Inspiration ...

Green's functions I 1
Comprehensive treatment of correlations at different energy scales in nuclei using Green’s functions

Lecture 1: 8/28/07  Propagator description of single-particle motion and the link with experimental data
Lecture 2: 8/29/07  From Hartree-Fock to spectroscopic factors < 1: inclusion of long-range correlations
Lecture 3: 8/29/07  Role of short-range and tensor correlations associated with realistic interactions
Lecture 4: 8/30/07  Dispersive optical model and predictions for nuclei towards the dripline

Adv. Lecture 1: 8/30/07  Saturation problem of nuclear matter & pairing in nuclear and neutron matter
Adv. Lecture 2: 8/31/07  Quasi-particle density functional theory

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Some questions ...

What does a nucleon do in the nucleus?
Is this a legitimate question?
Speculations ...
What is the dependence on $N$ and $Z$?

Energy scales:  As high as a realistic $V_{NN}$ will take you
...  $\Delta$-isobars, pions
...  As low as the first excited state

⇒ ALL OF THEM!  HOW?
⇒ Time-dependent formulation not surprising
Description of the nuclear many-body problem

Ingredients: Nucleons interacting by “realistic interactions"
Nonrelativistic many-body problem

Method: Green’s functions (Propagators)
⇒ amplitudes instead of wave functions
keep track of all nucleons, including the high-momentum ones

Book: Dimitri Van Neck & W.D.

Why: Physical insight and useful for all many-body systems
Link between experiment and theory clear
Can include all energy scales
Efficient: generates amplitudes not wave functions

Lecture notes: http://www.nscl.msu.edu/~brown/theory-group/lecture-notes.html
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Physics of this picture requires different approach
Outline

• What is a propagator
• Propagator in the many-body problem
• Information contained in propagator
• Spectral functions
• Relation with experimental data
• Experimental results
• Outline of perturbation theory
What is a propagator or Green's function?

Time evolution is governed by the Hamiltonian $H$. For a single particle the state

$$|\alpha, t_0; t \rangle = e^{-\frac{i}{\hbar}H(t-t_0)} |\alpha, t_0 \rangle$$

is indeed a solution of

$$i\hbar \frac{\partial}{\partial t} |\alpha, t_0; t \rangle = H |\alpha, t_0; t \rangle$$

Relation between wave function at $t$ and $t_0$ can then be written as

$$\psi(\vec{r}, t) = \langle \vec{r} | \alpha, t_0; t \rangle = \langle \vec{r} | e^{-\frac{i}{\hbar}H(t-t_0)} |\alpha, t_0 \rangle = \int d\vec{r}' \langle \vec{r} | e^{-\frac{i}{\hbar}H(t-t_0)} |\vec{r}' \rangle \langle \vec{r}' | \alpha, t_0 \rangle$$

$$= i\hbar \int d\vec{r}' G(\vec{r}, \vec{r}'; t-t_0) \psi(\vec{r}', t_0)$$

with the propagator or Green's function defined by

$$G(\vec{r}, \vec{r}'; t-t_0) = -\frac{i}{\hbar} \langle \vec{r} | e^{-\frac{i}{\hbar}H(t-t_0)} |\vec{r}' \rangle$$

Recall Huygens' principle!
Alternative expressions

Using \( \theta(t-t_0) = -\int \frac{dE}{2\pi i} \frac{e^{-\frac{i}{\hbar}E(t-t_0)}}{E+i\eta} \) (Note \( \frac{d}{dt} \theta(t-t_0) = \delta(t-t_0) \))

the Fourier transform of the propagator can be written as

\[
G(\vec{r},\vec{r}';E) = \int_{-\infty}^{\infty} d(t-t_0) e^{\frac{i}{\hbar}E(t-t_0)} G(\vec{r},\vec{r}';t-t_0) \theta(t-t_0)
\]

\[
= \sum_n \frac{\langle 0|a_{\vec{r}}|n\rangle \langle n|a_{\vec{r}}^+|0\rangle}{E-\varepsilon_n+i\eta} \]

\[
= \langle 0|a_{\vec{r}} \frac{1}{E-H+i\eta} a_{\vec{r}}^+|0\rangle \quad \text{with} \quad H|n\rangle = \varepsilon_n |n\rangle
\]

Also \( \langle 0|a_{\vec{r}}|n\rangle = \langle \vec{r}|n\rangle = u_n(\vec{r}) \)

So numerator yields information on wave functions and denominator on eigenvalues of \( H \).
How is $G$ calculated?

