Introduction to Green functions

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Outline

- Green functions in mathematics
- Many-particle Green functions in equilibrium
  - Zero temperature formalism
    - One-particle Green function
    - Response functions and two-particle Green functions
  - Finite temperature formalism
- Non-equilibrium Green functions
  - Keldysh contour and Kadanoff-Baym equations
- Summary

Green functions in mathematics

consider inhomogeneous differential equation (1D for simplicity)

$$\hat{D}_x y(x) = f(x)$$

where $\hat{D}_x$ is linear differential operator in x.

Example: damped harmonic oscillator $\hat{D}_x = \frac{\mathrm{d}^2}{\mathrm{d}x^2} + \gamma \frac{\mathrm{d}}{\mathrm{d}x} + \omega^2$

general solution of inhomogeneous equation:

$$y(x) = y_{\mathrm{hom}}(x) + y_{\mathrm{spec}}(x)$$

where y_{hom} is solution of the homogeneous eqn. $\hat{D}_x y_{\mathrm{hom}}(x) = 0$
and $y_{\mathrm{spec}}(x)$ is any special solution of the inhomogeneous equation.

Green functions in mathematics (cont.)

how to obtain a special solution of the inhomogeneous equation for *any* inhomogeneity $f(x)$?
first find the solution of the following equation

$$\hat{D}_x G(x, x') = \delta(x - x')$$

This defines the Green function $G(x, x')$ corresponding to the operator $\hat{D}_x$.

Once $G(x, x')$ is found, a special solution can be constructed by

$$y_{\rm spec}(x) = \int \mathrm{d}x' \; G(x, x') f(x')$$

check: $\hat{D}_x \int \mathrm{d}x' \; G(x, x') f(x') = \int \mathrm{d}x' \; \delta(x - x') f(x') = f(x)$

Hamiltonian of interacting electrons

consider system of interacting electrons in static external potential $v_{ext}(\mathbf{r})$ described by Hamiltonian $\hat{H}$

$$\hat{H} = \hat{T} + \hat{V}_{ext} + \hat{W} = \int \mathrm{d}^3x \; \hat{\psi}^\dagger(\mathbf{x}) \left(-\frac{\nabla^2}{2} + v_{ext}(\mathbf{r}) \right) \hat{\psi}(\mathbf{x})$$

$$+ \frac{1}{2} \int \mathrm{d}^3x \int \mathrm{d}^3x' \; \hat{\psi}^\dagger(\mathbf{x}) \hat{\psi}^\dagger(\mathbf{x}') \frac{1}{|\mathbf{r} - \mathbf{r}'|} \hat{\psi}(\mathbf{x}') \hat{\psi}(\mathbf{x})$$

- $\mathbf{x} = (\mathbf{r}, \sigma)$: space-spin coordinate
- $\hat{\psi}^\dagger(\mathbf{x})$, $\hat{\psi}(\mathbf{x})$: electron creation and annihilation operators

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One-particle Green functions at zero temperature

Time-ordered 1-particle Green function at zero temperature

$$iG(\mathbf{x},t;\mathbf{x}',t') = \frac{\langle\Psi_0^N|\hat{T}[\hat{\psi}(\mathbf{x},t)_H\hat{\psi}^\dagger(\mathbf{x}',t')_H]|\Psi_0^N\rangle}{\langle\Psi_0^N|\Psi_0^N\rangle}$$

- $|\Psi_0^N\rangle$: N-particle ground state of $\hat{H}$: $\hat{H}|\Psi_0^N\rangle = E_0^N|\Psi_0^N\rangle$
- $\hat{\psi}(\mathbf{x},t)_H = \exp(i\hat{H}t)\hat{\psi}(\mathbf{x})\exp(-i\hat{H}t)$:
  electron annihilation operator in Heisenberg picture
- $\hat{T}$: time-ordering operator
  $\hat{T}[\hat{\psi}(\mathbf{x},t)_H\hat{\psi}(\mathbf{x}',t')_H^\dagger] =$
  $\theta(t-t')\hat{\psi}(\mathbf{x},t)_H\hat{\psi}(\mathbf{x}',t')_H^\dagger - \theta(t'-t)\hat{\psi}(\mathbf{x}',t')_H^\dagger\hat{\psi}(\mathbf{x},t)_H$

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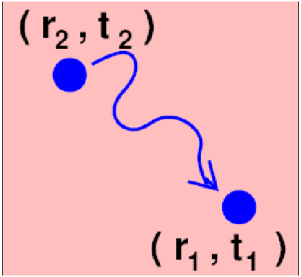
Green functions as propagator

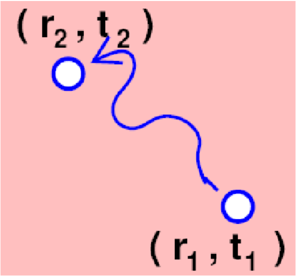
$t_1 < t_2$

create electron at time t_2 at position $\mathbf{r}_2$ and propagate; then annihilate electron at time t_1 at position $\mathbf{r}_1$



