The GW approximation

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Outline

References


L. Hedin
Phys. Rev. **139**, A796 (1965).


L. Hedin and S. Lundqvist
Solid State Physics **23** (Academic, New York, 1969).


G. Strinati
Rivista del Nuovo Cimento **11**, (12)1 (1988).


G. Onida, L. Reining, and A. Rubio
Rev. Mod. Phys. **74**, 601 (2002).

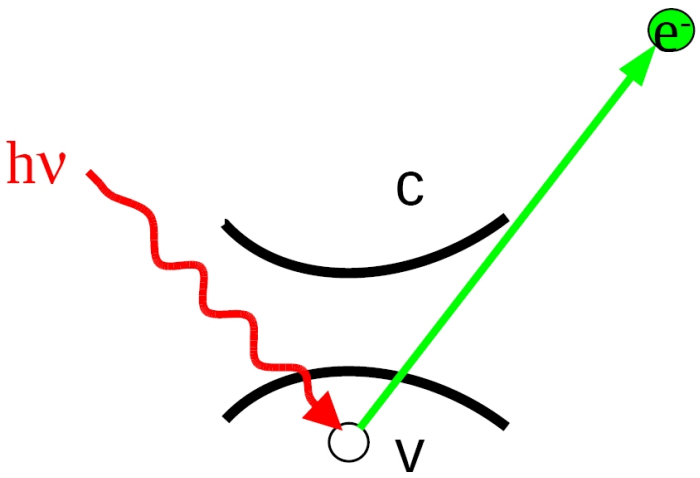

F. Bruneval and M. Gatti
Topics in Current Chemistry, in press


F. Bruneval
PhD thesis, Ecole Polytechnique (2005)
`http://theory.polytechnique.fr/people/bruneval/bruneval_these.pdf`

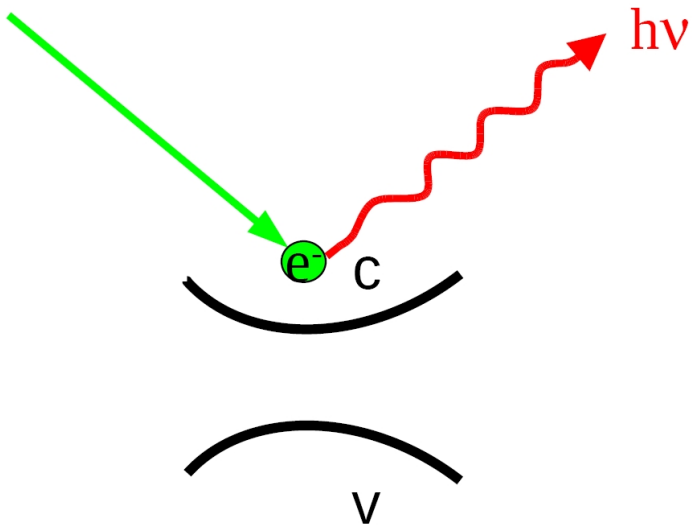
Outline

Photoemission

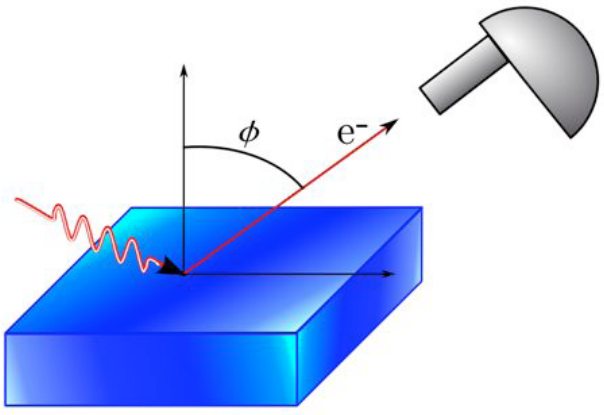
Direct Photoemission



Inverse Photoemission



Direct Photoemission

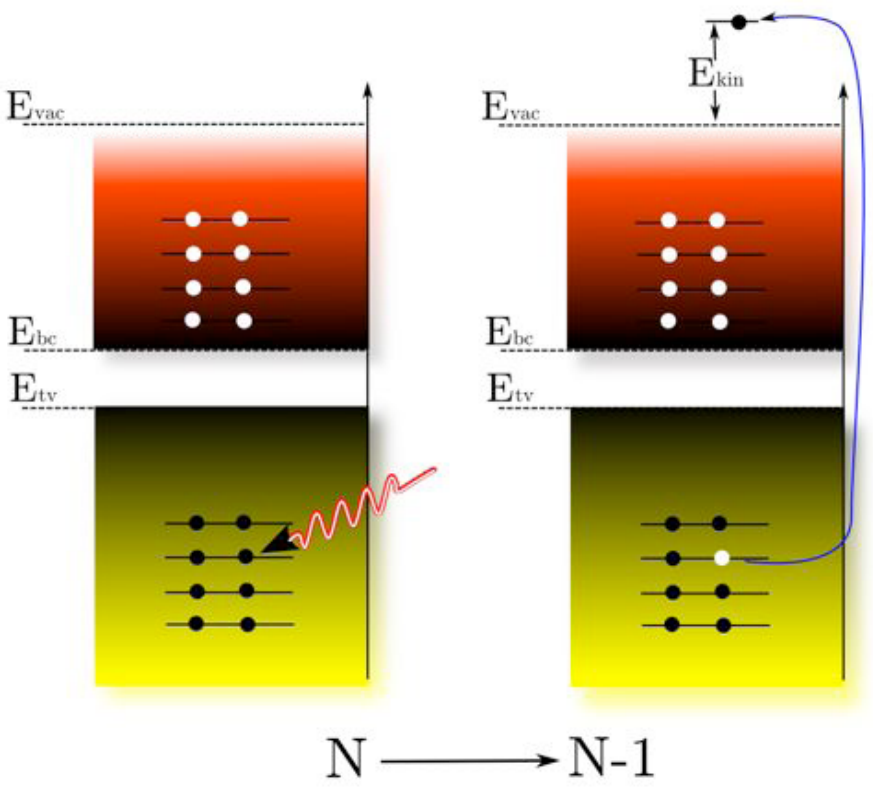


photon in - electron out

$$E(N) + h\nu = E(N-1, i) + E_{kin}$$

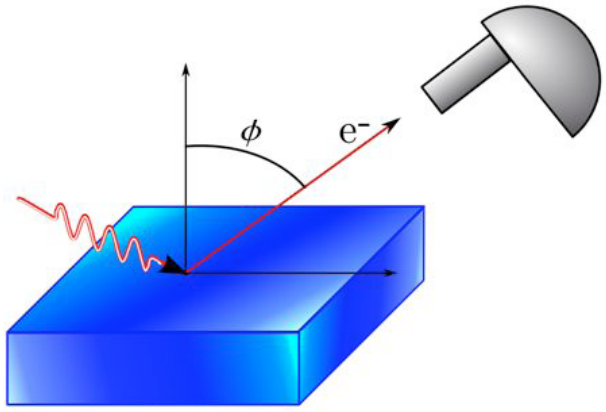
$$E_i = E(N) - E(N-1, i) = E_{kin} - h\nu$$

...plus momentum conservation $\Rightarrow$ ARPES



occupied states

Direct Photoemission



photon in - electron out

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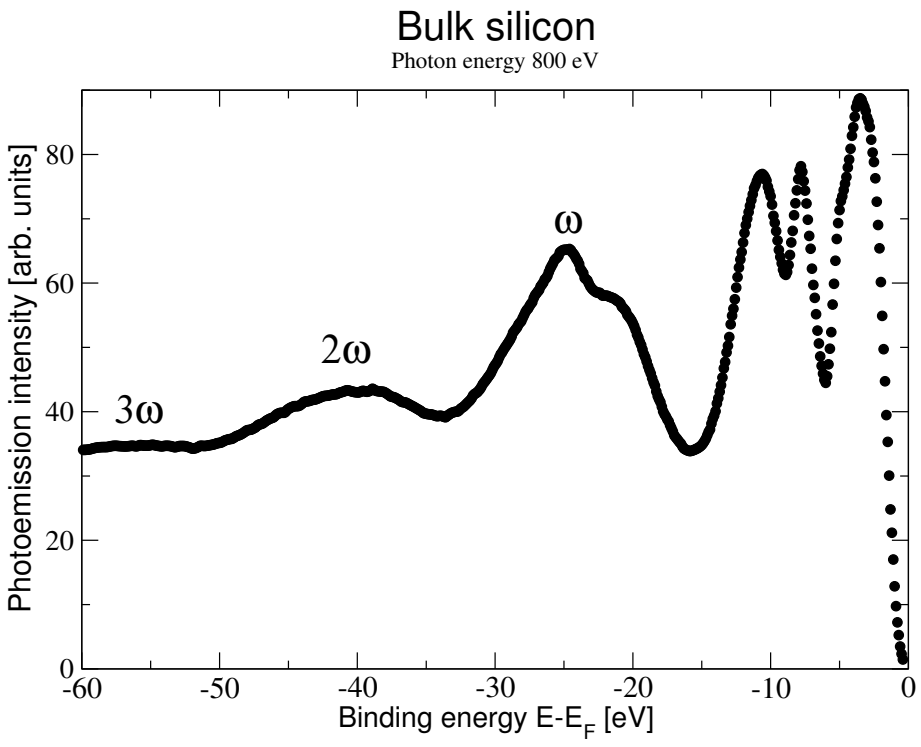
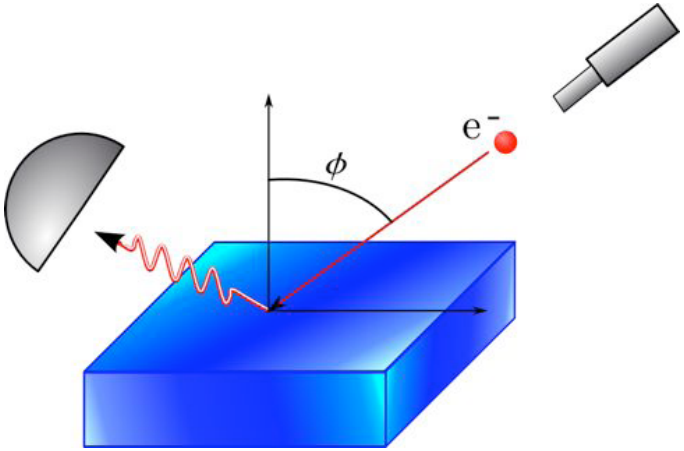


M. Guzzo *et al.*, PRL 107 (2011).

Inverse Photoemission

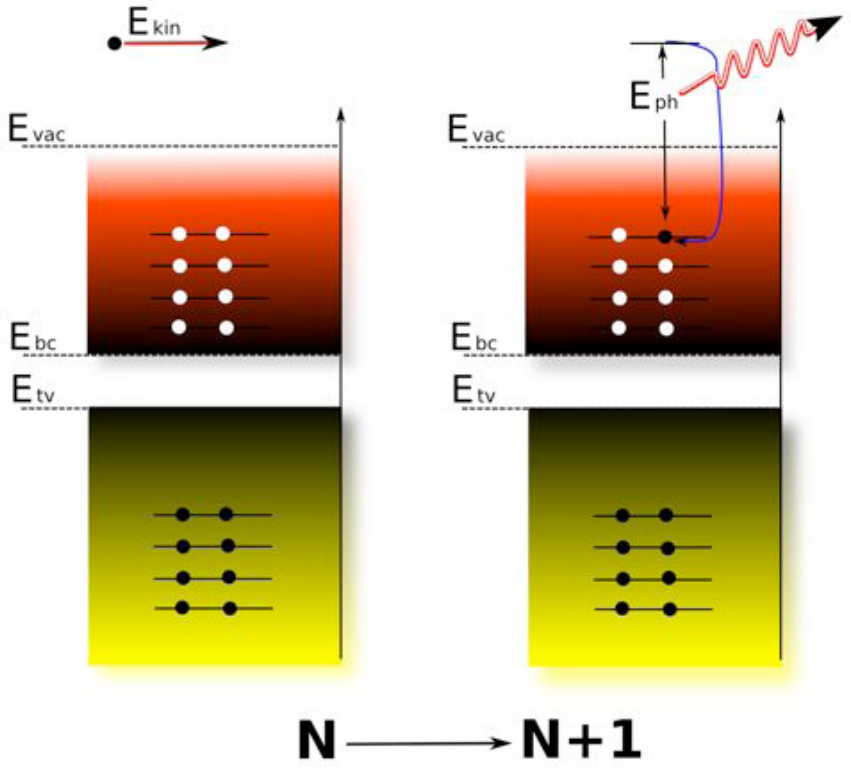


electron in - photon out

$$E(N) + E_{kin} = E(N+1, i) + h\nu$$

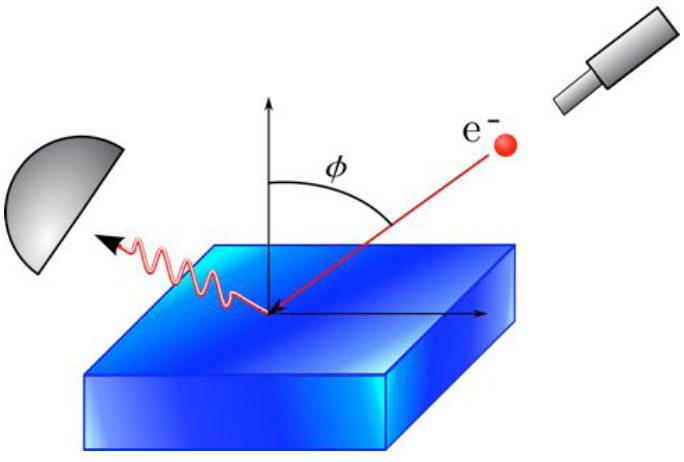
$$E_i = E(N+1, i) - E(N) = E_{kin} - h\nu$$

aka Bremsstrahlung
isochromat spectroscopy (BIS)

