Green's Functions Theory for Quantum Many-Body Systems
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Lectures website: http://ribf.riken.jp/~barbieri/mbgf.html
Many-body Green's functions (MBGF) are a set of techniques that originated in quantum field theory but have then found wide applications to the many-body problem.

In this case, the focus are complex systems such as crystals, molecules, or atomic nuclei.

*Development of formalism: late 1950s/1960s → imported from quantum field theory*

*1970s - today → applications and technical developments...*
Many-body Green's functions are a VAST formalism. They have a wide range of applications and contain a lot of information that is accessible from experiments.

Here we want to give an introduction:

- Teach the basic definitions and results
- Make connection with experimental quantities → gives insight into physics
- Discuss some specific application to many-bodies
Purpose and organization

Most of the material covered here is found on

(covers both formalism and recent applications
very large → 700+ pages)

I will provide:

• notes on formalism discussed (partial)
• the slides of the lectures

→ Download from the website:

  http://ribf.riken.jp/~barbieri/mbgf.html
Books on many-body Green’s Functions:

- J. W. Negele and H. Orland, *Quantum Many-Particle Systems,* (Benjamin, Redwood City CA, 1988)
- ...
Recent reviews:


(Some) classic papers on formalism:

### Schedule (4 weeks)

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<td><strong>Basics and link to spectroscopy</strong></td>
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<td>4/6 (月)</td>
<td>15:00-16:30</td>
<td>second quantization (review), definitions of GF</td>
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<td>4/9 (木)</td>
<td>14:00-15:30</td>
<td>Basic properties and sum rules</td>
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<td>Link to experimental quantities</td>
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<td>4/13 (月)</td>
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<td>Equation of motion method, expansion of the self-energy</td>
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<td>4/16 (木)</td>
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<td>Introduction to Feynman diagrams</td>
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<td>Self-consistency and RPA</td>
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## Schedule (4 weeks)

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<td>4/27 (月)</td>
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<td>4/27 (木)</td>
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<td>5/14 (木)</td>
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<td>Superfluidity, BCS/BEC cross over</td>
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<td>5/14 (木)</td>
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<td>Cold atoms</td>
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<td>5/18 (月)</td>
<td>15:00-16:30</td>
<td>Finite temperature/nucleonic matter (time permitting)</td>
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• \textbf{Green's functions}
• \textbf{Propagators}
• \textbf{Correlation functions}

\{ names for the same objects \}

• \textbf{Many-body Green's functions} $\leftarrow$ \textbf{Green's functions} applied to the \textbf{MB} problem

• \textbf{Self-consistent Green's functions (SCGF)} $\leftarrow$ \textbf{a particular approach to calculate GFs}
In Green's Function Monte Carlo one starts with a “trial” wave function, and lets it propagate in time:

\[ \Psi^N(t) = e^{-iH(r_1, r_2, \ldots, r_N)t/\hbar} \Psi_{\text{trial}}^N \]

For \( t \to -\infty \), this goes to the gs wave function!

Better to break the time in many little intervals \( \Delta t \),

\[ |\Psi^N(t)\rangle = \int \int \ldots \int \langle r_1'', r_2'', \ldots, r_N'' | e^{-H\Delta \tau/\hbar} | r_1'', r_2'', \ldots, r_N'' \rangle \cdot \cdot \cdot \]

\[ \ldots \langle r_1', r_2', \ldots, r_N' | e^{-H\Delta \tau/\hbar} | r_1, r_2, \ldots, r_N \rangle \langle r_1, r_2, \ldots, r_N | \Psi_{\text{trial}}^N \rangle \]

GFMC is a method to compute the exact wave function.
(typically works for few bodies, \( A \leq 12 \) in nuclei).
MBGF is a method that DO NOT compute the wave function:
It assumes that the system is in its ground state and attempts at calculating simple excitation on from it directly

• Large N (number of particles)

• The N-body ground state plays the role of vacuum (of excitations)

• Degrees of freedom are a few particles (or holes) on top of this vacuum

• It is a microscopic method (and capable of “ab-initio” calculations)
Don’t get confused:

Green’s function Monte Carlo (GFMC) and

Many-body Green’s Functions

are NOT the same method!!!!!!
One-hole spectral function -- example

\[ S^{(h)}(p_m, E_m) = \sum_n |\langle \Psi^{-1}_n | c_{P_m} | \Psi^A_0 \rangle|^2 \delta(E_m - (E^A_0 - E^{-1}_n)) \]

\[ \rightarrow \text{distribution of momentum (} p_m \text{) and energies (} E_m \text{)} \]
Examples of quasiparticles – Nuclei-I

The nuclear force has strong repulsive behavior at short distances.