$t_2 < t_1$

annihilate electron (create hole) at time t_1 at position $\mathbf{r}_1$; then create electron (annihilate hole) at time t_2 at position $\mathbf{r}_2$



Observables from Green functions

Information which can be extracted from Green functions

- ground-state expectation values of any single-particle operator $\hat{O} = \int d^3x \; \hat{\psi}^\dagger(\mathbf{x}) o(\mathbf{x}) \hat{\psi}(\mathbf{x})$
  e.g., density operator $\hat{n}(\mathbf{r}) = \sum_\sigma \hat{\psi}^\dagger(\mathbf{r}\sigma)\hat{\psi}(\mathbf{r}\sigma)$
- ground-state energy of the system

Galitski-Migdal formula

$$E_0^N = -\frac{i}{2} \int d^3x \lim_{t' \to t^+} \lim_{\mathbf{r}' \to \mathbf{r}} \left(i \frac{\partial}{\partial t} - \frac{\nabla^2}{2} \right) G(\mathbf{r}\sigma, t; \mathbf{r}'\sigma, t')$$

- spectrum of system: direct photoemission, inverse photoemission

Other kind of Green functions

Retarded and advanced Green functions

$$iG^R(\mathbf{x},t;\mathbf{x}',t') = \theta(t-t')\langle\Psi_0^N|\{\hat{\psi}(\mathbf{x},t)_H,\hat{\psi}^\dagger(\mathbf{x}',t')_H^\dagger\}|\Psi_0^N\rangle$$

$$iG^A(\mathbf{x},t;\mathbf{x}',t') = -\theta(t'-t)\langle\Psi_0^N|\{\hat{\psi}(\mathbf{x},t)_H,\hat{\psi}^\dagger(\mathbf{x}',t')_H\}|\Psi_0^N\rangle$$

Spectral (Lehmann) representation of Green function

use completeness relation $1 = \sum_{N,k} |\Psi_k^N\rangle\langle\Psi_k^N| \longrightarrow$

$$iG(\mathbf{x},t;\mathbf{x}',t') = \theta(t-t')\sum_k \exp\left(i(E_0^N - E_k^{N+1})(t-t')\right) g_k(\mathbf{x})g_k^*(\mathbf{x}') - \theta(t'-t)\sum_k \exp\left(i(E_0^N - E_k^{N-1})(t'-t)\right) f_k(\mathbf{x}')f_k^*(\mathbf{x})$$

with quasiparticle amplitudes

$$f_k(\mathbf{x}) = \langle\Psi_k^{N-1}|\hat{\psi}(\mathbf{x})|\Psi_0^N\rangle$$

$$g_k(\mathbf{x}) = \langle\Psi_0^N|\hat{\psi}(\mathbf{x})|\Psi_k^{N+1}\rangle$$

note: G depends only on $t-t' \longrightarrow$ Fourier transform w.r.t. $t-t'$

Lehmann representation of Green function

Lehmann representation

$$G(\mathbf{x},\mathbf{x}';\omega)$$
$$= \sum_k \frac{g_k(\mathbf{x})g_k^*(\mathbf{x}')}{\omega - (E_k^{N+1} - E_0^N) + i\eta} + \sum_k \frac{f_k(\mathbf{x})f_k^*(\mathbf{x}')}{\omega + (E_k^{N-1} - E_0^N) - i\eta}$$

similarly for retarded/advanced Green functions

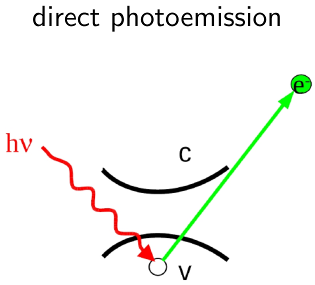
Lehmann representation for retarded and advanced GF

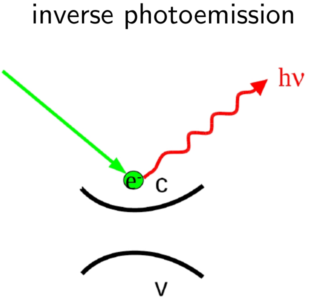
$$G^{R/A}(\mathbf{x},\mathbf{x}';\omega)$$
$$= \sum_k \frac{g_k(\mathbf{x})g_k^*(\mathbf{x}')}{\omega - (E_k^{N+1} - E_0^N) \pm i\eta} + \sum_k \frac{f_k(\mathbf{x})f_k^*(\mathbf{x}')}{\omega + (E_k^{N-1} - E_0^N) \pm i\eta}$$

where $''+''$ applies for G^R and $''-''$ for G^A

Spectral information contained in Green function

Green function contains spectral information on single-particle excitations changing the number of particles by one! The poles of the GF give the corresponding excitation energies.