“Simple” for the case of one particle. Can proceed by splitting

$$H = H_0 + V$$

and using the operator identity

$$\frac{1}{A-B} = \frac{1}{A} + \frac{1}{A} \frac{1}{A-B}$$

for the operator

$$G = \frac{1}{E - H + i\eta}$$

with

$$A = E - H_0 + i\eta$$

and

$$B = V$$

to obtain $G$ in terms of $G^{(0)}$ and $V$:

$$G = G^{(0)} + G^{(0)}VG$$

$$= G^{(0)} + G^{(0)}VG^{(0)} + G^{(0)}VG^{(0)}VG^{(0)} + \cdots$$

or in a particular basis

$$G(\alpha, \beta; E) = G^{(0)}(\alpha, \beta; E) + \sum \gamma \delta G^{(0)}(\alpha, \gamma; E) \langle \gamma | V | \delta \rangle G(\delta, \beta; E)$$

with

$$G(\alpha, \beta; E) = \langle \alpha | \frac{1}{E - H + i\eta} | \beta \rangle$$

and

$$G^{(0)}(\alpha, \beta; E) = \langle \alpha | \frac{1}{E - H_0 + i\eta} | \beta \rangle$$
Diagrams

Lowest order

First order

All orders summed by

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Single-particle propagator in the medium

Definition

\[
G(\alpha, \beta; t - t') = -\frac{i}{\hbar} \langle \Psi_0^N | T [ a_{\alpha_{H}}(t) a_{\beta_{H}}^+(t') ] | \Psi_0^N \rangle 
\]

with

\[
\hat{H} | \Psi_0^N \rangle = E_0^N | \Psi_0^N \rangle
\]

for the exact ground state

and

\[
a_{\alpha_{H}}(t) = e^{\frac{i}{\hbar} \hat{H}_t} a_{\alpha} e^{-\frac{i}{\hbar} \hat{H}_t}
\]

(Heisenberg picture)

while \( T \) orders the operators with larger time on the left including a sign change

\[
G(\alpha, \beta; t - t') = -\frac{i}{\hbar} \left\{ \theta(t-t') e^{\frac{i}{\hbar} E_0^N (t-t')} \left\langle \Psi_0^N | a_{\alpha} e^{-\frac{i}{\hbar} \hat{H}_t} a_{\beta}^+ | \Psi_0^N \right\rangle 
- \theta(t'-t) e^{\frac{i}{\hbar} E_0^N (t'-t)} \left\langle \Psi_0^N | a_{\beta} e^{-\frac{i}{\hbar} \hat{H}_t} a_{\alpha}^+ | \Psi_0^N \right\rangle \right\}
\]

particle

hole

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Fourier transform of $G$ (Lehmann representation)

$$G(\alpha, \beta; E) = \sum_m \frac{\langle \Psi_0^N | a_\alpha | \Psi_m^{N+1} \rangle \langle \Psi_m^{N+1} | a_\beta^+ | \Psi_0^N \rangle}{E - (E_m^{N+1} - E_0^N) + i\eta}$$

$$+ \sum_n \frac{\langle \Psi_0^N | a_{\beta}^+ | \Psi_n^{N-1} \rangle \langle \Psi_n^{N-1} | a_\alpha | \Psi_0^N \rangle}{E - (E_0^N - E_n^{N-1}) - i\eta}$$

