Photoemission spectroscopy from the three-body Green's function.

GABRIELE RIVA, PINA ROMANIELLO, ARJAN BERGER

Université Toulouse III-Paul Sabatier

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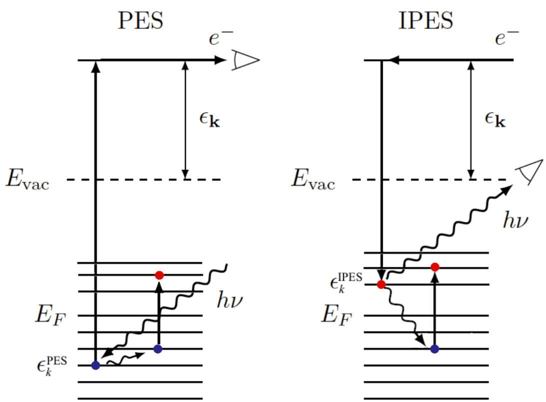
Outline

- Physics of the photoemission spectroscopy;
- one and three-body Green's function;
- application to the symmetric Hubbard dimer;
- conclusion and future development.

Direct and inverse photoemission

•*hole / hole / electron* •*electron / electron / hole*



$N \rightarrow N-1$ $N \rightarrow N+1$

One-body Green's function

The one-body Green's function is defined as

$$iG_1(1,1') = \langle \Psi_0^N | T[\hat{\psi}(1)\hat{\psi}^\dagger(1')] | \Psi_0^N \rangle$$

where $(1) = (\mathrm{r}_1, \sigma_1, t_1)$ and

$$T[\hat{\psi}(1)\hat{\psi}^\dagger(1')] = \theta(t_1 - t_{1'})\hat{\psi}(1)\hat{\psi}^\dagger(1') - \theta(t_{1'} - t_1)\hat{\psi}^\dagger(1')\hat{\psi}(1).$$

It is possible to write G_1 in the well known spectral representation

$$G_1(\omega) = \sum_n \frac{\langle \Psi_0^N | \hat{\psi} | \Psi_n^{N+1} \rangle \langle \Psi_n^{N+1} | \hat{\psi}^\dagger | \Psi_0^N \rangle}{\omega - (E_n^{N+1} - E_0^N) + i\eta} + \sum_n \frac{\langle \Psi_0^N | \hat{\psi}^\dagger | \Psi_n^{N-1} \rangle \langle \Psi_n^{N-1} | \hat{\psi} | \Psi_0^N \rangle}{\omega - (E_0^N - E_n^{N-1}) - i\eta}$$

To calculate G_1 we use the Dyson equation

$$G_1(\omega) = G_{01}(\omega) + G_{01}(\omega)\Sigma_1(\omega)G_1(\omega)$$

Why a three-body Green's function

$$G_1(\omega) = G_{01}(\omega) + G_{01}(\omega)\Sigma_1(\omega)G_1(\omega)$$

- $G_{01}(\omega)$ contains only quasi-particle poles;
- $\Sigma_1(\omega)$ creates satellites and moves all the poles correctly.
- $\Sigma_1(\omega = 0)$ moves the QP poles. No satellites are created (important at strong correlation).

$$G_3(\omega) = G_{03}(\omega) + G_{03}(\omega)\Sigma_3(\omega)G_3(\omega)$$

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Three-body Green's function

The three-body Green's function is defined as

$$G_3(1,2,3,1',2',3') = i\langle\Psi_0^N|T[\hat{\psi}(1)\hat{\psi}(2)\hat{\psi}(3)\hat{\psi}^\dagger(3')\hat{\psi}^\dagger(2')\hat{\psi}^\dagger(1')]|\Psi_0^N\rangle$$

where $(1) = (\mathrm{r}_1, \sigma_1, t_1)$. Thanks to the T-ordering operator

$$T[\hat{\psi}_1(1)...\hat{\psi}_n(n)] = \sum_p \theta(t_{p_1} > ... > t_{p_n})(-1)^P \hat{\psi}_{p_1}(p_1)...\hat{\psi}_{p_n}(p_n)$$

and adding a completeness $\sum_n |\Psi_n^N\rangle\langle\Psi_n^N| = 1$, it describes

