similarly for the adjoint operator.

Step 2: Fourier Transform and the Lehmann Representation

After writing the time dependence explicitly and performing the Fourier transform with respect to the time difference $t = t_1 - t_2$, one obtains a representation of the greater and lesser propagators as sums over delta functions:

$$G^>(x_1,x_2,\omega) = -2\pi i\sum_{\alpha,\lambda} w_\alpha\, f_{\alpha\lambda}(x_1)f^*_{\alpha\lambda}(x_2)\,\delta(\omega+E_\alpha-E_\lambda)\,, \tag{28}$$

$$G^<(x_1,x_2,\omega) = +2\pi i\sum_{\alpha,\lambda} w_\lambda\, f_{\alpha\lambda}(x_1)f^*_{\alpha\lambda}(x_2)\,\delta(\omega+E_\alpha-E_\lambda)\,. \tag{29}$$

Step 3: Definition of the Spectral Function

The spectral function is defined in terms of these two propagators by

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

Substituting the expressions from above, we obtain

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

Physical Interpretation:

- The delta function $\delta(\omega + E_\alpha - E_\lambda)$ enforces energy conservation and indicates that the Green's function has poles (or spectral weight) at the excitation energies corresponding to adding or removing a particle.
- The Dyson amplitudes $f_{\alpha\lambda}(x)$ provide the spatial (and spin) structure of the transition between the many-body states $|\alpha\rangle$ and $|\lambda\rangle$.
- The statistical factors w_α and w_λ weight the contributions from the initial and final states in the ensemble.

Thus, the general expression for the spectral function in an interacting system,

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

encapsulates the full spectrum of excitations (both electron addition and removal processes) of the interacting system, including all many-body effects.

Spectral Function, Retarded and Time-Ordered Green's Functions at $T = 0$

At zero temperature ($T = 0$) and fixed particle number N, the time-ordered Green's function $G_T(\omega)$ can also be analytically continued uniquely. However, because of the Fermi occupation factors becoming step functions at $T = 0$, the analytic continuation differs depending on whether the frequency is above or below the chemical potential μ:

$$G_T(\omega) = \begin{cases} G(\omega + i\eta) = G_R(\omega), & \omega > \mu, \\ G(\omega - i\eta) = G_A(\omega), & \omega < \mu. \end{cases}$$

This means that for $\omega > \mu$ the time-ordered function coincides with the retarded function, while for $\omega < \mu$ it coincides with the advanced function.

Because of this, the relation between the spectral function and $G_T(\omega)$ involves a sign change. One finds that:

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

In contrast, the retarded Green's function is defined uniformly as $G_R(\omega) = G(\omega + i\eta)$ for all ω, so its relation with the spectral function is simply

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

Summary:

- In the general case, the spectral function is defined by

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

  where $G_R(\omega)$ is the retarded Green's function obtained by analytic continuation $z = \omega + i\eta$.

- At $T = 0$ and fixed N, the time-ordered Green's function $G_T(\omega)$ requires separate analytic continuations:

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

  Thus, the expression for the spectral function in terms of $G_T(\omega)$ becomes

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

- The difference in sign arises because for $\omega < \mu$ the analytic continuation gives the advanced Green's function, whose imaginary part has the opposite sign compared to the retarded one.

Why is the Time-Ordered Green's Function Useful?

While the **retarded Green's function** $G_R(x_1, t_1; x_2, t_2)$ is directly related to physical response—being causal (i.e. nonzero only for $t_1 > t_2$) and directly measurable in linear response experiments—the **time-ordered (or Feynman) Green's function** $G_T(x_1, t_1; x_2, t_2)$ plays a central role in many-body theoretical calculations for several reasons:

1. **Perturbation Theory and Diagrammatic Techniques:** The time-ordered Green's function is the natural object that appears in the perturbative expansion of many-body systems. Its definition,

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

   allows one to apply Wick's theorem, which is essential for systematically organizing and summing Feynman diagrams. This simplifies calculations, even in interacting systems.

2. **Matsubara Formalism at Finite Temperature:** In finite-temperature many-body theory, one often works with imaginary (Matsubara) time. The time-ordered Green's function is naturally defined in this context and provides a smooth function on the imaginary time axis. Physical (real-time) quantities can then be obtained via analytic continuation.

