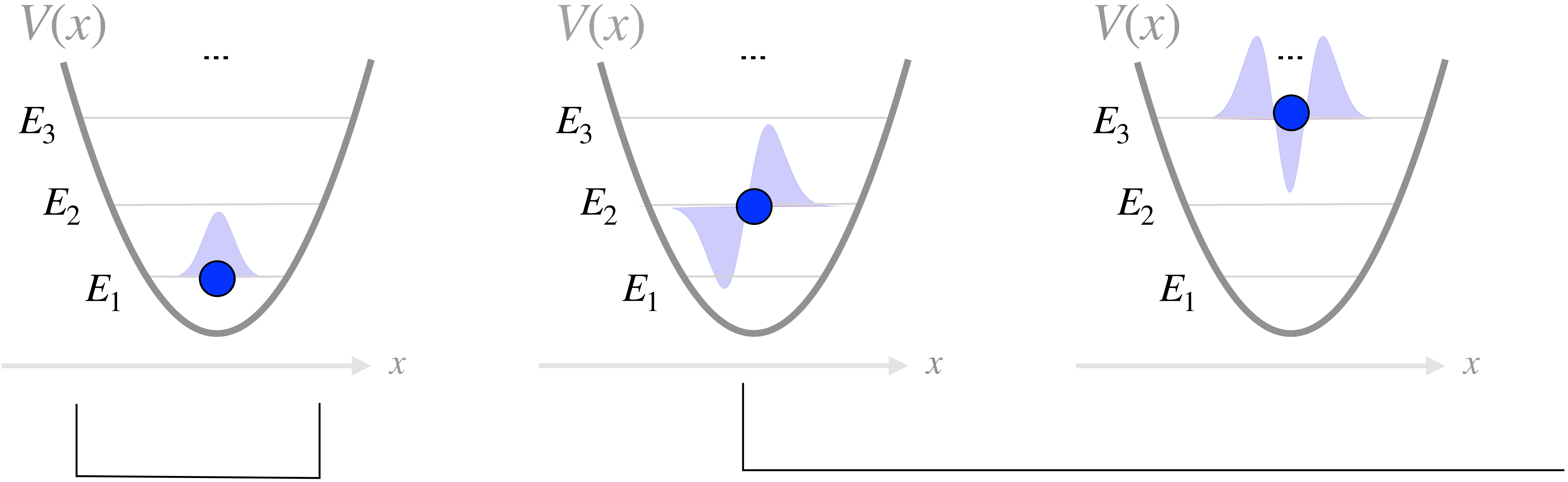
Excited states

Andrey Geondzhian

Skoltech

Excited states

$$\hat{h}|\phi> = E|\phi>$$

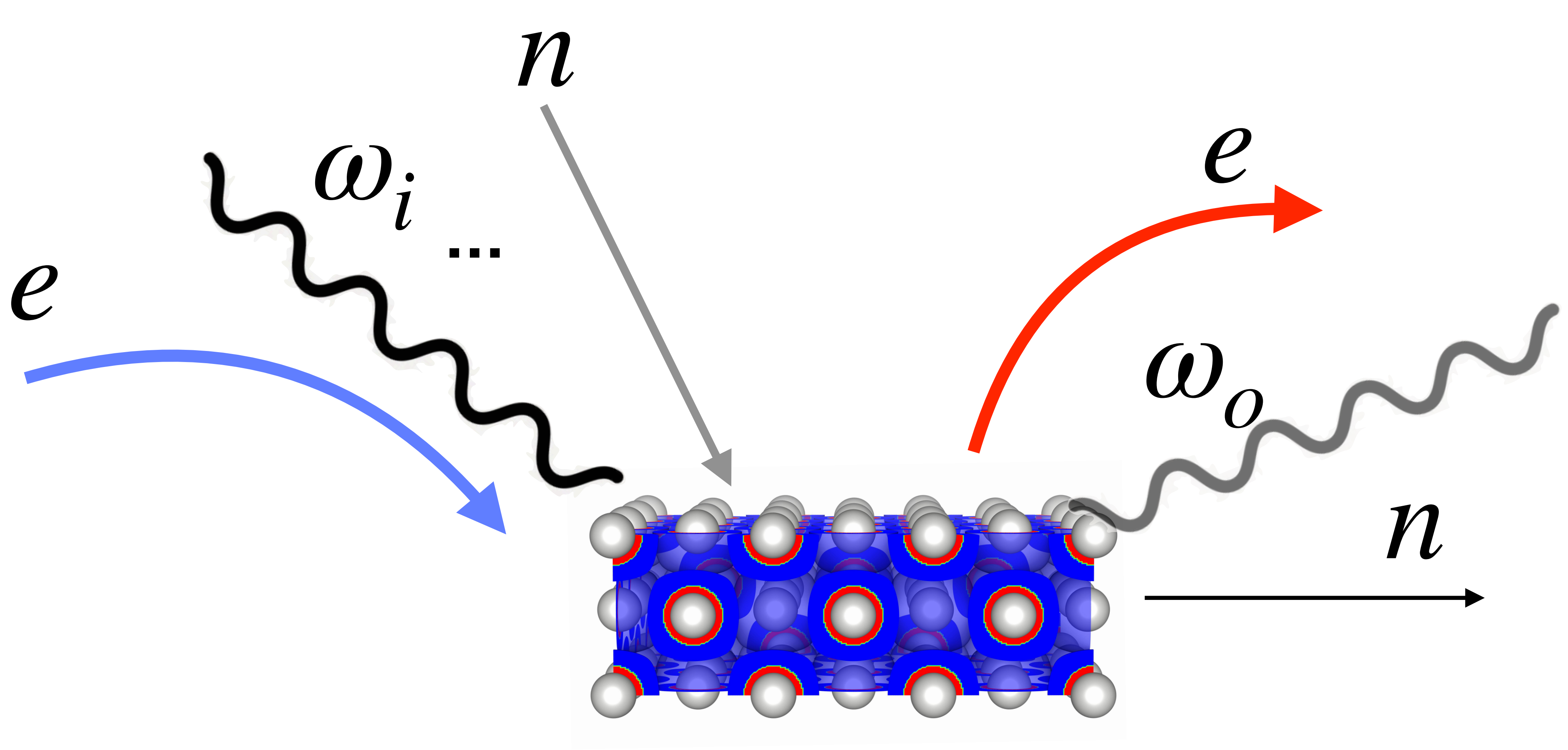


GS

Excited States

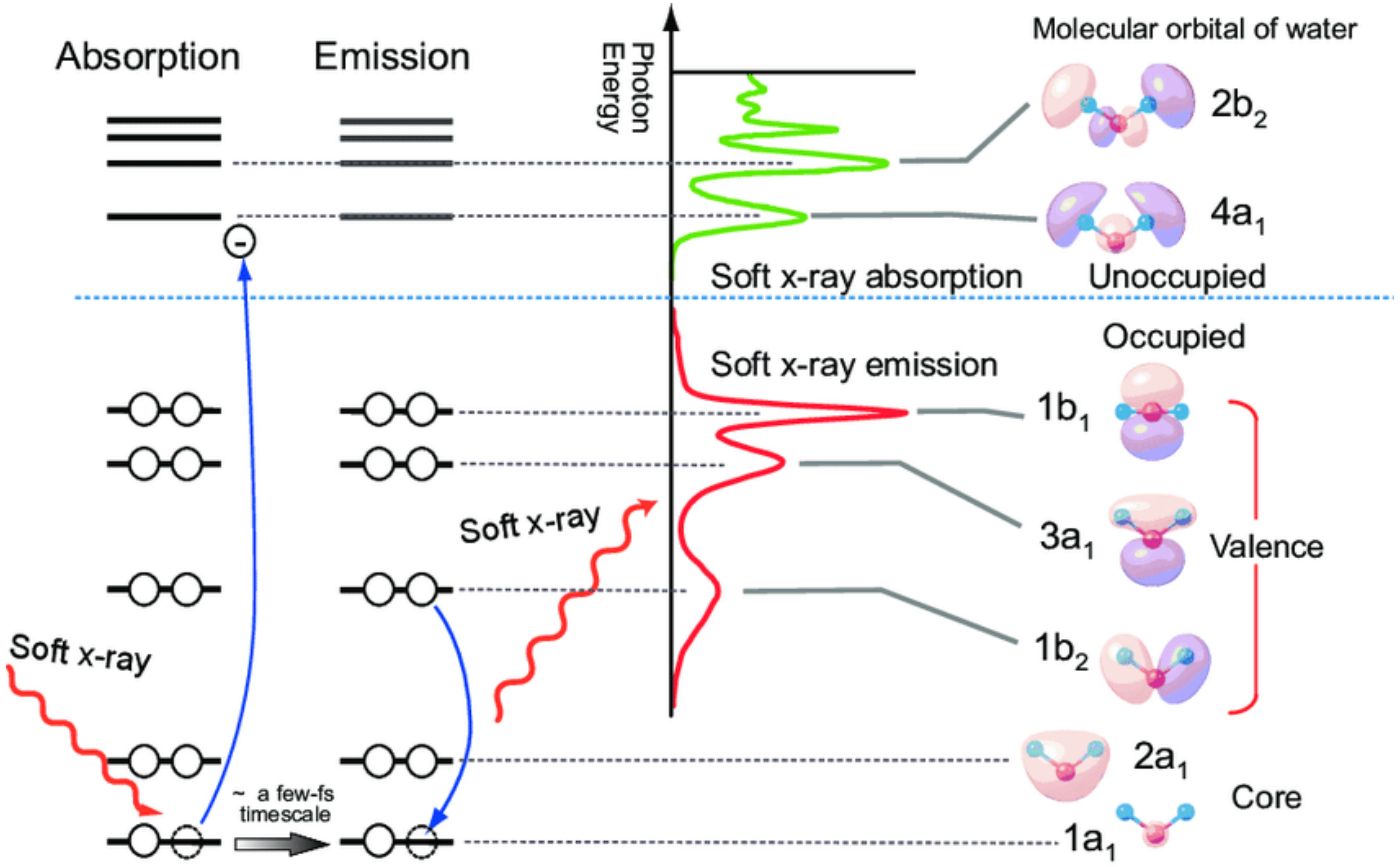
Why? (motivation)

- To predict the response of the system



- Understand electronic structure

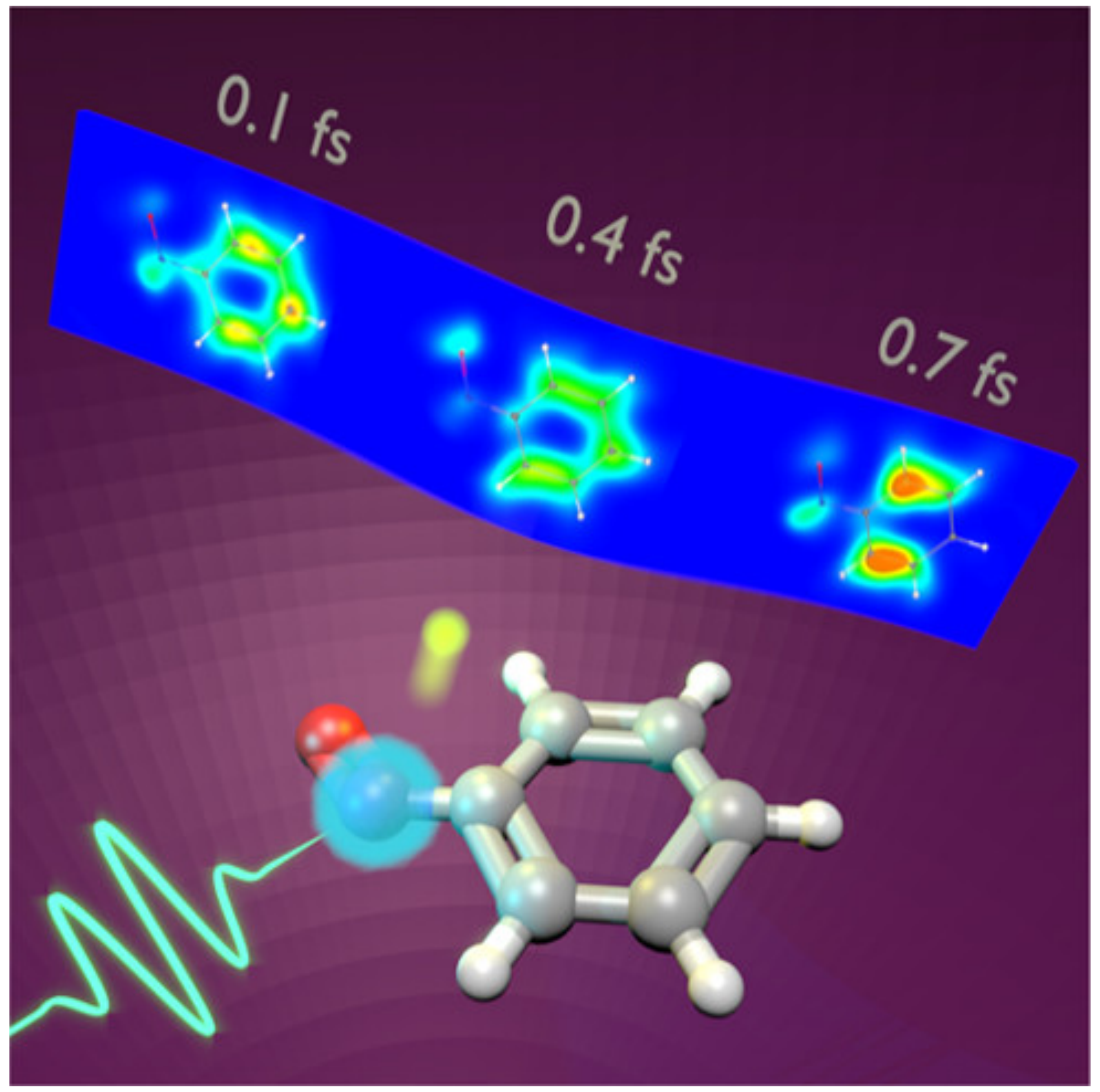
Light absorption/emission spectroscopy

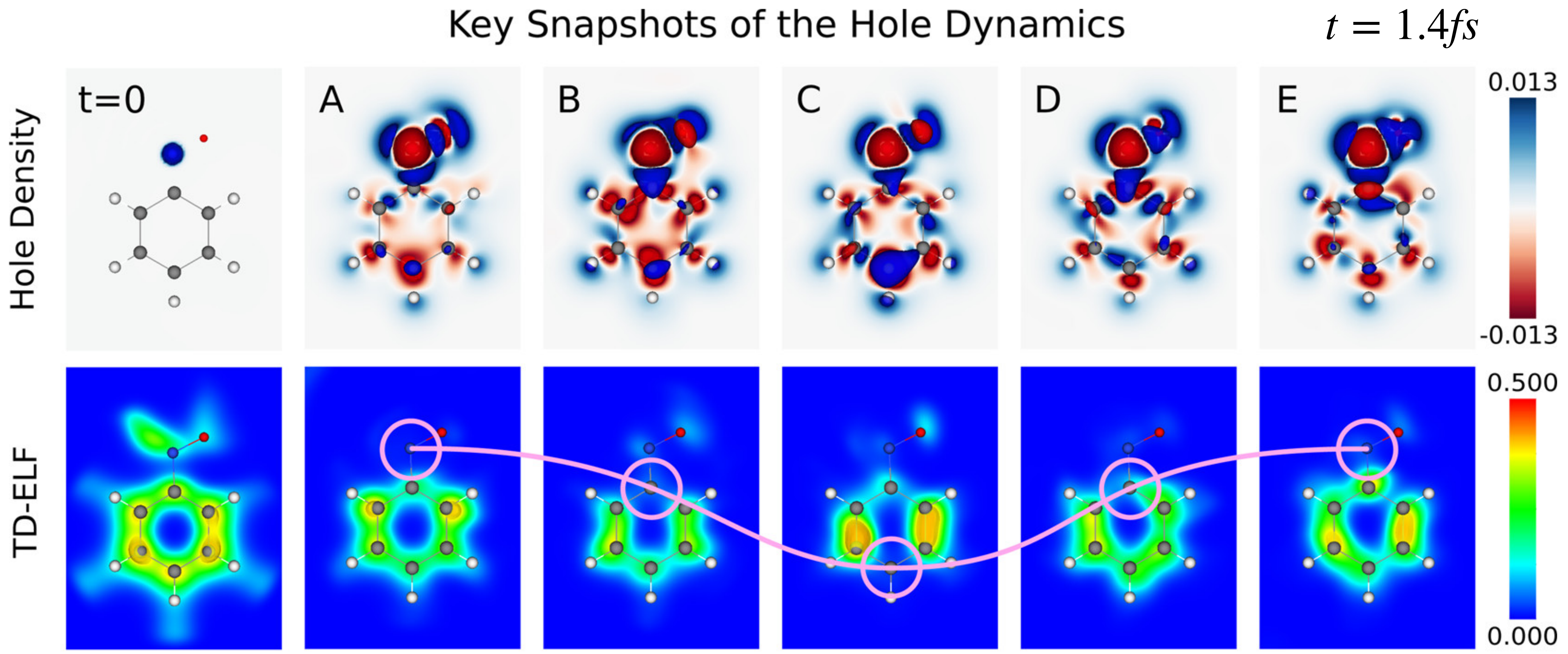


Takashi. Molecular Science (2015)

Why? (motivation)

- Understand dynamics of the process



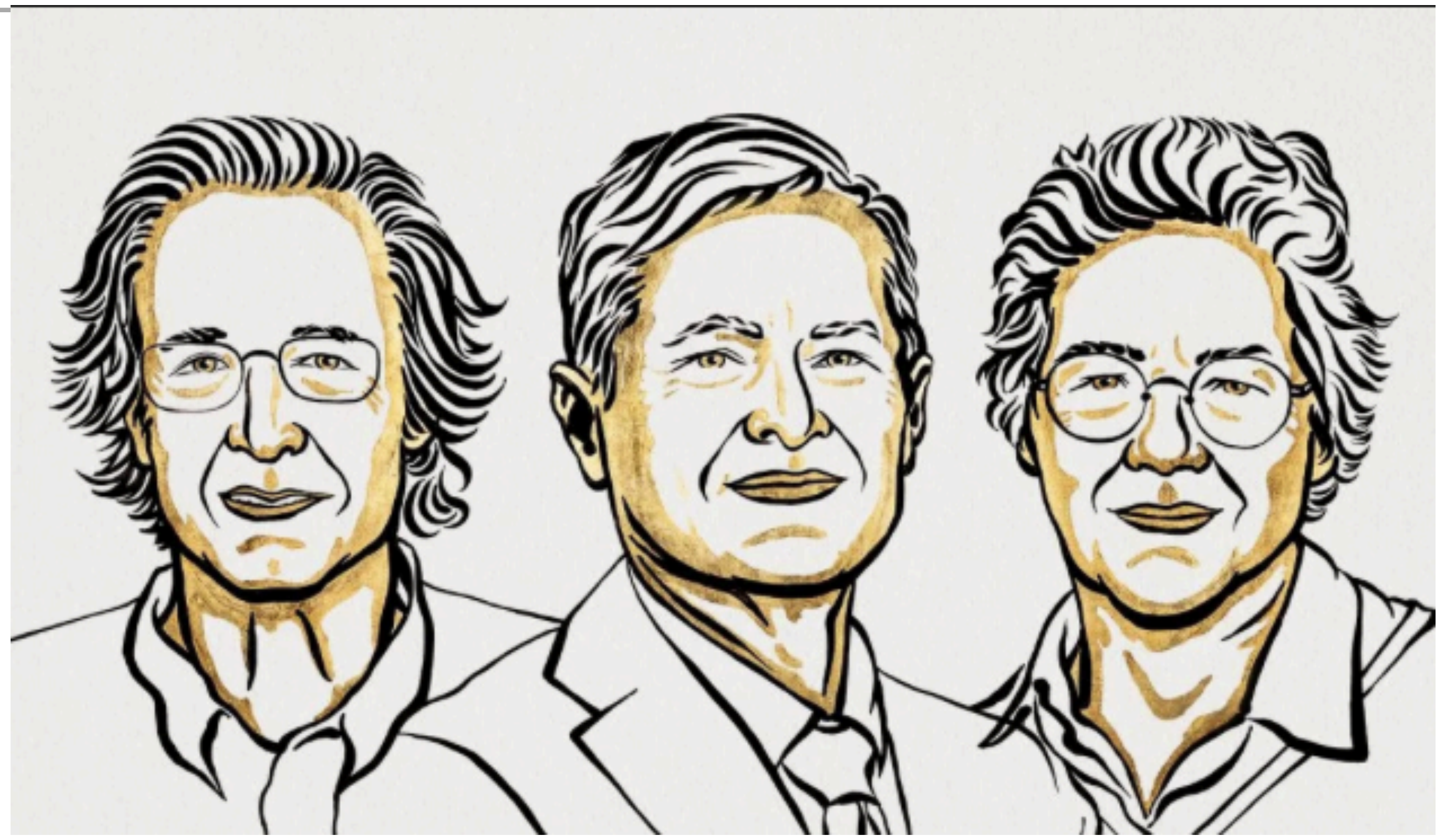


Bruner et al. JPCL (2017)

- Fast (ultra-fast) (<1fs)

Is it important?

- Fast (ultra-fast) (<1fs)



The Royal Swedish Academy of Sciences has decided to award
the Nobel Prize in Physics 2023 jointly to

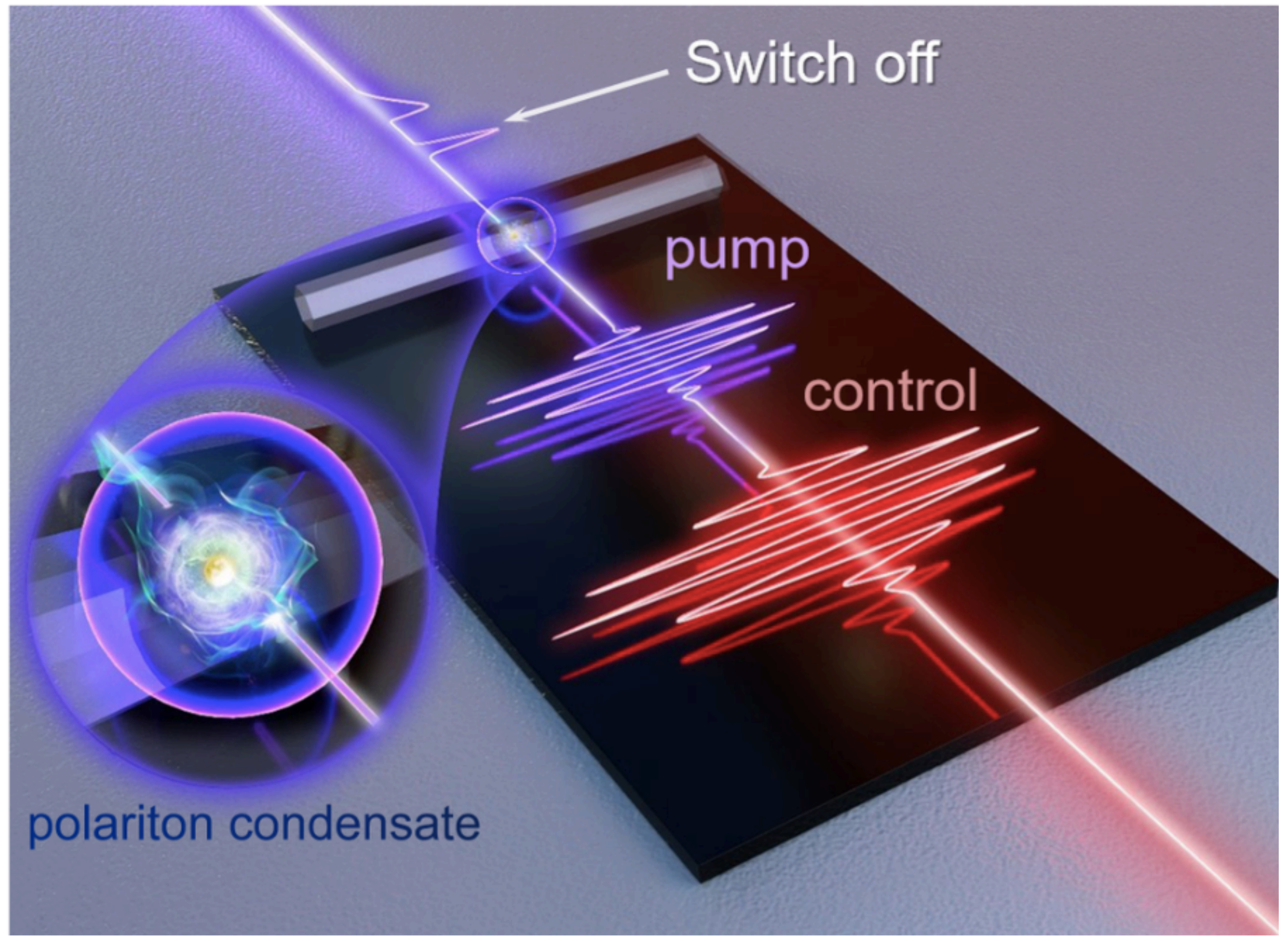
Pierre Agostini, Ferenc Krausz and **Anne L'Huillier**

"for experimental methods that generate attosecond pulses of light for the study of electron dynamics in matter"

Why? (motivation)