- $e/e/h$ $\quad\langle\Psi_0^N|\hat{\psi}\hat{\psi}^\dagger\hat{\psi}|\Psi_n^{N+1}\rangle\langle\Psi_n^{N+1}|\hat{\psi}^\dagger\hat{\psi}\hat{\psi}^\dagger|\Psi_0^N\rangle$
- $h/h/e$ $\quad\langle\Psi_0^N|\hat{\psi}^\dagger\hat{\psi}\hat{\psi}^\dagger|\Psi_n^{N-1}\rangle\langle\Psi_n^{N-1}|\hat{\psi}\hat{\psi}^\dagger\hat{\psi}|\Psi_0^N\rangle$
- $e/e/e$ $\quad\langle\Psi_0^N|\hat{\psi}\hat{\psi}\hat{\psi}|\Psi_n^{N+3}\rangle\langle\Psi_n^{N+3}|\hat{\psi}^\dagger\hat{\psi}^\dagger\hat{\psi}^\dagger|\Psi_0^N\rangle$
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Meaning of the time differences

Each e/e/h term has a form similar to

$$\sum_n e^{i\tau(E_0^N - E_n^{N+1})} \langle \Psi_0^N | \hat{\psi}(x_1) e^{-i\hat{H}\tau_{13'}} \hat{\psi}^\dagger(x_{3'}) e^{-i\hat{H}\tau_{3'2}} \hat{\psi}(x_2) | \Psi_n^{N+1} \rangle$$

$$\langle \Psi_n^{N+1} | \hat{\psi}^\dagger(x_{2'}) e^{-i\hat{H}\tau_{2'3}} \hat{\psi}(x_3) e^{-i\hat{H}\tau_{31'}} \hat{\psi}^\dagger(x_{1'}) | \Psi_0^N \rangle$$

where τ corresponds to the time of the combined propagation of the added particle and the electron-hole pair

$$\tau = \frac{1}{3}(t_1 + t_2 + t_{3'}) - \frac{1}{3}(t_3 + t_{1'} + t_{2'}) \quad \text{and} \quad \tau_{ij} = t_i - t_j.$$

The time differences τ_{ij} are instantaneous: $\tau_{ij} \to 0$.

Electron-electron-hole and hole-hole-electron parts

The e/e/h and h/h/e parts of G_3 in the spectral representation read as

$$
\begin{aligned}
{G_3}^{e+h}(x_1, x_2, x_3, x_{1'}, x_{2'}, x_{3'}; \omega) &= G_3^e(x_1, ..., x_{3'}; \omega) + G_3^h(x_1, ..., x_{3'}; \omega) \\
&= \sum_n \frac{\langle \Psi_0^N | \hat{\psi}(x_1) \hat{\psi}^\dagger(x_{3'}) \hat{\psi}(x_2) | \Psi_n^{N+1} \rangle \langle \Psi_n^{N+1} | \hat{\psi}^\dagger(x_{2'}) \hat{\psi}(x_3) \hat{\psi}^\dagger(x_{1'}) | \Psi_0^N \rangle}{\omega - (E_n^{N+1} - E_0^N) + i\eta} \\
&+ \sum_n \frac{\langle \Psi_0^N | \hat{\psi}^\dagger(x_{2'}) \hat{\psi}(x_3) \hat{\psi}^\dagger(x_{1'}) | \Psi_n^{N-1} \rangle \langle \Psi_n^{N-1} | \hat{\psi}(x_1) \hat{\psi}^\dagger(x_{3'}) \hat{\psi}(x_2) | \Psi_0^N \rangle}{\omega - (E_0^N - E_n^{N-1}) - i\eta}
\end{aligned}
$$