The short range core is:
• required by elastic NN scattering
• supported by high-energy electron scattering (Jlab)
• and supported by Lattice-QCD (Ishii now in 東大)

Repulsive core: 500 - 600 MeV

Attractive pocket: about 30 MeV

Yukawa tail $\propto e^{-m_r/r}$

Nucleons attract themselves at intermediate distances and scatter like billiard balls:
→ Naively, nuclei cannot be treated as orbits structures

“BAD” model of a nucleus

“GOOD” model of a nucleus
Examples of quasiparticles - Nuclei-III

...BUT, understanding binding energies and magic number DOES require a shell structure!!!

→ Single particle orbits?


→ Nobel prize (1963)!
Examples of quasiparticles - ions in liquid

Ions in a liquid screen each other’s charge and interact weakly

[Picture adapted from Mattuck]
Examples of quasiparticles - ions in liquid

Ions in a liquid screen each other's charge and interact weakly

[Picture adapted from Mattuck]
Examples of quasiparticles - ions in liquid

Ions in a liquid screen each other’s charge and interact weakly

[Picture adapted from Mattuck]
Examples of quasiparticles - electron in gas

[Picture adapted form Mattuck]
Choose an orthonormal single-particle basis \( \{ \alpha \} \) and use it to build bases for the many-body states. 
E.g.,

\[
| n_{\alpha_1} = 3, \ n_{\alpha_2} = 0, \ n_{\alpha_3} = 2, \ n_{\alpha_4} = 2, \ n_{\alpha_5} = 0, \ldots \rangle \equiv \mathcal{S}[\phi_{\alpha_1}(r_1)\phi_{\alpha_1}(r_2)\phi_{\alpha_1}(r_3)\phi_{\alpha_3}(r_4)\phi_{\alpha_3}(r_5)\phi_{\alpha_4}(r_6)\phi_{\alpha_4}(r_7)]
\]

Need states of different particle number \( N \)

\[ \Rightarrow \text{use the Fock space:} \]

\[
I = \sum_{n_1=0}^{n_{\text{max}}} \sum_{n_2=0}^{n_{\text{max}}} \sum_{n_3=0}^{n_{\text{max}}} \ldots \sum_{n_\alpha=0}^{n_{\text{max}}} \ldots
\]

\[
|n_1, \ n_2, \ n_3, \ldots \ n_\alpha, \ldots \rangle \langle n_1, \ n_2, \ n_3, \ldots \ n_\alpha, \ldots |
\]

It must include the vacuum state: \( |0\rangle \langle 0| \)

\( n_{\text{max}} = 1 \) for fermions
\( = \infty \) for bosons
Second quantization

Basis states for bosons are constructed as

\[ |n_1, n_2, \ldots, n_\alpha, \ldots \rangle = \frac{1}{\sqrt{n_1!\, n_2! \cdots n_\alpha! \cdots}} (c_1^\dagger)^{n_1} (c_2^\dagger)^{n_2} \cdots (c_\alpha^\dagger)^{n_\alpha} \cdots |0\rangle \]

creation and annihilation operators give

\[ c_\alpha^\dagger |n_1, n_2, \ldots n_\alpha, \ldots \rangle = \sqrt{n_\alpha + 1} |n_1, n_2, \ldots n_\alpha + 1, \ldots \rangle \]
\[ c_\alpha |n_1, n_2, \ldots n_\alpha, \ldots \rangle = \sqrt{n_\alpha} |n_1, n_2, \ldots n_\alpha - 1, \ldots \rangle \]

