Many-body perturbation theory: I. Introduction to diagrammatics

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Outline

1. Green's function: Definition and Physics
2. Green's function: Some Mathematical Properties
3. Basics of MBPT: Introduction to Feynman diagrams
4. More on diagrammatics: GW, Hedin, etc...
5. GW in practice
6. Literature

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Quantum many-body problem

Main object: System of many (N) interacting electrons

$$\hat{H} = \hat{T} + \hat{V}_{ext} + \hat{W} = \int d\mathbf{x}\, \hat{\psi}^\dagger(\mathbf{x}) \left(-\frac{\nabla^2}{2} + v_{ext}(\mathbf{r}) \right) \hat{\psi}(\mathbf{x})$$
$$+ \frac{1}{2} \int d\mathbf{x} d\mathbf{x}'\, \hat{\psi}^\dagger(\mathbf{x}) \hat{\psi}^\dagger(\mathbf{x}') \frac{1}{|\mathbf{r} - \mathbf{r}'|} \hat{\psi}(\mathbf{x}') \hat{\psi}(\mathbf{x})$$

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

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$$\hat{H}|\Psi_n^N\rangle = E_n^N |\Psi_n^N\rangle,$$

$|\Psi_0^N\rangle$ is the ground state (GS) wave function

Equilibrium (GS at $T = 0$) MBPT is aimed at studying ground state properties and some simple/typical weakly exited states

Formal definition of one-particle Green function

Time-ordered 1-particle Green function at zero temperature

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

- $|\Psi_0^N\rangle$: N-particle ground state of $\hat{H}$: $\hat{H}|\Psi_0^N\rangle = E_0^N|\Psi_0^N\rangle$
- $\hat{\psi}_H(\mathbf{x},t) = e^{i\hat{H}t}\hat{\psi}(\mathbf{x})e^{-i\hat{H}t}$ and $\hat{\psi}_H^\dagger(\mathbf{x},t) = e^{i\hat{H}t}\hat{\psi}^\dagger(\mathbf{x})e^{-i\hat{H}t}$: electron field operators in Heisenberg picture
- $\hat{T}$: time-ordering operator

$$\hat{T}[\hat{\psi}_H(\mathbf{x},t)\hat{\psi}_H^\dagger(\mathbf{x}',t')] = \begin{cases} \hat{\psi}_H(\mathbf{x},t)\hat{\psi}_H^\dagger(\mathbf{x}',t'), & t > t' \\ -\hat{\psi}_H^\dagger(\mathbf{x}',t')\hat{\psi}_H(\mathbf{x},t), & t < t' \end{cases}$$

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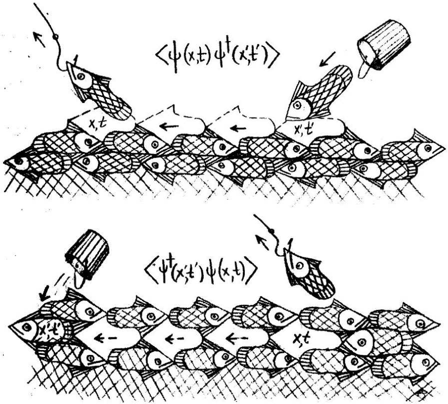
$$\begin{aligned} G(\mathbf{x},t;\mathbf{x}',t') = &-\theta(t-t')i\langle\Psi_0^N|\hat{\psi}_H(\mathbf{x},t)\hat{\psi}_H^\dagger(\mathbf{x}',t')|\Psi_0^N\rangle \\ &+\theta(t'-t)i\langle\Psi_0^N|\hat{\psi}_H^\dagger(\mathbf{x}',t')\hat{\psi}_H(\mathbf{x},t)|\Psi_0^N\rangle \end{aligned}$$

Physical meaning of Green function: Propagator

$$iG(t,t') = \theta(t-t')\langle\hat{\psi}_H(\mathbf{x},t)\hat{\psi}^\dagger_H(\mathbf{x}',t')\rangle - \theta(t'-t)\langle\hat{\psi}^\dagger_H(\mathbf{x}',t')\hat{\psi}_H(\mathbf{x},t)\rangle$$



[Taken from “Quantum Theory of Many-Body Systems” by A. M. Zagoskin, Springer 1998]

$t > t'$:

Propagation of a particle added to the system

$t < t'$

Propagation of a hole after one particle is removed

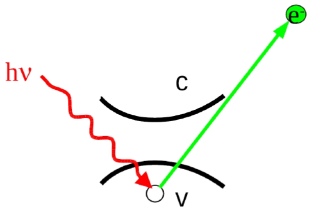
Spectral information contained in Green function

Time evolution/propagation in QM is described by $e^{-i\hat{H}t} \Longrightarrow$

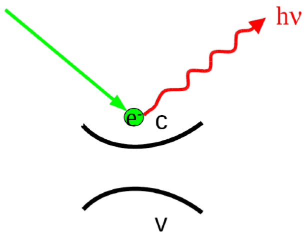
$$G(t) \sim e^{-i\epsilon_l t} e^{-\gamma_l t} \xrightarrow{\text{Fourier}} G(\omega) \sim \frac{1}{\omega - \epsilon_l + i\gamma_l}$$

Poles of $G(\omega)$ should correspond to the energies of particle/hole excitations propagating through the system.