while the addition and the removal parts of G_1 are

$$
\begin{aligned}
G_1(x_1, x_{1'}; \omega) &= G_1^e(x_1, x_{1'}; \omega) + G_1^h(x_1, x_{1'}; \omega) \\
&= \sum_n \frac{\langle \Psi_0^N | \hat{\psi}(x_1) | \Psi_n^{N+1} \rangle \langle \Psi_n^{N+1} | \hat{\psi}^\dagger(x_{1'}) | \Psi_0^N \rangle}{\omega - (E_n^{N+1} - E_0^N) + i\eta} \\
&+ \sum_n \frac{\langle \Psi_0^N | \hat{\psi}^\dagger(x_{1'}) | \Psi_n^{N-1} \rangle \langle \Psi_n^{N-1} | \hat{\psi}(x_1) | \Psi_0^N \rangle}{\omega - (E_0^N - E_n^{N-1}) - i\eta}
\end{aligned}
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The e/e/h and h/h/e parts of G_3 in the spectral representation read as

$$G_3{}^{e+h}(x_1, x_2, x_3, x_{1'}, x_{2'}, x_{3'}; \omega) = G_3^e(x_1, ..., x_{3'}; \omega) + G_3^h(x_1, ..., x_{3'}; \omega)$$

$$= \sum_n \frac{\langle \Psi_0^N | \hat{\psi}(x_1) \hat{\psi}^\dagger(x_{3'}) \hat{\psi}(x_2) | \Psi_n^{N+1} \rangle \langle \Psi_n^{N+1} | \hat{\psi}^\dagger(x_{2'}) \hat{\psi}(x_3) \hat{\psi}^\dagger(x_{1'}) | \Psi_0^N \rangle}{\omega - (E_n^{N+1} - E_0^N) + i\eta}$$

$$+ \sum_n \frac{\langle \Psi_0^N | \hat{\psi}^\dagger(x_{2'}) \hat{\psi}(x_3) \hat{\psi}^\dagger(x_{1'}) | \Psi_n^{N-1} \rangle \langle \Psi_n^{N-1} | \hat{\psi}(x_1) \hat{\psi}^\dagger(x_{3'}) \hat{\psi}(x_2) | \Psi_0^N \rangle}{\omega - (E_0^N - E_n^{N-1}) - i\eta}$$

while the addition and the removal parts of G_1 are

$$G_1(x_1, x_{1'}; \omega) = G_1^e(x_1, x_{1'}; \omega) + G_1^h(x_1, x_{1'}; \omega)$$

$$= \sum_n \frac{\langle \Psi_0^N | \hat{\psi}(x_1) | \Psi_n^{N+1} \rangle \langle \Psi_n^{N+1} | \hat{\psi}^\dagger(x_{1'}) | \Psi_0^N \rangle}{\omega - (E_n^{N+1} - E_0^N) + i\eta}$$

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Link between G_3 and G_1

With appropriate contractions and integrations it is possible to recover G_1 from G_3

$$\int dx_2 dx_3 G_3^e(x_1, x_2, x_3, x_{1'}, x_3, x_2, \omega) = (N+1)^2 G_1^e(x_1, x_{1'}, \omega)$$

$$\int dx_2 dx_3 G_3^h(x_1, x_2, x_3, x_{1'}, x_3, x_2, \omega) = N^2 G_1^h(x_1, x_{1'}, \omega)$$

Dyson equation and self-energy for G_3

$$G_3^{e+h}(\omega) = G_{03}^{e+h}(\omega) + G_{03}^{e+h}(\omega)\Sigma_3(\omega)G_3^{e+h}(\omega)$$

where G_{03}^{e+h} is the non-interacting electron/hole three-body Green's function. It contains both quasi-particle and satellite poles

$$G_{03}^{e+h}(\omega) = \frac{\phi\phi\phi\phi^*\phi^*\phi^*}{\omega - \epsilon^c + i\eta} + \frac{\phi\phi\phi\phi^*\phi^*\phi^*}{\omega - \epsilon^c - \epsilon^{e/h} + i\eta} + \dots$$

where ϵ^c is the one-particle energy of a conduction band, and $\epsilon^{e/h}$ is the energy of the electron/hole pair.