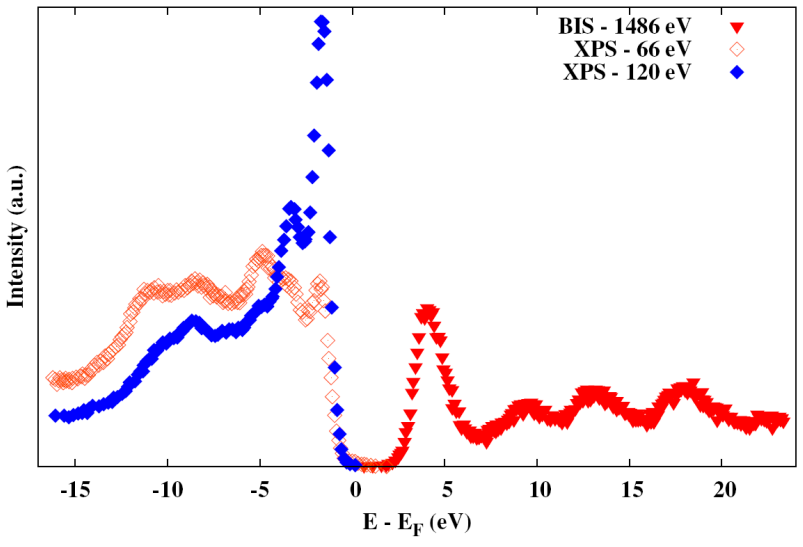


empty states

Inverse Photoemission

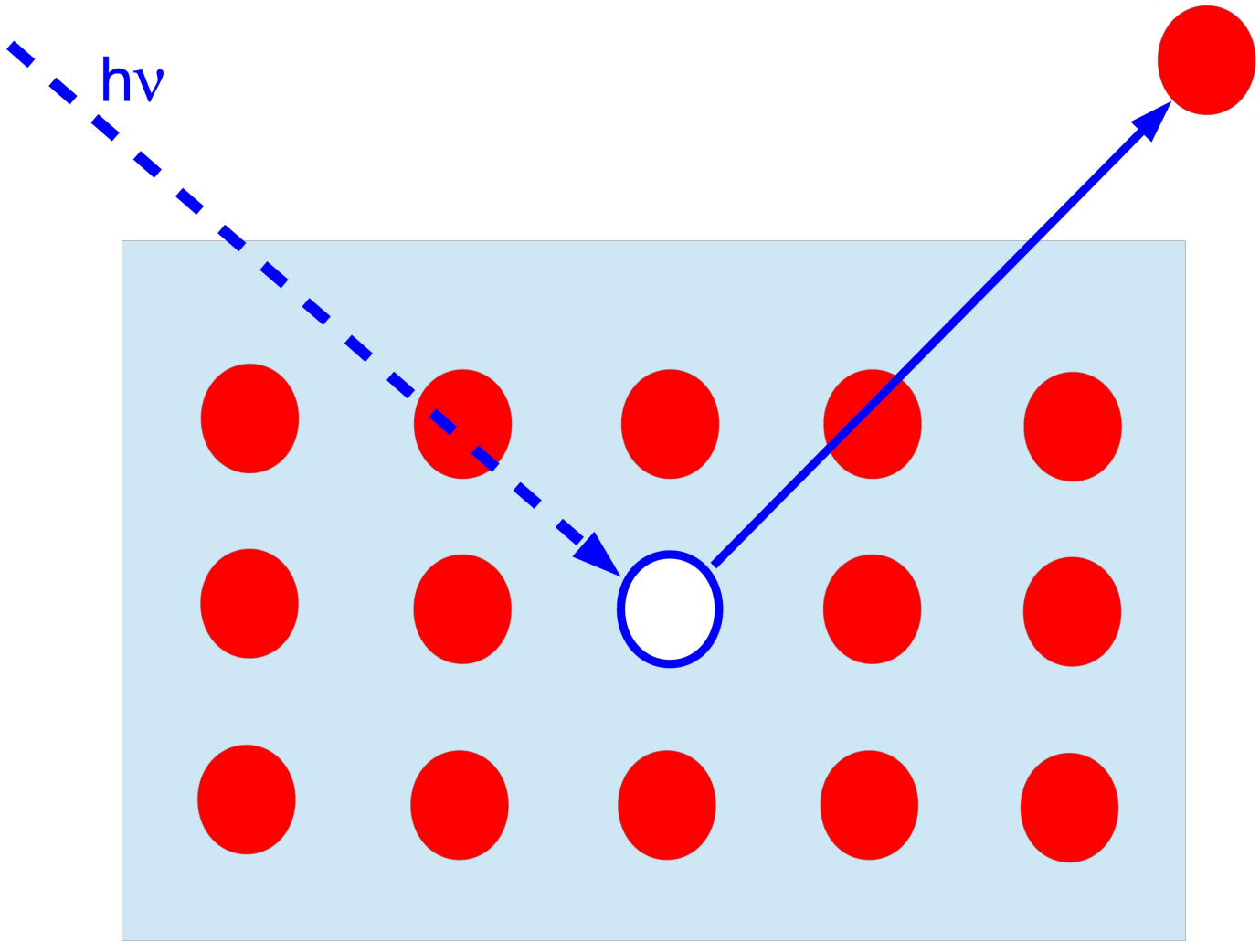


electron in - photon out

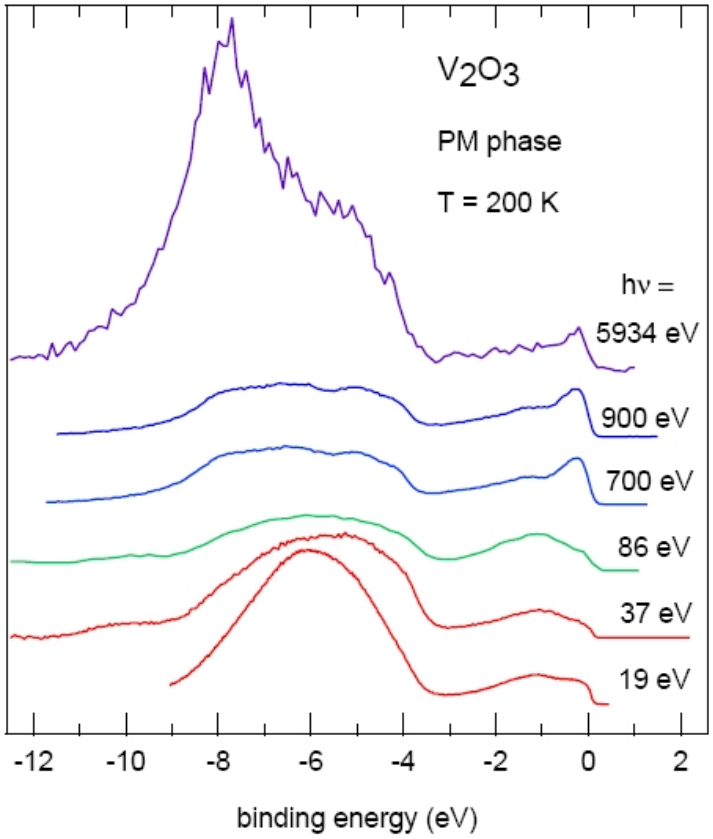


Nickel oxide
Sawatzky and Allen PRL 53 (1984)

Photoemission



Photoemission



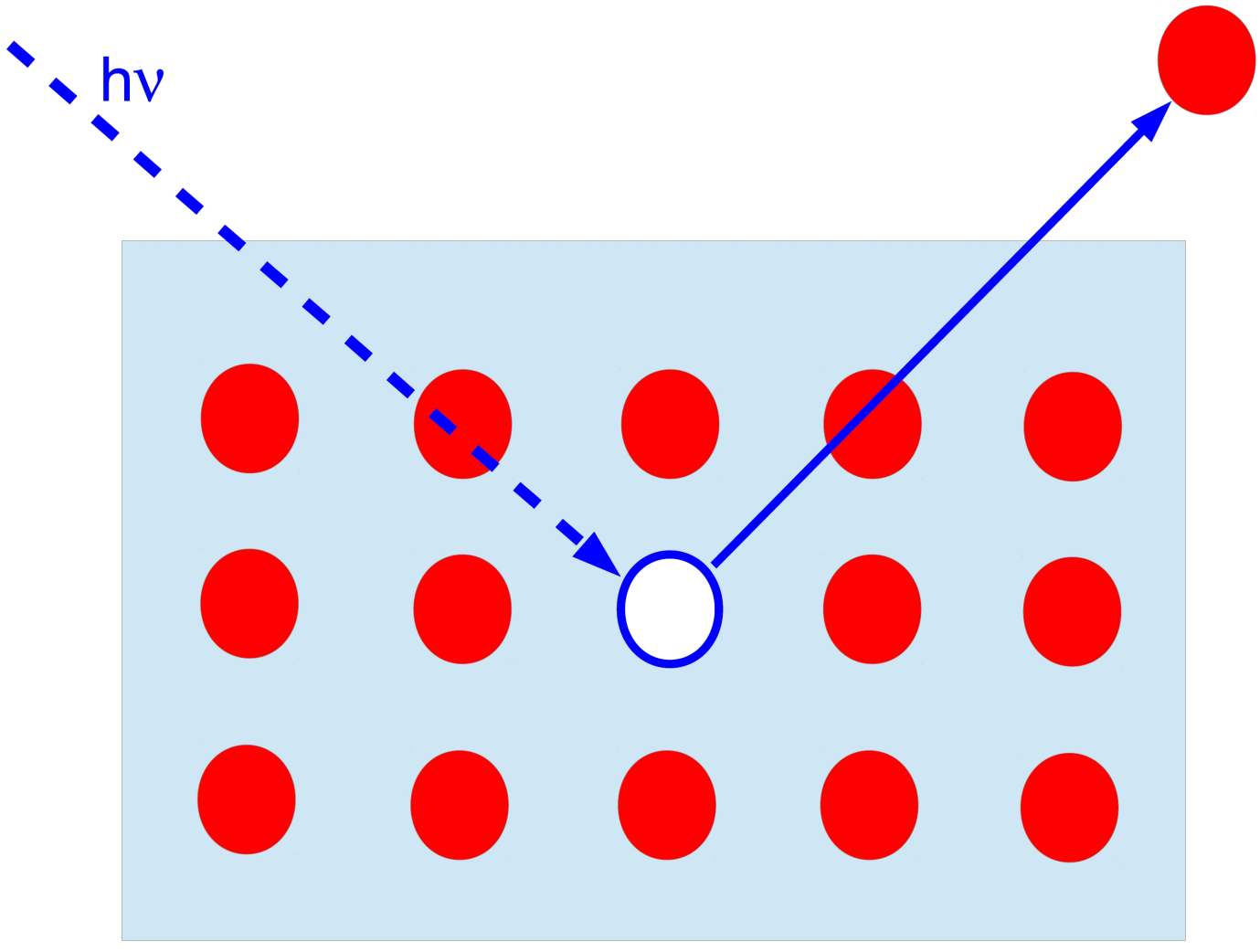
E. Papalazarou *et al.*, PRB 80 (2009)

Not discussed here:

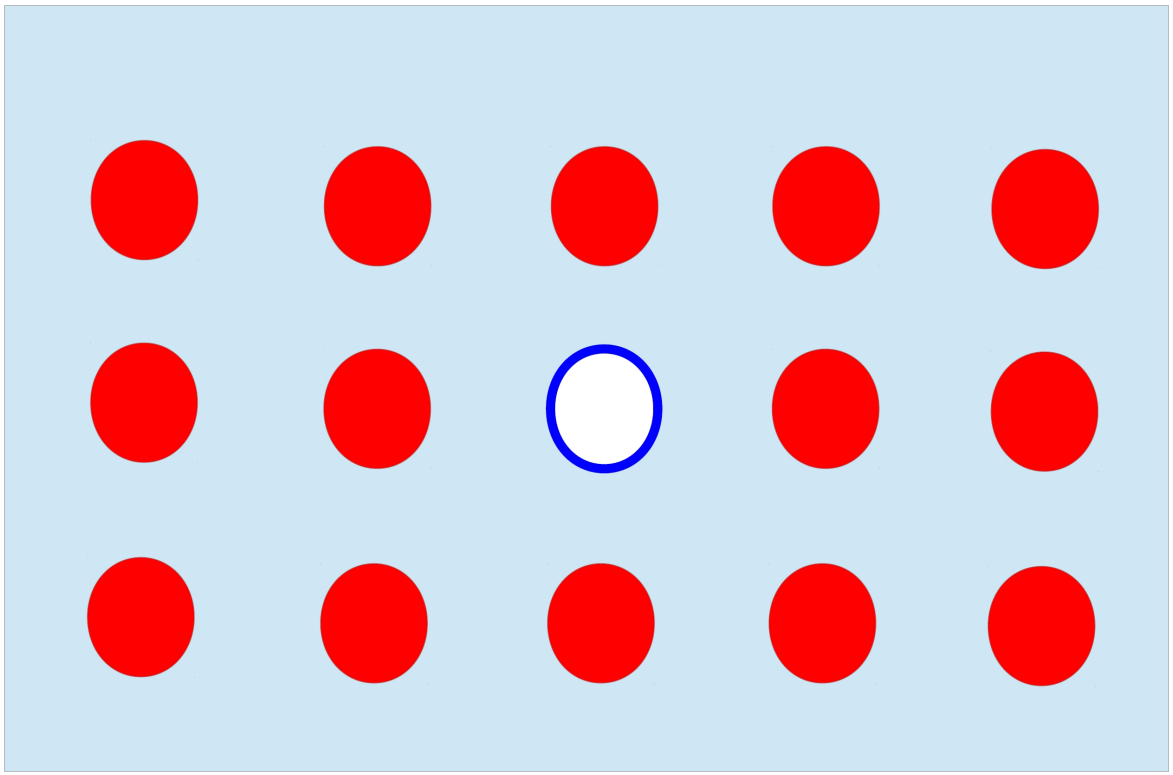
- matrix elements - cross sections (dependence on photon energy / photon polarization)
- sudden approximation vs. interaction photoelectron - system
- surface sensitivity
- ...

S. Hüfner, *Photoelectron spectroscopy* (1995)

Photoemission: additional charge

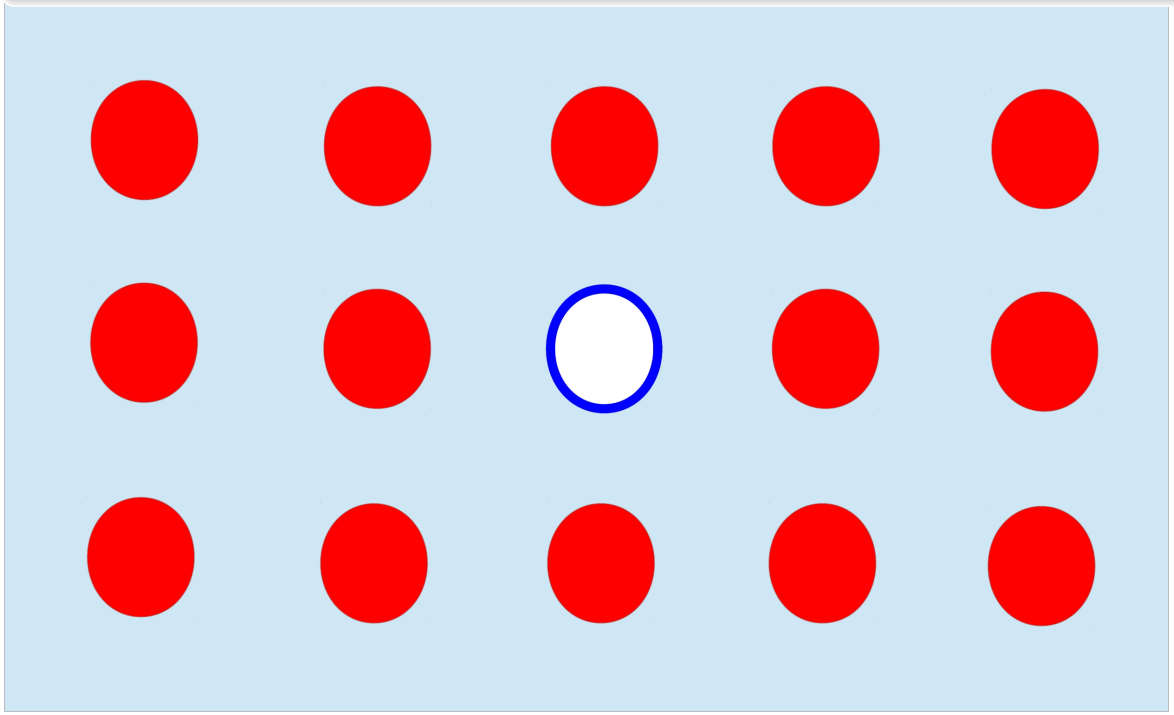


Photoemission: additional charge



Photoemission: additional charge

What happens?



Outline

One-particle Green's function

What is the one-particle Green's function $G(1,2) = G(\mathbf{x_1}, \mathbf{x_2}, t_1 - t_2)$?

One-particle Green's function

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The one-particle Green's function G

1. Propagation of one additional particle in the system

$$iG(\mathbf{x_1}, \mathbf{x_2}, t_1 - t_2) = \langle N| T\left[\psi(\mathbf{x_1}, t_1)\psi^\dagger(\mathbf{x_2}, t_2)\right] |N\rangle$$

How to calculate G?

One-particle Green's function

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How to calculate G?

2. Resolvent of $H(\omega) = H_0 + \Sigma(\omega) = h_0 + V_H + \Sigma(\omega)$:

$$G^{-1}(\omega) = (\omega - H_0 - \Sigma(\omega)) = (G_0^{-1}(\omega) - \Sigma(\omega))$$

What is $H(\omega)$? What is $\Sigma(\omega)$?

One-particle Green's function

The one-particle Green's function G

Definition and meaning of G:

$$iG(\mathbf{x_1}, t_1; \mathbf{x_2}, t_2) = \langle N| T\left[\psi(\mathbf{x_1}, t_1)\psi^\dagger(\mathbf{x_2}, t_2)\right]|N\rangle$$

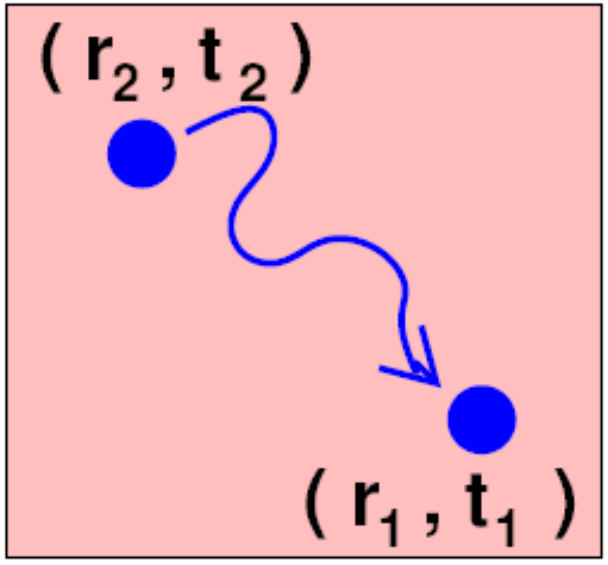
$$\text{for} \quad t_1 > t_2 \Rightarrow iG(\mathbf{x_1}, t_1; \mathbf{x_2}, t_2) = \langle N|\psi(\mathbf{x_1}, t_1)\psi^\dagger(\mathbf{x_2}, t_2)|N\rangle$$

$$\text{for} \quad t_1 < t_2 \Rightarrow iG(\mathbf{x_1}, t_1; \mathbf{x_2}, t_2) = -\langle N|\psi^\dagger(\mathbf{x_2}, t_2)\psi(\mathbf{x_1}, t_1)|N\rangle$$

One-particle Green's function

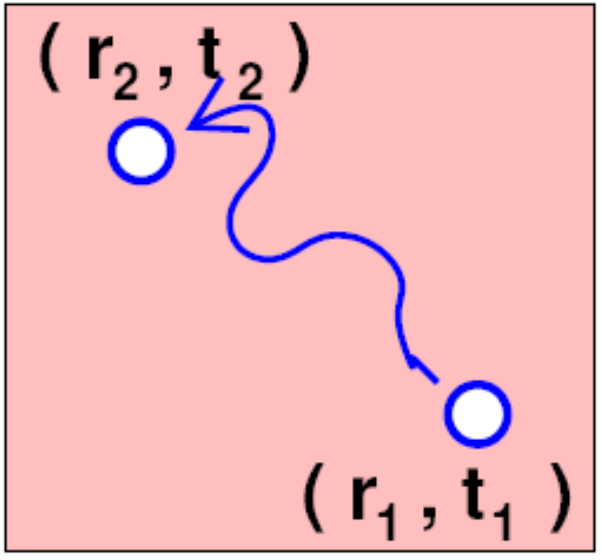
$t_1 > t_2$

$\langle N|\psi(\mathbf{r_1}, t_1)\psi^\dagger(\mathbf{r_2}, t_2)|N\rangle$



$t_1 < t_2$

$-\langle N|\psi^\dagger(\mathbf{r_2}, t_2)\psi(\mathbf{r_1}, t_1)|N\rangle$



One-particle Green's function

What is G ?