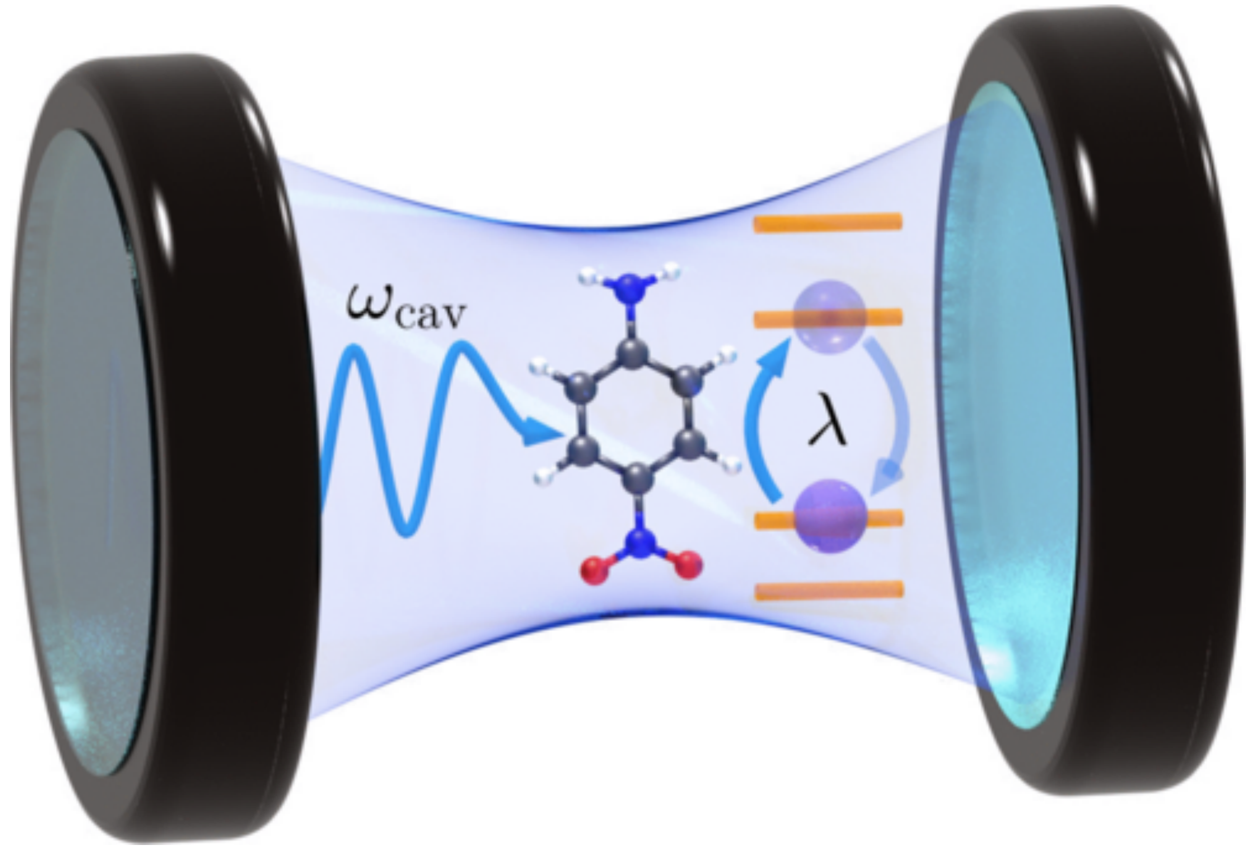
- To create and control new states

Polaritons



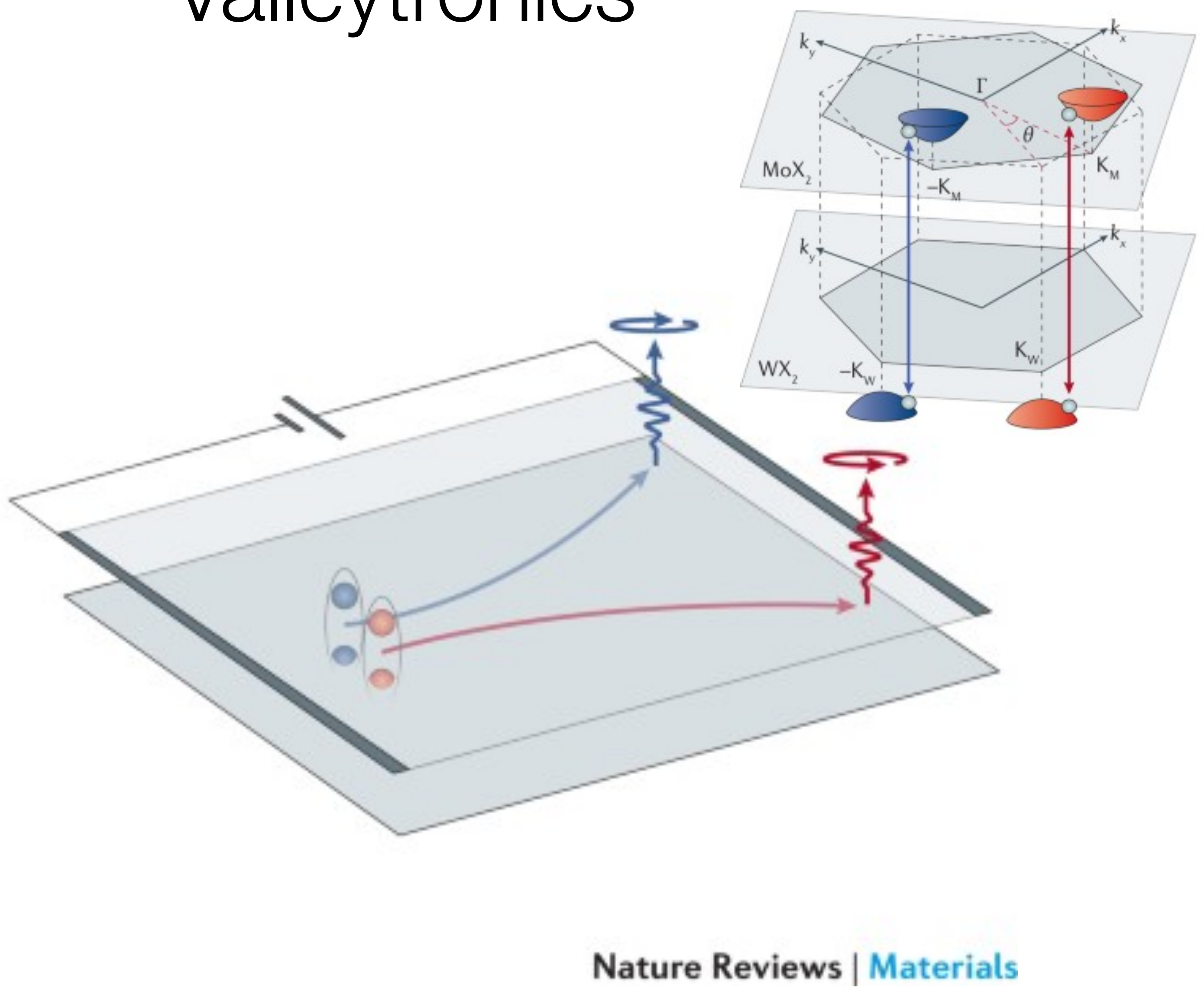
Chen et al. PRL 2022

Cavity engineering



Haugland et al. PRX 2020

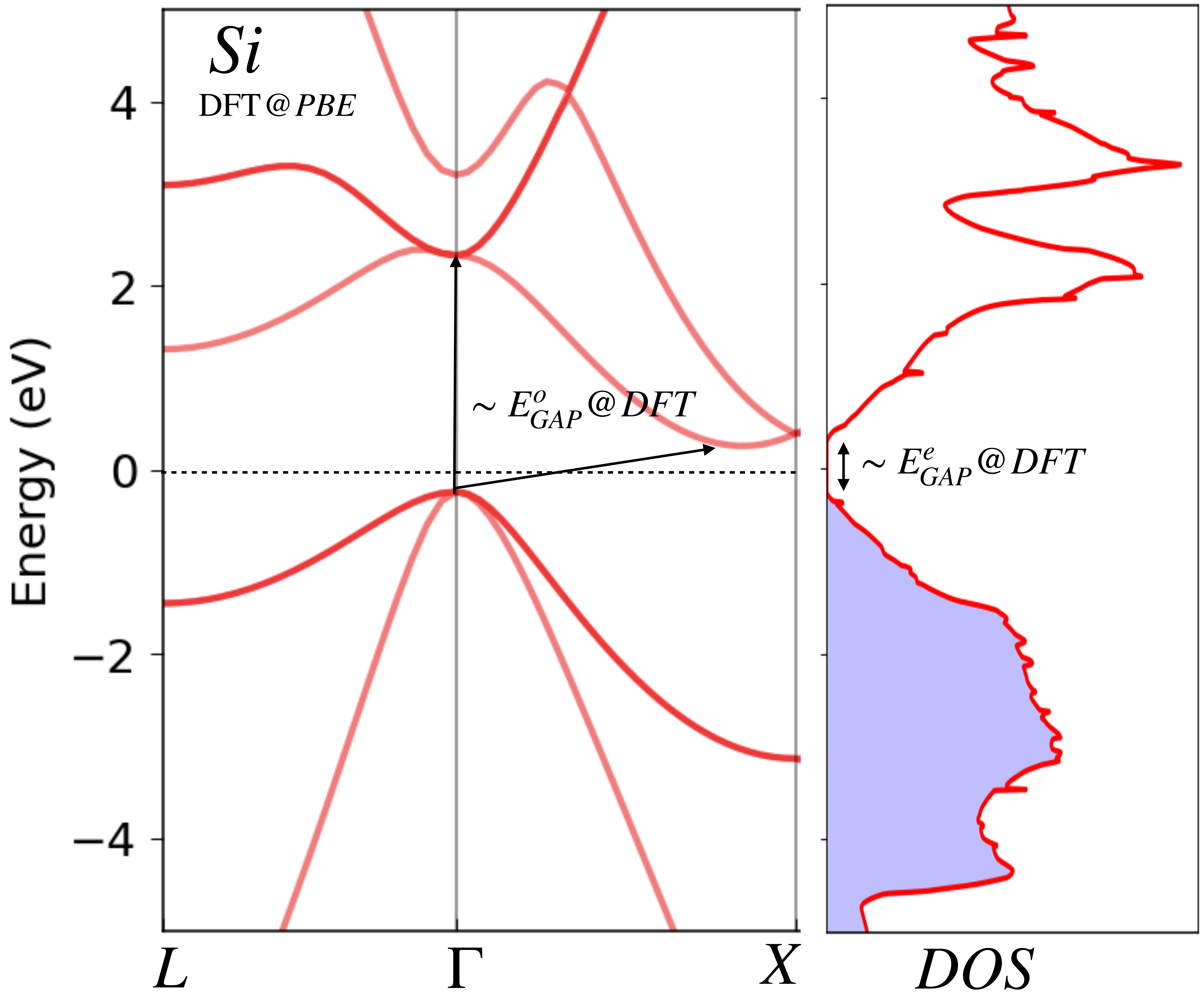
Valleytronics

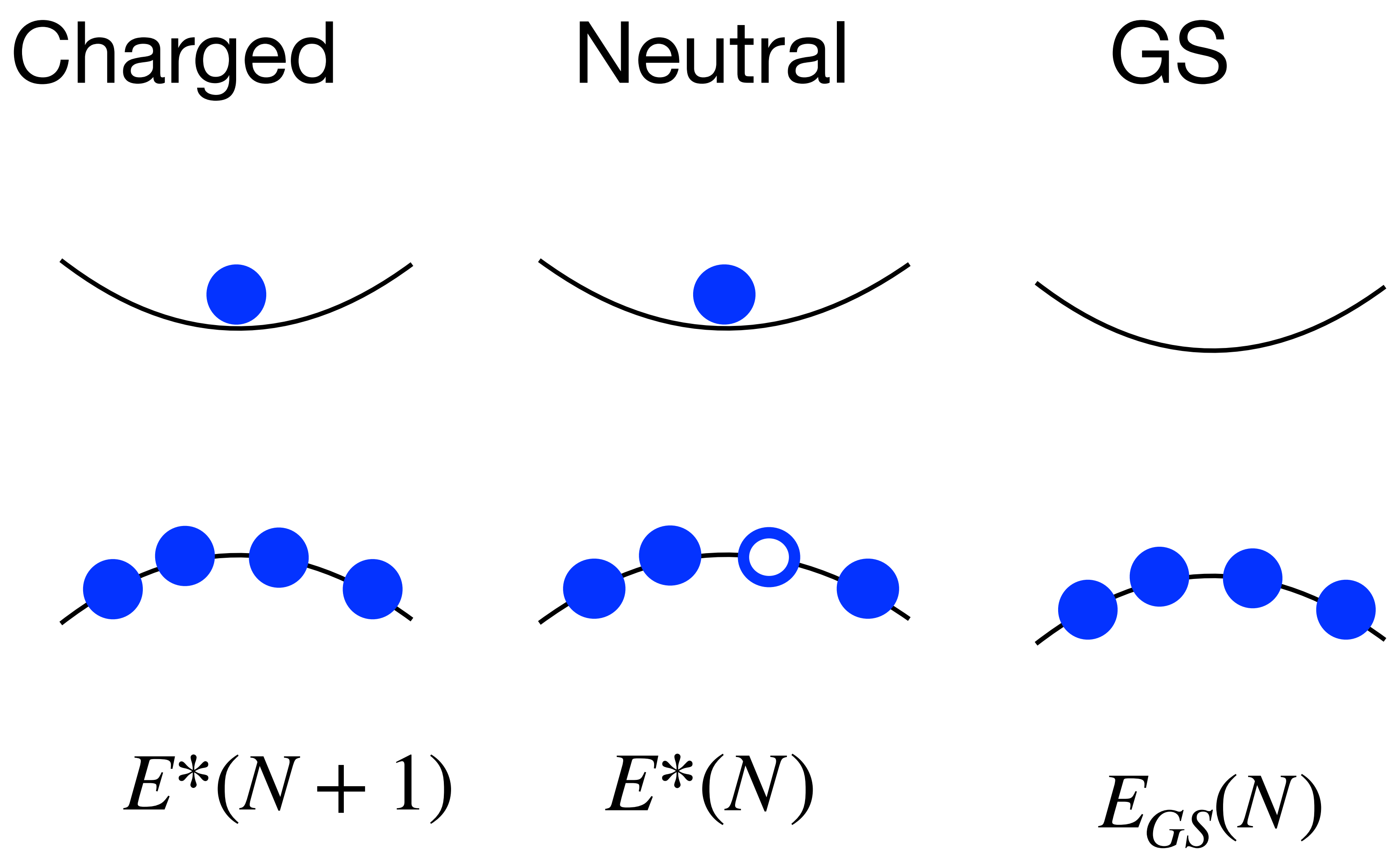


Schaibley et al. Nature Mat 2016

etc

Electronic Gap and Optical Gap



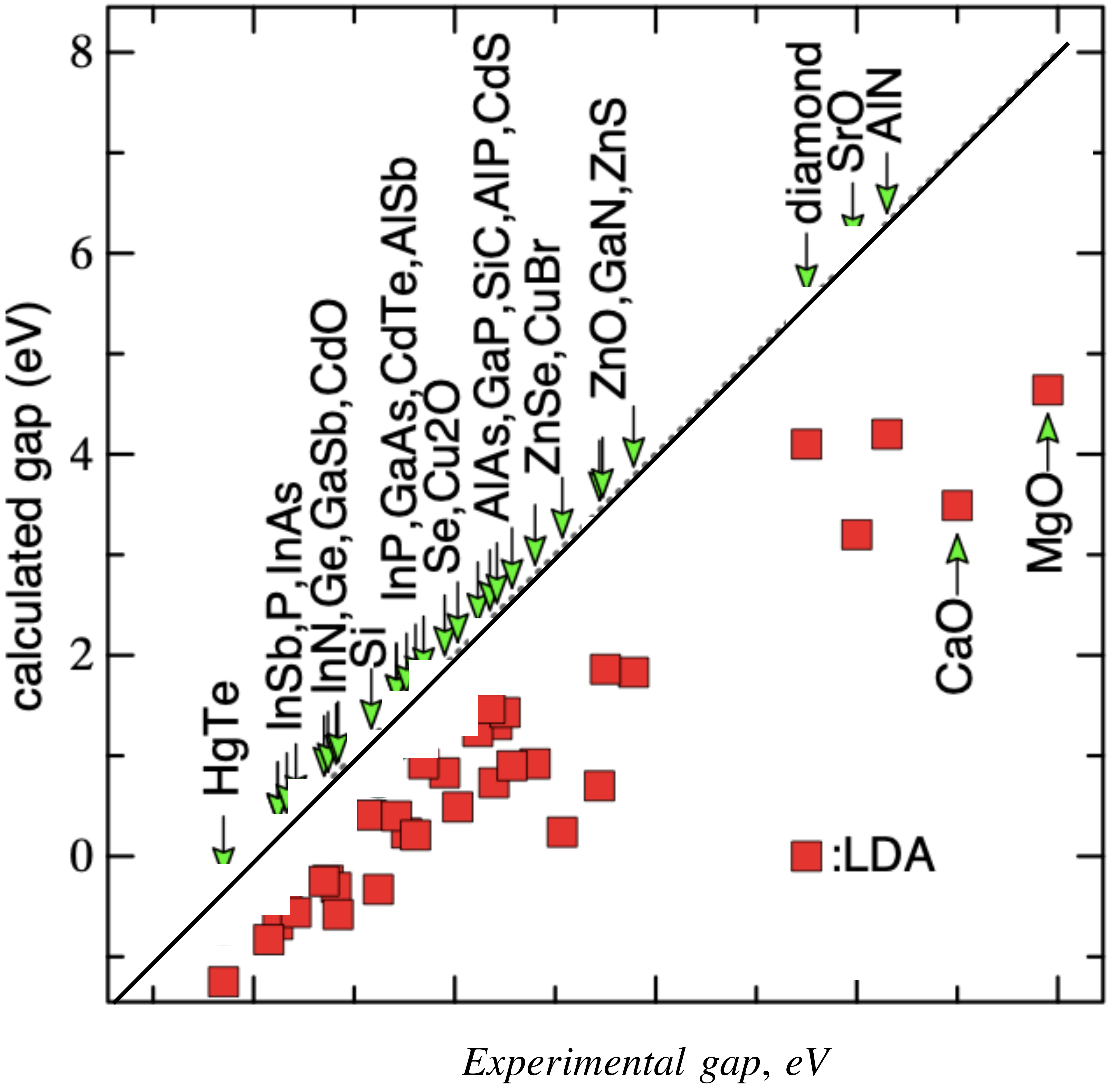


ϵ_{LU} ϵ_{HO}

$$E^*(N+1) - E_{GS}(N) - (E_{GS}(N) - E^*(N-1)) = E^e_{GAP}$$

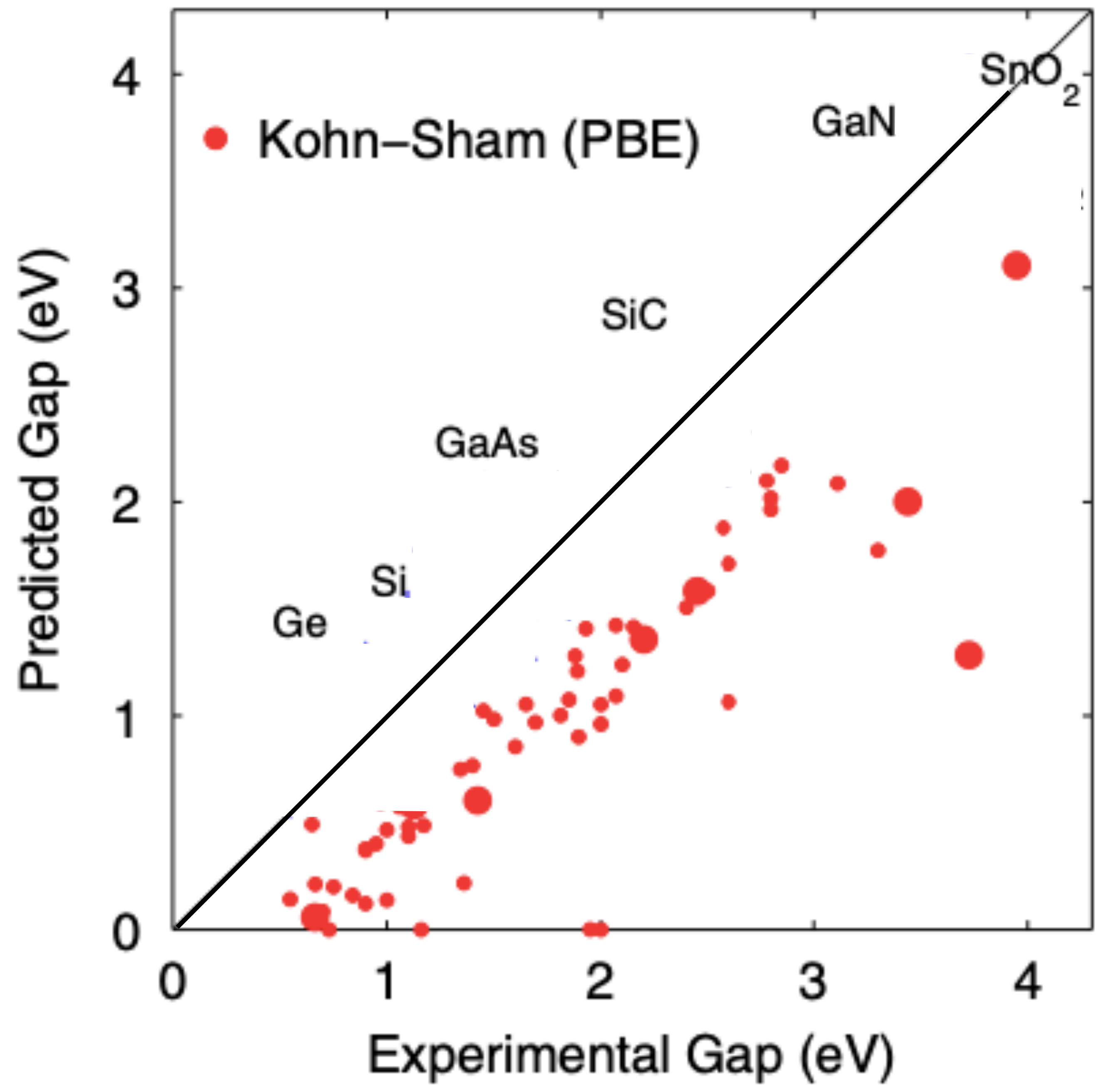
$$E^*(N) - E_{GS}(N) = E^o_{GAP}$$

Fundamental gap (electronic gap)



adapted from van Schilfgraade et al. PRL 2006

Consistent underestimation of the gap DFT@(LDA/GGA)



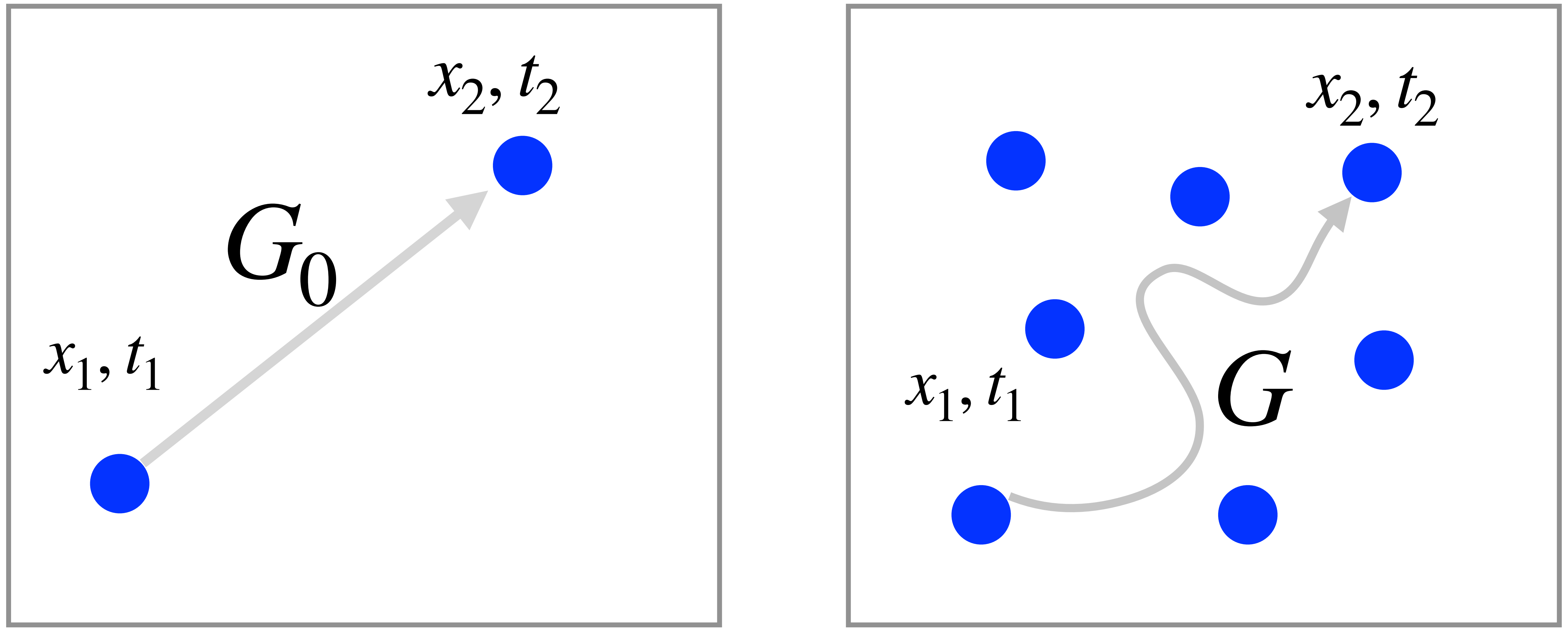
adapted from Chen et al. PRL 2010

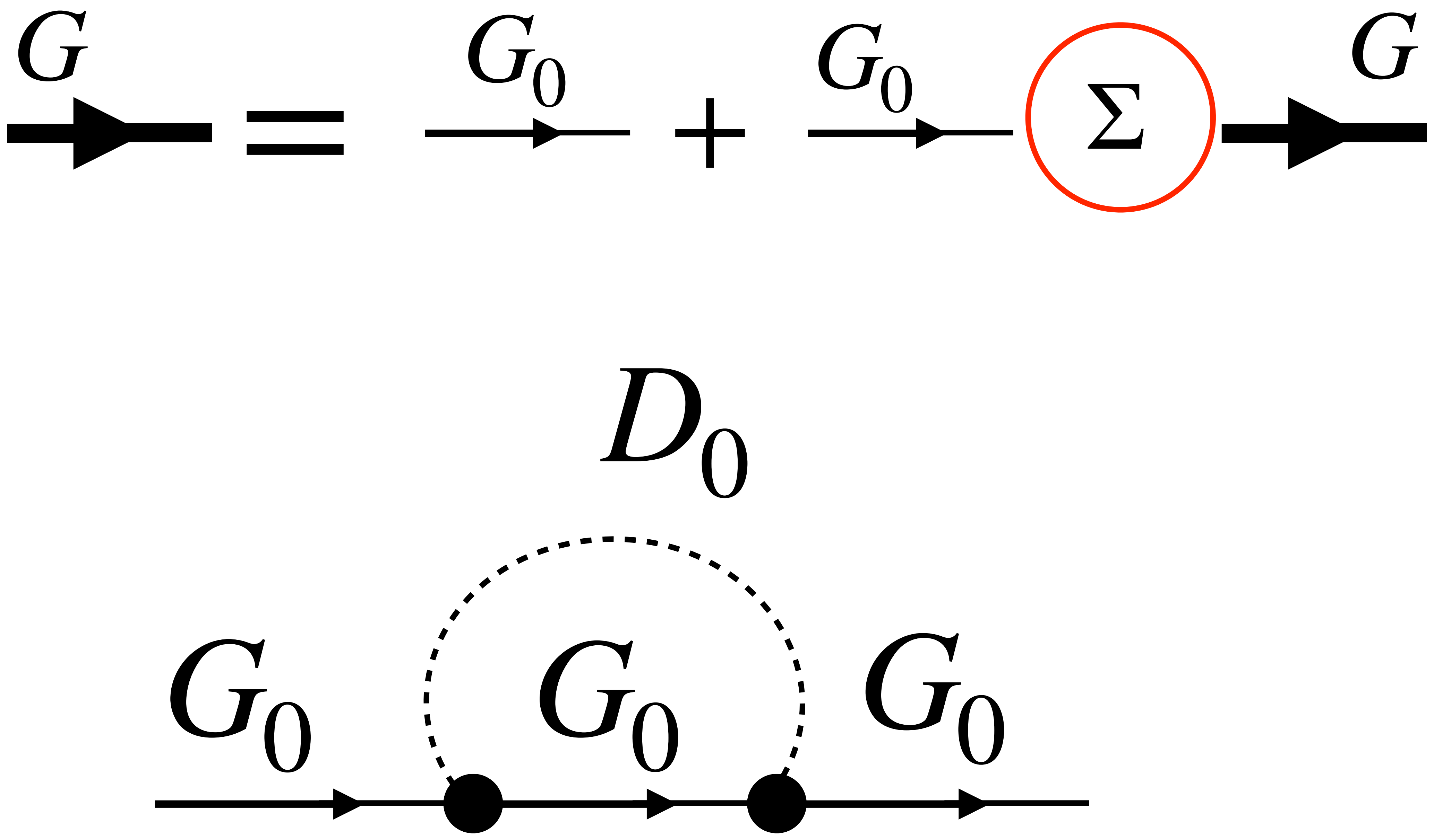
Many-body perturbation theory

- Green's functions (propagators (correlation functions))
- Feynman et al.

non-interacting

interacting



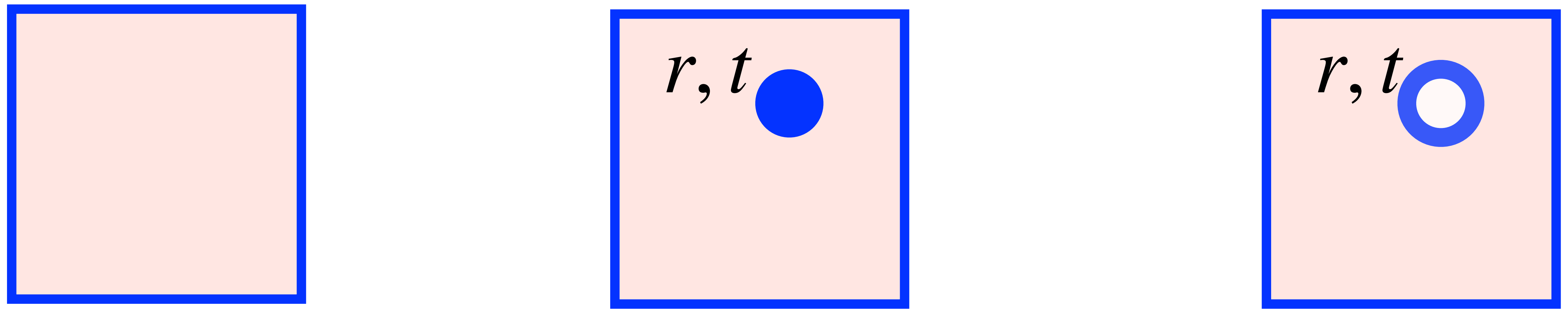


Green's function as a propagator

$$\hat{H}|\Psi> = E|\Psi>$$

$|\Psi>$ exact state of N particles

$|\Psi>$ $\hat{\psi}^{+}(r,t)|\Psi>$ $\hat{\psi}^{+}(r,t)|\Psi>$



N $N+1$ $N-1$

creation operator of the particle at r,t

$\hat{\psi}^{+}(r,t)$

distraction operator of the particle at r,t

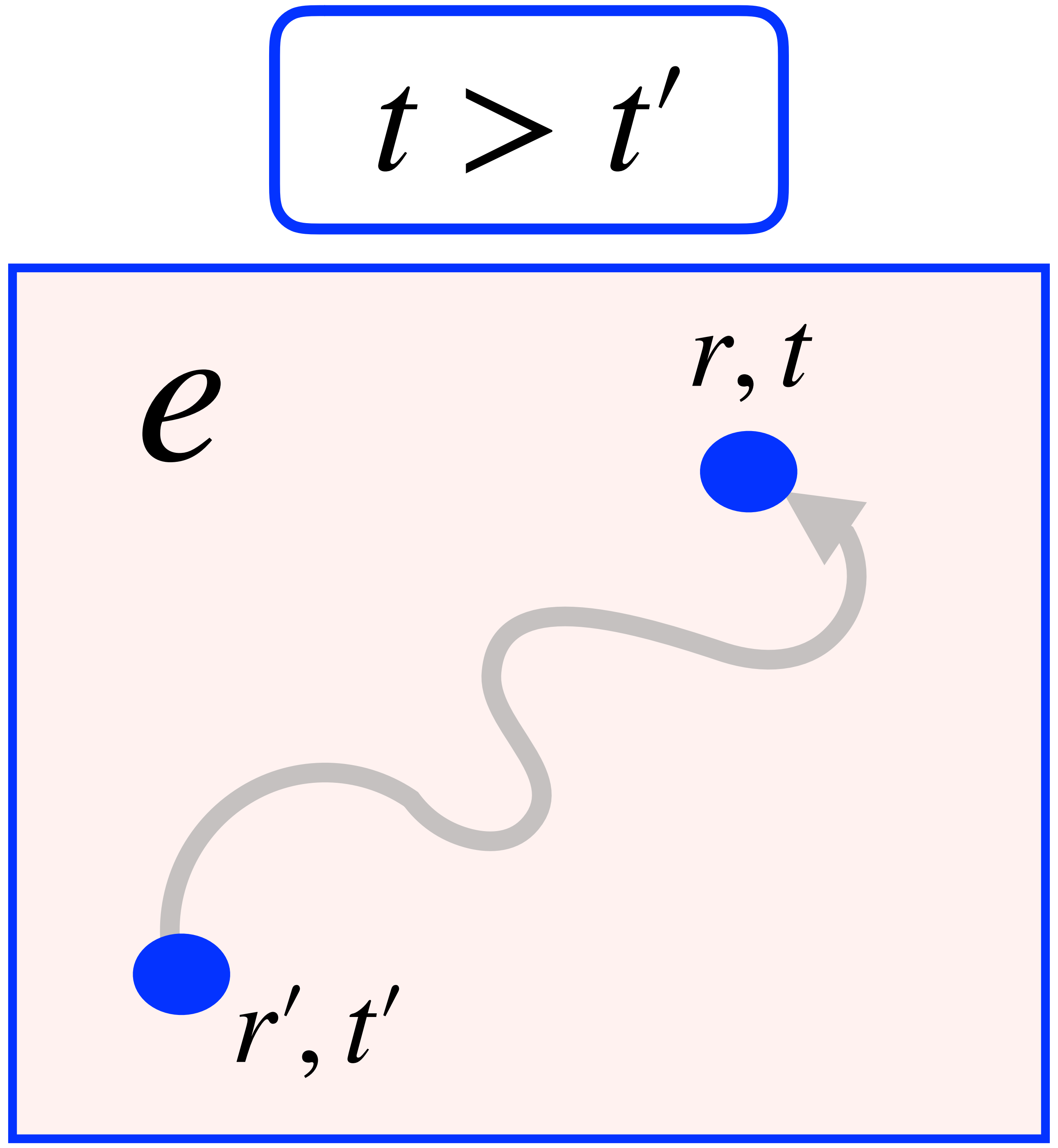
$\hat{\psi}(r,t)$

$$\{\hat{\psi}^{+}(r), \psi(r')\} = \delta(r-r')$$

$$[\hat{\psi}^{+}(r), \psi(r')] = \delta(r-r')$$

Green's function as a propagator

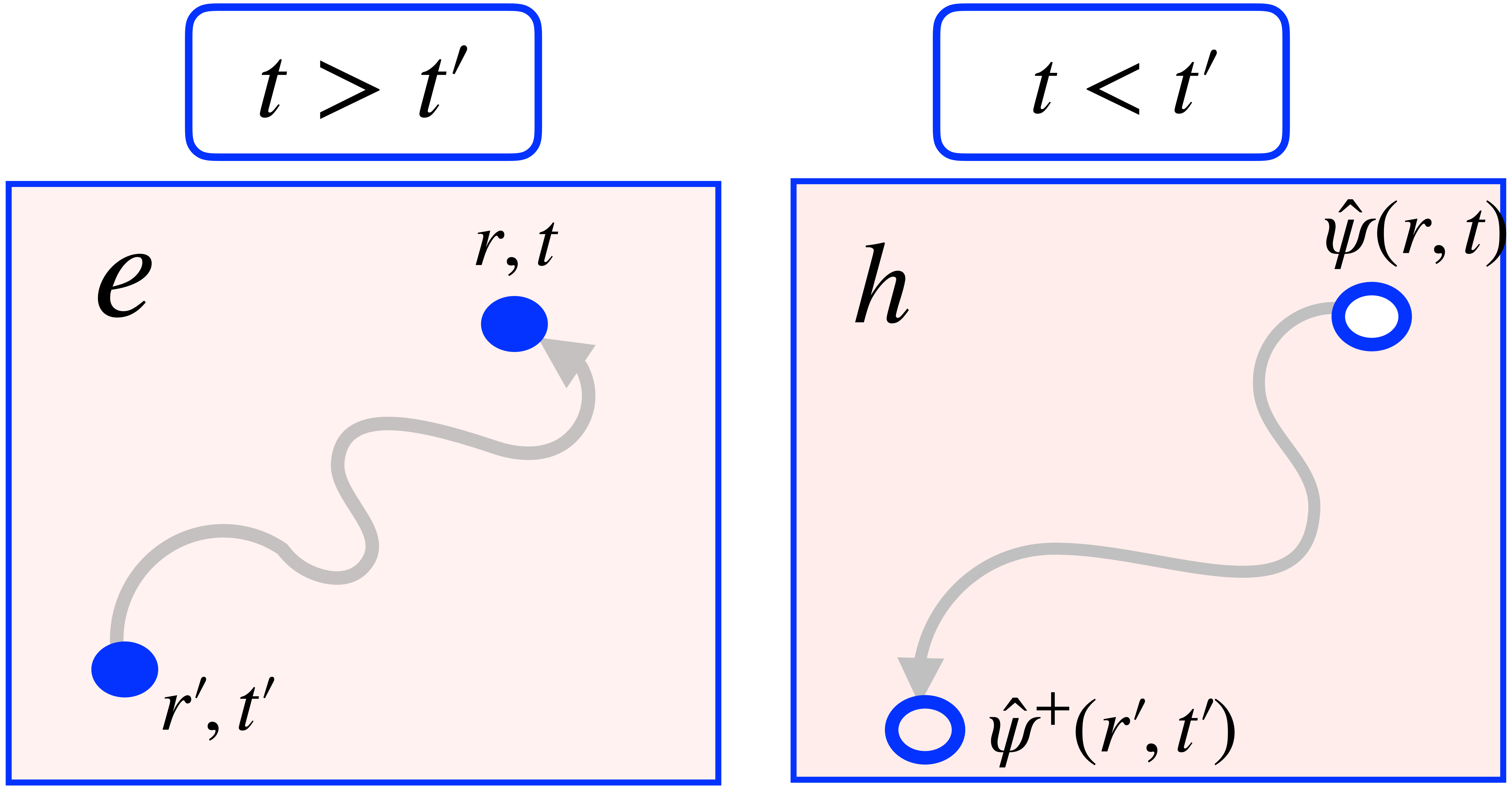
$$G^{>}(r', t', r, t) = -i < \Psi \,|\, \hat{\psi}(r,t)\hat{\psi}^{+}(r',t') \,|\, \Psi >$$



describes propagation of single particle (electron) from t' to t

Green's function as a propagator

$$G(r', t', r, t) = -i < \Psi | T\hat{\psi}(r, t)\hat{\psi}^{+}(r', t') | \Psi >$$



Time ordering

$$G(r',t',r,t) = -i < \Psi | T\hat{\psi}(r,t)\hat{\psi}^{+}(r',t') | \Psi >$$

$$T = \begin{cases} \hat{A}(t)\hat{B}(t') & t > t' \\ \pm\hat{B}(t')\hat{A}(t) & t < t' \end{cases}$$

$$G(r',t',r,t) = -i\theta(t-t') < \Psi | \hat{\psi}(r,t)\hat{\psi}^{+}(r',t') | \Psi > + i\theta(t'-t) < \Psi | \hat{\psi}(r,t)\hat{\psi}^{+}(r',t') | \Psi >$$

$$G(r',t',r,t) = \theta(t-t')G^{>}(r,t,r',t') + i\theta(t'-t)G^{<}(r,t,r',t')$$

FT

FT

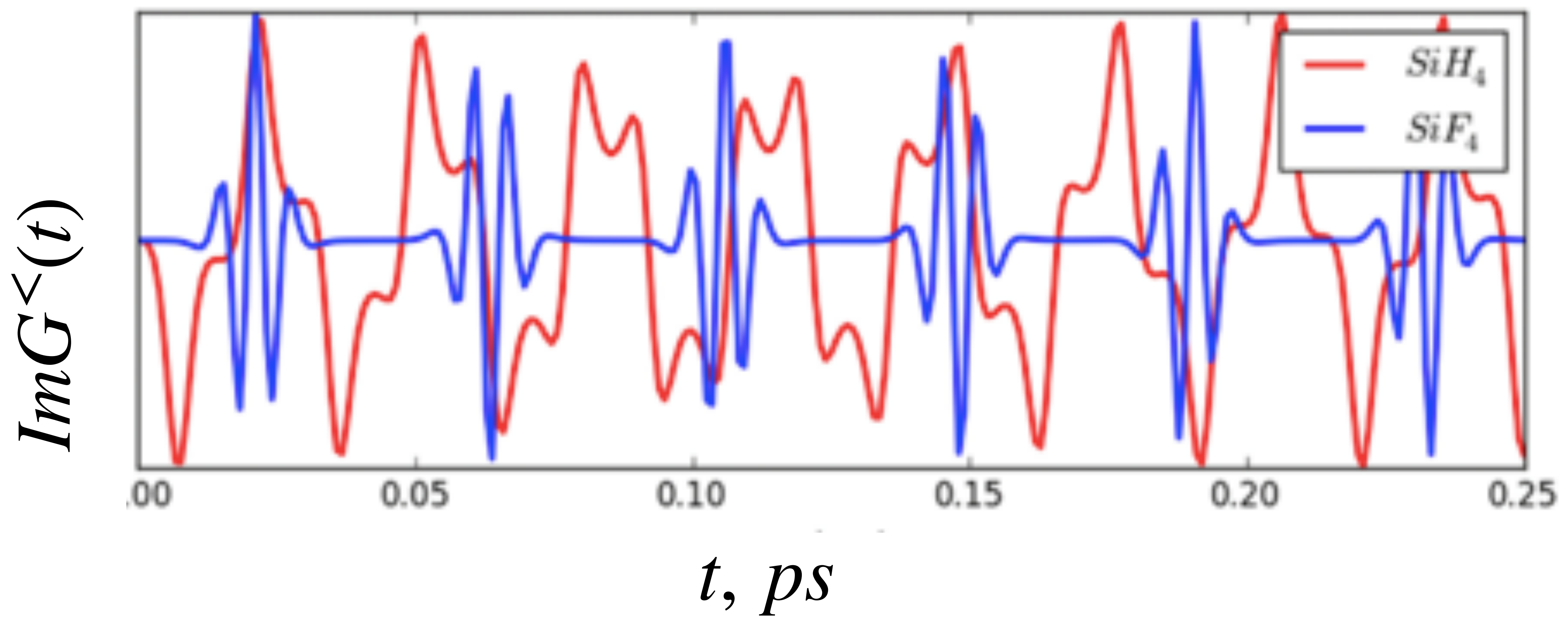
$\hat{\psi}^{+}(r,t) -> \hat{c}^{+}_{\alpha}(t)$

