ISTITUTO NANOSCIENZE CONSIGLIO NAZIONALE DELLE RICERCHE

Istituto Nanoscienze
S3 center, Modena, Italy

Theory: Foundations of the GW approximation

Andrea Ferretti

06 May 2026
Yambo tutorial

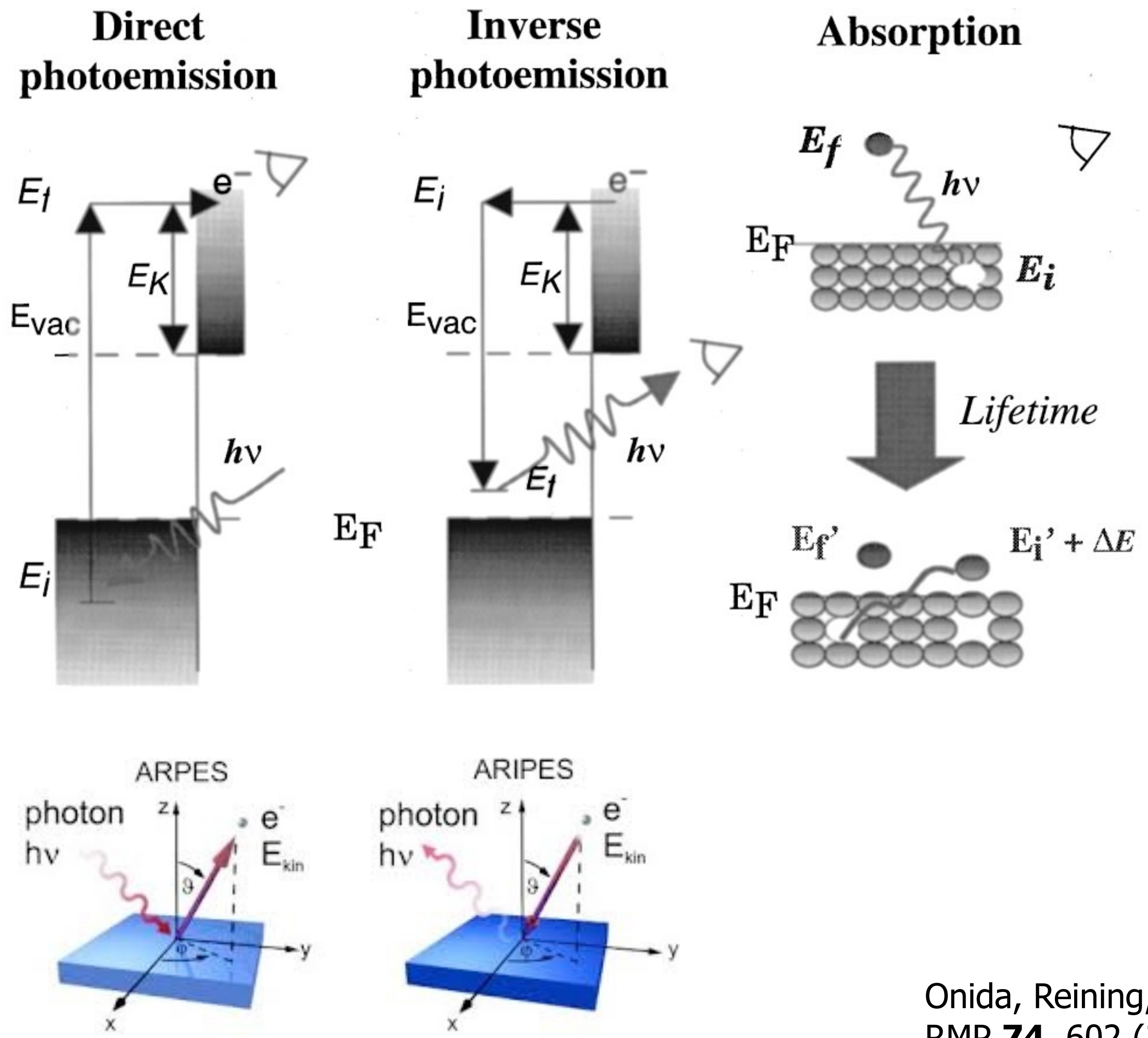
outline

- **ARPES** from a theory perspective
- Connection to the **Green's function theory**
- The **GW self-energy**

outline

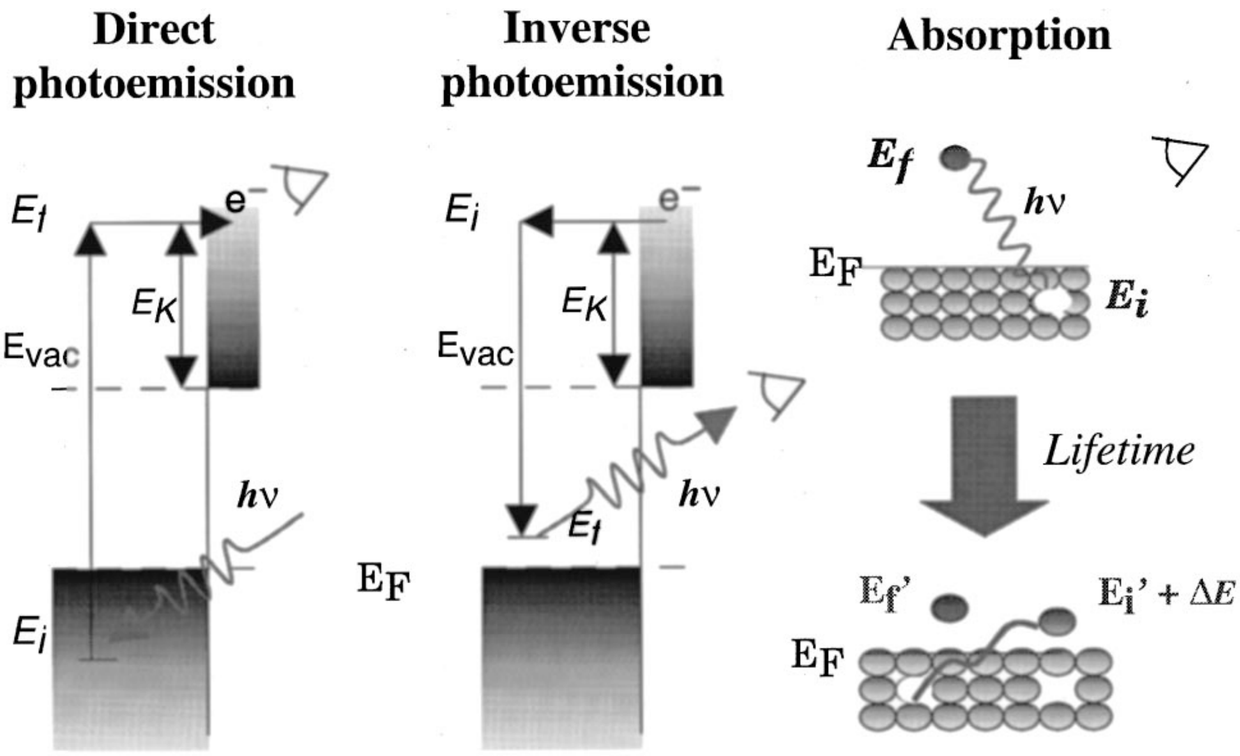
- **ARPES** from a theory perspective
- Connection to the **Green's function theory**
- The **GW self-energy**

excitations



Onida, Reining, Rubio,
RMP **74**, 602 (2002)

excitations



N-1 electrons

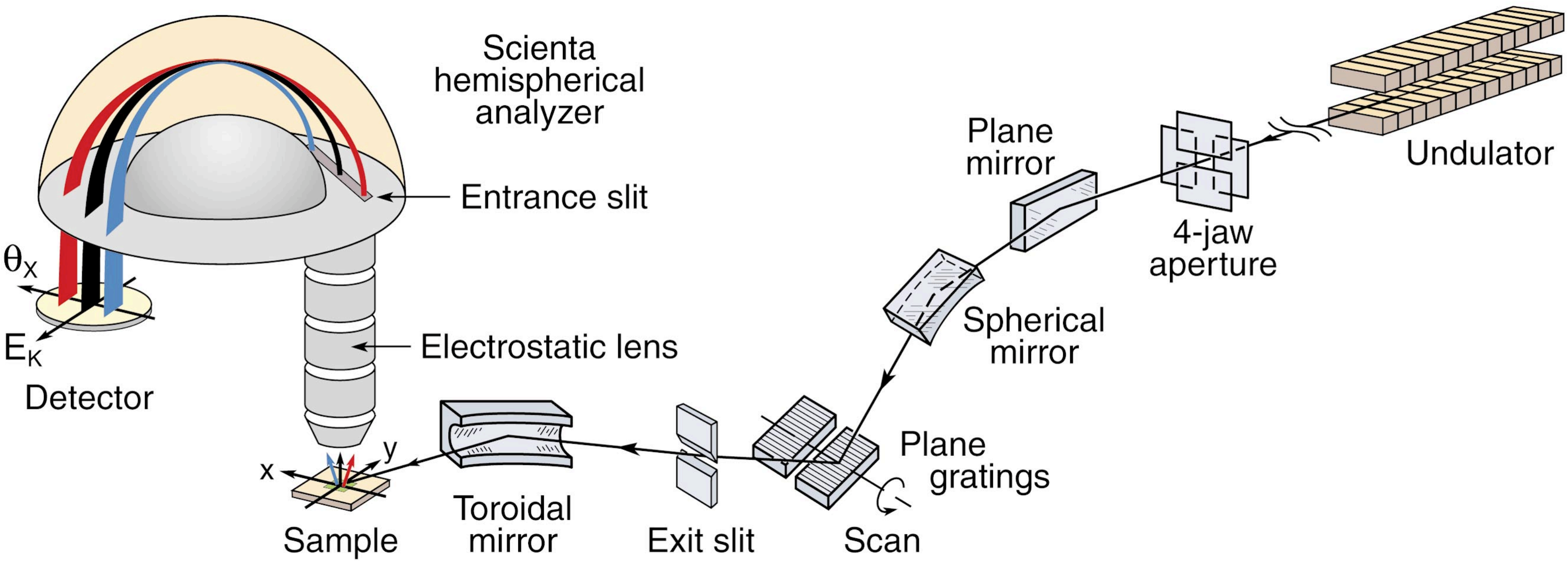
N+1 electrons

N electrons

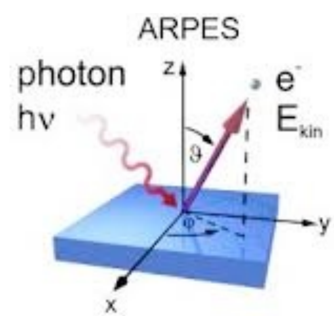
Onida, Reining, Rubio, RMP **74**, 602 (2002)

the ARPES experiment

Damascelli, Hussain, Shen, Rev. Mod. Phys. **75**, 473 (2003)