On experimental side $G(\omega)$ is expected to be related to the spectra of direct/inverse photoemission (experimental electron removal/addition)



direct photoemission



inverse photoemission

Observables from the Green function

Green function is directly related to the 1-particle density matrix

$$\rho(\mathbf{x},\mathbf{x}') = \langle \Psi_0 | \hat{\psi}^\dagger(\mathbf{x}) \hat{\psi}(\mathbf{x}') | \Psi_0 \rangle = -i \lim_{t' \to t+0} G(\mathbf{x},t;\mathbf{x}',t') \equiv -iG(\mathbf{x},t;\mathbf{x}',t^+)$$

In general from 1-particle Green function we can extract:

- ground-state expectation values of any single-particle operator $\hat{O} = \int d\mathbf{x}d\mathbf{x}' \; \hat{\psi}^\dagger(\mathbf{x}) \hat{o}(\mathbf{x},\mathbf{x}') \hat{\psi}(\mathbf{x}')$
  e.g., the ground state density $n(\mathbf{r}) = -i \sum_\sigma G(\mathbf{r}\sigma,t;\mathbf{r}\sigma,t^+)$
- ground-state energy of the system

Galitski-Migdal formula

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

- spectrum of system: direct/inverse photoemission

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Green function of noninteracting system I

For noninteracting system $\hat{H} = \sum_{j=0}^{N} \hat{h}(\mathbf{r}_j) = \sum_{j=0}^{N} \left[-\frac{\nabla_j^2}{2} + v_{ext}(\mathbf{r}_j) \right]$

Particles occupy single-particle states $\varphi_l(\mathbf{r})$ with energies ε_l up to E_F

$$\hat{h}(\mathbf{r})\varphi_l(\mathbf{r}) = \varepsilon_l \varphi_l(\mathbf{r})$$

Examples:

- Homogeneous system [$v_{ext}(\mathbf{r}) = 0$]: plane wave states $l = \mathbf{k}$
  $\varphi_l(\mathbf{r}) = \frac{1}{\sqrt{V}} e^{i\mathbf{k}\mathbf{r}}$
- Periodic system [$v_{ext}(\mathbf{r} + \mathbf{R}) = v_{ext}(\mathbf{r})$]: Bloch states $l = n, \mathbf{k}$
  $\varphi_l(\mathbf{r}) = \frac{1}{\sqrt{V}} u_{\mathbf{k}n}(\mathbf{r}) e^{i\mathbf{k}\mathbf{r}}$

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Time dependence of field operators is very simple (no interactions!):

$$\hat{\psi}_H(\mathbf{r},t) = \sum_l e^{-i\varepsilon_l t}\varphi_l(\mathbf{r})\hat{a}_l, \quad \hat{\psi}_H^\dagger(\mathbf{r},t) = \sum_l e^{i\varepsilon_l t}\varphi_l^*(\mathbf{r})\hat{a}_l^\dagger$$

$$\{\hat{a}_l^\dagger, \hat{a}_{l'}\} = \delta_{l.l'}$$

Green function of noninteracting system II

$$iG_0(\mathbf{r},t;\mathbf{r}',t') = \langle 0|\hat{T}[\hat{\psi}_H(\mathbf{r},t)\hat{\psi}_H^\dagger(\mathbf{r}',t')]|0\rangle$$

$$= \sum_l \left[\theta(t-t')\langle 0|\hat{a}_l\hat{a}_l^\dagger|0\rangle - \theta(t'-t)\langle 0|\hat{a}_l^\dagger\hat{a}_l|0\rangle\right]\varphi_l(\mathbf{r})\varphi_l^*(\mathbf{r}')e^{-i\varepsilon_l(t-t')}$$

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$$= \theta(t-t')\underbrace{\sum_l^{\mathrm{unocc}}\varphi_l(\mathbf{r})\varphi_l^*(\mathbf{r}')e^{-i\varepsilon_l(t-t')}}_{\text{propagation of extra particle}} - \theta(t'-t)\underbrace{\sum_l^{\mathrm{occ}}\varphi_l(\mathbf{r})\varphi_l^*(\mathbf{r}')e^{-i\varepsilon_l(t-t')}}_{\text{propagation of extra hole}}$$

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Using the completeness relation $\sum_l \varphi_l(\mathbf{r})\varphi^*_l(\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}')$ we find

$$\left[i\partial_t - \hat{h}(\mathbf{r})\right] G_0(\mathbf{r},t;\mathbf{r}',t') = \delta(t-t')\delta(\mathbf{r}-\mathbf{r}')$$

For noninteracting system $G_0(\mathbf{r},t;\mathbf{r}',t')$ is the usual “mathematical” Green’s function of the Schrödinger operator $\hat{L} = i\partial_t - \hat{h}(\mathbf{r})$

Green function of noninteracting system III

Fourier transform: $G(\mathbf{x},\mathbf{x}',\omega) = \int_{-\infty}^{\infty} d(t-t')G(\mathbf{x},\mathbf{x}',t-t')e^{i\omega(t-t')}$

Spectral representation of noninteracting Green function

$$G_0(\mathbf{r},\mathbf{r}',\omega) = \underbrace{\sum_l^{\text{unocc}} \frac{\varphi_l(\mathbf{r})\varphi_l^*(\mathbf{r}')}{\omega-\varepsilon_l+i\eta}}_{\text{electron part}} + \underbrace{\sum_l^{\text{occ}} \frac{\varphi_l(\mathbf{r})\varphi_l^*(\mathbf{r}')}{\omega-\varepsilon_l-i\eta}}_{\text{hole part}}$$