Commutation rules:

\[ [c_\alpha, c_\beta^\dagger] = \delta_{\alpha,\beta}, \quad [c_\alpha, c_\beta] = [c_\alpha^\dagger, c_\beta^\dagger] = 0 \]
Many-Body Green's Functions

Second quantization

Basis states for fermions are constructed as

$$|n_1, n_2, \ldots, n_\alpha, \ldots\rangle = (c_1^\dagger)^{n_1} (c_2^\dagger)^{n_2} \cdots (c_\alpha^\dagger)^{n_\alpha} \cdots |0\rangle$$

creation and annihilation operators give

$$c_\alpha^\dagger |n_1, n_2, \ldots n_\alpha, \ldots\rangle = \delta_{0,n_\alpha} (-)^{s_\alpha} \sqrt{n_\alpha + 1} |n_1, n_2, \ldots n_\alpha + 1, \ldots\rangle$$

$$c_\alpha |n_1, n_2, \ldots n_\alpha, \ldots\rangle = \delta_{1,n_\alpha} (-)^{s_\alpha} \sqrt{n_\alpha} |n_1, n_2, \ldots n_\alpha - 1, \ldots\rangle$$

with: $s_\alpha = n_1 + n_2 + n_3 + \cdots + n_{\alpha-1}$

Commutation rules: $\{c_\alpha, c_\beta^\dagger\} = \delta_{\alpha,\beta}$, $\{c_\alpha, c_\beta\} = \{c_\alpha^\dagger, c_\beta^\dagger\} = 0$
Consider an N-body system in a state $|\Psi_{t_0}\rangle$ at time $t=t_0$. The time evolution operator is

$$U \equiv U(t,t_0) = e^{-iH(t-t_0)/\hbar}$$

### Schrödinger pict.

**Time evolution equation:**

$$i\hbar \frac{d}{dt} |\Psi^S(t)\rangle = H |\Psi^S(t)\rangle$$

**Solutions:**

$$|\Psi^S(t)\rangle = U|\Psi_{t_0}\rangle$$

$O^S$ does not evolve

### Heisenberg pict.

**Time-indep. $O^S$:**

$$i\hbar \frac{d}{dt} O^H(t) = [O^H(t), H]$$

for a time-indep. $O^S$.

**Solutions:**

$$|\Psi^H\rangle = U^\dagger |\Psi^S(t)\rangle = |\Psi_{t_0}\rangle$$

$$O^H(t) = U^\dagger O^S U$$

$$[A^H(t), B^H(t)]_\mp = U^\dagger [A^S, B^S]_\mp U$$

same time!
Many-Body Green's Functions

Propagating a free particle

Consider a free particle with Hamiltonian

\[ h_1 = t + U(r) \]

the eigenstates and eigenenergies are

\[ h_1 \left| \phi_n \right> = \varepsilon_n \left| \phi_n \right> \]

The time evolution is

\[ i\hbar \frac{d}{dt} \left| \psi(t) \right> = h_1 \left| \psi(t) \right> \quad \Rightarrow \quad \left| \psi(t) \right> = e^{-i h_1 t / \hbar} \left| \psi_{tr} \right> \]

\[ \left< r \left| \psi(t) \right> \right> = \left< r \left| e^{-i h_1 t / \hbar} \left| \psi_{tr} \right> \right> \]

\[ = \int dr' \left< r \left| e^{-i h_1 t / \hbar} \left| r' \right> \right> \left< r' \left| \psi_{tr} \right> \right> \]

with:

\[ \left< r \left| \psi_{tr} \right> \right> \text{ wave fnct. at } t=0 \]

\[ \left< r \left| \psi(t) \right> \right> \text{ wave fnct. at time } t \]
Green's function (=propagator) for a free particle:

\[ G(r, r'; t) \equiv \langle r | e^{-i \frac{\hbar}{\hbar} t} | r' \rangle \]

\[ \langle r | \psi(t) \rangle = \int dr' G(r, r'; t) \psi_{tr}(r') \]
Green's function (=propagator) for a free particle:

\[ G(r, r'; t) \equiv \langle r | e^{-iH_1 t/\hbar} | r' \rangle \]

\[ = \sum_n \langle r | \phi_n \rangle e^{-i\varepsilon_n t/\hbar} \langle \phi_n | r' \rangle \]

