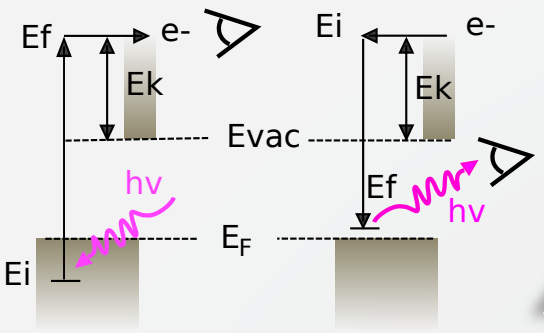
What is the key strategy of Density-Functional-Theory to attack the many-body problem?

What is the key strategy of Density-Functional-Theory to attack the many-body problem?

Reduce the degrees of freedom

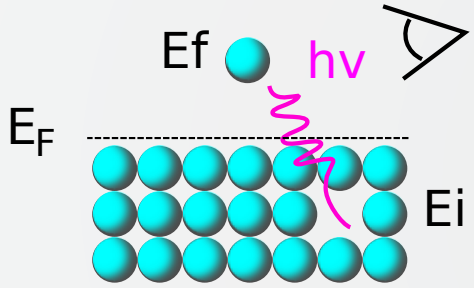
$$n(\mathbf{r}) = N \sum_{s} \int d\mathbf{x}_2 \cdots d\mathbf{x}_N |\Psi(\mathbf{r}s \cdots \mathbf{x}_M, \mathbf{x}_{M+1} \cdots \mathbf{x}_N)|^2$$

(Access only part of the information: ground state properties)



Target charged excitations in electronic system:

Reduce to
a 2-point 1 particle 'correlation function'



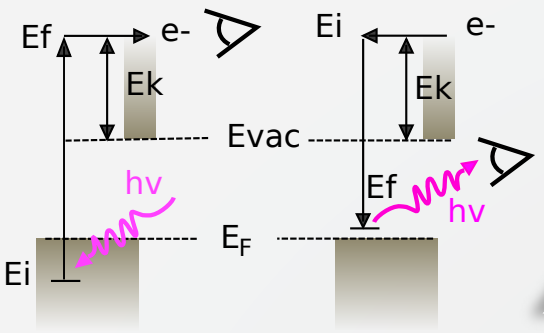
Target neutral excitations in electronic system:

Reduce to
a 4-point 2 particles 'correlation function'

Derive equation of motion for the correlation functions
(under certain assumptions)

Look briefly at practical implementations

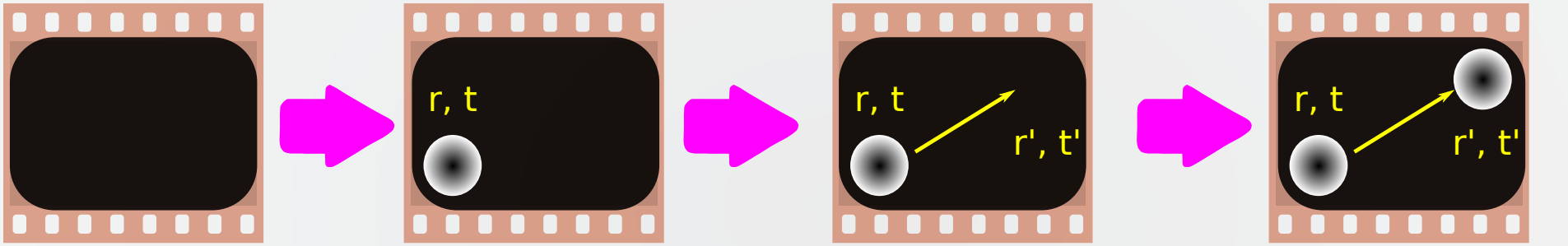
Discuss the assumptions...



Target charged excitations in electronic system:

Reduce to
a 2-point 1 particle 'correlation function'

Let's "watch" the propagation of an added electron:



$|\Psi_0^N\rangle$ $\hat{\psi}^\dagger(\mathbf{r})|\Psi_0^N\rangle$ $\hat{U}(t',t)\hat{\psi}^\dagger(\mathbf{r})|\Psi_0^N\rangle$ $\hat{\psi}(\mathbf{r}')\hat{U}(t',t)\hat{\psi}^\dagger(\mathbf{r})|\Psi_0^N\rangle$

with:

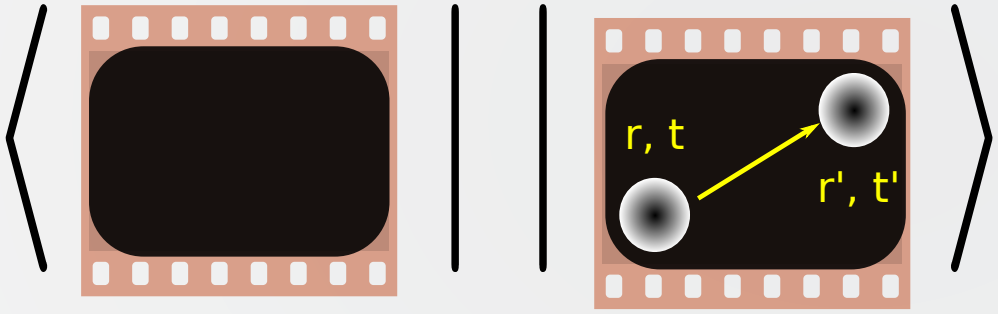
$|\Psi_0^N\rangle$ N-electron ground state

$\hat{\psi}(\mathbf{r}),\ \hat{\psi}^\dagger(\mathbf{r})$ field operators of annihilation/creation electron at r

$U(t',t) = \exp\left(-i\hat{H}(t'-t)\right)$ evolution operator from t to t'> t

Probability amplitude for propagation of additional electron from (r,t) to (r',t') in a many electron system:

=overlap final/initial states:



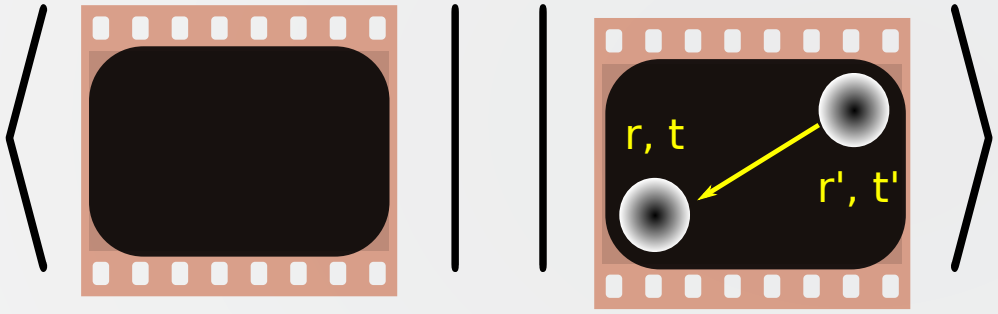
$$\langle \Psi_0^N | \qquad \hat{\psi}(\mathbf{r}')\hat{U}(t',t)\hat{\psi}^\dagger(\mathbf{r})|\Psi_0^N\rangle \equiv \hat{\psi}(\mathbf{r}',t')\psi^\dagger(\mathbf{r},t)|\Psi_0^N\rangle$$

=definition of Green's function:

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

Probability amplitude for propagation of additional hole from (r,t) to (r',t') in a many electron system:

=overlap final/initial states:



$$\langle \Psi_0^N | \qquad \hat{\psi}^\dagger(\mathbf{r}')\hat{U}(t',t)\hat{\psi}(\mathbf{r})|\Psi_0^N\rangle \equiv \hat{\psi}^\dagger(\mathbf{r}',t')\psi(\mathbf{r},t)|\Psi_0^N\rangle$$

=definition of Green's function:

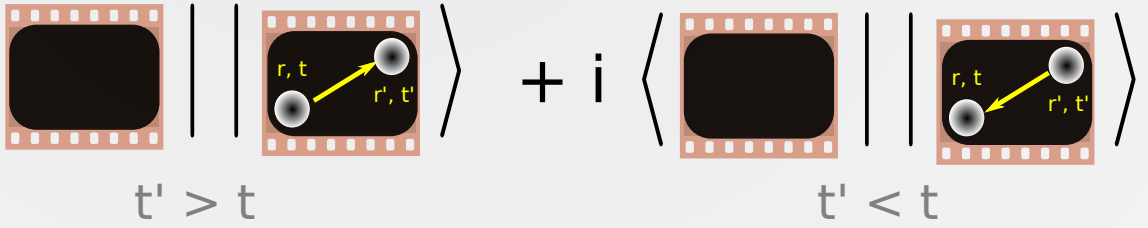
$$iG^h(\mathbf{r},t;\mathbf{r}',t') = \langle \Psi_0^N|\hat{\psi}^\dagger(\mathbf{r},t)\hat{\psi}(\mathbf{r}',t')|\Psi_0^N\rangle\theta(t-t')$$

We can so define the time-ordered Green's function

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

$$= G^e(\mathbf{r}',t';\mathbf{r},t) - G^h(\mathbf{r},t;\mathbf{r}',t')$$

$$= -i \left\langle \quad \middle| \quad \right\rangle + i \left\langle \quad \middle| \quad \right\rangle$$



t' > t t' < t

$\hat{T}$ **time ordering operator:** re-arranges a series of field operators in order of ascending time. Each permutation = x(-1)

Which information is contained in the Green's function?

$$n(\mathbf{r}t) = \langle \Psi_0^N | \psi^\dagger(\mathbf{r},t)\psi(\mathbf{r},t) | \Psi_0^N \rangle = -iG(\mathbf{r},t;\mathbf{r},t+\eta)$$

η infinitesimal positive number

It reduces to the ground state density:
all ground state observables (by Hohenberg-Kohn theorem)

Which information is contained in the Green's function?

Lehmann representation:

$$G(\mathbf{r}',\mathbf{r}) = \sum_s \frac{\psi_s^{N+1}(\mathbf{r}')[\psi_s^{N+1}(\mathbf{r})]^*}{\omega - \varepsilon_s^{N+1} + i\eta} + \sum_s \frac{\psi_s^{N-1}(\mathbf{r})[\psi_s^{N-1}(\mathbf{r}')]^*}{\omega - \varepsilon_s^{N-1} - i\eta}$$

obtained from GF definition by inserting:

$$1 = \sum_s |\Psi_s^{N\pm1}\rangle\langle\Psi_s^{N\pm1}|$$

sum over all states of N+1 (N -1) system

and Fourier transforming (time)

Which information is contained in the Green's function?