$\Leftarrow$ Particle part

$\Leftarrow$ Hole part

Numerator contains information about “wave functions”

$$\langle \Psi_{n}^{N-1} | a_\alpha | \Psi_0^N \rangle \quad \text{and} \quad \langle \Psi_{m}^{N+1} | a_\beta^+ | \Psi_0^N \rangle$$

while denominator identifies eigenvalues of $H$ for the $N \pm 1$ states

Note

$$\hat{H} \left| \Psi_n^{N \pm 1} \right\rangle = E_n^{N \pm 1} \left| \Psi_n^{N \pm 1} \right\rangle$$

has been used for exact $N \pm 1$ states of $H$
Spectral functions

Probability density for the removal of a particle with quantum numbers represented by $\alpha$ from the ground state, while leaving the remaining system at an energy $E_{n}^{N-1} = E_{0}^{N} - E$

$$S_h(\alpha; E) = \sum_{n} \left| \left\langle \Psi_{n}^{N-1} | a_{\alpha} | \Psi_{0}^{N} \right\rangle \right|^2 \delta(E - (E_{0}^{N} - E_{n}^{N-1}))$$

for energies $E \leq \varepsilon_{F} = E_{0}^{N} - E_{0}^{N-1}$

Relation of “hole” spectral function to propagator

$$S_h(\alpha; E) = \frac{1}{\pi} \text{Im} \ G(\alpha,\alpha; E)$$

based on $\frac{1}{x \pm i\eta} = P \frac{1}{x} \mp i \pi \delta(x)$

Occupation number:

$$n(\alpha) = \int_{-\infty}^{\varepsilon_{F}} S_h(\alpha; E) \, dE = \left\langle \Psi_{0}^{N} | a_{\alpha}^\dagger a_{\alpha} | \Psi_{0}^{N} \right\rangle$$
Relation with experimental data

Direct knockout reaction:
Transfer a large amount of momentum and energy to a bound $N$-particle system leaving an ejected fast particle and a bound $N-1$ system. By observing the momentum of the ejected particle one can reconstruct the hole spectral function.

Initial state $|\Psi_i\rangle = |\Psi_0^N\rangle$  
Final state $|\Psi_f\rangle = a_\vec{p}^+ |\Psi_{n}^{N-1}\rangle$

External probe transfers momentum

$\hat{\rho}(\vec{q}) = \sum_{\vec{p}} a_{\vec{p}}^+ a_{\vec{p} - \vec{q}}$

Transition matrix element

$\langle \Psi_f | \hat{\rho}(\vec{q}) | \Psi_i \rangle \approx \langle \Psi_{n}^{N-1} | a_{\vec{p} - \vec{q}} | \Psi_0^N \rangle$

(Plane Wave) Impulse Approximation $\Rightarrow$ ejected particle absorbs $\vec{q}$

Cross section from Fermi’s Golden Rule

$d\sigma \propto \sum |\langle \Psi_f | \hat{\rho}(\vec{q}) | \Psi_i \rangle|^2 \delta(E + E_i - E_f) = S_h (\vec{p}_{miss};E_{miss})$

with $\vec{p}_{miss} = \vec{p} - \vec{q}$ and $E_{miss} = \frac{\vec{p}^2}{2m} - E = E_0^N - E_{n}^{N-1}$
Basic idea of (e,2e) or (e,e',p)

\[ d\sigma_L \propto \left| \langle \Psi_f | \hat{\rho}_c (\vec{q}) | \Psi_i \rangle \right|^2 \delta(E - E_i - E_f) \]

Simplest case:  \[ \langle \vec{p}, \Psi^{N-1}_n | \hat{\rho}_c (\vec{q}) | \Psi^N_0 \rangle \Rightarrow \langle \Psi^{N-1}_n | a^{+}_{\vec{p}-\vec{q}} | \Psi^N_0 \rangle \]

\Rightarrow d\sigma_L \propto \sum_n \langle \Psi^N_0 | a^{+}_{\vec{p}-\vec{q}} | \Psi^{N-1}_n \rangle \langle \Psi^{N-1}_n | a_{\vec{p}-\vec{q}} | \Psi^N_0 \rangle \delta(E_{\text{miss}} - (E^N_0 - E^{N-1}_n))

Realistic case: distorted waves / more realistic description of knocked out particle

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Atoms studied with the (e,2e) reaction

\[ \phi_{1s}(p) = 2^{3/2} \pi \frac{1}{(1 + p^2)^2} \]


And so on for other atoms ...

Spectroscopic factors in atoms

For a bound final $N-1$ state the spectroscopic factor is given by

$$S = \int dp \left| \langle \Psi_{n}^{N-1} | a_{p} | \Psi_{0}^{N} \rangle \right|^{2}$$

For H and He the 1s electron spectroscopic factor is 1
For Ne the valence 2p electron has $S=0.92$ with two additional fragments, each carrying 0.04, at higher energy.