3. **Computational Convenience:** The time-ordered Green's function is easier to compute directly using the standard techniques of quantum field theory. Although its physical interpretation is less immediate than that of the retarded function, it encapsulates all the information of the system. One can extract the retarded (or advanced) Green's function by performing an analytic continuation:

$$G_R(\omega) = \lim_{\eta \to 0^+} G_T(\omega + i\eta) \quad (\text{for } \omega > \mu),$$

and similarly for $G_A(\omega)$ for frequencies below the chemical potential.

4. **Universality of the Formalism:** Many-body techniques (including the Dyson equation and self-energy corrections) are naturally formulated in terms of the time-ordered Green's function. Once these quantities are computed, one can relate them to experimentally accessible quantities (such as the spectral function) using established relations.

Useful Quantities Derived from the One-Particle Green's Function

We will use the time ordered Green's function defined as

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

where $\psi(x, t)$ and $\psi^\dagger(x, t)$ are the field operators that annihilate and create particles, respectively, and T is the time-ordering operator. From this fundamental object, several useful physical quantities can be extracted.

1. Electron Density

The electron density $n(x)$ at point x is given by the expectation value of the density operator

$$\hat{n}(x) = \psi^\dagger(x, t)\psi(x, t) .$$

Using the time-ordered Green's function, one can show that

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

where t^+ indicates a time infinitesimally later than t to preserve the proper ordering.

For zero temperature it can be shown that:

The time-ordered Green's function can be written in the Lehmann representation as

$$G_T(x, x', \omega) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \, \frac{A(x, x', \omega')}{\omega - \omega' + i\eta \, \mathrm{sgn}(\omega' - \mu)} ,$$

where $A(x, x', \omega)$ is the spectral function. For a many-body system at $T = 0$, the spectral function has the form

$$A(x, x', \omega) = \sum_\lambda f_\lambda(x) f_\lambda^*(x') \, \delta(\omega - \epsilon_\lambda) ,$$

with:

- ϵ_λ being the excitation energies (i.e. the difference between the energy of the state with one particle removed or added and the ground state energy),
- $f_\lambda(x) \equiv f_{0\lambda}(x) = \langle 0|\psi(x)|\lambda\rangle$ are the Dyson amplitudes, which give the probability amplitude for removing a particle from the ground state $|0\rangle$ to reach the state $|\lambda\rangle$.

The general relation for the density is obtained by integrating the spectral function weighted by the Fermi-Dirac distribution $f(\omega)$:

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

At $T = 0$, the Fermi function becomes a step function:

$$f(\omega) = \theta(\mu - \omega)\,,$$

where μ is the chemical potential. Thus,

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

Substitute the expression for the spectral function:

$$A(x, x, \omega) = \sum_\lambda |f_\lambda(x)|^2\, \delta(\omega - \epsilon_\lambda)\,.$$

Thus,

$$n(x) = \sum_\lambda |f_\lambda(x)|^2 \int_{-\infty}^{\infty} d\omega\, \delta(\omega - \epsilon_\lambda)\, \theta(\mu - \omega)\,.$$

The δ-function picks out $\omega = \epsilon_\lambda$, so the integral yields:

$$\int_{-\infty}^{\infty} d\omega\, \delta(\omega - \epsilon_\lambda)\, \theta(\mu - \omega) = \theta(\mu - \epsilon_\lambda)\,.$$

Thus, we obtain:

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

This equation shows that the density is given by a sum over the probabilities (the squared Dyson amplitudes) for removing a particle from the ground state, but only those excitations with energy ϵ_λ below the chemical potential (i.e. corresponding to occupied states) contribute.

2. One-Particle Density Matrix

The one-particle density matrix is defined as

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

Its diagonal part $\rho(x,x)$ gives the density $n(x)$, and its off-diagonal part carries information about the coherence and correlations in the system.

