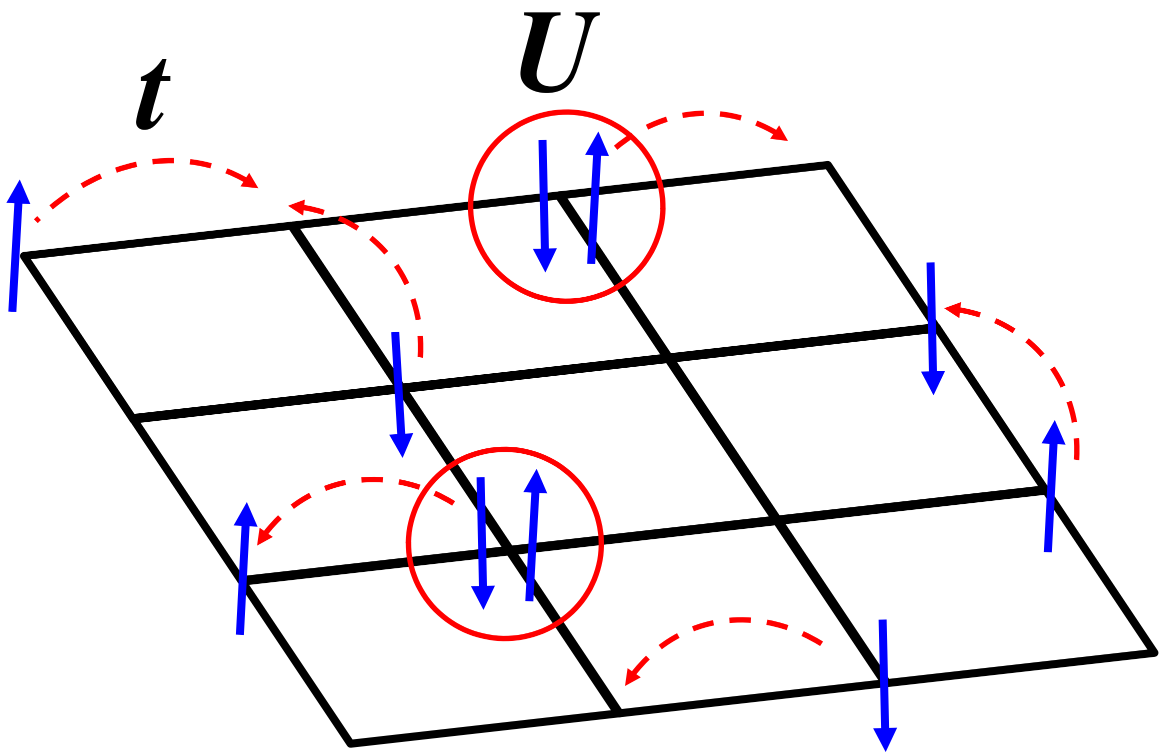
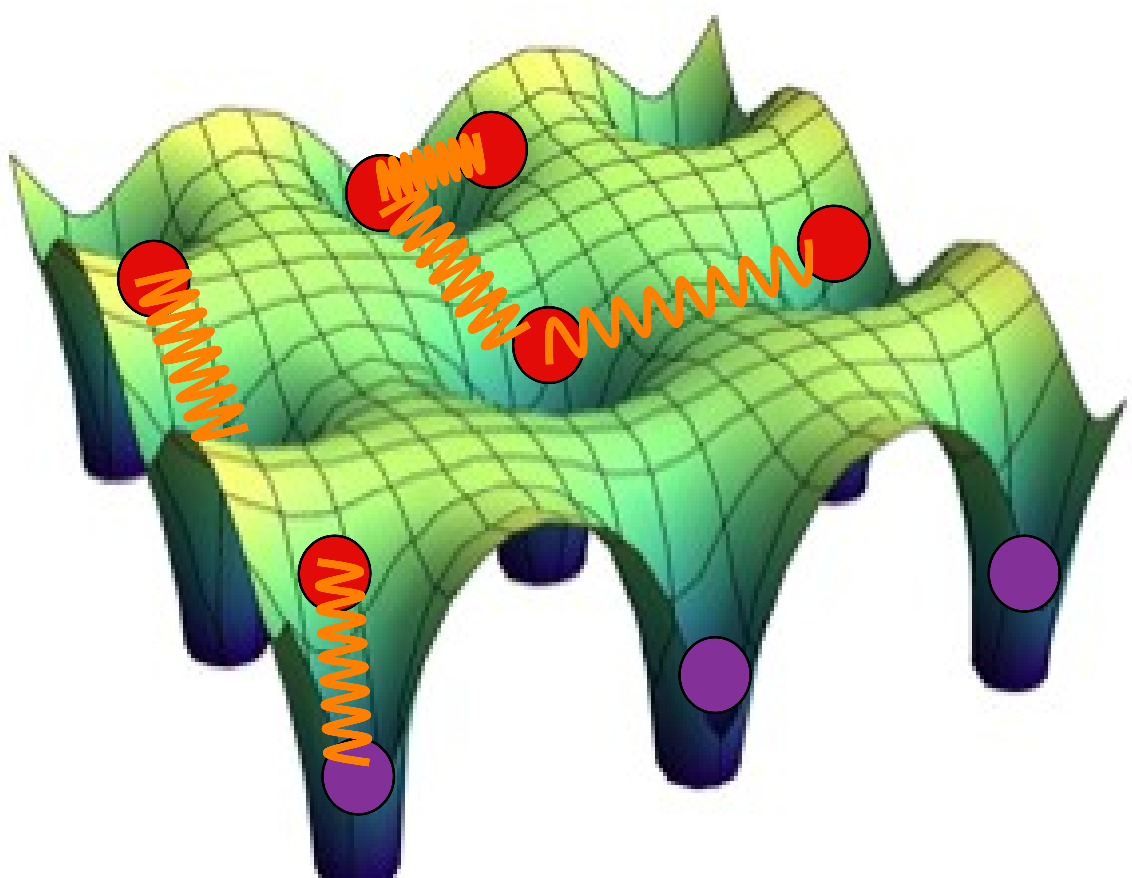
Hubbard model