Spectral functions (spectral densities) of particle and hole excitations:

$$A_e(\mathbf{r},\mathbf{r}',\omega) = \sum_l^{\text{unocc}} \varphi_l(\mathbf{r})\varphi_l^*(\mathbf{r}')\delta(\omega-\varepsilon_l+\mu)$$

$$A_h(\mathbf{r},\mathbf{r}',\omega) = \sum_l^{\text{occ}} \varphi_l(\mathbf{r})\varphi_l^*(\mathbf{r}')\delta(\omega+\varepsilon_l-\mu)$$

$$G_0(\mathbf{r},\mathbf{r}',\omega) = \int_0^{\infty} d\omega' \left[\frac{A_e(\mathbf{r},\mathbf{r}',\omega')}{\omega-\mu-\omega'+i\eta} + \frac{A_h(\mathbf{r},\mathbf{r}',\omega')}{\omega-\mu+\omega'-i\eta}\right]$$

Green function of interacting many-particle system

use completeness relation $1 = \sum_{N\pm1,k} |\Psi_k^{N\pm1}\rangle\langle\Psi_k^{N\pm1}| \longrightarrow$

$$\begin{aligned} iG(\mathbf{x},t;\mathbf{x}',t') &= \langle\Psi_0^N|\hat{T}[\hat{\psi}_H(\mathbf{r},t)\hat{\psi}_H^\dagger(\mathbf{r}',t')]|\Psi_0^N\rangle \\ &= \theta(t-t')\sum_k g_k(\mathbf{x})g_k^*(\mathbf{x}')e^{-i(E_k^{N+1}-E_0^N)(t-t')} \\ &\quad -\theta(t'-t)\sum_k f_k^*(\mathbf{x}')f_k(\mathbf{x})e^{-i(E_0^N-E_k^{N-1})(t-t')} \end{aligned}$$

with quasiparticle amplitudes

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

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

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In the noninteracting limit $g_k(\mathbf{x})$ and $f_k(\mathbf{x})$ reduce to the orbitals $\varphi_k(\mathbf{x})$

$$g_k(\mathbf{x}) = \varphi_k^{\mathrm{unocc}}(\mathbf{x})\,, \qquad f_k(\mathbf{x}) = \varphi_k^{\mathrm{occ}}(\mathbf{x})$$

Lehmann representation of Green function

$$G(\mathbf{x},\mathbf{x}';t-t') \xrightarrow{\text{Fourier}} G(\mathbf{x},\mathbf{x}';\omega)$$

Spectral (Lehmann) representation

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

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Rewrite energy differences in the denominators:

$$E_k^{N+1} - E_0^N = (E_k^{N+1} - E_0^{N+1}) - (E_0^N - E_0^{N+1}) = \varepsilon_k^{N+1} - \mathcal{A},$$

$$E_0^N - E_k^{N-1} = -(E_k^{N-1} - E_0^{N-1}) - (E_0^{N-1} - E_0^N) = -\varepsilon_k^{N-1} - \mathcal{I}$$

Here $\mathcal{A}$ – electron affinity, and $\mathcal{I}$ – ionization potential

"Thermodynamic" fundamental energy gap: $E_g = \mathcal{I} - \mathcal{A}$

Chemical potential at $T \to 0$: $\mu = -\frac{1}{2}(\mathcal{I} + \mathcal{A})$

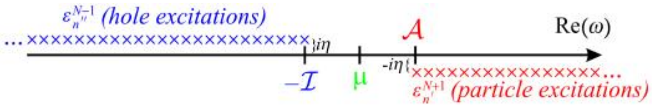
Analytic structure of Green function

Spectral functions of particle and hole excitations:

$$A_e(\mathbf{r},\mathbf{r}',\omega) = \sum_k^{\text{part}} g_k(\mathbf{r}) g_k^*(\mathbf{r}') \delta\left(\omega - \varepsilon_k^{N+1} - \tfrac{1}{2}E_g\right)$$

$$A_h(\mathbf{r},\mathbf{r}',\omega) = \sum_k^{\text{hole}} f_k(\mathbf{r}) f_k^*(\mathbf{r}') \delta\left(\omega - \varepsilon_k^{N-1} - \tfrac{1}{2}E_g\right)$$

$$G(\mathbf{r},\mathbf{r}',\omega) = \int_0^\infty d\omega' \left[\frac{A_e(\mathbf{r},\mathbf{r}',\omega')}{\omega - \mu - \omega' + i\eta} + \frac{A_h(\mathbf{r},\mathbf{r}',\omega')}{\omega - \mu + \omega' - i\eta}\right]$$



In extended systems poles merge into branch cut

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Perturbation theory for Green functions

Green function $G(\mathbf{x},t;\mathbf{x}',t') = -i\langle\Psi_0^N|\hat{T}[\hat{\psi}_H(\mathbf{x},t)\hat{\psi}_H(\mathbf{x}',t')^\dagger]|\Psi_0^N\rangle$ is a very complicated object, it involves many-body ground state $|\Psi_0^N\rangle$

$\longrightarrow$ perturbation theory to calculate Green function:

1. split Hamitonian in two parts

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

2. 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

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On the other hand, Green function is a very intuitive object (propagator) and the structure of the perturbation theory can be easily understood from qualitative/physical arguments

Scattering of noninteracting particles by a potential I

$$\hat{h}(r) = -\frac{\nabla^2}{2} + v_0(r) + v_1(r) = \hat{h}_0 + v_1$$

$\longrightarrow$ treat additional potential $v_1(r)$ as a perturbation

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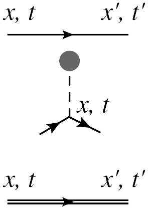
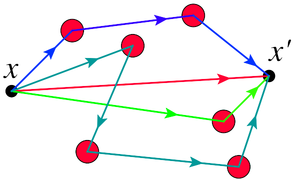
I. Qualitative consideration