Fourier transform of the eigenspectrum!

\[ \langle r | \phi_n \rangle \rightarrow \text{states} \]

\[ \varepsilon_n \rightarrow \text{energies} \]

The spectrum of the Hamiltonian is separated by the FT because the time evolution is driven by \( H \):

\[ e^{-iH(t-t_0)/\hbar} \]
Definitions of Green’s functions

Take a generic the Hamiltonian $H$ and its static Schrödinger equation

$$H = H_0 + V$$

$$H \left| \Psi_N^N \right> = E_N^N \left| \Psi_N^N \right>$$

We evolve in time the field operators instead of the wave function by using the Heisenberg picture

$$\psi_s^\dagger(r, t) = e^{iHt/\hbar} \psi_s^\dagger(r) e^{-iHt/\hbar}$$

$$\psi_s(r, t) = e^{iHt/\hbar} \psi_s(r) e^{-iHt/\hbar}$$

(creation/annihilation of a particle in $\vec{r}$ at time $t$)
Definitions of Green’s functions

The one body propagator (≡ Green’s function) associated to the ground state \(|\Psi_0^N\rangle\) is defined as

\[
g_{ss'}(r, t; r', t') = -\frac{i}{\hbar} \langle \Psi_0^N | T[\psi_s(r, t)\psi_{s'}^\dagger(r', t')] | \Psi_0^N \rangle
\]

with the time ordering operator

\[
T[\psi_s(r, t)\psi_{s'}^\dagger(r', t')] = \begin{cases} 
\psi_s(r, t)\psi_{s'}^\dagger(r', t') , & t > t' \text{ adds a particle} \\
\pm\psi_{s'}^\dagger(r', t')\psi_s(r, t) , & t' > t \text{ removes a particle}
\end{cases}
\]

(+ for bosons, 
- for fermions)

Expand t-dep in operators: \(\psi_s(r, t) = e^{iHt/\hbar} \psi_s(r) e^{-iHt/\hbar}\)
Definitions of Green's functions

With explicit time dependence:

\[ g_{ss'}(r, r'; t - t') = -\frac{i}{\hbar} \theta(t - t') \langle \Psi_0^N | \psi_s(r) e^{-i(H-E_0^N)(t-t')/\hbar} \psi_{s'}^\dagger(r') | \Psi_0^N \rangle \]

\[ + \frac{i}{\hbar} \theta(t' - t) \langle \Psi_0^N | \psi_{s'}^\dagger(r') e^{i(H-E_0^N)(t-t')/\hbar} \psi_s(r) | \Psi_0^N \rangle . \]

- \( t > t' \) adds a particle
- \( t' > t \) removes a particle
Definitions of Green's functions

Green's function can be defined in any single-particle basis (not just \( r \) or \( k \) space). So let's call \( \{\alpha\} \) a general orthonormal basis with wave functions \( \{u_\alpha(r)\} \)

\[
\psi^\dagger(r) = \sum_\alpha c_\alpha^\dagger u_\alpha^*(r)
\]

The Heisenberg operators are:

\[
c_\alpha^\dagger(t) = e^{iHt/\hbar} c_\alpha^\dagger e^{-iHt/\hbar}
\]

\[
c_\alpha(t) = e^{iHt/\hbar} c_\alpha e^{-iHt/\hbar}
\]

and

\[
g_{ss'}(r, t; r', t') = \sum_{\alpha\beta} u_\alpha(r, s) g_{\alpha\beta}(t, t') u_\beta^*(r', s')
\]
Definitions of Green's functions