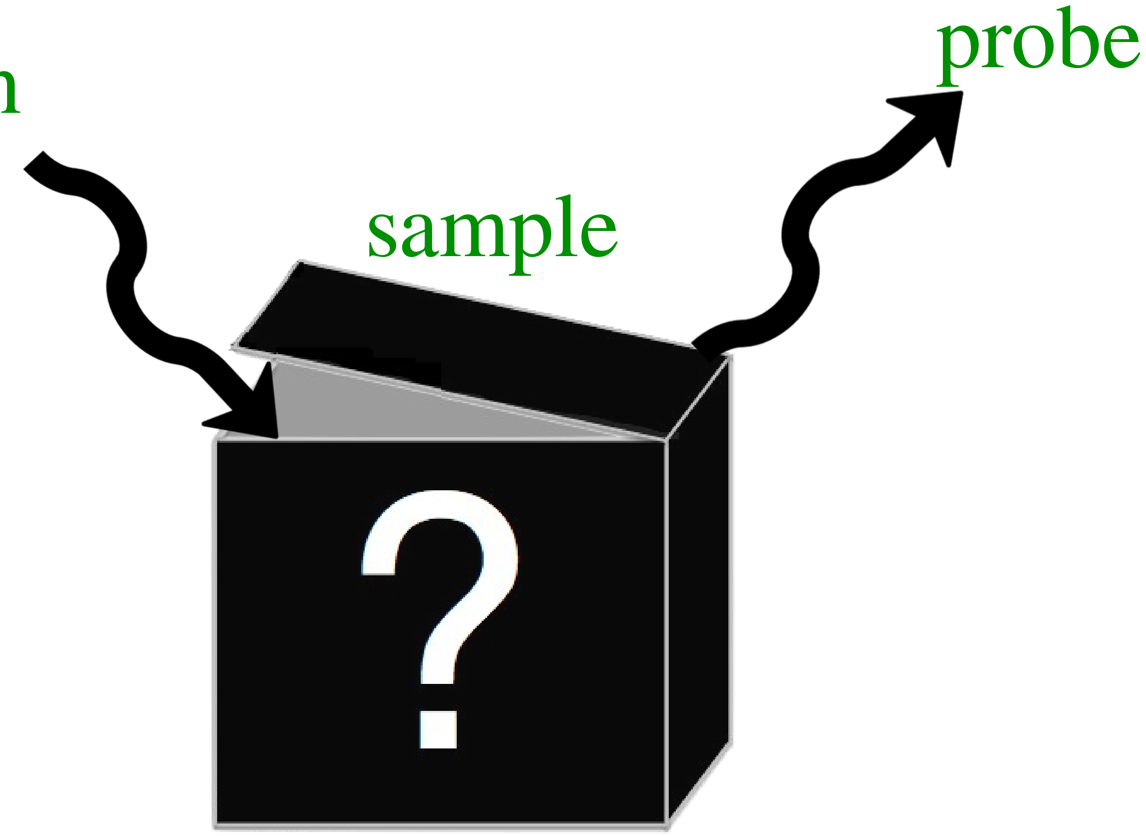


Hubbard model



Electrons in crystal

How do we describe materials?



$\langle c^\dagger(t)c(t')\rangle$ photoemission

$\langle \vec{j}(t)\vec{j}(t')\rangle$ transport

$\langle \vec{S}(t)\vec{S}(t')\rangle$ magnetism

$\vec{S}, \vec{j} \sim c^\dagger c$ 2-particle properties

Weakly correlated electrons:

$$\langle c_i^\dagger c_j c_k^\dagger c_l\rangle = \langle c_i^\dagger c_j\rangle\langle c_k^\dagger c_l\rangle - \langle c_i^\dagger c_l\rangle\langle c_k^\dagger c_j\rangle + \mathrm{small\_correction}$$

Strongly correlated electrons:

'small_correction' is not small !

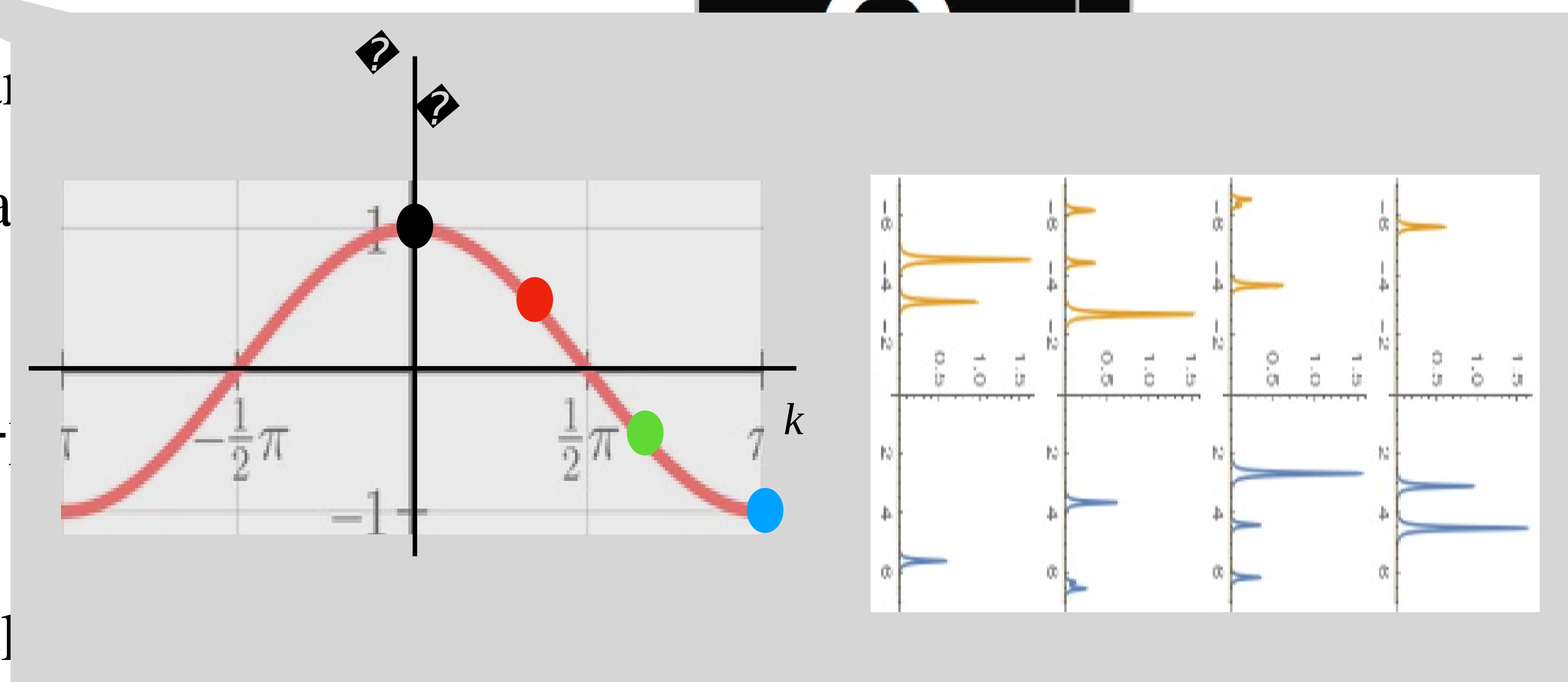
How do we describe materials?

