GW, ARPES, and lifetimes: a theory overview

Andrea Ferretti

27-31 Jan 2020
Yambo tutorial
- ARPES from a theory perspective
- Connection to the Green’s function theory
- The GW self-energy
ARPES from a theory perspective

Connection to the Green’s function theory

The GW self-energy
Excitations

**Direct photoemission**

- Energy level $E_f$ to $E_{K}$
- $h\nu$ photon absorbed

**Inverse photoemission**

- Energy level $E_f$ to $E_{K}$
- $h\nu$ photon emitted

**Absorption**

- Energy level $E_f$ to $E_i$ with $\Delta E$
- Lifetime

**ARPES**

- Photon absorption
- Electron emission
This process looks, at first glance, like the sum of a photoexcited electron from an occupied state into a conduction state. In absorption experiments, an electron is transferred from an occupied state to an unoccupied state, which corresponds to a change in the density of occupied states. By analogy, inverse photoemission measures the density of states that were formerly occupied by the photoelectron. Hence, as a first approximation, one can state that photoemission measures the density of states below the Fermi level, i.e., the energy level that was formerly occupied by the photoelectron. Point (iii) constitutes the main difficulty for a direct description of this type of experiment.

In every spectroscopic experiment one perturbs the system (by incoming photons, electrons, etc.) and measures the response of the system to this perturbation. In absorption, the joint density of occupied and unoccupied states, respectively, one realizes that (i) electronic excitations can be well described by the density of occupied states, whereas direct and inverse photoemission results are often already well described by the density of occupied states. Moreover, it is clear that, in the case of absorption, even over a small range of excitation energies, transition probabilities can vary considerably and must be taken into account, and one must consider both occupied and unoccupied states, respectively, one realizes that (i) electronic excitations can be well described by the density of occupied states, whereas direct and inverse photoemission results are often already well described by the density of occupied states. Moreover, it is clear that, in the case of absorption, even over a small range of excitation energies, transition probabilities can vary considerably and must be taken into account, and one must consider both occupied and unoccupied states.

**Excitations**

**Direct photoemission**
- $E_f$ to $E_i$
- Excitation energy: $E_K$
- Electron: $E_i$, $E_f$
- Vacuum: $E_vac$
- Energy level: $E_K$

**Inverse photoemission**
- $E_i$ to $E_f$
- Excitation energy: $E_K$
- Electron: $E_f$, $E_i$
- Vacuum: $E_vac$
- Energy level: $E_K$

**Absorption**
- $E_i$ to $E_f$
- Excitation energy: $E_f - E_i$
- Electron: $E_f$, $E_i$
- Vacuum: $E_vac$
- Energy level: $E_f$

N-1 electrons
N+1 electrons
N electrons

*Rev. Mod. Phys., Vol. 74, No. 2, April 2002*
**the ARPES experiment**


- **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**
imply that, in general, even experiments performed for
served across the sample surface due to the lack of
neglected at the low photon energies typically used in
scheme. Upon going to larger
dicular to the sample surface are obtained from the po-
energy distribution produced by incoming photons and mea-
FIG. 2. Energetics of the photoemission process. The electron
trons (right) is more conveniently expressed in terms of the
Within the noninteracting electron picture, and by
E
mE
E
h
E
k
k
h

Binding energy (eV)
Wave vector \( k_{\parallel x} \) (1/Å)
Binding energy (eV)
PES intensity (arb. un.)

Varykhalov et al, PRX 2, 041017 (2012)
Photocurrent $J$ by using the **Fermi golden rule**:

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

$$\Delta = A \cdot p + p \cdot A$$

**Kinetic energy** of the outcoming electron excitation left over

$$\epsilon_k = k^2 / 2$$

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

**Final state**

$$|\Psi_{k,s}\rangle = \left[ 1 + \frac{1}{E - H - i\eta} (H - E) \right] c_k^\dagger |N - 1, s\rangle$$
the 3 step model

- (1) **photoexcitation** intrinsic losses are accounted for (satellite structures)