Lehmann representation:

$$G(\mathbf{r}',\mathbf{r}) = \sum_s \frac{\psi_s^{N+1}(\mathbf{r}')[\psi_s^{N+1}(\mathbf{r})]^*}{\omega - \varepsilon_s^{N+1} + i\eta} + \sum_s \frac{\psi_s^{N-1}(\mathbf{r})[\psi_s^{N-1}(\mathbf{r}')]^*}{\omega - \varepsilon_s^{N-1} - i\eta}$$

where

$$\psi_s^{N+1}(\mathbf{r}) = \langle \Psi_0^N | \hat{\psi}(\mathbf{r}) | \Psi_s^{N+1} \rangle \qquad \varepsilon_s^{N+1} = E_s^{N+1} - E_0^N$$

with

$$\psi_s^{N-1}(\mathbf{r}) = \langle \Psi_0^N | \hat{\psi}^\dagger(\mathbf{r}) | \Psi_s^{N-1} \rangle \qquad \varepsilon_s^{N-1} = E_0^N - E_s^{N-1}$$

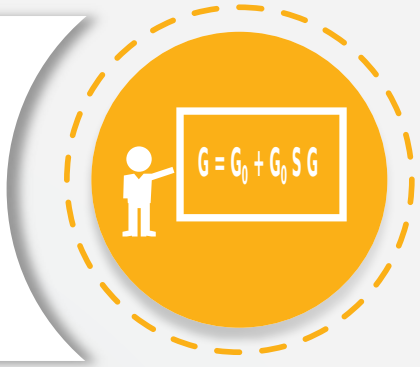
Which information is contained in the Green's function?

$$G(\mathbf{r}',\mathbf{r}) = \sum_s \frac{\psi_s^{N+1}(\mathbf{r}')[\psi_s^{N+1}(\mathbf{r})]^*}{\omega - \varepsilon_s^{N+1} + i\eta} + \sum_s \frac{\psi_s^{N-1}(\mathbf{r})[\psi_s^{N-1}(\mathbf{r}')]^*}{\omega - \varepsilon_s^{N-1} - i\eta}$$

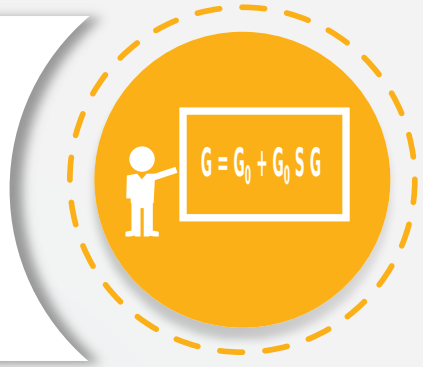
$$\varepsilon_s^{N+1} = E_s^{N+1} - E_0^N \qquad \varepsilon_s^{N-1} = E_0^N - E_s^{N-1}$$

Poles of Green's function give
energies of added/removed electron
(charged excitations)

How can we obtain the Green's function of a given many electron system?



From the equation of motion (EOM) for the annihilation field operator:



$$i\partial_t \hat{\psi}(\mathbf{r},t) = \left[\hat{\psi}(\mathbf{r},t), \hat{H}\right]$$

with Hamiltonian (in term of field operators)

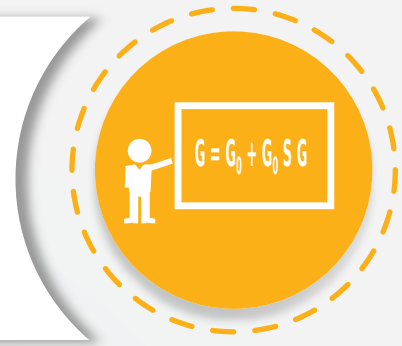
$$\hat{H} = \int d\mathbf{r}\hat{\psi}^\dagger(\mathbf{r})h(\mathbf{r})\hat{\psi}(\mathbf{r}) +$$

ONE PARTICLE OPERATOR = KINETIC + EXTERNAL

$$\frac{1}{2}\iint d\mathbf{r}d\mathbf{r}'\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r}')v(\mathbf{r},\mathbf{r}')\hat{\psi}(\mathbf{r})\hat{\psi}(\mathbf{r}')$$

TWO-PARTICLE OPERATOR (COULOMB)

We obtain an EOM for the Green's function



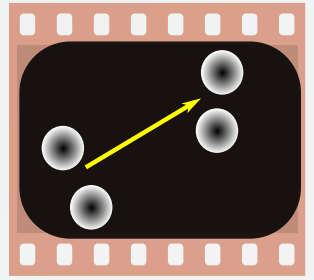
Using time-ordered Green's function definition:

$$i\partial_t G(\mathbf{r},t;\mathbf{r}',t') = \delta(\mathbf{r}-\mathbf{r}')\delta(t-t') + h(\mathbf{r})G(\mathbf{r},t;\mathbf{r}',t') - i\int d\mathbf{r}''\, v(\mathbf{r},\mathbf{r}'')\langle\Psi_0^N|\hat{T}[\hat{\psi}^\dagger(\mathbf{r}'',t+2\eta)\hat{\psi}(\mathbf{r}'',t+\eta)\hat{\psi}(\mathbf{r},t)\hat{\psi}^\dagger(\mathbf{r}',t')|\Psi_0^N\rangle|_{\eta\to 0^+}$$

which however depends on 2-particles Green's function

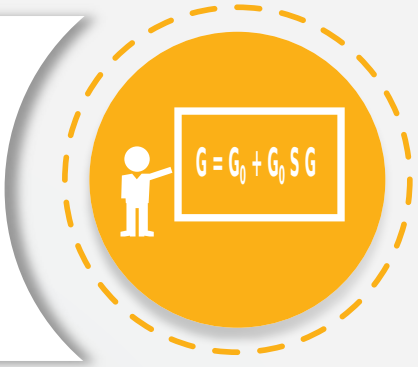
$$G_2(1,2,3,4) = (i)^2\langle\Psi_0^N|\hat{T}[\hat{\psi}(1)\hat{\psi}(2)\hat{\psi}^\dagger(4)\hat{\psi}^\dagger(3)]|\Psi_0^N\rangle$$

$$1 \equiv (\mathbf{r}_1, t_1)$$



infinite hierarchy of n-particles Green's function...

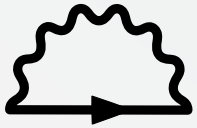
Let's introduce the mass operator



$$i\partial_t G(\mathbf{r},t;\mathbf{r}',t') = \delta(\mathbf{r}-\mathbf{r}')\delta(t-t') + h(\mathbf{r})G(\mathbf{r},t;\mathbf{r}',t') + \int d\mathbf{r}''\, M(\mathbf{r},t;\mathbf{r}''t'')G(\mathbf{r}'',t;\mathbf{r}',t')$$

$$\int d\mathbf{r}''\, M(\mathbf{r},t;\mathbf{r}''t'')G(\mathbf{r}'',t;\mathbf{r}',t') = -i\int d\mathbf{r}''\, v(\mathbf{r},\mathbf{r}'')\langle\Psi_0^N|\hat{T}[\hat{\psi}^\dagger(\mathbf{r}'',t)\hat{\psi}(\mathbf{r}'',t)\hat{\psi}(\mathbf{r},t)\hat{\psi}^\dagger(\mathbf{r}',t')]|\Psi_0^N\rangle$$

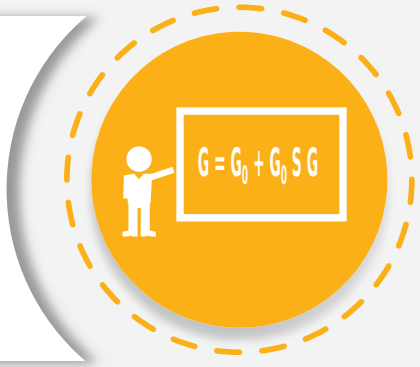
We need to find an operative expression



Many-Body perturbation theory

$+V \to 0$ Schwinger functional derivative

Following the Schwinger functional derivative method



Change of Green's function to addition of 'fake' external potential

$$\left.\frac{\delta G(1,2)}{\delta V(3)}\right|_{V=0} = G(1,2)\underbrace{G(3,3^+)}_{n(3)} - G_2(1,2,3,3^+)$$

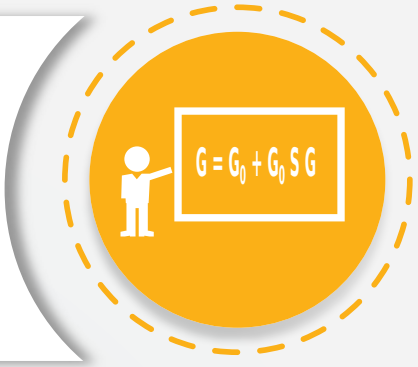
allows to define: $M(\mathbf{r},t;\mathbf{r}''t'') = \underbrace{\int d\mathbf{r}' n(\mathbf{r}') v(\mathbf{r}-\mathbf{r}')}_{v_H(\mathbf{r})}\,\delta(\mathbf{r}-\mathbf{r}'') + \underbrace{\Sigma(\mathbf{r},t;\mathbf{r}''t'')}_{\Sigma(12)=v(13)\frac{\delta G(34)}{\delta V(5)}G^{-1}(52)}$

= HARTREE POTENITAL + SELF-ENERGY

and rewrite: $i\partial_t G(\mathbf{r},t;\mathbf{r}',t') = \delta(\mathbf{r}-\mathbf{r}')\delta(t-t') + \underbrace{\left(h(\mathbf{r})+v_H(\mathbf{r})\right)}_{h_0(\mathbf{r})} G(\mathbf{r},t;\mathbf{r}',t')$

$$+ \int d\mathbf{r}''\,\Sigma(\mathbf{r},t;\mathbf{r}''t'')G(\mathbf{r}'',t;\mathbf{r}',t')$$

Taking the Fourier transform (time to frequency space)



$$i\partial_t G(\mathbf{r},t;\mathbf{r}',t') = \delta(\mathbf{r}-\mathbf{r}')\delta(t-t') + h_0(\mathbf{r})G(\mathbf{r},t;\mathbf{r}',t') + \int d\mathbf{r}''\,\Sigma(\mathbf{r},t;\mathbf{r}''t'')G(\mathbf{r}'',t;\mathbf{r}',t')$$