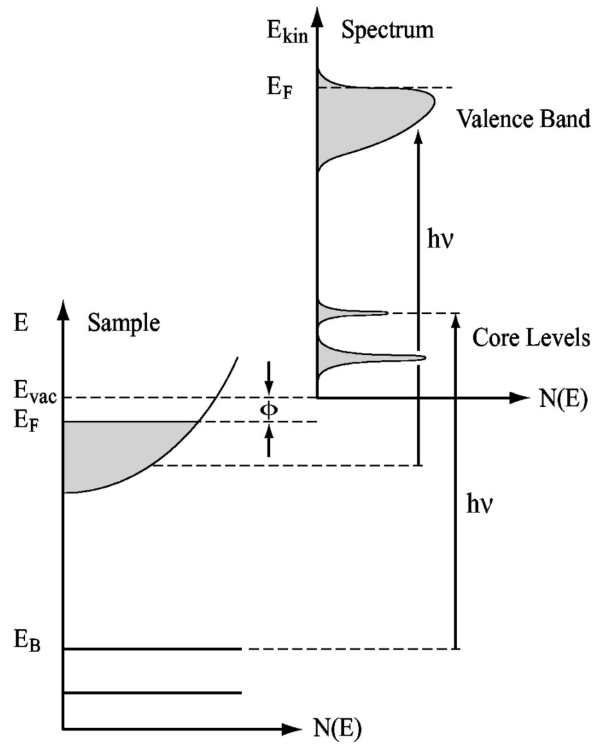


- **incident photons** (hw, angle, polarization)
- the method measures the **kinetic energy** (and the exit **angle,** and/or **spin**) of out-coming electrons
- allows one to access **electronic (band) structures**



the ARPES experiment

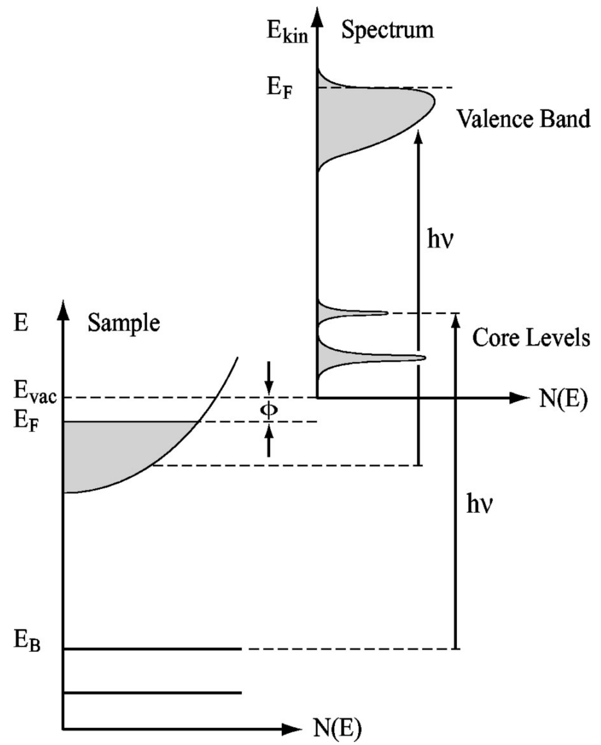
model



Rev. Mod. Phys. **75**, 473 (2003)

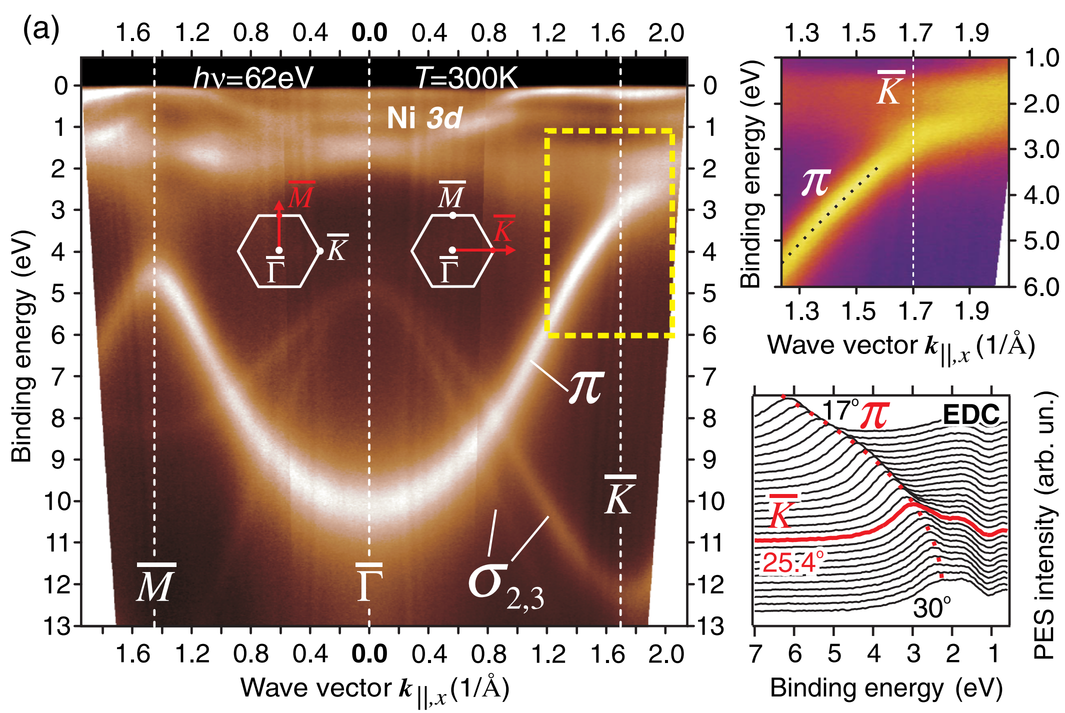
the ARPES experiment

model



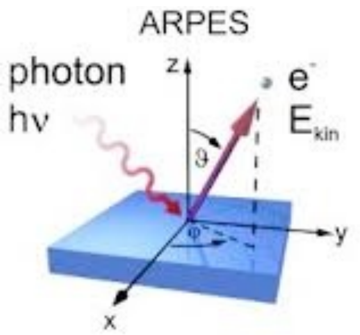
Rev. Mod. Phys. **75**, 473 (2003)

realistic system



Varykhalov et al, PRX **2**, 041017 (2012)

theoretical treatment



see Hedin, Michiels, Inglesfield, PRB **58**, 15565 (1998)
Damascelli et al, RMP **75**, 473 (2003)

Photocurrent J by using the **Fermi golden rule:**

$$J_{\mathbf{k}}(\omega) = \sum_s |\langle \Psi_{\mathbf{k},s} | \Delta | \Psi_i \rangle|^2 \; \delta(\omega - \epsilon_{\mathbf{k}} + \epsilon_s)$$

$$\Delta = \mathbf{A} \cdot \mathbf{p} + \mathbf{p} \cdot \mathbf{A}$$

Kinetic energy of the extracted electron

$$\epsilon_{\mathbf{k}} = \mathbf{k}^2/2$$

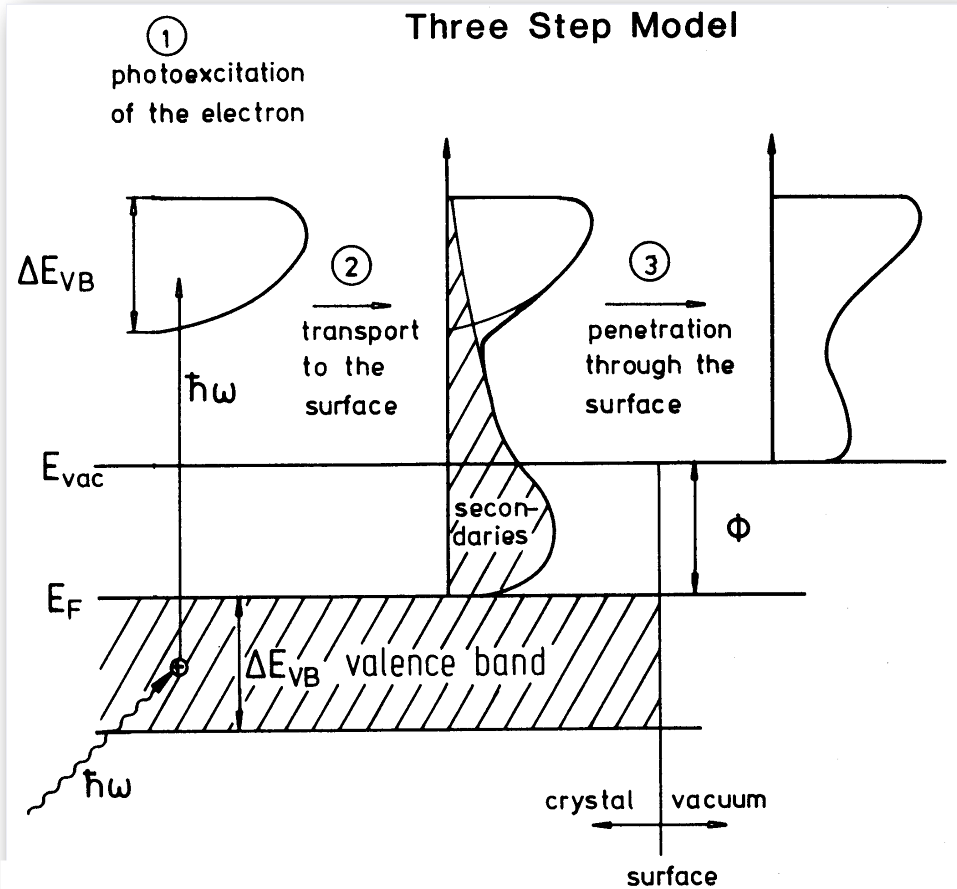
excitation left over

$$\epsilon_s = E(N,0) - E(N-1,s)$$

final state

$$|\Psi_{\mathbf{k},s}\rangle = \left[1 + \frac{1}{E - H - i\eta}(H - E)\right] \; c^\dagger_{\mathbf{k}} |N-1, s\rangle$$