At zero temperature in the Lehmann representation (or using Dyson amplitudes), it can be written as

$$\rho(x_1,x_2) = \sum_\lambda \theta(\mu-\epsilon_\lambda)\, f_\lambda(x_1) f_\lambda^*(x_2)\,,$$

where:

- $\theta(\mu-\epsilon_\lambda)$ selects only those excitations with energy ϵ_λ below the chemical potential μ (i.e., corresponding to occupied states),
- $f_\lambda(x) \equiv \langle 0|\psi(x)|\lambda\rangle$ is the Dyson amplitude describing the probability amplitude for removing a particle from the ground state $|0\rangle$ to reach the $(N-1)$-particle state $|\lambda\rangle$.

To obtain the momentum distribution, we project the density matrix onto the basis of plane waves. In a homogeneous system the plane-wave basis functions are

$$\psi_k(x) = \frac{1}{\sqrt{V}} e^{i\mathbf{k}\cdot\mathbf{x}}\,,$$

where V is the normalization volume. The momentum distribution $\rho(k)$ is given by the diagonal elements of the density matrix in this basis:

$$\rho(k) = \langle c_k^\dagger c_k\rangle = \int d^3x\, d^3x'\, \psi_k^*(x)\, \rho(x,x')\, \psi_k(x')\,.$$

Substitute the Lehmann representation for $\rho(x,x')$:

$$\rho(k) = \sum_\lambda \theta(\mu-\epsilon_\lambda) \int d^3x\, d^3x'\, \psi_k^*(x)\, f_\lambda(x) f_\lambda^*(x')\, \psi_k(x')\,.$$

Recognize that the integrals yield the projection of the Dyson amplitude $f_\lambda(x)$ onto the plane-wave state:

$$\langle k|f_\lambda\rangle \equiv \int d^3x\, \psi_k^*(x)\, f_\lambda(x)\,.$$

Thus, the expression becomes

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

This equation shows that the momentum distribution is given by a sum over the probabilities (the squared amplitudes) for finding a particle with momentum k, where the contribution from each excitation $|\lambda\rangle$ is weighted by the factor $\theta(\mu-\epsilon_\lambda)$ to include only the occupied states.

4. Kinetic Energy

The kinetic energy can be derived from the Green's function using its equation of motion. If the single-particle kinetic energy operator is

$$\hat{T} = -\frac{\nabla^2}{2m}\,,$$

one can show that

$$\langle T \rangle = -\int d^3x \, \lim_{x' \to x} \left[\frac{\nabla^2}{2m} \, G(x,t;x',t^+) \right] \,.$$

This expression is obtained by applying the differential operator to the Green's function and taking the equal-space limit as follows:

At zero temperature and fixed particle number, the kinetic energy operator is given by

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

so that its expectation value is

$$\langle T \rangle = \langle \hat{T} \rangle = -\frac{1}{2} \int d^3x \, \langle \psi^\dagger(x) \, \nabla^2 \psi(x) \rangle \,.$$

This expectation value can be expressed in terms of the one-particle time-ordered Green's function G_T by using the relation

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

where t^+ indicates a time infinitesimally later than t to ensure proper ordering.

Thus, the density matrix is given by

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

The expectation value of the kinetic energy becomes

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

Substituting the expression for $\rho(x,x')$, we have

$$\langle T \rangle = -\frac{1}{2} \int d^3x \, \lim_{x' \to x} \nabla_x^2 \Big[-i \, G_T(x,t;x',t^+) \Big].$$

Noting that the factors of i combine (i.e. $-\frac{1}{2} \times (-i) = \frac{i}{2}$) and then cancel when we reinsert the appropriate i from the definition, we write

$$\langle T \rangle = \frac{i}{2} \int d^3x \, \lim_{x' \to x} \nabla_x^2 \, G_T(x,t;x',t^+).$$

At $T = 0$, the one-body density matrix (or equivalently, the Green's function at equal times) can be expressed in terms of the Dyson amplitudes:

$$-i\, G_T(x, t; x', t^+) = \rho(x, x') = \sum_\lambda \theta(\mu - \epsilon_\lambda)\, f_\lambda(x) f_\lambda^*(x')\,,$$

where

- $f_\lambda(x) = \langle 0|\psi(x)|\lambda\rangle$ is the Dyson amplitude (with $|0\rangle$ the ground state and $|\lambda\rangle$ an eigenstate of the $N-1$ particle system),
- $\theta(\mu - \epsilon_\lambda)$ is the Heaviside function ensuring that only states with energy ϵ_λ below the chemical potential contribute.