Definition and meaning of G:

$$G(\mathbf{x_1}, \mathbf{x_2}, t_1 - t_2) = -i < N| T\left[\psi(\mathbf{x_1}, t_1)\psi^\dagger(\mathbf{x_2}, t_2)\right] |N >$$

Insert a complete set of $N+1$ or $N-1$-particle states and Fourier transform. This yields:

$$G(\mathbf{x_1}, \mathbf{x_2}, \omega) = \sum_j \frac{f_j(\mathbf{x_1}) f_j^*(\mathbf{x_2})}{\omega - E_j + i\eta sgn(E_j - \mu)}.$$

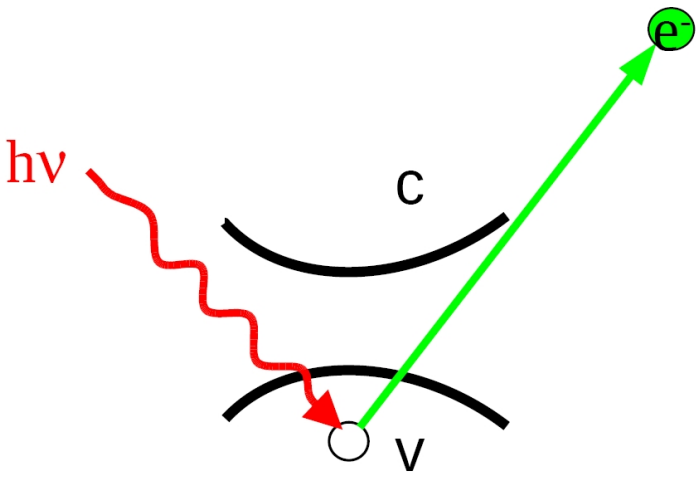
where:

$$E_j = \begin{cases} E(N+1, j) - E(N), & E_j > \mu \\ E(N) - E(N-1, j), & E_j < \mu \end{cases}$$

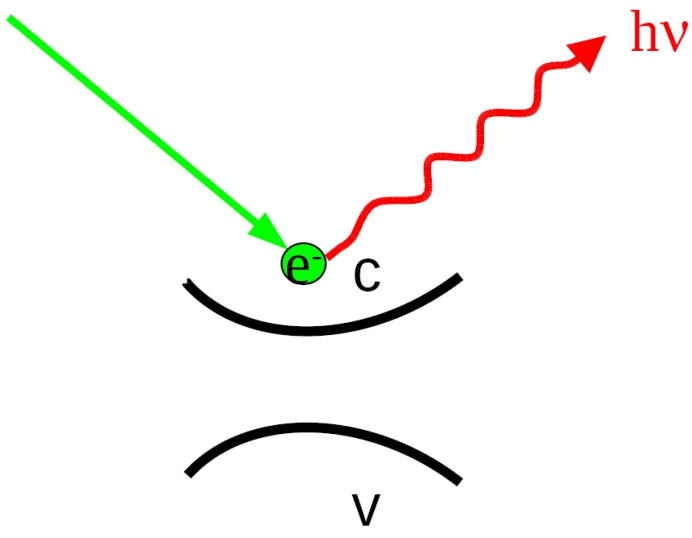
$$f_j(\mathbf{x_1}) = \begin{cases} \langle N | \psi(\mathbf{x_1}) | N+1, j \rangle, & E_j > \mu \\ \langle N-1, j | \psi(\mathbf{x_1}) | N \rangle, & E_j < \mu \end{cases}$$

Photoemission

Direct Photoemission



Inverse Photoemission



One-particle excitations $\rightarrow$ poles of one-particle Green's function G

One-particle Green's function

Spectral function

A useful definition: the spectral function

$$A(\mathbf{x}, \mathbf{x}'; \omega) = \frac{1}{\pi} \mid \mathrm{Im} G(\mathbf{x}, \mathbf{x}'; \omega) \mid = \sum_j f_j(\mathbf{x}) f_j^*(\mathbf{x}') \delta(\omega - E_j).$$

One particle excitations $\rightarrow$ peaks of spectral function A

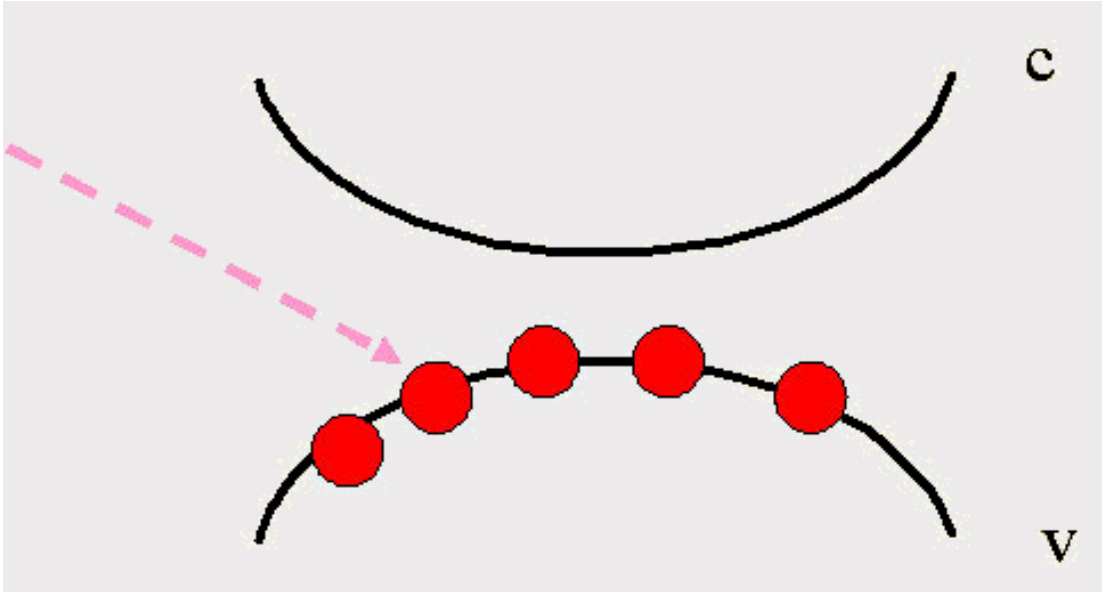
One-particle Green's function

One-particle Green's function

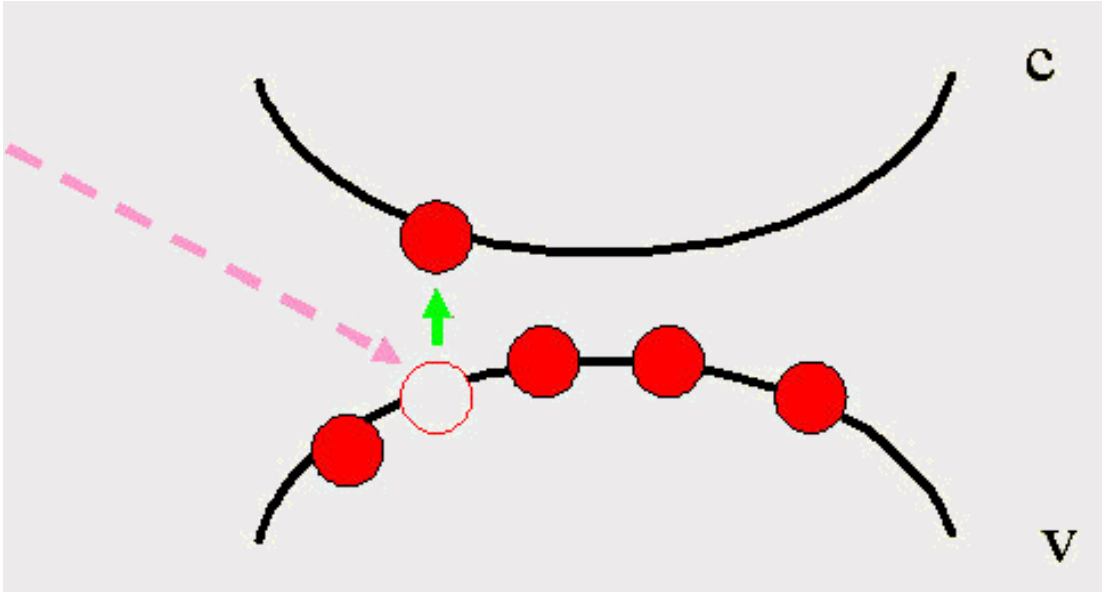
From one-particle G we can obtain:

- one-particle excitation spectra
- ground-state expectation value of any one-particle operator: e.g. density ρ or density matrix γ:
  $\rho(\mathbf{r}, t) = -iG(\mathbf{r}, \mathbf{r}, t, t^+)$ $\gamma(\mathbf{r}, \mathbf{r}', t) = -iG(\mathbf{r}, \mathbf{r}', t, t^+)$
- ground-state total energy (e.g. Galitskii-Migdal)

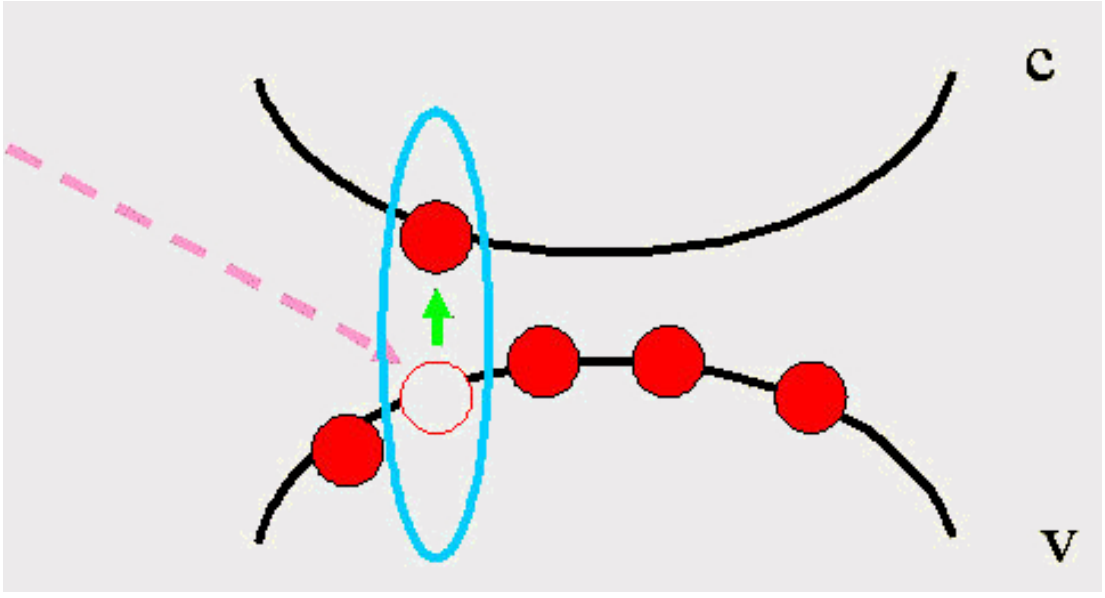
One-particle Green's function: absorption?



One-particle Green's function: absorption?



One-particle Green's function: absorption?



How to calculate G?

Straightforward?

$$iG(\mathbf{x_1}, t_1; \mathbf{x_2}, t_2) = \langle N| T\left[\psi(\mathbf{x_1}, t_1)\psi^\dagger(\mathbf{x_2}, t_2)\right]|N\rangle$$

How to calculate G?

Straightforward?

$$iG(\mathbf{x_1}, t_1; \mathbf{x_2}, t_2) = \langle N| T\left[\psi(\mathbf{x_1}, t_1)\psi^\dagger(\mathbf{x_2}, t_2)\right]|N\rangle$$

$|N> = ???$ Interacting ground state!

See e.g. A.L. Fetter and J.D. Walecka, *Quantum Theory of Many-Particle Systems*

How to calculate *G*?

G as the solution of a differential equation (with boundary conditions)

Equation of motion

$$\left[i\frac{\partial}{\partial t_1} - h_0(1)\right] G(1,2) = \delta(1,2) - i\int d3v(1,3)G_2(1,3,2,3^+)$$

where $h_0 = -\frac{1}{2}\nabla^2 + v_{ext}$

Interaction $\rightarrow$ two-particle excitations

How to calculate G?

G as the solution of a differential equation (with boundary conditions)

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Interaction $\rightarrow$ two-particle excitations

Unfortunately, hierarchy of equations

$$\begin{array}{ccc} G(1,2) & \leftarrow & G_2(1,2;3,4) \\ G_2(1,2;3,4) & \leftarrow & G_3(1,2,3;4,5,6) \\ \vdots & \vdots & \vdots \end{array}$$

Self-energy

$$\left[i\frac{\partial}{\partial t_1} - h_0(1)\right] G(1,2) = \delta(1,2) - i\int d3v(1,3)G_2(1,3,2,3^+)$$

Self-energy

$$\left[i\frac{\partial}{\partial t_1} - h_0(1) - V_H(1)\right] G(1,2) = \delta(1,2) + \int d3\Sigma(1,3)G(3,2)$$

- Σ = non-local effective potential (exchange and correlation)
- $\Sigma = \Sigma[G]$: self-consistency

Self-energy

$$\left[i\frac{\partial}{\partial t_1} - h_0(1) - V_H(1)\right] G(1,2) = \delta(1,2) + \int d3\Sigma(1,3)G(3,2)$$

Fourier transform: G as resolvent

$$\left[\omega - h_0(\mathbf{r}_1) - V_H(\mathbf{r}_1)\right] G(\mathbf{r}_1,\mathbf{r}_2,\omega) = \int d\mathbf{r}_3 \Sigma(\mathbf{r}_1,\mathbf{r}_3,\omega)G(\mathbf{r}_3,\mathbf{r}_2,\omega)$$

$$(\omega - H_0)G(\omega) = \Sigma(\omega)G(\omega) \quad \Rightarrow \quad G^{-1}(\omega) = (\omega - H_0 - \Sigma(\omega))$$

$\Sigma = \Sigma(\omega)$: folding of higher-order excitations

Dyson equation

$$\left[i\frac{\partial}{\partial t_1} - h_0(1) - V_H(1)\right] G(1,2) = \delta(1,2) + \int d3\Sigma(1,3)G(3,2)$$

$$\left[i\frac{\partial}{\partial t_1} - h_0(1) - V_H(1)\right] G_0(1,2) = \delta(1,2)$$

Dyson equation

$$G(1,2) = G_0(1,2) + \int d34 G_0(1,3)\Sigma(3.4)G(4.2)$$

Dyson equation

Dyson equation

$$G(1,2) = G_0(1,2) + \int d34 G_0(1,3)\Sigma(3.4)G(4.2)$$

Two general properties:

1.

$$\begin{aligned} G &= G_0 + G_0\Sigma G \\ &= G_0 + G_0\Sigma G_0 + G_0\Sigma G_0\Sigma G_0 + ... \\ &= (G_0^{-1} - \Sigma)^{-1} \end{aligned}$$