Analytic structure of Green function

rewrite denominator of first term for Green function:

$$\omega - (E_k^{N+1} - E_0^N) + i\eta = \omega - (E_k^{N+1} - E_0^{N+1}) - (E_0^{N+1} - E_0^N) + i\eta$$
$$\approx \omega - (E_k^{N+1} - E_0^{N+1}) - \mu + i\eta$$

similarly for second denominator:

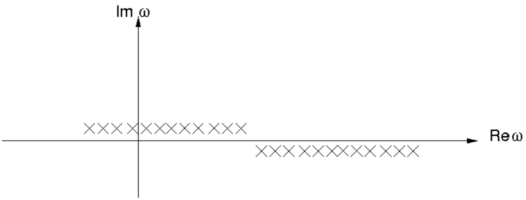
$$\omega + (E_k^{N-1} - E_0^N) - i\eta = \omega + (E_k^{N-1} - E_0^{N-1}) - \mu - i\eta$$

where we used (valid for large N and for *metallic* systems)

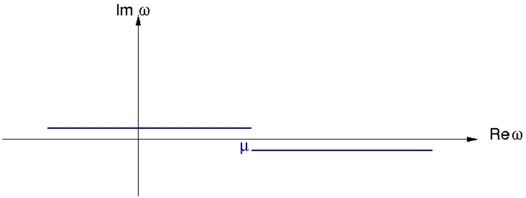
$$\frac{E_0^{N+1} - E_0^N}{1} \approx \left.\frac{\mathrm{d}E_0}{\mathrm{d}N}\right|_N = \mu(N) \approx \mu(N-1) := \mu$$

Analytic structure of Green function

pole structure of Green function



for extended systems: single poles merge to branch cuts



Spectral function

Spectral function

$$A(\mathbf{x},\mathbf{x}';\omega) = -\frac{1}{\pi}\mathrm{Im}\, G^R(\mathbf{x},\mathbf{x}';\omega) =$$

$$\sum_k g_k(\mathbf{x}) g_k^*(\mathbf{x}')\delta(\omega + E_0^N - E_k^{N+1}) + f_k(\mathbf{x}) f_k^*(\mathbf{x}')\delta(\omega + E_k^{N-1} - E_0^N)$$

$A(\mathbf{x},\mathbf{x}';\omega)$: local density of states

Perturbation Theory for Green function

Green function $G(\mathbf{x},t;\mathbf{x}',t') = -i\langle\Psi_0^N|\hat{T}[\hat{\psi}(\mathbf{x},t)_H\hat{\psi}(\mathbf{x}',t')_H^\dagger]|\Psi_0^N\rangle$ is a complicated object, it involves many-body ground state $|\Psi_0^N\rangle$ $\longrightarrow$ perturbation theory to calculate Green function: split Hamitonian in two parts

$$\hat{H} = \hat{H}_0 + \hat{W} = \hat{T} + \hat{V}_{ext} + \hat{W}$$

treat interaction $\hat{W}$ as perturbation $\longrightarrow$ machinery of many-body perturbation theory: Wick's theorem, Gell-Mann-Low theorem, and, most importantly, Feynman diagrams

Feynman diagrams

Feynman diagrams: graphical representation of perturbation series

elements of diagrams:

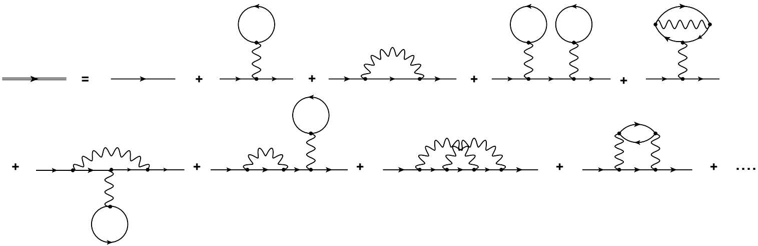
Green function G_0 of noninteracting system ($\hat{H}_0$)

Green function G of interacting system

Coulomb interaction $v_{\text{Clb}}(\mathbf{x}, t; \mathbf{x}', t') = \frac{\delta(t-t')}{|\mathbf{r}-\mathbf{r}'|}$

Diagrammatic series for Green function

Perturbation series for G: sum of all *connected* diagrams

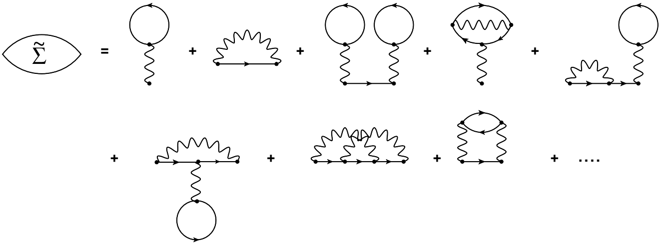


Lots of diagrams!