– free propagation

– scattering event

– full propagation



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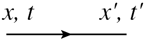

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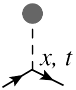
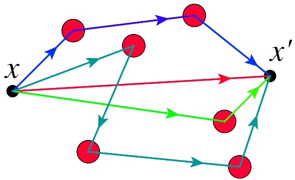
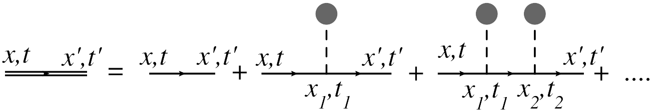


– scattering event

– full propagation





Integration over all intermediate coordinates $\equiv$ summing up all trajectories connecting points $(\mathbf{x}, t)$ and $(\mathbf{x}', t')$

Scattering of noninteracting particles by a potential II

II. Where diagrams formally come from

$$\Big[\underbrace{i\partial_t - \hat{h}_0(\mathbf{x})}_{G_0^{-1}} - v_1(\mathbf{x})\Big]G(\mathbf{x},t;\mathbf{x}',t') = \delta(t-t')\delta(\mathbf{x}-\mathbf{x}')$$

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Equivalent integral equation:

$$G(\mathbf{x},t;\mathbf{x}',t') = G_0(\mathbf{x},t;\mathbf{x}',t') + \int dt_1 d\mathbf{x}_1 G_0(\mathbf{x},t;\mathbf{x}_1,t_1) v_1(\mathbf{x}_1) G(\mathbf{x}_1,t_1;\mathbf{x}',t')$$

$$[i\partial_t - \hat{h}_0 - v_1]G = I \quad \rightarrow \quad G = G_0 + G_0 v_1 G$$

Scattering of noninteracting particles by a potential II

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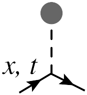
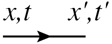
$$G = G_0 + G_0 v_1 G_0 + G_0 v_1 G_0 v_1 G_0 + G_0 v_1 G_0 v_1 G_0 v_1 G_0 + \dots$$



$= v_1(x)$

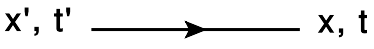


$= G_0(x,t;x',t')$

Feynman diagrams in interacting system

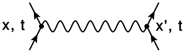
Feynman diagrams: graphical representation of perturbation series

elements of diagrams:



Green function G_0 of noninteracting system

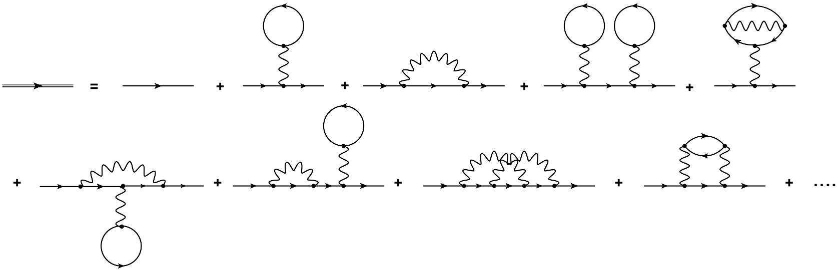
Green function G of interacting system



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

Perturbation series for Green function

Perturbation series for $G(\mathbf{x}, t; \mathbf{x}', t')$: sum of all <u>connected</u> diagrams



to each elementary vertex  we assign a space-time point $(\mathbf{x}, t)$ and integrate over coordinates of all intermediate points

- Mathematically each diagram is a multidimensional integral
- Physically it corresponds to a particular propagation “path”

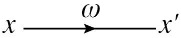
Feynman diagrams for Fourier transformed G

In equilibrium all functions depend only on time difference:

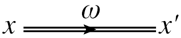
$$G(\mathbf{x},t;\mathbf{x}',t') = G(\mathbf{x},\mathbf{x}',t-t')\,,\;\; v_{\mathrm{C}}(\mathbf{x},t;\mathbf{x}',t') = \delta(t-t')v_{\mathrm{C}}(|\mathbf{x}-\mathbf{x}'|)$$

$\longrightarrow$ Fourier transform in time: $G(\mathbf{x},\mathbf{x}',\omega)\,,\;\; v_{\mathrm{C}}(|\mathbf{x}-\mathbf{x}'|)$

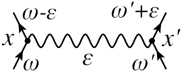
Elements of Fourier transformed diagrams:



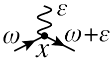
noninteracting Green function $G_0(\mathbf{x},\mathbf{x}',\omega)$



Green function $G(\mathbf{x},\mathbf{x}',\omega)$ of interacting system

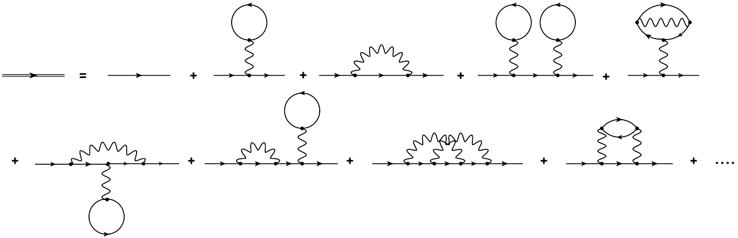


Coulomb interaction $v_{\mathrm{C}}(\mathbf{x},\mathbf{x}',\omega) = \frac{1}{|\mathbf{r}-\mathbf{r}'|}$