Dyson equation

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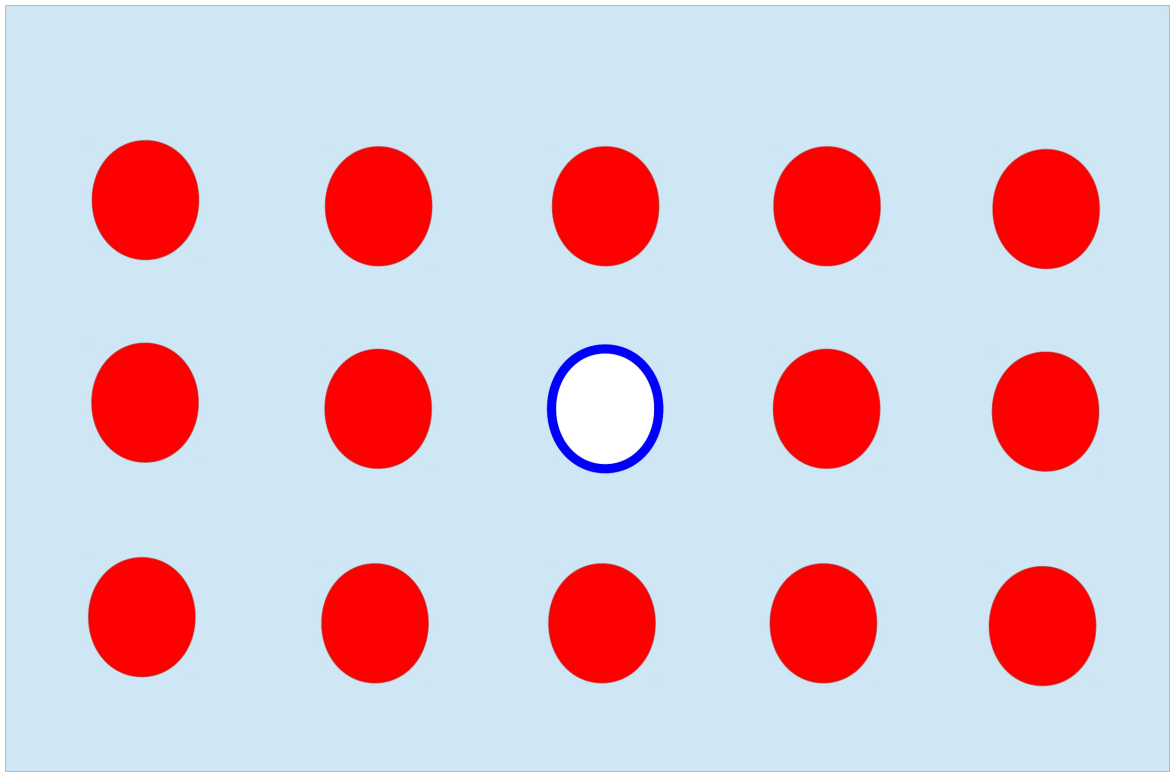
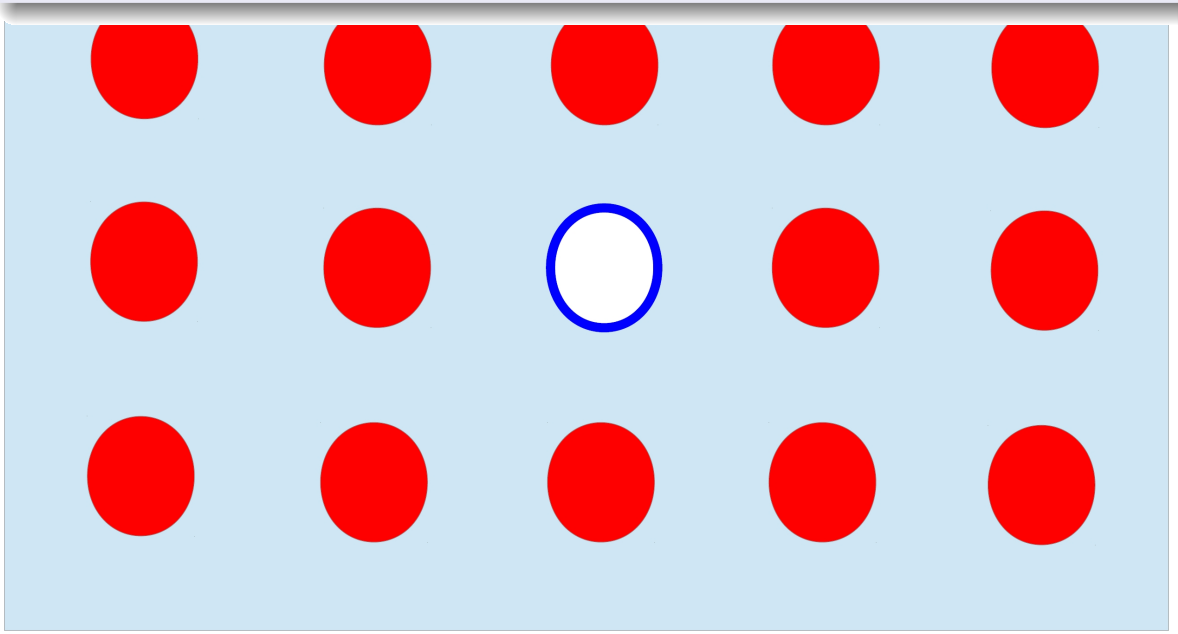
2. $$G = G_0 + G_0\Sigma G \Rightarrow \begin{cases} G_1 = G_0 + G_0\Sigma_1 G_1 \\ G = G_1 + G_1\Sigma_2 G \end{cases}$$

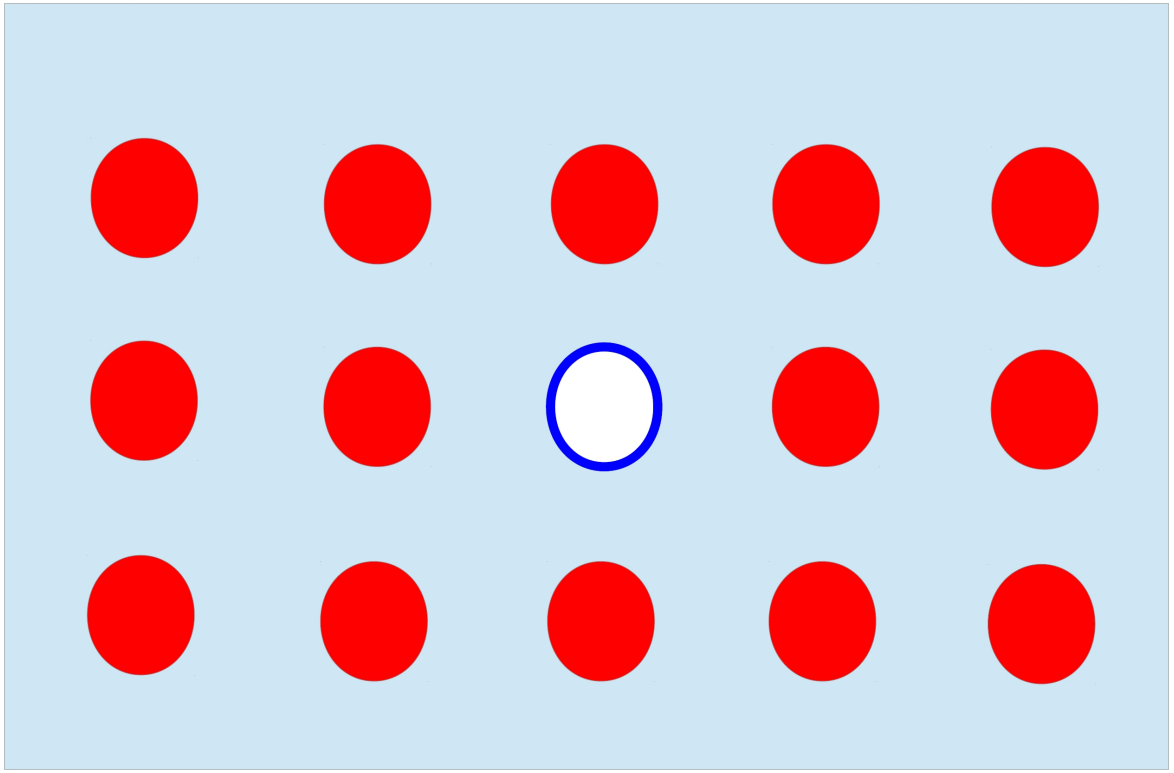
Outline

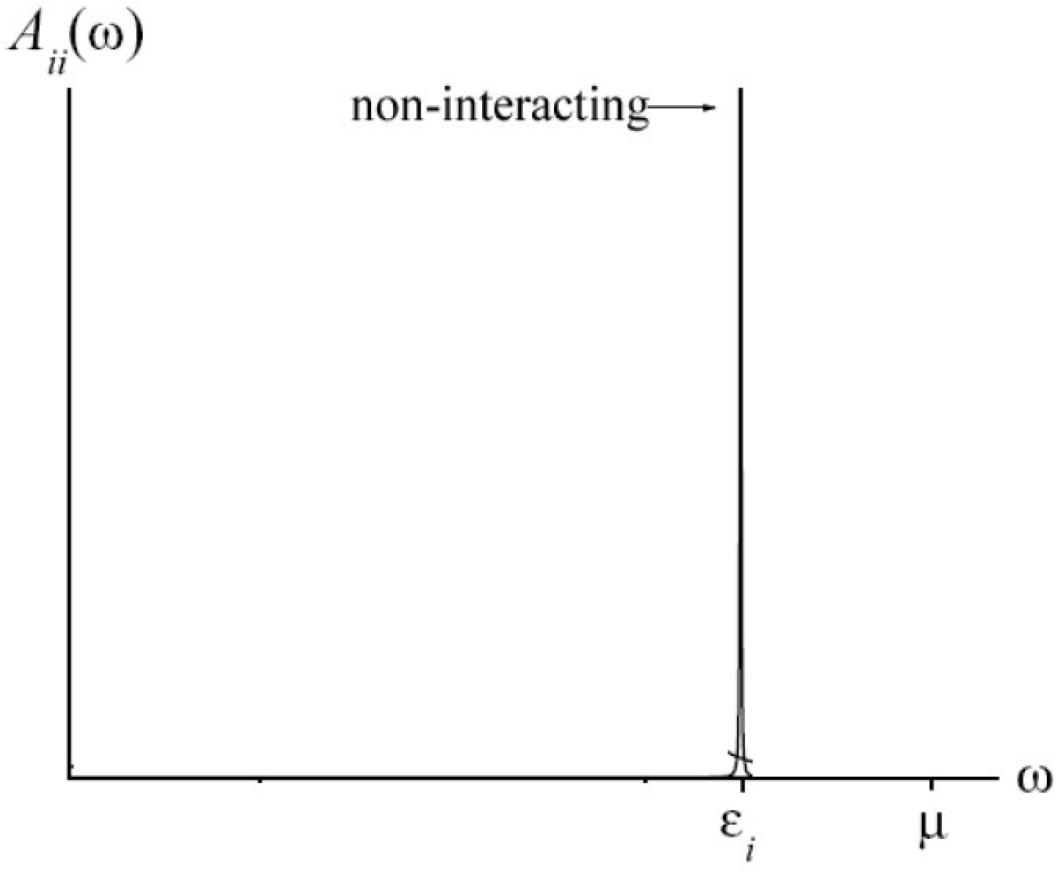


What happens?