We defined Σ_3 as the three-body self-energy. Its task is to shift the poles from non-interacting to interacting ones. A static self-energy is enough to do that

$$G_{3static}^{-1}(\omega) = G_{03}^{-1}(\omega) - \Sigma_3(\omega = 0)$$

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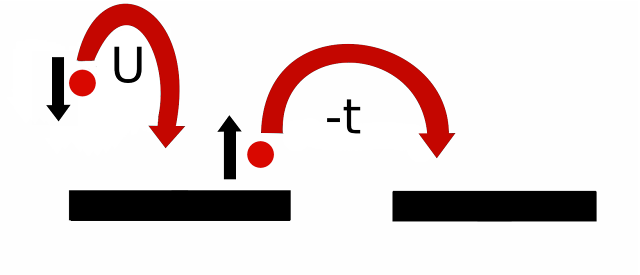
$$G_{3static}^{-1}(\omega) = G_{03}^{-1}(\omega) - \Sigma_3(\omega = 0)$$

Symmetric Hubbard dimer

The Hamiltonian of the model is

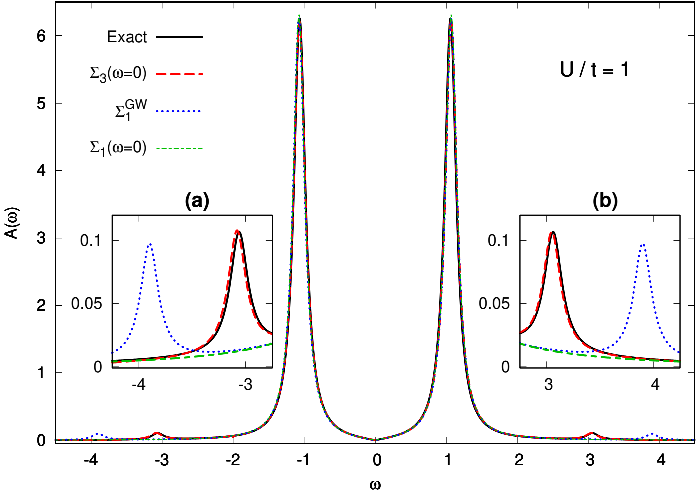
$$H = -t \sum_{i \neq j = 1,2} \sum_{\sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + \frac{U}{2} \sum_{i=1,2} \sum_{\sigma\sigma'} c^{\dagger}_{i\sigma} c^{\dagger}_{i\sigma'} c_{i\sigma'} c_{i\sigma} - \epsilon_0 \sum_{i=1,2} \sum_{\sigma} n_{i\sigma}.$$

Where $-t$ and U represents the hopping kinetic energy and the on-site (spin-independent) interaction.



Spectral function of the half filling Hubbard dimer

Weak interaction



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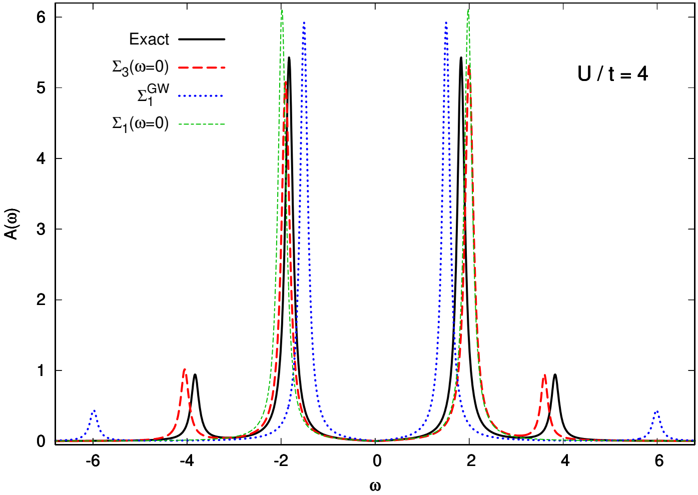


Conclusions and future developments

In conclusion:

- We developed a new strategy, based on the three-body Green's function and static three-body self-energy, to obtain the direct and inverse photo-emission spectra;
- Our model was tested on the symmetric Hubbard dimer giving very encouraging results;
- We need a strategy to find an approximate three-body self-energy that can be applied to real system.