In general it is possible to define propagators for more particles and different times:

\[ g^{2-\text{pt}}_{\alpha\beta}(t, t') = -\frac{i}{\hbar} \langle \Psi_0^N | T [c_\alpha(t)c_\beta^\dagger(t')] | \Psi_0^N \rangle \]

\[ g^{4-\text{pt}}_{\alpha\beta,\gamma\delta}(t_1, t_2; t'_1, t'_2) = -\frac{i}{\hbar} \langle \Psi_0^N | T [c_\beta(t_2)c_\alpha(t_1)c_\gamma^\dagger(t'_1)c_\delta^\dagger(t'_2)] | \Psi_0^N \rangle \]

\[ g^{6-\text{pt}}_{\alpha\beta\gamma,\mu\nu\lambda}(t_1, t_2, t_3; t'_1, t'_2, t'_3) = \]

\[ -\frac{i}{\hbar} \langle \Psi_0^N | T [c_\gamma(t_3)c_\beta(t_2)c_\alpha(t_1)c_\mu^\dagger(t'_1)c_\nu^\dagger(t'_2)c_\lambda^\dagger(t'_3)] | \Psi_0^N \rangle \]

\[ \vdots \]
Definitions of Green's functions

**Graphic conventions:**

$$g_{\alpha\beta}(t>t')$$  
(quasi)particle

$$g_{\alpha\beta}(t'>t)$$  
(quasi)hole

$$g^{4-\text{pt}}_{\alpha\beta,\gamma\delta}(t_1, t_2; t'_1, t'_2) = -\frac{i}{\hbar}\langle\Psi_0^N | T[c_\beta(t_2)c_\alpha(t_1)c_\gamma^\dagger(t'_1)c_\delta^\dagger(t'_2)] | \Psi_0^N \rangle$$

Many-Body Green's Functions
Definitions of Green's functions

Graphic conventions:

\[ g_{\alpha\beta}(t > t') \]
\( \text{(quasi)particle} \)

\[ g_{\alpha\beta}(t' > t) \]
\( \text{(quasi)hole} \)

\[ g_{4\text{-pt}}^{\alpha\beta,\gamma\delta}(t_1, t_2; t'_1, t'_2) = \]
\[ -\frac{i}{\hbar} \langle \Psi^N_0 | T[c_{\beta}(t_2)c_{\alpha}(t_1)c_{\gamma}^\dagger(t'_1)c_{\delta}^\dagger(t'_2)] | \Psi^N_0 \rangle \]
Definitions of Green's functions

With explicit time dependence:

\[
g_{ss'}(\mathbf{r}, \mathbf{r}'; t - t') = -\frac{i}{\hbar} \theta(t - t') \langle \Psi_0^N | \psi_s(\mathbf{r}) e^{-i(H - E_0^N)(t - t')/\hbar} \psi_{s'}(\mathbf{r}') | \Psi_0^N \rangle + \frac{i}{\hbar} \theta(t' - t) \langle \Psi_0^N | \psi_{s'}(\mathbf{r}') e^{i(H - E_0^N)(t - t')/\hbar} \psi_s(\mathbf{r}) | \Psi_0^N \rangle.
\]
Expand on the eigenstates of $N \pm 1$

$$g_{\alpha\beta}(t - t') = -\frac{i}{\hbar} \theta(t - t') \langle \Psi_0^N | c_{\alpha} e^{-i(H - E_0^N)(t - t')/\hbar} c_{\beta}^\dagger | \Psi_0^N \rangle$$

$$\mp \frac{i}{\hbar} \theta(t' - t) \langle \Psi_0^N | c_{\beta}^\dagger e^{i(H - E_0^N)(t - t')/\hbar} c_{\alpha} | \Psi_0^N \rangle$$

$$= -\frac{i}{\hbar} \theta(t - t') \sum_n \langle \Psi_0^N | c_{\alpha} | \Psi_n^{N+1} \rangle \langle \Psi_n^{N+1} | c_{\beta}^\dagger | \Psi_0^N \rangle e^{-i(E_0^{N+1} - E_0^N)(t - t')/\hbar}$$

$$\mp \frac{i}{\hbar} \theta(t' - t) \sum_k \langle \Psi_0^N | c_{\beta}^\dagger | \Psi_k^{N-1} \rangle \langle \Psi_k^{N-1} | c_{\alpha} | \Psi_0^N \rangle e^{i(E_0^{N-1} - E_0^N)(t - t')/\hbar}$$

$\rightarrow$ Fourier transform to energy representation...