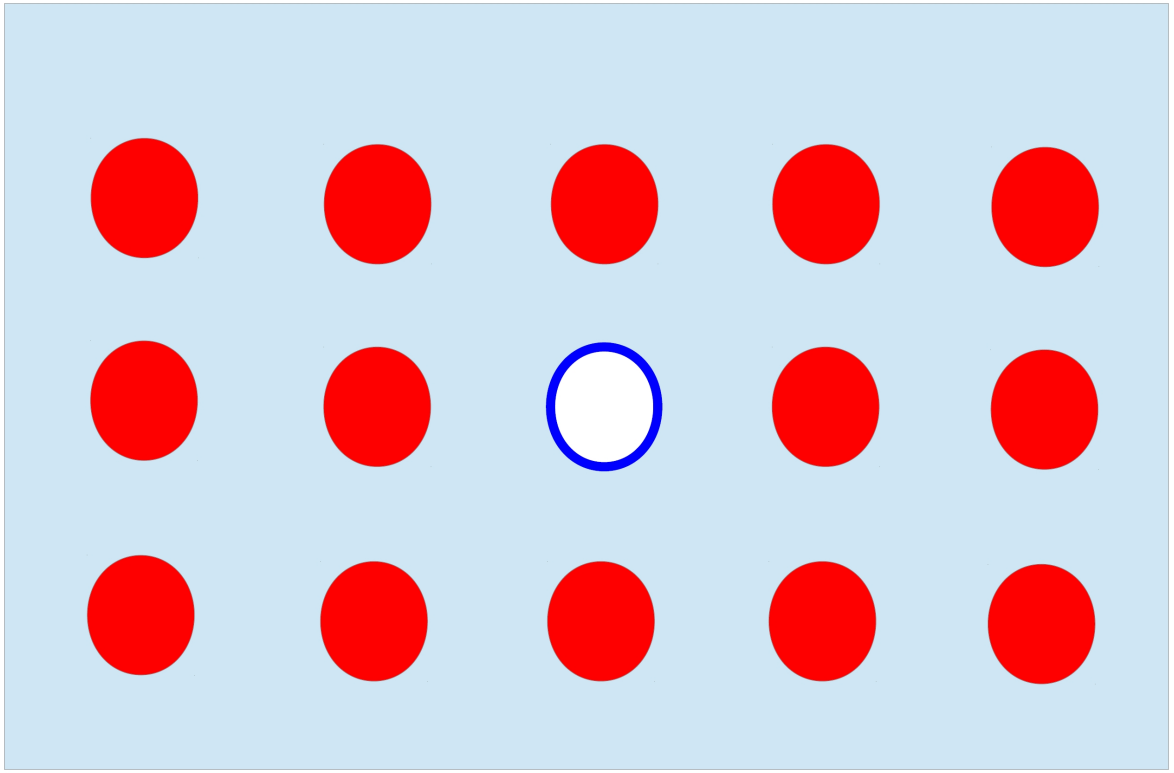


Non-interacting particles

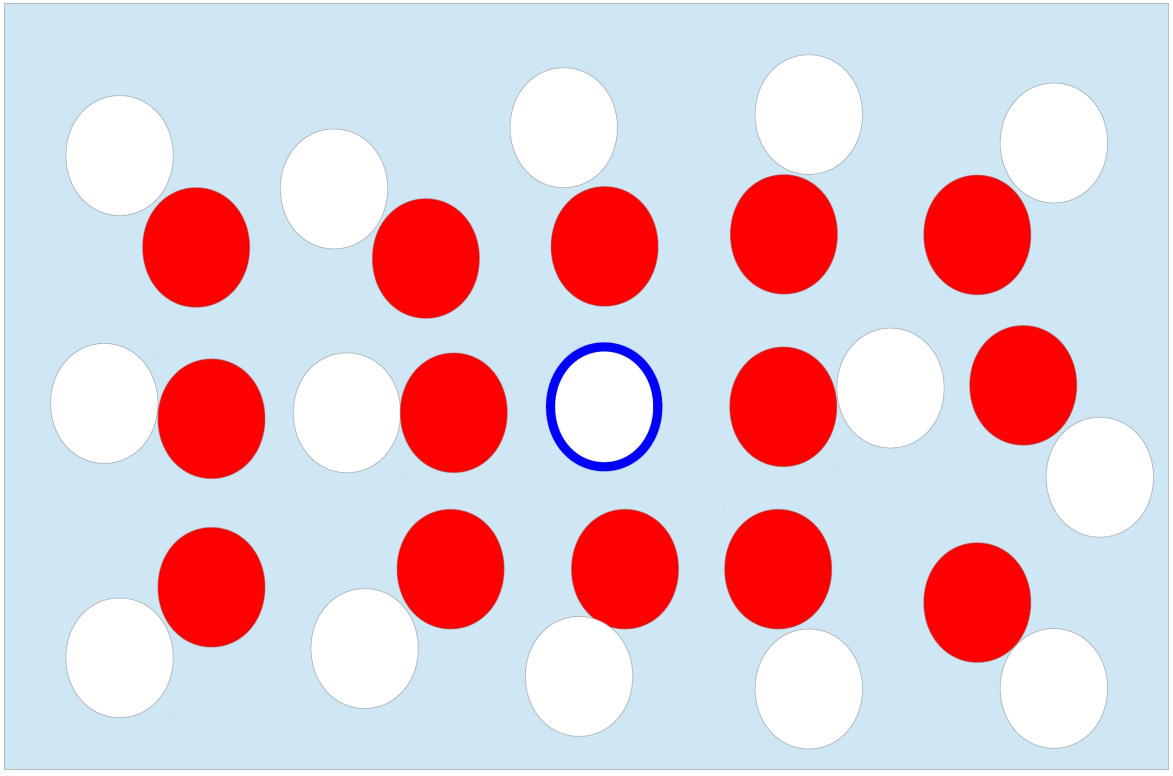



$A_{ii}(\omega)$
non-interacting
ω
ε_i
μ

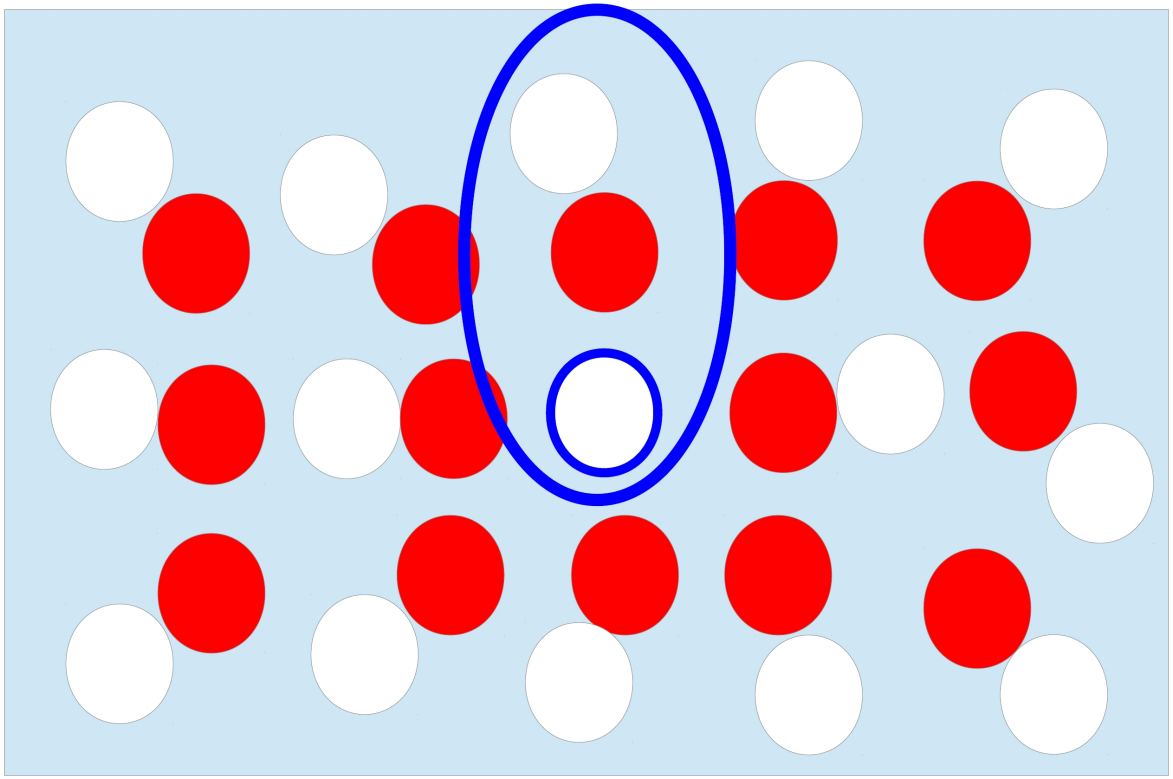
Interacting particles



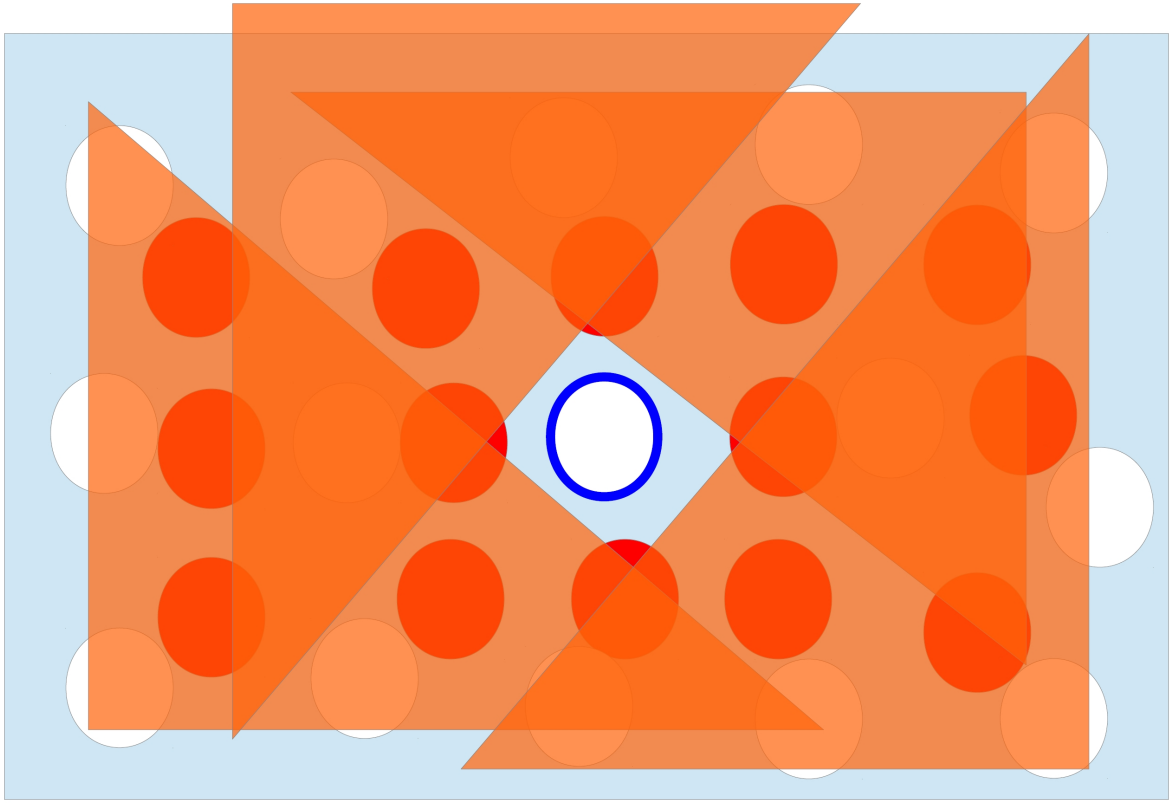
Interacting particles



Interacting particles



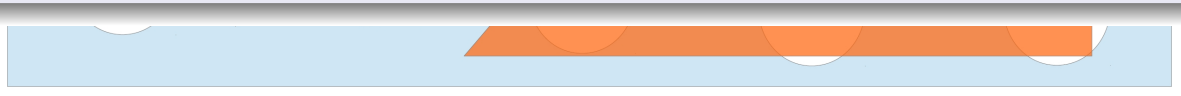
Interacting particles



Interacting particles

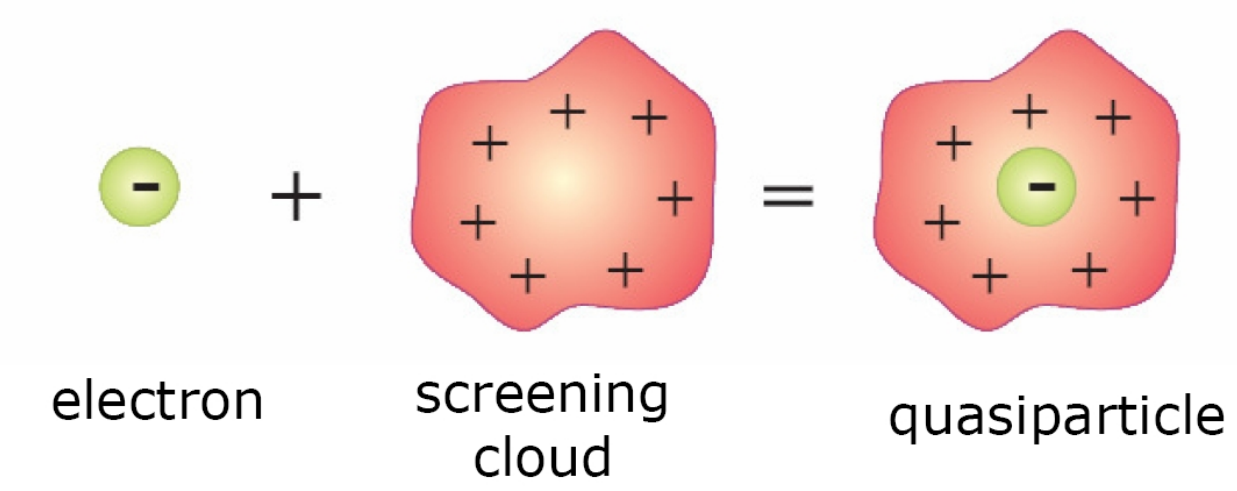
Screening

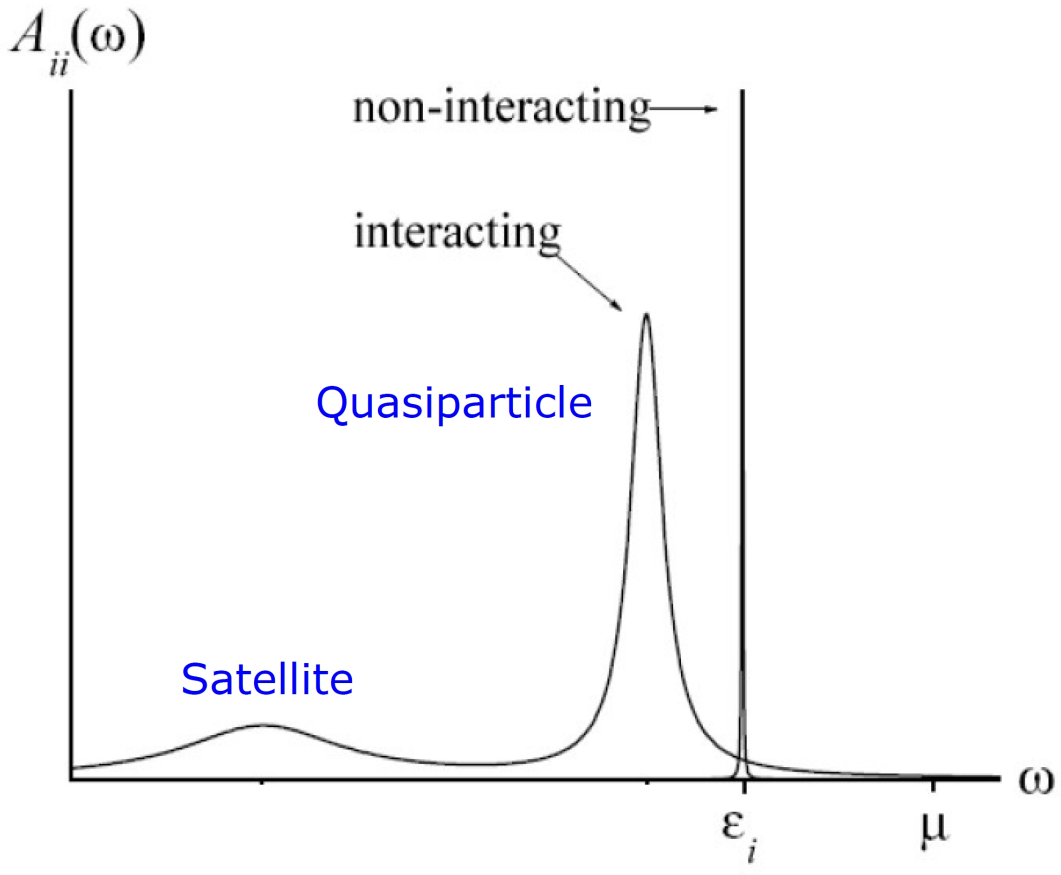
$$W(\mathbf{r}_1, \mathbf{r}_2, \omega) = \int d\mathbf{r}_3 \epsilon^{-1}(\mathbf{r}_1, \mathbf{r}_3, \omega) v(\mathbf{r}_3, \mathbf{r}_2)$$



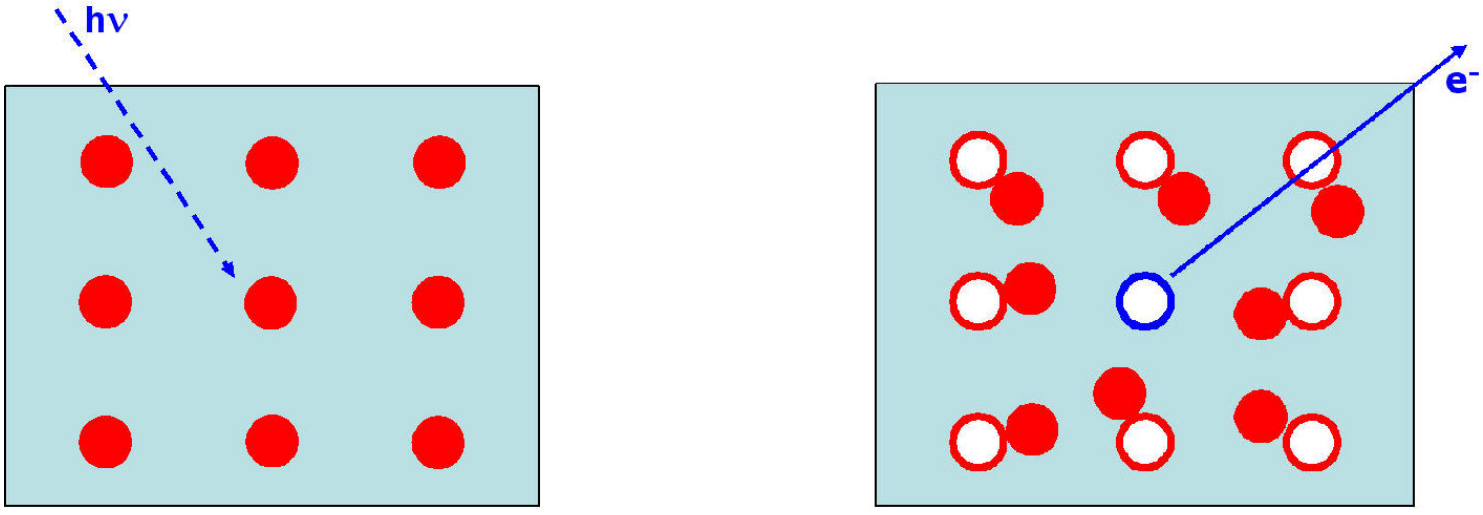
Screening: quasiparticles

Quasiparticle




$A_{ii}(\omega)$
non-interacting
interacting
Quasiparticle
Satellite
ω
ε_i
μ

GW approximation



additional charge $\rightarrow$ reaction: polarization, screening

GW approximation

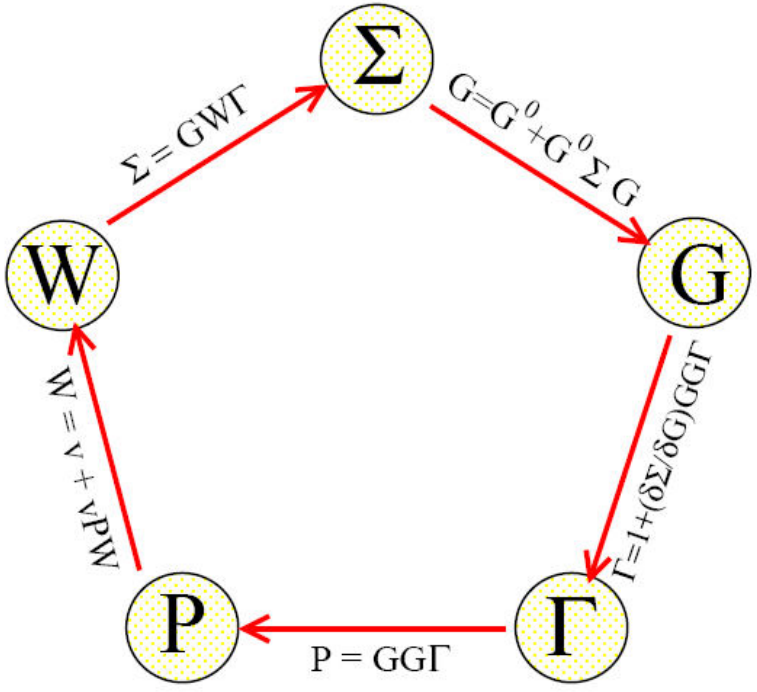
1. polarization made of noninteracting electron-hole pairs (RPA)
2. classical (Hartree) interaction between additional charge and polarization charge

GW approximation

Hedin's equation and GW

Hedin's equations

$$\Sigma = iGW\Gamma$$
$$G = G_0 + G_0\Sigma G$$
$$\Gamma = 1 + \frac{\delta\Sigma}{\delta G} GG\Gamma$$
$$P = -iGG\Gamma$$
$$W = v + vPW$$



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

Hedin's equation and GW

GW approximation: $\Gamma = 1$

$$\Sigma = iGW$$
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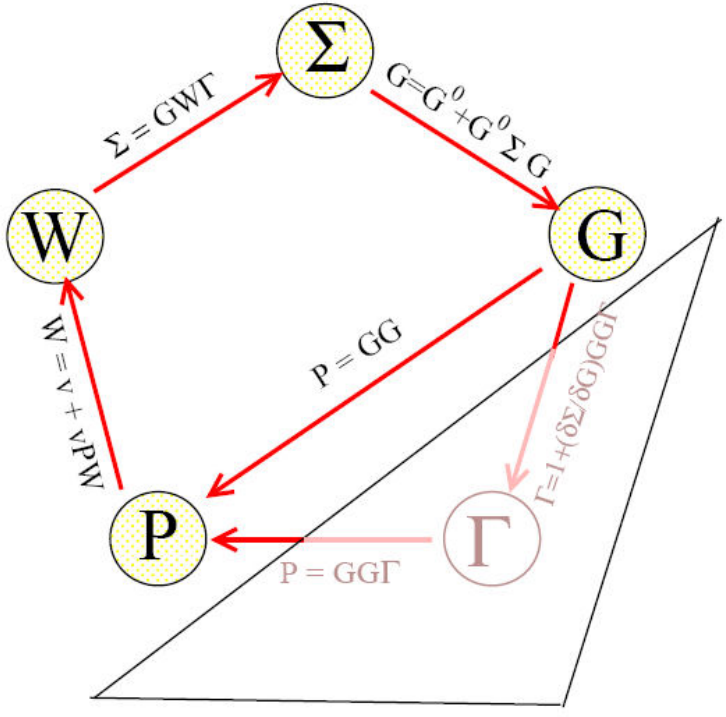

L. Hedin, Phys. Rev. **139** (1965)

Self-energy and GW

The self-energy

Self-energy = exchange + induced Hartree + induced exchange-correlation

$$\Sigma(12) = iG(12)v(12) + iG(12)W_p(12) + iG(1\bar{4})\frac{\delta\Sigma(\bar{4}2)}{\delta\rho(\bar{5})}\chi(\bar{5}\bar{3})v(\bar{3}1)$$

$$W_p(12) = W(12) - v(12) = v(1\bar{3})\chi(\bar{3}\bar{4})v(\bar{4}2)$$

GW = exchange + induced Hartree (with RPA χ)