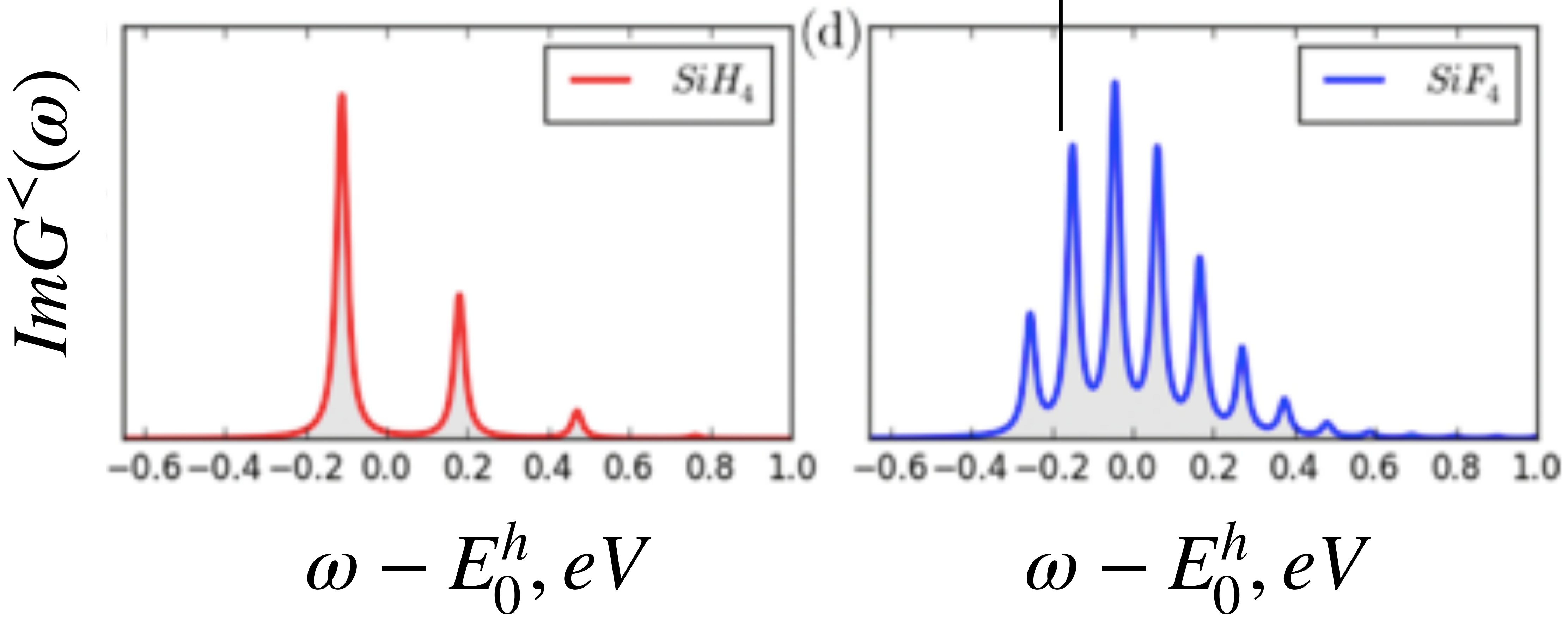
$t, t' -> t - t'$

$g_{s,k}$

$$iG^{<}(\mathbf{k}, t'-t) = <\Psi_{GS}|\hat{c}_{\mathbf{k}}{}^{+}(t)\hat{c}_{\mathbf{k}}(t')|\Psi_{GS}>$$

$$G^{<}(\mathbf{k},\omega) = \sum_{s} \frac{|<\Psi_s|c_{\mathbf{k}}|\Psi_{GS}>|^2}{(\omega - E^h_s - i\eta)}$$



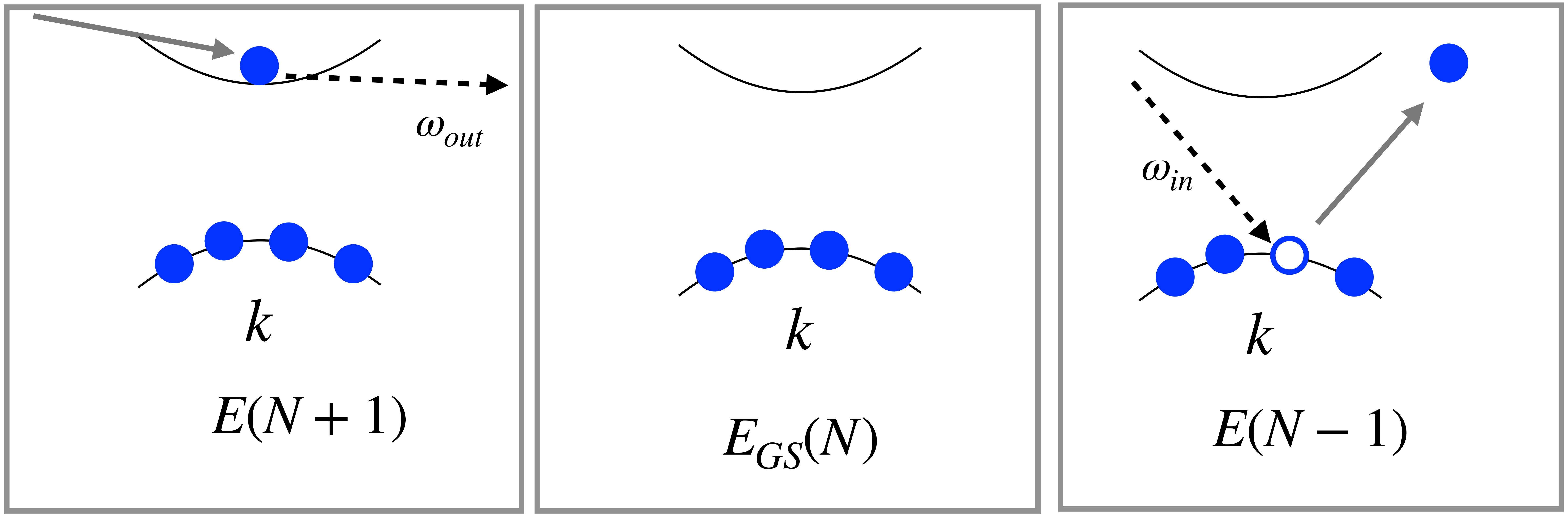


Inverse

$$G(\mathbf{k}, \omega) = \sum_s \frac{|f_{s,k}|^2}{(\omega - E_s^h - i\eta)} + \sum_\beta \frac{|g_{s,k}|^2}{(\omega - E_s^e + i\eta)}$$

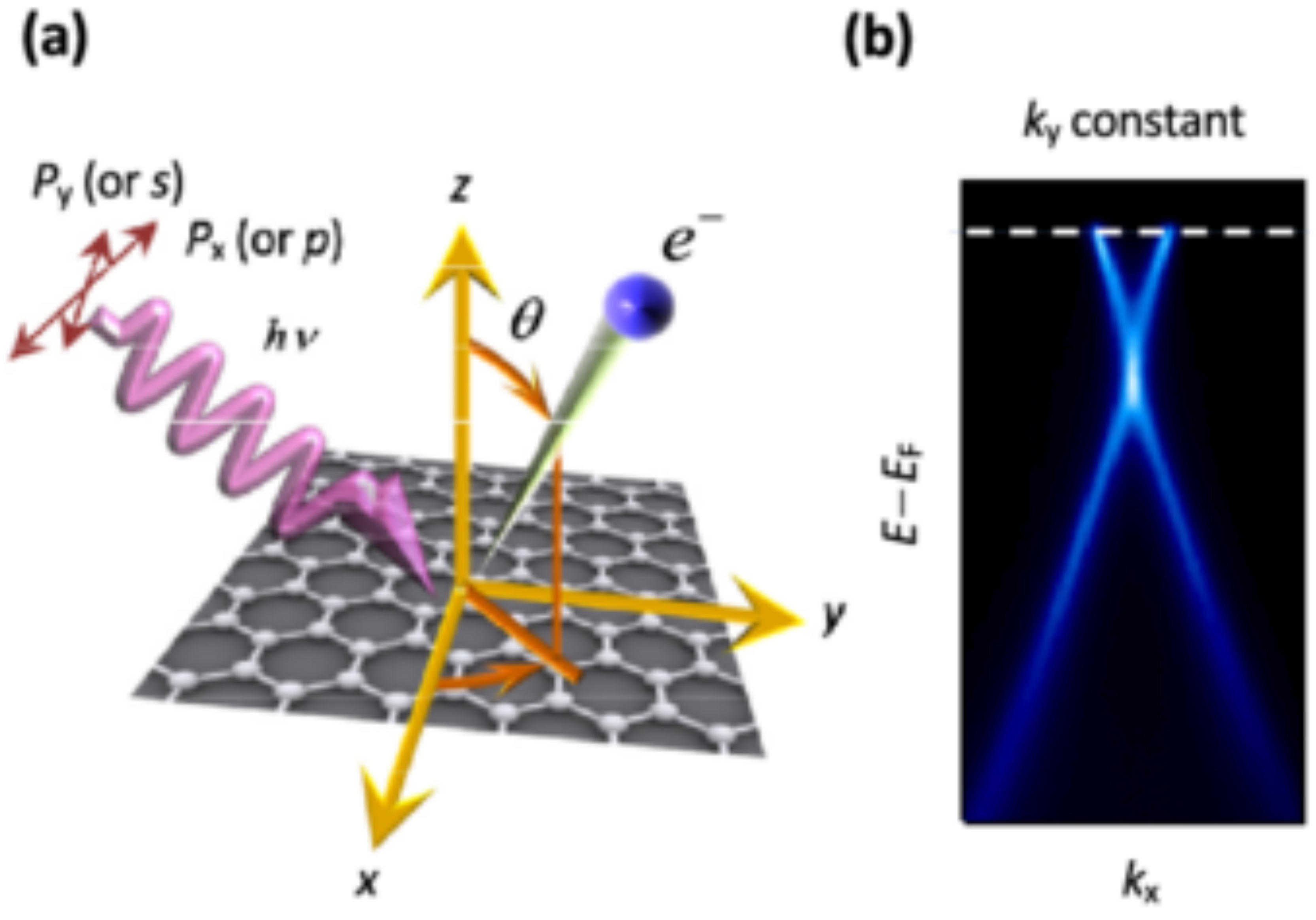
$E_s^e = E_s(N+1) - E_{GS}(N)$

$E_s^h = E_{GS}(N) - E_s(N-1)$



Spectral

Angular resolved photo-emission spectroscopy (ARPES)



Hwang et al. CAPh (2021)

Spectral function

$$A(\omega) = -\frac{1}{\pi} ImG(\omega)$$

Photoemission

$$J_{ps}(\mathbf{k}, \omega) \sim A^{<}_{\mathbf{k}}(\omega) = -\frac{1}{\pi}\sum_s |g_{s\mathbf{k}}|^2 \delta(\omega - E^h_{\mathbf{k}})$$

Inverse Photoemission

$$J_{ips}(\mathbf{k}, \omega) \sim A^{>}_{\mathbf{k}}(\omega) = -\frac{1}{\pi}\sum_s |f_s|^2 \delta(\omega - E^e_{\mathbf{k}})$$

Recup

Q: What is the advantage?

$$G^{<}(\mathbf{k},\omega) = \sum_s \frac{|<\Psi_s|c_{\mathbf{k}}|\Psi_{GS}>|^2}{(\omega - E_s^h - i\eta)} \quad \Longleftrightarrow \quad H|\Psi_s> = E_s|\Psi_s>$$

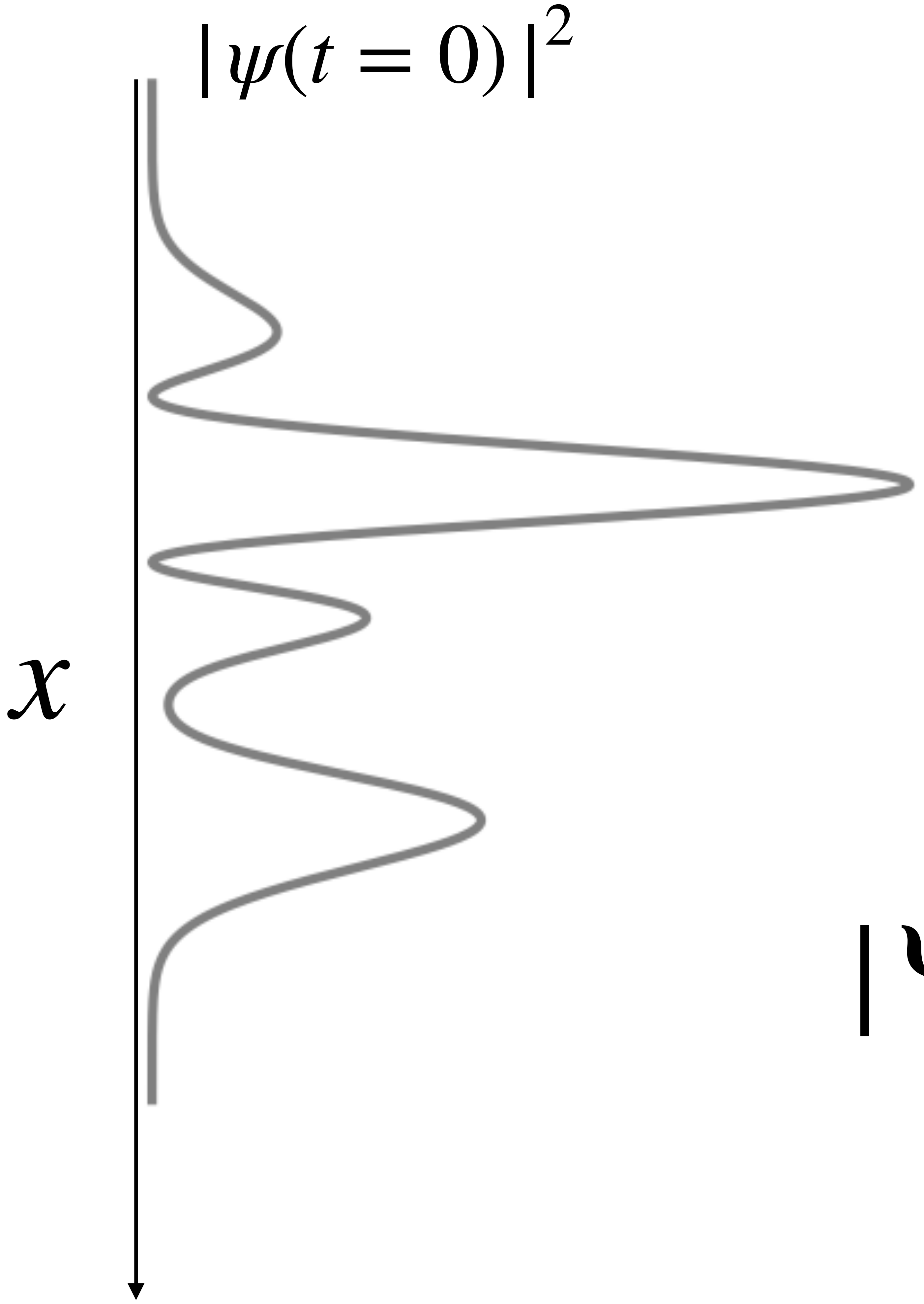
A: Many-body perturbation theory (time-dependent)

$$H_0 \rightarrow G_0$$

$$H = H_0 + V \rightarrow G$$

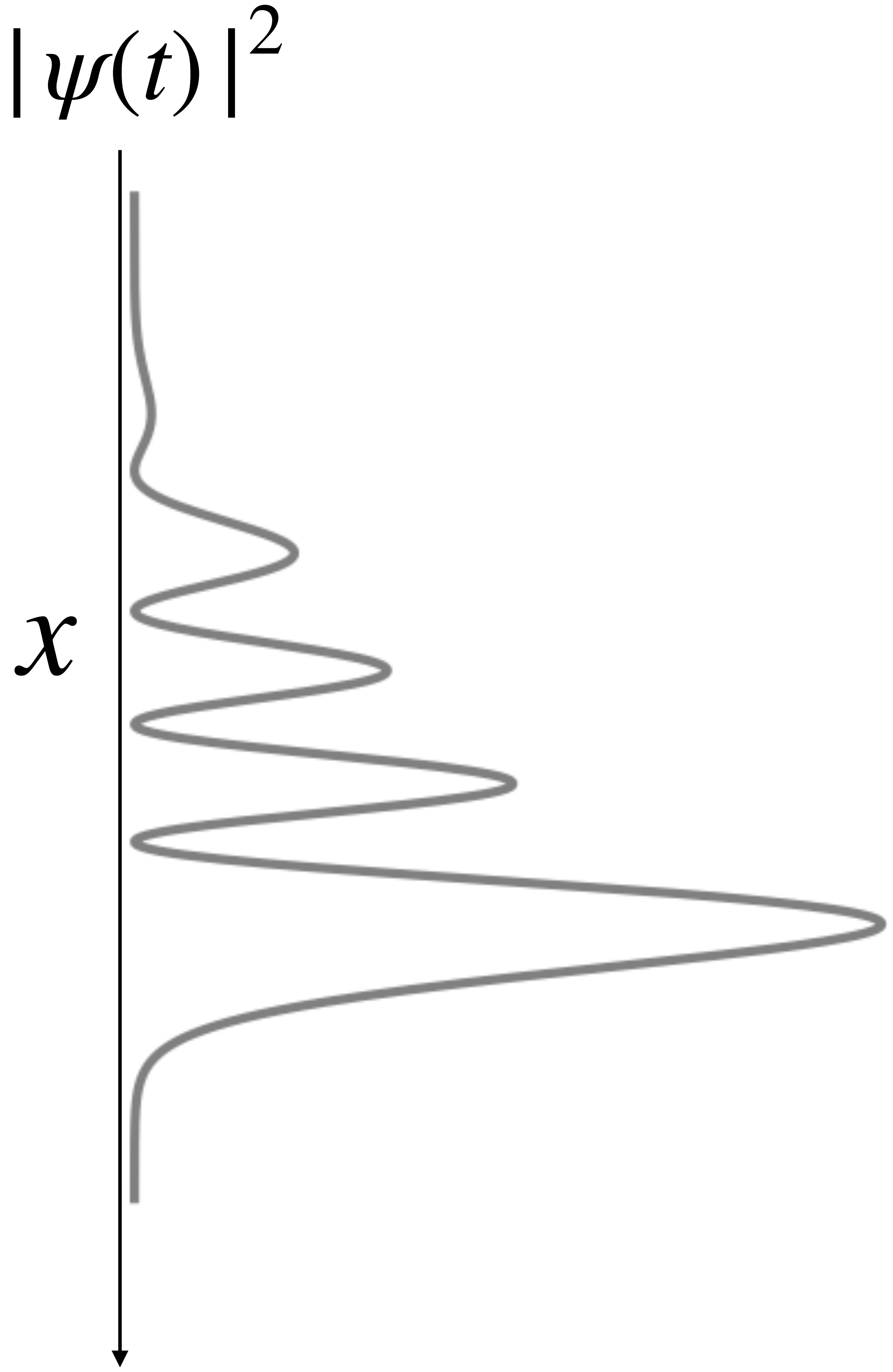
$$G[G_0]?$$

Time evolution



$$U(t)$$

$$|\Psi(t)> = U(t)|\Psi(0)>$$

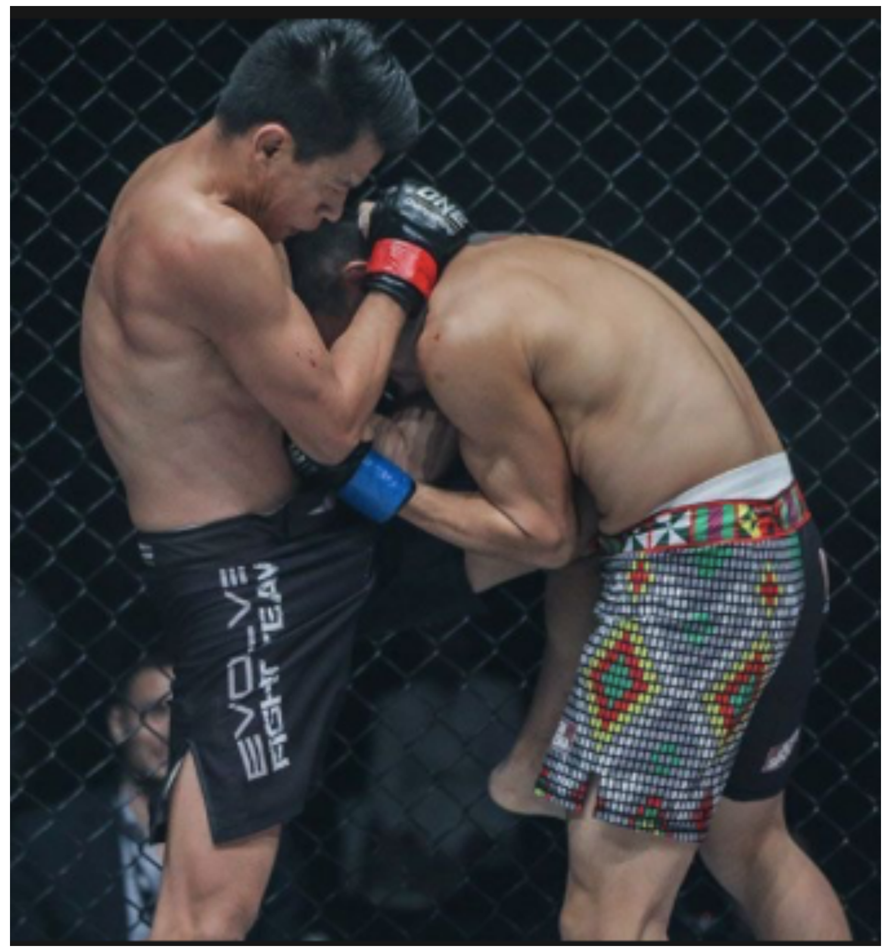


Time evolution pictures

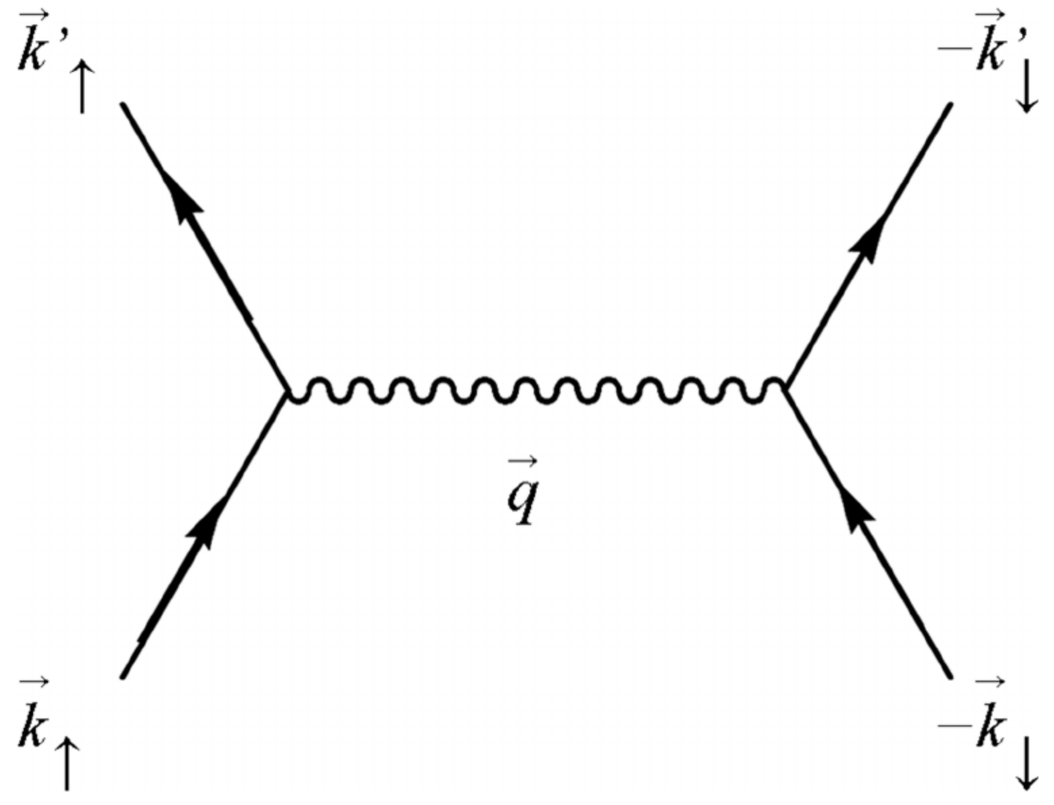
Schrödinger

Heisenberg

Interaction



Time evolution pictures

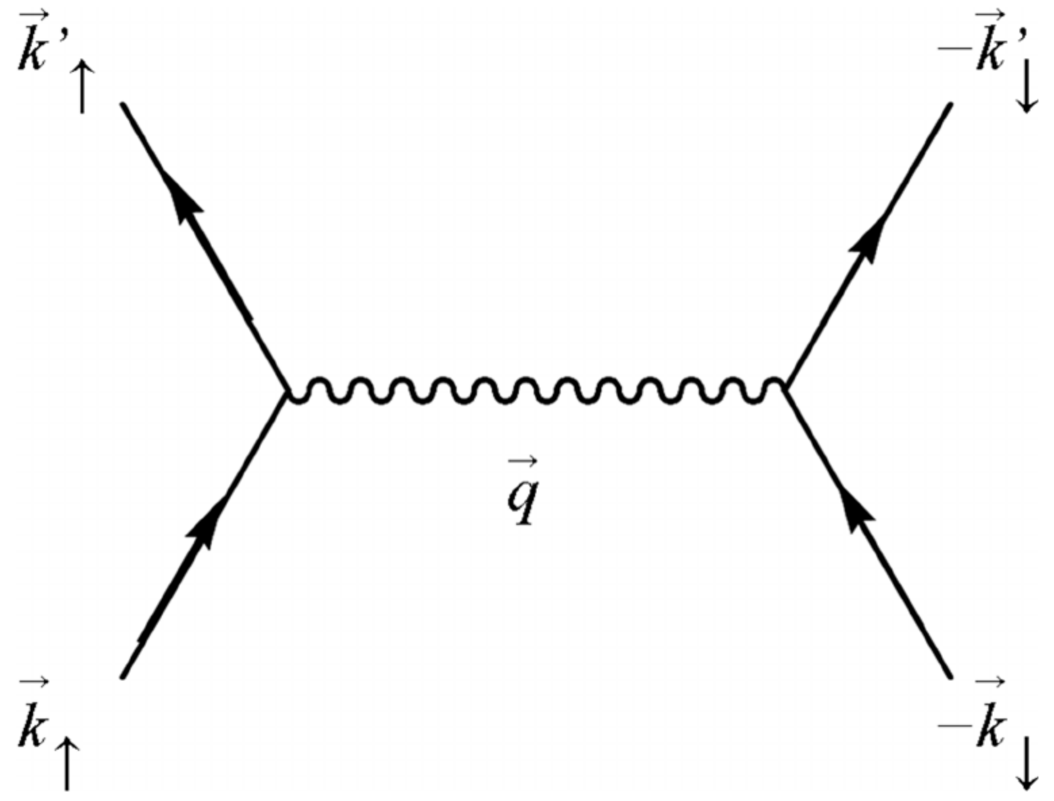
	Schrödinger	Heisenberg	Interaction picture
			
State	$\lvert\psi(t) >$	$\lvert\psi >$	$\lvert\psi_I(t) >$
Operator	$\hat{O}$	$\hat{O}(t)$	$\hat{O}_I(t)$
Evolution	$i\frac{d}{dt}\psi(t) = H\psi(t)$	$-i\frac{d}{dt}\hat{O} = [\hat{H}, \hat{O}]$	$i\frac{d}{dt}\psi_I(t) = V_I\psi_{(}t)$ $-i\frac{d}{dt}\hat{O} = [\hat{H}_0, \hat{O}]$

Time evolution pictures

Schrodinger

Heisenberg

Interaction picture



Theory *Exp*

$$< \psi(t) | \hat{O} | \psi(t) > = < \psi | \hat{O}(t) | \psi > = < \psi_I(t) | \hat{O}_I(t) | \psi_I(t) > = < \hat{O}(t) >$$

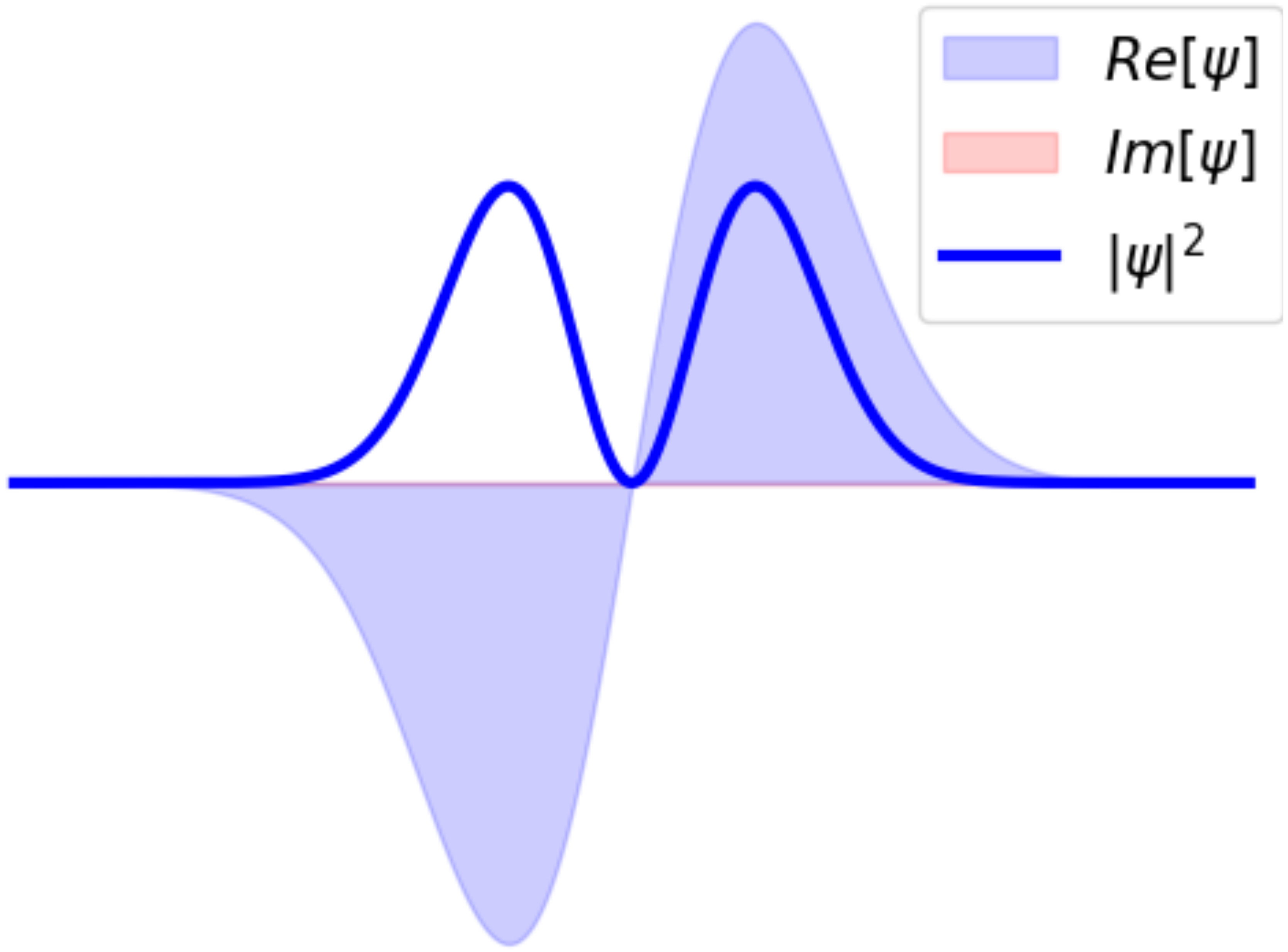
Time evolution: H0

Time-independent Hamiltonian

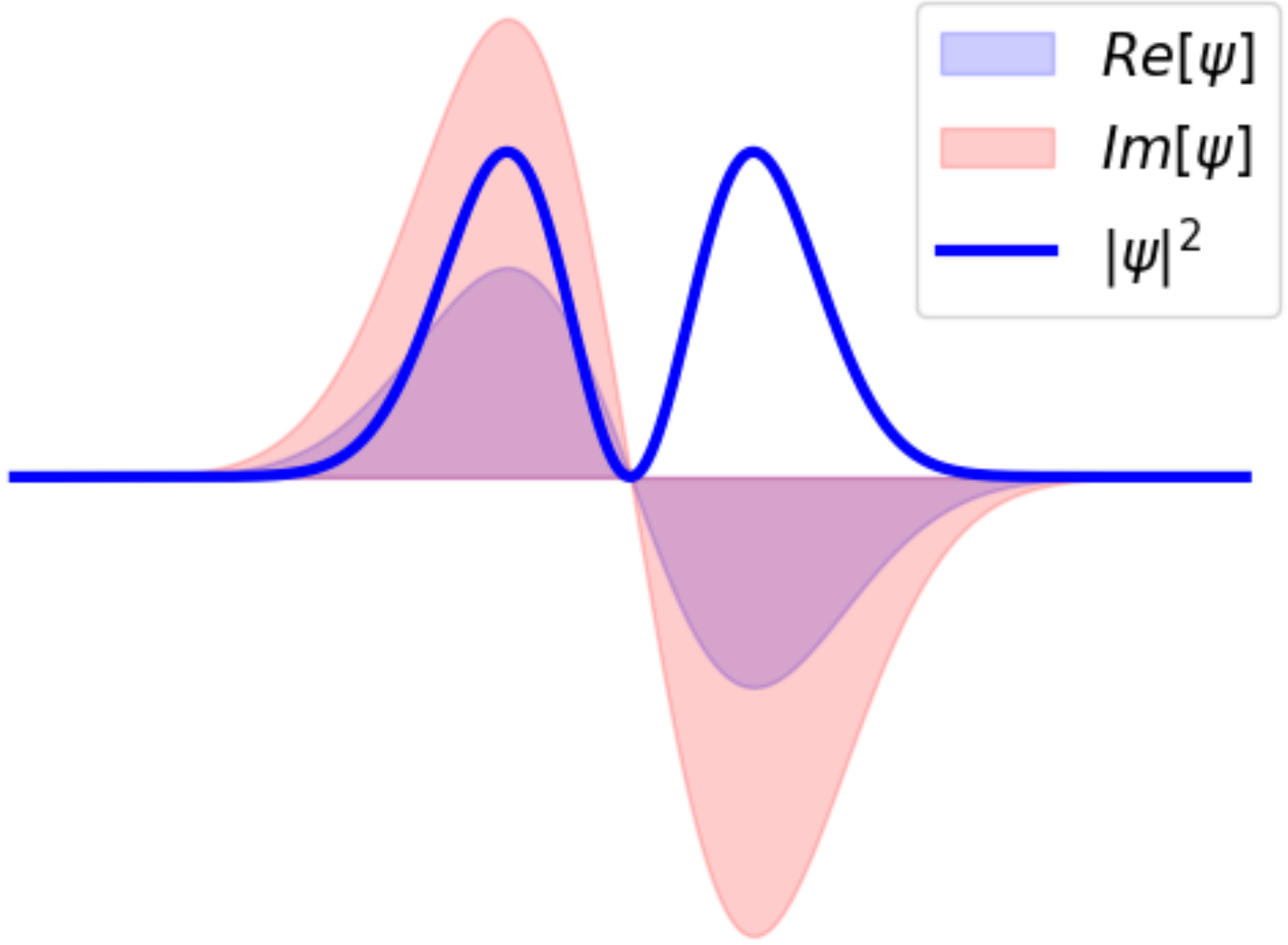
$$i\frac{d}{dt}|\psi(t)> = H_0|\psi(t)>$$