Self energy: reducible and irreducible

Self energy insertion and reducible self energy

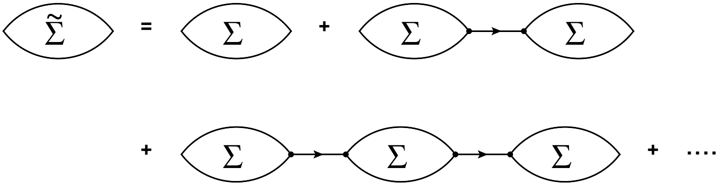
- Self energy insertion: any part of a diagram which is connected to the rest of the diagram by two G_0-lines, one incoming and one outgoing
- Reducible self energy $\tilde{\Sigma}$: sum of all self-energy insertions



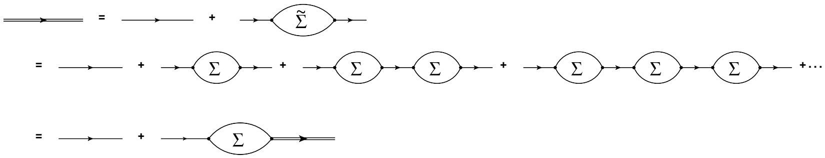
Self energy: reducible and irreducible

Proper self energy insertion and irreducible (proper) self energy

- Proper self energy insertion: any self energy insertion which cannot be separated in two pieces by cutting a single G_0-line
- Irreducible self energy Σ: sum of all *proper* self-energy insertions



Dyson equation



Dyson equation

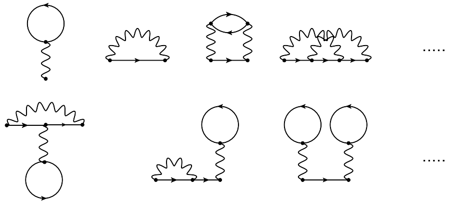
$$G(\mathbf{x},\mathbf{x}';\omega) = G_0(\mathbf{x},\mathbf{x}';\omega) + \int d^3y \int d^3y' G_0(\mathbf{x},\mathbf{y};\omega)\Sigma(\mathbf{y},\mathbf{y}';\omega)G(\mathbf{y}',\mathbf{x}';\omega)$$

Skeletons and dressed skeletons

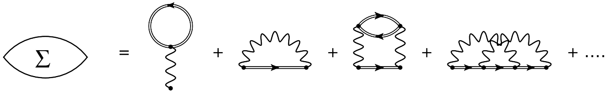
Skeleton diagram: self-energy diagram which does contain no other self-energy insertions except itself

Skeletons:

No skeletons:



Dressed skeleton: replace all G_0-lines in a skeleton by G-lines $\longrightarrow$ irreduzible self energy: sum of all dressed skeleton diagrams



$\longrightarrow$ Σ becomes functional of G: $\Sigma = \Sigma[G]$

Equation of motion for Green function

Lehmann representation for G_0

$$G_0(\mathbf{x},\mathbf{x}';\omega)$$
$$= \sum_k \frac{\theta(\varepsilon_k - \varepsilon_F)\varphi_k(\mathbf{x})\varphi_k^*(\mathbf{x}')}{\omega - \varepsilon_k + i\eta} + \sum_k \frac{\theta(\varepsilon_F - \varepsilon_k)\varphi_k(\mathbf{x})\varphi_k^*(\mathbf{x}')}{\omega - \varepsilon_k - i\eta}$$

act with operator $\omega - \hat{h}_0(\mathbf{x}) = \omega - (-\frac{\nabla_\mathbf{x}^2}{2} + v_{ext}(\mathbf{x}))$ on G_0

Equation of motion for non-interacting Green function G_0

$$(\omega - \hat{h}_0(\mathbf{x}))G_0(\mathbf{x},\mathbf{x}';\omega) = \sum_k \varphi_k(\mathbf{x})\varphi_k^*(\mathbf{x}') = \delta(\mathbf{x}-\mathbf{x}')$$

$\longrightarrow$ G_0 is a mathematical Green function !

Equation of motion for Green function (cont.)

act with $\omega - \hat{h}_0(\mathbf{x})$ on Dyson equation for G

Equation of motion for interacting Green function G

$$(\omega - \hat{h}_0(\mathbf{x}))G(\mathbf{x},\mathbf{x}';\omega) = \delta(\mathbf{x}-\mathbf{x}') + \int \mathrm{d}^3y'\ \Sigma(\mathbf{x},\mathbf{y}';\omega)G(\mathbf{y}',\mathbf{x}';\omega)$$

or with time arguments

$$\left(i\frac{\partial}{\partial t} - \hat{h}_0(\mathbf{x})\right)G(\mathbf{x},t;\mathbf{x}',t') = \delta(\mathbf{x}-\mathbf{x}')\delta(t-t')$$

$$+ \int \mathrm{d}^3y' \int \mathrm{d}t''\, \Sigma(\mathbf{x},t;\mathbf{y}',t'')G(\mathbf{y}',t'',\mathbf{x}';t')$$