$\langle c^\dagger(t)c(t')\rangle$ photoemission

$\langle \vec{j}(t)\vec{j}(t')\rangle$ tra

$\langle \vec{S}(t)\vec{S}(t')\rangle$ ma

$\vec{S}, \vec{j} \sim c^\dagger c$ 2-



Weakly correlated el

$$\langle c_i^\dagger c_j c_k^\dagger c_l\rangle = \langle c_i^\dagger c_j\rangle\langle c_k^\dagger c_l\rangle - \langle c_i^\dagger c_l\rangle\langle c_k^\dagger c_j\rangle + \mathrm{small\_correction}$$

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How do we describe materials?

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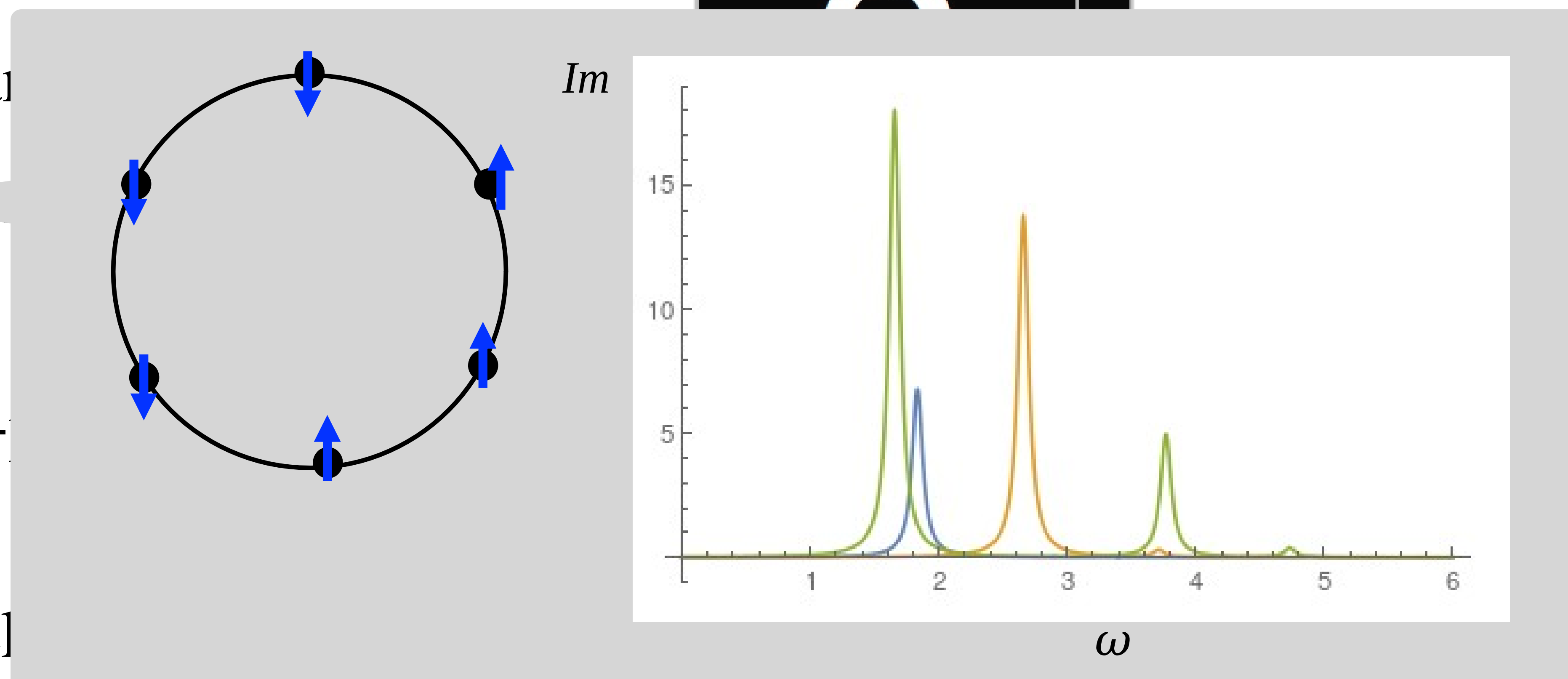

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Weakly correlated el

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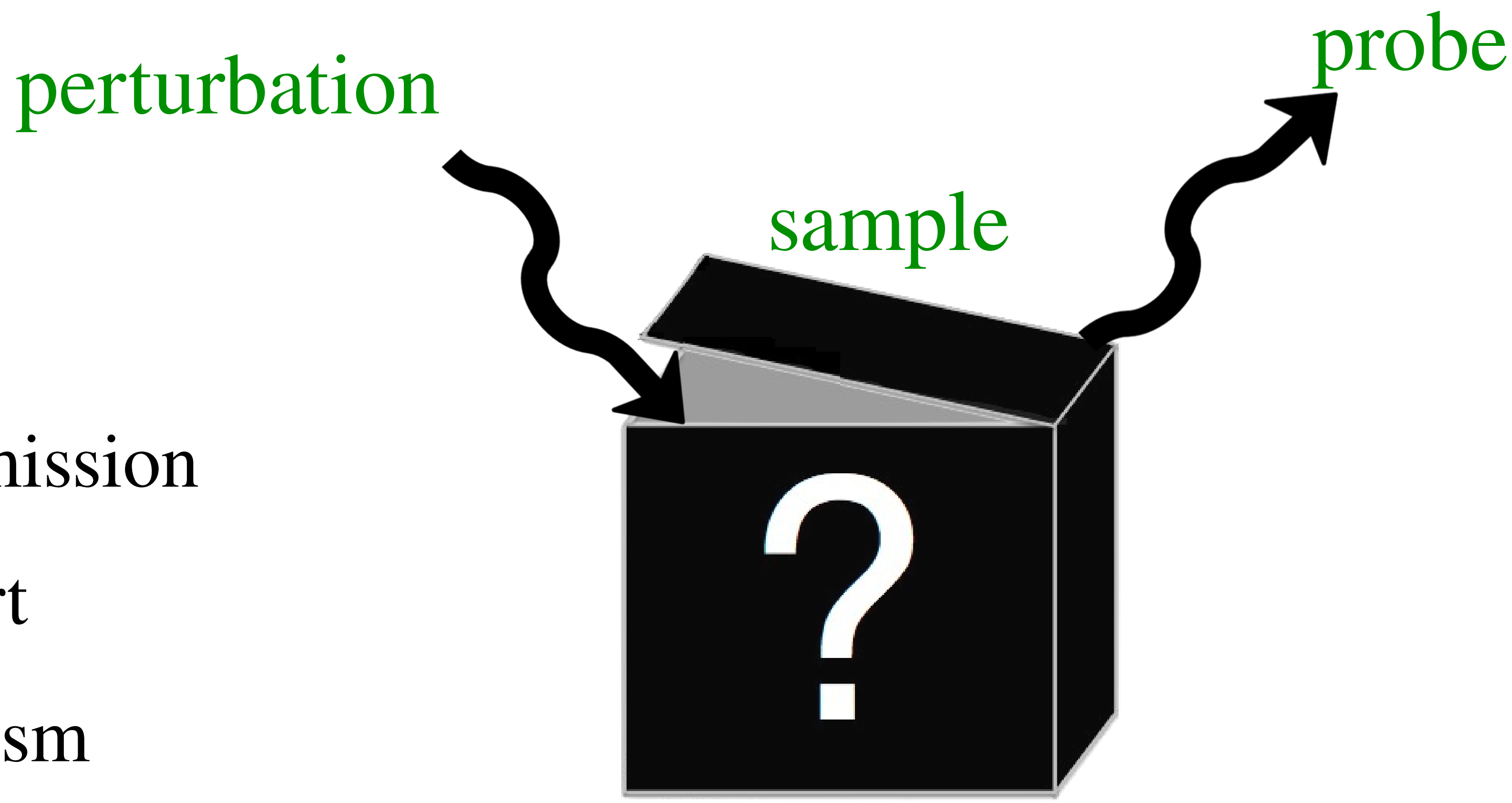
How do we calculate correlation functions?