- at each vertex  frequency is conserved
- integral over all intermediate coordinates and frequencies

Self energy and Dyson equation

Sorting out diagrams: 1-particle irreducible/reducible



Self energy and Dyson equation

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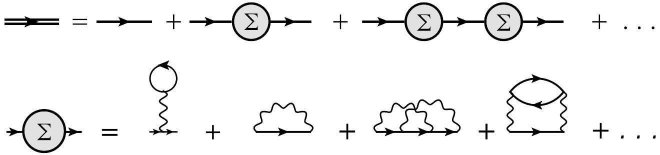
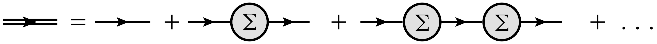
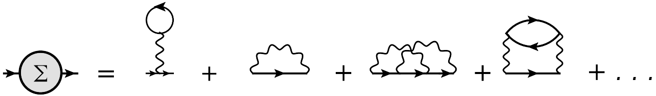


$\Sigma(\mathbf{x}, \mathbf{x}', \omega)$ – sum of all 1-particle irreducible (1PI) diagrams

Self energy and Dyson equation

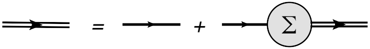
Sorting out diagrams: 1-particle irreducible/reducible





$\Sigma(\mathbf{x}, \mathbf{x}', \omega)$ – sum of all 1-particle irreducible (1PI) diagrams

Dyson equation:



$$G(\mathbf{x}, \mathbf{x}', \omega) = G_0(\mathbf{x}, \mathbf{x}', \omega) + \int d\mathbf{x}_1 d\mathbf{x}_2 G_0(\mathbf{x}, \mathbf{x}_1, \omega)\Sigma(\mathbf{x}_1, \mathbf{x}_2, \omega)G(\mathbf{x}_2, \mathbf{x}', \omega)$$

Dyson equation and quasiparticle energies

$$G(\mathbf{x},\mathbf{x}',\omega) = G_0(\mathbf{x},\mathbf{x}',\omega) + \int d\mathbf{x}_1 d\mathbf{x}_2 G_0(\mathbf{x},\mathbf{x}_1,\omega)\Sigma(\mathbf{x}_1,\mathbf{x}_2,\omega)G(\mathbf{x}_2,\mathbf{x}',\omega)$$

Energies ε_n of 1-particle excitations:
poles of $G(\omega)$ or, equivalently, zeros of $G^{-1}(\omega) = [G_0^{-1}(\omega) - \Sigma(\omega)]^{-1}$

$$[\underbrace{\varepsilon_n - \hat{h}_0(\mathbf{x})}_{G_0^{-1}(\varepsilon_n)}]\phi_n(\mathbf{x}) - \int d\mathbf{x}'\Sigma(\mathbf{x},\mathbf{x}',\varepsilon_n)\phi_n(\mathbf{x}') = 0$$

$\Sigma(\mathbf{x},\mathbf{x}',\omega)$ – interaction correction to effective 1-particle Hamiltonian

Dyson equation and quasiparticle energies

$$G(\mathbf{x},\mathbf{x}',\omega) = G_0(\mathbf{x},\mathbf{x}',\omega) + \int d\mathbf{x}_1 d\mathbf{x}_2 G_0(\mathbf{x},\mathbf{x}_1,\omega)\Sigma(\mathbf{x}_1,\mathbf{x}_2,\omega)G(\mathbf{x}_2,\mathbf{x}',\omega)$$

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$\Sigma(\mathbf{x},\mathbf{x}',\omega)$ – interaction correction to effective 1-particle Hamiltonian

Approximation strategies

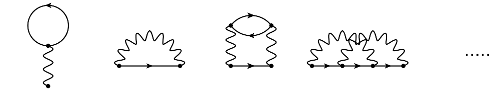
- Approximate $\Sigma(\omega)$ (e.g., by truncating diagrammatic series)
- Solve Dyson equation for $G(w)$

By keeping a few diagrams for Σ we generate infinite series for G
$\longrightarrow$ “partial summation” – most useful diagrammatic trick

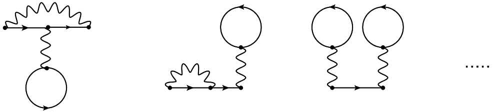
Skeletons and dressed skeletons

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

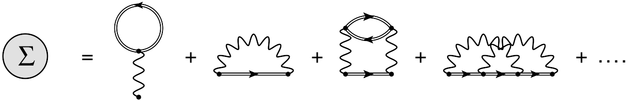
Skeletons:



No skeletons:



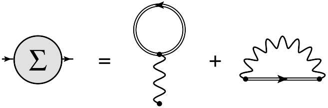
Dressed skeleton: replace all G_0-lines in a skeleton by G-lines $\longrightarrow$ Self energy $\Sigma(\omega)$: sum of all dressed skeleton diagrams



$\longrightarrow$ Σ becomes functional of G: $\Sigma = \Sigma[G]$ (to be approximated)

Hartree-Fock approximation

First order skeleton diagrams for $\Sigma \longrightarrow$ Hartree-Fock



$\Sigma_{HF}(\mathbf{r},\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}')v_H(\mathbf{r}) + \Sigma_x(\mathbf{r},\mathbf{r}')$ is frequency independent

$$v_H(\mathbf{r}) = \int d\mathbf{r}' v_C(\mathbf{r}-\mathbf{r}')n(\mathbf{r}') = \int d\mathbf{r}' \frac{n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}$$ – Hartree potential

second term $\Sigma_x(\mathbf{r},\mathbf{r}')$ – nonlocal Fock exchange potential