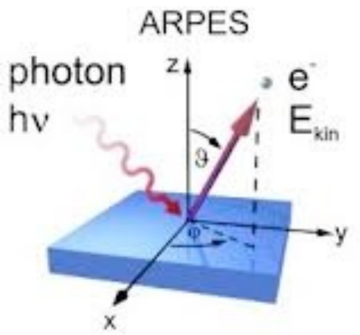
the 3 step model



S. Hufner, Photoelectron Spectroscopy, Third Edition.
see also Slides from Matthias Kreier, Humboldt Uni (2007)

- (1) **photoexcitation**
intrinsic losses are accounted for (satellite structures)
- (2) transport to the surface
extrinsic losses
- (3) transmission through the surface

sudden approximation



see Hedin, Michiels, Inglesfield, PRB **58**, (1998)
Damascelli et al, RMP **75**, 473 (2003)

$$|\Psi_{\mathbf{k},s}\rangle = \left[1 + \frac{1}{E - H - i\eta}(H - E)\right] c^\dagger_{\mathbf{k}}|N-1,s\rangle$$

↓

k fast enough

sudden approx

$$|\Psi_{\mathbf{k},s}\rangle = c^\dagger_{\mathbf{k}}\,|N-1,s\rangle$$

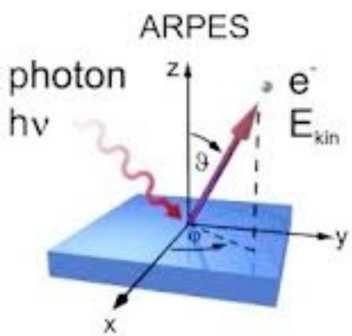
extrinsic losses neglected

↓

spectral function

$$J_{\mathbf{k}}(\omega) = \sum_{ij} \Delta_{\mathbf{k}i}\, A_{ij}(\epsilon_{\mathbf{k}} - \omega)\, \Delta_{j\mathbf{k}}$$

sudden approximation



see Hedin, Michiels, Inglesfield, PRB **58**, (1998)
Damascelli et al, RMP **75**, 473 (2003)

$$|\Psi_{\mathbf{k},s}\rangle = \left[1 + \frac{1}{E - H - i\eta}(H - E)\right] c^\dagger_{\mathbf{k}} |N-1, s\rangle$$

extrinsic losses neglected

spectral function

sudden approx

k fast enough

$$J_{\mathbf{k}}(\omega) = \sum_{ij} \Delta_{\mathbf{k}i}\, A_{ij}(\epsilon_{\mathbf{k}} - \omega)\, \Delta_{j\mathbf{k}}$$

$$A_{ij}(\omega) = \sum_s^{\epsilon_s < \mu} \langle N | c_i^\dagger | N-1, s\rangle \langle N-1, s | c_j | N\rangle\, \delta(\omega - \epsilon_s)$$

connecting to the GF's

In this context, angle-resolved photoemission spectroscopy (ARPES) plays a major role because it is the most direct method of studying the electronic structure of solids (see Sec. II). Its large impact on the development of many-body theories stems from the fact that this technique provides information on the single-particle Green's function, which can be calculated starting from a

the **Green's function** contains info about the **spectral function** → **ARPES**

outline

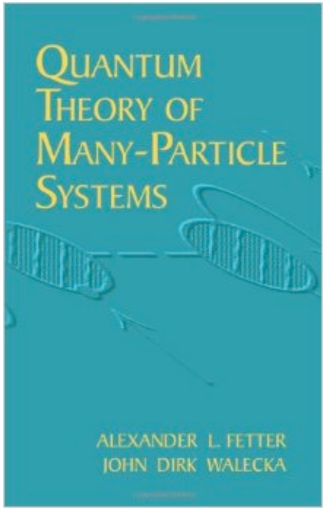
- **ARPES** from a theory perspective
- Connection to the **Green's function theory**
- The **GW self-energy**

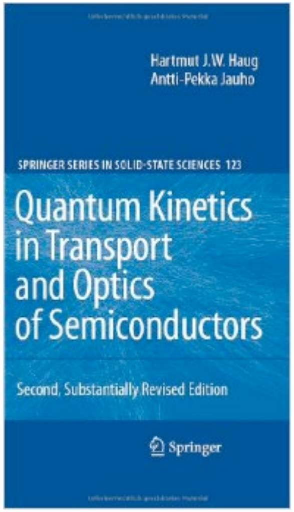
the Green's function

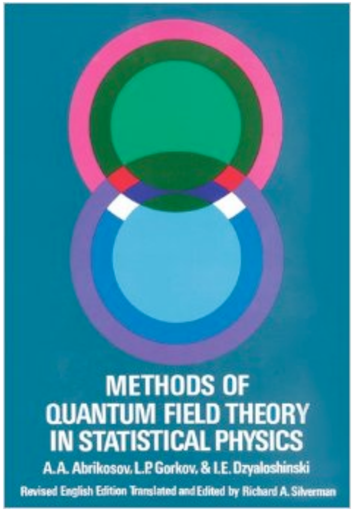
$$iG(\mathbf{x}_1, \mathbf{x}_2, t_1 - t_2) = \langle N| \, T \left[\psi(\mathbf{x}_1 t_1), \psi^\dagger(\mathbf{x}_2 t_2) \right] | \, N \rangle$$

$$= \theta(t_1 - t_2) \langle N | \psi(\mathbf{x}_1 t_1) \psi^\dagger(\mathbf{x}_2 t_2) | N \rangle$$

$$- \, \theta(t_2 - t_1) \langle N | \psi^\dagger(\mathbf{x}_2 t_2) \psi(\mathbf{x}_1 t_1) | N \rangle$$







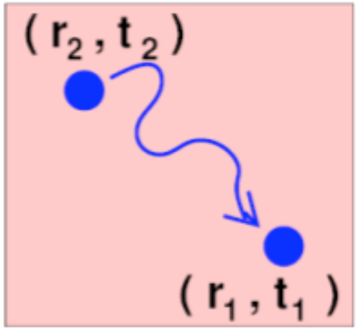
CNRNANO
ISTITUTO NANOSCIENZE CONSIGLIO NAZIONALE DELLE RICERCHE

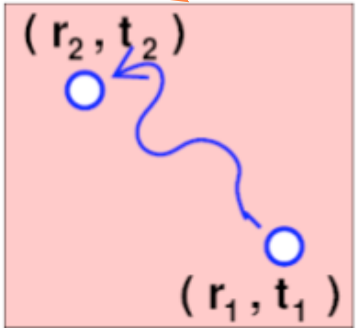
the Green's function

$$iG(\mathbf{x}_1, \mathbf{x}_2, t_1 - t_2) = \langle N | \, T \left[\psi(\mathbf{x}_1 t_1), \psi^\dagger(\mathbf{x}_2 t_2) \right] | \, N \rangle$$

$$= \theta(t_1 - t_2) \langle N | \psi(\mathbf{x}_1 t_1) \psi^\dagger(\mathbf{x}_2 t_2) | N \rangle$$

$$- \theta(t_2 - t_1) \langle N | \psi^\dagger(\mathbf{x}_2 t_2) \psi(\mathbf{x}_1 t_1) | N \rangle$$





the Lehmann representation

- Using the **completeness** of the eigenvectors at **N+1 and N-1 electrons**

$$G(\mathbf{x},\mathbf{x}',\omega) = \sum_s \frac{f_s(\mathbf{x})\, f_s^*(\mathbf{x}')}{\omega - \epsilon_s + i\eta_s}$$

as for non-interacting systems

- **Charged excitations**

$$\epsilon_s = E_0^N - E_s^{N-1} \qquad \eta_s = -i0^+$$

$$\epsilon_s = E_s^{N+1} - E_0^N \qquad \eta_s = \quad i0^+$$

plays the role of the non-int **eigenvalues**

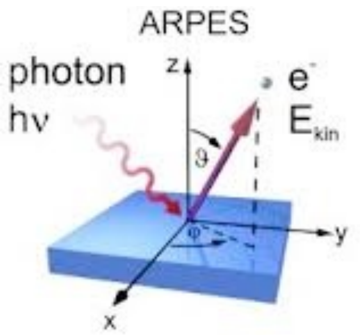
- **Dyson** orbitals

$$\epsilon_s < \mu \qquad f_s(\mathbf{x}) = \langle N-1, s|\, \hat{\psi}(\mathbf{x})\, |N, 0\rangle$$

$$\epsilon_s \geq \mu \qquad f_s(\mathbf{x}) = \langle N, 0|\, \hat{\psi}(\mathbf{x})\, |N+1, s\rangle$$

plays the role of the non-int **eigenvectors**

sudden approximation



see Hedin, Michiels, Inglesfield, PRB **58**, (1998)
Damascelli et al, RMP **75**, 473 (2003)

$$|\Psi_{\mathbf{k},s}\rangle = \left[1 + \frac{1}{E - H - i\eta}(H - E)\right] c^\dagger_{\mathbf{k}} |N-1, s\rangle$$

extrinsic losses neglected

spectral function

sudden approx

k fast enough

$$J_{\mathbf{k}}(\omega) = \sum_{ij} \Delta_{\mathbf{k}i}\, A_{ij}(\epsilon_{\mathbf{k}} - \omega)\, \Delta_{j\mathbf{k}}$$

$$A_{ij}(\omega) = \sum_{s}^{\epsilon_s<\mu} \langle N|c^\dagger_i|N-1,s\rangle\langle N-1,s|c_j|N\rangle\, \delta(\omega - \epsilon_s)$$

the Lehmann representation

- Using the **completeness** of the eigenvectors at **N+1 and N-1 electrons**

$$G(\mathbf{x},\mathbf{x}',\omega) = \sum_s \frac{f_s(\mathbf{x})\, f_s^*(\mathbf{x}')}{\omega - \epsilon_s + i\eta_s}$$

- The **spectral function**

$$A(\mathbf{x},\mathbf{x}',\omega) = \frac{1}{2\pi i}\left[G(\omega) - G^\dagger(\omega)\right]_{\mathbf{x},\mathbf{x}'} \mathrm{sgn}(\mu - \omega)$$

$$G(\mathbf{x},\mathbf{x}',\omega) = \int \frac{A(\mathbf{x},\mathbf{x}',\omega')}{\omega - \omega' \pm i0^+} d\omega'$$