$$U_0(t) = e^{-iH_0 t}$$

$$|\psi(t=0)> = |\phi_1>$$



$$\psi(t) = e^{-iE_1 t}|\phi_1>$$



Time evolution: interaction picture

Time-dependent part $V(t)$

From S picture to I: $|\Psi_I(t)> = U_0(t)^+ |\Psi_S(t)>$

$$|\Psi_I(t)> = U_I(t)^+ |\Psi_I(0)>$$

$$i\frac{d}{dt}U_I(t) = V_I(t)U_I(t)$$

$$U_I(t) = Te^{-i\int_0^t V(t_1)dt_1}$$

Time evolution: interaction picture

$$i\frac{d}{dt}U_I(t) = V_I(t)U_I(t)$$

$$U_I(t) - U_I(0) = -i\int_0^t dt_1 \hat{V}(t_1)U_I(t_1)$$

Chain rule: $$U_I(t) = 1 - i\int_0^t dt_1 \hat{V}(t_1)U_I(t_1)$$

$$U_I(t) = I - \sum_n^{\infty}\int_0^t dt_1 \ldots \int_0^{t_{n-1}} dt_n \hat{V}(t_1)\ldots\hat{V}(t_n) = I - T\sum_n \frac{i^n}{n!}\int_0^t dt_1 \ldots \int_0^t dt_n \hat{V}(t_1)\ldots\hat{V}(t_n)$$

$$U_I(t) = Te^{-i\int_0^t V(t_1)dt_1}$$

Time evolution

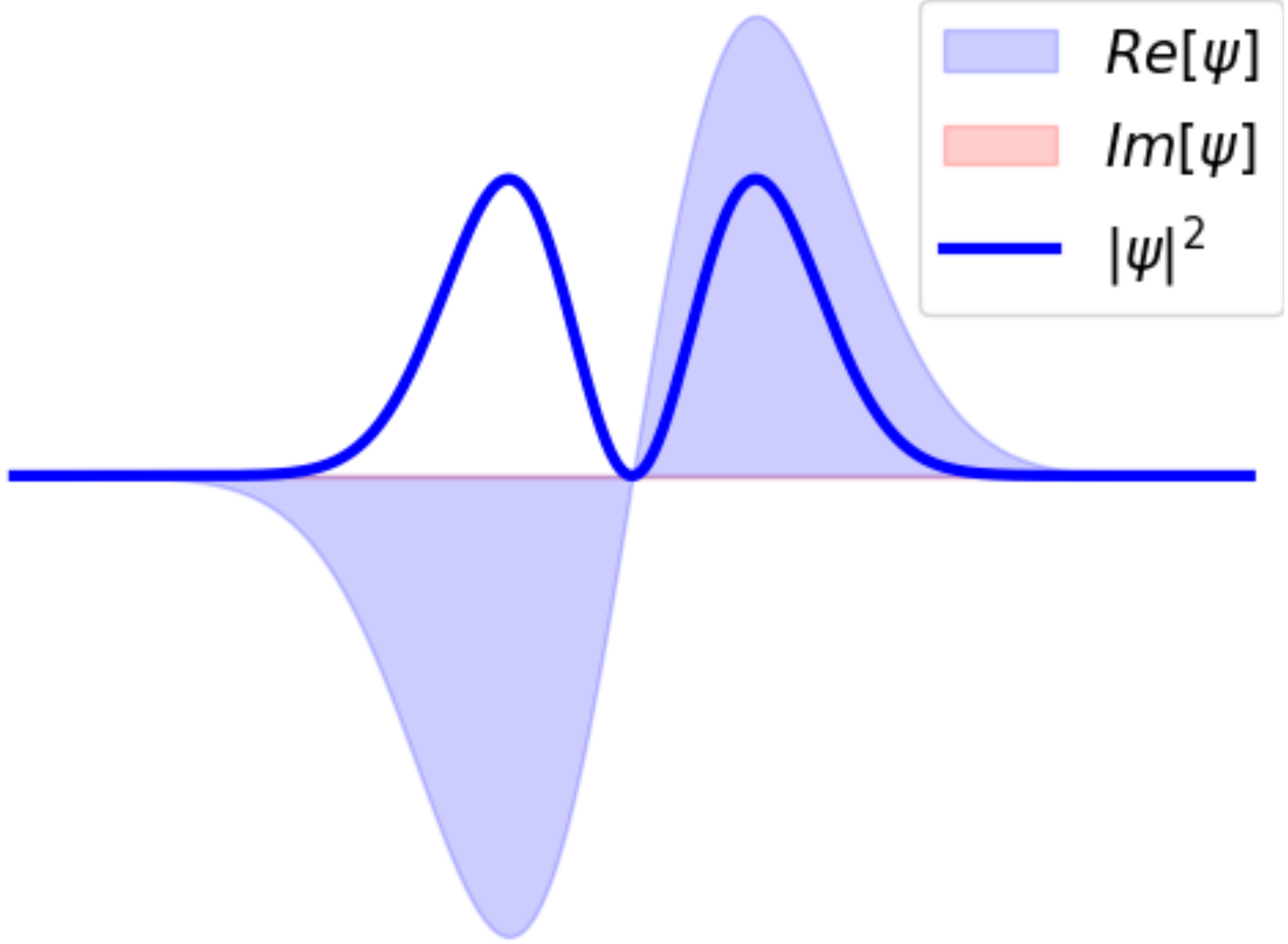
Time-dependent part

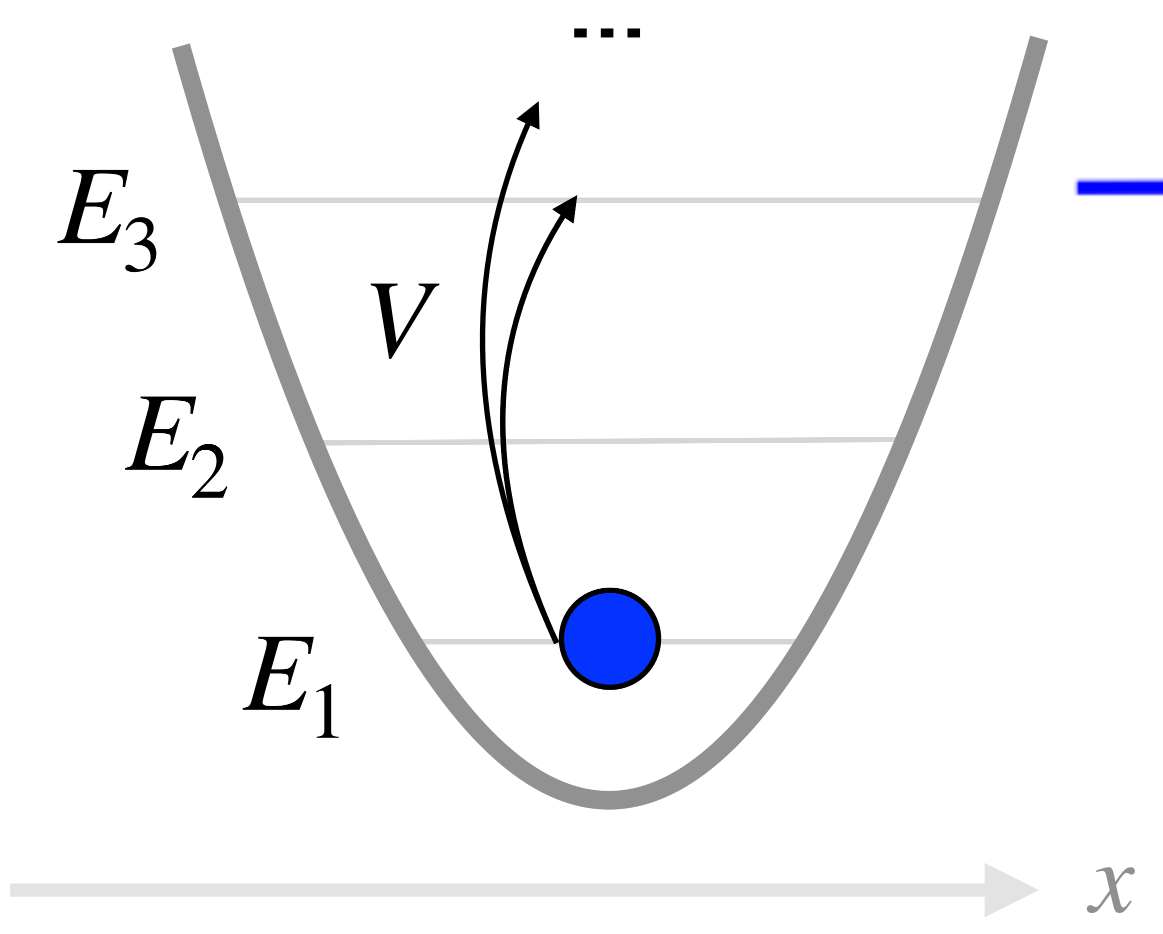
$$i\frac{d}{dt}|\psi(t)> = H|\psi(t)>$$

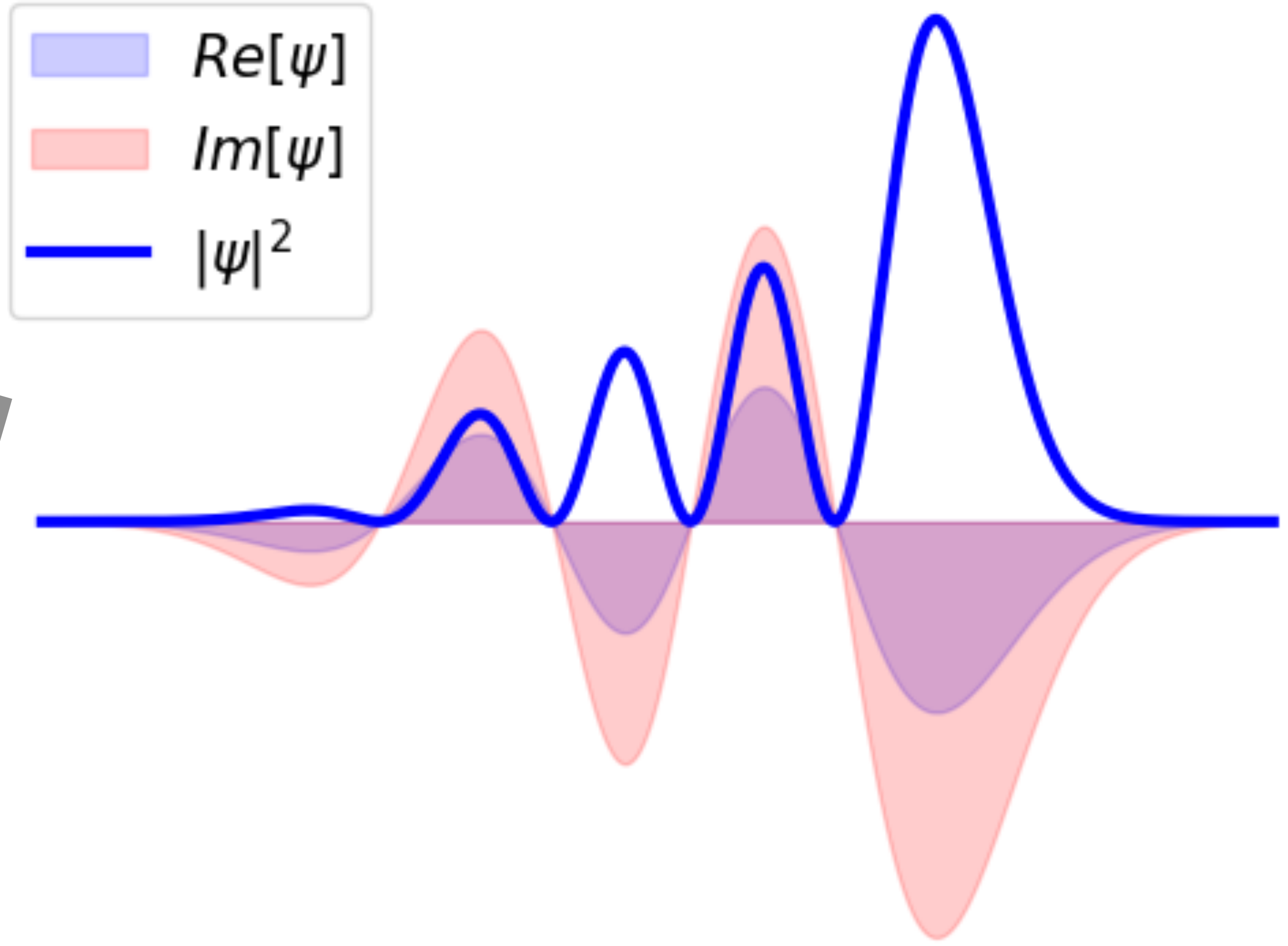
$$U_I(t) = Te^{-i\int_0^t V(t_1)dt_1}$$

$$|\psi(t=0)> = |\phi_1>$$

$$\psi_I(t) = U_I(t)|\psi(0)>$$







$$\alpha|\phi_3(t)> + \beta|\phi_4(t)>$$

Scattering matrix

$$S(t, t') = U(t)U^{+}(t')$$

$$S(t, t) = 1$$

$$S^{+}(t, t') = S(t', t)$$

$$S(t, t')S(t', t'') = S(t', t'')$$

Interacting Green's function

$$(H_0 + \lambda V)\Psi = E\Psi$$

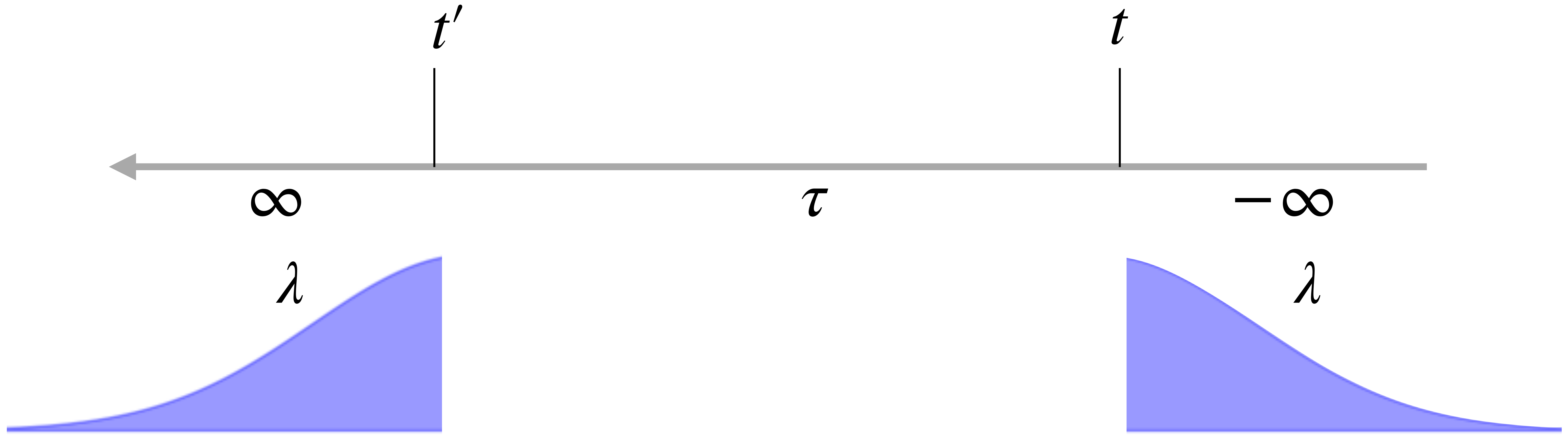
$$H_0 \phi_\alpha = E_\alpha \phi$$

$$G(\alpha, t, t') = -i < \Psi(0) | T c_{h,\alpha}(t) c^+_{h,\alpha}(t') | \Psi(0) >$$

$$e^{iL} < \phi_0 | S(\infty, 0) = < \Psi(0) |$$

$$c_{h,\alpha}(t) = U(t) c_\alpha(t) U^+(t)$$

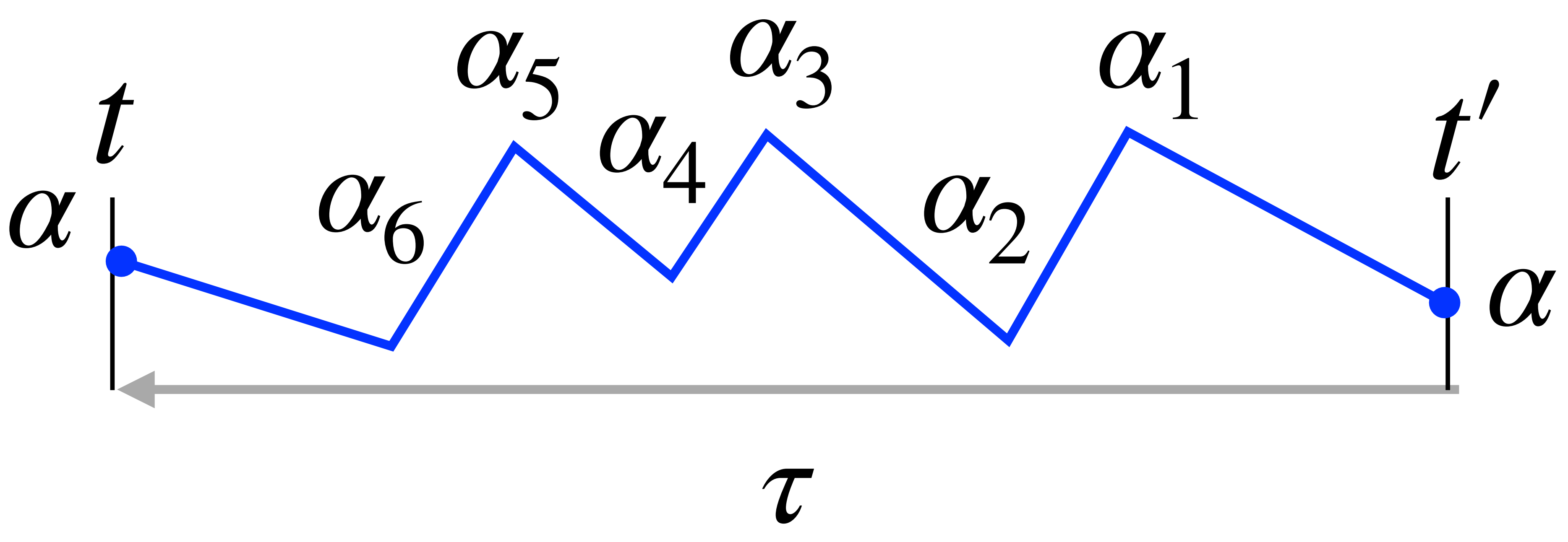
$$| \Psi(0) > = S(0, -\infty) | \phi_0 >$$



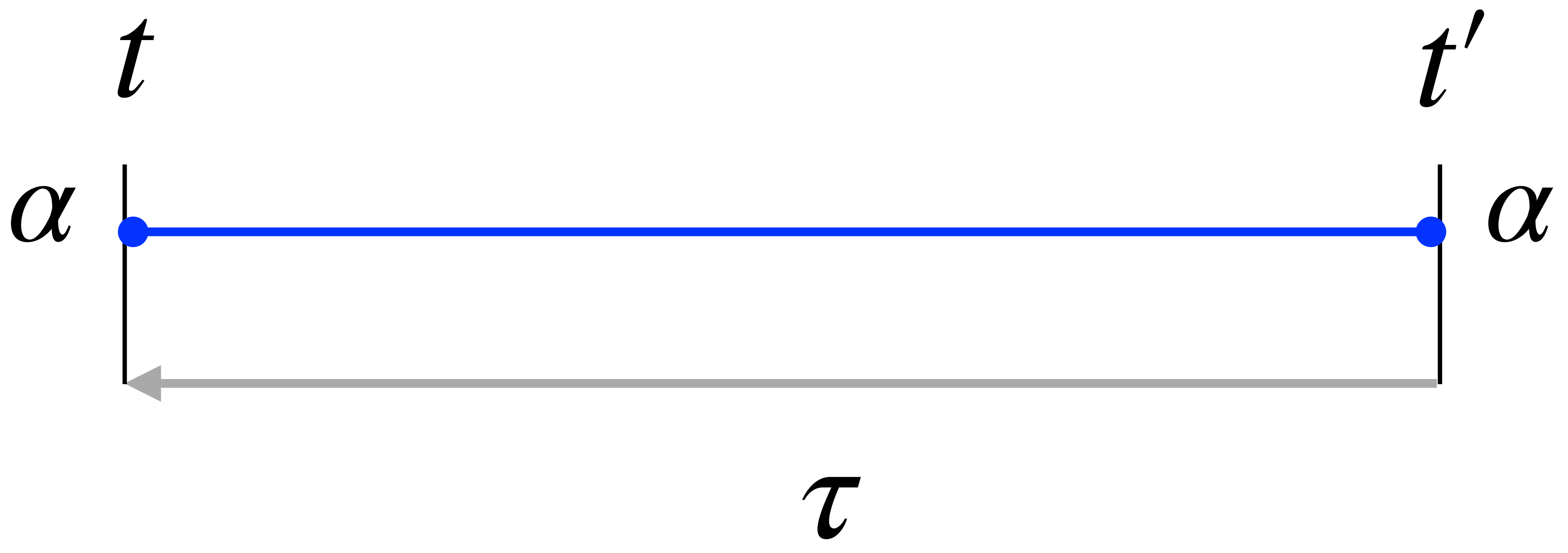
Interacting Green's function

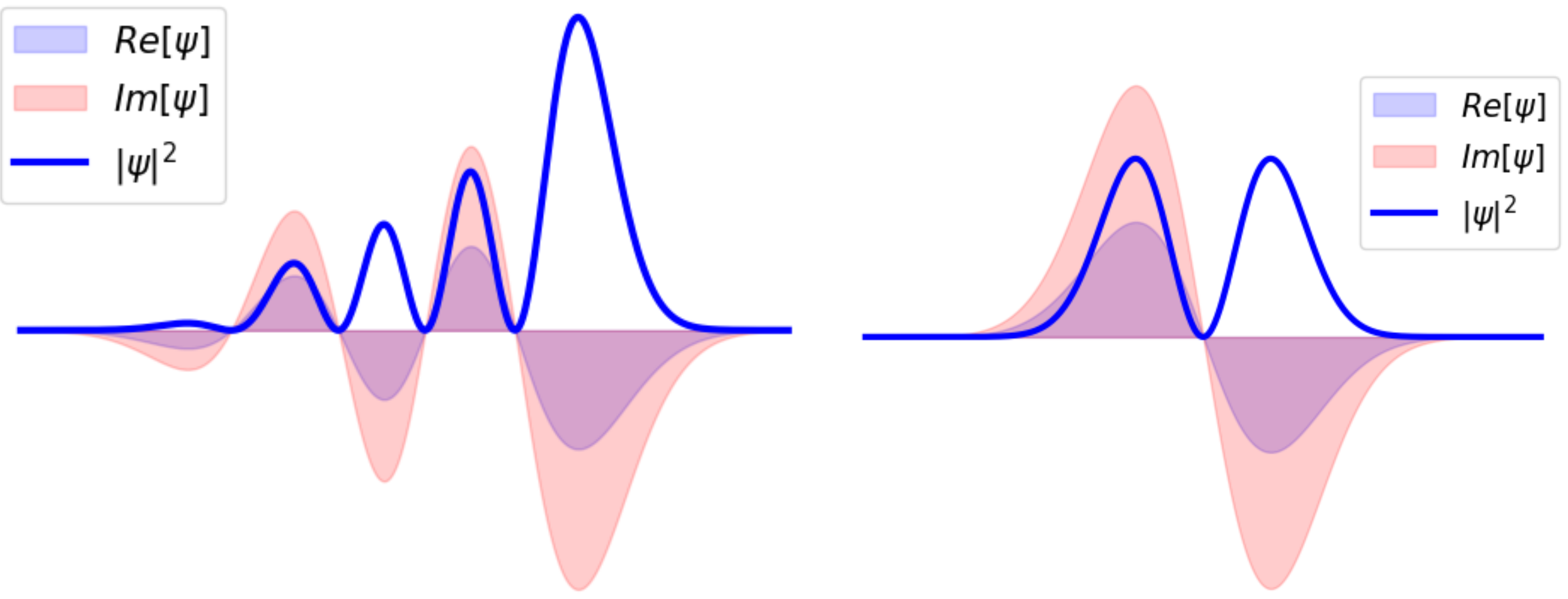
$$G(\alpha, t, t') = -i < \phi_0 | TS(-\infty, t) c_\alpha(t) S(t, t') c_\alpha^+(t') S(t', \infty) | \phi_0 > e^{iL}$$

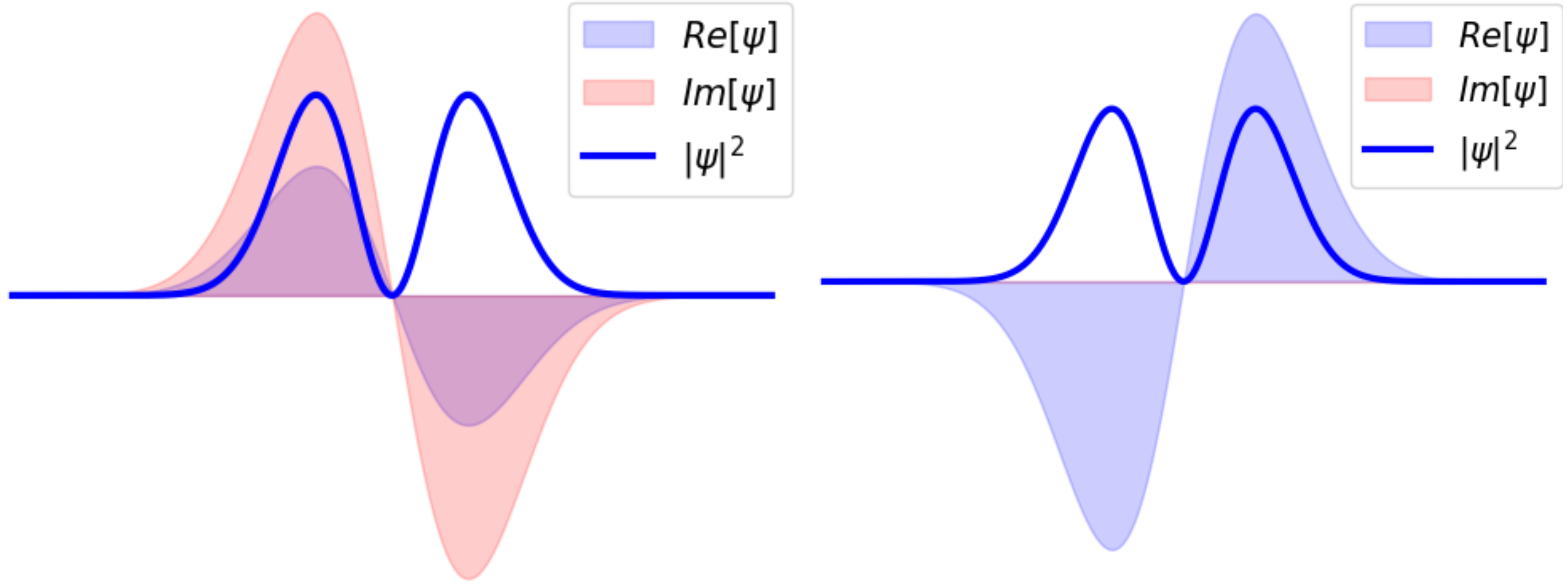
$S(t, t')$



$S(t, t') = 1$







Dyson series

$$G(\alpha, t, t') = -i < \phi_0 | TS(-\infty, \infty) c_\alpha(t) c_\alpha^+(t') | \phi_0 >_c$$

$$S(-\infty, \infty) = T \sum_n \frac{i^n}{n!} \int_{-\infty}^{\infty} dt_1 \dots \int_{-\infty}^{\infty} dt_n \hat{V}(t_1) \dots \hat{V}(t_n)$$

Key ingredients

Wick's theorem

$$< 0 | Ta(t_1) b(t_2) a^+(t_3) b^+(t_4) | 0 > = < 0 | Ta(t_1) a^+(t_3) | 0 > < 0 | Tb(t_2) b^+(t_4) | 0 >$$

$$G_0(t_1, t_2, t_3, t_4) = G_0(t_1, t_3) G_0(t_3, t_4)$$

Dyson series

$$G(\alpha, t, t') = G_0(\alpha, t - t') + (-i)^2 \int_{-\infty}^{\infty} dt_1 < 0 | Tc_\alpha(t) V(t_1) c_\alpha^+(t') | 0 >$$

$$+(-i)^3 \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dt_1 dt_2 < 0 | Tc_\alpha(t) V(t_1) V(t_2) c_\alpha^+(t') | 0 > \ldots$$

e.g. electron-phonon(photon) interaction $V(t) = \sum_{\gamma\gamma'\lambda} M_{\gamma\gamma'} c_\gamma^+(t) c_{\gamma'}(t) A_\lambda(t)$

$$G(\alpha, t, t') = G_0(\alpha, t - t') + (-i)^2 \int_{-\infty}^{\infty} dt_1 < 0 | Tc_\alpha(t) \sum_{\beta\beta'\lambda} M_{\beta\beta'} c_\beta^+(t_1) c_{\beta'}(t_1) A_\lambda(t_1) c_\alpha^+(t') | 0 >$$

$$+(-i)^3 \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dt_1 dt_2 < 0 | Tc_\alpha(t) \sum_{\beta,\beta'} M_{\beta\beta'\lambda} c_\beta^+(t_1) c_{\beta'}(t_1) A_\lambda(t_1) \sum_{\gamma\gamma'\lambda} M_{\gamma\gamma'} c_\gamma^+(t_2) c_{\gamma'}(t_2) A_\lambda(t_2) c_\alpha^+(t') | 0 > \ldots$$

Dyson series

$$G(\alpha,t,t') = G_0(\alpha,t-t') + (-i)^2\int_{-\infty}^{\infty} dt_1 < 0\,|\,Tc_\alpha(t)V(t_1)c_\alpha^+(t')\,|\,0 >$$

$$+(-i)^3\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dt_1 dt_2 < 0\,|\,Tc_\alpha(t)V(t_1)V(t_2)c_\alpha^+(t')\,|\,0 > \dots$$

We know all parts

$$G = F[G_0, M, D_0]$$

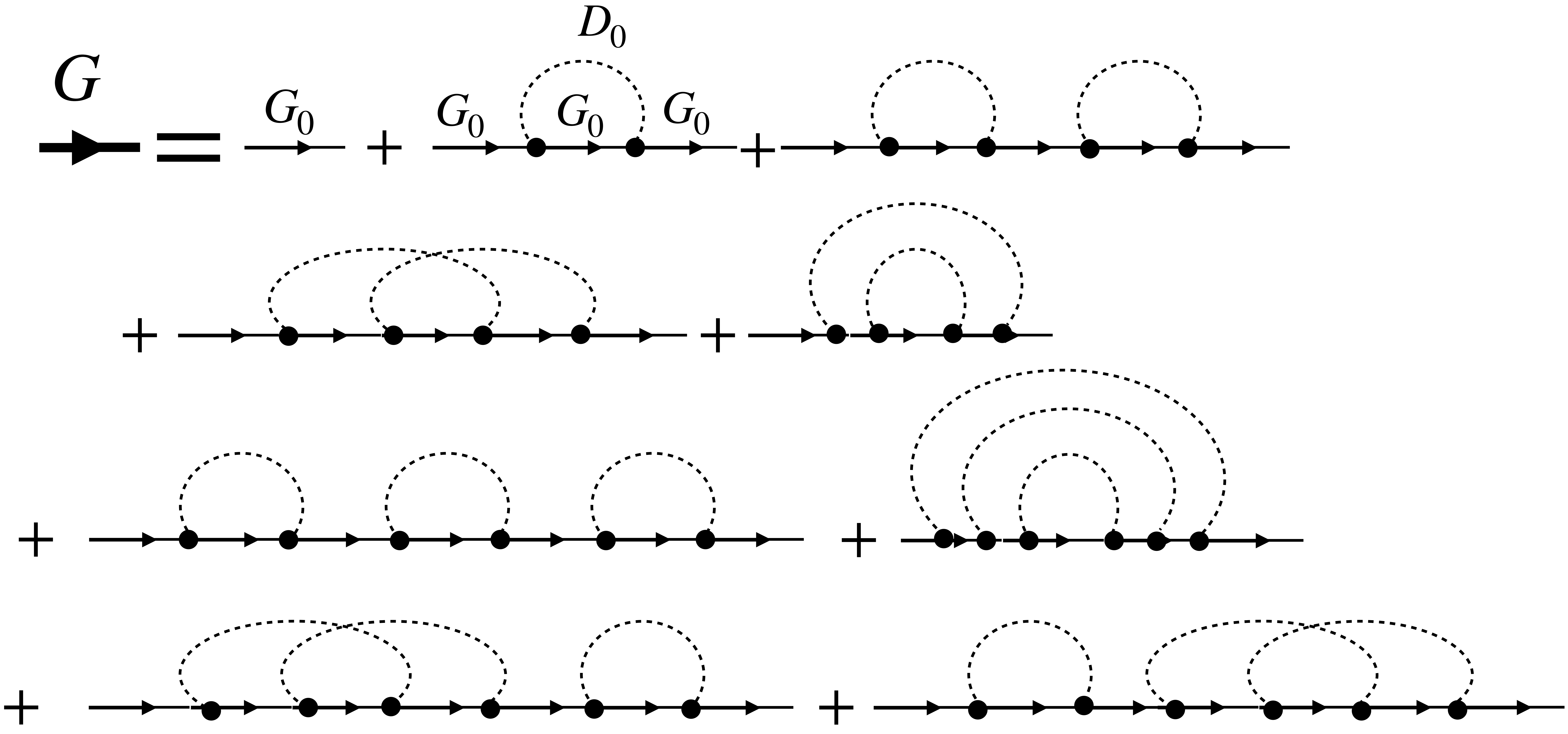
e.g. electron-phonon(photon) interaction $V(t) = \sum_{\gamma\gamma'\lambda} M_{\gamma\gamma'}c_\gamma^+(t)c_{\gamma'}(t)A_\lambda(t)$

interacting

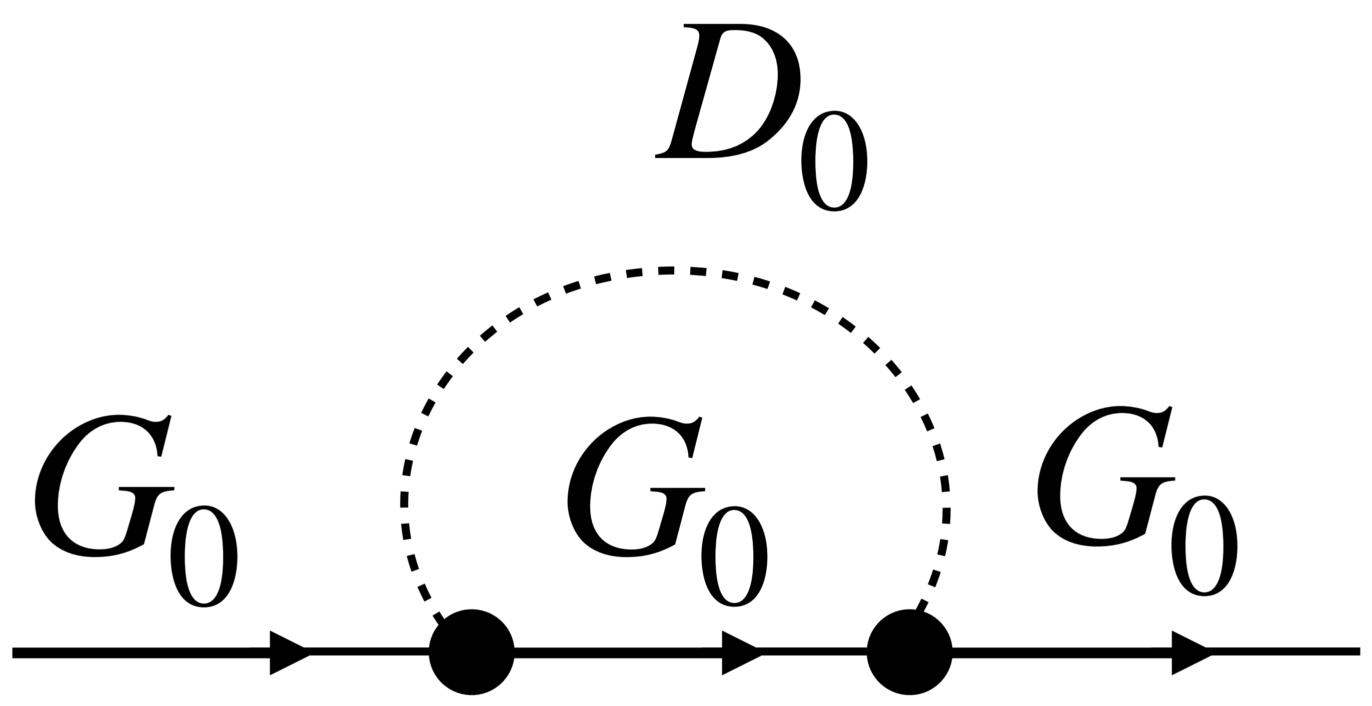
$$G(\alpha,t,t') = G_0(\alpha,t-t') + (-i)^2\int_{-\infty}^{\infty} dt_1 < 0\,|\,Tc_\alpha(t)\sum_{\beta\beta'\lambda} M_{\beta\beta'}c_\beta^+(t_1)c_{\beta'}(t_1)A_\lambda(t_1)c_\alpha^+(t')\,|\,0 >$$

$$+(-i)^3\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dt_1 dt_2 < 0\,|\,Tc_\alpha(t)\sum_{\beta,\beta'} M_{\beta\beta'\lambda}c_\beta^+(t_1)c_{\beta'}(t_1)A_\lambda(t_1)\sum_{\gamma\gamma'\lambda} M_{\gamma\gamma'}c_\gamma^+(t_2)c_{\gamma'}(t_2)A_\lambda(t_2)c_\alpha^+(t')\,|\,0 > \dots$$