$$g_{\alpha\beta}(\omega) = \int d\tau e^{i\omega\tau} g_{\alpha\beta}(\tau)$$

$$\theta(\pm \tau) = \mp \lim_{\eta \to 0^+} \frac{1}{2\pi i} \int_{-\infty}^{+\infty} d\omega \frac{e^{-i\omega\tau}}{\omega \pm i\eta}$$
The Lehman representation of $g_{\alpha\beta}(\omega)$ is:

$$
g_{\alpha\beta}(\omega) = \sum_n \frac{\langle \Psi_0^N | c_\alpha | \Psi_{n}^{N+1} \rangle \langle \Psi_{n}^{N+1} | c_\beta^\dagger | \Psi_0^N \rangle}{\hbar \omega - (E_{n}^{N+1} - E_{0}^N) + i\eta} + \sum_k \frac{\langle \Psi_0^N | c_\beta^\dagger | \Psi_{k}^{N-1} \rangle \langle \Psi_{k}^{N-1} | c_\alpha | \Psi_0^N \rangle}{\hbar \omega - (E_{0}^N - E_{k}^{N-1}) - i\eta}
$$

Poles $\rightarrow$ energy absorbed/released in particle transfer

Residues:

$$\left| \langle \Psi_{n}^{N+1} | c_\alpha^\dagger | \Psi_0^N \rangle \right|^2 \quad \text{particle addition}$$

$$\left| \langle \Psi_{k}^{N-1} | c_\alpha | \Psi_0^N \rangle \right|^2 \quad \text{particle ejected}$$
The Lehman representation of $g_{\alpha\beta}(\omega)$ is:

$$
g_{\alpha\beta}(\omega) = \sum_n \frac{\langle \Psi_0^N | c_\alpha | \Psi_{n}^{N+1} \rangle \langle \Psi_{n}^{N+1} | c_\beta^\dagger | \Psi_0^N \rangle}{\hbar \omega - (E_n^{N+1} - E_0^N) + i\eta} \\
\mp \sum_k \frac{\langle \Psi_0^N | c_\beta^\dagger | \Psi_{k}^{N-1} \rangle \langle \Psi_{k}^{N-1} | c_\alpha | \Psi_0^N \rangle}{\hbar \omega - (E_0^N - E_k^{N-1}) - i\eta} \leftarrow (\text{quasi})\text{particles}
\leftarrow (\text{quasi})\text{holes}
$$

(- bosons, + fermions)

To extract the imaginary part:

$$
\frac{1}{x \pm i\eta} = \mathcal{P} \frac{1}{x} \mp i\pi \delta(x)
$$
The spectral function is the Im part of $g_{\alpha\beta}(\omega)$

$$S_{\alpha\beta}(\omega) = S_{\alpha\beta}^p(\omega) + S_{\alpha\beta}^h(\omega)$$

$$S_{\alpha\beta}^p(\omega) = -\frac{1}{\pi} \text{Im} \ g_{\alpha\beta}^p(\omega) \quad \leftrightarrow \text{(quasi)particles}$$

$$= \sum_n \langle \Psi_0^N | c_\alpha | \Psi_{n}^{N+1} \rangle \langle \Psi_{n}^{N+1} | c_\beta^\dagger | \Psi_0^N \rangle \ \delta \left( \hbar \omega - (E_{n}^{N+1} - E_0^N) \right)$$

$$S_{\alpha\beta}^h(\omega) = \frac{1}{\pi} \text{Im} \ g_{\alpha\beta}^h(\omega) \quad \leftrightarrow \text{(quasi)holes}$$

$$= \sum_k \langle \Psi_0^N | c_\beta^\dagger | \Psi_{k}^{N-1} \rangle \langle \Psi_{k}^{N-1} | c_\alpha | \Psi_0^N \rangle \ \delta \left( \hbar \omega - (E_0^N - E_k^{N-1}) \right)$$

\(-\) bosons, \(+\) fermions

\(\rightarrow\) Contains the same information as the Lehmann rep.
Lehmann representation and spectral function

$g_{\alpha \beta}(\omega)$ is fully constrained by its imaginary part:

$$g_{\alpha \beta}(\omega) = \int d\omega' \frac{S^p_{\alpha \beta}(\omega')}{\omega - \omega' + i\eta} + \int d\omega' \frac{S^h_{\alpha \beta}(\omega')}{\omega - \omega' - i\eta}$$