HF-Dyson equation is solved by the HF Green function G_{HF}:

$$G_{HF}(\mathbf{r},\mathbf{r}',\omega) = \sum_l^{\mathrm{unocc}} \frac{\varphi_l(\mathbf{r})\varphi_l^*(\mathbf{r}')}{\omega - \varepsilon_l + i\eta} + \sum_l^{\mathrm{occ}} \frac{\varphi_l(\mathbf{r})\varphi_l^*(\mathbf{r}')}{\omega - \varepsilon_l - i\eta}$$

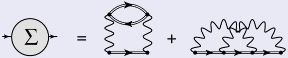
where $\varphi_l(\mathbf{r})$ and ε_l – HF orbitals and energies

Outline

1. Green's function: Definition and Physics
2. Green's function: Some Mathematical Properties
3. Basics of MBPT: Introduction to Feynman diagrams
4. More on diagrammatics: GW, Hedin, etc...
5. GW in practice
6. Literature

Approximations beyond Hartree-Fock

I. Simplest ω-dependent Σ: 2nd-order Born approximation



Strictly valid for dilute gases with short-range interaction

Approximations beyond Hartree-Fock

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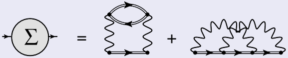
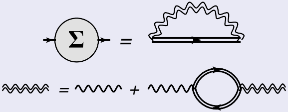


Strictly valid for dilute gases with short-range interaction

II. Dynamically screened interaction and GW approximation



$$\longrightarrow \Sigma = GW, \quad W = v_\mathrm{C} + v_\mathrm{C} GGW$$

GW $\equiv$ “dynamically screened exchange”:
Interaction is screened by virtual e-h pairs (series of e-h bubbles)
Screening is extremely important in extended Coulomb systems like plasmas and solids (more on practical GW comes soon).

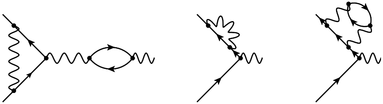
Vertex insertions

Diagrams missing in GW: interaction lines in the “corners”

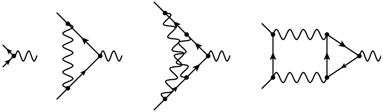
Vertex insertion

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

Reducible vertex insertions:

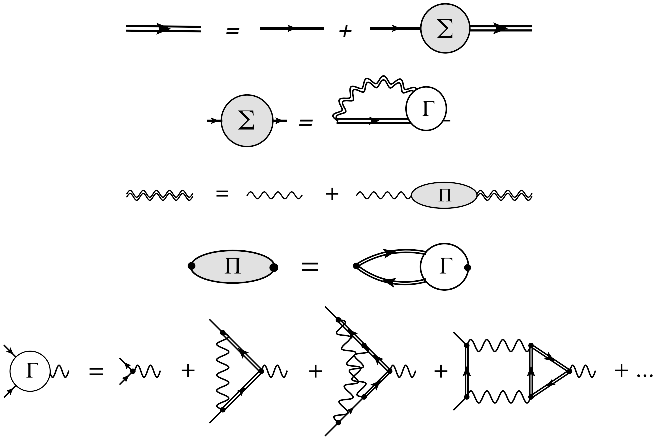


Irreducible vertex insertions:

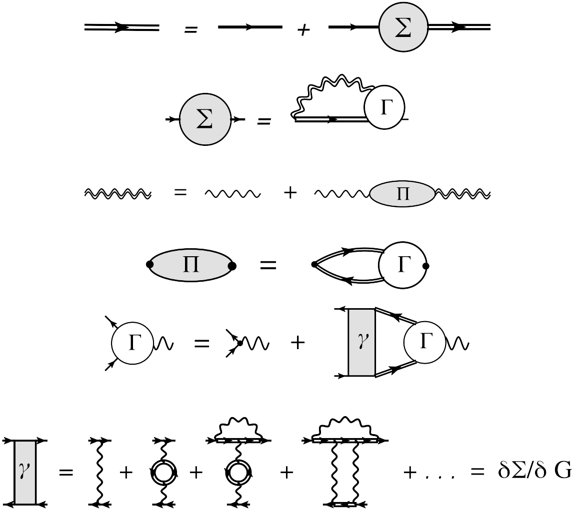


Only irreducible vertex insertions are missing in GW approximation!

Hedin's equations (exact!)



Hedin’s equations (exact!)



$\gamma = \frac{\delta\Sigma}{\delta G}$ – effective irreducible electron-hole interaction

GW from Hedin's equations

Full system of Hedin's equations

$$G = G_H + G_H \Sigma G$$

$$\Sigma = G W \Gamma$$

$$W = v_{\mathrm{C}} + v_{\mathrm{C}} \Pi W$$

$$\Pi = G G \Gamma$$

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

Hedin's equations can be "solved" iteratively by setting $\gamma = \frac{\delta \Sigma}{\delta G} = 0$ on the first step of iterations. On this step we recover GW approximation

Initial step of Hedin's iterations – GW approximation

$$\Gamma = 1 \longrightarrow \quad \Sigma = GW, \quad \Pi = GG$$

Concluding remarks

Beyond the scope of this lecture:

- Finite temperature (Matsubara) Green functions
- Nonequilibrium (Keldysh) Green functions

Both in Matsubara and in Keldysh formalisms the structure of diagrammatic series remains the same.