Diagrams



Many-body physics in examples



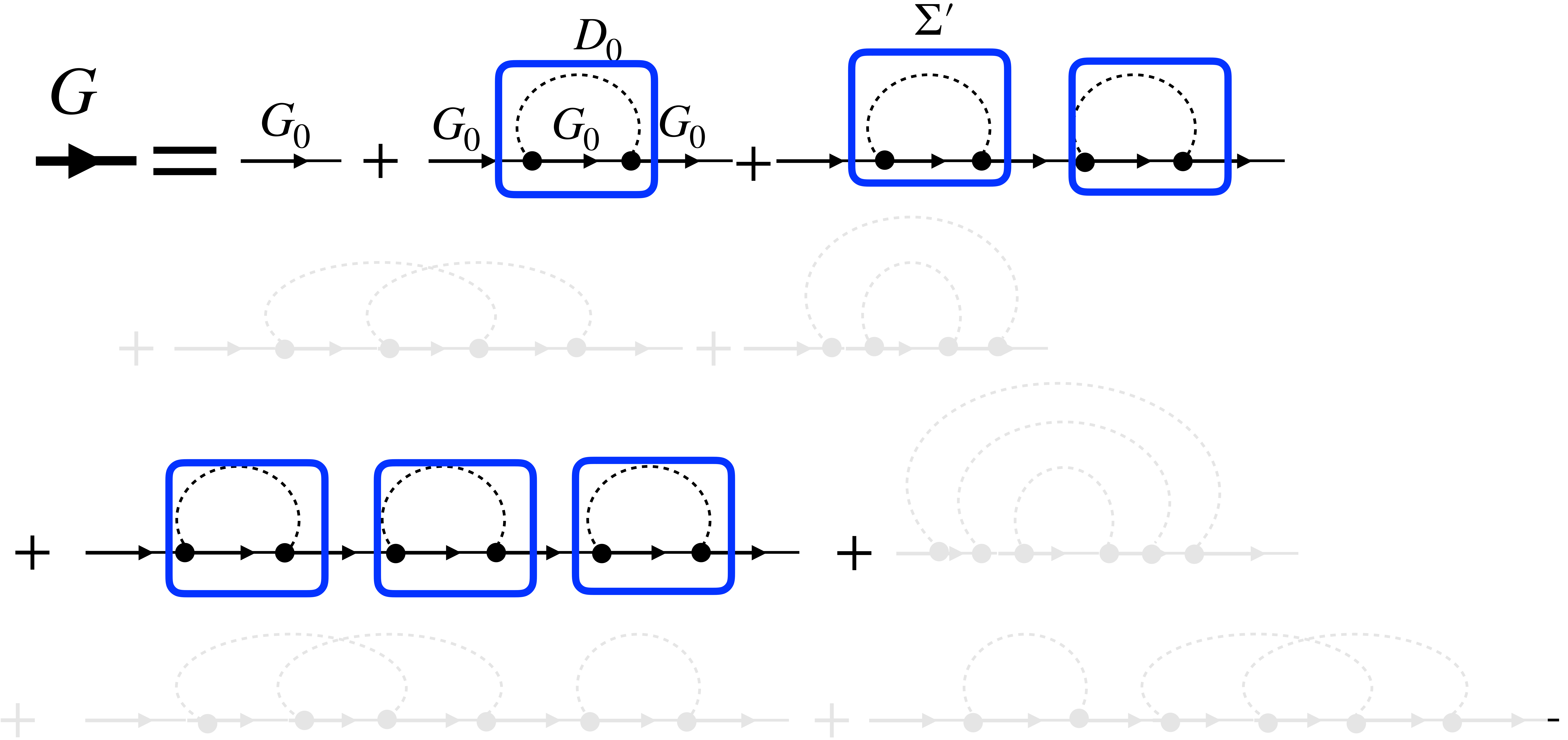
Time domain:

$$-\int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 \sum_{\beta\beta'\lambda} |M_{\beta\beta'}|^2 G_0(\beta, t, t_1) G_0(\beta', t_1, t_2) D_0(\lambda, t_1, t_2) G_0(\beta, t_2, t)$$

Energy domain:

$$-G_0(\omega, \beta) \sum_{\beta,\beta'} |M_{\beta,\beta'}|^2 \int \frac{d\omega'}{2\pi} D(\omega') G_0(\omega' - \omega) G_0(\omega, \beta) = \boxed{G_0(\omega)\Sigma'(\omega)G_0(\omega)}$$

GW correction

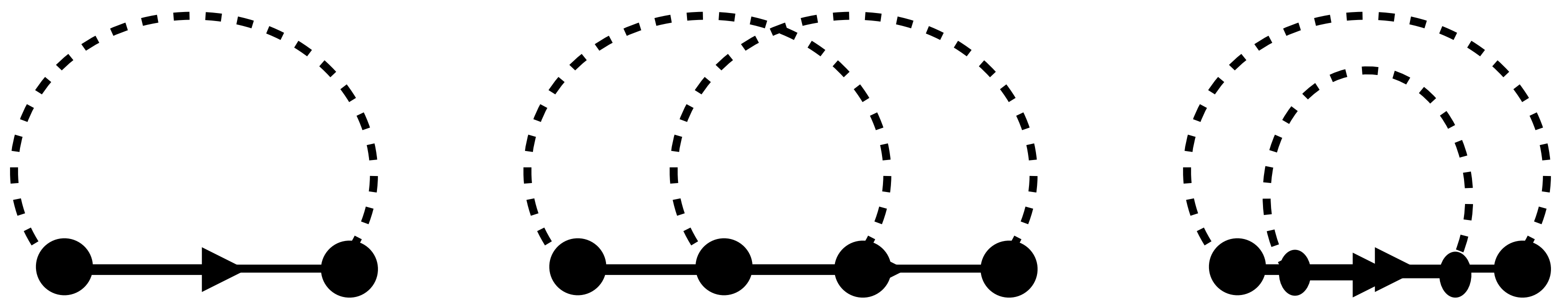


Dyson equation

$$G = G_0 + G_0 \Sigma G_0 + G_0 \Sigma G_0 \Sigma G_0 + G_0 \Sigma G_0 \Sigma G_0 \Sigma G_0 + \dots$$

$$G = G_0 + G_0 \Sigma G$$

$$\Sigma$$



Sum of all irreducible diagrams

Second order truncation

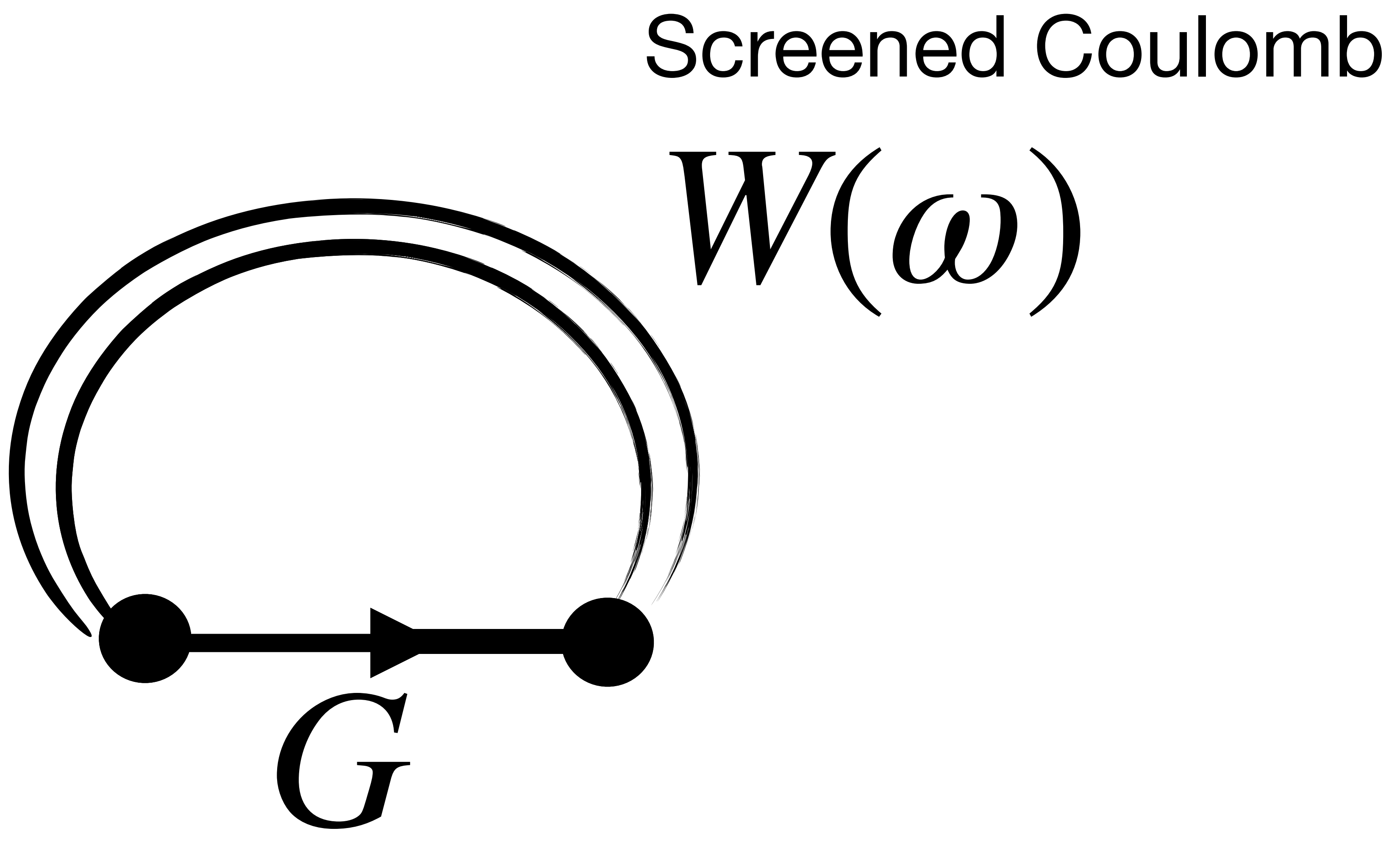
$$G = G_0 + G_0 \Sigma^{(2)} G_0$$

All orders for some diagrams

$$G = \frac{G_0}{1 - G_0 \Sigma^{(2)}}$$

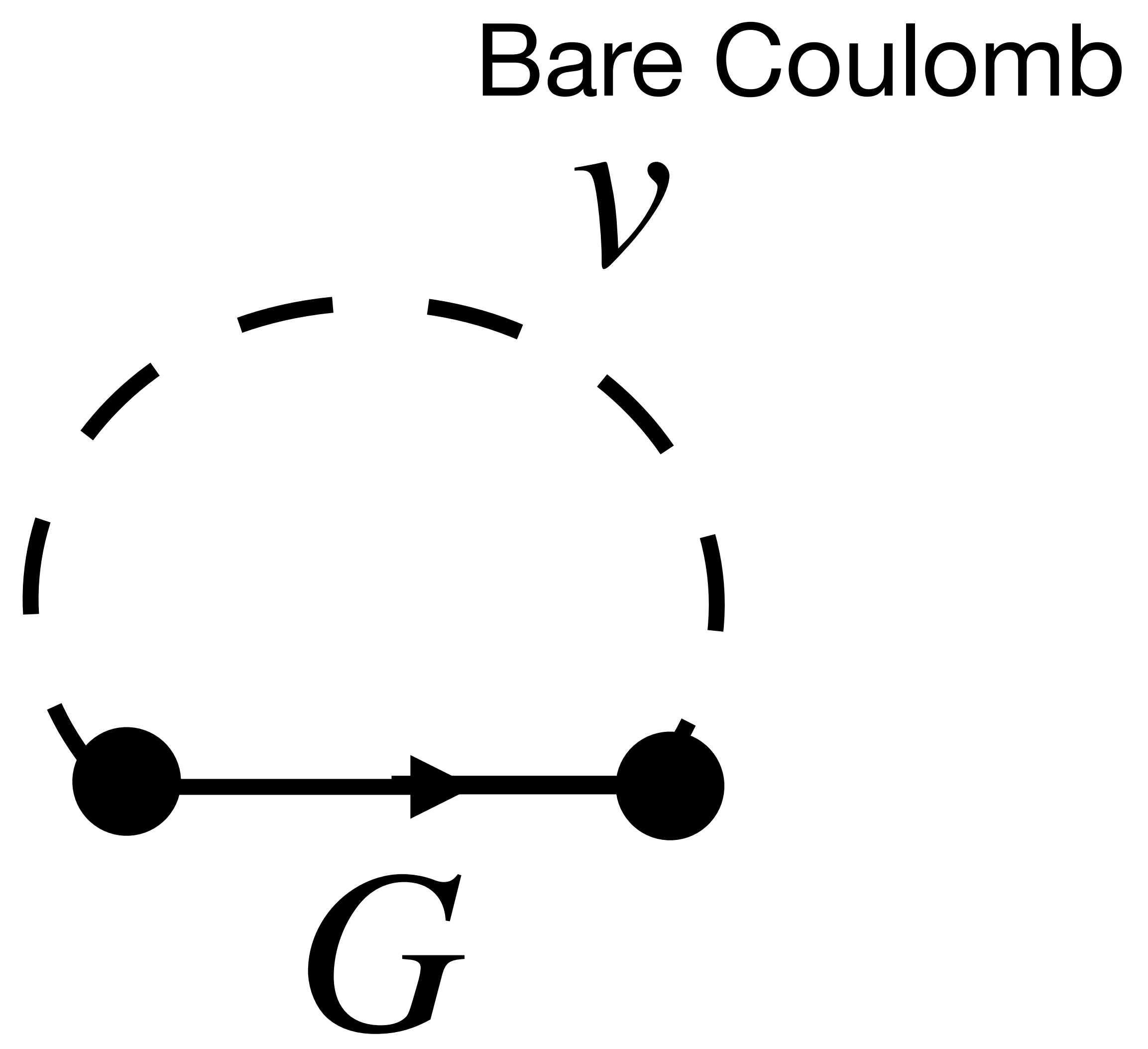
GW approximation

$$\Sigma(r, r', \omega) \sim i \int G(r, r, \omega' - \omega) W(r, r', \omega) d\omega'$$



Hartree-Fock

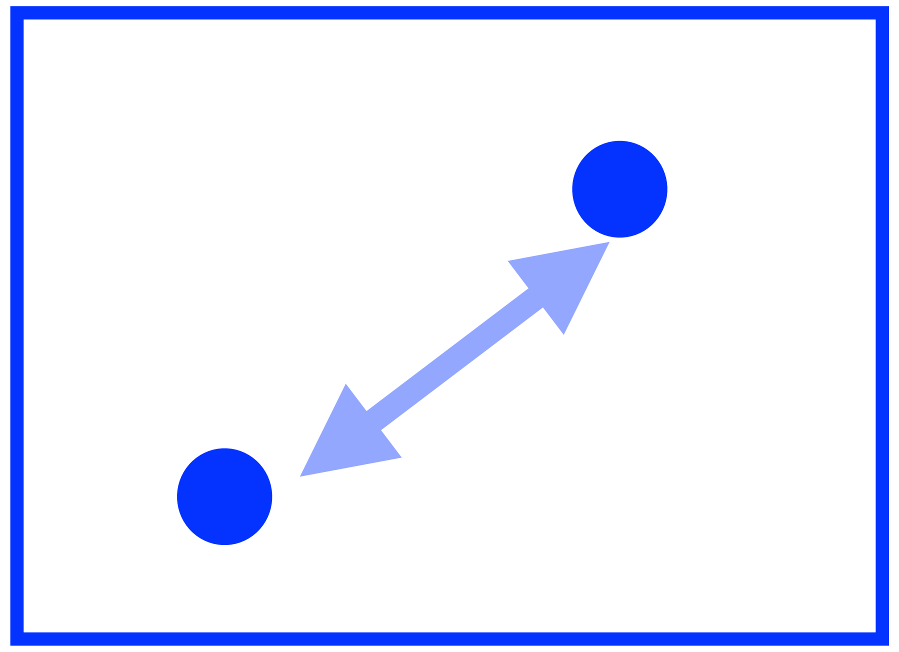
$$\Sigma(r, r') \sim i \int G(r, r, \omega') v(r, r') d\omega'$$



Screened Coulomb interaction

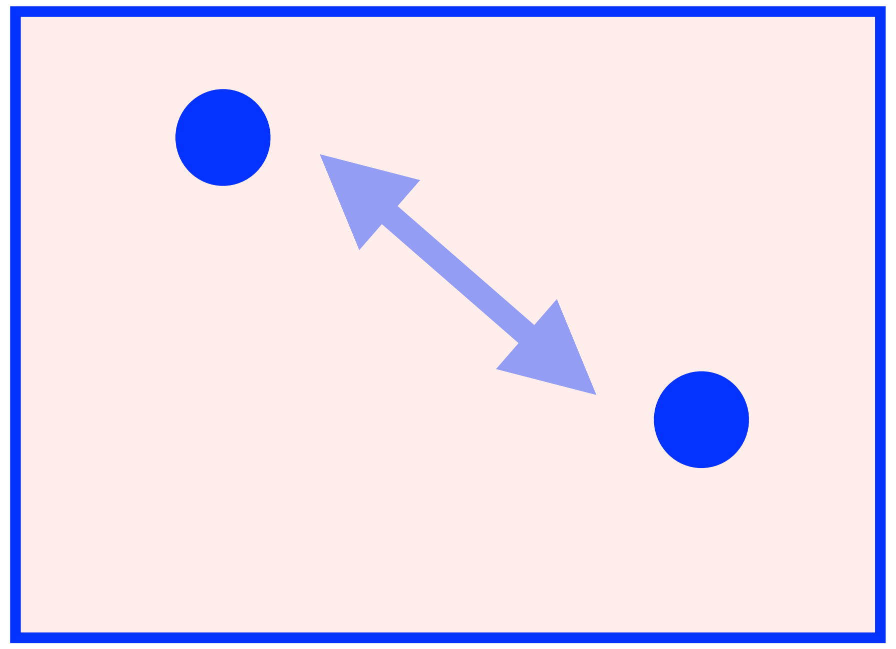
Interaction in vacuum

$$v(r,r') \sim \frac{1}{4\pi\epsilon_0}\frac{1}{|r'-r|}$$



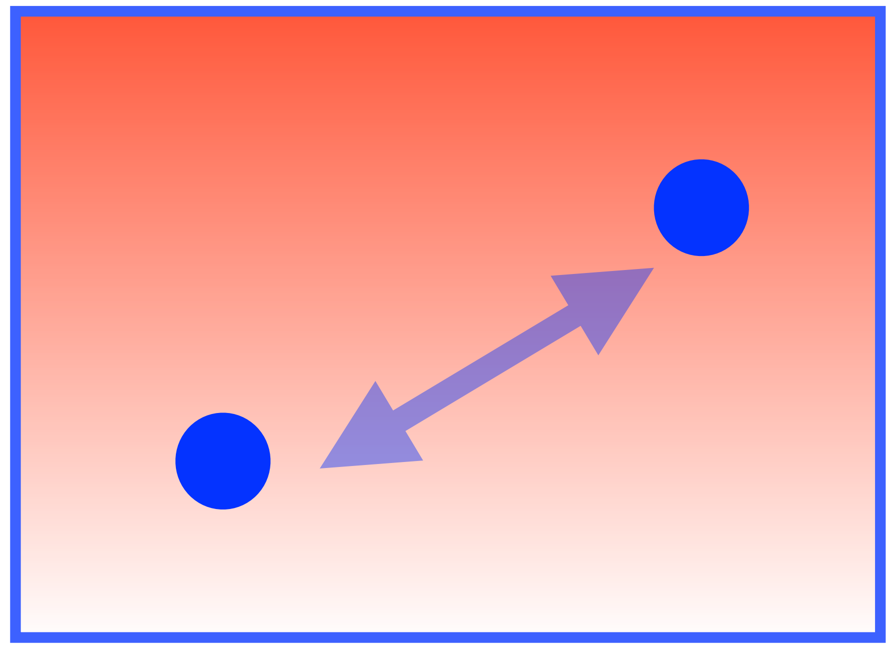
Constant screening

$$W(r,r') \sim \frac{1}{4\pi\epsilon_0}\frac{\epsilon_r^{-1}}{|r'-r|}$$

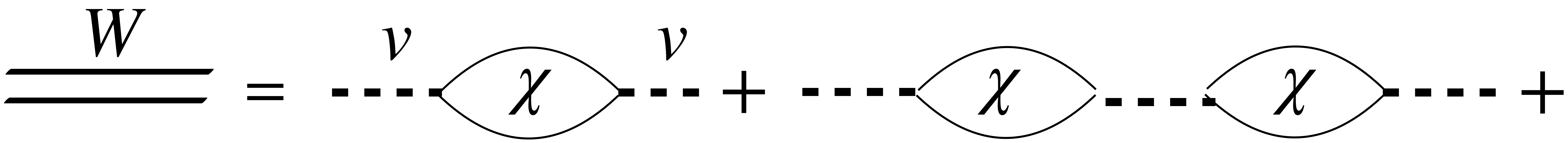


Dynamic screening

$$W(r,r',\omega) \sim \frac{1}{4\pi\epsilon_0}\int\frac{\epsilon^{-1}(r,r',\omega)}{|r'-r_1|}dr_1$$