**Argon**

3p and 3s strength

**Closed-shell atoms**

$n(\alpha) = 0$ or 1

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(e,e' p) cross sections for closed-shell nuclei
Removal probability for valence protons from NIKHEF data

Note:
We have seen mostly data for removal of valence protons
and ...

Quasi-hole strength or spectroscopic factor $Z(2s_{1/2}) = 0.65$
$n(2s_{1/2}) = 0.75$
from elastic electron scattering

Strong fragmentation of deeply-bound states

E. Quint, Ph.D. thesis NIKHEF, 1988
Many-body perturbation theory for $G$

- Identify solvable problem by considering
  $$\hat{H}_0 = \hat{T} + \hat{U}$$
  where $U$ is a suitable auxiliary potential.
- Develop expansion in
  $$\hat{H}_1 = \hat{V} - \hat{U}$$
- Employs time-evolution, Heisenberg, Schrödinger, and interaction picture of quantum mechanics.
- Once established, this expansion (expressed in Feynman diagrams) is organized in such a way that nonperturbative results can be obtained leading to the Dyson equation. The Dyson equation describes sp motion in the medium under the influence of the self-energy which is an energy-dependent complex sp potential.
- Further insight into the proper description of sp motion in the medium is obtained by studying the relation between sp and two-particle propagation. This allows the selection of appropriate choices of the relevant ingredients for the system under study.
How to calculate $G$?

Rearrange Hamiltonian

$$\hat{H} = \hat{T} + \hat{V} = (\hat{T} + \hat{U}) + (\hat{V} - \hat{U}) = \hat{H}_0 + \hat{H}_1$$

Many-body problem with $H_0$ can be exactly solved when $U$ is a one-body potential like a Woods-Saxon or HO potential. Corresponding sp propagator (replace $H$ by $H_0$)

$$G^{(0)}(\alpha, \beta; E) = \sum_m \frac{\langle \Phi^N_0 | a_\alpha | \Phi^{N+1}_m \rangle \langle \Phi^{N+1}_m | a_\beta | \Phi^N_0 \rangle}{E - \left( E_{m+1}^A - E_{\Phi^N_0} \right) + i\eta} + \sum_n \frac{\langle \Phi^N_0 | a_\beta | \Phi^{N-1}_n \rangle \langle \Phi^{N-1}_n | a_\alpha | \Phi^N_0 \rangle}{E - \left( E_{\Phi^N_0} - E_{n+1}^A \right) - i\eta}
$$

$$= \delta_{\alpha, \beta} \left[ \frac{\theta(\alpha - F)}{E - \varepsilon_{\alpha} + i\eta} + \frac{\theta(F - \alpha)}{E - \varepsilon_{\alpha} - i\eta} \right]$$

using the sp basis associated with $H_0$. Note that

$$\hat{H}_0 a_\alpha | \Phi^N_0 \rangle = (E_{\Phi^N_0} + \varepsilon_{\alpha}) a_\alpha | \Phi^N_0 \rangle$$

$$\hat{H}_0 a_\alpha | \Phi^N_0 \rangle = (E_{\Phi^N_0} - \varepsilon_{\alpha}) a_\alpha | \Phi^N_0 \rangle$$

So that e.g.

$$S_h^{(0)}(\alpha; E) = \frac{1}{\pi \Im G^{(0)}(\alpha, \alpha; E) = \delta(E - \varepsilon_{\alpha}) \theta(F - \alpha)$$

$$\sim \text{like in atoms}$$

and

$$n^{(0)}(\alpha) = \int dE \delta(E - \varepsilon_{\alpha}) \theta(F - \alpha) = \theta(F - \alpha)$$

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Perturbation expansion using $G^{(0)}$ and $H_1$

Use "interaction picture"  \[
\hat{H}_1(t) = e^{\frac{i}{\hbar} \hat{H}_0 t} \hat{H}_1 e^{-\frac{i}{\hbar} \hat{H}_0 t}
\]

then ……

\[
G(\alpha, \beta; t-t') = -\frac{i}{\hbar} \sum \left( \frac{-i}{\hbar} \right)^m \frac{1}{m!} \int dt_1 \cdots \int dt_m \langle \Phi_0^N | T[\hat{H}_1(t_1) \cdots \hat{H}_1(t_m) a_\alpha(t) a_\beta^+(t')] \rangle_{\text{connected}} \]

Can be calculated order by order using diagrams and Wick's theorem. Yields expressions involving $G^{(0)}$ and matrix elements of the two-body interaction $V$ (and the auxiliary potential $U$)

Simple diagram rules in time formulation.