- (2) transport to the surface **extrinsic losses**

- (3) transmission through the surface

see also Slides from Matthias Kreier, Humboldt Uni (2007)
sudden approximation

see Hedin, Michiels, Inglesfield, PRB 58, (1998)

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

\[ J_k(\omega) = \sum_{ij} \Delta_{ki} A_{ij} (\epsilon_k - \omega) \Delta_{jk} \]
sudden approximation

see Hedin, Michiels, Inglesfield, PRB 58, (1998)

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

extrinsic losses neglected

\[ J_k(\omega) = \sum_{ij} \Delta_{ki} A_{ij}(\epsilon_k - \omega) \Delta_{jk} \]

k fast enough

\[ A_{ij}(\omega) = \sum_{s} \frac{\epsilon_s < \mu}{\langle N | c_i^\dagger | N - 1, s\rangle \langle N - 1, s | c_j | N \rangle \delta(\omega - \epsilon_s)} \]
Angle-resolved photoemission studies of the cuprate superconductors

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(Published 17 April 2003)

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

\[ iG(x_1, x_2, t_1 - t_2) = \langle N | T [\psi(x_1 t_1), \psi^\dagger(x_2 t_2)] | N \rangle \]
\[ = \theta(t_1 - t_2) \langle N | \psi(x_1 t_1) \psi^\dagger(x_2 t_2) | N \rangle \]
\[ - \theta(t_2 - t_1) \langle N | \psi^\dagger(x_2 t_2) \psi(x_1 t_1) | N \rangle \]
the Green's function

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

\[ = \theta(t_1 - t_2) \langle N | \psi(x_1 t_1) \psi^{\dagger}(x_2 t_2) | N \rangle \]

\[ - \theta(t_2 - t_1) \langle N | \psi^{\dagger}(x_2 t_2) \psi(x_1 t_1) | N \rangle \]
the Lehmann representation

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

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

as for non-interacting systems

• **charged excitations**

\[ \epsilon_s = E_0^N - E_s^{N-1} \quad \eta_s = -i0^+ \]
\[ \epsilon_s = E_s^{N+1} - E_0^N \quad \eta_s = i0^+ \]

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

• **Dyson** orbitals

\[ \epsilon_s < \mu \quad f_s(x) = \langle N - 1, s | \hat{\psi}(x) | N, 0 \rangle \]
\[ \epsilon_s \geq \mu \quad f_s(x) = \langle N, 0 | \hat{\psi}(x) | N + 1, s \rangle \]

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

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

extrinsic losses neglected

\[ J_k(\omega) = \sum_{ij} \Delta_{ki} A_{ij}(\epsilon_k - \omega) \Delta_{jk} \]

\[ A_{ij}(\omega) = \sum_{s} \langle N | c_i^\dagger |N - 1, s\rangle \langle N - 1, s | c_j | N \rangle \delta(\omega - \epsilon_s) \]

see Hedin, Michiels, Inglesfield, PRB 58, (1998)

sudden approx

k fast enough
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**

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

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

**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**

\[
G(x, x', \omega) = \sum_s \frac{f_s(x) f^*_s(x')}{\omega - \epsilon_s + i\eta_s}
\]

• The **spectral function**

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

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

\[
\rho(x, \omega) = \sum_s |f_s(x)|^2 \delta(\omega - \epsilon_s)
\]

Kramers-Kronig transform

spectral info
the Lehmann representation

Assuming we knew the self-energy

\[
G(\omega) = G_0(\omega) + G_0(\omega)\Sigma(\omega)G(\omega)
\]

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

\[
G(x, x', \omega) = \sum_s \frac{f_s(x) f^*_s(x')}{\omega - \epsilon_s + i\eta_s}
\]

Assuming discrete states:

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

- frequency (orbital) dependent potential
- see Onida, Reining, Rubio, Rev. Mod. Phys. 74, 602 (2002)
the QP representation

the **Dyson** Equation

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

by direct **diagonalization**

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

**QP approximation**

\[ E_s(z_{mQ}) = z_{mQ} \]