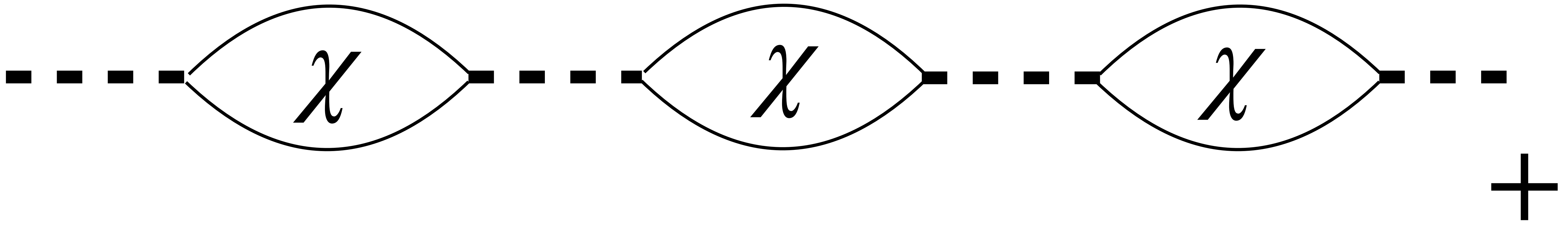


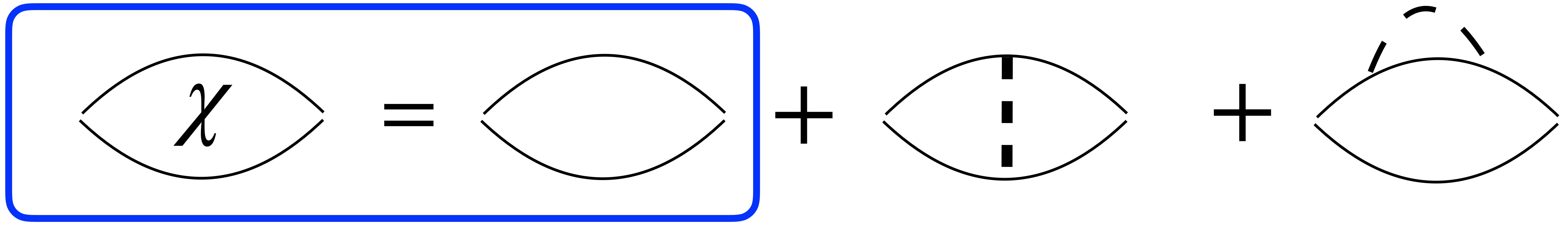
Random Phase Approximation



$$W = \frac{v}{1 - v\chi}$$

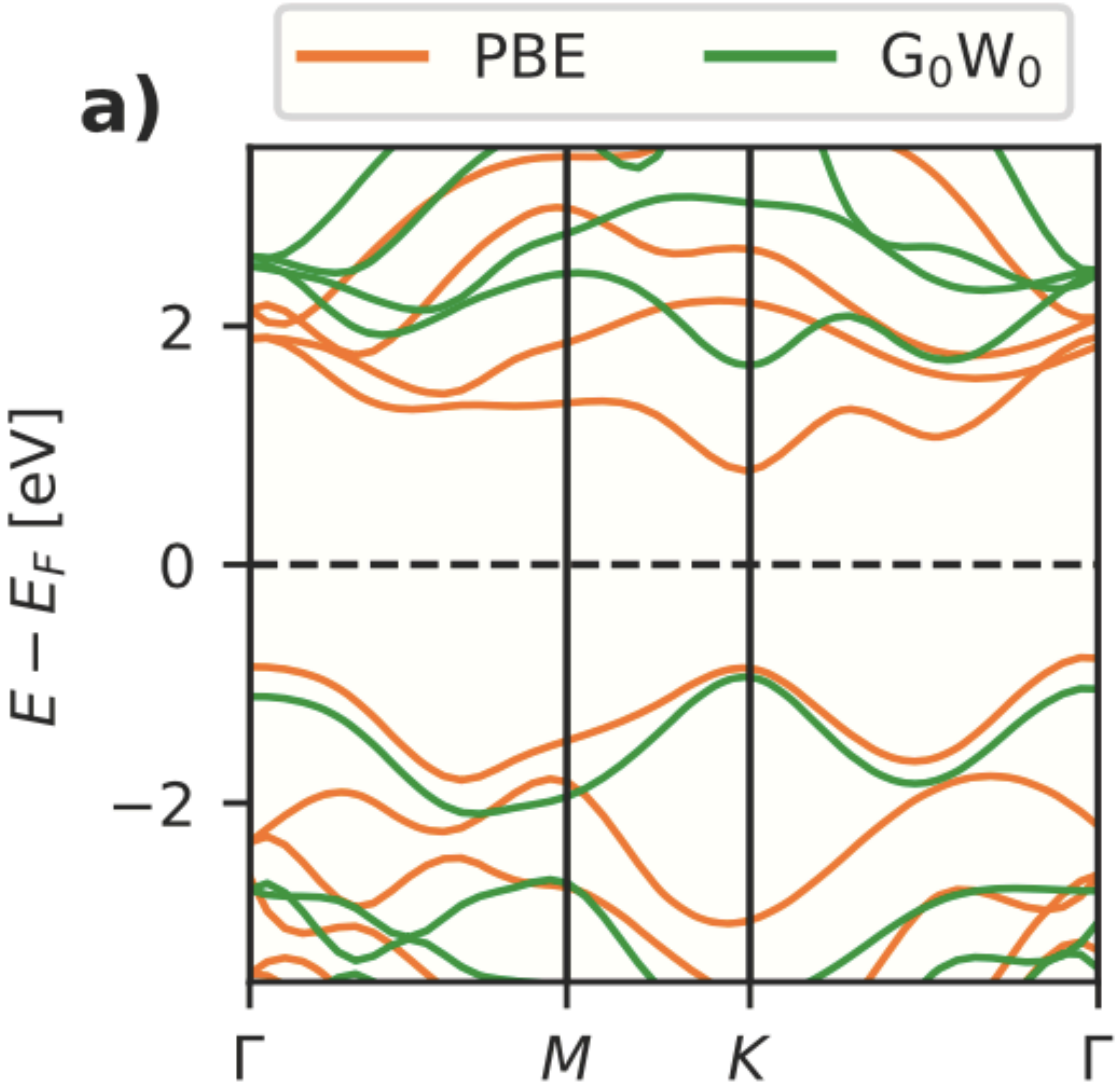
ϵ_{RPA}



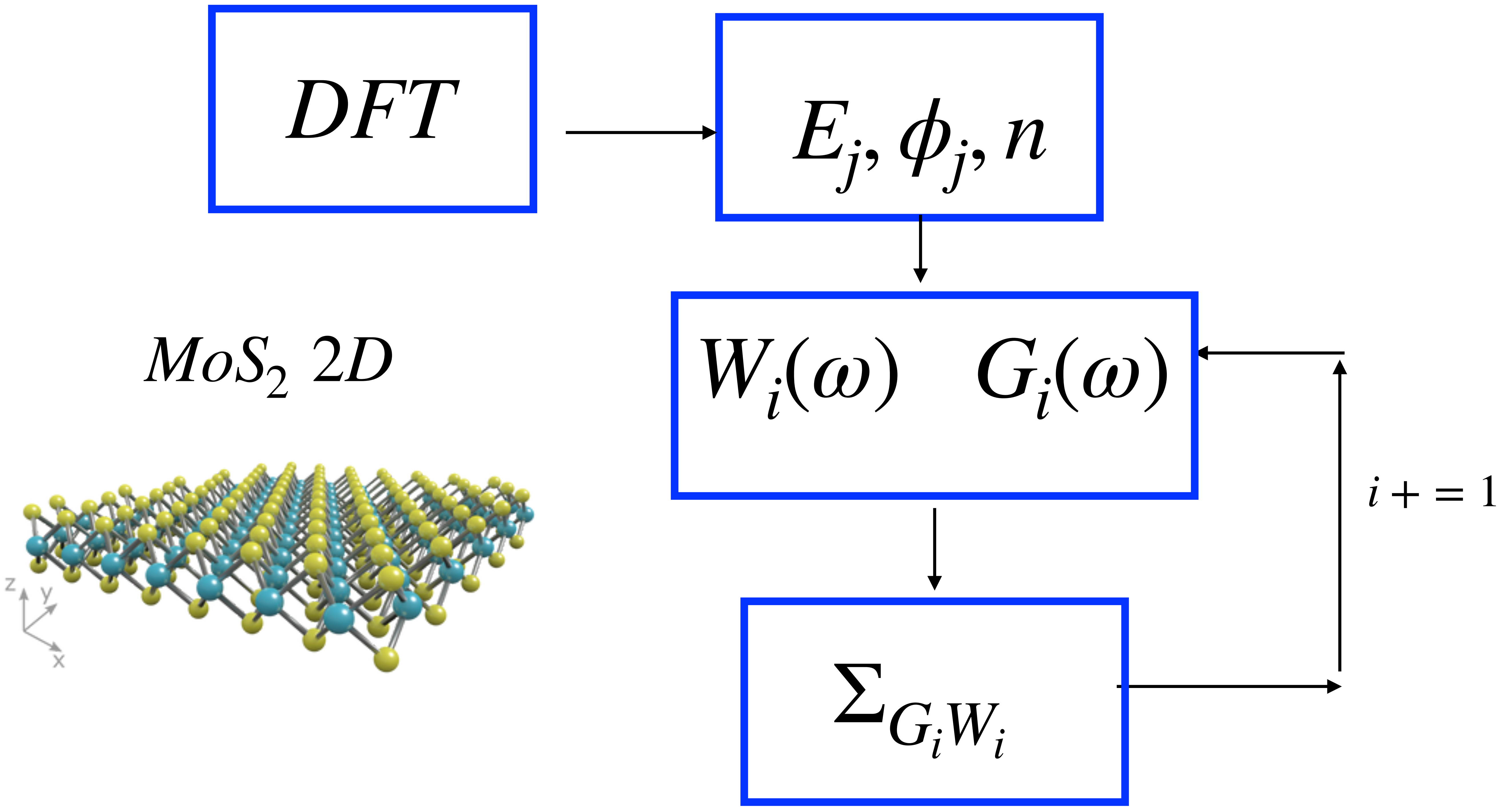


$$\chi_{RPA}(t -' t) = -iG(t - t')G(t' - t)$$

Band structure corrections

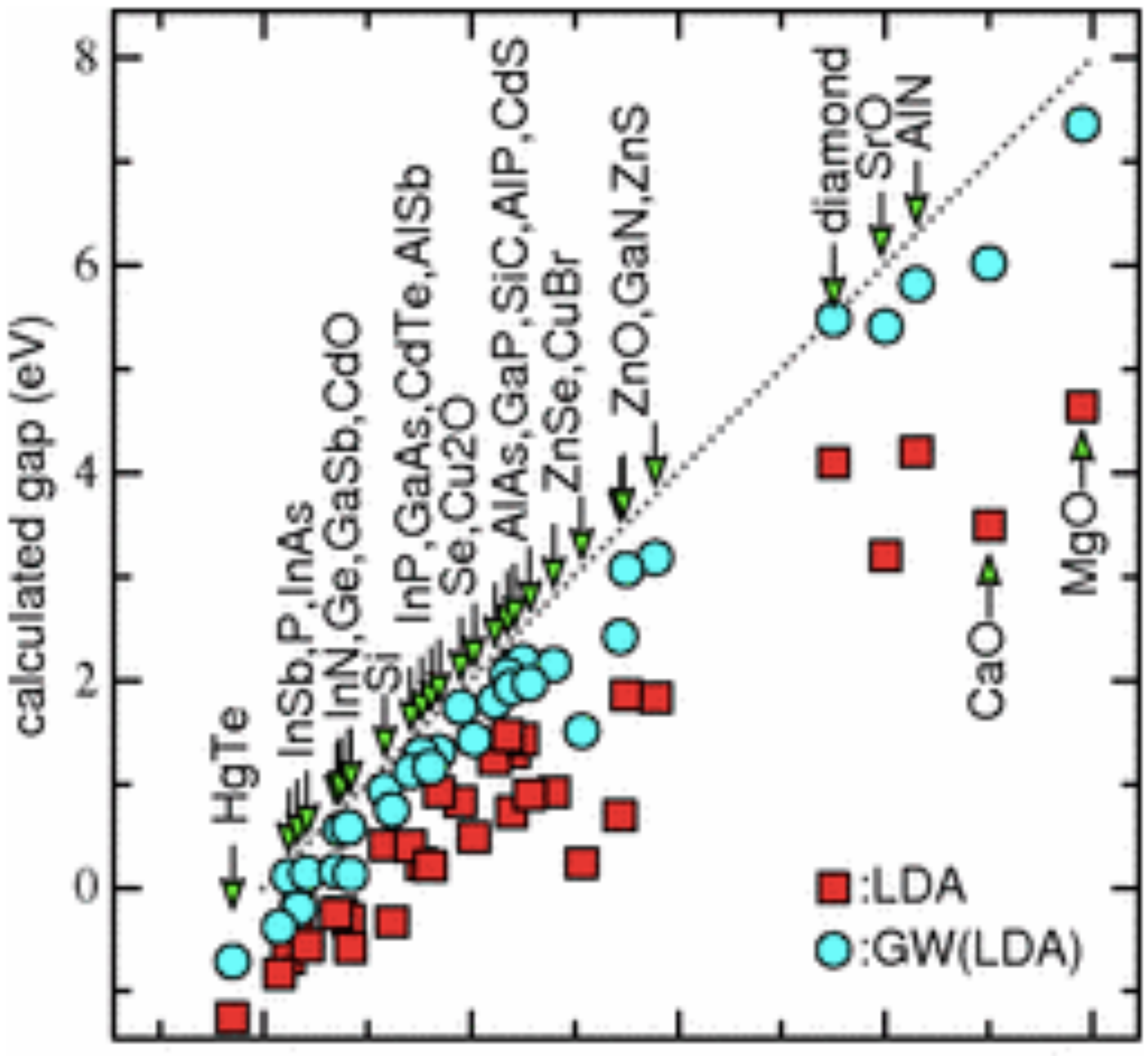


Knøsgaard et al. NatCom 2022

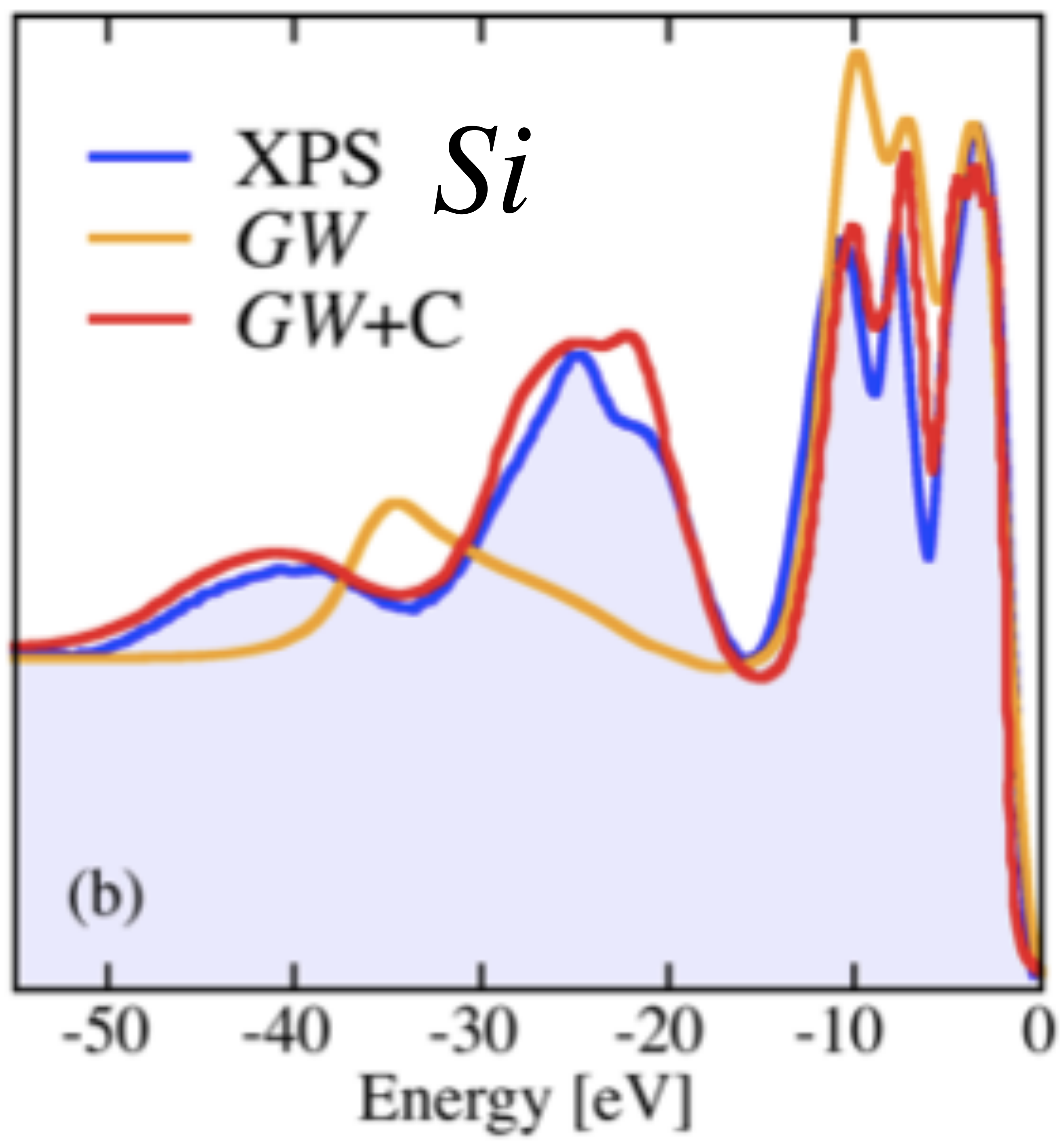


$$E^i_{qp} = E^i_{DFT} + E^i_{GW}$$

GW

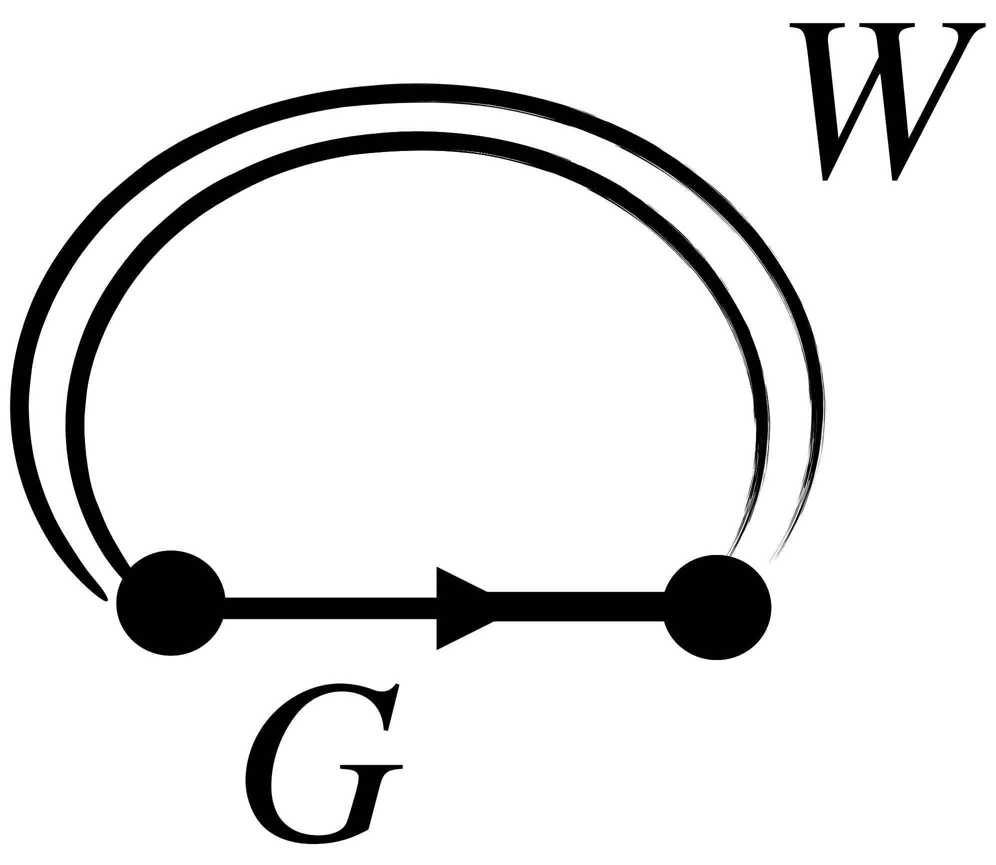


van Schilfgaarde PRL 2008

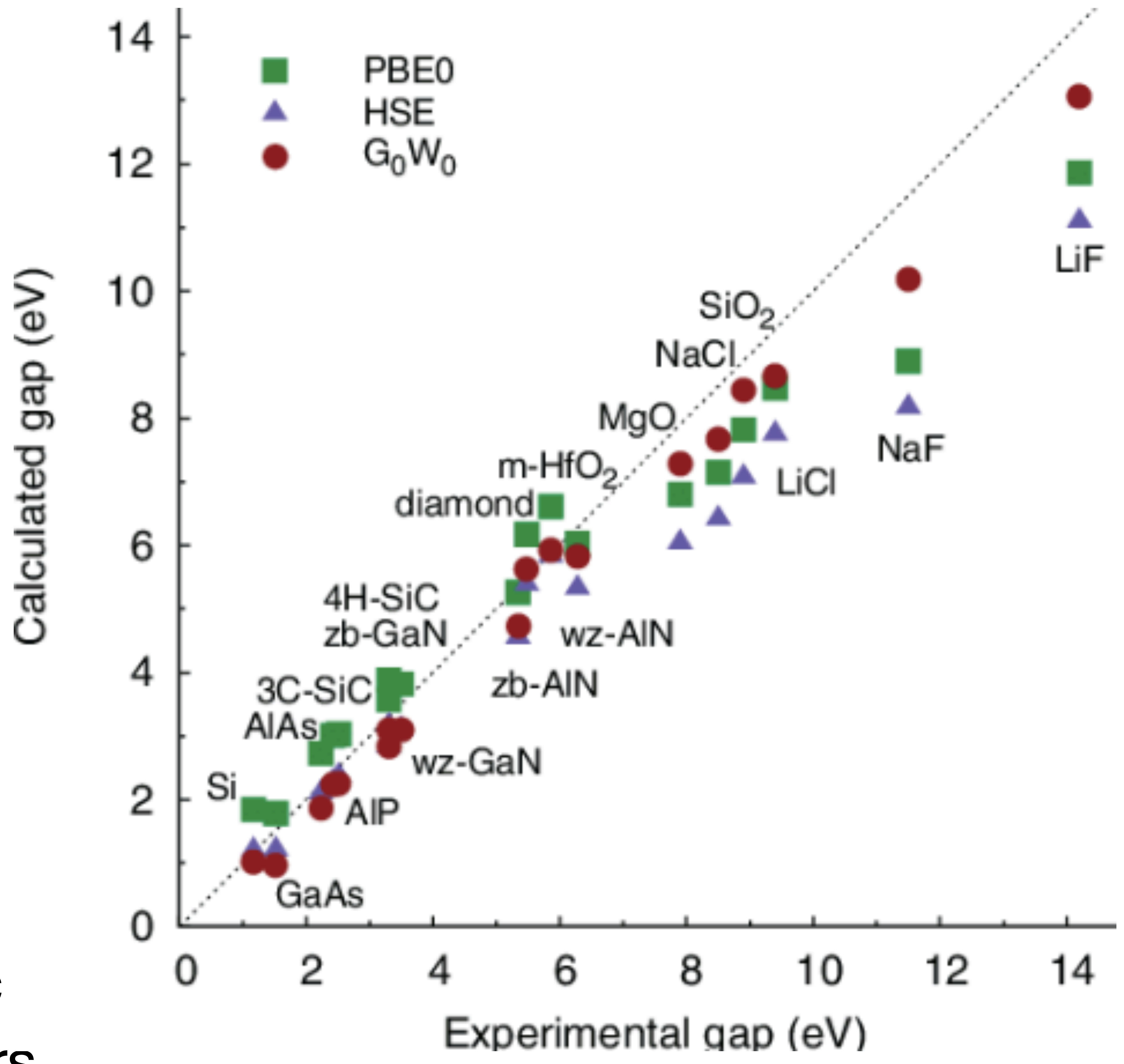


Caruso et al. 2018

- Reasonable gap
- Problems with dynamical contributions

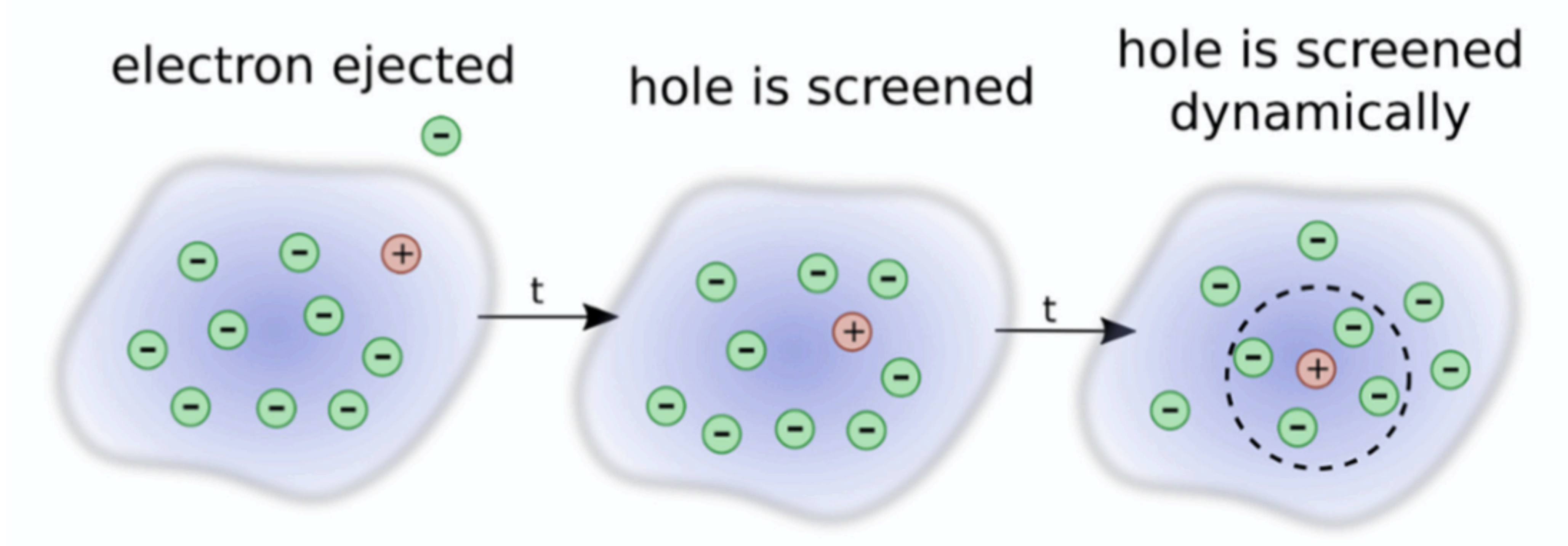


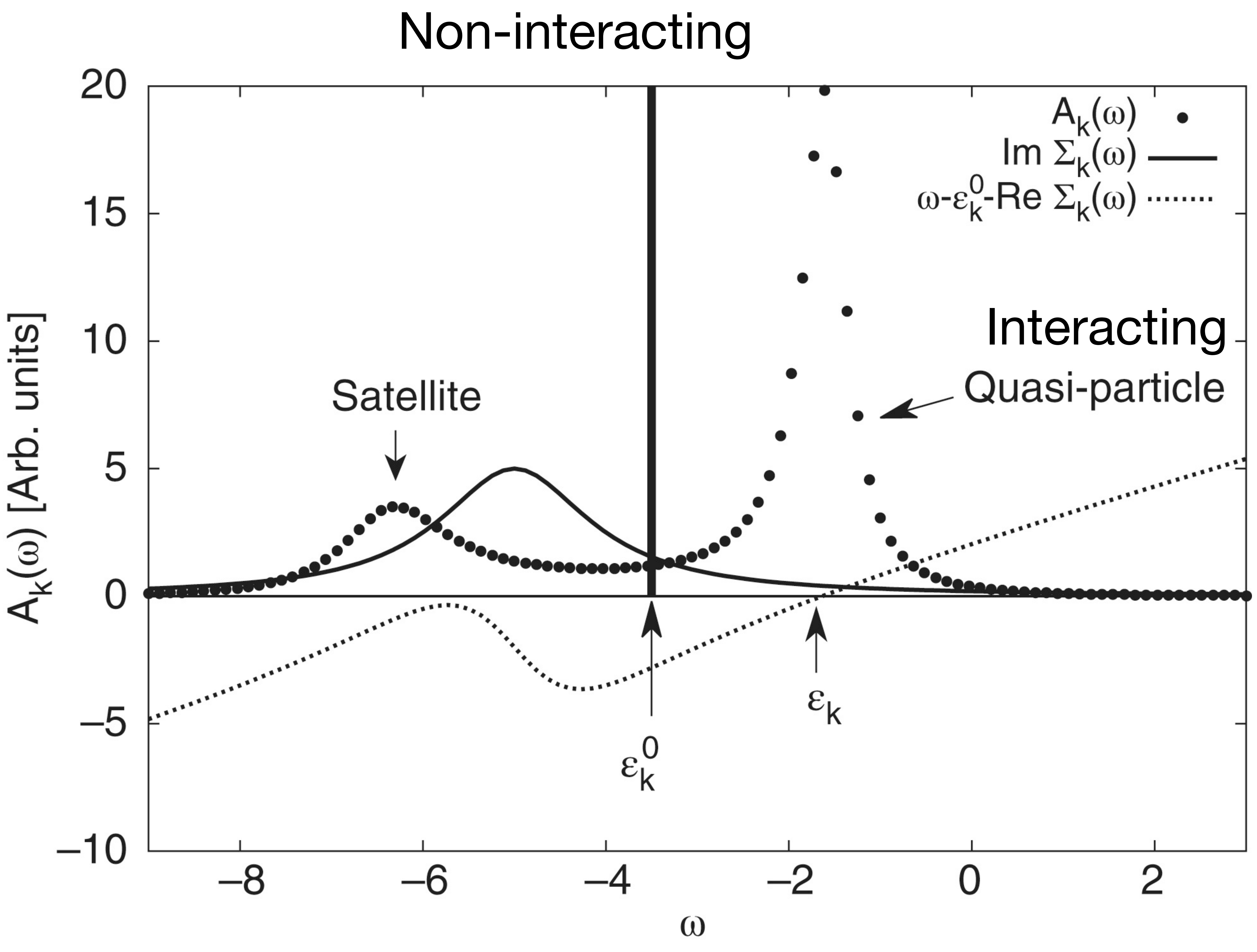
- Better then LDA/GGA
- Better then HF
- More consistent then hybrids (and some times better)
- But also more computationally expensive
- Different flavours G0W0, scGW, evGW, etc
- Results varies (overestimations) wrt flavours



Chen et al. PRB 2012

Quasiparticles

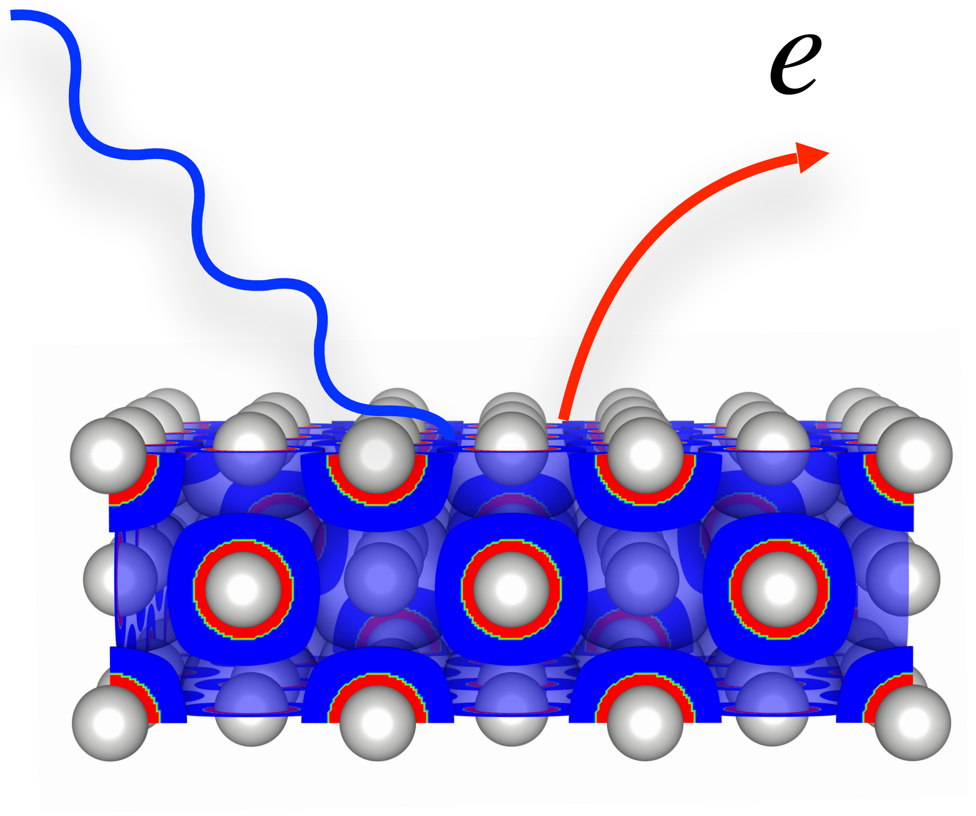


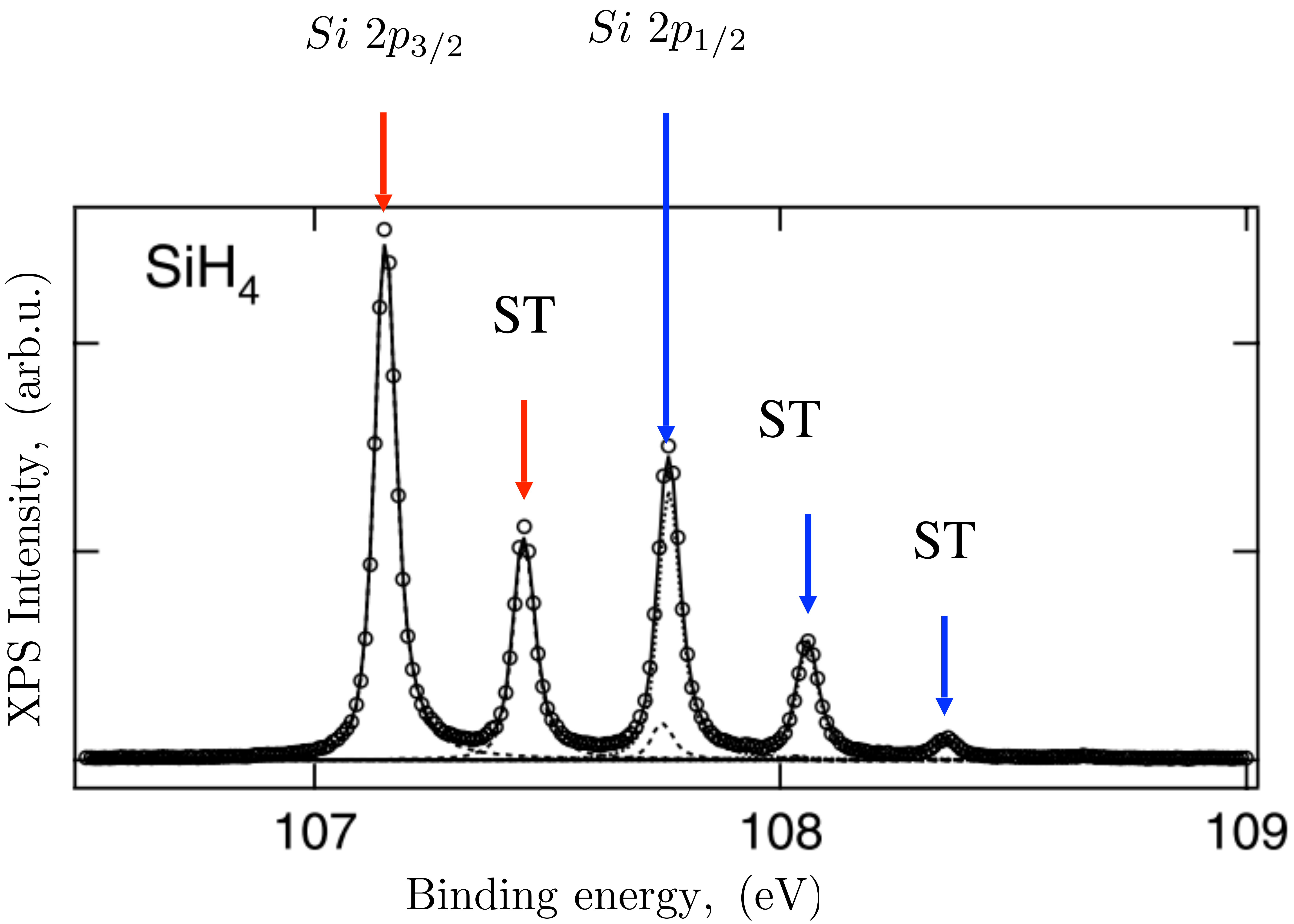


Reining ComMolSc 2017

Charged excitations / XPS

X-ray Photoemission Spectroscopy (XPS)





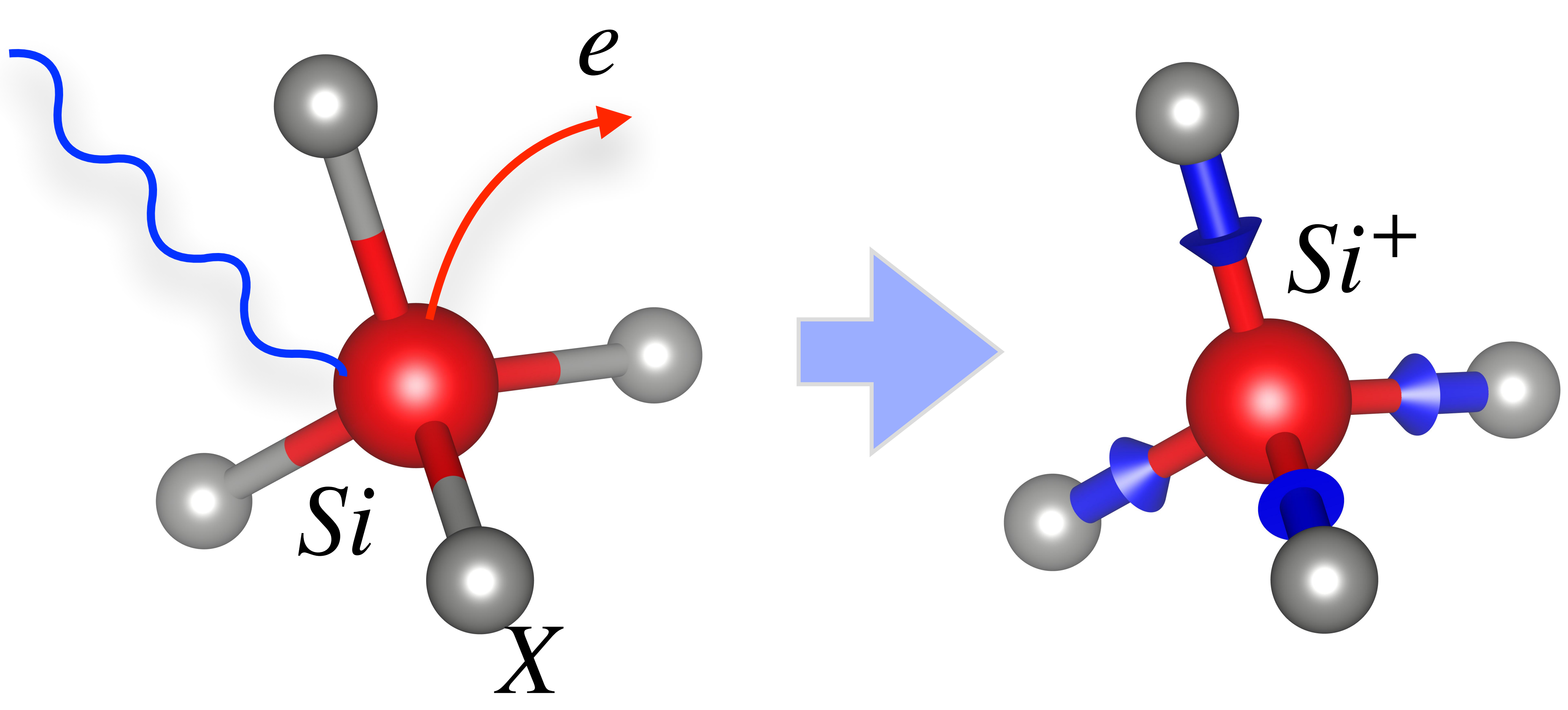
Bound state - continuum transitions

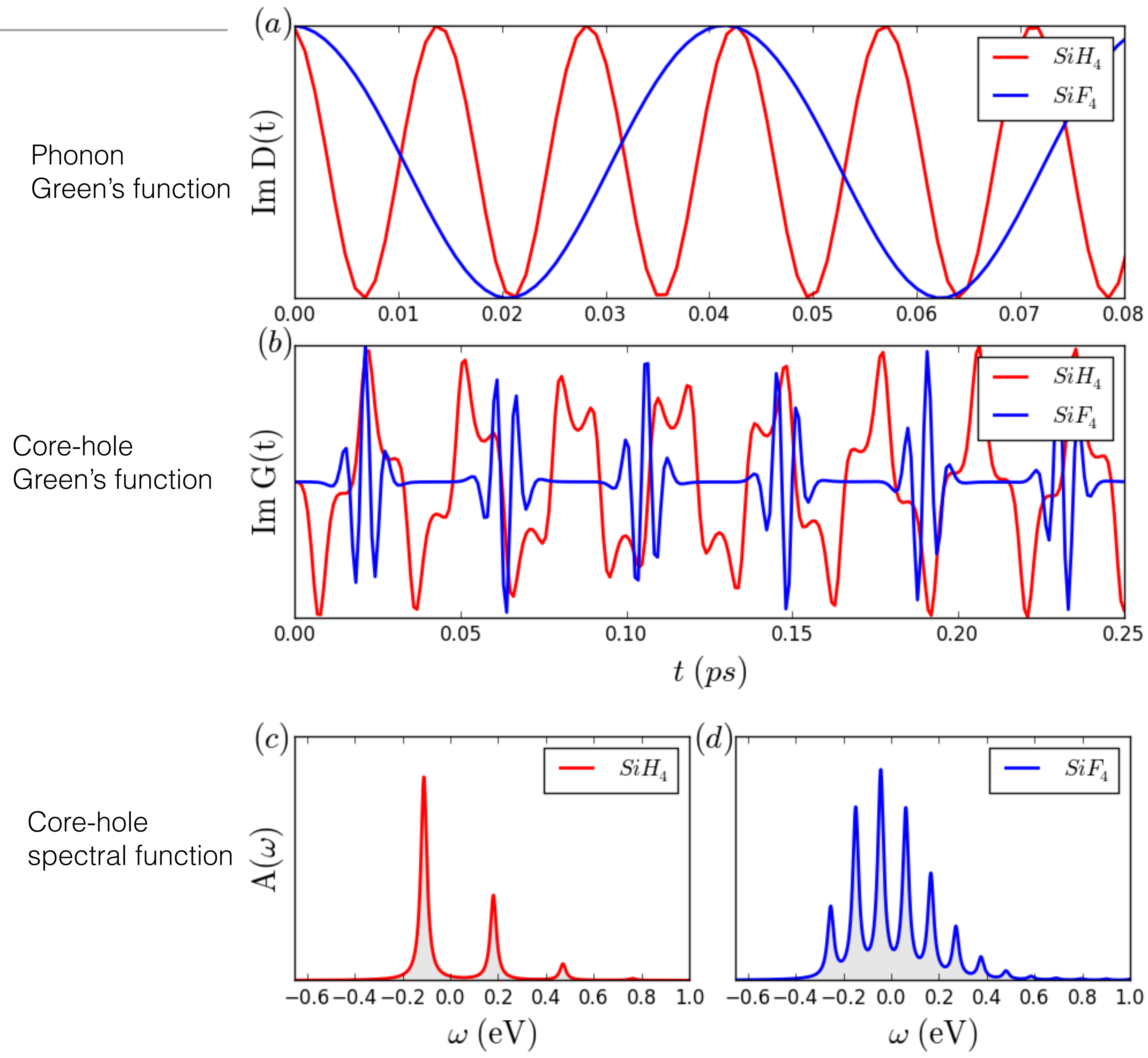
First-order process in X-ray-matter interaction

$$J_\alpha(\omega) \approx |d_\alpha|^2 \mathrm{Im}\ G_\alpha(\omega) \sim \mathrm{oc.DOS}$$

Thomas et al. Phys. Rev. Lett. (2002)