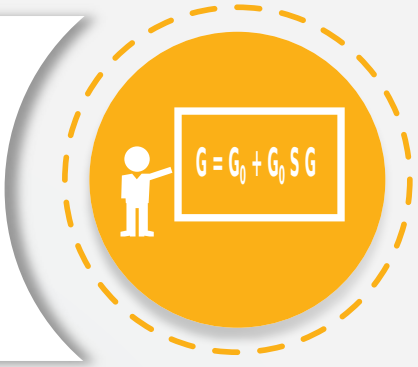
defining $(i\partial_t - h_0(1))\,G_0(1,2) = \delta(12)$

& assuming steady state (dependence on t-t' only)

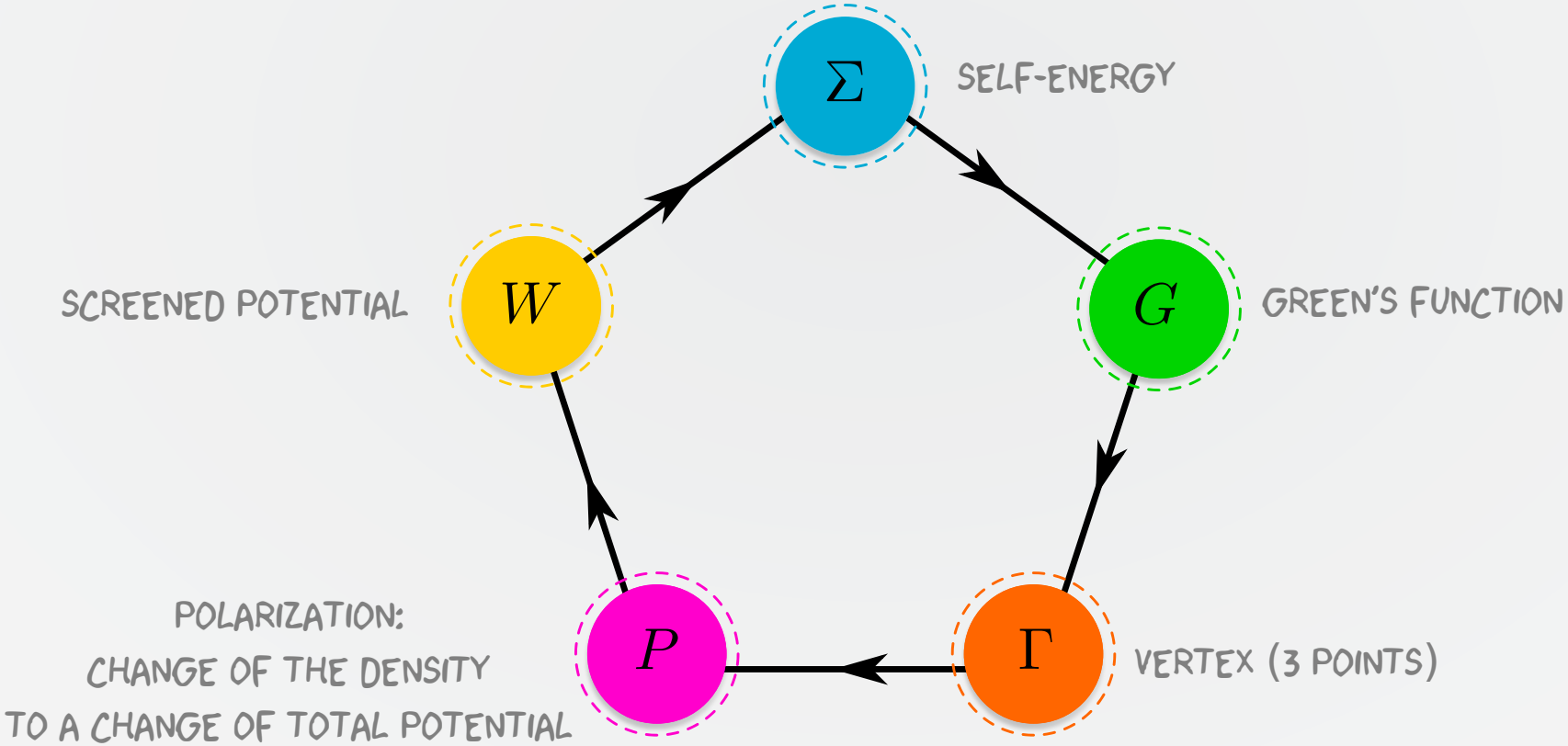
$$G(\mathbf{r},\mathbf{r}';\omega) = G_0(\mathbf{r},\mathbf{r}';\omega) + \iint d\mathbf{r}''d\mathbf{r}'''\,G_0(\mathbf{r};\mathbf{r}'';\omega)\Sigma(\mathbf{r}'',\mathbf{r}''';\omega)G(\mathbf{r}''',\mathbf{r}';\omega)$$

INTERACTING = NON-INTERACTING + SELF-ENERGY CORRECTIONS

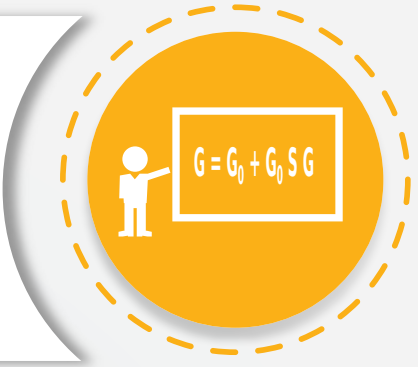
Carrying on with Schwinger functional derivative method eventually obtain Hedin equations



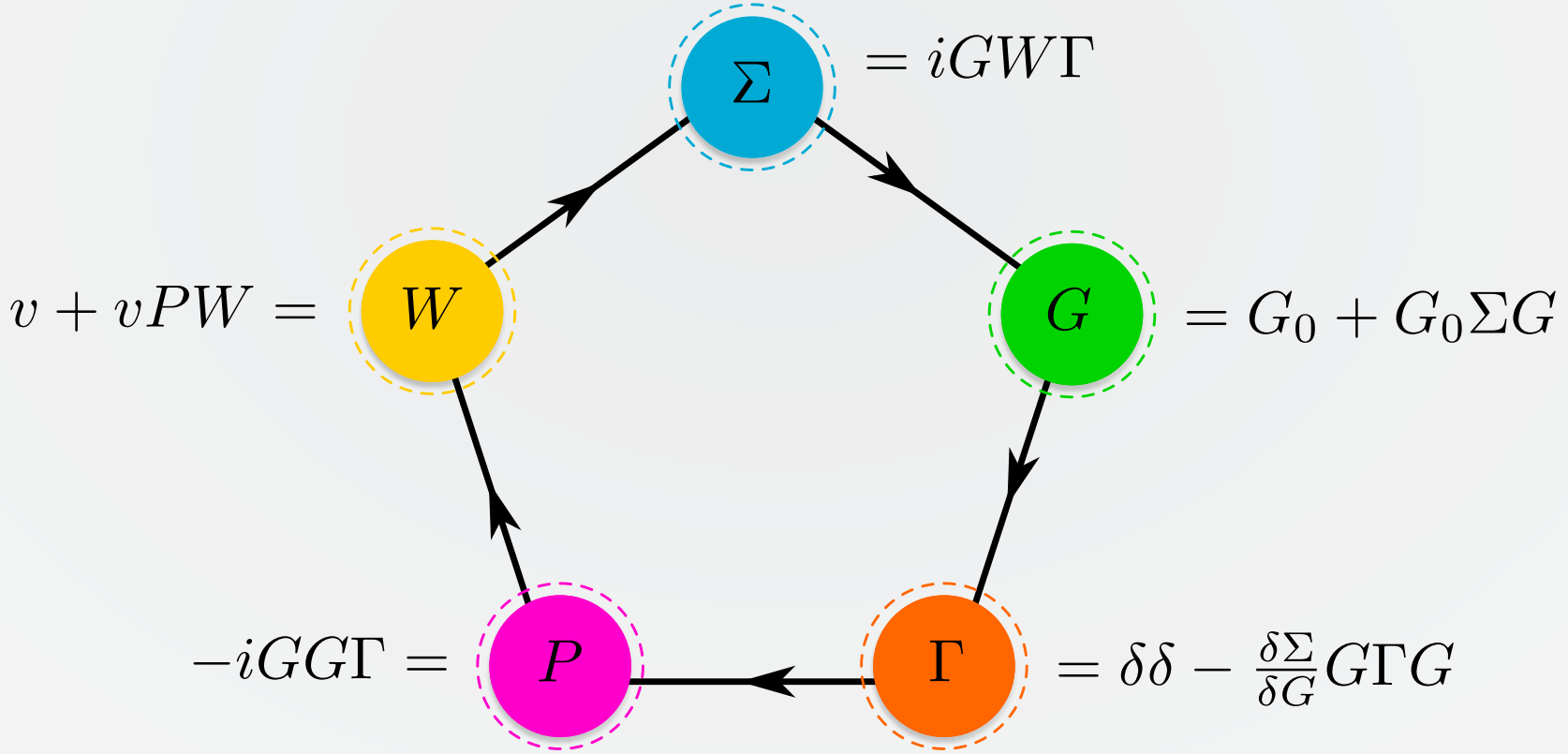
set of coupled integro-differential equation for:

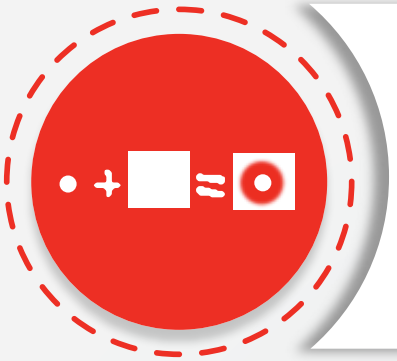


Carrying on with Schwinger functional derivative method eventually obtain Hedin equations

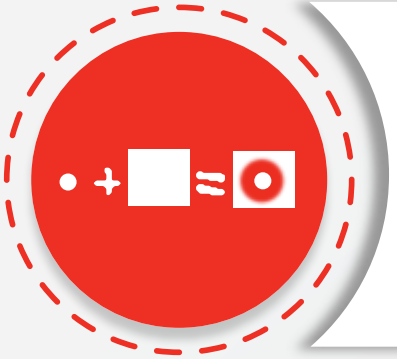


can be iterated analytically:



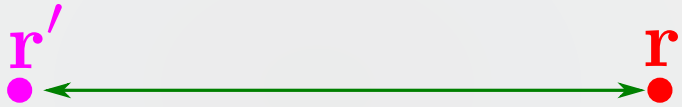


What is the physics we need to "put into" the self-energy?