Linear density response function

Suppose we expose our interacting many-electron system to an external, time-dependent perturbation $\hat{V}(t) = \int d^3x\, \delta v(\mathbf{x},t)\hat{n}(\mathbf{x})$ we are interested in the change of the density

$$\delta n(\mathbf{x},t) = \langle \Psi^N(t)|\hat{n}(\mathbf{x})|\Psi^N(t)\rangle - \langle \Psi_0^N|\hat{n}(\mathbf{x})|\Psi_0^N\rangle$$

to linear order in $\delta v(\mathbf{x},t)$

time-dependent Schrödinger equation

$$i\frac{\partial}{\partial t}|\Psi^N(t)\rangle = \left(\hat{H} + \hat{V}(t)\right)|\Psi^N(t)\rangle$$

in Heisenberg picture $|\Psi^N(t)\rangle_H = \exp(i\hat{H}t)|\Psi^N(t)\rangle \longrightarrow$

$$i\frac{\partial}{\partial t}|\Psi^N(t)\rangle_H = \hat{V}(t)_H|\Psi^N(t)\rangle_H$$

Linear density response function (cont.)

$\longrightarrow$ to linear order in $\delta v(\mathbf{x},t)$ we have

$$|\Psi^N(t)\rangle = \exp(-i\hat{H}t)\left(1 - i\int_0^t \mathrm{d}t'\ \hat{V}(t')_H\right)|\Psi_0^N\rangle$$

and for $\delta n(\mathbf{x},t) = \int \mathrm{d}^3x' \int_0^\infty \mathrm{d}t'\ \chi(\mathbf{x},t;\mathbf{x}',t')\delta v(\mathbf{x}',t')$ with

linear density response function

$$i\chi(\mathbf{x},t;\mathbf{x}',t') = i\Pi^R(\mathbf{x},t;\mathbf{x}',t')$$

$$= \theta(t-t')\frac{\langle\Psi_0^N|[\hat{\tilde{n}}(\mathbf{x},t)_H, \hat{\tilde{n}}(\mathbf{x}',t')_H]|\Psi_0^N\rangle}{\langle\Psi_0^N|\Psi_0^N\rangle}$$

with $\hat{\tilde{n}}(\mathbf{x},t)_H = \hat{n}(\mathbf{x},t)_H - \langle\Psi_0^N|\hat{n}(\mathbf{x})|\Psi_0^N\rangle$

Linear density response function (cont.)

Lehmann representation of linear density response function

$$\chi(\mathbf{x},\mathbf{x}';\omega) = \Pi^R(\mathbf{x},\mathbf{x}';\omega) = \sum_k \frac{\langle\Psi_0^N|\hat{\tilde{n}}(\mathbf{x})|\Psi_k^N\rangle\langle\Psi_k^N|\hat{\tilde{n}}(\mathbf{x}')|\Psi_0^N\rangle}{\omega-(E_k^N-E_0^N)+i\eta} - \sum_k \frac{\langle\Psi_0^N|\hat{\tilde{n}}(\mathbf{x}')|\Psi_k^N\rangle\langle\Psi_k^N|\hat{\tilde{n}}(\mathbf{x})|\Psi_0^N\rangle}{\omega+(E_k^N-E_0^N)+i\eta}$$

note: the poles of χ are at the *optical* excitation energies of the system, i.e., excitations for which the number of particles does not change!

Two-particle Green function and polarization propagator

Two-particle Green function

$$i^2 G^{(2)}(\mathbf{x}_1, t_1; \mathbf{x}_2, t_2; \mathbf{x}_3, t_3; \mathbf{x}_4, t_4) = \frac{1}{\langle \Psi_0^N | \Psi_0^N \rangle}$$

$$\langle \Psi_0^N | \hat{T}[\hat{\psi}(\mathbf{x}_1, t_1)_H \hat{\psi}(\mathbf{x}_2, t_2)_H \hat{\psi}^\dagger(\mathbf{x}_3, t_3)_H \hat{\psi}^\dagger(\mathbf{x}_4, t_4)_H] | \Psi_0^N \rangle$$

Polarization propagator

$$i\Pi(\mathbf{x}, t; \mathbf{x}', t') = \frac{\langle \Psi_0^N | \hat{T}[\hat{\tilde{n}}(\mathbf{x}, t)_H \hat{\tilde{n}}(\mathbf{x}', t')_H] | \Psi_0^N \rangle}{\langle \Psi_0^N | \Psi_0^N \rangle}$$

relation between the two:

$$i^2 G^{(2)}(\mathbf{x}_1, t_1; \mathbf{x}_2, t_2; \mathbf{x}_1, t_1^+; \mathbf{x}_2, t_2^+) = i\Pi(\mathbf{x}_1, t_1; \mathbf{x}_2, t_2) + n(\mathbf{x}_1) n(\mathbf{x}_2)$$