Remember: $v = \delta V_H/\delta\rho$

Correlation = coupling of excitations

Dynamical screening

Convolution in frequency domain

$$\Sigma_c(\mathbf{r}_1, \mathbf{r}_2, \omega) = \frac{i}{2\pi} \int d\omega' e^{i\eta\omega'} G(\mathbf{r}_1, \mathbf{r}_2, \omega + \omega') W_p(\mathbf{r}_1, \mathbf{r}_2, \omega')$$

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$$W_p(\mathbf{r}_1, \mathbf{r}_2, \omega) = 2 \sum_s \frac{\omega_s W_s(\mathbf{r}_1, \mathbf{r}_2)}{\omega^2 - (\omega_s - i\eta)^2}$$

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$$\Sigma_c(\mathbf{r}_1, \mathbf{r}_2, \omega) = \frac{i}{2\pi} \int d\omega' e^{i\eta\omega'} G(\mathbf{r}_1, \mathbf{r}_2, \omega + \omega') W_p(\mathbf{r}_1, \mathbf{r}_2, \omega')$$

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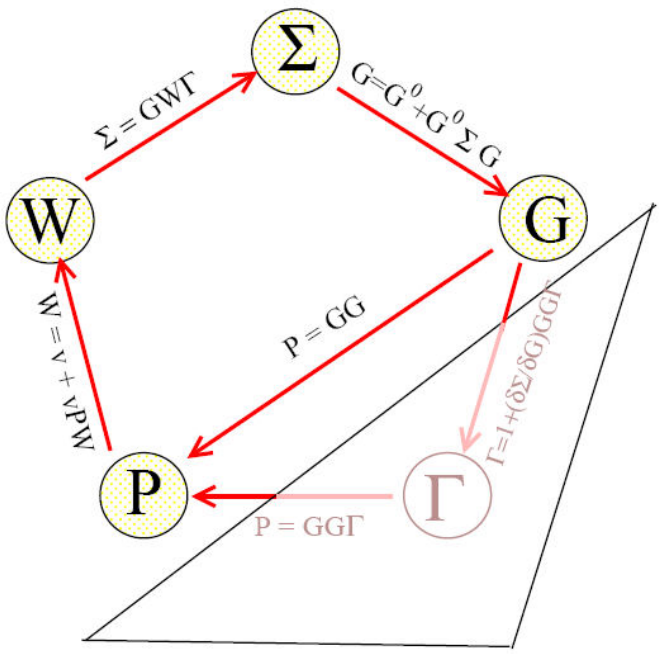
$$\Sigma_c(\mathbf{r}_1, \mathbf{r}_2, \omega) = \sum_{j,s\neq 0} \frac{f_j(\mathbf{r}_1) f_j^*(\mathbf{r}_2) W_s(\mathbf{r}_1, \mathbf{r}_2)}{\omega - E_j + \omega_s \mathrm{sgn}(\mu - E_j)}$$

Coupling of addition/removal E_i and neutral excitations ω_s

Outline

GW: Self-consistent solution

$$G = G_0 + G_0\,\Sigma[G]\,G$$



Self-consistent GW

- bad for spectral properties in solids
- OK for atoms, small molecules
- necessary for total energy (conserving approximation)
- computationally very heavy!

G_0W_0: Quasiparticle corrections

Standard perturbative G_0W_0

$$H_0(\mathbf{r})\phi_i(\mathbf{r}) + \int d\mathbf{r}' \; \Sigma(\mathbf{r}, \mathbf{r}', \omega = E_i) \; \phi_i(\mathbf{r}') = E_i \, \phi_i(\mathbf{r})$$

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$$H_0(\mathbf{r})\varphi_i(\mathbf{r}) + V_{xc}(\mathbf{r})\varphi_i(r) = \epsilon_i\varphi_i(\mathbf{r})$$

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First-order perturbative corrections with $\Sigma = iGW$:

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

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First-order perturbative corrections with $\Sigma = iGW$:

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

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

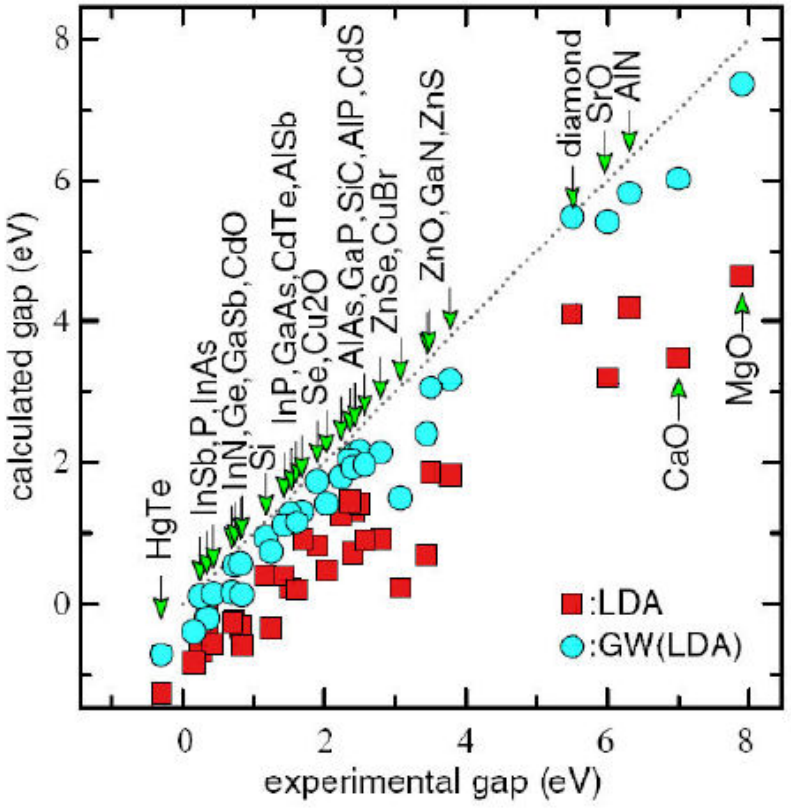
Quasiparticle energies

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

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

Hybersten and Louie, PRB **34** (1986); Godby, Schlüter and Sham, PRB **37** (1988)

G_0W_0: QP results



M. van Schilfgaarde *et al.*, PRL **96** (2006)

G_0W_0 results

Great improvement over LDA.

Drawback: dependency on the starting point

G_0W_0 results

- OK for *sp* electron systems
- questionable for *df* electron systems (and whenever LDA is bad)

Beyond G_0W_0: alternative starting points

Looking for a better starting point

- Kohn-Sham with other functionals (EXX, LDA+U) - e.g. Rinke 2005, Miyake 2006, Jiang 2009,...
- Generalized Kohn-Sham: hybrid functionals (HSE06) - e.g. Fuchs 2006,...
- effective quasiparticle Hamiltonians
  - QSGW scheme - Faleev 2004
  - Hedin's COHSEX approximation - Bruneval 2005

Beyond G_0W_0: alternative starting points

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  - QSGW scheme - Faleev 2004
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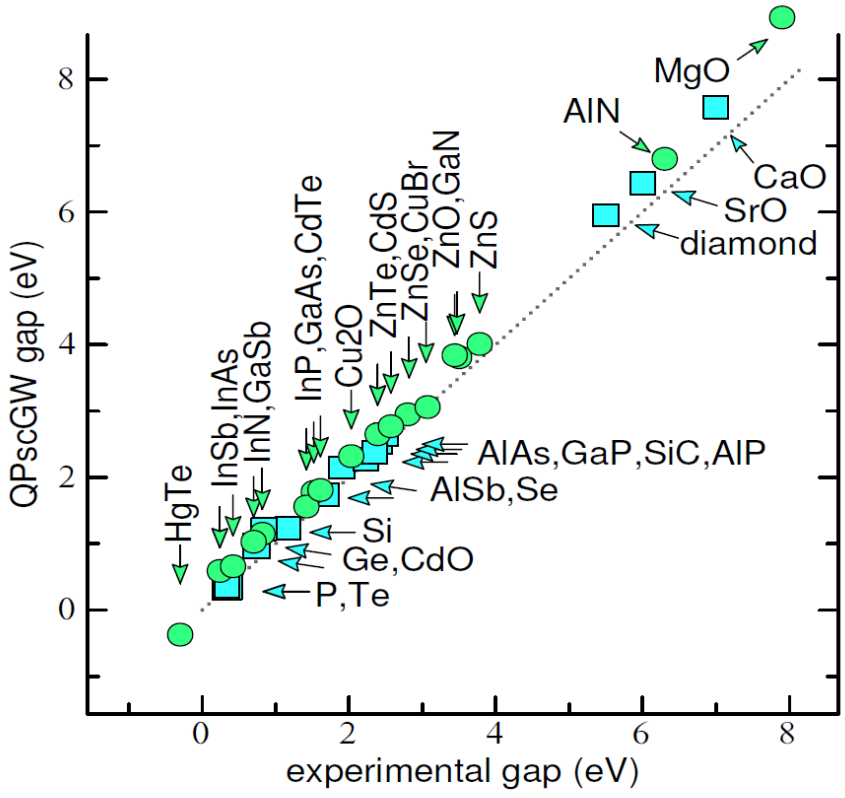
Beyond G_0W_0: QSGW scheme

Only retain hermitian part of GW Σ and iterate QP:

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



S. V. Faleev, M. van Schilfgaarde, and T. Kotani, PRL 93 (2004)

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

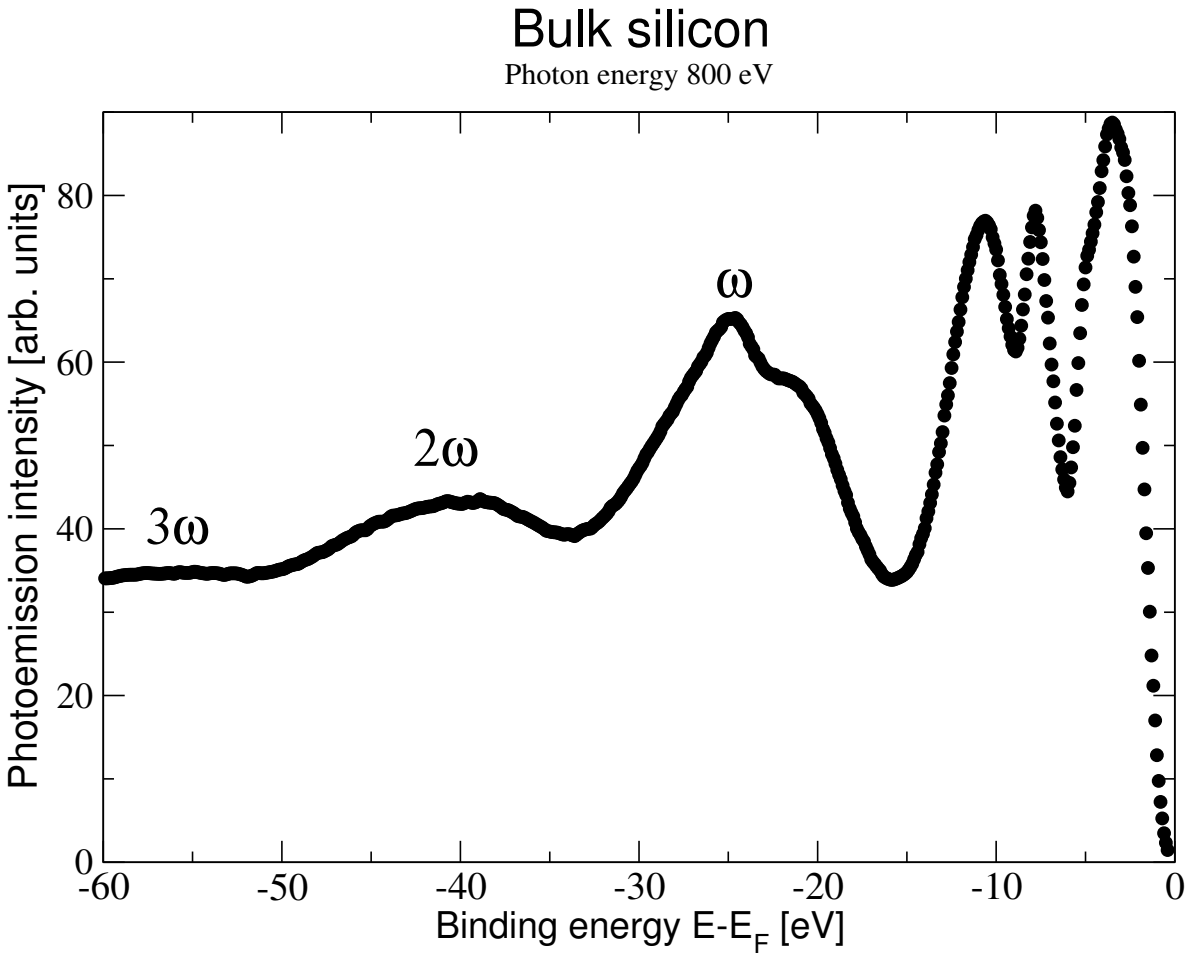
Outline

Beyond GW: vertex corrections

Beyond GW

- multiple plasmon satellites: cumulant expansion
- self-screening
- atomic limit
- additional interactions: T matrix