Kramers-Kronig transform

$$A(\mathbf{x},\mathbf{x}',\omega) = \sum_s f_s(\mathbf{x}) f_s^*(\mathbf{x}')\, \delta(\omega - \epsilon_s)$$

spectral info

the Lehmann representation

- Using the **completeness** of the eigenvectors at **N+1 and N-1 electrons**

$$G(\mathbf{x},\mathbf{x}',\omega) = \sum_s \frac{f_s(\mathbf{x})\, f_s^*(\mathbf{x}')}{\omega - \epsilon_s + i\eta_s}$$

- The **spectral function**

$$A(\mathbf{x},\mathbf{x}',\omega) = \frac{1}{2\pi i}\left[G(\omega) - G^\dagger(\omega)\right]_{\mathbf{x},\mathbf{x}'} \mathrm{sgn}(\mu - \omega)$$

$$G(\mathbf{x},\mathbf{x}',\omega) = \int \frac{A(\mathbf{x},\mathbf{x}',\omega')}{\omega - \omega' \pm i0^+} d\omega'$$

Kramers-Kronig transform

$$\rho(\mathbf{x},\omega) = \sum_s |f_s(\mathbf{x})|^2\, \delta(\omega - \epsilon_s)$$

spectral info

the Lehmann representation

Dyson equation

$$G(\omega) = G_0(\omega) + G_0(\omega)\Sigma(\omega)G(\omega)$$

$$G(\omega) = \big[\omega - H_0 - \Sigma(\omega)\big]^{-1}$$

$$G(\mathbf{x},\mathbf{x}',\omega) = \sum_s \frac{f_s(\mathbf{x})\, f_s^*(\mathbf{x}')}{\omega - \epsilon_s + i\eta_s}$$

Assuming discrete states:

$$\big[H_0 + \Sigma(\epsilon_s)\big]|f_s\rangle = \epsilon_s|f_s\rangle$$

$$\langle f_s|f_s\rangle = Z_s = \left[1 - \langle\frac{\partial\Sigma}{\partial\omega}\rangle_s\right]^{-1}_{\omega=\epsilon_s}$$

- **Non-linear eigenvalue problem** (NLEP)
- Frequency (orbital) dependent potential
- fs need to be normalized to Zs
- See Onida, Reining, Rubio, Rev. Mod. Phys. **74**, 602 (2002)

the QP representation

Dyson Equation

$$G(\omega) = \left[\omega - H_0 - \Sigma(\omega)\right]^{-1}$$

by direct **diagonalization**

$$\left[h_0 + \Sigma(\omega)\right] |\psi_{s\omega}\rangle = E_s(\omega)|\psi_{s\omega}\rangle$$

$$G(\omega) = \sum_s \frac{|\psi_{s\omega}\rangle\langle\psi^{s\omega}|}{\omega - E_s(\omega)}$$

- Sgm is **non-hermitian**
- diag leads to left and right (dual) eigenvectors
- $E_s(\omega)$ can be **complex**
- **Relevant poles** can be selected according to the condition

see Onida et al, RMP **74**, 602 (2002)
Farid preprint cond-mat/0110481 (2001)
phyl mag B **82**, 1413 (2002)

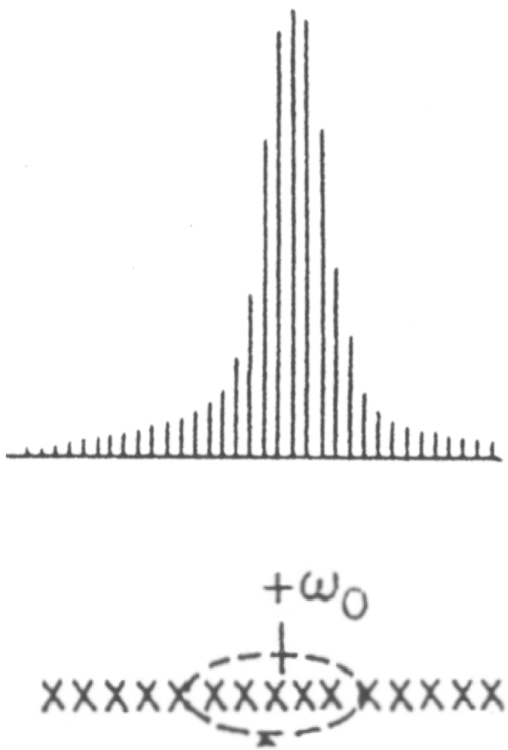
QP approximation

$$E_s(z_m^{\mathrm{QP}}) = z_m^{\mathrm{QP}}$$

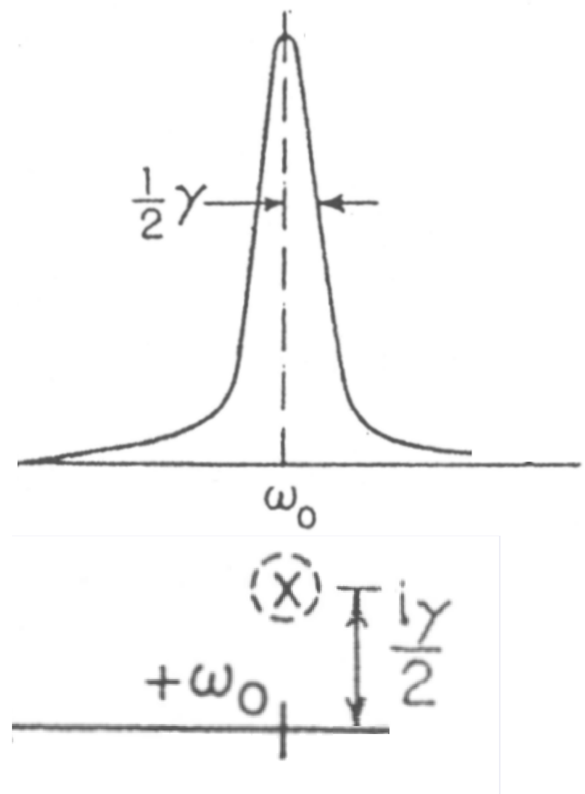
Lehmann vs QP

$$G(\mathbf{x},\mathbf{x}',\omega) = \sum_s \frac{f_s(\mathbf{x})\, f_s^*(\mathbf{x}')}{\omega - \epsilon_s + i\eta_s}$$

$$G(\mathbf{x},\mathbf{x}',\omega) = \sum_m \frac{\langle \mathbf{x}|\psi_m^{\mathrm{QP}}\rangle\langle\psi^{\mathrm{QP}m}|\mathbf{x}'\rangle}{\omega - z_m^{\mathrm{QP}}}$$



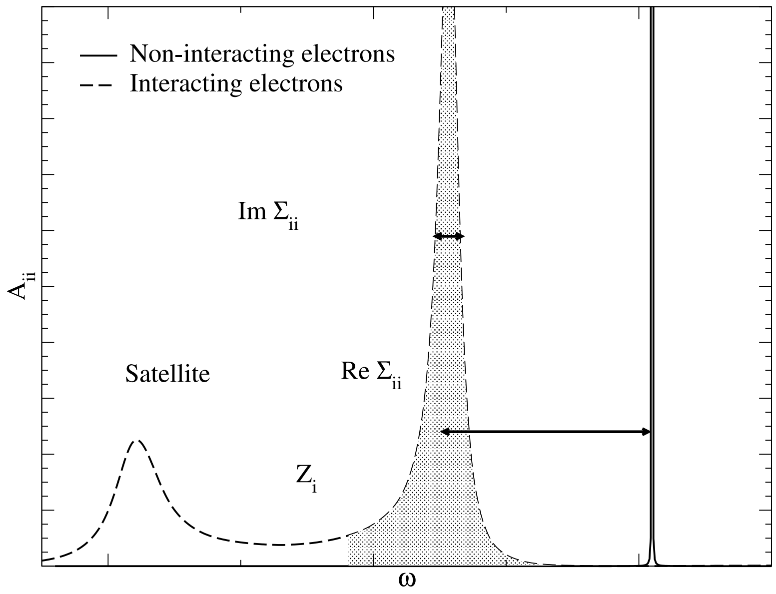
Farid preprint cond-mat/0110481 (2001)
phyl mag B **82**, 1413 (2002)



Figures adapted from M. Gatti PhD thesis

the spectral function

Figure from F. Bruneval PhD thesis



Let's **assume**:

Σ and G are **diagonal** on the basis of the **non-int Hamiltonian**

$$H_0|\phi_i\rangle = \epsilon_i|\phi_i\rangle$$

$$\Sigma_{ii}(\omega) = \langle\phi_i|\Sigma(\omega)|\phi_i\rangle$$

$$G_{ii}(\omega) = [\omega - \epsilon_i - \Sigma_{ii}(\omega)]^{-1}$$

Making a Taylor expansion of Σ(**ω**) around $E_i = \epsilon_i + \mathrm{Re}\Sigma_{ii}(E_i)$

$$\Sigma_{ii}(\omega) = \Sigma_{ii}(E_i) + \frac{\partial\Sigma_{ii}}{\partial\omega}(\omega - E_i)$$

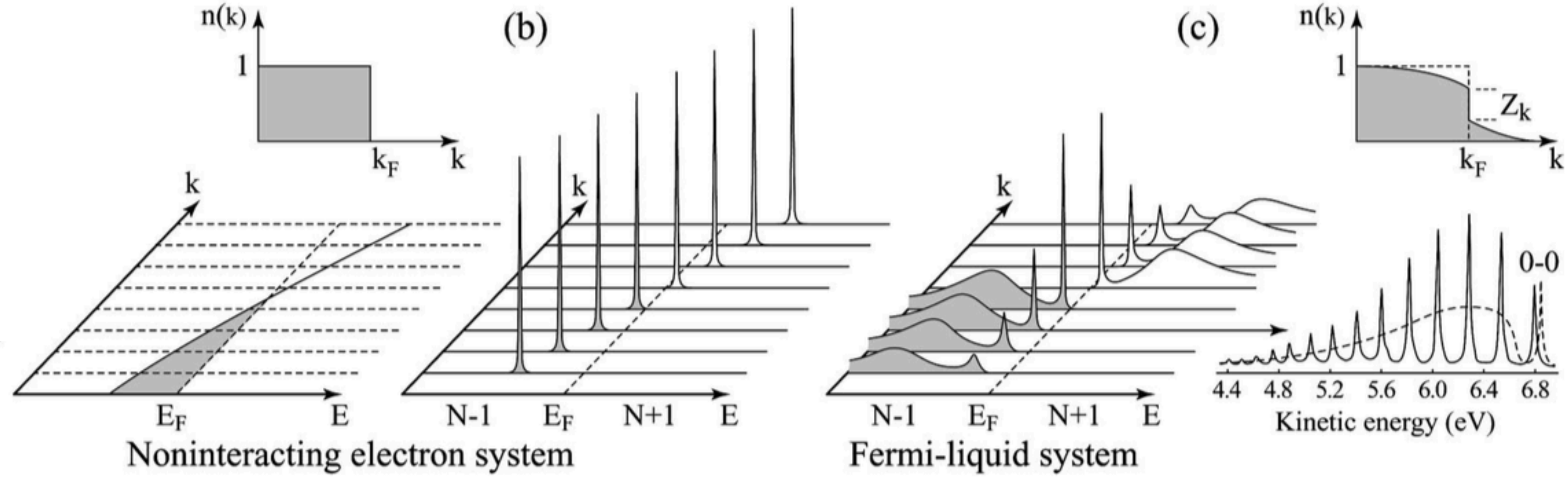
$$G_i(\omega) = \frac{Z_i}{\omega - E_i - i\Gamma_i}$$

renormalization factor

$$Z_i = (1 - \frac{\partial\Sigma_{ii}}{\partial\omega}_{|E_i})^{-1}$$

$$\Gamma_i = \mathrm{Im}\Sigma_{ii}(E_i)$$

the spectral function



Manybody features include

- **satellites**
- **lifetimes**
- **renormalization**

All the above features depend on the **dynamical** and **non-hermitian** nature of **Σ(ω)**