$\langle c^\dagger(t) c(t') \rangle$ photoemission

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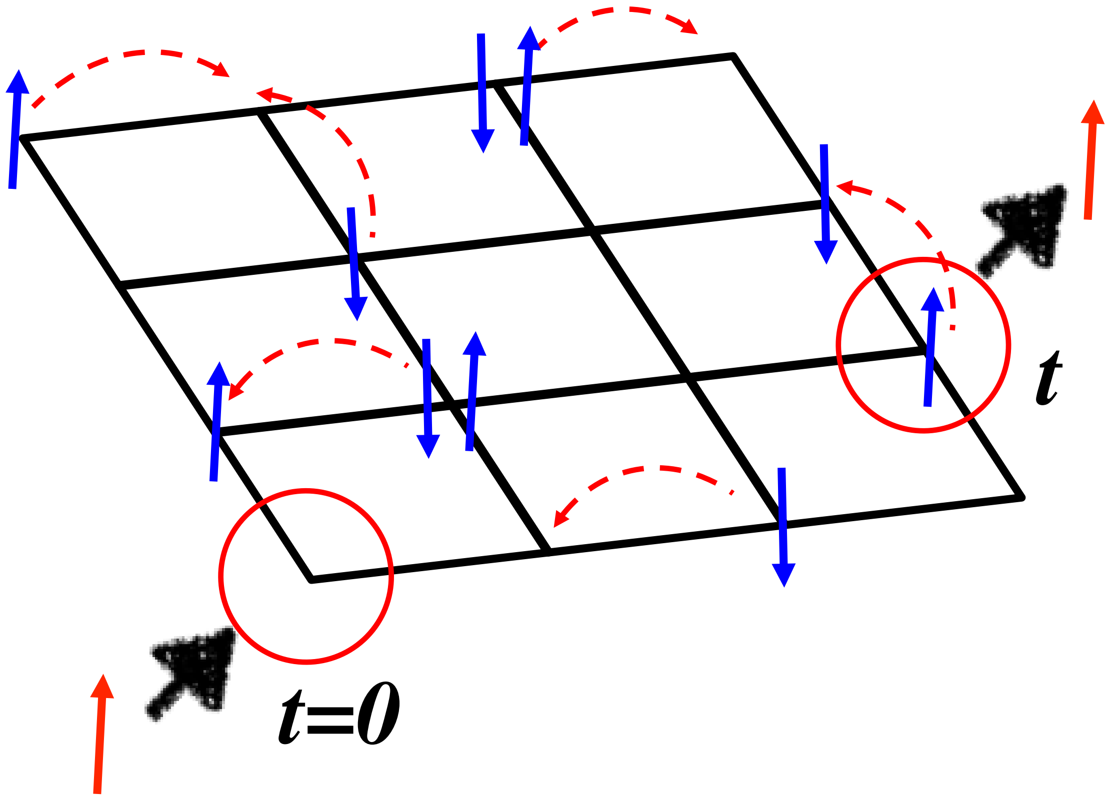
Electron self-energy

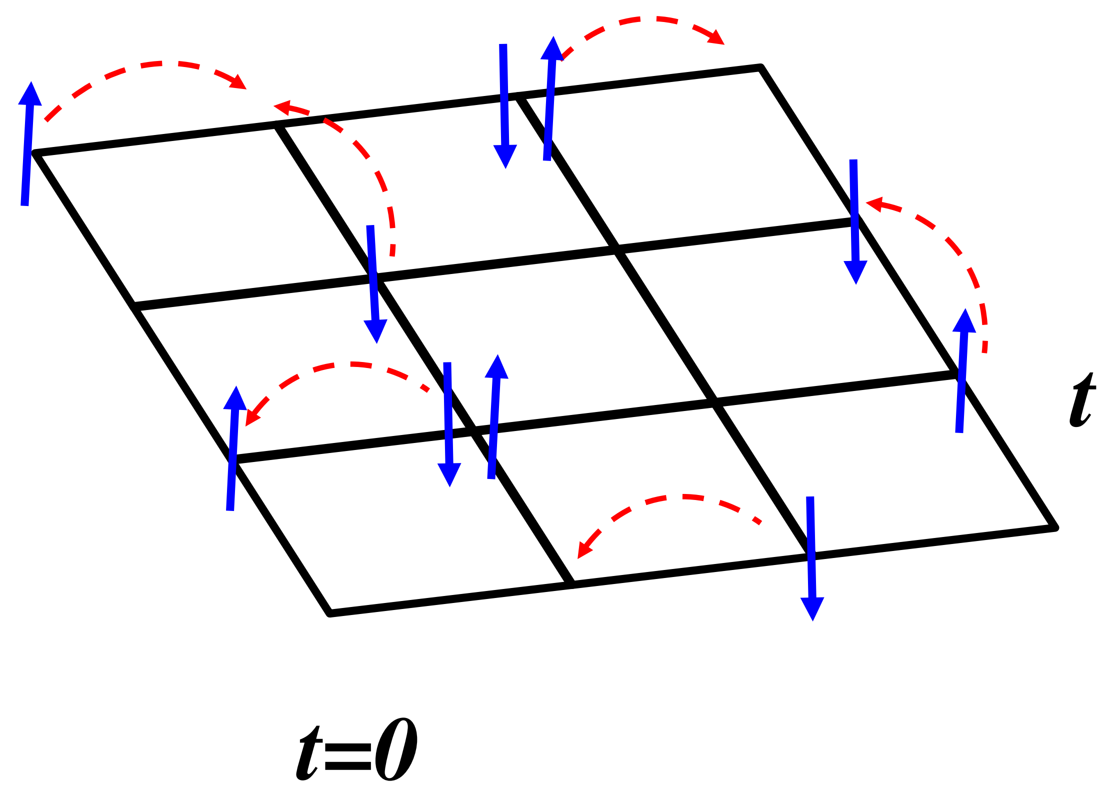
How does coupling to phonons affect electrons?