- 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)
Lehmann vs QP

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

\[ G(x, x', \omega) = \sum_m \frac{\langle x|\psi_m^{QP}\rangle \langle \psi_m^{QP}|x'\rangle}{\omega - z_m^{QP}} \]

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

Figures adapted from M. Gatti 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 \( \Sigma(\omega) \) around renormalization factor

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

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

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

\[ \Gamma_i = \text{Im} \Sigma_{ii}(E_i) \]
Manybody features include

- satellites
- lifetimes
- renormalization

All the above features depend on the dynamical and non-hermitian nature of $\Sigma(\omega)$

Figure from: Damascelli, Hussain, Shen, Rev. Mod. Phys. 75, 473 (2003)
- ARPES from a theory perspective
- Connection to the Green’s function theory
- The GW self-energy
Hedin's equations

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

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

\[ H = H_0 + H_1, \]

\[ H_0 = \int \psi^\dagger(x) h(x) \psi(x) dx \]

\[ + \frac{1}{2} \int \psi^\dagger(x) \psi^\dagger(x') v(x,x') \psi(x') \psi(x) dx dx', \quad (A1) \]

\[ H_1 = \int \rho(x) w(x,t) dx, \quad \rho(x) = \psi^\dagger(x) \psi(x), \]
Hedin’s equations

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

\[ G(12) = G_0(12) + \int d34 G_0(13) \Sigma(34) G(42) \]

\[ W(12) = v(12) + \int d34 v(13) P(34) W(42) \]

\[ \Sigma(12) = i \int d34 G(13) W(41) \Gamma(324) \]

\[ P(12) = -i \int d34 G(13) G(41) \Gamma(342) \]

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

\[ 1 \equiv x_1 t_1 \]

\[ G_0 \longleftrightarrow H_0 = T + V_{\text{ext}} + V_H \]
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:

\[ W = v + vPv + vPvPv + vPvPvPv + \ldots \]

\[ = \sum_{n=0}^{\infty} (vP)^n v \quad \text{formal solution} \]

\[ = [1 - vP]^{-1} v \quad \text{summation using the geometric series} \]

\[ = \epsilon^{-1} v \]
Hedin’s equations

L. Hedin, Phys. Rev. 139, A796 (1965)
Hedin's Eq to GW

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

\[ G(12) = G_0(12) + \int d34 G_0(13) \Sigma(34) G(42) \]

\[ W(12) = v(12) + \int d34 v(13) P(34) W(42) \]

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\[ \Gamma(123) = \delta(12) \delta(13) + \int d4567 \frac{\delta\Sigma(12)}{\delta G(45)} G(46) G(75) \Gamma(673) \]
the GW approximation


\[ G(12) = G_0(12) + \int d34 G_0(13) \Sigma(34) G(42) \]

\[ W(12) = v(12) + \int d34 v(13) P(34) W(42) \]

\[ \Sigma(12) = iG(12)W(21) \]

\[ P(12) = -iG(12)G(21) \]

\[ \Gamma(123) = \delta(12)\delta(13) \]

**Independent particle polarisability**

(\(\rightarrow\) reducible polarisability at RPA level)

the GW approximation
the GW approximation

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

\[ \Sigma(12) = iG(12)W(21) \]
\[ P(12) = -iG(12)G(21) \]
\[ \Gamma(123) = \delta(12)\delta(13) \]

\[ \Sigma^{GW}(12) = \]

\[ = \]

Indep particle bubble

RPA screening
The GW approximation

\[ \Sigma(12) = iG(12)W(21) \]

\[ P(12) = -iG(12)G(21) \]

\[ \Gamma(123) = \delta(12)\delta(13) \]

\[ \Sigma^{GW}(12) = \]

\[ = W + \]

\[ = + \]

\[ = + \ldots \]

**beware**: GW is not the whole story

e.g. 2nd order exchange is not there

Indep particle bubble
**related approximations**

**Hartree-Fock**

\[ \Sigma^\text{HF}(12) = iG(12)v(21) \]

\[ \Sigma^\text{GW}(12) = iG(12)W(21) \]