CNRNANO ISTITUTO NANOSCIENZE CONSIGLIO NAZIONALE DELLE RICERCHE

Figure from: Damascelli, Hussain, Shen, Rev. Mod. Phys. **75**, 473 (2003)

outline

- **ARPES** from a theory perspective
- Connection to the **Green's function theory**
- The **GW self-energy**

L. Hedin, Phys. Rev. **139**, A796 (1965)
L. Reining, WIREs Comput. Mol. Sci. **8**, e1344 (2018).
D. Golze, M. Dvorak, P. Rinke, Front. Chem. **7**, 377 (2019).

Hedin's equations

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

New Method for Calculating the One-Particle Green's Function with Application to the Electron-Gas Problem*

LARS HEDIN†
Argonne National Laboratory, Argonne, Illinois
(Received 8 October 1964; revised manuscript received 2 April 1965)

We write the Schrödinger representation of the Hamiltonian for the system to be considered as

$$H = H_0 + H_1 ,$$

$$H_0 = \int \psi^\dagger(\mathbf{x}) h(\mathbf{x}) \psi(\mathbf{x}) d\mathbf{x} + \frac{1}{2} \int \psi^\dagger(\mathbf{x}) \psi^\dagger(\mathbf{x}') v(\mathbf{x},\mathbf{x}') \psi(\mathbf{x}') \psi(\mathbf{x}) d\mathbf{x} d\mathbf{x}' , \quad \text{(A1)}$$

$$H_1 = \int \rho(\mathbf{x}) w(\mathbf{x},t) d\mathbf{x} , \quad \rho(\mathbf{x}) = \psi^\dagger(\mathbf{x}) \psi(\mathbf{x}) ,$$

Hedin's equations

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

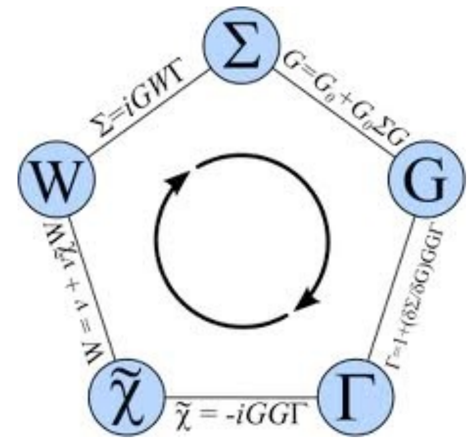
$$G(12) = G_0(12) + \int d34\, G_0(13)\Sigma(34)G(42)$$

$$W(12) = v(12) + \int d34\, v(13)P(34)W(42)$$

$$\Sigma(12) = i \int d34\, G(13)W(41)\Gamma(324)$$

$$P(12) = -i \int d34\, G(13)G(41)\Gamma(342)$$

$$\Gamma(123) = \delta(12)\delta(13) + \int d4567\, \frac{\delta\Sigma(12)}{\delta G(45)} G(46)G(75)\Gamma(673)$$



$$\Gamma(123) = -\frac{\delta G^{-1}(12)}{\delta v(3)}$$

$$1 \equiv x_1 t_1$$

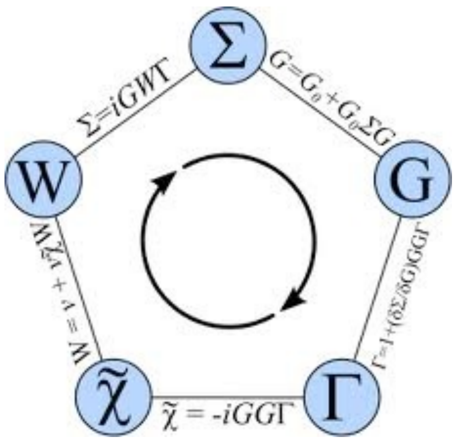
$$G_0 \longleftrightarrow H_0 = T + V_{\text{ext}} + V_H$$

Hedin's equations

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

$$G(12) = G_0(12) + \int d34\, G_0(13)\Sigma(34)G(42)$$

$$W(12) = v(12) + \int d34\, v(13)P(34)W(42)$$



Dyson-like equations:

$$W = v + vPv + vPvPv + vPvPvPv + \dots$$

$$= \sum_{n=0}^{\infty} (vP)^n\, v$$

formal solution

$$= [1 - vP]^{-1} v$$

summation using the **geometric series**

$$= \epsilon^{-1} v$$

Hedin's Eq to GW

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

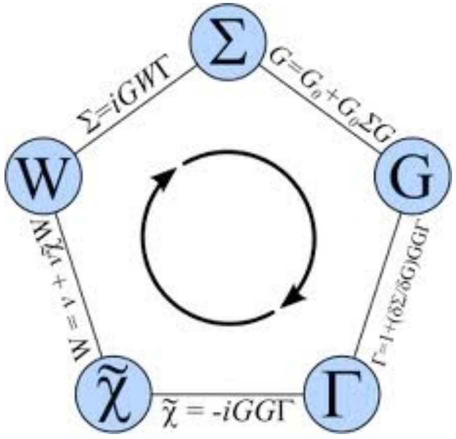
$$G(12) = G_0(12) + \int d34\, G_0(13)\Sigma(34)G(42)$$

$$W(12) = v(12) + \int d34\, v(13)P(34)W(42)$$

$$\Sigma(12) = i\int d34\, G(13)W(41)\Gamma(324)$$

$$P(12) = -i\int d34\, G(13)G(41)\Gamma(342)$$

$$\Gamma(123) = \delta(12)\delta(13) + \int d4567\, \frac{\delta\Sigma(12)}{\delta G(45)} G(46)G(75)\Gamma(673)$$



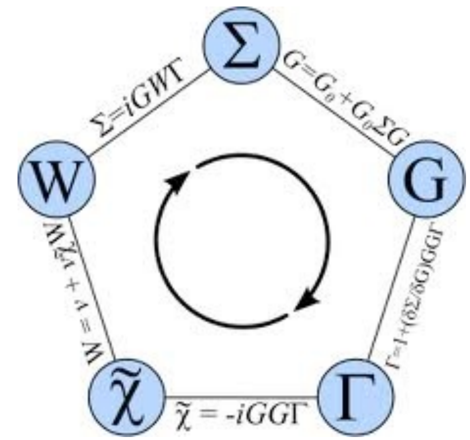
$$\Gamma(123) = -\frac{\delta G^{-1}(12)}{\delta v(3)}$$

the GW approximation

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

$$G(12) = G_0(12) + \int d34\, G_0(13)\Sigma(34)G(42)$$

$$W(12) = v(12) + \int d34\, v(13)P(34)W(42)$$



$$\Sigma(12) = \quad iG(12)W(21)$$

$$P(12) = -iG(12)G(21)$$

$$\Gamma(123) = \quad \delta(12)\delta(13)$$

the GW approximation

Independent particle polarisability
(-> reducible polarisability at RPA level)