Electron propagator: $\langle c_{j\uparrow}(t)c^{\dagger}_{i\uparrow}(0)\rangle \equiv \langle\psi_g|e^{itH}c_{j\uparrow}e^{-itH}c^{\dagger}_{i\uparrow}|\psi_g\rangle$

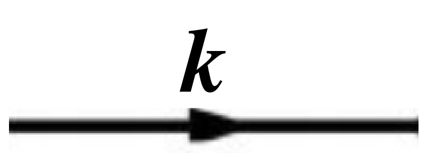
$c_{j\uparrow}e^{-itH}c^{\dagger}_{i\uparrow}|\psi_g\rangle$



$\langle\psi_g|e^{itH}$



In a non-interacting system:



$$G(\omega,k) \equiv G_{kk}(\omega) = \frac{1}{\omega - \epsilon_k}$$

Self-energy and Dyson equation

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

$$G^{-1}(\omega, k) = \omega - h_k - \Sigma(\omega, k)$$

effective potential

perturbation theory (diagrams)

$$\Sigma =$$

Quasiparticle construction:

$$G(\omega) = \frac{1}{\omega - \epsilon - \mathrm{Re}\,\Sigma(\omega) - i\,\mathrm{Im}\,\Sigma(\omega)}$$

Non-interacting particle is a pole of $G(\omega)$.

equation for approx. pole ω^* with a linewidth

$$\omega^* - \epsilon - \mathrm{Re}\,\Sigma(\omega^*) = 0$$

$$\sim \mathrm{Im}\,\Sigma(\omega^*)$$

Self-energy and Dyson equation

Quasiparticle construction:

$$G(\omega) = \frac{1}{\omega - \epsilon - \mathrm{Re}\,\Sigma(\omega) - i\,\mathrm{Im}\,\Sigma(\omega)}$$

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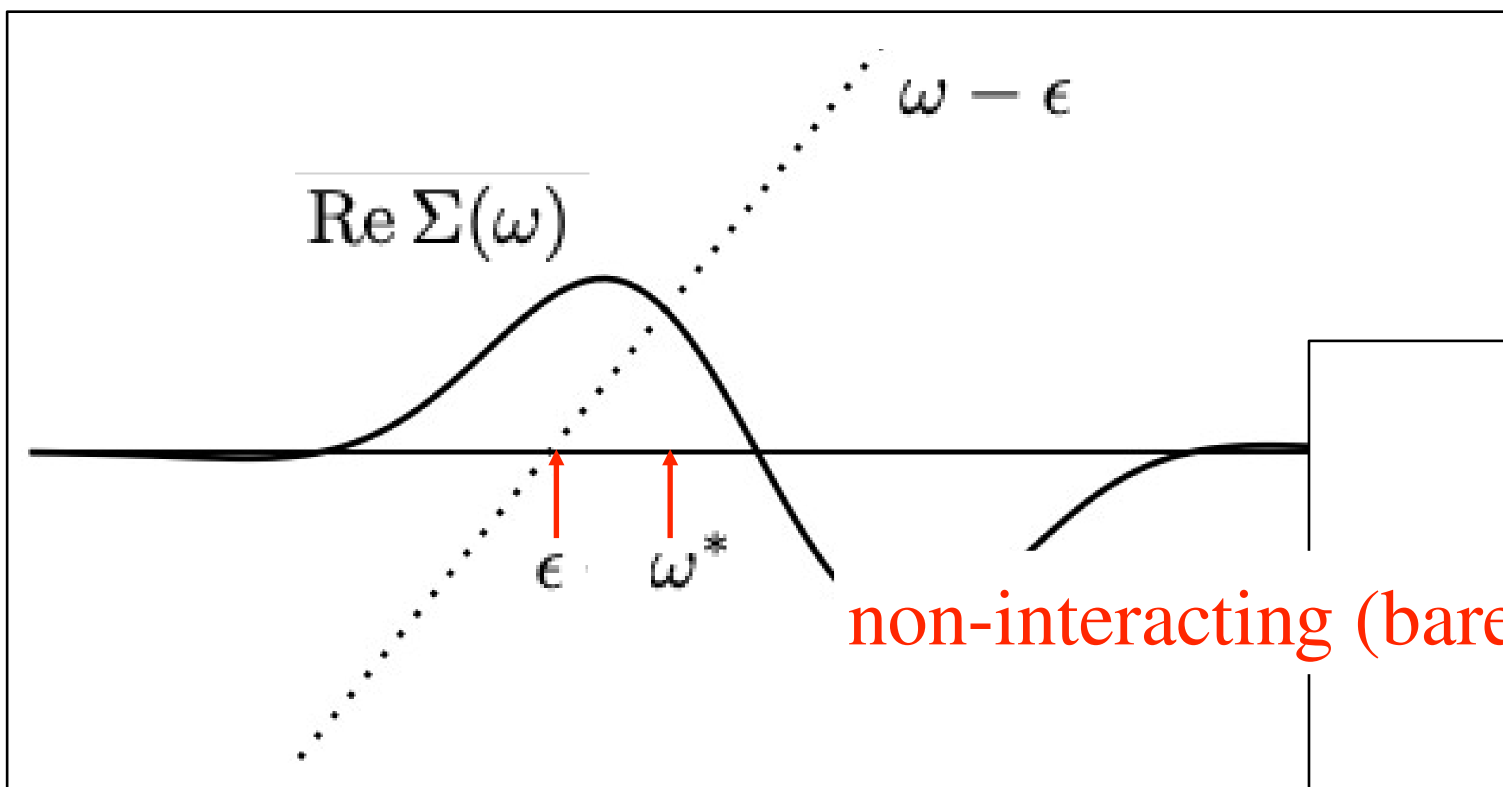
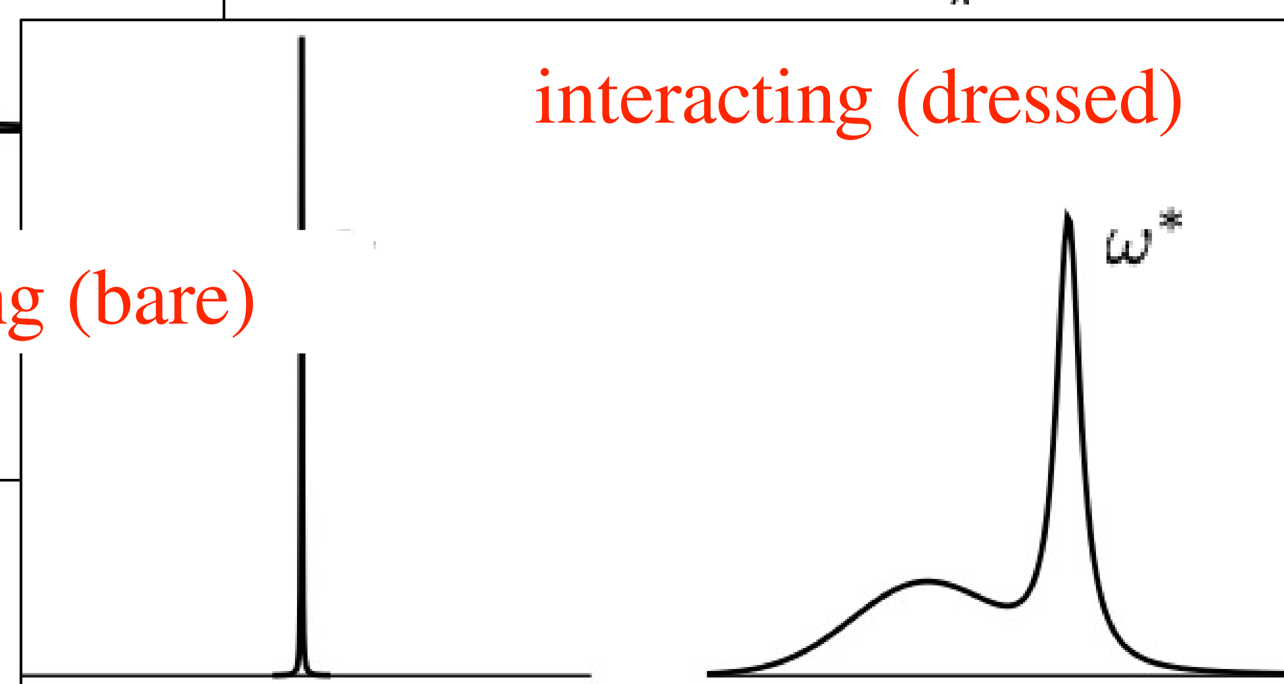
equation for approx. pole * with a linewidth