Response function



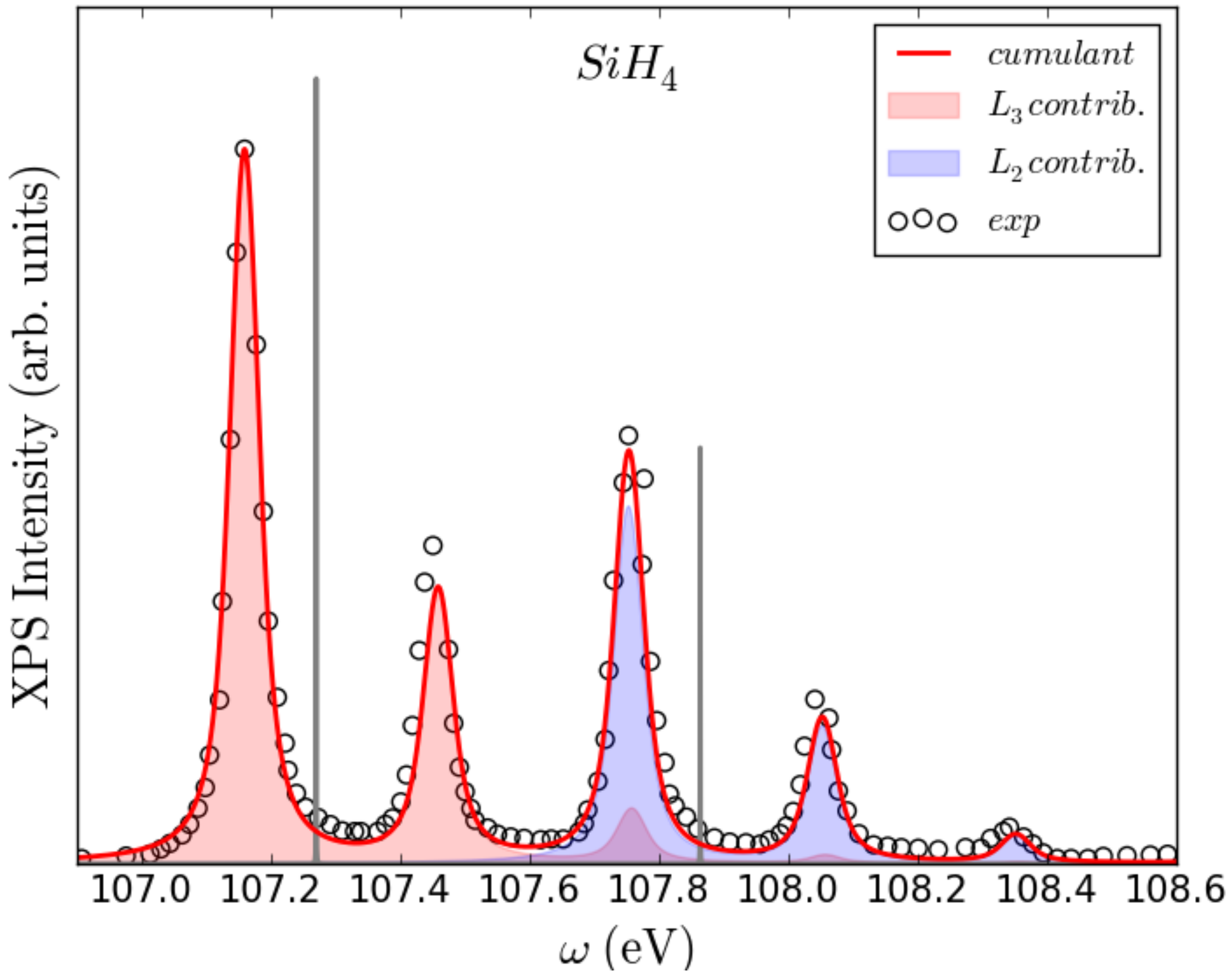


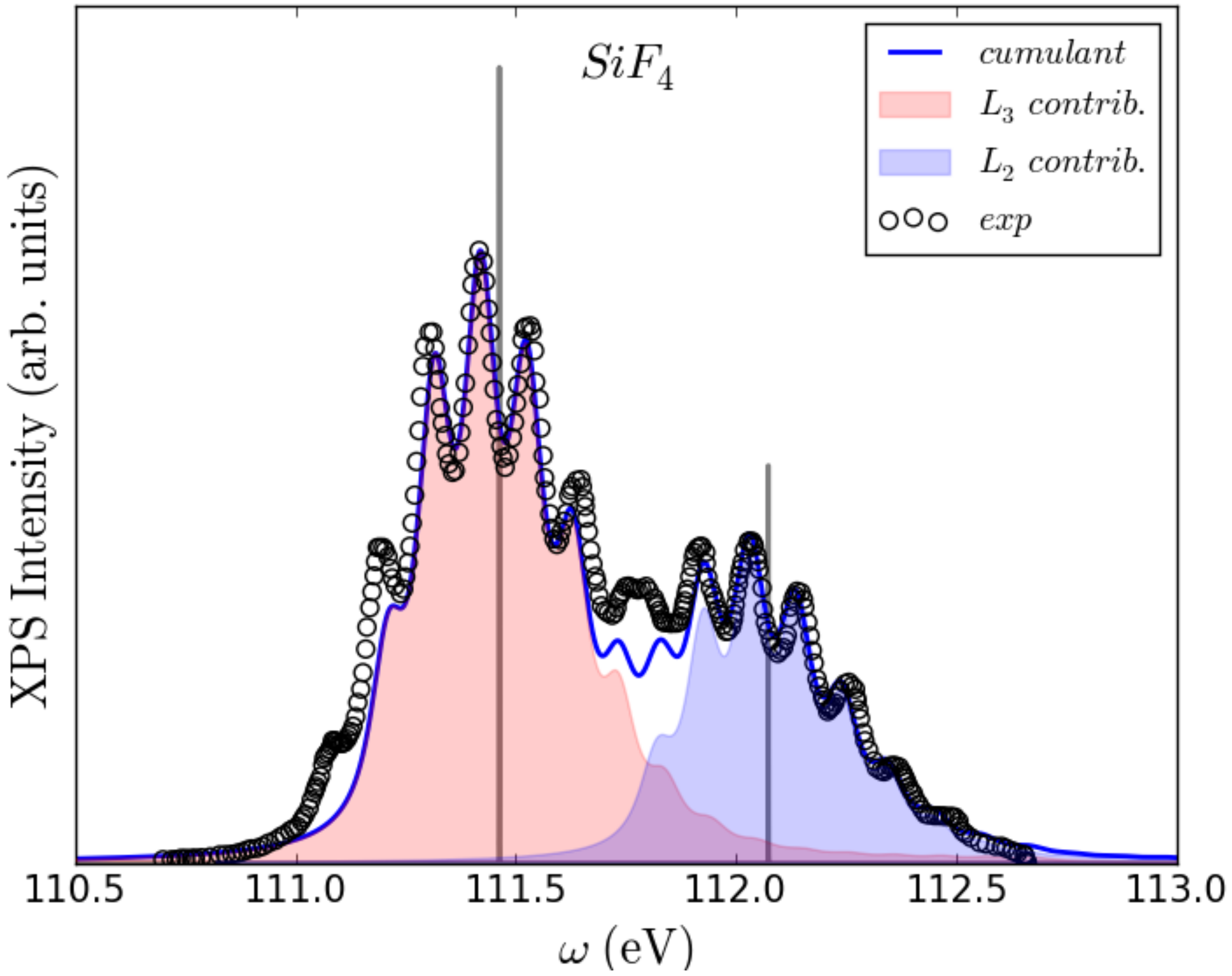
$$\chi(t) \longrightarrow C_2(t) \longrightarrow G(t) = G_0(t)e^{C(t)}$$

- Adiabatic calculation within the ab-initio MD
- Phonon Green's function from displacement autocorrelation function
- Coupling constant - from real space forces

Geondzhian and Gilmore PRB (2018)

Charge excitations : Results



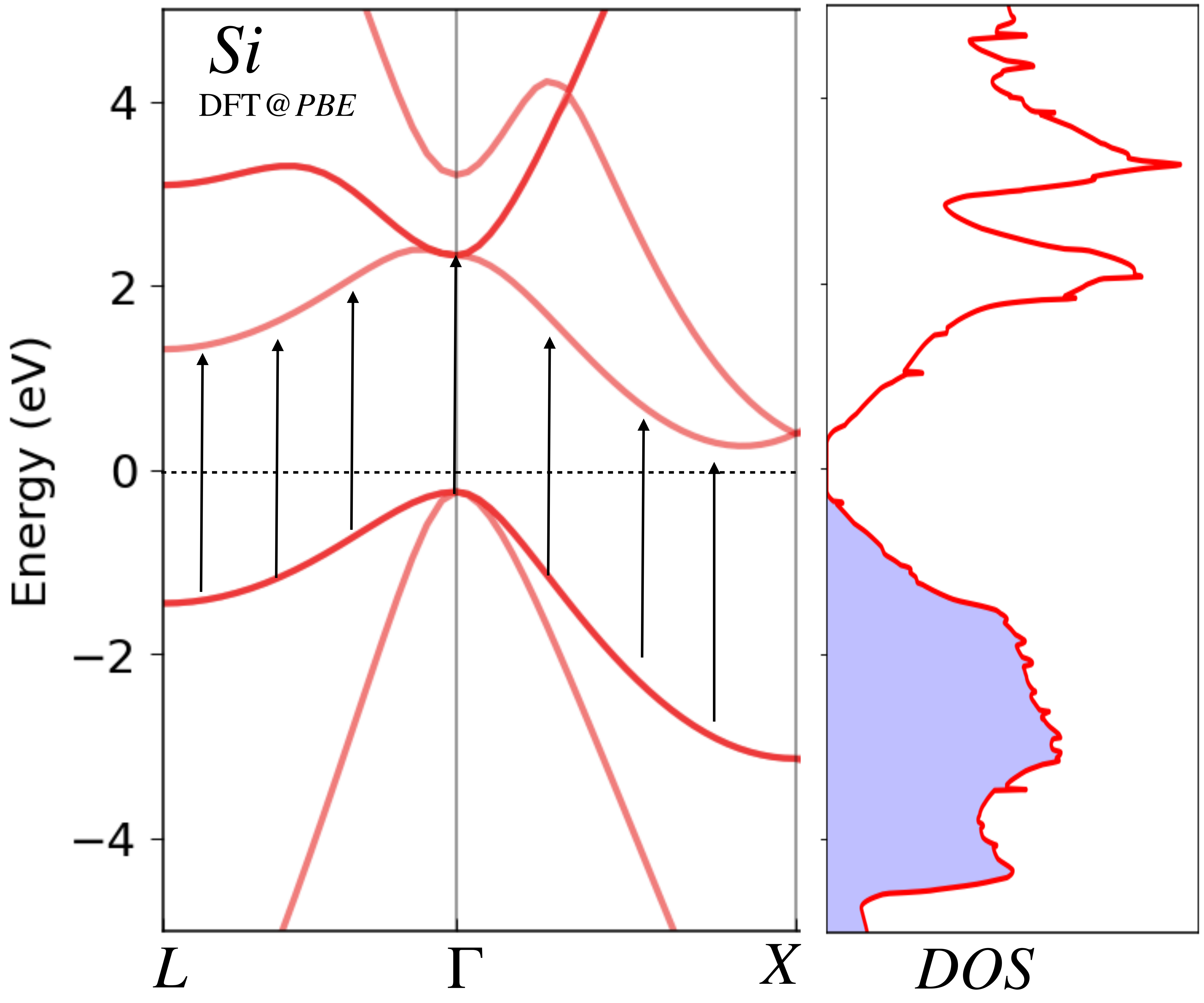


- **Cumulant** ansatz works well reproducing phonon side-bands in core-excitations spectra
- Directly applicable to crystalline materials

Calc: Geondzhian and Gilmore PRB (2018)

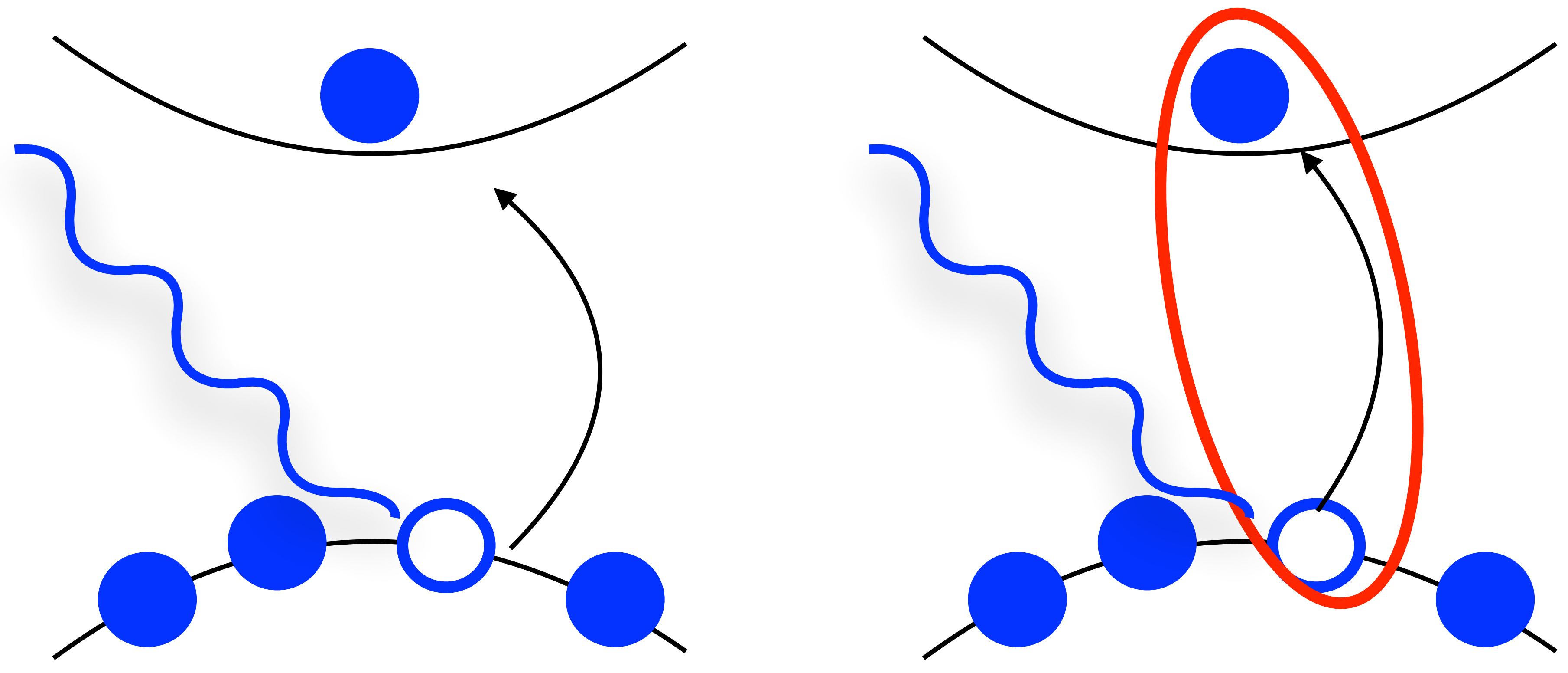
Exp: Thomas et al. Phys. Rev. Lett. (2002)

What about other excited states?



Independent particles

interacting particles

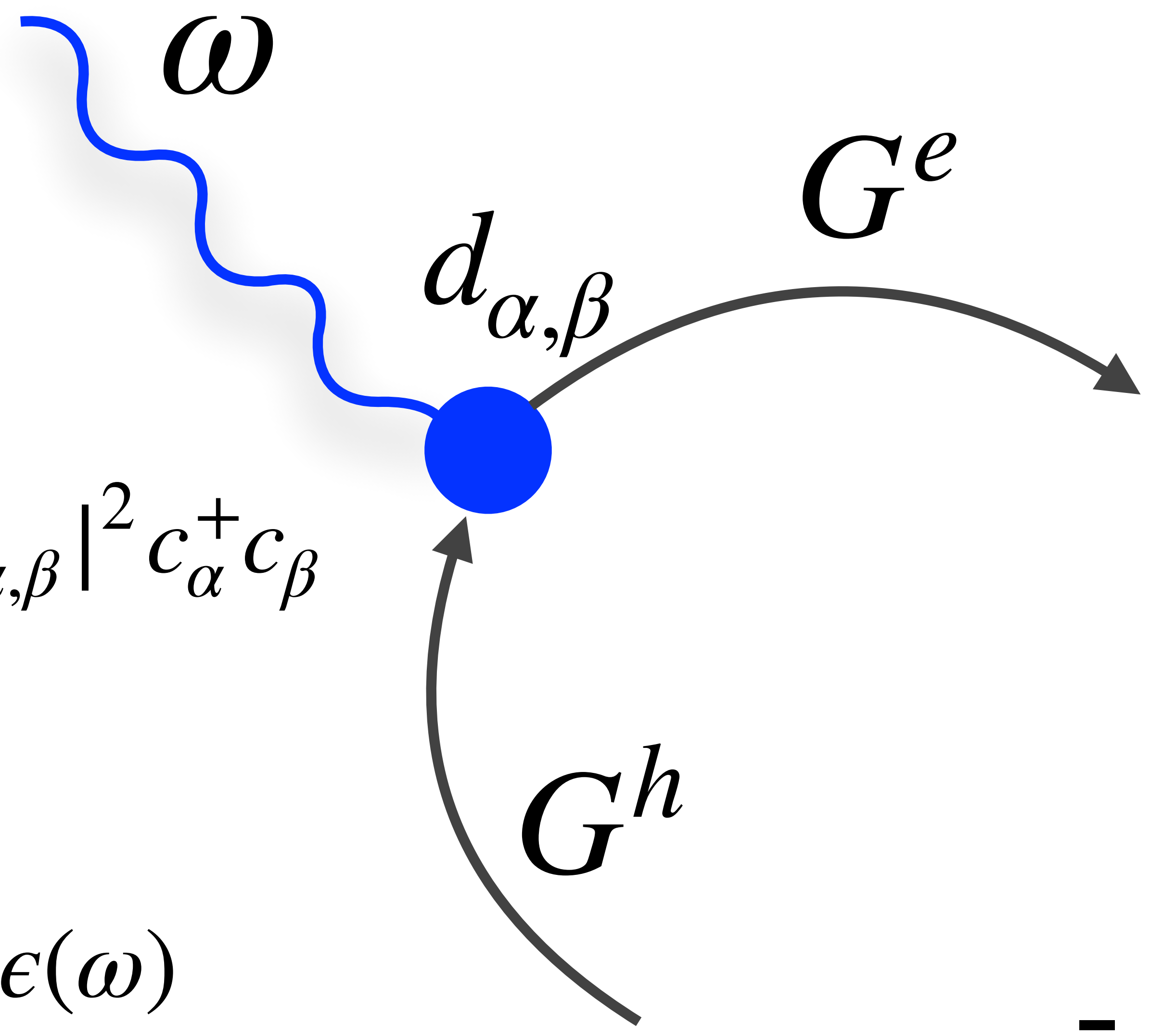


$$E^{o}_{DFT} > E^{o}_{ex}$$

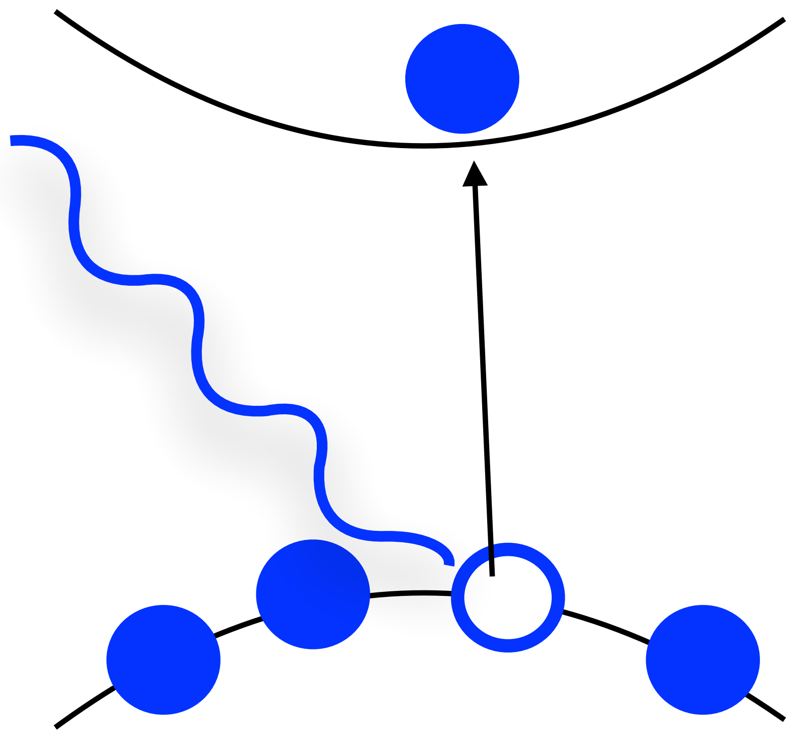
Absorption process

Fermi's Golden rule

$$W_{fi}(\omega) \sim |<\Psi_f|\hat{V}|\Psi_i>|^2 \delta(\omega - (E_f - E_i))$$

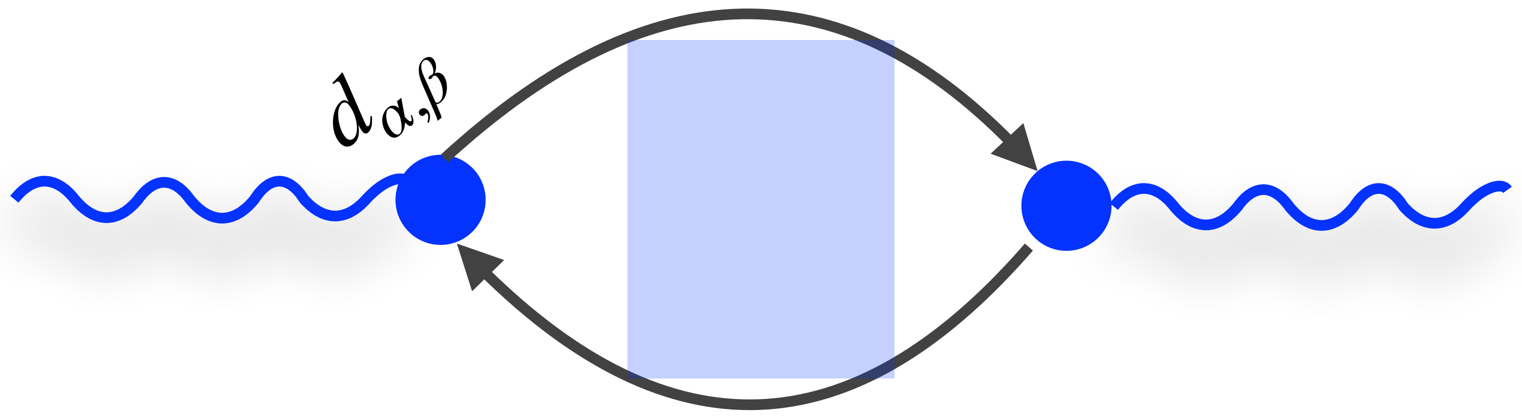


$$\hat{V} \sim \sum_{\alpha,\beta} |d_{\alpha,\beta}|^2 c_\alpha^+ c_\beta$$

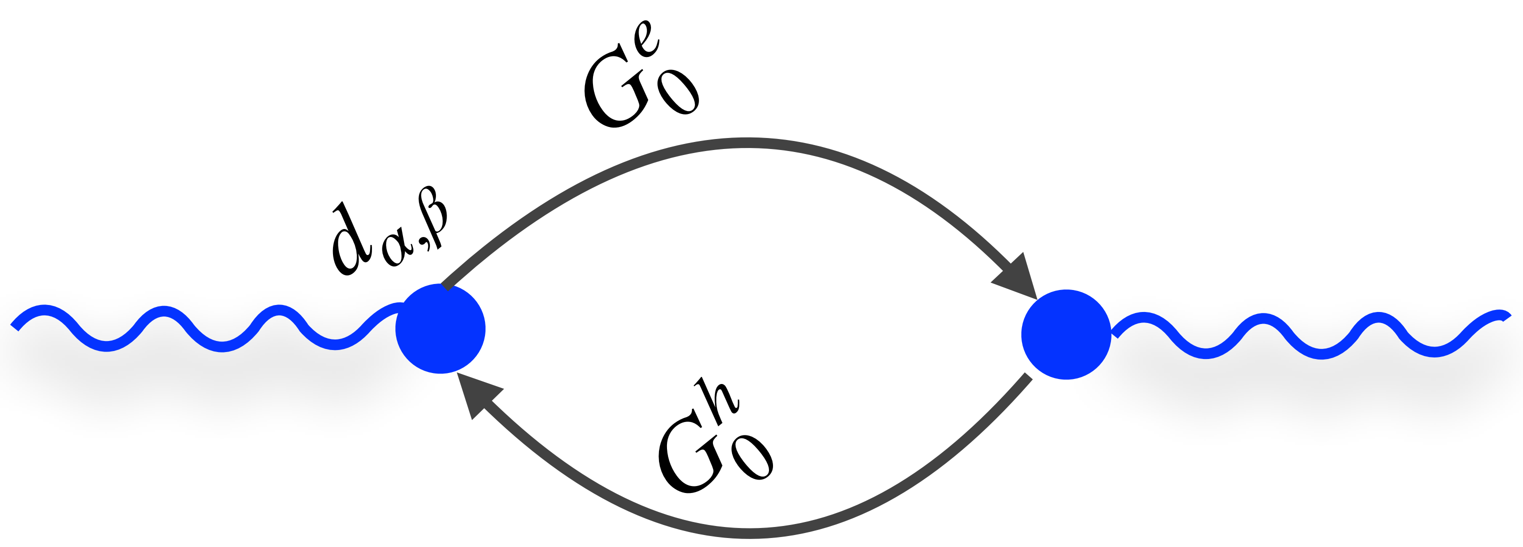


$$\sigma(\omega) \sim \sum_f |<\Psi_f|\hat{V}|\Psi_i>|^2 \delta(\omega - (E_f - E_i)) \sim Im\epsilon(\omega)$$