For practical calculations use energy formulation. Diagrams
Diagram rules in energy formulation

**Rule 1** Draw all topologically distinct (direct) and connected diagrams with $m$ horizontal interaction lines for $V$ (dashed) and $2m + 1$ directed (using arrows) Green’s functions $G^{(0)}$.

**Rule 2** Label external points only with sp quantum numbers, e.g. $\alpha$ and $\beta$.

Label each interaction with sp quantum numbers:

\[
\alpha \quad \beta \\
\gamma \quad \delta
\]

\[\Rightarrow \langle \alpha \beta | V | \gamma \delta \rangle = (\alpha \beta | V | \gamma \delta) - (\alpha \beta | V | \delta \gamma)\]

For each arrow line one writes:

\[
\mu \quad \nu
\]

\[\Rightarrow G^{(0)}(\mu, \nu; E)\]

but in such a way that energy is conserved for each $V$.

**Rule 3** Sum (integrate) over all internal sp quantum numbers and integrate over all $m$ internal energies.

For each closed loop an independent energy integration occurs over the contour $C$.

**Rule 4** Include a factor $(i/2\pi)^m$ and $(-1)^F$ where $F$ is the number of closed fermion loops.

**Rule 5** Include a factor of $\frac{1}{2}$ for each equivalent pair of lines.
Examples of diagrams

\[ \sum_{\gamma \delta} G^{(0)}(\alpha, \gamma; E) \]
\[ \times \quad -i \int_{C} \frac{dE'}{2\pi} G^{(0)}(\theta, \epsilon; E') \]
\[ \times \quad G^{(0)}(\delta, \beta; E) \]

\[ \sum_{\gamma \delta} G^{(0)}(\alpha, \gamma; E) \]
\[ \times \quad (-1)^2 i^2 \int_{C} \frac{dE''}{2\pi} \langle \gamma \lambda \mid V \mid \epsilon \theta \rangle G^{(0)}(\theta, \lambda; E') \]
\[ \times \quad G^{(0)}(\epsilon, \zeta; E) \sum_{\xi \mu} \int_{C} \frac{dE'}{2\pi} \langle \zeta \xi \mid V \mid \delta \mu \rangle G^{(0)}(\mu, \xi; E'') \]
\[ \times \quad G^{(0)}(\delta, \beta; E) \]
More diagrams

\[ \Rightarrow \sum_{\gamma \delta} G^{(0)}(\alpha, \gamma; E) \times i^2 \sum_{\epsilon \theta} \sum_{\lambda \zeta} \int_{C^\uparrow} \frac{dE'}{2\pi} \times \langle \gamma \epsilon | V | \delta \theta \rangle G^{(0)}(\lambda, \epsilon; E') G^{(0)}(\theta, \zeta; E') \times \sum_{\mu \xi} \int_{C^\uparrow} \frac{dE''}{2\pi} \langle \zeta \xi | V | \lambda \mu \rangle G^{(0)}(\mu, \xi; E'') \times G^{(0)}(\delta, \beta; E) \]

\[ \Rightarrow \sum_{\gamma \delta} G^{(0)}(\alpha, \gamma; E) \times (-1)^{i^2} \frac{1}{2} \int \frac{dE_1}{2\pi} \int \frac{dE_2}{2\pi} \sum_{\lambda, \epsilon, \theta} \sum_{\zeta, \xi, \mu} \langle \gamma \lambda | V | \epsilon \theta \rangle \times G^{(0)}(\epsilon, \zeta; E_1) G^{(0)}(\mu, \lambda; E_1 + E_2 - E) \times G^{(0)}(\theta, \xi; E_2) \langle \zeta \xi | V | \delta \mu \rangle \times G^{(0)}(\delta, \beta; E) \]
Diagram organization