$$\omega^* - \epsilon - \mathrm{Re}\,\Sigma(\omega^*) = 0 \qquad \sim \mathrm{Im}\,\Sigma(\omega^*)$$



$$A(\omega) = -\frac{1}{\pi}\,\mathrm{Im}\,G(\omega)$$



Self-energy and Dyson equation

Quasiparticle construction:

$$G(\omega) = \frac{1}{\omega - \epsilon - \mathrm{Re}\,\Sigma(\omega) - i\,\mathrm{Im}\,\Sigma(\omega)}$$

Non-interacting particle is a pole of *G*( ).

equation for approx. pole * with a linewidth

$$\omega^* - \epsilon - \mathrm{Re}\,\Sigma(\omega^*) = 0 \qquad \sim \mathrm{Im}\,\Sigma(\omega^*)$$

For ω close to 0: Re$\boldsymbol{\Sigma}(\omega)$ is linear (in FL, not in general)

$$G(\omega, k) = \frac{1}{\omega - \epsilon_k - \omega \frac{\partial\,\mathrm{Re}\,\Sigma}{\partial\omega}|_{\omega=0}} = \frac{Z}{\omega - Z\epsilon_k}$$

Quasi-particles are Z^{-1} heavier than bare particles.

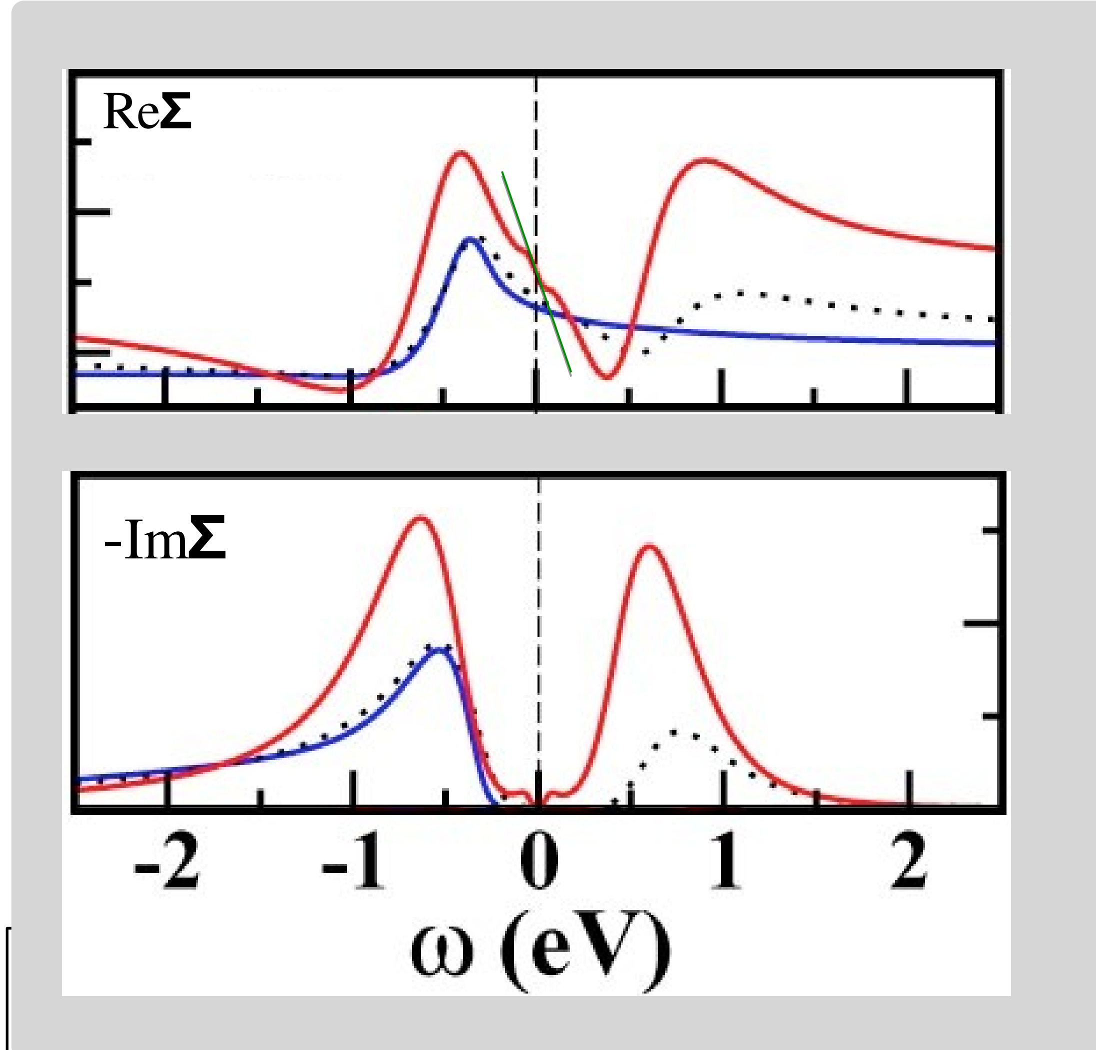
$$Z = \frac{1}{1 - \frac{\partial\,\mathrm{Re}\,\Sigma}{\partial\omega}|_{\omega=0}}$$