Lehmann representation of polarization propagator

$$\Pi(\mathbf{x},\mathbf{x}';\omega) = \sum_k \frac{\langle \Psi_0^N | \hat{\tilde{n}}(\mathbf{x}) | \Psi_k^N \rangle \langle \Psi_k^N | \hat{\tilde{n}}(\mathbf{x}') | \Psi_0^N \rangle}{\omega - (E_k^N - E_0^N) + i\eta} - \sum_k \frac{\langle \Psi_0^N | \hat{\tilde{n}}(\mathbf{x}') | \Psi_k^N \rangle \langle \Psi_k^N | \hat{\tilde{n}}(\mathbf{x}) | \Psi_0^N \rangle}{\omega + (E_k^N - E_0^N) - i\eta}$$

compare with Lehmann representation of linear density response

$$\chi(\mathbf{x},\mathbf{x}';\omega) = \Pi^R(\mathbf{x},\mathbf{x}';\omega) = \sum_k \frac{\langle \Psi_0^N | \hat{\tilde{n}}(\mathbf{x}) | \Psi_k^N \rangle \langle \Psi_k^N | \hat{\tilde{n}}(\mathbf{x}') | \Psi_0^N \rangle}{\omega - (E_k^N - E_0^N) + i\eta} - \sum_k \frac{\langle \Psi_0^N | \hat{\tilde{n}}(\mathbf{x}') | \Psi_k^N \rangle \langle \Psi_k^N | \hat{\tilde{n}}(\mathbf{x}) | \Psi_0^N \rangle}{\omega + (E_k^N - E_0^N) + i\eta}$$

Lehmann representation of polarization propagator

$$\Pi(\mathbf{x},\mathbf{x}';\omega) = \sum_k \frac{\langle\Psi_0^N|\hat{\tilde{n}}(\mathbf{x})|\Psi_k^N\rangle\langle\Psi_k^N|\hat{\tilde{n}}(\mathbf{x}')|\Psi_0^N\rangle}{\omega-(E_k^N-E_0^N)+i\eta} - \sum_k \frac{\langle\Psi_0^N|\hat{\tilde{n}}(\mathbf{x}')|\Psi_k^N\rangle\langle\Psi_k^N|\hat{\tilde{n}}(\mathbf{x})|\Psi_0^N\rangle}{\omega+(E_k^N-E_0^N)-i\eta}$$

compare with Lehmann representation of linear density response

$$\chi(\mathbf{x},\mathbf{x}';\omega) = \Pi^R(\mathbf{x},\mathbf{x}';\omega) = \sum_k \frac{\langle\Psi_0^N|\hat{\tilde{n}}(\mathbf{x})|\Psi_k^N\rangle\langle\Psi_k^N|\hat{\tilde{n}}(\mathbf{x}')|\Psi_0^N\rangle}{\omega-(E_k^N-E_0^N)+i\eta} - \sum_k \frac{\langle\Psi_0^N|\hat{\tilde{n}}(\mathbf{x}')|\Psi_k^N\rangle\langle\Psi_k^N|\hat{\tilde{n}}(\mathbf{x})|\Psi_0^N\rangle}{\omega+(E_k^N-E_0^N)+i\eta}$$

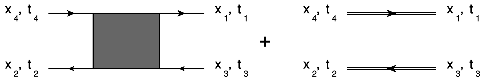
Particle-hole propagator: diagrammatic representation

Definition of particle-hole propagator

The particle-hole propagator is the two-particle Green function with a time-ordering such that both the two latest and the two earliest times correspond to one creation and one annihilation operator

Diagrammatic representation:

$G^{(2)}(x_1,t_1;x_2,t_2;x_3,t_3;x_4,t_4) =$



Diagrammatic representation of polarization propagator:

$i\,\Pi\,(x_1,t_1;x_2,t_2) =$

$=:$

Polarization propagator and irreducible polarization insertions

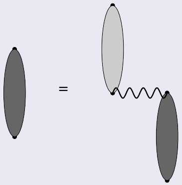
Irreducible polarization insertion

A diagram for the polarization propagator which cannot be reduced to lower-order diagrams for Π by cutting a single interaction line

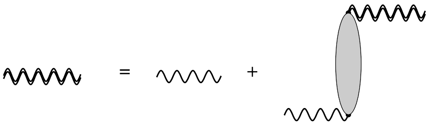
Def: $i\,P(x_1,t_1;x_2,t_2)$ =

= sum of all irreducible polarization insertions

$\longrightarrow$ Dyson-like eqn. for full polarization propagator



Effective interaction and dielectric function



Effective interaction

$$v_{\rm eff} =: \varepsilon^{-1} v_{\rm Clb} = v_{\rm Clb} + v_{\rm Clb} P v_{\rm eff}$$

Dielectric function

$$\varepsilon = 1 - v_{\rm Clb} P$$

Inverse dielectric function

$$\varepsilon^{-1} = 1 + v_{\rm Clb} \Pi$$

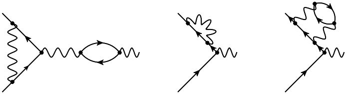
Vertex insertions

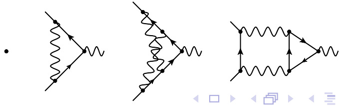
Vertex insertion

(part of a) diagram with one external in- and one outgoing G_0-line and one external interaction line

Irreducible vertex insertion

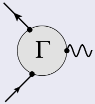
A vertex insertion which has no self-energy insertions on the in- and outgoing G_0-lines and no polarization insertion on the external interaction line

Reducible vertex insertions:  .....