THANKS FOR YOUR ATTENTION

Link G_3-G_1

$$G_3{}^{e+h}(x_1, x_2, x_3, x_{1'}, x_3, x_2; \omega) =$$

$$= \sum_n \frac{\langle \Psi_0^N | \hat{\psi}(x_1) \hat{\psi}^\dagger(x_2) \hat{\psi}(x_2) | \Psi_n^{N+1} \rangle \langle \Psi_n^{N+1} | \hat{\psi}^\dagger(x_3) \hat{\psi}(x_3) \hat{\psi}^\dagger(x_{1'}) | \Psi_0^N \rangle}{\omega - (E_n^{N+1} - E_0^N) + i\eta}$$

$$+ \sum_n \frac{\langle \Psi_0^N | \hat{\psi}^\dagger(x_3) \hat{\psi}(x_3) \hat{\psi}^\dagger(x_{1'}) | \Psi_n^{N-1} \rangle \langle \Psi_n^{N-1} | \hat{\psi}(x_1) \hat{\psi}^\dagger(x_2) \hat{\psi}(x_2) | \Psi_0^N \rangle}{\omega - (E_0^N - E_n^{N-1}) - i\eta}$$

Using $\int dx \hat{\psi}^\dagger(x) \hat{\psi}(x) | \Psi_n^N \rangle = N | \Psi_n^N \rangle$ and $\int dx \langle \Psi_n^N | \hat{\psi}^\dagger(x) \hat{\psi}(x) = \langle \Psi_n^N | N$

$$\int dx_2 dx_3 G_3^e(x_1, x_2, x_3, x_{1'}, x_3, x_2, \omega) = (N+1)^2 G_1^e(x_1, x_{1'}, \omega)$$

$$\int dx_2 dx_3 G_3^h(x_1, x_2, x_3, x_{1'}, x_3, x_2, \omega) = N^2 G_1^h(x_1, x_{1'}, \omega)$$

G_{03}

the non-interacting three-body Green's function is a sum of two types of terms

$$G_{01}(\omega)G_{01}G_{01} = \sum_{n,m,t} \frac{\phi_n\phi_n^*\phi_m\phi_m^*\phi_t\phi_t^*}{\omega - \epsilon_n^{c/v} + i\eta\text{sign}(\omega-\mu)}$$

$$\int d\omega' d\omega'' G_{01}(\omega+\omega'-\omega'')G_{01}(\omega')G_{01}(\omega'') =$$

$$= \sum_{n,m,t} \frac{\phi_n\phi_n^*\phi_m\phi_m^*\phi_t\phi_t^*}{\omega - \epsilon_n^{c/v} - \epsilon_m^{c/v} + \epsilon_t^{v/c} + i\eta\text{sign}(\omega-\mu)}$$

Total electron/electron/hole contribution

$$G_3{}^e(x_1, x_2, x_3, x_{1'}, x_{2'}, x_{3'}; \tau_{12}, \tau_{23'}, \tau_{1'2'}, \tau_{2'3}, \omega) =$$
$$= -\sum_n e^{-i[\omega-(E_n^{N+1}-E_0^N)]F(\tau_{12},\tau_{3'1},\tau_{1'2'},\tau_{31'})}$$
$$\frac{\mathrm{X}_n(x_1, x_2, x_{3'}; \tau_{12}, \tau_{23'})\tilde{\mathrm{X}}_n(x_{1'}, x_{2'}, x_3; \tau_{1'2'}, \tau_{2'3})}{\omega - (E_n^{N+1} - E_0^N) + i\eta}$$