All changes can be attributed to time integration – extension to a complex “time” plane and integration over different time-contours.

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Dyson equation

$$[\omega - \hat{h}_0(\mathbf{x}_1)]G(\mathbf{x}_1, \mathbf{x}_2, \omega) - \int d\mathbf{x}_3 \Sigma(\mathbf{x}_1, \mathbf{x}_3, \omega) G(\mathbf{x}_3, \mathbf{x}_2, \omega) = \delta(\mathbf{x}_1 - \mathbf{x}_2)$$

Analytic continuation of G: Biorthonormal representation

$$G(\mathbf{x}_1, \mathbf{x}_2, z) = \sum_\lambda \frac{\Phi_\lambda(\mathbf{x}_1, z)\tilde{\Phi}_\lambda(\mathbf{x}_2, z)}{z - E_\lambda(z)}$$

$$\hat{h}_0(\mathbf{x}_1)\Phi_\lambda(\mathbf{x}_1, z) + \int d\mathbf{x}_2 \Sigma(\mathbf{x}_1, \mathbf{x}_2, z)\Phi_\lambda(\mathbf{x}_2, z) = E_\lambda(z)\Phi_\lambda(\mathbf{x}_1, z)$$

$$\hat{h}_0(\mathbf{x}_1)\tilde{\Phi}_\lambda(\mathbf{x}_1, z) + \int d\mathbf{x}_2 \tilde{\Phi}_\lambda(\mathbf{x}_2, z)\Sigma(\mathbf{x}_2, \mathbf{x}_1, z) = E_\lambda(z)\tilde{\Phi}_\lambda(\mathbf{x}_1, z)$$

$$\int d\mathbf{x} \tilde{\Phi}_\lambda(\mathbf{x}, z)\Phi_{\lambda'}(\mathbf{x}, z) = \delta_{\lambda\lambda'}$$

Dyson equation

Complex poles of $G \mapsto$ Quasiparticles

$$\varepsilon_n - E_\lambda(\varepsilon_n) = 0 \quad \Rightarrow \quad \varepsilon_n = E_\lambda(\varepsilon_n)$$

$$\phi_n(\mathbf{x}) = \Phi_\lambda(\mathbf{x}, \varepsilon_n)$$

Analytic continuation of G: Biorthonormal representation

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$$\hat{h}_0(\mathbf{x}_1)\tilde{\Phi}_\lambda(\mathbf{x}_1, z) + \int d\mathbf{x}_2 \tilde{\Phi}_\lambda(\mathbf{x}_2, z)\Sigma(\mathbf{x}_2, \mathbf{x}_1, z) = E_\lambda(z)\tilde{\Phi}_\lambda(\mathbf{x}_1, z)$$

$$\int d\mathbf{x} \tilde{\Phi}_\lambda(\mathbf{x}, z)\Phi_{\lambda'}(\mathbf{x}, z) = \delta_{\lambda\lambda'}$$

G_0W_0: Perturbative QP corrections

Standard perturbative G_0W_0 corrections to the KS-DFT spectrum

$$\hat{h}_0(\mathbf{x})\varphi_i(\mathbf{x}) + V_{\mathrm{xc}}(\mathbf{x})\varphi_i(\mathbf{x}) = \varepsilon_n\varphi_i(\mathbf{x})$$

$$\hat{h}_0(\mathbf{x})\phi_i(\mathbf{x}) + \int d\mathbf{x}'\Sigma(\mathbf{x},\mathbf{x}',\omega = E_i)\phi_i(\mathbf{x}') = E_i\phi_i(\mathbf{x})$$

First order perturbative correction with $\Sigma = GW$

$$E_i - \varepsilon_i = \langle\varphi_i|\Sigma(E_i) - V_{\mathrm{xc}}|\varphi_i\rangle$$

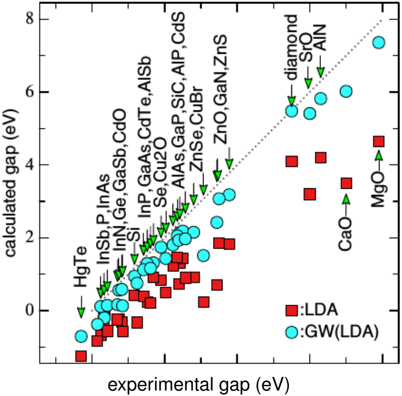
$$\Sigma(E_i) = \Sigma(\varepsilon_i) + (E_i - \varepsilon_i)\partial_\omega\Sigma(\omega)|_{\varepsilon_i}$$

$$E_i = \varepsilon_i + Z_i\langle\varphi_i|\Sigma(\varepsilon_i) - V_{\mathrm{xc}}|\varphi_i\rangle$$

$$Z_i = (1 - \langle\varphi_i|\partial_\omega\Sigma(\omega)|_{\varepsilon_i}|\varphi_i\rangle)^{-1}$$

Hybertsen and Louie, PRB **34**, 5390 (1986)
Godby, Schlüter, and Sham, PRB **37**, 10159 (1988)

G_0W_0: Results for the fundamental gap



M. van Schilfgaarde, T. Kotani, and S. Faleev, PRL **96**, 226402 (2006)

G_0W_0 results

Great improvement over LDA.