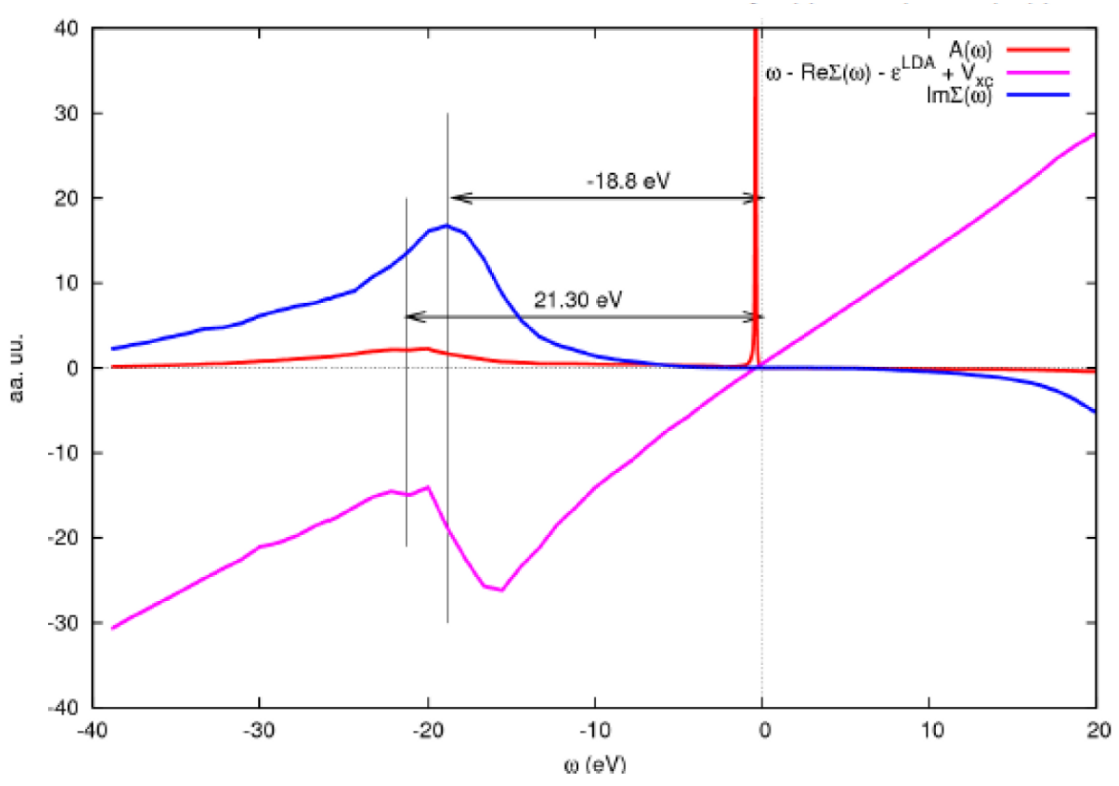
Multiple satellites in silicon: PES



M. Guzzo *et al.*, PRL 107 (2011).

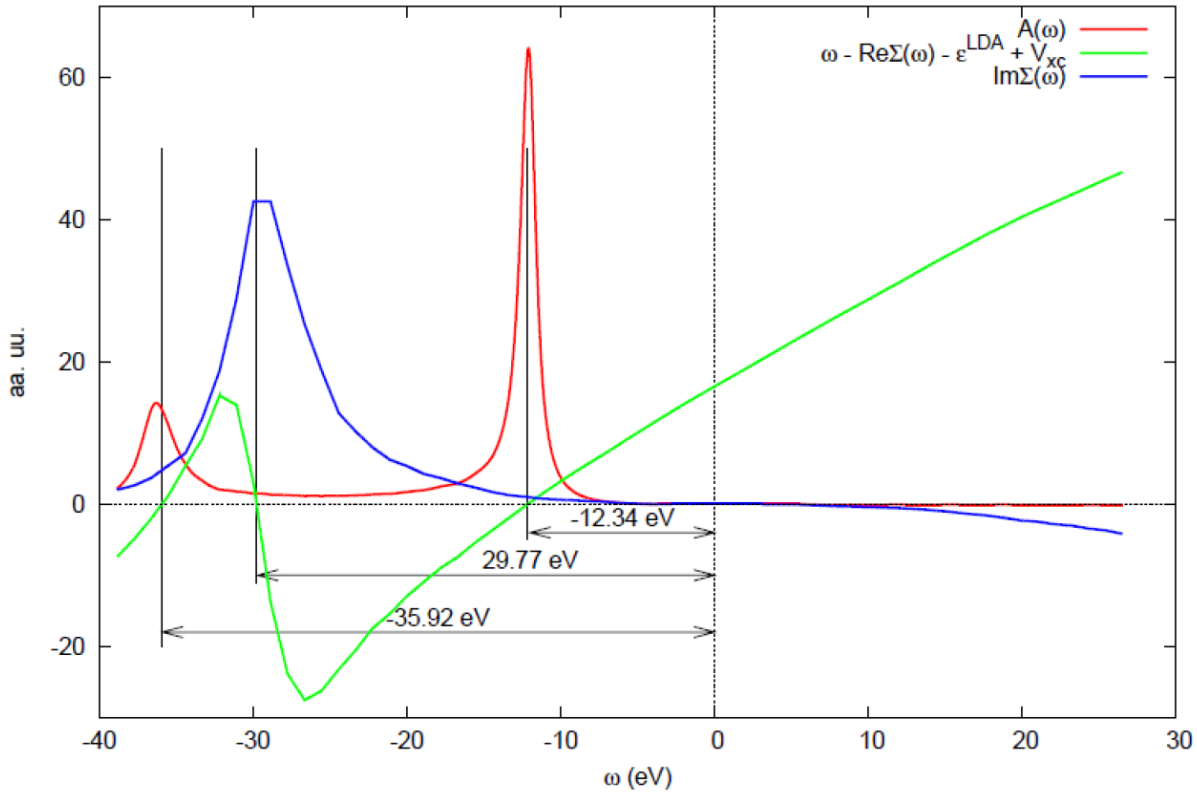
Multiple satellites in silicon: GW

GW spectral function: top valence at Γ
A very weak plasmon satellite



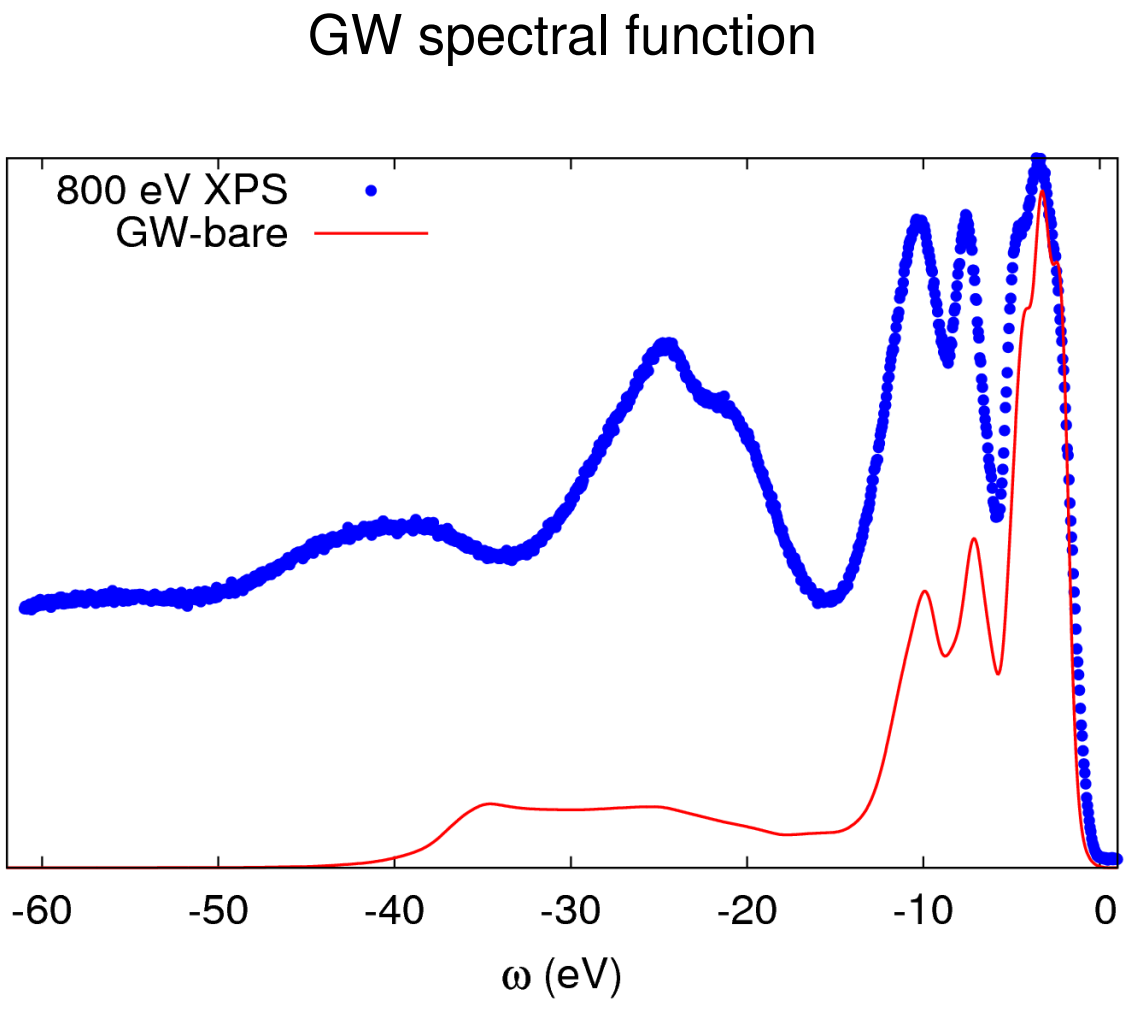
Multiple satellites in silicon: GW

GW spectral function: bottom valence at Γ
A plasmaron satellite



B. I. Lundqvist, Phys. Kondens. Mater. 6 (1967)

Multiple satellites in silicon: GW



Decoupling approximation: exponential solution

Equation of motion of G :

$$G = \tilde{G}_0 + \tilde{G}_0 V_H G + \tilde{G}_0 U G + i\tilde{G}_0 v \frac{\delta G}{\delta U} \quad \text{with} \quad \tilde{G}_0 = (\omega - h_0)^{-1}$$

1. Linearize: $V_H = V_H^0 + v\chi U + ...$

$$G = G_0 + G_0 \bar{U} G + iG_0 W \frac{\delta G}{\delta \bar{U}} \quad \text{with} \quad \bar{U} = \epsilon^{-1} U, G_0 = (\omega - h_0 - V_H^0)^{-1}$$

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2. Optimize QP such that G and G_{QP} are diagonal in the basis $|k\rangle$:

$$\text{holes:} \quad G_k^{QP}(\tau) = i\theta(-\tau) e^{-i\epsilon_k^{QP}\tau}$$

$$\forall k : G = G^{QP} + G^{QP}(\bar{U} - \Delta^{QP})G + iG^{QP} W \frac{\delta G}{\delta \bar{U}}$$

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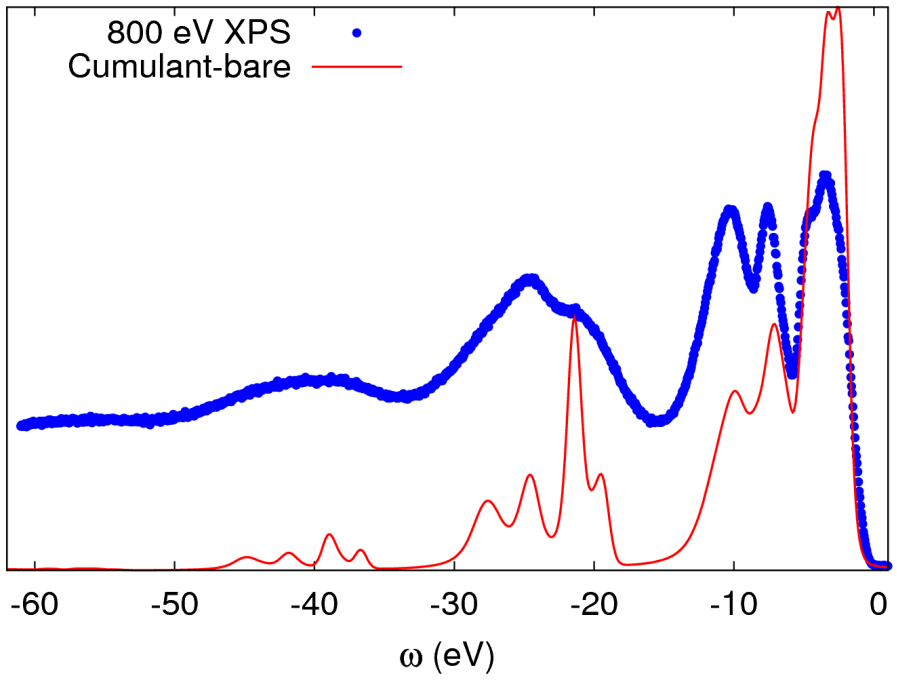
Exact solution:

$$G(t_1, t_2) = G^{QP}(t_1 - t_2) e^{i\Delta^{QP}(t_1 - t_2)} e^{i\int_{t_1}^{t_2} dt' \left[U(t') - \int_{t'}^{t_2} dt'' W(t', t'')\right]}$$

Multiple satellites in silicon: exponential solution

Plasmon-pole approximation to W: $W(\tau) = -i\lambda_k \left[\theta(\tau)e^{-i\tilde{\omega}_k\tau} + \theta(-\tau)e^{i\tilde{\omega}_k\tau}\right]$

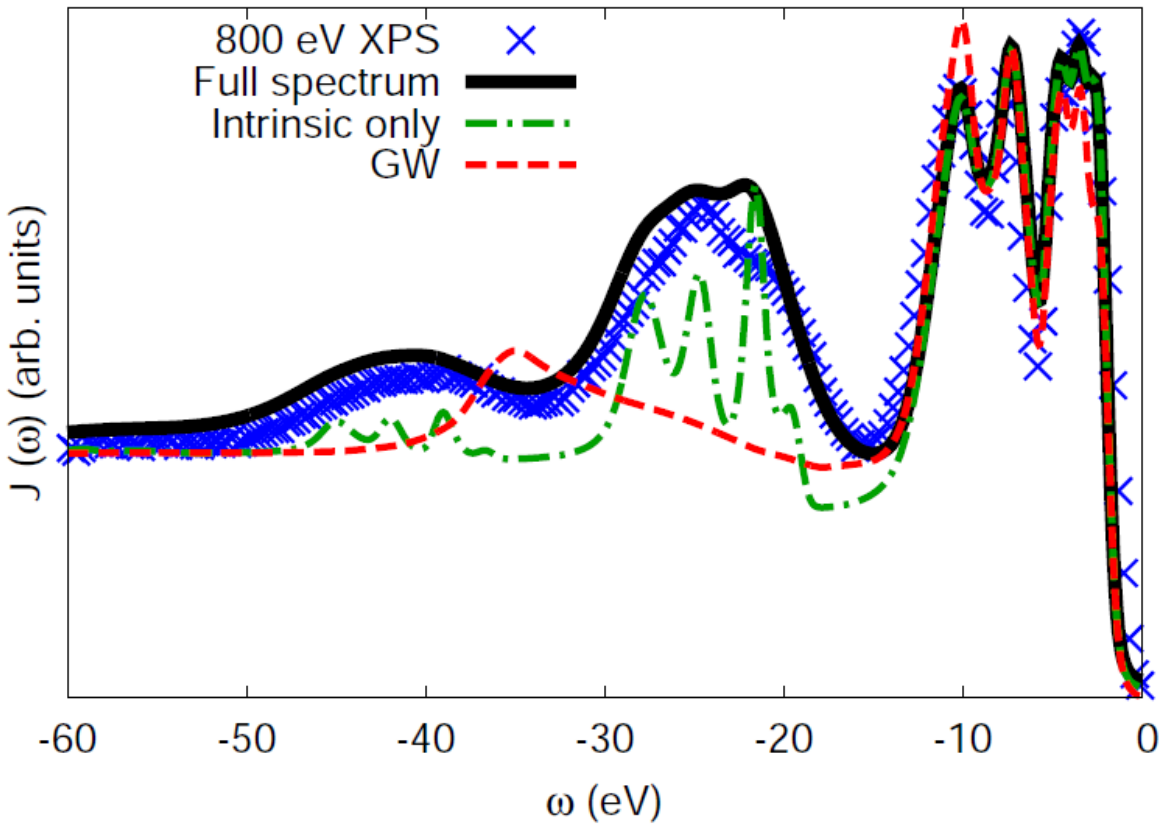


Exponential solution - cumulant expansion

$$A_k(\omega) = \frac{e^{-a_k}}{\pi} \sum_{n=0}^{\infty} \frac{a_k^n}{n!} \frac{\mathrm{Im}\epsilon_k^{QP}}{(\omega - \mathrm{Re}\epsilon_k^{QP} + n\tilde{\omega}_k)^2 + (\mathrm{Im}\epsilon_k^{QP})^2},$$

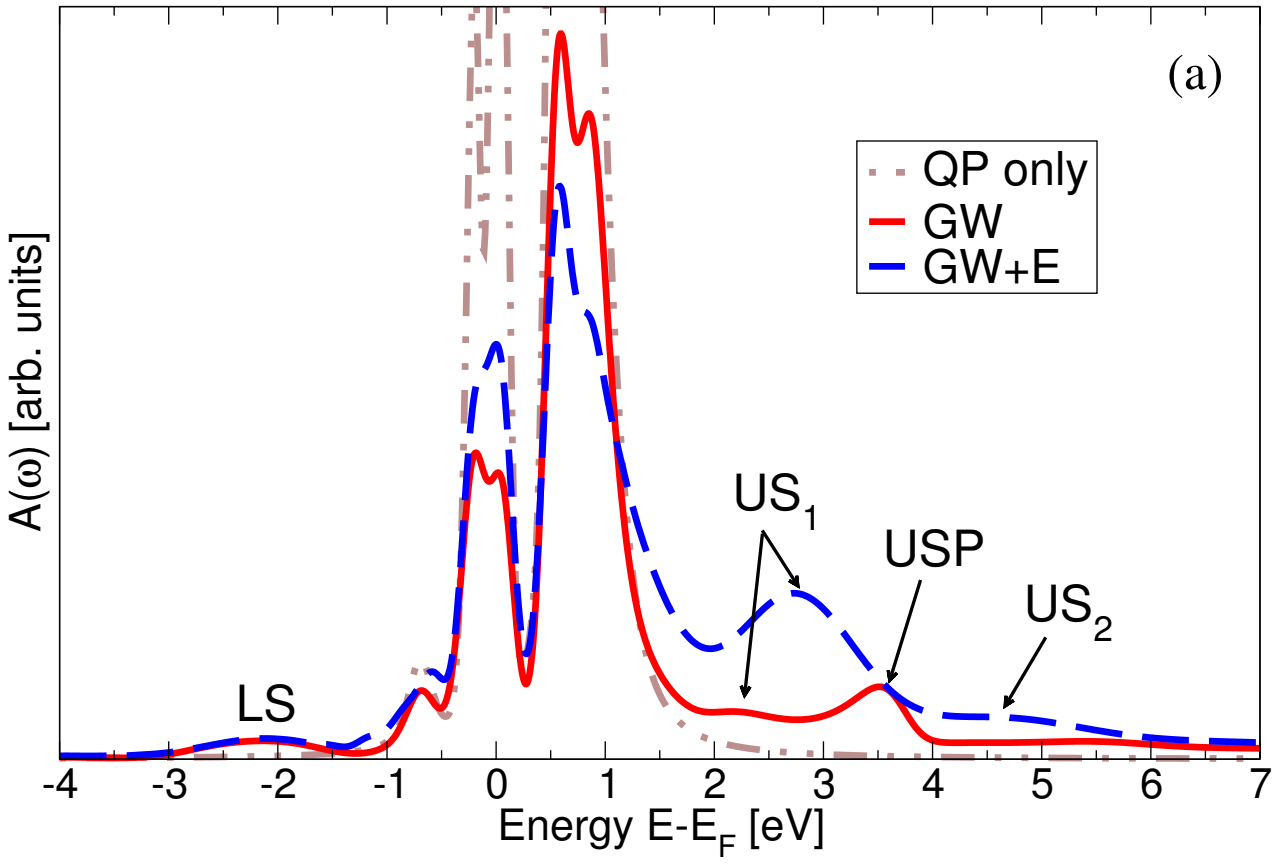
Multiple satellites in silicon: exponential solution

Plus contributions from:
extrinsic effects, interference effects, cross sections, background



M. Guzzo *et al.*, PRL 107 (2011)

Satellites in strongly correlated materials: $SrVO_3$



M. Gatti and M. Guzzo, PRB 87 (2013)

GW approximation

Self-screening

Particle in a box: add or remove

$(-\nabla^2/2 + V_{box})\phi = \varepsilon\phi$

$\varepsilon = -(E_{N=0} - E_{N=1}) = E_{N=1} - E_{N=0}$

Self-screening

Particle in a box: add or remove

$(-\nabla^2/2 + V_{box})\phi = \varepsilon\phi$

$\varepsilon = -(E_{N=0} - E_{N=1}) = E_{N=1} - E_{N=0}$

- Kohn-Sham

  $(-\nabla^2/2 + V_{box} + \rho v - \rho v)\phi = \varepsilon\phi$

- Hartree-Fock

  $(-\nabla^2/2 + V_{box} + \rho v)\phi - \phi^*\phi v\phi = \varepsilon\phi$

- GW

  $(-\nabla^2/2 + V_{box} + \rho v)\phi - \phi^*\phi v\phi + \Sigma_c\phi = \varepsilon\phi$

  $W = v + W_p = v + v\chi^{RPA}v$ W_p should be zero!