Sum of all diagrams can be written as

\[ G = G^{(0)} + \Sigma G^{(0)} \]
Introducing some self-energy diagrams

First order

\[
\begin{align*}
\gamma & \quad \bullet \quad \epsilon \quad \delta \quad \theta & \quad \Rightarrow & \quad -i \sum_{\epsilon \theta} \langle \gamma \epsilon | V | \delta \theta \rangle \int_{C} \frac{dE'}{2\pi} G^{(0)}(\theta, \epsilon; E') \\
E' & \quad \Rightarrow & \quad \Rightarrow & \quad (-1)i^{2} \frac{1}{2} \int \frac{dE_{1}}{2\pi} \int \frac{dE_{2}}{2\pi} \sum_{\lambda, \epsilon, \theta} \sum_{\zeta, \xi, \mu} \langle \gamma \lambda | V | \epsilon \theta \rangle \\
E_{1} & \quad \Rightarrow & \quad \Rightarrow & \quad \times G^{(0)}(\epsilon, \zeta; E_{1}) G^{(0)}(\mu, \lambda; E_{1} + E_{2} - E) \\
E_{2} & \quad \Rightarrow & \quad \Rightarrow & \quad \times G^{(0)}(\theta, \xi; E_{2}) \langle \zeta \xi | V | \delta \mu \rangle
\end{align*}
\]

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The irreducible self-energy

The following self-energy diagram is reducible (previous two were irreducible), i.e. can be obtained from lower order self-energy terms by iterating with $G^{(0)}$

\[
\begin{align*}
\gamma & \rightarrow \lambda \\
\epsilon & \rightarrow \theta \\
\Rightarrow & \quad (-1)^2 i^2 \sum_{\epsilon, \zeta} \sum_{\lambda, \theta} \int_{C^\uparrow} \frac{dE'}{2\pi} \langle \gamma \lambda | V | \epsilon \theta \rangle G^{(0)}(\theta, \lambda; E') \\
& \quad \times G^{(0)}(\epsilon, \zeta; E) \sum_{\xi, \mu} \int_{C^\uparrow} \frac{dE''}{2\pi} \langle \zeta \xi | V | \delta \mu \rangle G^{(0)}(\mu, \xi; E'')
\end{align*}
\]

Sum of all irreducible diagrams is denoted by $\Sigma^*$. All diagrams can then be obtained by summing

\[
G(\alpha, \beta; E) = G^{(0)}(\alpha, \beta; E) + \sum_{\gamma, \delta} G^{(0)}(\alpha, \gamma; E) \Sigma^* (\gamma, \delta; E) G^{(0)}(\delta, \beta; E) + \cdots
\]

Diagrammatically ...
Towards the Dyson equation

Can be summed by

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Dyson equation

Looks like the propagator equation for a single particle

\[ G(\alpha,\beta;E) = G^{(0)}(\alpha,\beta;E) + \sum_{\gamma,\delta} G^{(0)}(\alpha,\gamma,E)\Sigma^*(\gamma,\delta,E)G(\delta,\beta;E) \]

with the irreducible self-energy acting as the in-medium (complex) potential.
Homework

Recover the time-independent Schrödinger equation for bound states from

\[ G(\alpha, \beta; E) = G^{(0)}(\alpha, \beta; E) + \sum_{\gamma \delta} G^{(0)}(\alpha, \gamma; E) \langle \gamma | V | \delta \rangle G(\delta, \beta; E) \]

in momentum space for a particle without spin

\[ G^{(0)}(\alpha, \beta; E) = \langle \alpha | \frac{1}{E - H_0 + i\eta} | \beta \rangle \]

\[ G^{(0)}(\vec{p}, \vec{p}'; E) = \langle \vec{p} | \frac{1}{E - \frac{p_{\text{op}}^2}{2m} + i\eta} | \vec{p}' \rangle = \delta(\vec{p} - \vec{p}') \frac{1}{E - \frac{p^2}{2m} + i\eta} \]

Strategy:

• Introduce complete set of eigenstates of \( H \) in \( G \)

• Calculate \( \lim_{E \to \epsilon \eta} (E - \epsilon \eta) [G = G^{(0)} + G^{(0)}VG] \)

with \( H | n \rangle = \epsilon_n | n \rangle \) and \( \epsilon_n < 0 \)