Irreducible vertex insertions:  .....

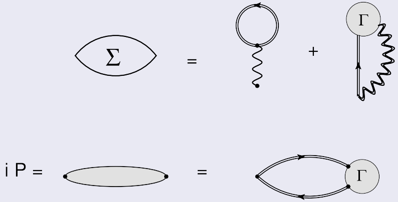
Irreducible vertex and Hedin's equations

Irreducible vertex



= sum of all irreducible vertex insertions

Hedin's equations (exact!)



L. Hedin, Phys. Rev. **139** (1965)

Hedin's equations

$$\Sigma = v_{\mathrm{Hart}} + iGW\Gamma$$

$$iP = GG\Gamma$$

$$G = G_0 + G_0 \Sigma G$$

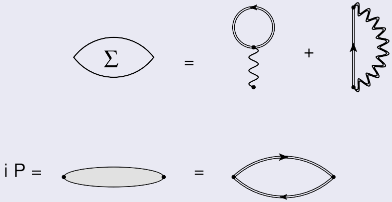
$$W = v_{\mathrm{Clb}} + v_{\mathrm{Clb}} P W$$

$$\Gamma = 1 + \frac{\delta \Sigma}{\delta G} GG\Gamma$$

GW approximation

In the GW approximation the vertex is approximated as: $\Gamma \approx 1$

GW approximation



GW approximation

$$\Sigma = v_{\rm Hart} + iGW$$

$$iP = GG$$

$$G = G_0 + G_0 \Sigma G$$

$$W = v_{\rm Clb} + v_{\rm Clb} P W$$

$$\Gamma = 1$$

Finite-temperature Green functions in equilibrium

system described by Hamiltonian $\hat{H}$ in equilibrium at inverse temperature $\beta = 1/T$

grand partition function and statistical operator

$$Z_G = \mathrm{Tr}\left\{\exp(-\beta(\hat{H} - \mu\hat{N}))\right\}$$

$$\hat{\rho}_G = \frac{\exp(-\beta(\hat{H} - \mu\hat{N}))}{Z_G}$$

modified Heisenberg picture for operator $\hat{O}(\mathbf{x})$

$$\hat{O}(\mathbf{x}, \tau)_H = \exp((\hat{H} - \mu\hat{N})\tau)\hat{O}(\mathbf{x})\exp(-(\hat{H} - \mu\hat{N})\tau)$$

Finite-temperature Green functions (cont.)

Equilibrium Green function at finite temperature

$$G(\mathbf{x},\tau;\mathbf{x}',\tau') = -\mathrm{Tr}\left\{\hat{\rho}_G \hat{T}_\tau[\hat{\psi}(\mathbf{x},\tau)_H \hat{\psi}^\dagger(\mathbf{x}',\tau')_H]\right\}$$

where time-ordering operator T_τ orders w.r.t. τ:

$$\hat{T}_\tau[\hat{\psi}(\mathbf{x},\tau)_H \hat{\psi}(\mathbf{x}',\tau')_H^\dagger] =$$
$$\theta(\tau-\tau')\hat{\psi}(\mathbf{x},\tau)_H \hat{\psi}(\mathbf{x}',\tau')_H^\dagger - \theta(\tau'-\tau)\hat{\psi}(\mathbf{x}',\tau')_H^\dagger \hat{\psi}(\mathbf{x},\tau)_H$$

periodicity of finite-T Green function: assume $0<\tau'<\beta$

$$\begin{aligned}
G(\mathbf{x},0;\mathbf{x}',\tau') &= -\mathrm{Tr}\left\{\hat{\rho}_G \hat{\psi}^\dagger(\mathbf{x}',\tau')_H \hat{\psi}(\mathbf{x},0)_H\right\} \\
&= -Z_G^{-1}\mathrm{Tr}\left\{\hat{\psi}(\mathbf{x},0)_H \exp(-\beta(\hat{H}-\mu\hat{N}))\hat{\psi}^\dagger(\mathbf{x}',\tau')_H\right\} \\
&= -Z_G^{-1}\mathrm{Tr}\left\{\exp(-\beta(\hat{H}-\mu\hat{N}))\hat{\psi}(\mathbf{x},\beta)_H \hat{\psi}^\dagger(\mathbf{x}',\tau')_H\right\} \\
&= G(\mathbf{x},\beta;\mathbf{x}',\tau')
\end{aligned}$$

Finite-temperature Green functions (cont.)