Self-screening

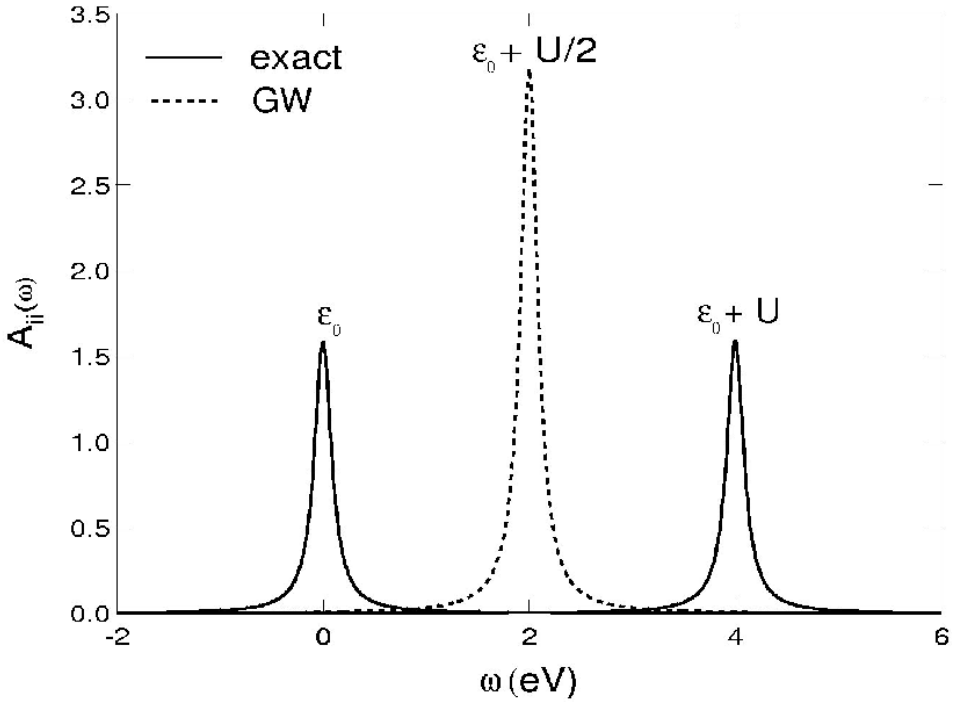
Corrections to GW

- W test-charge
  use exact χ instead of $\chi^{RPA} \Rightarrow \chi = \chi_0$
  $\Rightarrow W_p = v\chi_0 v \neq 0$
- W test-electron
  local vertex: $W_p = (v + f_{xc})\chi_0 v = 0 \qquad (f_{xc} = -v)$

W. Nelson, P. Bokes, P. Rinke, and R. W. Godby, Phys. Rev. A 75 (2007)
P. Romaniello, S. Guyot, and L. Reining, JCP 131 (2009)
F. Aryasetiawan, R. Sakuma, and K. Karlsson, arXiv:1110.6765

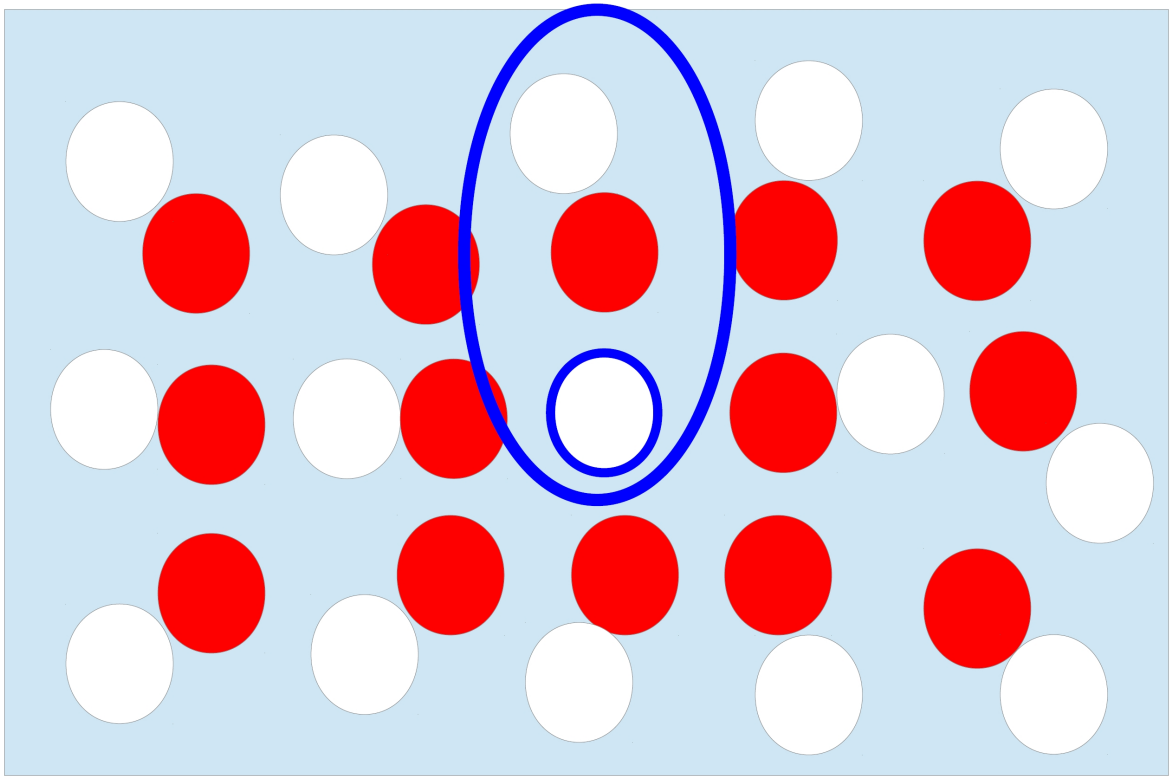
Atomic limit

One electron in two-site Hubbard model

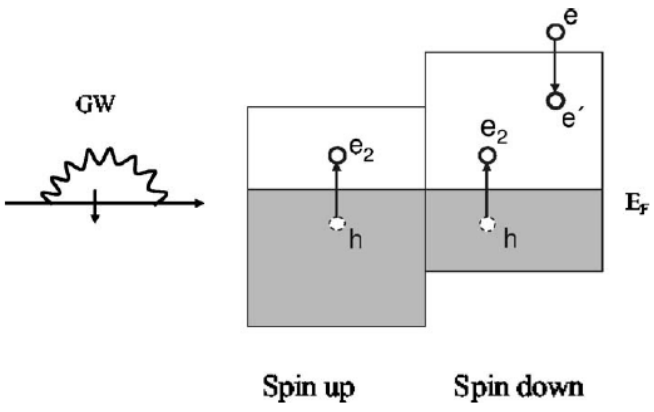


P. Romaniello, S. Guyot, and L. Reining, JCP 131 (2009)

Interacting particles



GW and T matrix



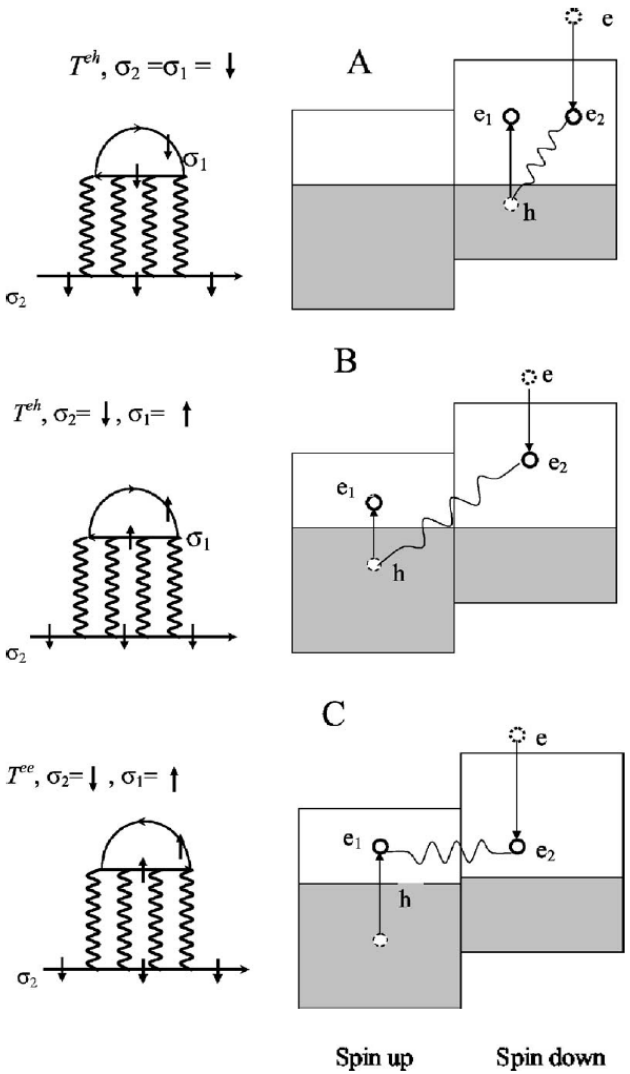
GW

- Add one primary electron e, spin $\downarrow$
- Disexcitation $(e, \downarrow) \rightarrow (e', \downarrow)$
- Creation of electron-hole pairs e_2-h in both spin channels.

Note

- primary electron: final spin = initial spin (no spin flips)
- no interaction between primary electron and secondary particles
- analogously for additional hole

GW and T matrix



T matrix

- Add one primary electron e, spin $\downarrow$
- Disexcitation $(e, \downarrow) \rightarrow (e_2, \downarrow)$
- Creation of electron-hole pairs e_1-h in both spin channels
- Interaction between primary electron and hole of electron-hole pair (A,B)
- Interaction between primary electron and electron of electron-hole pair (C)

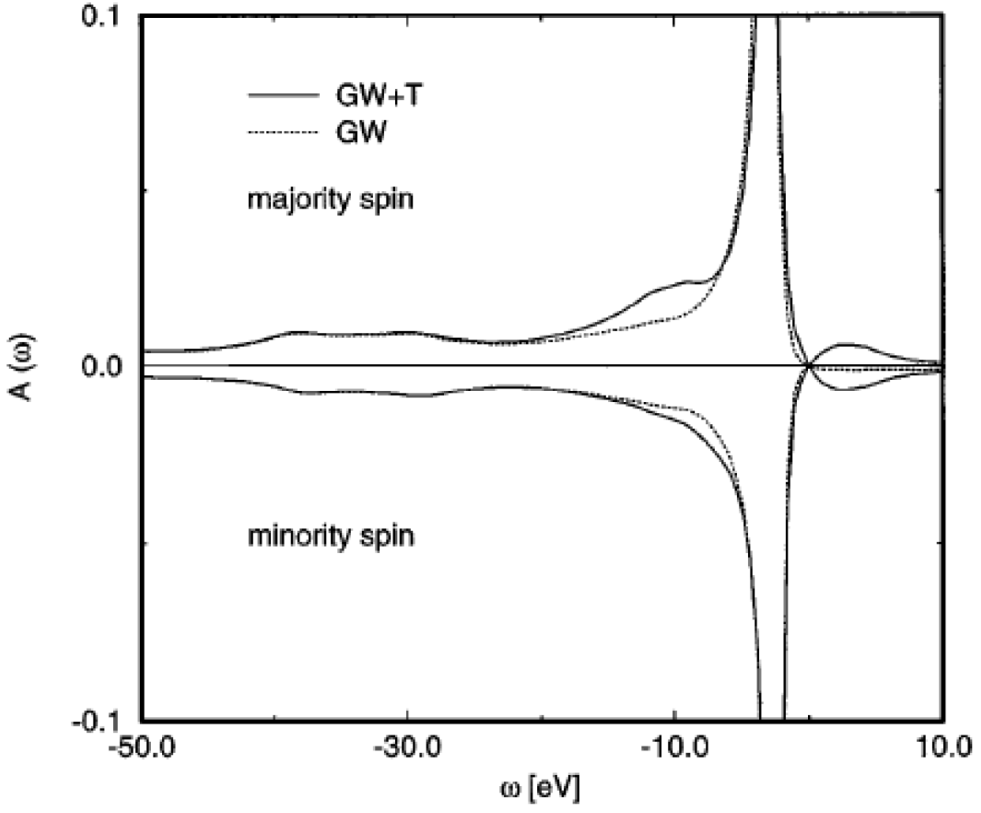
Note

- (B) spin flips: coupling with spin-waves, magnons, paramagnons
- analogously for additional hole

V. P. Zhukov, E. V. Chulkov, and P. M. Echenique, PRB 72 (2005)

T matrix

T matrix: hole-hole interaction
6 eV satellite in Nickel



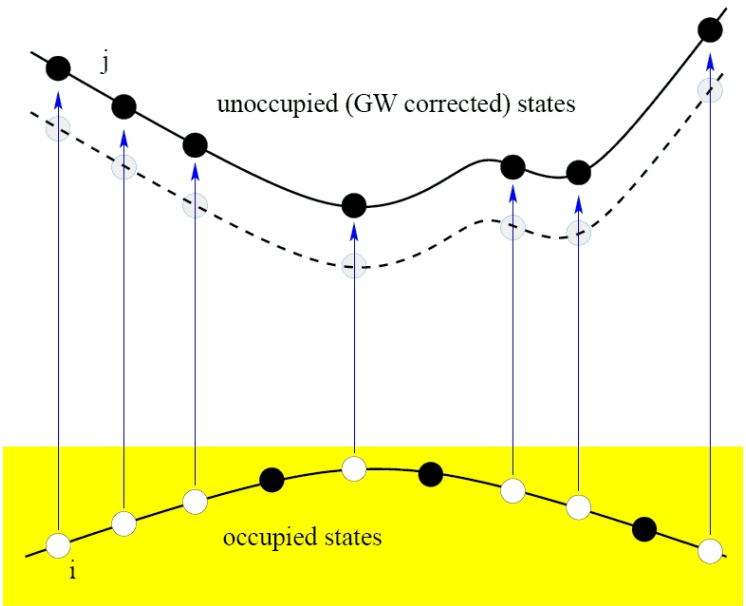
M. Springer, F. Aryasetiawan, and K. Karlsson, PRL 80 (1998)

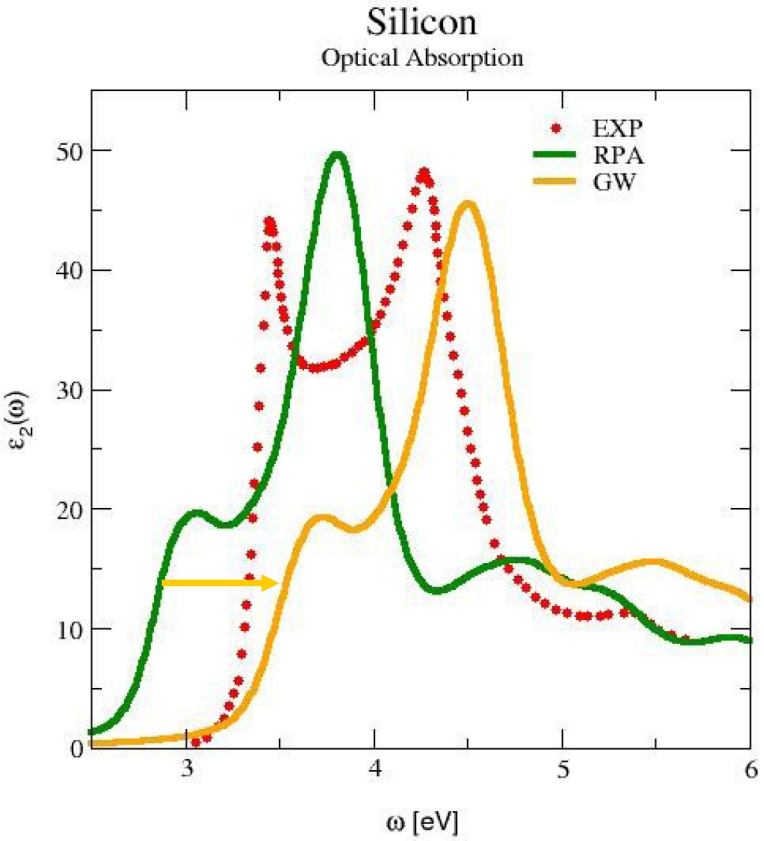
Outline

Independent (quasi)particles: GW

Independent transitions:

$$\epsilon_2(\omega) = \frac{8\pi^2}{\Omega\omega^2} \sum_{ij} |\langle\varphi_j|\mathbf{e}\cdot\mathbf{v}|\varphi_i\rangle|^2 \delta(E_j - E_i - \omega)$$





What is wrong?

What is missing?

What is wrong?

What is missing?

We need the BSE...

What is wrong?

What is missing?

We need the BSE... and Ilya.

Many thanks!

Acknowledgements

- Fabien Bruneval
- Rex Godby
- Valerio Olevano
- Lucia Reining
- Pina Romaniello
- Francesco Sottile