Let's look at the potential due to an additional electron

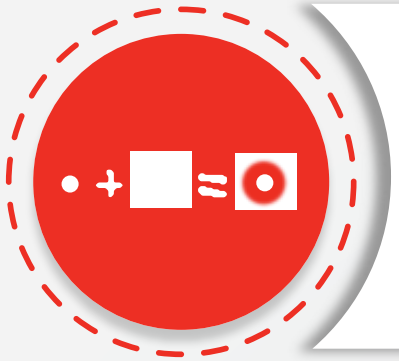
Let's neglect interaction between additional electron and electron system:



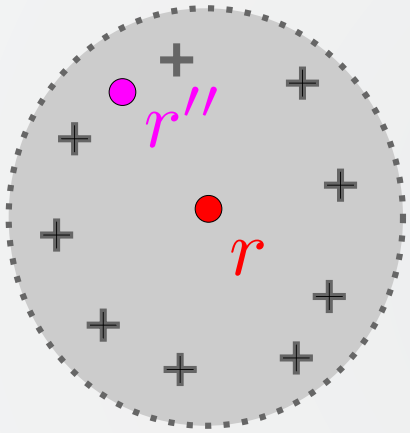
$$v(\mathbf{r},\mathbf{r}') = \frac{1}{|\mathbf{r}-\mathbf{r}'|}$$

This gives the Fock self-energy:

$$\Sigma_x(\mathbf{r},\mathbf{r}') = i\int d\omega\, G_0(\mathbf{r},\mathbf{r}';\omega)v(\mathbf{r},\mathbf{r}')$$



A test charge in an electron system induces a perturbation in the eletron density



electron gas +
positive background

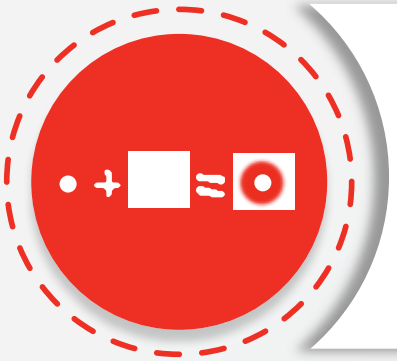
INDUCED CHARGE IN R'' DUE TO CHARGE IN R =

$$n^{\mathrm{ind}}(\mathbf{r}'', \mathbf{r}; \tau) = \int d\mathbf{r}' R(\mathbf{r}'', \mathbf{r}'; \tau) v(\mathbf{r}', \mathbf{r})$$

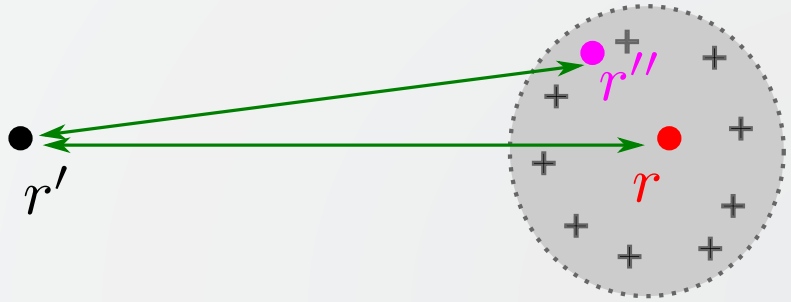
= DENSITY RESPONSE X POTENTIAL CHANGE IN R' DUE TO CHARGE IN R

where $$R(\mathbf{r}, t; \mathbf{r}', t') = \left. \frac{\delta n(\mathbf{r}, t)}{\delta V(\mathbf{r}', t')} \right|_{V=0}$$

DENSITY RESPONSE = CHANGE IN DENSITY AT R
DUE TO CHANGE IN POTENTIAL AT R'



In turn the induced charge changes (screens) the Coulomb potential



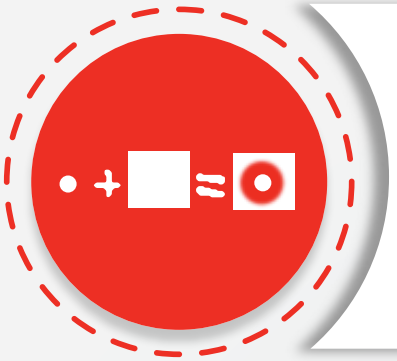
SCREENED POTENTIAL IN R' DUE TO TEST CHARGE IN R

$$W(\mathbf{r}',\mathbf{r};\tau) = v(\mathbf{r}',\mathbf{r}) + \int d\mathbf{r}'' v(\mathbf{r}',\mathbf{r}'') n^{\mathrm{ind}}(\mathbf{r}'',\mathbf{r};\tau)$$

$$= \int d\mathbf{r}'' \epsilon^{-1}(\mathbf{r}'',\mathbf{r};\tau) v(\mathbf{r}',\mathbf{r}'')$$

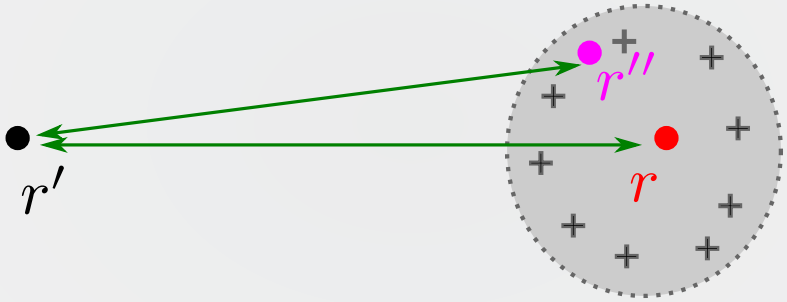
= BARE COULOMB + POTENTIAL DUE TO INDUCED CHARGE = INVERSE DIELECTRIC FUNCTION X BARE COULOMB POTENTIAL

with $$\epsilon^{-1}(\mathbf{r}'',\mathbf{r};\tau) = \delta(\mathbf{r}''-\mathbf{r}) + \int d\mathbf{r}_1 R(\mathbf{r}'',\mathbf{r}_1;\tau) v(\mathbf{r}_1,\mathbf{r})$$



Let's look at the potential due to an additional electron

when we consider the interaction between additional electron and electron system:



This gives the GW self-energy:

$$\Sigma_{xc}(\mathbf{r},\mathbf{r}';\omega) = i\int d\omega' \, G_0(\mathbf{r},\mathbf{r}';\omega')W(\mathbf{r},\mathbf{r}';\omega-\omega')$$

What effect on the calculated band gap do you expect when adding the screening?

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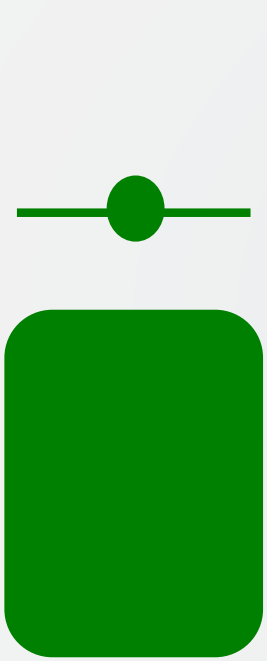


h_0

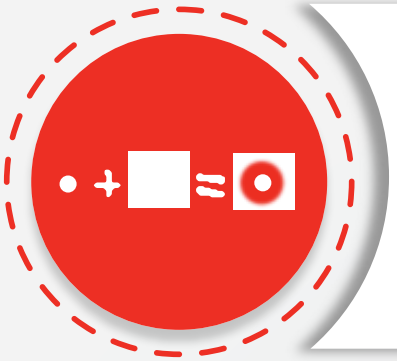
HARTREE
CLASSICAL MEAN FIELD POTENTIAL

Σ_x

FOCK EXCHANGE
PAULI CORRELATION

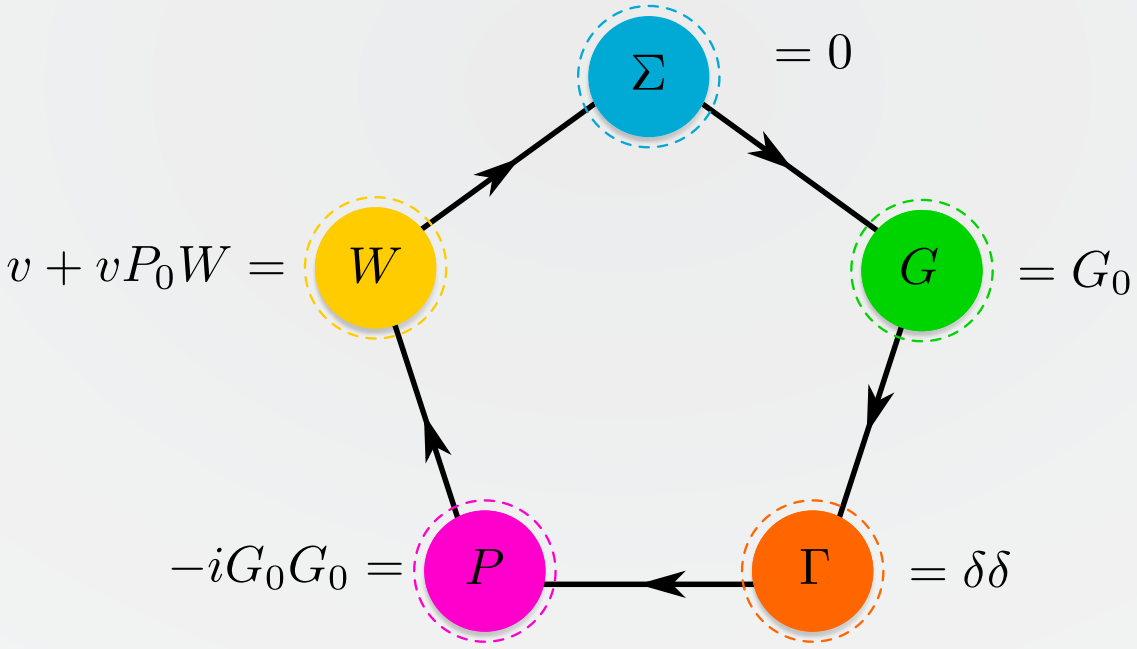
Σ_c

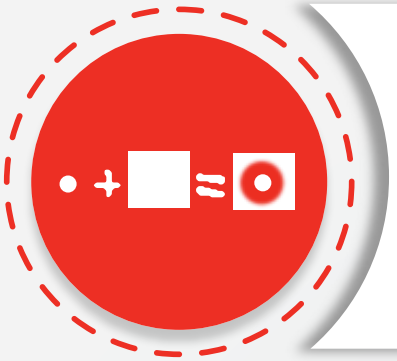
SCREENING
(LESS REPULSION)