Problem: Dependence on the starting point (LDA)

Quality of the results is tied to the quality of LDA wave functions

perturbative G_0W_0

- works reasonably well for sp electron systems
- questionable for df systems and whenever LDA is bad

Beyond G_0W_0

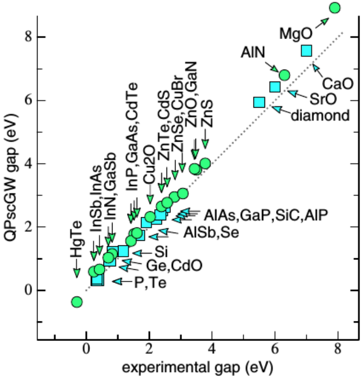
Alternative starting points and/or self-consistent QP schemes

- Looking for a better starting point:
  - Kohn-Sham with other functionals (EXX, LDA+U, ...)
  - hybrid functional (HSE06, ...)
- Effective quasiparticle Hamiltonians:
  - quasiparticle self-consistent GW (QPscGW) – Faleev 2004
  - Hedin's COHSEX approximation – Bruneval 2005

Beyond G_0W_0: QPscGW scheme

Retain only hermitian part of GW self-energy and iterate QP

$$\langle\phi_i|\Sigma|\phi_j\rangle \mapsto \frac{1}{2}\text{Re}[\langle\phi_i|\Sigma(E_i)|\phi_j\rangle + \langle\phi_i|\Sigma(E_j)|\phi_j\rangle]$$



S. Faleev, M. van Schilfgaarde, and T. Kotani, PRL **93**, 126406 (2004)
M. van Schilfgaarde, T. Kotani, and S. Faleev, PRL **96**, 226402 (2006)

Beyond LDA+G_0W_0: COHSEX approximation

GW self-energy with $G(\omega) = \sum_i \frac{|\phi_i\rangle\langle\phi_i|}{\omega - E_i + i\eta\cdot\mathrm{sgn}(\omega)}$

$\Sigma = \Sigma_1 + \Sigma_2$: contributions from poles of $G(\omega)$ or $W_p(\omega) = W(\omega) - v$

$$\Sigma_1(\mathbf{x}_1, \mathbf{x}_2, \omega) = -\sum_i^{\mathrm{occ}} \phi_i(\mathbf{x}_1)\phi_i^*(\mathbf{x}_2) W(\mathbf{x}_1, \mathbf{x}_2, \omega - E_i)$$

$$\Sigma_2(\mathbf{x}_1, \mathbf{x}_2, \omega) = -\sum_i \phi_i(\mathbf{x}_1)\phi_i^*(\mathbf{x}_2) \int_0^\infty \frac{d\omega'}{\pi} \frac{\mathrm{Im}\, W_p(\mathbf{x}_1, \mathbf{x}_2, \omega')}{\omega - E_i - \omega'}$$

COHSEX approximation: set $\omega - E_i = 0$

$$\Sigma_{\mathrm{SEX}}(\mathbf{x}_1, \mathbf{x}_2) = -\sum_i^{\mathrm{occ}} \phi_i(\mathbf{x}_1)\phi_i^*(\mathbf{x}_2) W(\mathbf{x}_1, \mathbf{x}_2, \omega = 0)$$

$$\Sigma_{\mathrm{COH}}(\mathbf{x}_1, \mathbf{x}_2) = \frac{1}{2}\delta(\mathbf{x}_1 - \mathbf{x}_2) W_p(\mathbf{x}_1, \mathbf{x}_2, \omega = 0)$$

COHSEX+G_0W_0 – F. Bruneval, N. Vast, and L. Reining, PRB **74**, 045102 (2006)

One-particle GF and physics

Physical information contained in $G(\mathbf{x}_1, \mathbf{x}_2, \omega)$

- $G \mapsto \rho(\mathbf{x}_1, \mathbf{x}_2) \mapsto$ ground state single-particle observables
- Ground state total energy via the Galitski-Migdal formula
- Poles of $G(\omega) \mapsto$ spectrum of single-particle excitations $\mapsto$ direct/inverse photoemission, fundamental gap $E_g = \mathcal{I} - \mathcal{A}$

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Importantly: the fundamental gap $\neq$ the optical gap

To describe optical experiments we need more!

Two-particles Green function and the Bethe-Salpeter equation
(comes in the next lecture)

Outline

1. Green's function: Definition and Physics
2. Green's function: Some Mathematical Properties
3. Basics of MBPT: Introduction to Feynman diagrams
4. More on diagrammatics: GW, Hedin, etc...
5. GW in practice
6. Literature

Literature: endless number of textbooks

Classics from 1960s - 1970s

- A.A. Abrikosov, L.P. Gor'kov, I.Ye. Dzyaloshinskii, *Quantum field theoretical methods in statistical physics* (Pergamon Press, 1965)
- A.L. Fetter, J.D. Walecka, *Quantum Theory of Many-Particle Systems* (McGraw-Hill, 1971) and later edition by Dover press
- R.D. Mattuck, *A guide to Feynman diagrams in the many-body problem* (McGraw-Hill, 1967), extended 2nd edition (1992)

More recent books with additional/new material

- J.W. Negele, H. Orland, *Quantum many-particle systems* (Westview Press, 1988, 1998)
- A.M. Zagoskin, *Quantum Theory of Many-Body Systems* (Springer, 1998)
- G. Stefanucci, R. van Leeuwen, *Nonequilibrium Many Body Theory of Quantum Systems: A Modern Introduction* (Cambridge University Press, 2013)
- R.M. Martin, L. Reining, D.M. Ceperley, *Interacting Electrons. Theory and Computational Approaches* (Cambridge University Press, 2016)