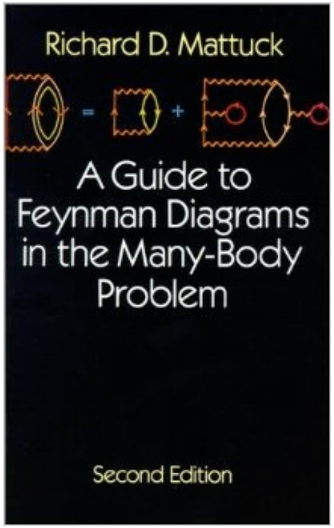
the GW approximation

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

$$\Sigma(12) = iG(12)W(21)$$

$$P(12) = -iG(12)G(21)$$

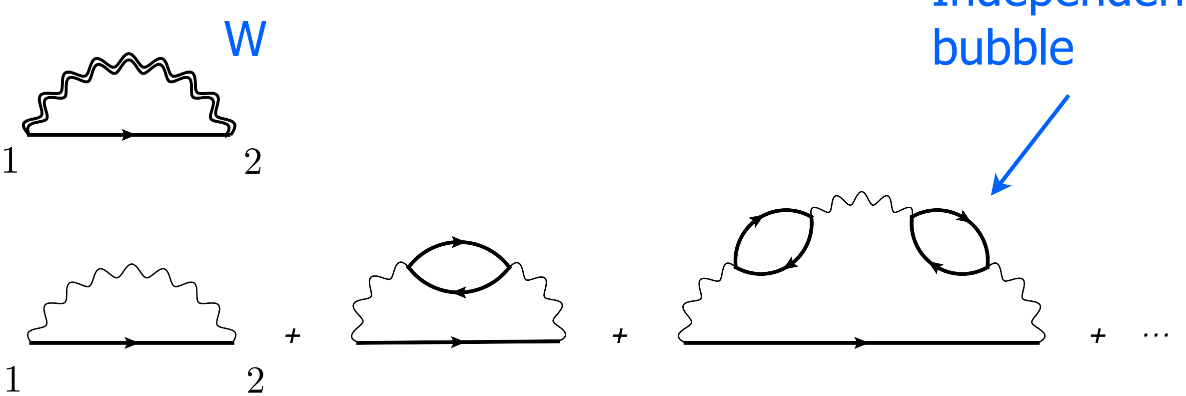
$$\Gamma(123) = \delta(12)\delta(13)$$



Independent particle bubble

$$\Sigma^{\mathrm{GW}}(12) =$$

$$=$$



RPA screening

the GW approximation

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

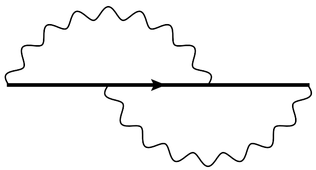
$$\Sigma(12) = iG(12)W(21)$$

$$P(12) = -iG(12)G(21)$$

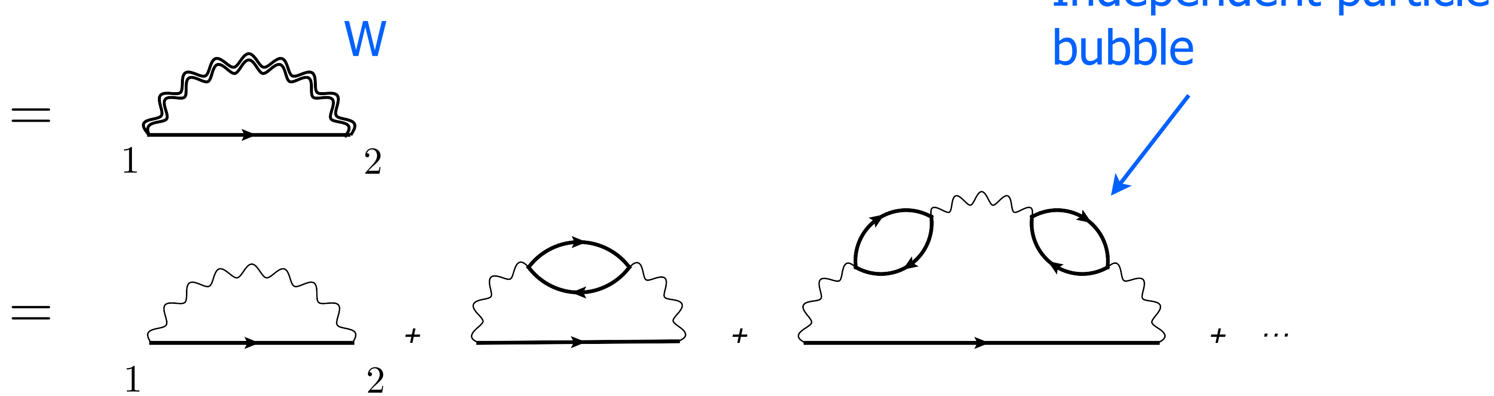
$$\Gamma(123) = \delta(12)\delta(13)$$

beware: GW is not the whole story

e.g. 2nd order exchange is not there



$$\Sigma^{\mathrm{GW}}(12) =$$

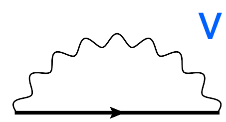


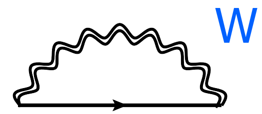
related approximations

Hartree-Fock

$$\Sigma^{\mathrm{HF}}(12) = \quad iG(12)v(21)$$

$$\Sigma^{\mathrm{GW}}(12) = \quad iG(12)W(21)$$

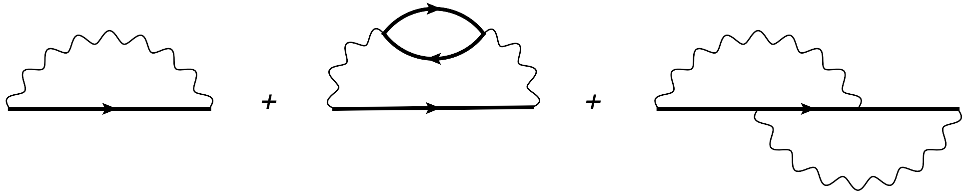




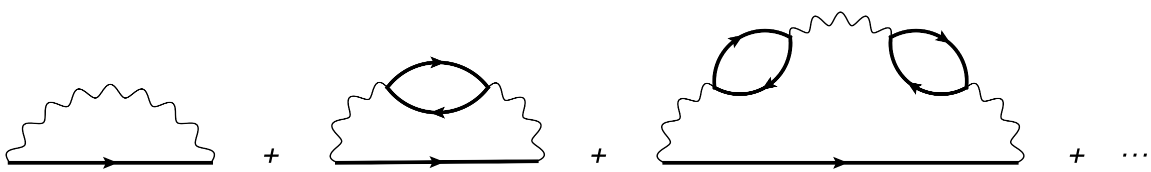
no screening

2nd Born approx (MP2)

$$\Sigma^{\mathrm{2B}}(12) =$$

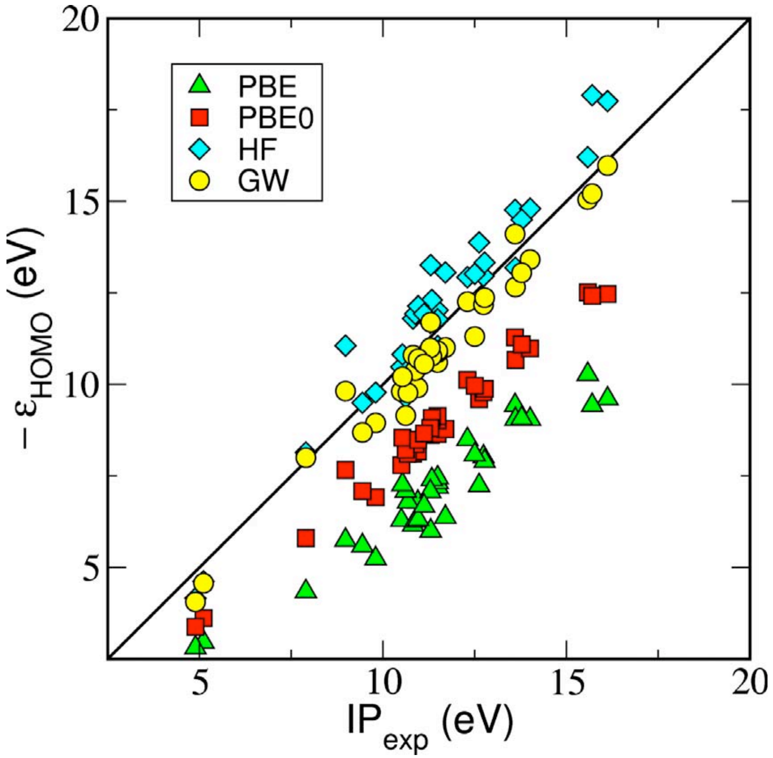


$$\Sigma^{\mathrm{GW}}(12) =$$



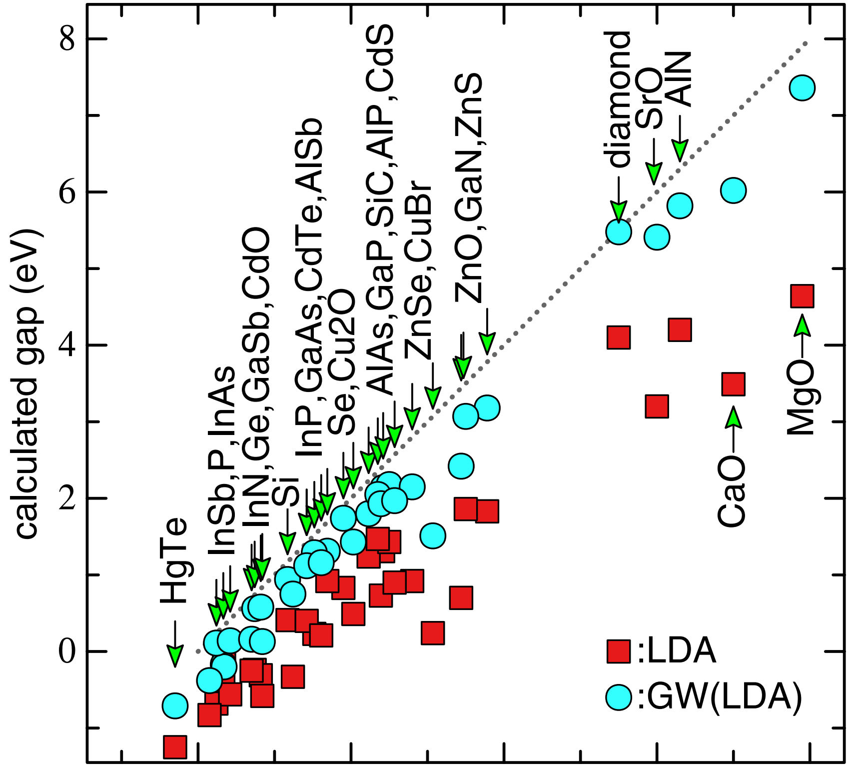
it works!

Molecules



C. Rostgaard, K. W. Jacobsen, and K. S. Thygesen, PRB **81**, 085103 (2010)

Solids



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

CNRNANO
ISTITUTO NANOSCIENZE CONSIGLIO NAZIONALE DELLE RICERCHE

but…

self-interaction in GW

PHYSICAL REVIEW A **75**, 032505 (2007)

Self-interaction in Green's-function theory of the hydrogen atom

W. Nelson,[1,*] P. Bokes,[2,3] Patrick Rinke,[3,4] and R. W. Godby[1,3,†]
[1]*Department of Physics, University of York, Heslington, York YO10 5DD, United Kingdom*
[2]*Department of Physics, Faculty of Electrical Engineering and Information Technology, Slovak University of Technology, Ilkovičova 3, 841 04 Bratislava, Slovak Republic*
[3]*European Theoretical Spectroscopy Facility (ETSF)*
[4]*Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany*
(Received 5 December 2006; published 14 March 2007)

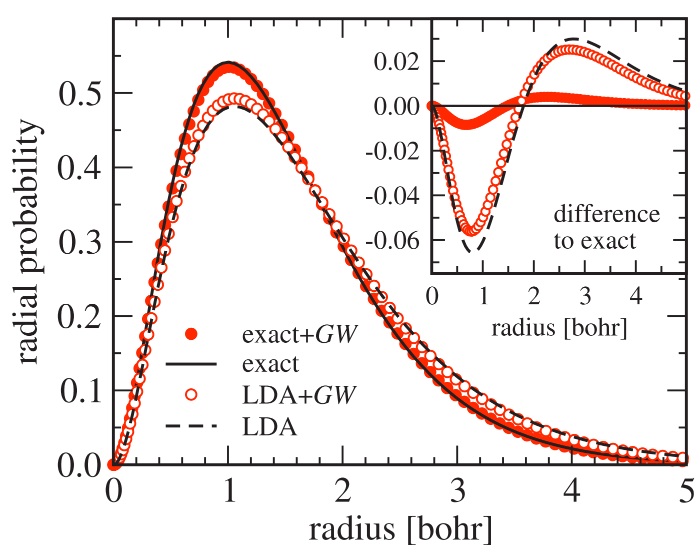
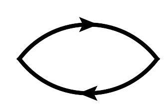


TABLE I. Quasiparticle energies (eV) for the 1*s* state of hydrogen (the ionization potential) obtained by diagonalizing the quasiparticle Hamiltonian (1). Two *GW* calculations are shown, starting from the LDA and from exact Kohn-Sham, respectively. For comparison, the Hartree-Fock (HF) and LDA eigenvalues are also shown.