GW approximation for the self-energy can be obtained rigorously from Hedin's equations

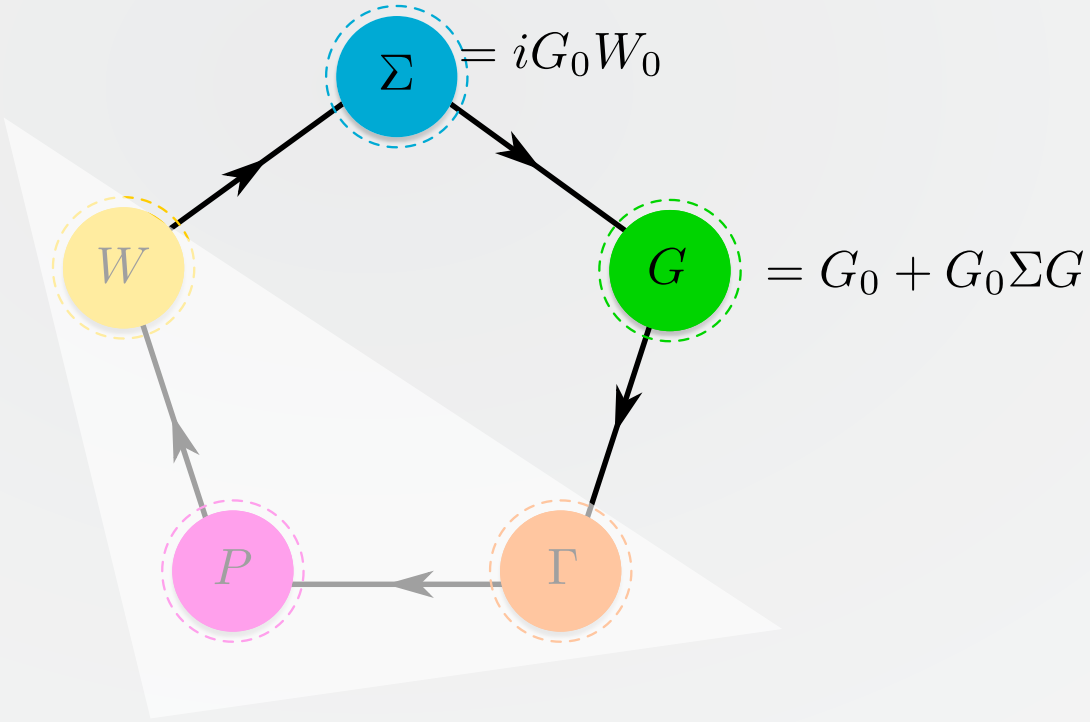
iteration 0:





GW approximation for the self-energy can be obtained rigorously from Hedin's equations

iteration 1:



How can we implement a feasible computational scheme?

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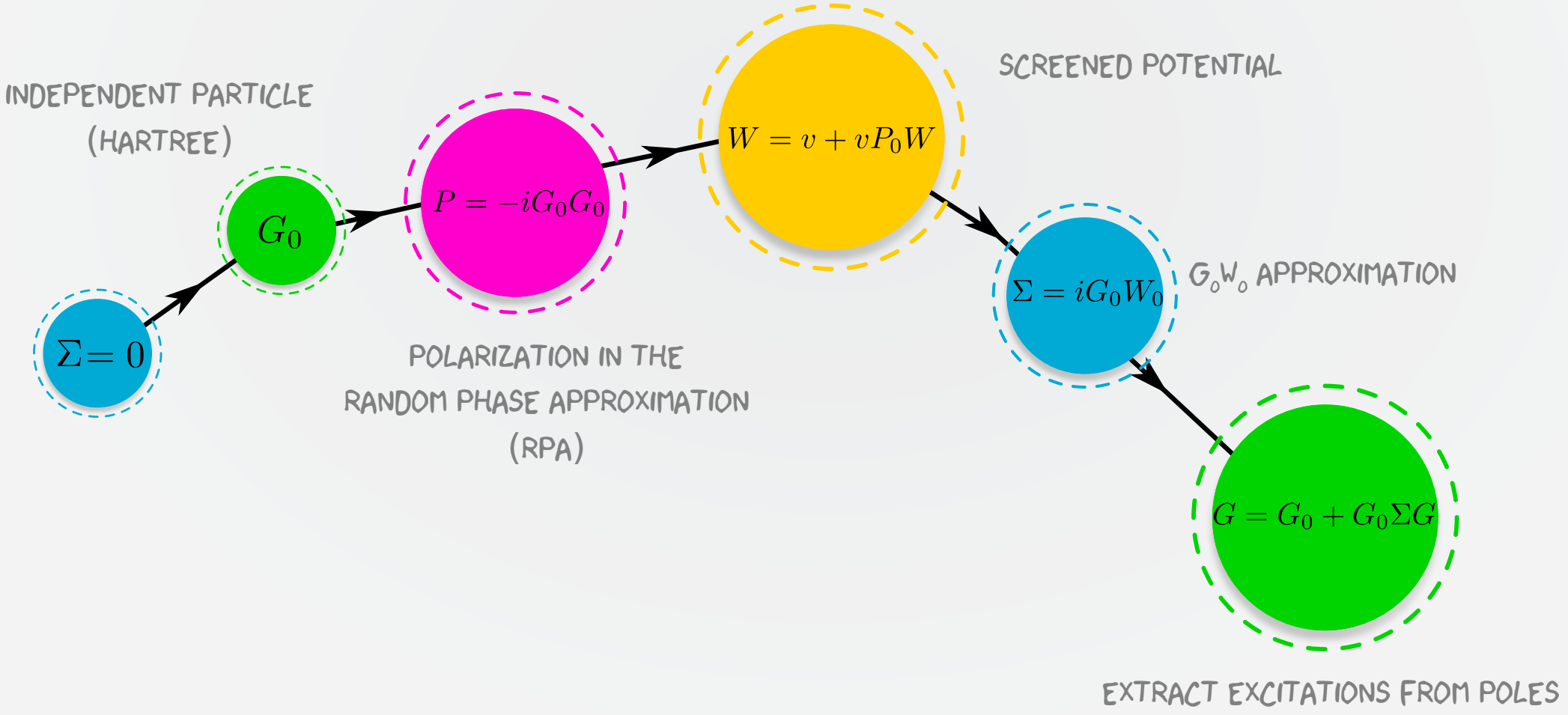
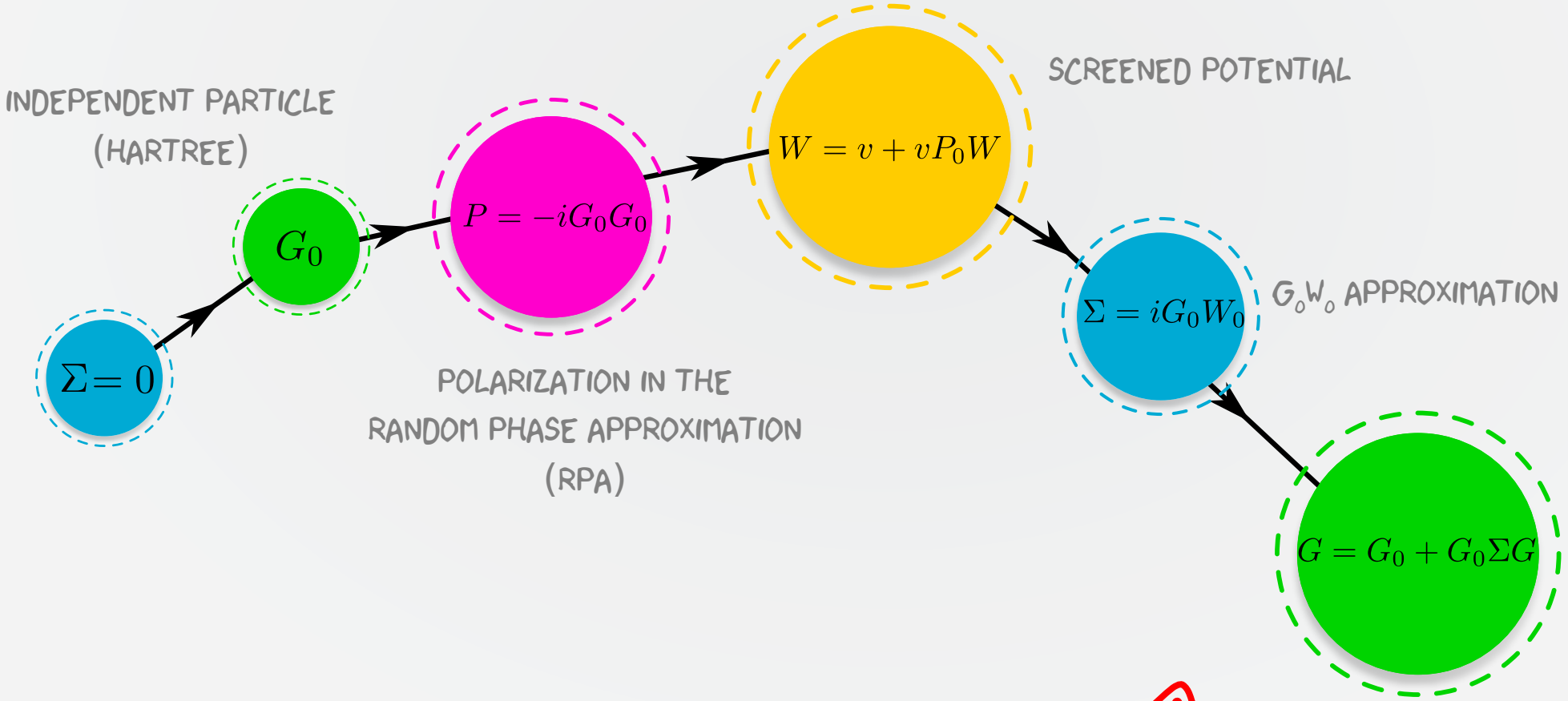
Recipe from Hedin's equations:



How can we implement a feasible computational scheme?