**2nd Born approx (MP2)**

\[ \Sigma^2\text{B}(12) = \]

\[ \Sigma^\text{GW}(12) = \]

\[ \rightarrow \text{chemistry} \]

\[ \rightarrow \text{solids} \]
find that the elements of procedure was used and validated for solids in Ref.

where sometimes estimated by where these valence-core interactions are not accessible. In a nonlinear functional of the density, this procedure is not is the valence electron density but as the local xc potential is closer to the experimental values. Numerical values are listed in errors while HF overestimates it slightly. The dynamical screening

sus experimental ionization potential. Both PBE and PBE0 systems

consistency is obtained when the difference between the non-exact theory, the one-body effective Hamiltonian was subtracted by hand from the calculations. The

The

96, Eq. (2), in bottom panel. The spin-orbit coupling subtracted by hand. The

is static and Hermitian but it can be

contribution.

with respect to experiments of 0.5 eV com-

 artyku.

mum

GW

AlAs,GaP,SiC,AlP

GaAs (left) and Na (right). Circles are experimental data, with

sp

GaAs (right).

We conclude that the amount of Fock

15% of the differences in the HOMO energies, we compare in Fig.

it works!


but...
Self-interaction in Green’s-function theory of the hydrogen atom

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(Received 5 December 2006; published 14 March 2007)

TABLE I. Quasiparticle energies (eV) for the 1s 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.

<table>
<thead>
<tr>
<th></th>
<th>Exact</th>
<th>HF</th>
<th>LDA</th>
<th>LDA+GW</th>
<th>Exact+GW</th>
</tr>
</thead>
<tbody>
<tr>
<td>Energy</td>
<td>−13.61</td>
<td>−13.61</td>
<td>−6.36</td>
<td>−12.66</td>
<td>−13.40</td>
</tr>
</tbody>
</table>

because of the RPA polarizability (self-screening)
The self-energy beyond GW: Local and nonlocal vertex corrections

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Ionization Potentials of Solids: The Importance of Vertex Corrections

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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-
• **GoWo (or GWo) satellites** tend to be located at the **wrong energies** (e.g., compared to GoWo+Cumulant, see next slides)

• **missing satellite replicas**, see e.g., PRB 62, 4858 (2000)

• **fully self-consistent GW fully damps the satellites**

• see **Tommaso Chiarotti poster** for more results about HEG
Beyond the quasiparticle approximation: Fully self-consistent GW calculations

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FIG. 4. Comparison of scGW (solid lines) and $G_0W_0$ (dashed lines) spectral functions of diamond for selected bands at $\Gamma$. Note that the signs of the spectral functions for unoccupied states such as $\Gamma_{15}$ and $\Gamma_2$ are intentionally reversed for clarity.
Valence Electron Photoemission Spectrum of Semiconductors: \textit{Ab Initio} Description of Multiple Satellites

Matteo Guzzo,\textsuperscript{1,2,*} Giovanna Lani,\textsuperscript{1,2} Francesco Sottile,\textsuperscript{1,2} Pina Romaniello,\textsuperscript{3,2} Matteo Gatti,\textsuperscript{4,2} Joshua J. Kas,\textsuperscript{5} John J. Rehr,\textsuperscript{5,2} Mathieu G. Silly,\textsuperscript{6} Fausto Sirotti,\textsuperscript{9} and Lucia Reining\textsuperscript{1,2,?}

\begin{itemize}
  \item \textbf{beyond GW} by using a cumulant-expansion like self-energy
  \item better photoemission modelling of \textbf{intrinsic losses}
  \item \textbf{extrinsic losses added} by ad hoc model
\end{itemize}

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.
Dispersing and non-dispersing satellites in the photoemission spectra of aluminum

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(Dated: November 30, 2018)

arXiv: 1811.12217v1

FIG. 1. (Left and right panels) Calculated spectral functions (shifted along k_x as detailed in [45]) and (middle panel) experimental ARPES image in the ΓL direction. The results of ab initio GW+C calculations are without (left panel) and with (right panel) the Debye-Waller contribution and extrinsic and interference effects.
thanks!

Designing the logo