- photon created e-h pair
- e-h pair - propagated
- e-h pair recombined

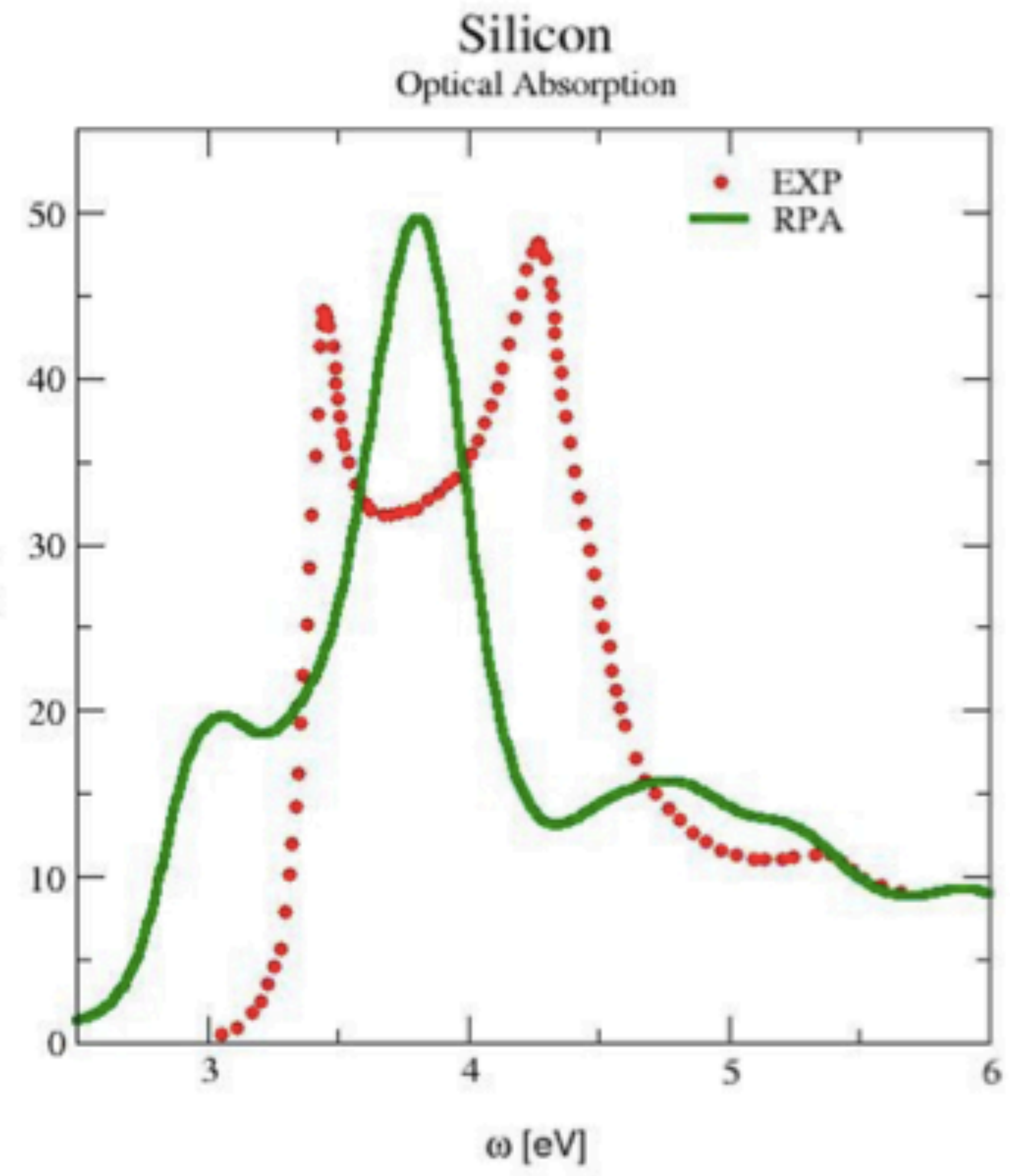


Independent particles



$$L(t,t') = G_0^e(t,t')G_0^h(t',t)$$

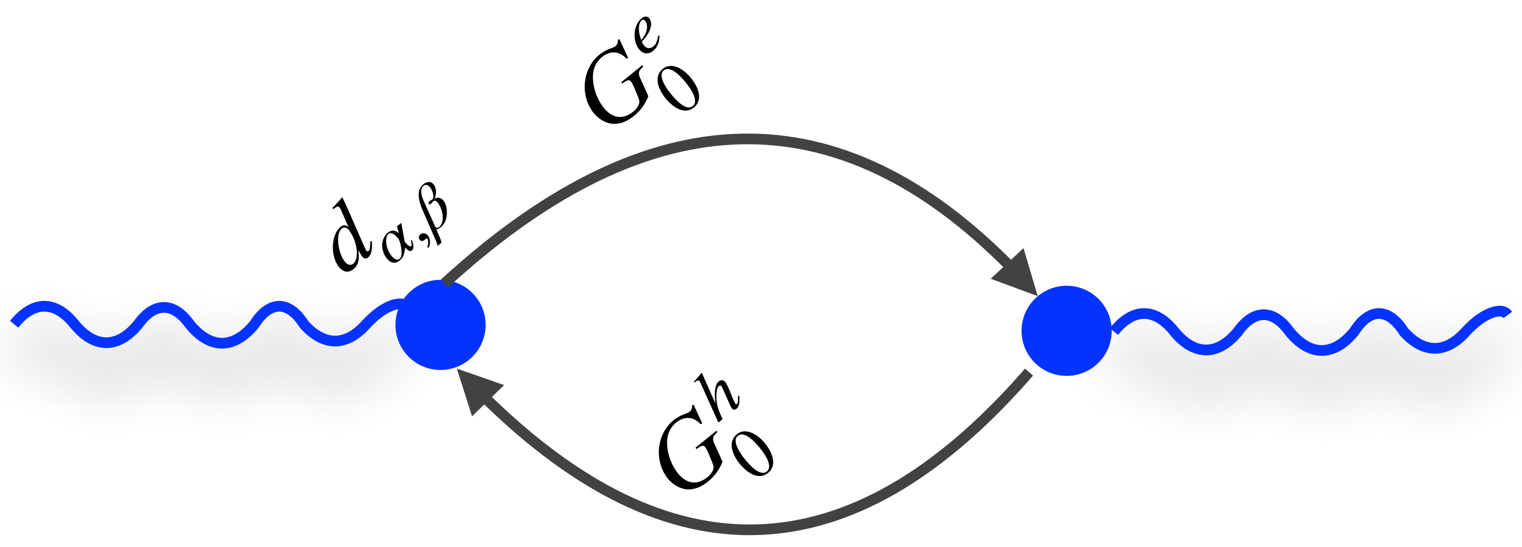
Non-interacting picture fails



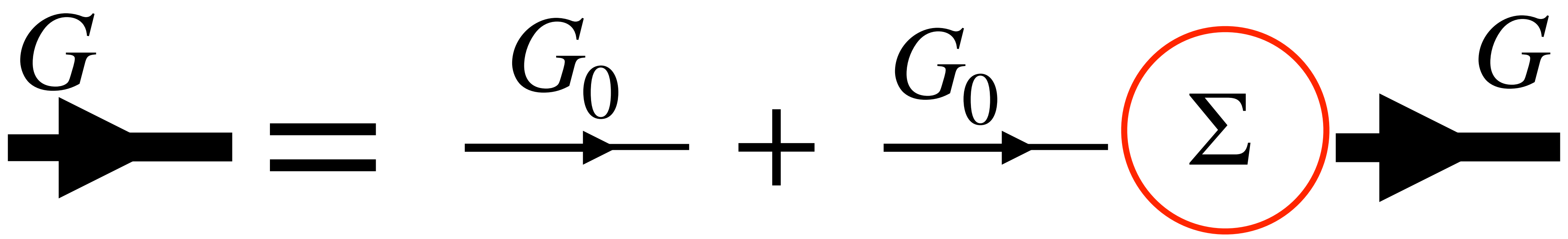
adapted from Onida et al. PR 2002

Dressed Green’s function

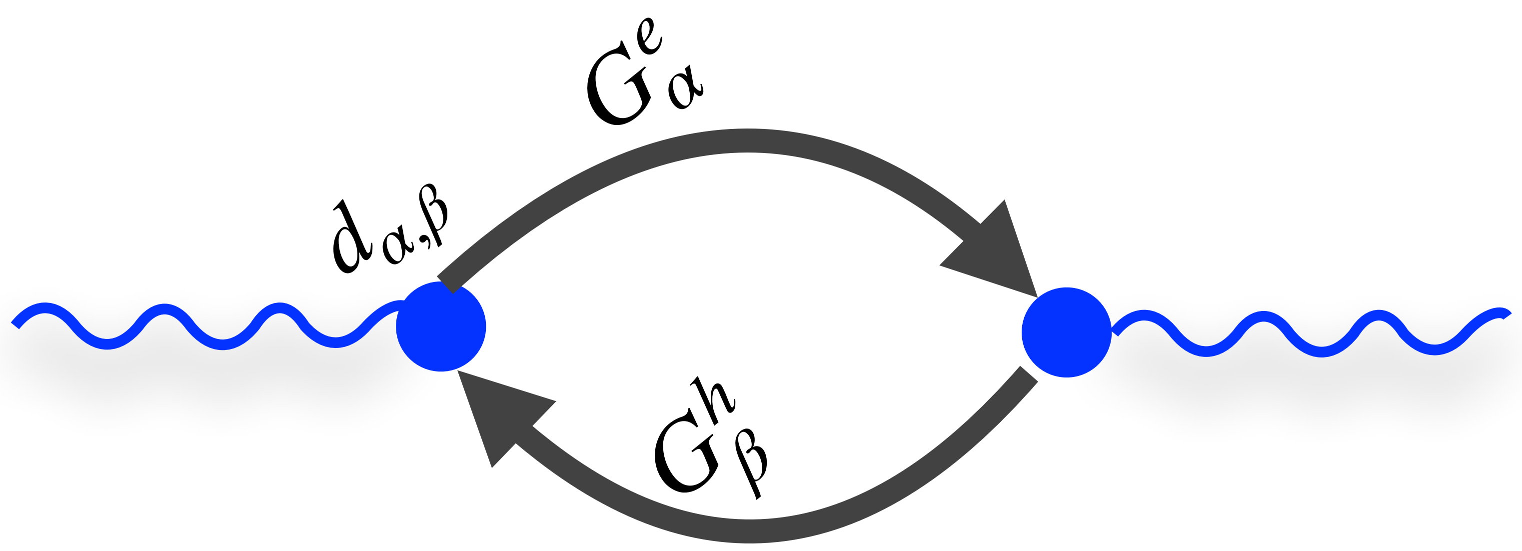
Before



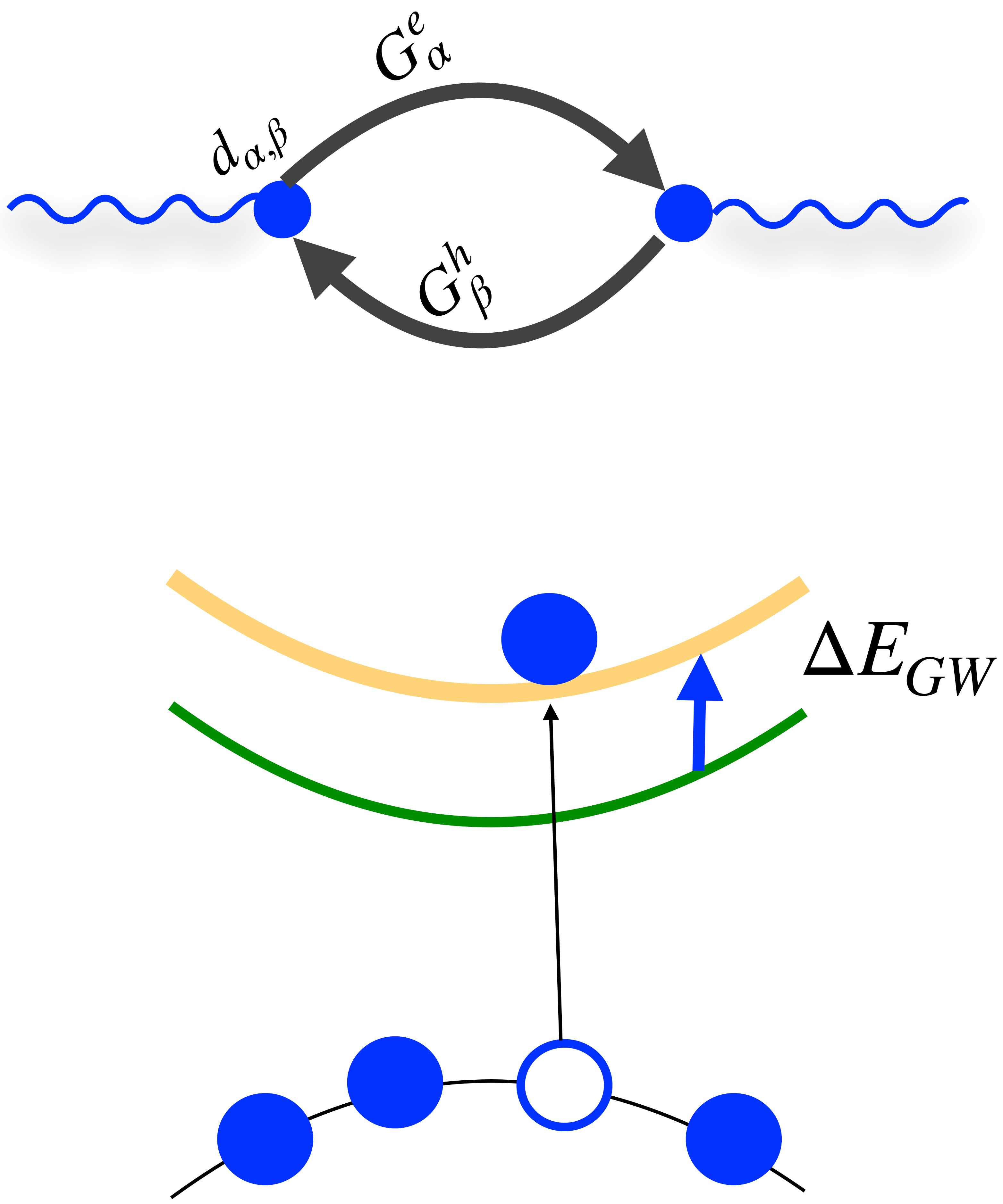
GW

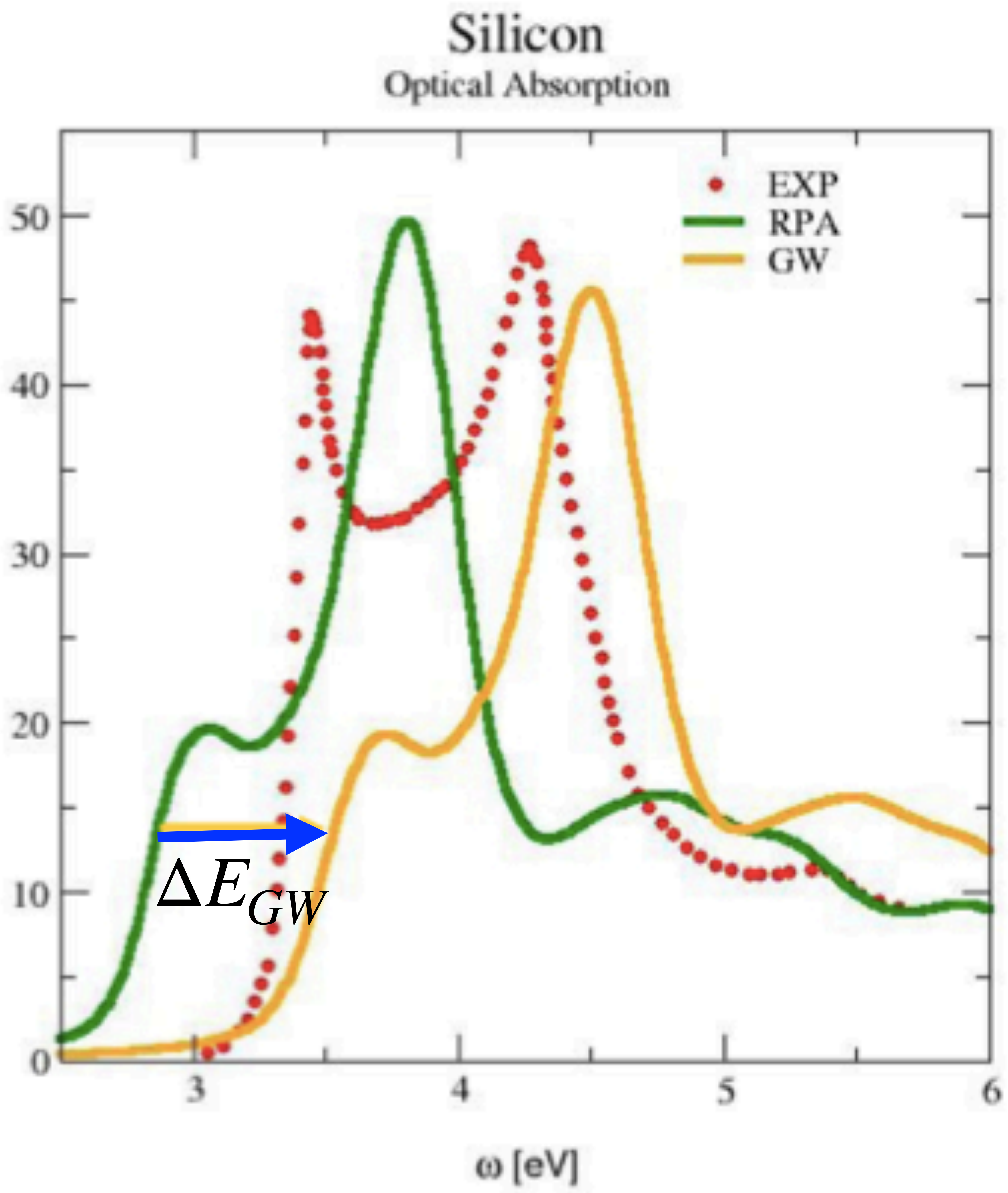


After



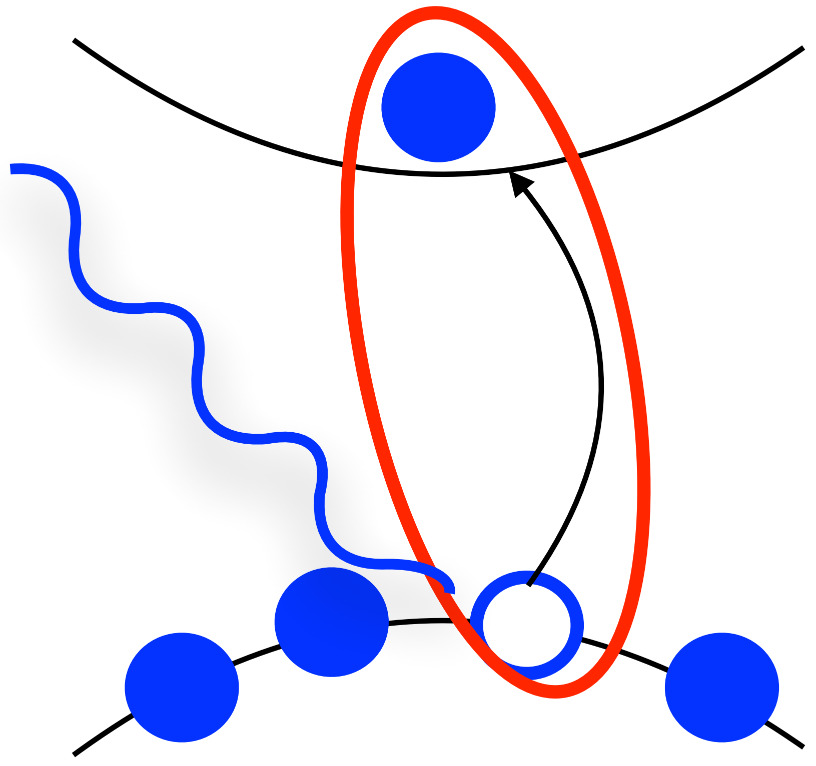
Dressed Green's function



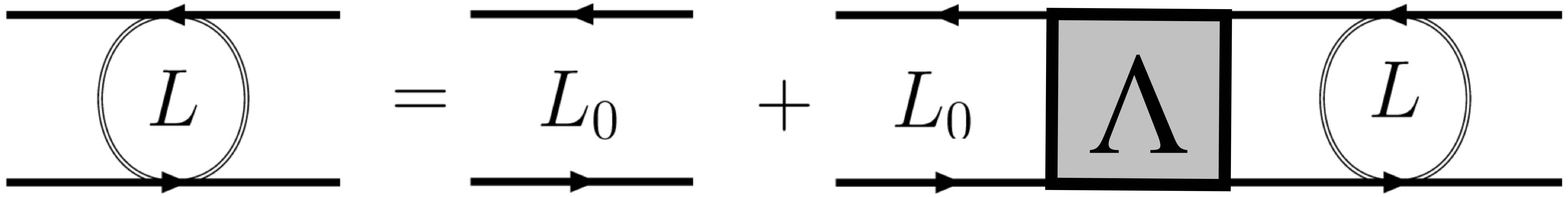


adapted from Onida et al. PR 2002

Electron-hole interactions



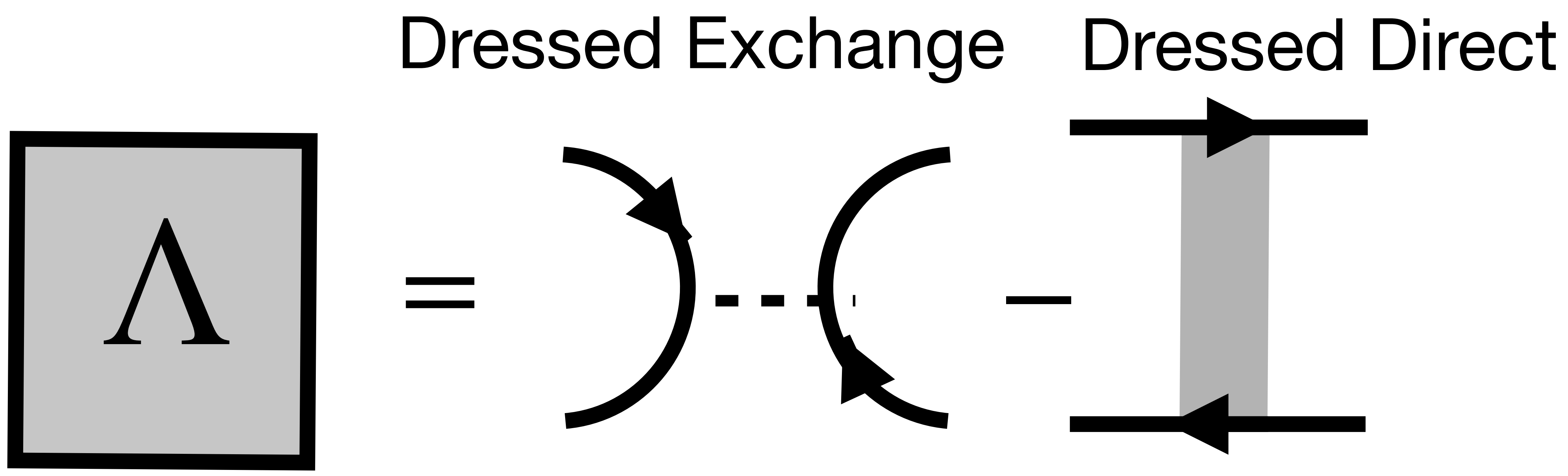
Bethe-Salpeter equation



Two interacting particles propagator: L

Two particles propagator: L_0

Interacting kernel: Λ



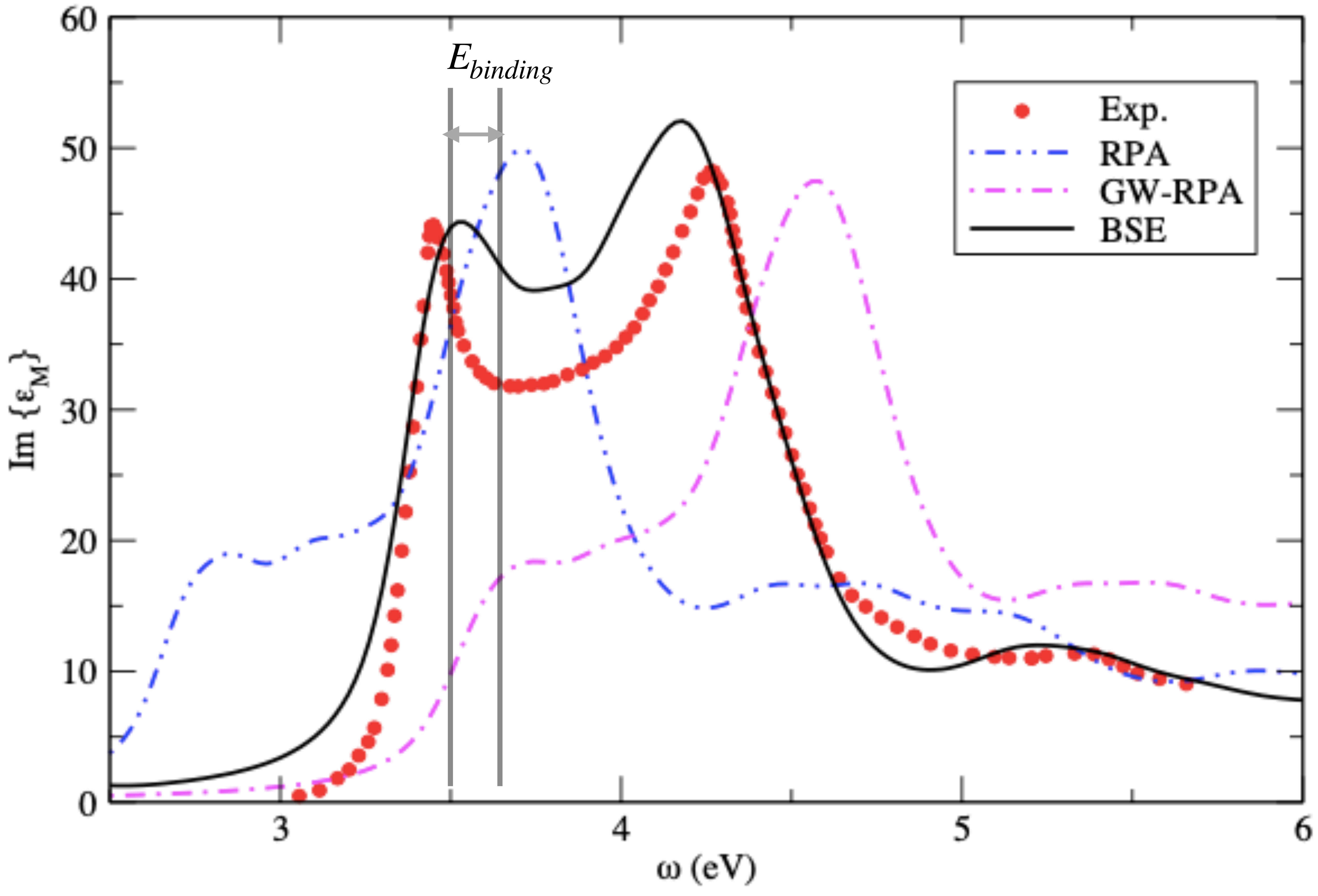
BSE results

Excitonic Green's function

$$L(x, x', \omega) = \sum_s \frac{A_s^+(x) A_s(x')}{\omega - E_s \pm i\gamma}$$

$$Im\epsilon(\omega) = Im \sum_{\alpha,\beta} d^+_{\alpha,\beta} L(\omega) d_{\alpha,\beta}$$

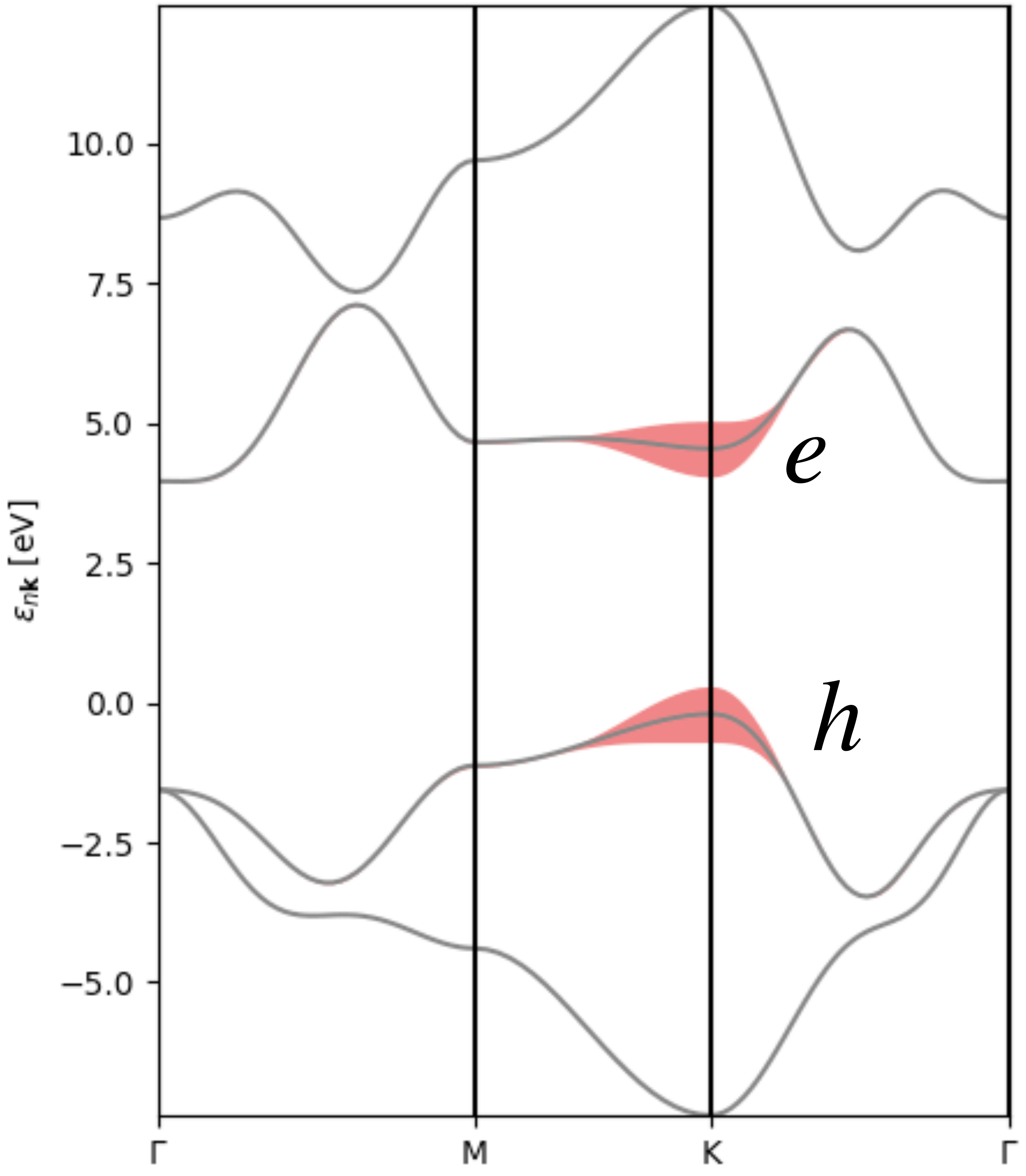
Enough to explain most of the features



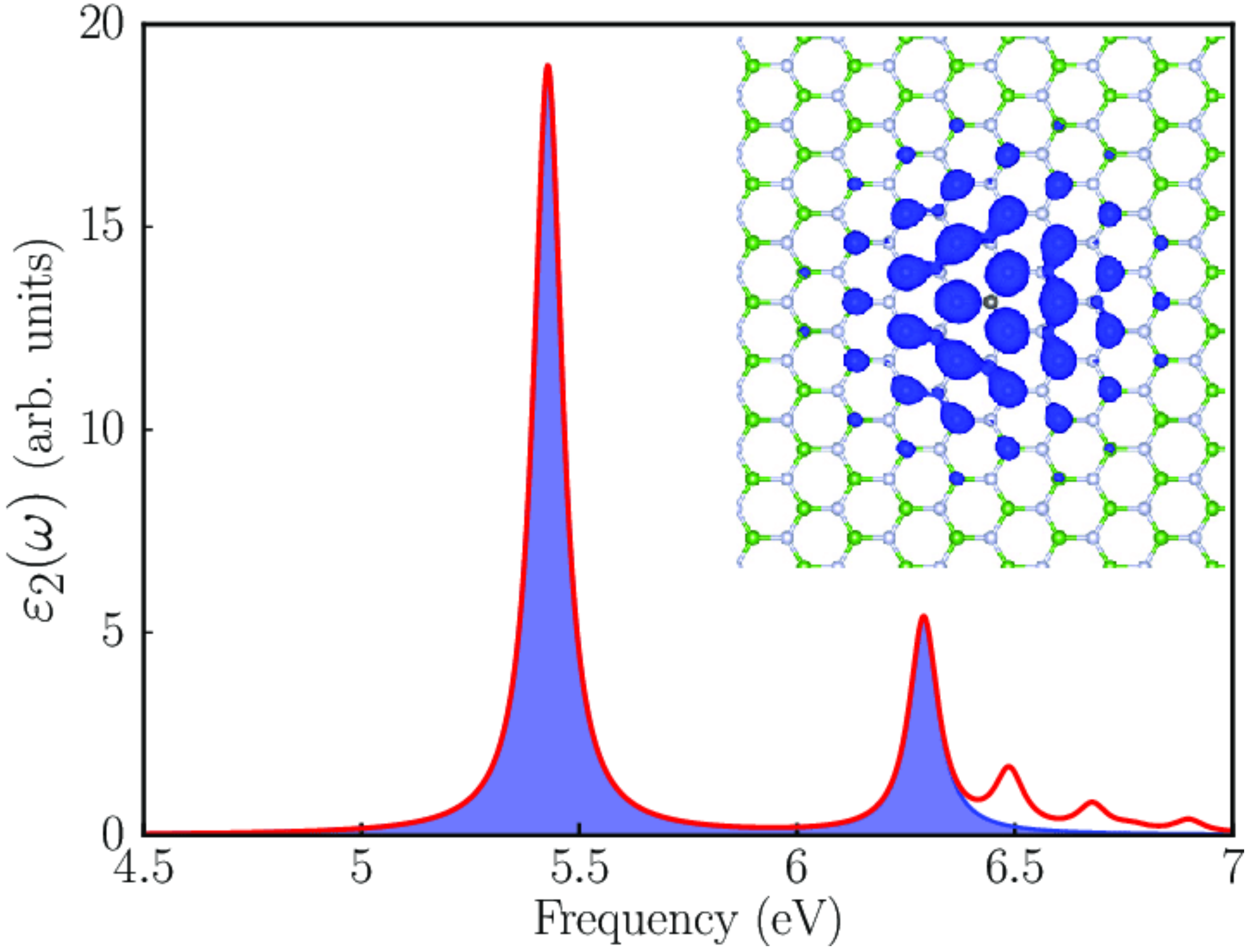
Sottile thesis 2003

Excitons

Exciton decomposition



Exciton wave-function $|\Psi(x, x')|^2$



Paleari et al. 2018

X-ray absorption

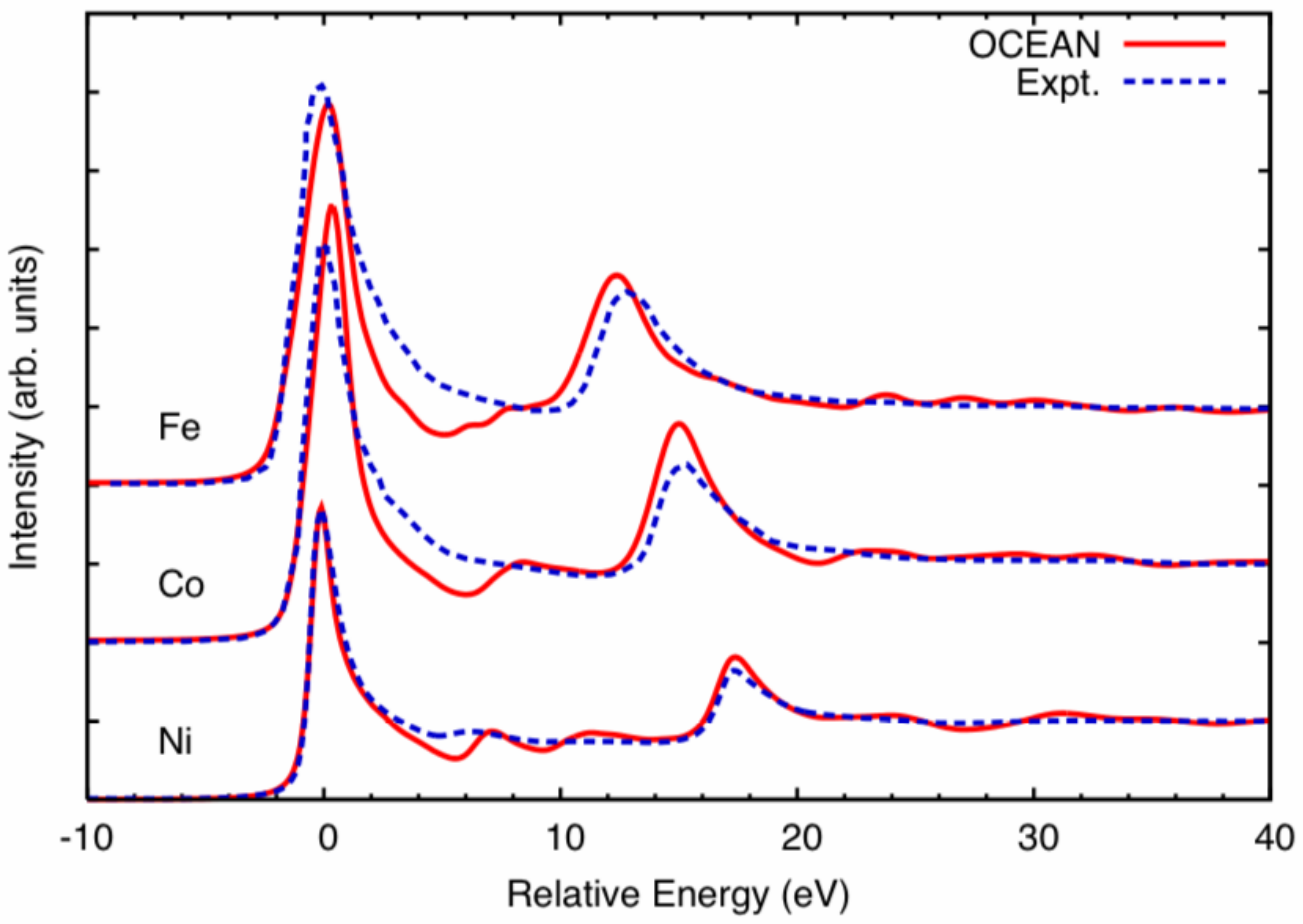


Figure 4.7: Calculations of the $L_{2,3}$ edge XAS of Fe, Co, and Ni metal compared with experiment [81, 82]. The calculations are scaled to match the high energy tails, and all the spectra are aligned at the L_3 edge to show the evolution of the spin-orbit splitting.

40

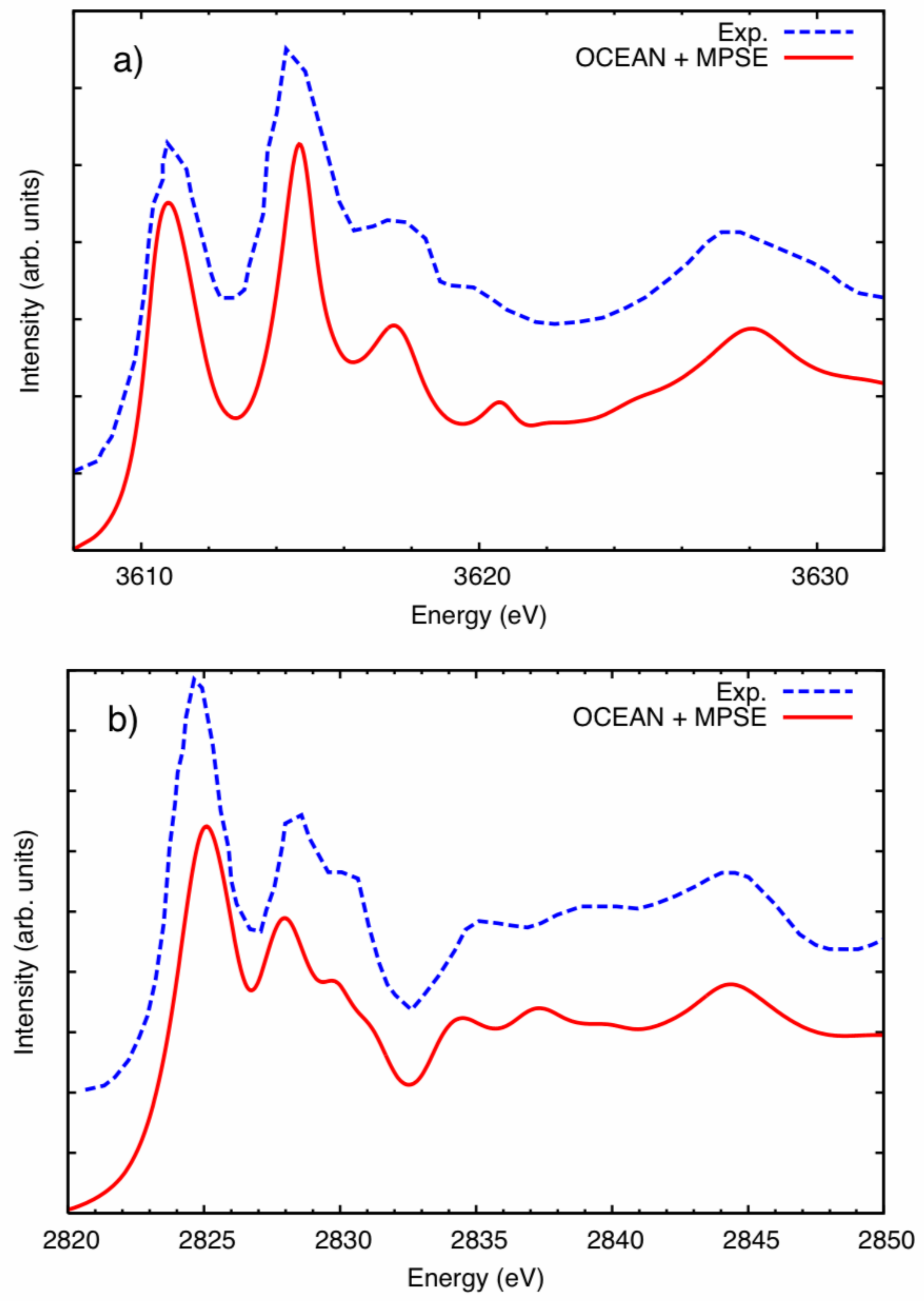


Figure 4.2: The XAS K edges in KCl for both a) potassium and b) chlorine as calculated in OCEAN compared to experiment [63]. For both the many-pole self-energy correction has been included. The spectra have been scaled to match each other and offset vertically for clarity.

Vinson et al. PRB 2012

Thank you for your patience!

Green's function (OG)

Homogeneous equation

$$L\phi_0 = 0$$

Green's function

$$LG(x, x') = \delta(x - x')$$

Inhomogeneous equation

$$L\phi = v$$

$$\phi = \phi_0 + \int dx' G(x, x') v(x')$$

$$(H - E)\Psi = 0 \qquad (H - E)G = I$$

$$G(E) = \sum_j \frac{|\Psi_j > < \Psi_j|}{E_j - E \pm i\eta}$$

Why Green's functions

$$G(E) = \sum_j \frac{|\Psi_j><\Psi_j|}{E_j - E \pm i\eta}$$

$$G(E) = \sum_j \frac{|\Psi_j><\Psi_j|}{E_j - E \pm i\eta}$$

$$G(E) = <\Psi'| \sum_j \frac{|\Psi_j><\Psi_j|}{E_j - E \pm i\eta} |\Psi'>$$

Spectral representation

Insert identity matrix

$$I = \sum_\beta |\Psi_\beta > < \Psi_\beta|$$

$$G(\mathbf{k}, t' - t) = -i < \Psi | T\hat{c}_\mathbf{k}(t) I \hat{c}^+_\mathbf{k}(t') | \Psi >$$

$$\hat{\psi}^+(r,t) -> \hat{c}^+_\alpha(t)$$

$$t, t' -> t - t'$$

$$H|\Psi_\beta> = E_\beta|\Psi_\beta>$$

Fourier transform

$$G(\mathbf{k}, \omega) = \int dt e^{i\omega t} G(\mathbf{k}, t)$$

Green's function in energy space

$$G(\mathbf{k}, \omega) = \sum_\beta \frac{| < \Psi_\beta | c^+_\mathbf{k} | \Psi_{GS} > |^2}{\omega - (E_\beta - E_{GS}) + i\eta} + \sum_\beta \frac{| < \Psi_\beta | c_\mathbf{k} | \Psi_{GS} > |^2}{\omega - (E_{GS} - E_\beta) - i\eta}$$

Green's function (OG)

Homogeneous equation

$$L\phi_0 = 0$$

Green's function

$$LG(x, x') = \delta(x - x')$$

Inhomogeneous equation

$$L\phi = v$$

$$\phi = \phi_0 + \int dx' G(x, x') v(x')$$

Quantum Mechanics:

$$(\hat{H} - E)\Psi = 0$$

$$(\hat{H} - E)G = I$$

linear operator

?