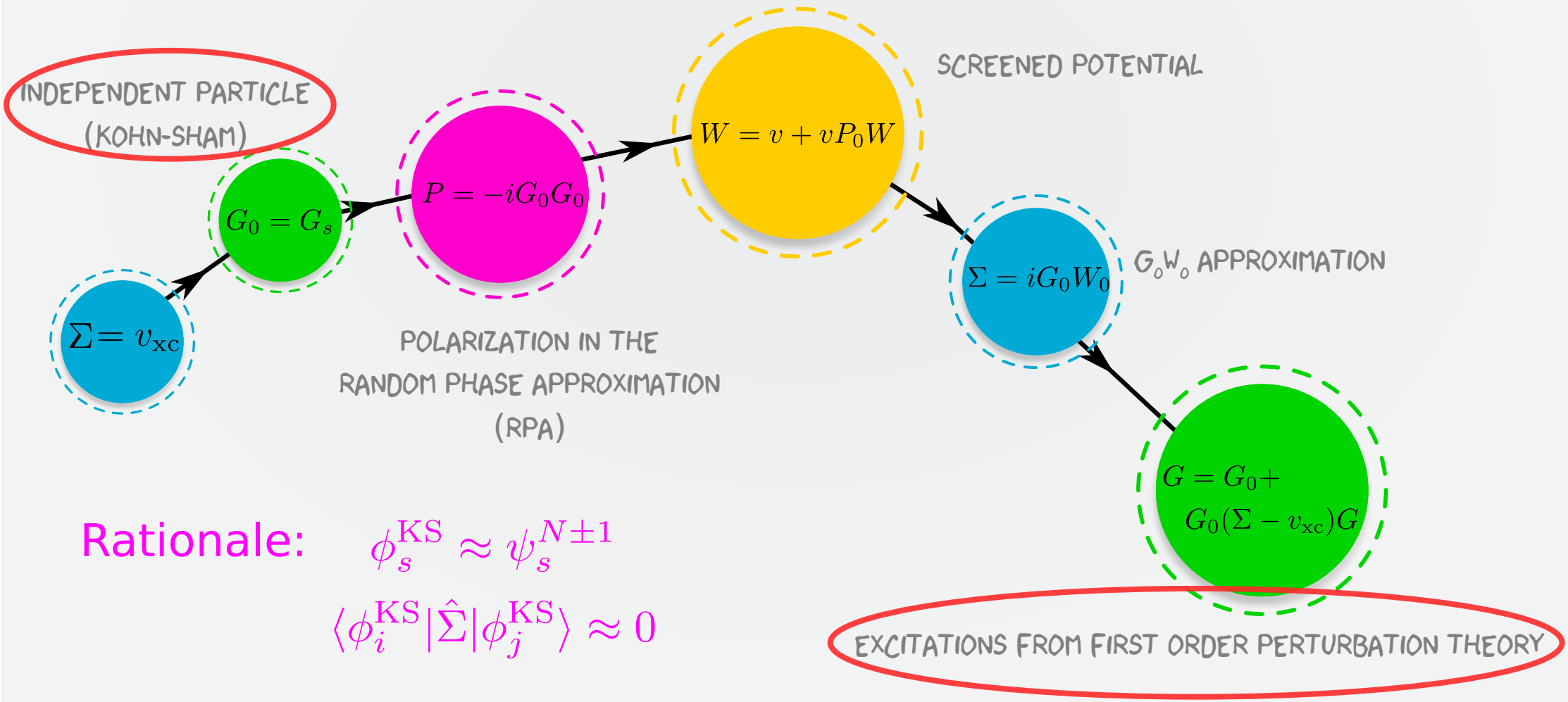
Recipe from Hedin's equations... problems!



How to solve this???

How can we implement a feasible computational scheme?

Modified recipe:



Rationale:

$$\phi_s^{\rm KS} \approx \psi_s^{N\pm1}$$

$$\langle \phi_i^{\rm KS} | \hat{\Sigma} | \phi_j^{\rm KS} \rangle \approx 0$$

In more detail one starts from a DFT calculation to obtain the Kohn-Sham eigensolutions

and calculate the non-interacting Green's function:

$$G_0(\mathbf{r},\mathbf{r}';\omega) = \sum_s^{\text{occ}} \frac{(\phi^{\text{KS}}(\mathbf{r}))^* \phi^{\text{KS}}(\mathbf{r}')}{\omega - \varepsilon_s^{\text{KS}} - i\eta} + \sum_s^{\text{unocc}} \frac{(\phi^{\text{KS}}(\mathbf{r}))^* \phi^{\text{KS}}(\mathbf{r}')}{\omega - \varepsilon_s^{\text{KS}} + i\eta}$$

solution of EOM:

$$\left(i\partial_t - \underbrace{h_0(1) - v_{\text{xc}}}_{h^{\text{KS}}} \right) G_0(1,2) = \delta(12)$$

Then evaluates the inverse dielectric function and screened potential

Polarisation:

$$P(\mathbf{r},\mathbf{r}';\omega) = \sum_{i}^{\text{occ}} \sum_{a}^{\text{unocc}} \phi_i(\mathbf{r})\phi_a^*(\mathbf{r})\phi_i^*(\mathbf{r}')\phi_a(\mathbf{r}') \times \left(\frac{1}{\omega + \varepsilon_i - \varepsilon_a + i\eta} - \frac{1}{\omega - \varepsilon_i + \varepsilon_a - i\eta} \right)$$

Dielectric matrix:

$$\epsilon(\mathbf{r},\mathbf{r}';\omega) = \delta(\mathbf{r}-\mathbf{r}') - \int d\mathbf{r}'' v(\mathbf{r},\mathbf{r}'') P_0(\mathbf{r}'',\mathbf{r}';\omega)$$

Inverse: $\epsilon^{-1}(\mathbf{r},\mathbf{r}';\omega),\ W(\mathbf{r},\mathbf{r}';\omega)$ IN A GIVEN BASIS (ALGEBRAIC PROBLEM!)

Then the self-energy matrix elements

EXCHANGE PART (FOCK), QUITE STRAIGHTFORWARD:

$$\langle \phi_s | \Sigma_x | \phi_s \rangle = \sum_i^{\text{occ}} \iint d\mathbf{r} d\mathbf{r}' \, \frac{\phi_i(\mathbf{r}) \phi_s^*(\mathbf{r}) \phi_i^*(\mathbf{r}') \phi_s(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}$$

CORRELATION PART (SCREENING), REQUIRES INTEGRATION OVER FREQUENCIES - EXPENSIVE...

$\langle \phi_s | \Sigma_c | \phi_s \rangle$ non trivial - numerical tricks/approximations needed to efficiently treat/reduce to analytical integral over frequencies

Finally calculates **perturbatively** the excitation energies

$$G(\mathbf{r},\mathbf{r}';\omega) = G_0(\mathbf{r},\mathbf{r}';\omega)$$
$$+ \iint d\mathbf{r}''d\mathbf{r}''' \, G_0(\mathbf{r};\mathbf{r}'';\omega)\left(\Sigma(\mathbf{r}'';\mathbf{r}''';\omega) - v_{\mathrm{xc}}(\mathbf{r}'')\delta(\mathbf{r}''-\mathbf{r}''')\right) G(\mathbf{r}''',t;\mathbf{r}',t')$$

PERTURBATION TO KS SOLUTION

At first order:

$$\phi_s^{\mathrm{KS}} \approx \psi_s^{N\pm1}$$
$$\langle\phi_i^{\mathrm{KS}}|\hat{\Sigma}|\phi_j^{\mathrm{KS}}\rangle \approx 0$$

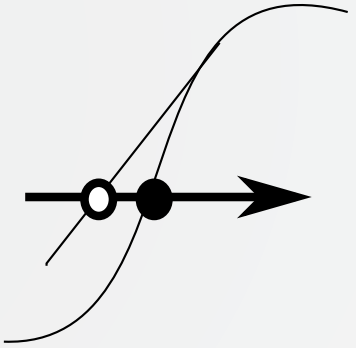
$$E_s = \varepsilon_s + \langle\phi_s|\Sigma(E_s) - v_{xc}|\phi_s\rangle$$

NONLINEAR!

Finally calculates **perturbatively** the excitation energies

$$E_s = \varepsilon_s + \langle \phi_s | \Sigma(E_s) - v_{xc} | \phi_s \rangle$$

Linearising (Newton): $\Sigma(E_s) \approx \Sigma(\varepsilon_s) + (E_s - \varepsilon_s) \frac{\partial \Sigma(\varepsilon)}{\partial \omega}$

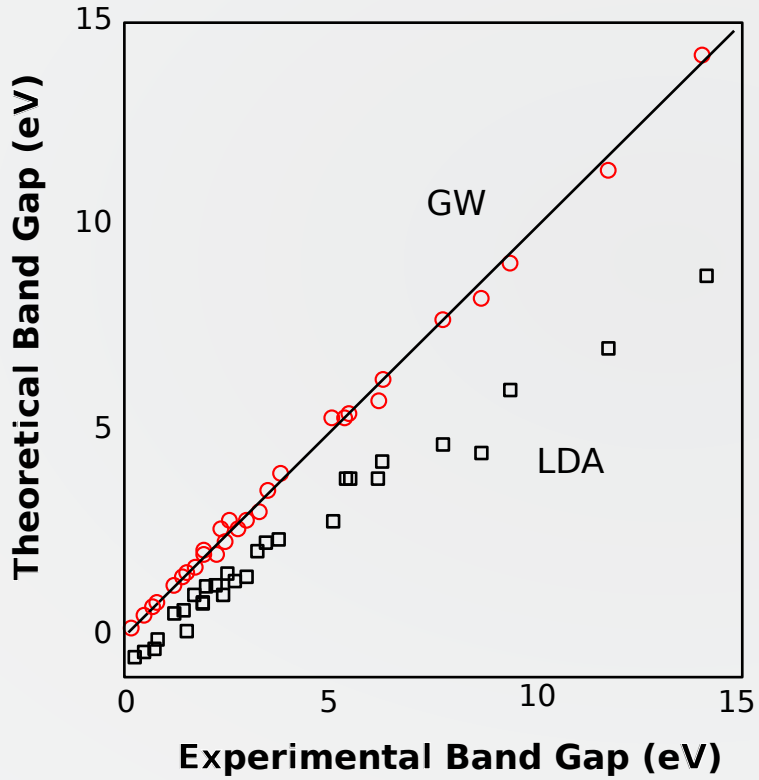


$$E_s = \varepsilon_s + Z_s \langle \phi_s | \Sigma(\varepsilon_s) - v_{xc} | \phi_s \rangle$$

$$Z_s = \left(1 - \langle \phi_s | \frac{\partial \Sigma(\omega)}{\partial \omega} |_{\omega=\varepsilon_s} | \phi_s \rangle\right)^{-1}$$

RENORMALIZATION FACTOR

How does this approach work?