Hamiltonian $\hat{H}$ time-independent $\longrightarrow$ G depends only on $\tau - \tau'$; use periodicity to write G as Fourier series

$$G(\mathbf{x},\tau;\mathbf{x}',\tau') = \frac{1}{\beta}\sum_n \exp(-i\omega_n(\tau-\tau'))G(\mathbf{x},\mathbf{x}';\omega_n)$$

$$G(\mathbf{x},\mathbf{x}';\omega_n) = \int_0^\beta \mathrm{d}\tau\ \exp(-i\omega_n(\tau-\tau'))G(\mathbf{x},\mathbf{x}';\tau-\tau')$$

$$\omega_n = \frac{(2n+1)\pi}{\beta} \qquad n \text{ integer}$$

Perturbation expansion for finite-T Green function structurally identical to the one for $T=0$: $\longrightarrow$ use same diagrammatic analysis with only small change when translating diagrams to equations

Non-equilibrium Green functions: Keldysh contour

now consider problem with *time-dependent* Hamiltonian $\hat{H}(t) \longrightarrow$ time evolution of an initial state as $|\Psi(t)\rangle = \hat{U}(t,0)|\Psi(0)\rangle$ with

Time evolution operator

$$\hat{U}(t,t') = \begin{cases} \hat{T}\exp(-i\int_t^{t'} \mathrm{d}\bar{t}\ \hat{H}(\bar{t})) & \text{for } t > t' \\ \hat{\bar{T}}\exp(-i\int_t^{t'} \mathrm{d}\bar{t}\ \hat{H}(\bar{t})) & \text{for } t < t' \end{cases}$$

where $\hat{T}$ is the time-ordering operator (orders operators with later times to left) and $\hat{\bar{T}}$ is anti-chronological time ordering operator (orders operators with earlier times to left)

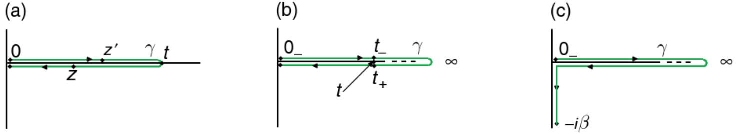
Keldysh contour

Expectation value of some operator

$$O(t) = \langle \Psi(0) | \hat{U}(0,t) \hat{O} \hat{U}(t,0) | \Psi(0) \rangle$$

$$= \left\langle \Psi(0) \middle| \hat{T}_\gamma \left[\exp\left(-i \int_\gamma \mathrm{d}\bar{z}\; \hat{H}(\bar{z}) \right) \hat{O}(t) \right] \middle| \Psi(0) \right\rangle$$

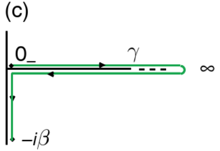
with contour a) (below) and contour ordering operator $\hat{T}_\gamma$ which moves operators with "later" contour variables to the left



extend contour to infinity as in b). For any physical time t: two points $z = t_-$ on the forward and $z = t_+$ on the backward branch
note: $O(t) = O(t_-) = O(t_+) = O(z)$!

Keldysh contour

If one is interested in the time-evolution of ensembles described by a statistical operator $\hat{\rho}(t) = \sum_m w_m |\Psi_m(t)\rangle\langle\Psi_m(t)|$, in particular if at $t = 0$ the system is in thermal equilibrium with statistical operator $\hat{\rho} = \exp(-\beta(\hat{H} - \mu\hat{N}))/Z_G \longrightarrow$ extend Keldysh contour



Ensemble expectation value of some operator

$$O(z) = \mathrm{Tr}\left\{\exp(\beta\mu\hat{N})\hat{T}_\gamma\left[\exp\left(-i\int_\gamma \mathrm{d}\bar{z}\;\hat{H}(\bar{z})\right)\hat{O}(z)\right]\right\}\Big/ Z_G$$

Non-equilibrium (Keldysh) Green function

Non-equilibrium (Keldysh) Green function

$$iG(\mathbf{x}, z; \mathbf{x}', z') =$$

$$\mathrm{Tr}\left\{\exp(\beta\mu\hat{N})\hat{T}_\gamma\left[\exp\left(-i\int_\gamma \mathrm{d}\bar{z}\ \hat{H}(\bar{z})\right)\hat{\psi}(\mathbf{x}, z)\hat{\psi}^\dagger(\mathbf{x}', z')\right]\right\}\Big/ Z_G$$

again diagrammatic analysis possible. Of course, the translation rules from diagrams to equations are more complicated!

Kadanoff-Baym equation

equation of motion for Keldysh Green function

Kadanoff-Baym equation

$$\left(i\partial_z - \hat{h}_0(z)\right) G(z;z') = \delta(z,z') + \int_\gamma \mathrm{d}\bar{z}\, \Sigma(z;\bar{z})\, G(\bar{z};z')$$

Summary

- Green functions: important concept in many-particle physics
- Diagrammatic analysis of Green function (deceptively) simple, actual calculation of specific diagrams much harder
- Green functions give access to spectroscopic properties of matter

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Literature

endless number of textbooks on Green functions

My favorites

- E.K.U. Gross, E. Runge, O. Heinonen, *Many-Particle Theory* (Hilger, Bristol, 1991)
- A.L. Fetter, J.D. Walecka, *Quantum Theory of Many-Particle Systems* (McGraw-Hill, New York, 1971) and later edition by Dover press

Thanks

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- YOU for your patience!

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