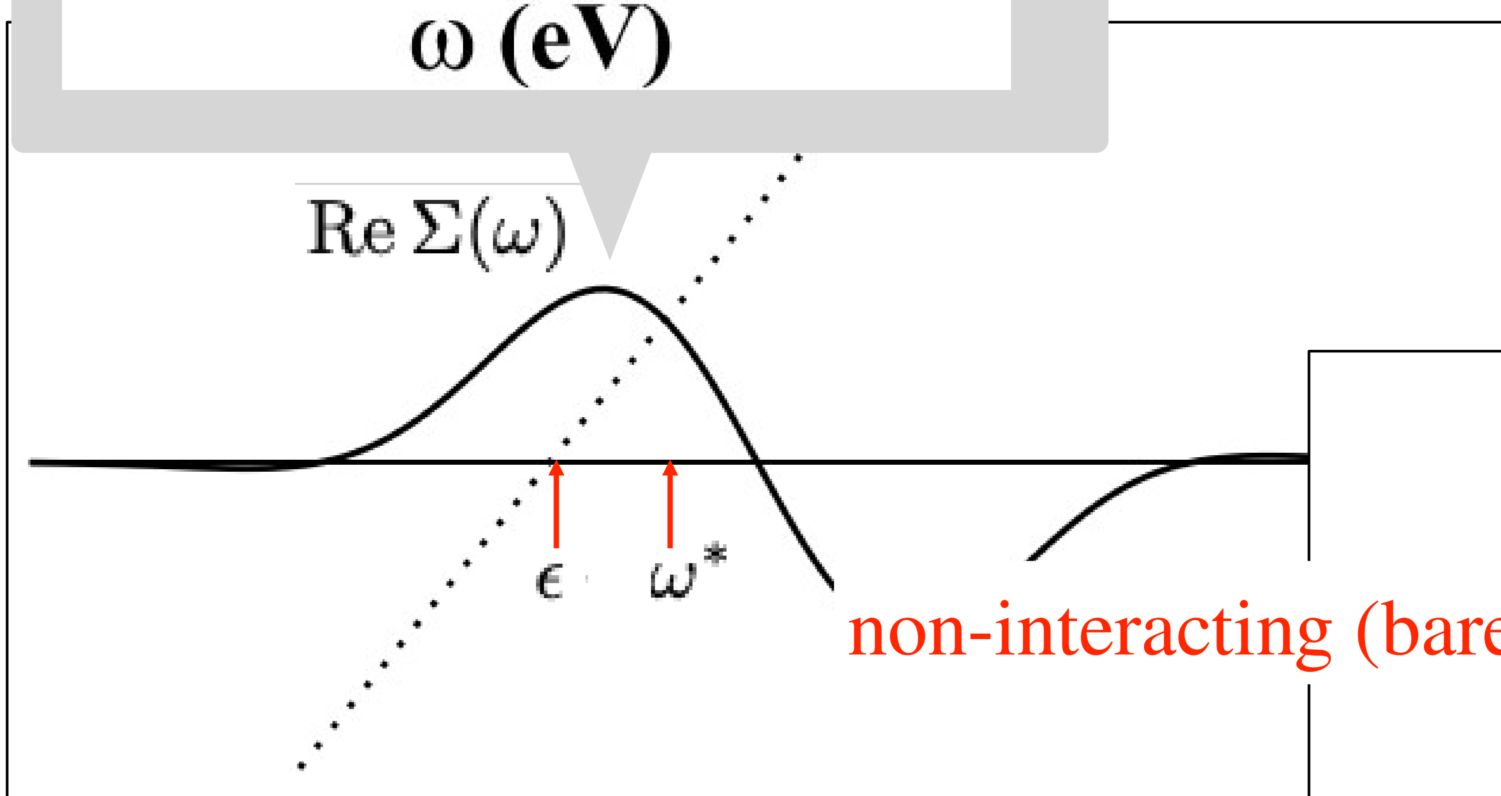
Quasi-particle residuum

gy and Dyson equation

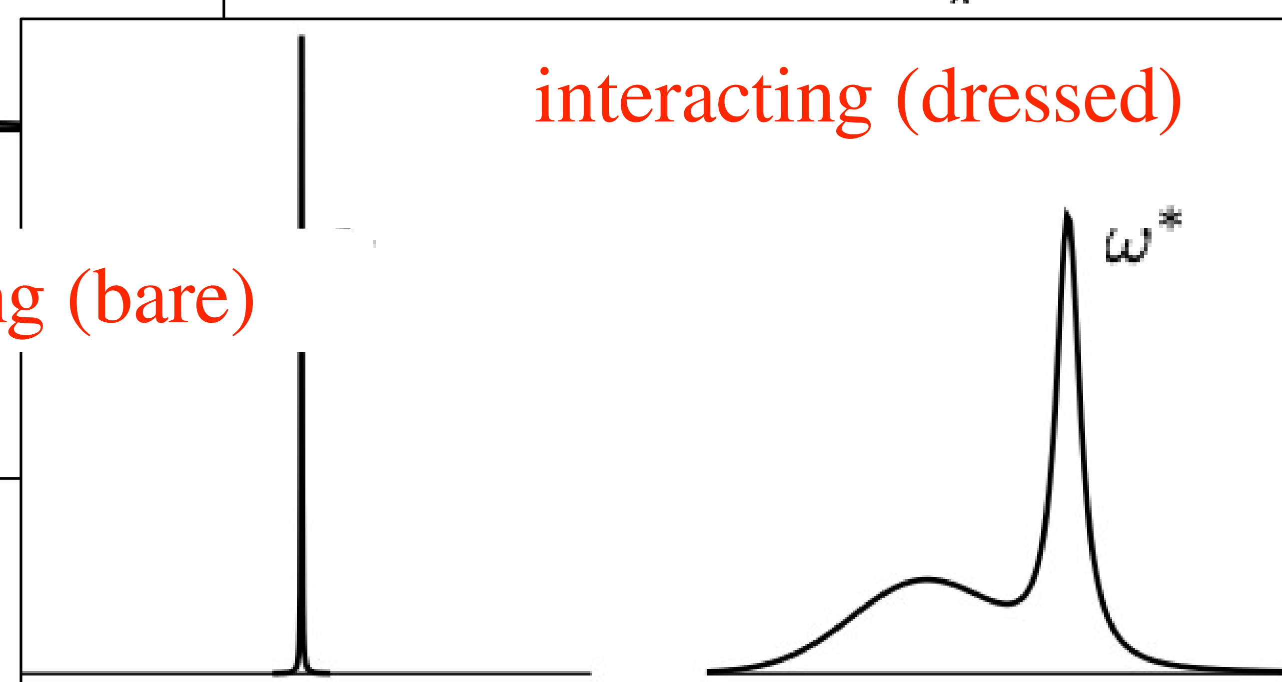
* with a linewidth

$\sim \operatorname{Im}\Sigma(\omega^*)$