Hedin, J. Phys. Cond Matt 11, R489 (1999)

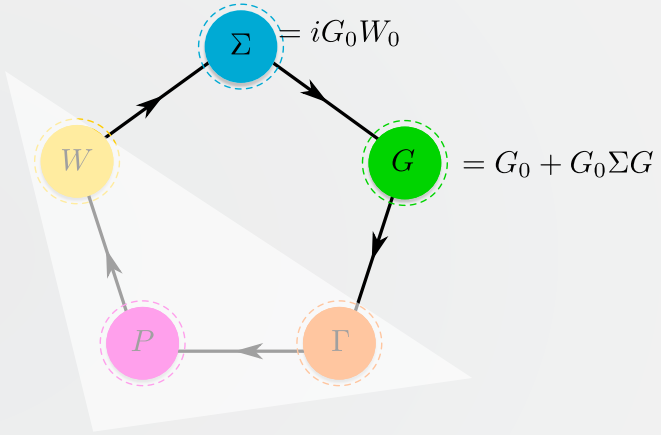
It corrects the underestimation of the LDA and takes calculated band-gaps close to the experimental values

$$E_s = \varepsilon_s + Z_s \langle \phi_s | \Sigma(\varepsilon_s) - v_{xc} | \phi_s \rangle$$

Can you trace back
all approximations we made
in obtaining the working equations?

Can you trace back all approximations we made in obtaining the working equations?

stopping at first iteration
(no vertex, RPA for polarization)



$$\phi_s^{\mathrm{KS}} \approx \psi_s^{N\pm1}$$

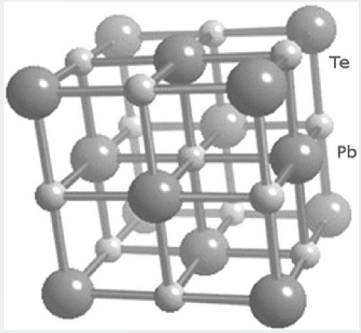
$$\langle \phi_i^{\mathrm{KS}} | \hat{\Sigma} | \phi_j^{\mathrm{KS}} \rangle \approx 0$$

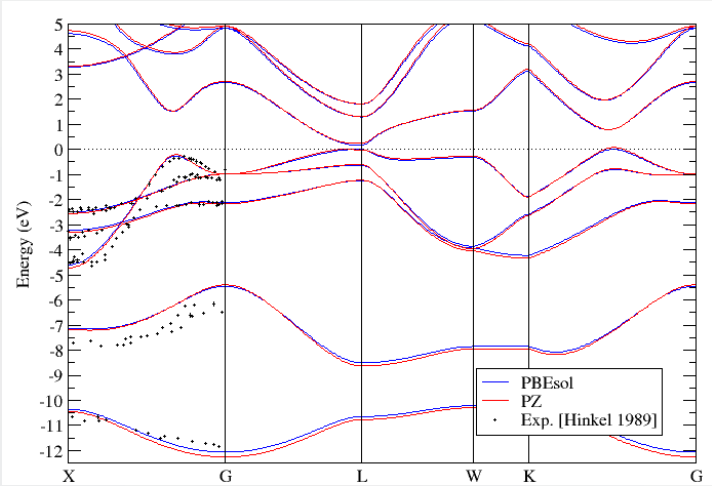
solving Dyson
within first-order PT

... more in numerical solutions

G0W0 is not enough...
...an example

lead telluride





	a (Ang)	B (Mbar)	Gap (eV)	SOS of VB @ Γ (eV)	SOS of CB @ L (eV)
Experiment	6.45	0.46	0.31	1.10 - 1.15	
Ours (PBEsol)	6.437	0.44	0.15(d)	1.14	0.51
Ours (PZ)	6.376	0.47	0.17(i)	1.17	0.51
Rabe & Joannopoulos (PZ)	6.29	0.45	0.4	1.2	
Hummer et al. (HSE03)	6.52	0.40	0.25	1.1	0.5

courtesy of Pablo Aguado-Puente

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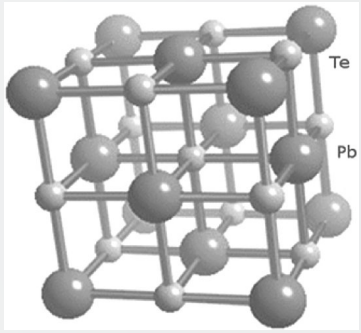
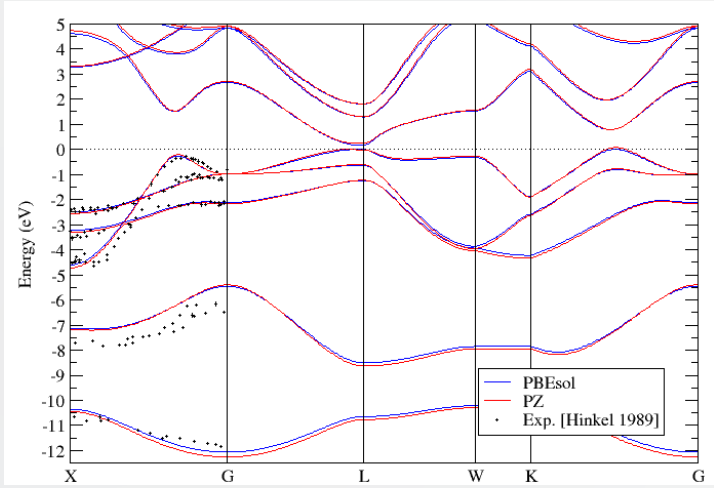
...an example

lead telluride



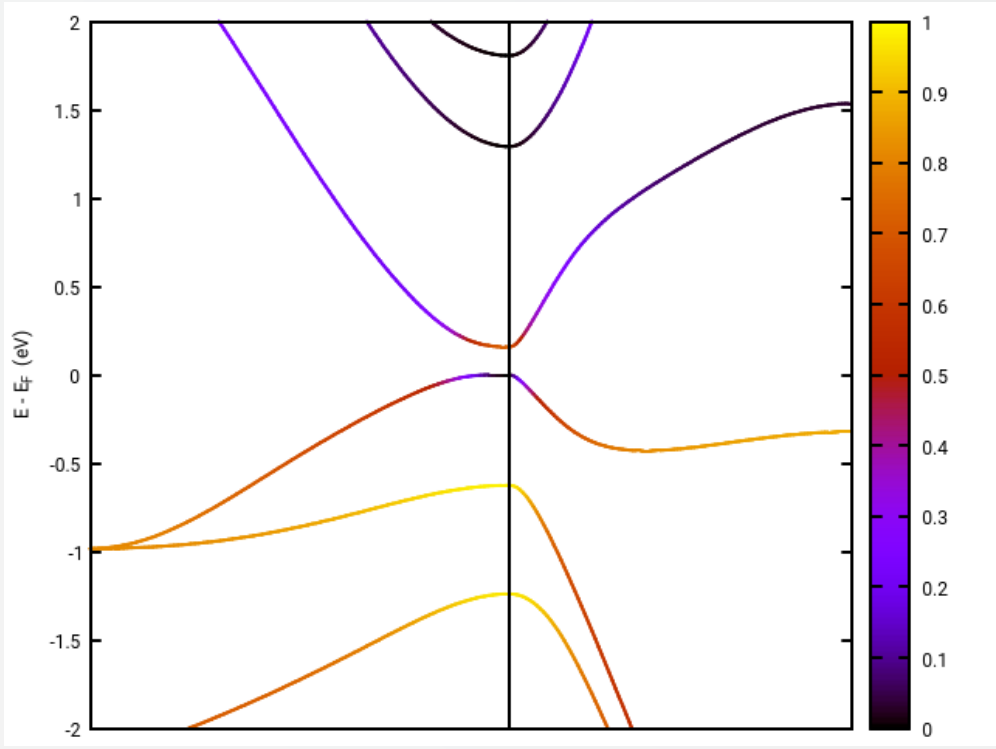


	$m^e_{\parallel}$	$m^e_{\perp}$	$m^h_{\parallel}$	$m^h_{\perp}$
Experiment	0.24	0.024	0.31	0.022
Ours (PBEsol+SO)	0.7	0.05	1.5	0.07
Svane et al. (scGW)	0.247	0.028	0.338	0.029
Hummer et al. (HSE03)	0.223	0.027	0.296	0.029

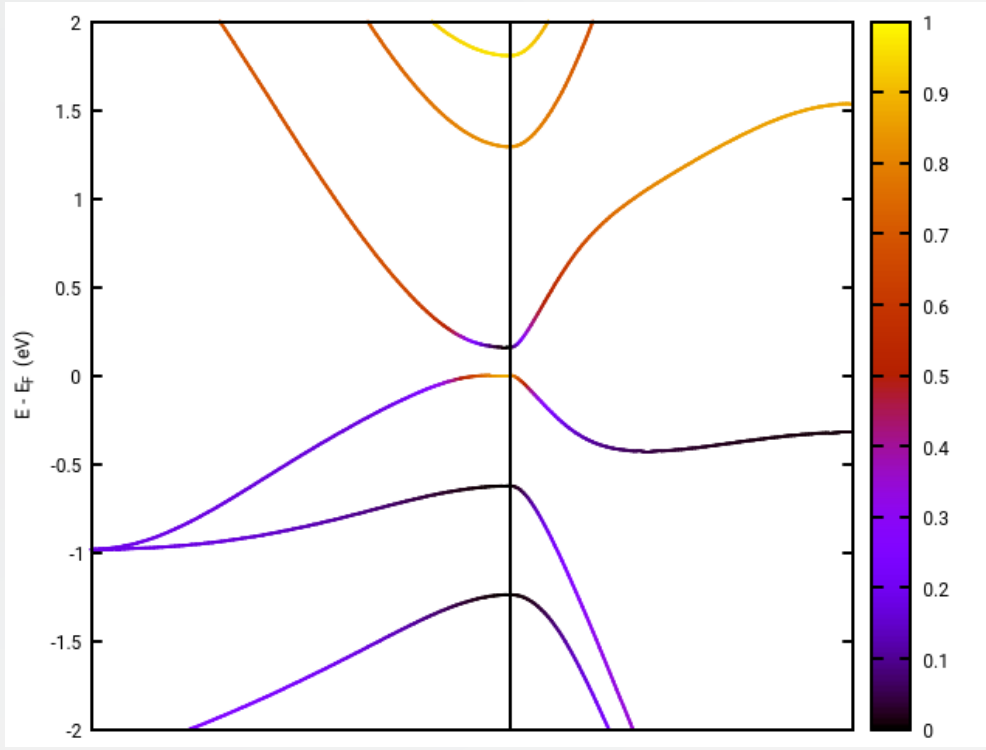
courtesy of Pablo Aguado-Puente

G0W0 is not enough...
...an example

projection of the bands on atomic-like wave functions:



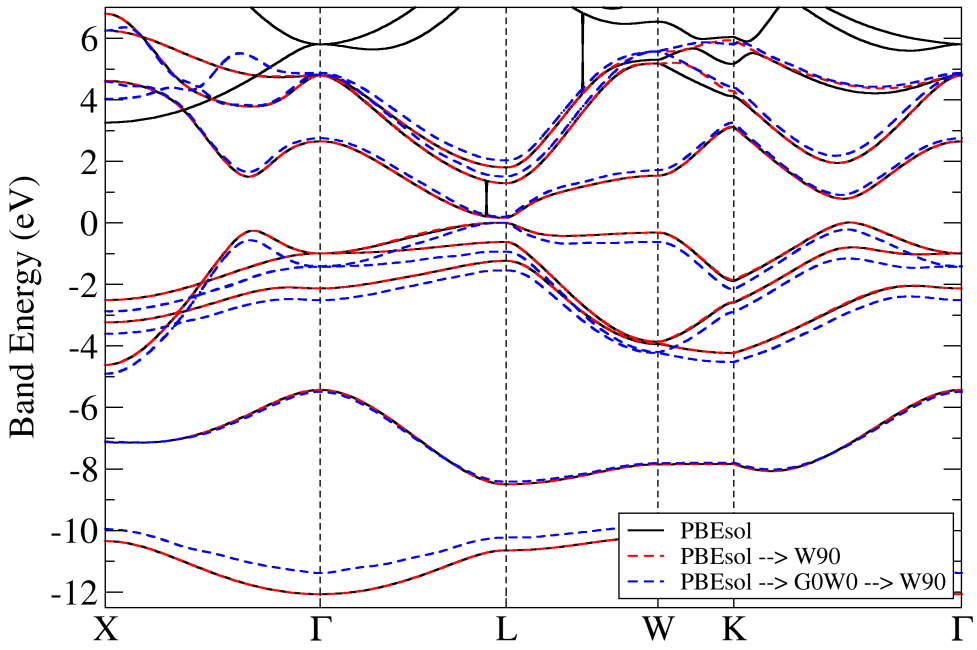
Te:5p L



Pb:6p L

courtesy of Pablo Aguado-Puente

G0W0 is not enough...
...an example



	$m^e_{\parallel}$	$m^e_{\perp}$	$m^h_{\parallel}$	$m^h_{\perp}$
Experiment	0.24	0.024	0.31	0.022
Ours (PBEsol)	0.7	0.05	1.5	0.07
Ours (PBEsol+G0W0)	0.30-0.35	0.021	0.44-0.62	0.022
Svane et al. (scGW)	0.247	0.028	0.338	0.029
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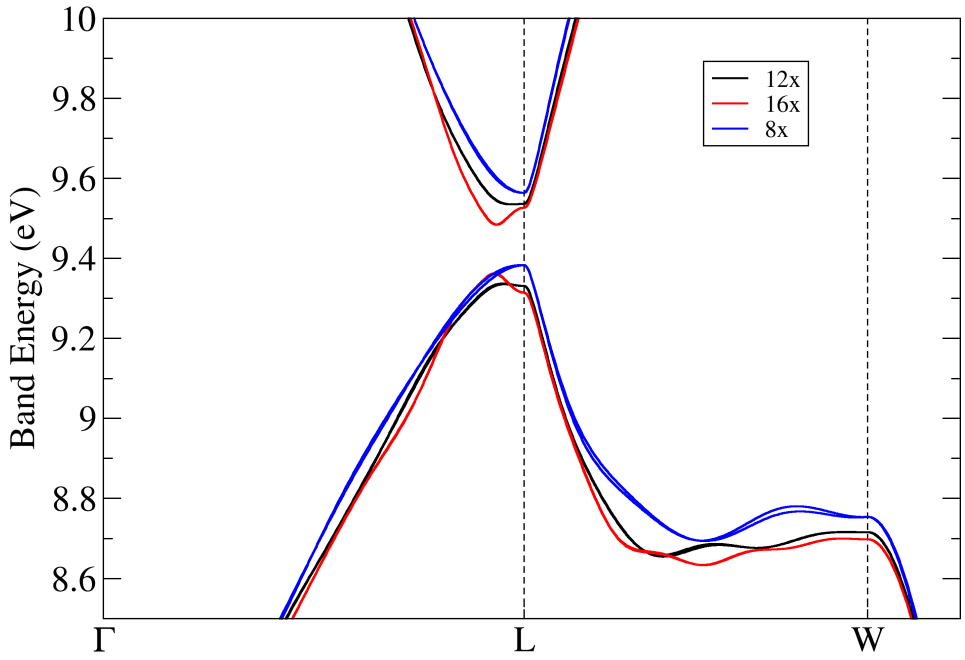

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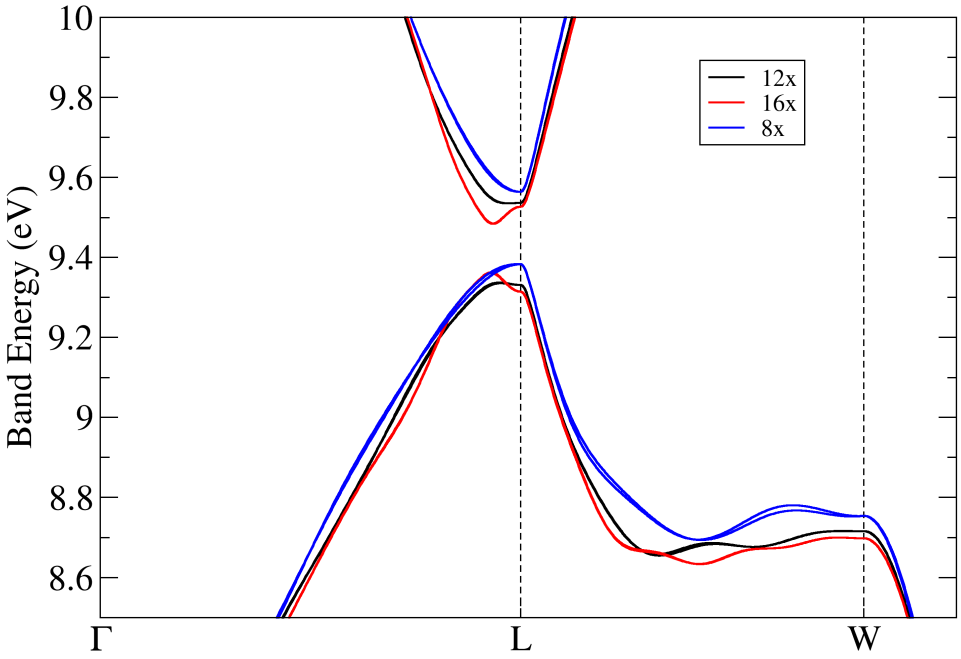
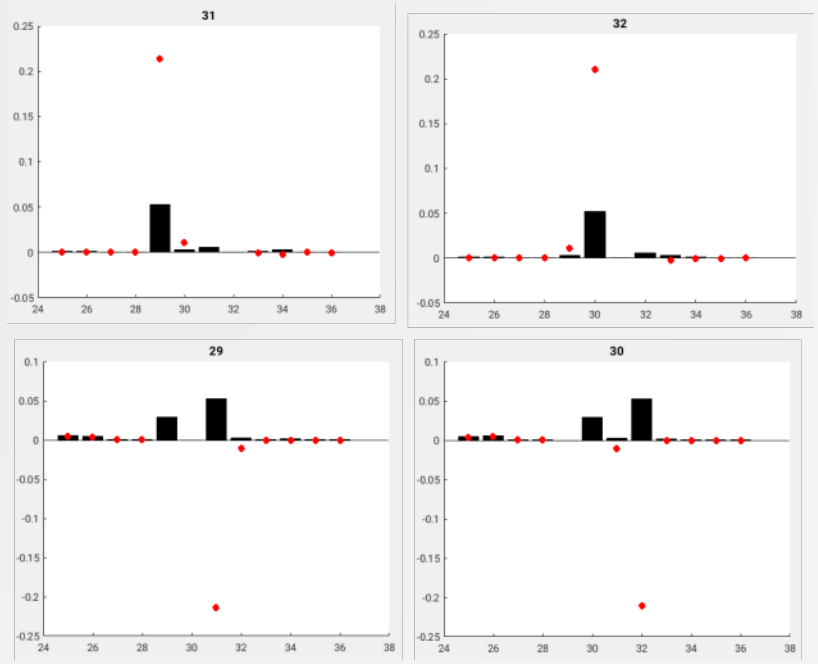


For the closest k to the L point:
in black $\Re\left(\langle n|\Sigma|m\rangle\langle m|\Sigma|n\rangle\right)$



The previous quantity weighted by the energy difference between states is plotted in red.

courtesy of Pablo Aguado-Puente

Bibliography:

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RM Martin, L. Reining and DM Ceperley - Cambridge University Press (2016)

Application of the Green’s functions method to the study
of the optical properties of semiconductors, G. Strinati
RIVISTA DEL NUOVO CIMENTO VOL. 11, N. 12 1988

Electronic Excitations: Density-Functional vs
Many-body Green's , G. Onida, L. Reining, A. Rubio
Rev. Modern Phys. 74, 601 (2002)

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