Exact	HF	LDA	LDA+*GW*	Exact+*GW*
−13.61	−13.61	−6.36	−12.66	−13.40

because of the **RPA polarizability** (self-screening)

P = $-i$ 

beyond the GW approx

THE JOURNAL OF CHEMICAL PHYSICS **131**, 154111 (2009)

The self-energy beyond *GW*: Local and nonlocal vertex corrections

P. Romaniello,[1,a)] S. Guyot,[2] and L. Reining[1]
[1]*Laboratoire des Solides Irradiés, École Polytechnique, CNRS-CEA/DSM, F-91128 Palaiseau, France and European Theoretical Spectroscopy Facility (ETSF), F-91128 Palaiseau, France*
[2]*LiSSi, E. A. 3956, Université Paris 12, 94010 Créteil, France*

(Received 13 July 2009; accepted 27 September 2009; published online 20 October 2009)

PRL **112,** 096401 (2014) PHYSICAL REVIEW LETTERS week ending 7 MARCH 2014

Ionization Potentials of Solids: The Importance of Vertex Corrections

Andreas Grüneis,[1] Georg Kresse,[1,*] Yoyo Hinuma,[2] and Fumiyasu Oba[2,3,†]
[1]*Faculty of Physics and Center for Computational Materials Science, University of Vienna, Sensengasse 8/12, A-1090 Vienna, Austria*
[2]*Department of Materials Science and Engineering, Kyoto University, Kyoto 606-8501, Japan*
[3]*Materials Research Center for Element Strategy, Tokyo Institute of Technology, Yokohama 226-8503, Japan*
(Received 12 September 2013; published 7 March 2014)

The ionization potential is a fundamental key quantity with great relevance to diverse material properties. We find that state of the art methods based on density functional theory and simple diagrammatic approaches as commonly taken in the *GW* approximation predict the ionization potentials of semiconductors and insulators unsatisfactorily. Good agreement between theory and experiment is obtained only when diagrams resulting from the antisymmetry of the many-electron wave function are taken into account via vertex corrections in the self-energy. The present approach describes both localized and delocalized states accurately, making it ideally suited for a wide class of materials and processes.

DOI: 10.1103/PhysRevLett.112.096401 PACS numbers: 71.10.-w, 31.15.A-

beyond the GW approx

JCTC Journal of Chemical Theory and Computation

Vacondio, Varsano, Ruini, Ferretti, JCTC **20**, 4718 (2024)

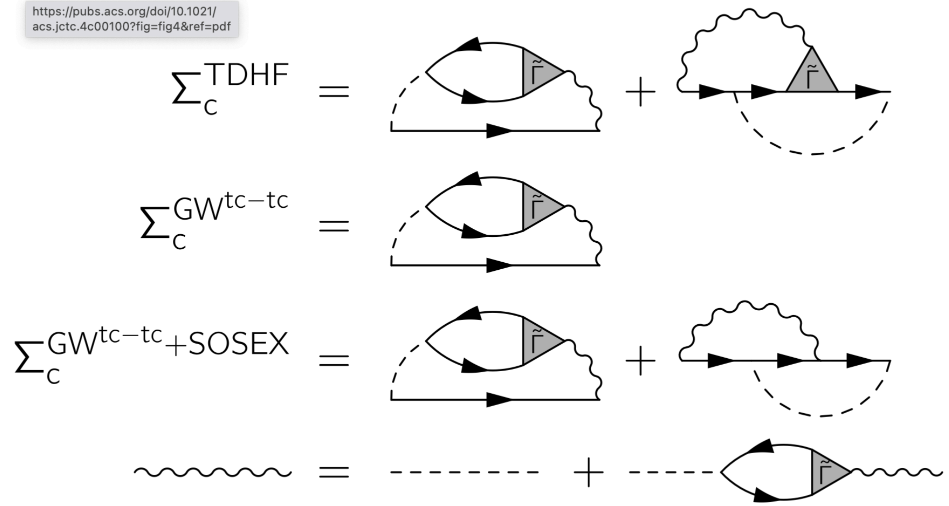
pubs.acs.org/JCTC Article

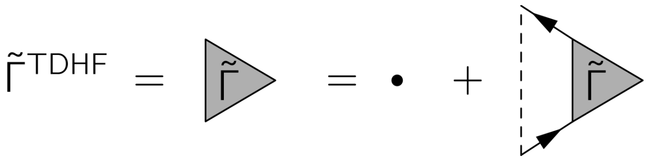
Going Beyond the GW Approximation Using the Time-Dependent Hartree–Fock Vertex

Simone Vacondio,* Daniele Varsano, Alice Ruini, and Andrea Ferretti

Cite This: https://doi.org/10.1021/acs.jctc.4c00100 Read Online

- Makes use of the **TD-HF vertex**
- Becomes the **BSE vertex** when including screening
- Assessment done on **spherical atoms**



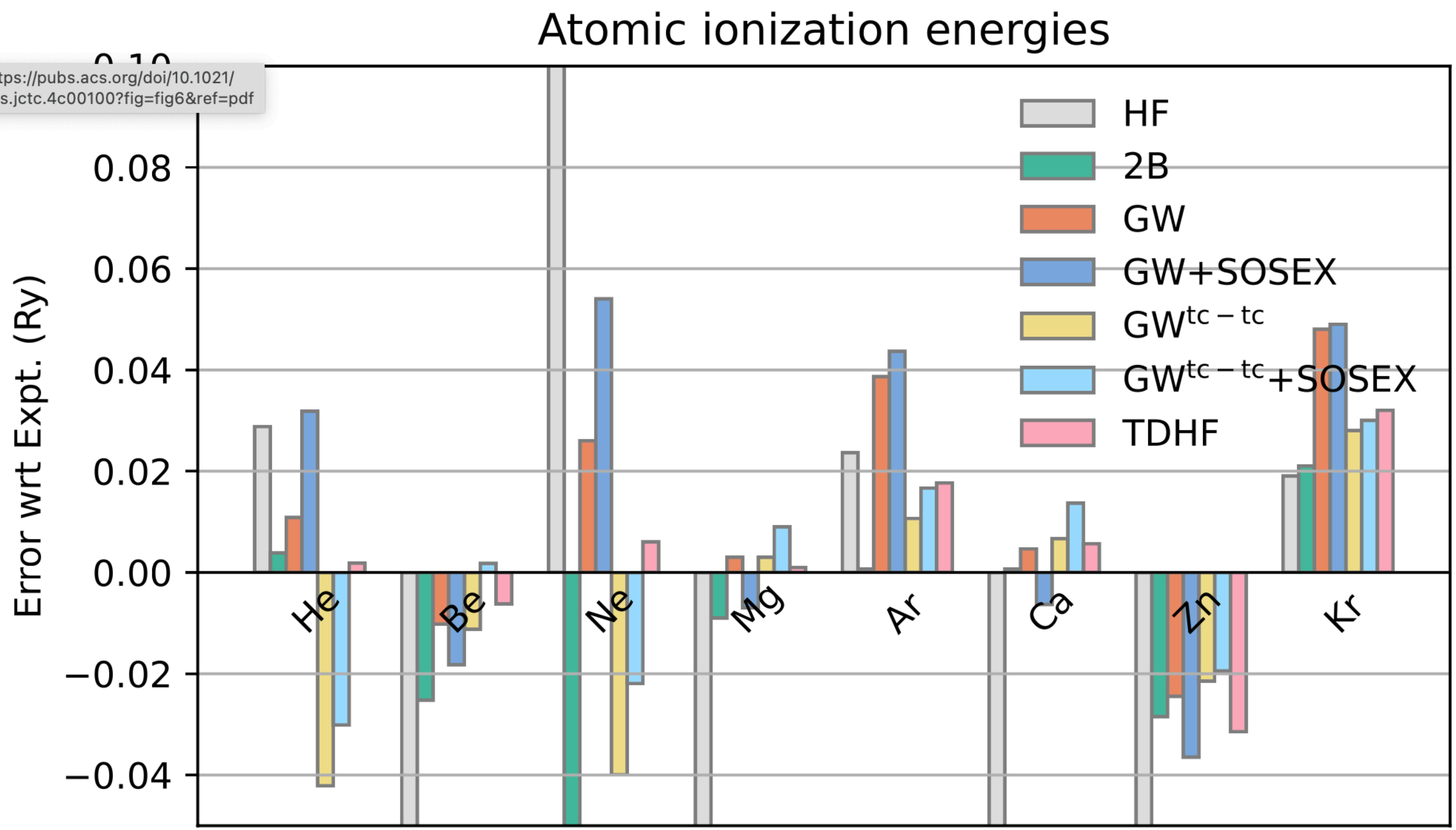


See also: Maggio, Kresse, JCTC **13**, 4765 (2017)
Kutepov, PRB **94**, 155101 (2016)

beyond the GW approx

Vacondio, Varsano, Ruini, Ferretti, JCTC **20**, 4718 (2024)

https://pubs.acs.org/doi/10.1021/acs.jctc.4c00100?fig=fig6&ref=pdf



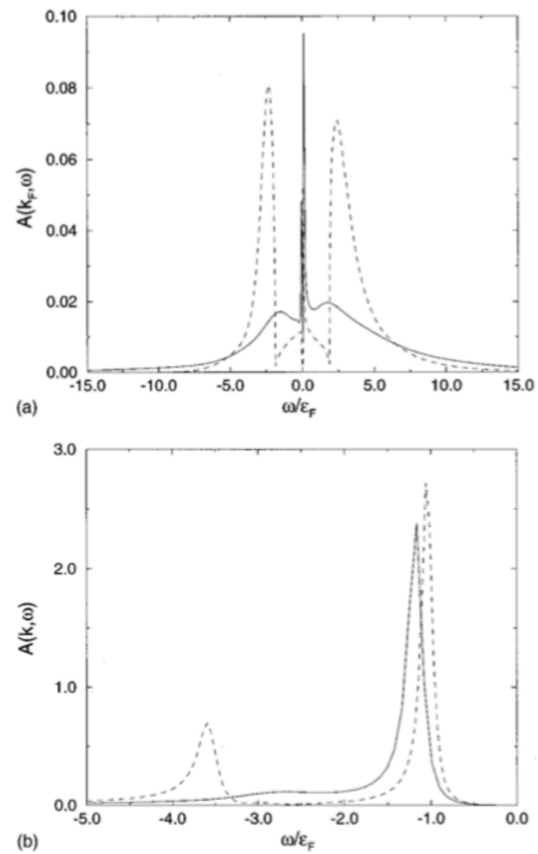
satellites in GW

PHYSICAL REVIEW B VOLUME 57, NUMBER 4

Fully self-consistent *GW* self-energy of the electron gas

B. Holm and U. von Barth
Department of Theoretical Physics, University of Lund, S-22362 Lund, Sweden
(Received 28 January 1997)