where

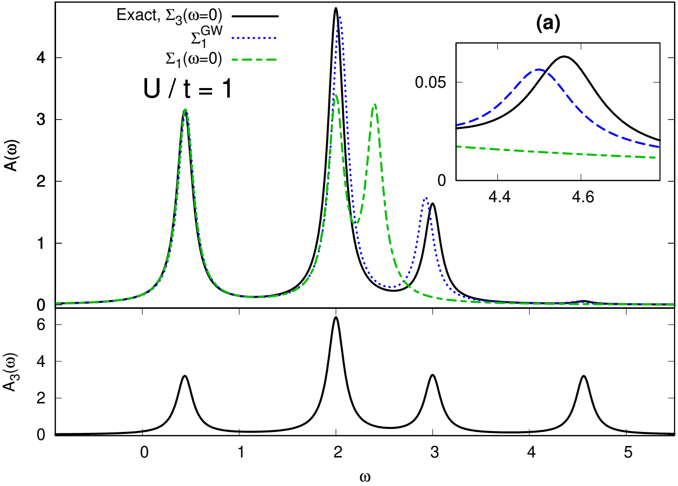
$$\mathrm{X}_n(x_1, x_2, x_{3'}; \tau_{12}, \tau_{23'}) = \sum_{i\neq j\neq k=1,2,3'} (-1)^P \theta(\tau_{ij})\theta(\tau_{jk}) \exp[\frac{i}{3} E_0^N (2\tau_{ij} + \tau_{jk})]$$
$$exp[\frac{i}{3} E_n^{N+1}(2\tau_{jk} + \tau_{ij})]\langle \Psi_0^N | \Upsilon(x_i) e^{-iH\tau_{ij}} \Upsilon(x_j) e^{-iH\tau_{jk}} \Upsilon(x_k) | \Psi_n^{N+1} \rangle$$

and

$$F(\tau_{12}, \tau_{3'1}, \tau_{1'2'}, \tau_{31'}) = \sum_{i\neq j\neq k=1,2,3'} (\tau_{ij} - \tau_{ki})\theta(\tau_{jk})\theta(\tau_{ki}) - \sum_{i\neq j\neq k=1',2',3} (\tau_{ij} - \tau_{ki})\theta(\tau_{jk})\theta(\tau_{ij})$$

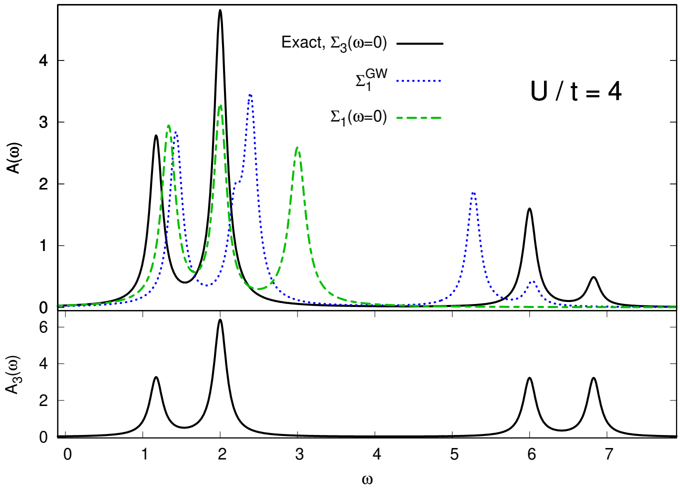
Spectral function of the 1/4 filling Hubbard dimer

Weak interaction



Spectral function of the 1/4 filling Hubbard dimer

Strong interaction



Spectral amplitude

$$G_3^{e+h}(\omega) = \int_{-\infty}^{\mu} d\omega' \frac{A_3(\omega')}{\omega - \omega' - i\eta} + \int_{\mu}^{+\infty} d\omega' \frac{A_3(\omega')}{\omega - \omega' + i\eta}$$

$$\begin{aligned} A_3(x_1, x_2, x_3, x_{1'}, x_{2'}, x_{3'}; \omega) \\ = \sum_n \mathrm{X}_n(x_1, x_2, x_{3'}) \mathrm{X}_n^*(x_{1'}, x_{2'}, x_3) \delta(\omega - (E_n^{N+1} - E_0^N)) \\ + \sum_n \mathrm{Z}_n(x_1, x_2, x_{3'}) \mathrm{Z}_n^*(x_{1'}, x_{2'}, x_3) \delta(\omega - (E_0^N - E_n^{N-1})) \end{aligned}$$