Thus,

$$G_T(x, t; x', t^+) = i \sum_\lambda \theta(\mu - \epsilon_\lambda)\, f_\lambda(x) f_\lambda^*(x').$$

Substitute the above expression into the formula for $\langle T\rangle$:

$$\langle T\rangle = \frac{i}{2} \int d^3x \lim_{x' \to x} \nabla_x^2 \left\{ i \sum_\lambda \theta(\mu - \epsilon_\lambda)\, f_\lambda(x) f_\lambda^*(x') \right\}.$$

Since $i \times i = -1$, this simplifies to

$$\langle T\rangle = -\frac{1}{2} \sum_\lambda \theta(\mu - \epsilon_\lambda) \int d^3x \lim_{x' \to x} \nabla_x^2 \Big[f_\lambda(x) f_\lambda^*(x') \Big]\,.$$

Assuming that the Dyson amplitudes are smooth enough, the limit $x' \to x$ yields

$$\lim_{x' \to x} \nabla_x^2 \Big[f_\lambda(x) f_\lambda^*(x') \Big] = f_\lambda^*(x)\, \nabla^2 f_\lambda(x)\,.$$

Thus, we obtain

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

This expresses the kinetic energy as a sum over the contributions from the occupied single-particle states, with the Dyson amplitudes $f_\lambda(x)$ providing the spatial profile of each state.

5. Relating the One-Particle Green's Function to the Coulomb Energy

The Coulomb (electron–electron) interaction energy is given by a two-body operator:

$$\hat{V}_{ee} = \frac{1}{2} \int d^3x\, d^3x'\, \psi^\dagger(x)\, \psi^\dagger(x')\, v(x - x')\, \psi(x')\, \psi(x),$$

where $v(x - x')$ is the Coulomb potential. Its expectation value involves the two-particle (or pair) probability,

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

with the pair probability (or pair correlation function) defined as

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

How Can the One-Particle Green's Function Be Sufficient?

Although $\langle \hat{V}_{ee} \rangle$ explicitly depends on a two-body quantity, there exists an important relation in many-body theory that allows one to express the total energy of the system (which includes $\langle \hat{V}_{ee} \rangle$) solely in terms of the one-particle Green's function. This is achieved via the *equation of motion* for the field operators.

The Heisenberg equation for the field operator $\psi(x, t)$ reads

$$i \frac{\partial}{\partial t} \psi(x, t) = \left[\psi(x, t), \hat{H} \right],$$

and when the Hamiltonian $\hat{H}$ includes both the kinetic energy and the interaction $\hat{V}_{ee}$, the time derivative of $\psi(x, t)$ picks up a term involving

$$\int d^3x' \, v(x - x') \, \psi^\dagger(x', t) \, \psi(x', t) \, \psi(x, t).$$

Taking the expectation value of this equation, with proper time ordering, relates the time derivative of the one-particle Green's function to both the kinetic energy and a term that involves the Coulomb interaction.

In practice, one obtains an expression for the total energy (for instance, via the Galitskii–Migdal formula) of the form

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

where $h(x)$ is the single-particle Hamiltonian (including kinetic and external potential terms). The derivative term implicitly contains the contributions from the interaction, because the equation of motion for $G(x, t; x', t')$ involves the self-energy—which itself encodes two-particle correlations.

- The Coulomb energy depends on the pair probability $n(x, x')$, a two-body quantity.
- However, the equation of motion for the field operators (and hence for the Green's function) includes the interaction terms.

- As a result, the one-particle Green's function (together with its self-energy) encapsulates the effects of two-body correlations.
- This allows one to derive expressions (e.g., via the Galitskii–Migdal formula) where the total energy—including the Coulomb energy—is written entirely in terms of the one-particle Green's function.

In this way, even though the Coulomb energy is conceptually a two-particle quantity, the one-particle Green's function contains the necessary information to determine it.