We present fully self-consistent results for the self-energy of the electron gas within the *GW* approximation. This means that the self-consistent Green's function *G*, as obtained from Dyson's equation, is used not only for obtaining the self-energy but also for constructing the screened interaction *W* within the random-phase approximation. Such a theory is particle and energy conserving in the sense of Kadanoff and Baym. We find an increase in the weight of the quasiparticle as compared to ordinary non-self-consistent calculations but also to calculations with partial self-consistency using a fixed *W*. The quasiparticle bandwidth is larger than that of free electrons and the satellite structure is broad and featureless; both results clearly contradict the experimental evidence. The total energy, though, is as accurate as that from quantum Monte Carlo calculations, and its derivative with respect to particle number agrees with the Fermi energy as obtained directly from the pole of the Green's function at the Fermi level. Our results indicate that, unless vertex corrections are included, non-self-consistent results are to be preferred for most properties except for the total energy.
[S0163-1829(97)04148-9]



- **GoWo (or GWo) satellites** tend to be located at the **wrong energies** (eg compared to GoWo+Cumulant, see next slides)
- **Missing satellite replicas**, see eg PRB **62**, 4858 (2000)
- fully self-consistent GW fully **damps the satellites**

satellites in GW

PHYSICAL REVIEW B **98**, 155143 (2018)

Editors' Suggestion

Beyond the quasiparticle approximation: Fully self-consistent *GW* calculations

Manuel Grumet,[1] Peitao Liu,[1,*] Merzuk Kaltak,[1] Jiří Klimeš,[2,3] and Georg Kresse[1,†]

[1]*University of Vienna, Faculty of Physics and Center for Computational Materials Science, Sensengasse 8/12, A-1090 Vienna, Austria*

[2]*J. Heyrovský Institute of Physical Chemistry, Academy of Sciences of the Czech Republic, Dolejškova 3, CZ-18223 Prague 8, Czech Republic*

[3]*Department of Chemical Physics and Optics, Faculty of Mathematics and Physics, Charles University, Ke Karlovu 3, CZ-12116 Prague 2, Czech Republic*

(Received 23 August 2018; revised manuscript received 9 October 2018; published 29 October 2018)

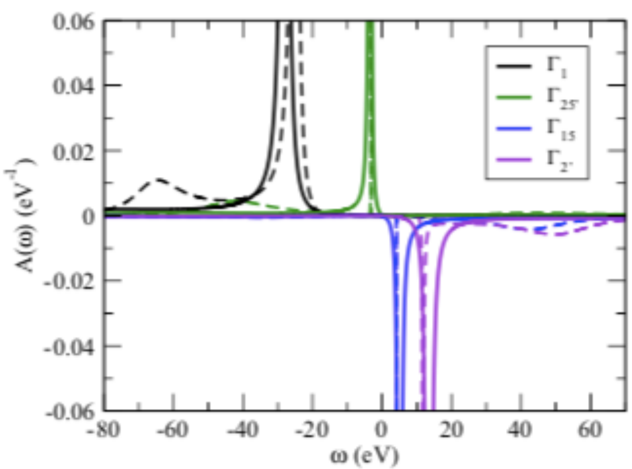


FIG. 4. Comparison of scGW (solid lines) and G_0W_0 (dashed lines) spectral functions of diamond for selected bands at Γ. Note that the signs of the spectral functions for unoccupied states such as Γ_{15} and $\Gamma_{2'}$ are intentionally reversed for clarity.

beyond the GW approx

PRL 107, 166401 (2011) PHYSICAL REVIEW LETTERS week ending 14 OCTOBER 2011

Valence Electron Photoemission Spectrum of Semiconductors: *Ab Initio* Description of Multiple Satellites

Matteo Guzzo,[1,2,*] Giovanna Lani,[1,2] Francesco Sottile,[1,2] Pina Romaniello,[3,2] Matteo Gatti,[4,2] Joshua J. Kas,[5] John J. Rehr,[5,2] Mathieu G. Silly,[6] Fausto Sirotti,[6] and Lucia Reining[1,2,†]

- **Beyond GW** by using a cumulant-expansion like self-energy
- Better photoemission modelling of **intrinsic losses**
- **Extrinsic losses added** by ad hoc model

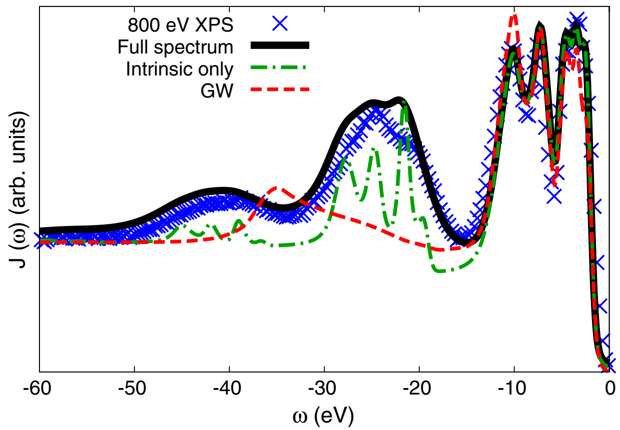


FIG. 1 (color online). Experimental XPS spectrum of Si at 800 eV photon energy (blue crosses), compared to the theoretical intrinsic $A(\omega)$ calculated from G_0W_0 (red dashed line), and from Eq. (4) (green dot-dashed line). On top of the latter the black solid line also includes extrinsic and interference effects. All spectra contain photoabsorption cross sections, a calculated secondary electron background and 0.4 eV Gaussian broadening to account for finite k-point sampling and experimental resolution. The Fermi energy is set to 0 eV.

CNRNANO
ISTITUTO NANOSCIENZE CONSIGLIO NAZIONALE DELLE RICERCHE

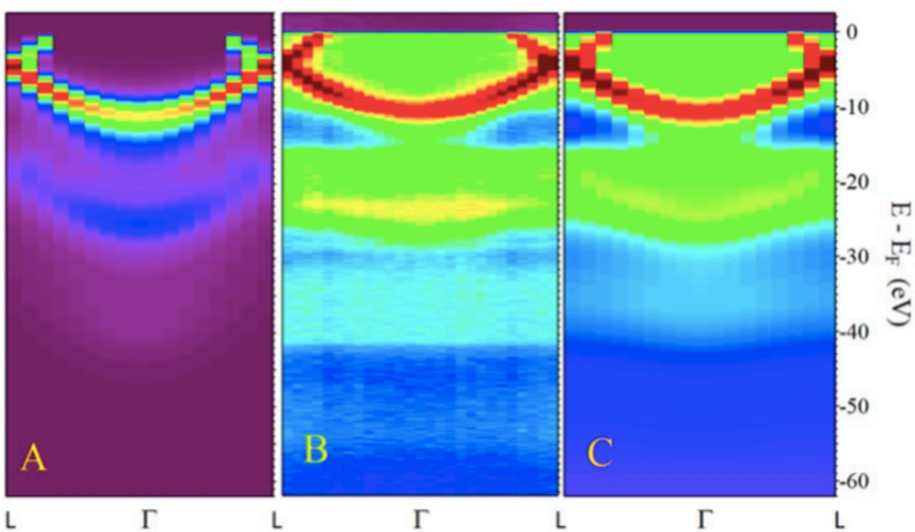
interpreting ARPES

Unraveling intrinsic correlation effects with angle-resolved photoemission spectroscopy

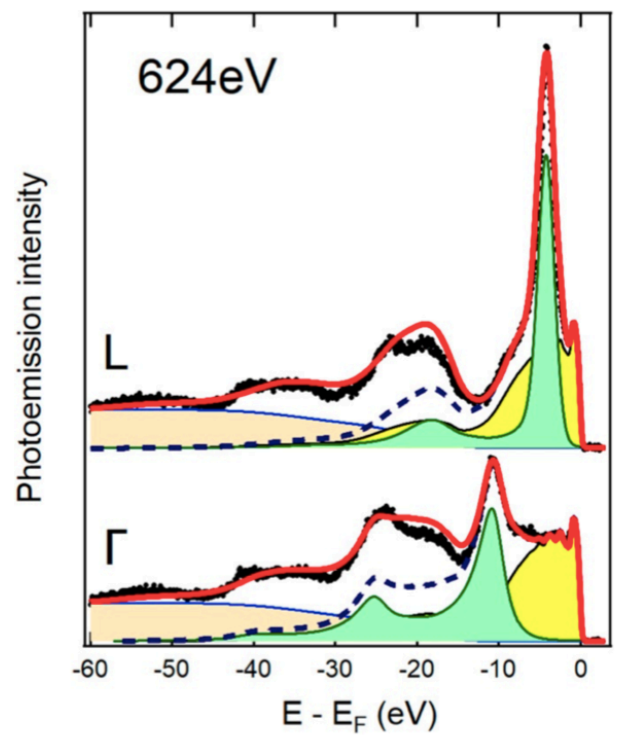
Jianqiang Sky Zhou[a,b,c], Lucia Reining[a,b,1], Alessandro Nicolaou[d], Azzedine Bendounan[d], Kari Ruotsalainen[d,2], Marco Vanzini[a,b,e], J. J. Kas[f], J. J. Rehr[f], Matthias Muntwiler[g], Vladimir N. Strocov[g], Fausto Sirotti[h,1], and Matteo Gatti[a,b,d,1]

PNAS **117**, 28596 (2020)

GW+C **ARPES** **GW+C +el-ph + extr**



Aluminum bulk



Yambo©

thanks!

MAX