$$A(\omega) = -\frac{1}{\pi}\operatorname{Im} G(\omega)$$



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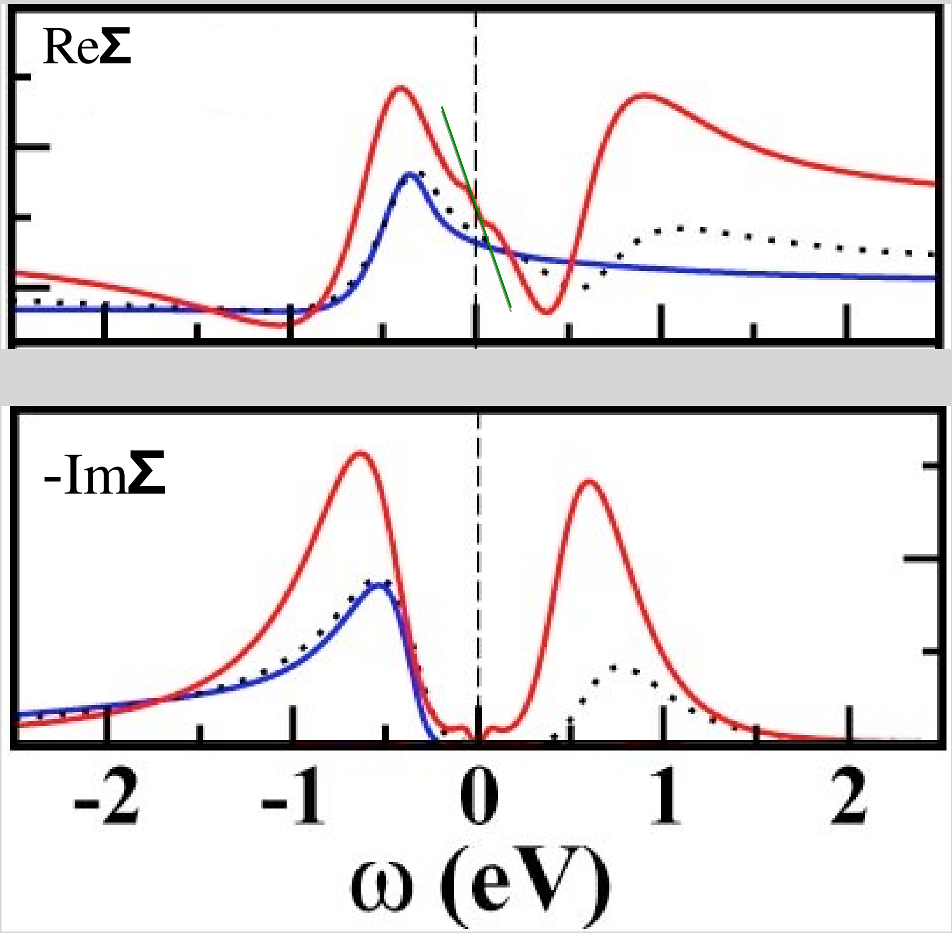
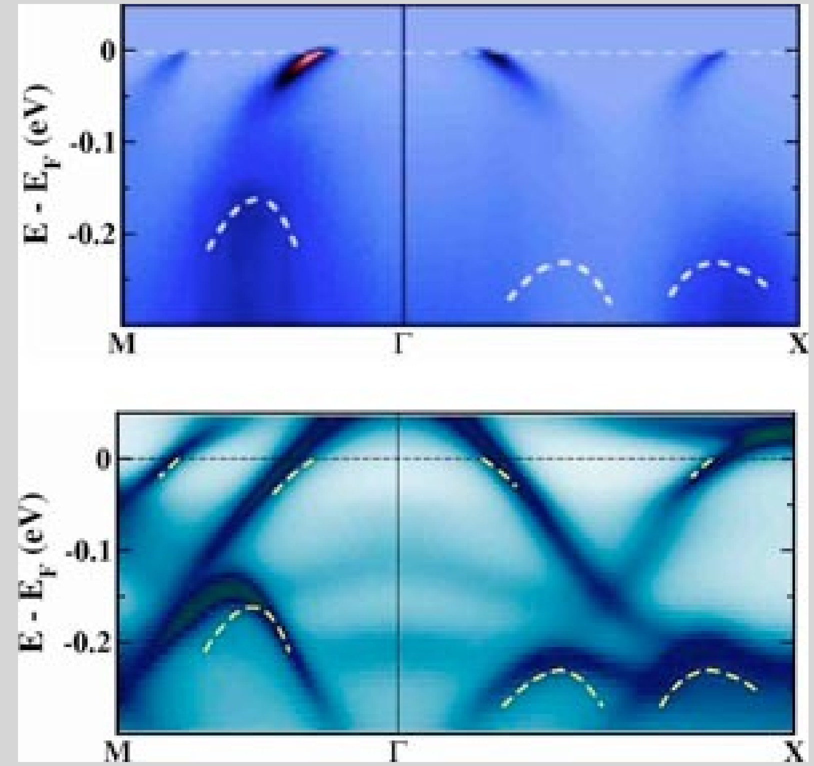


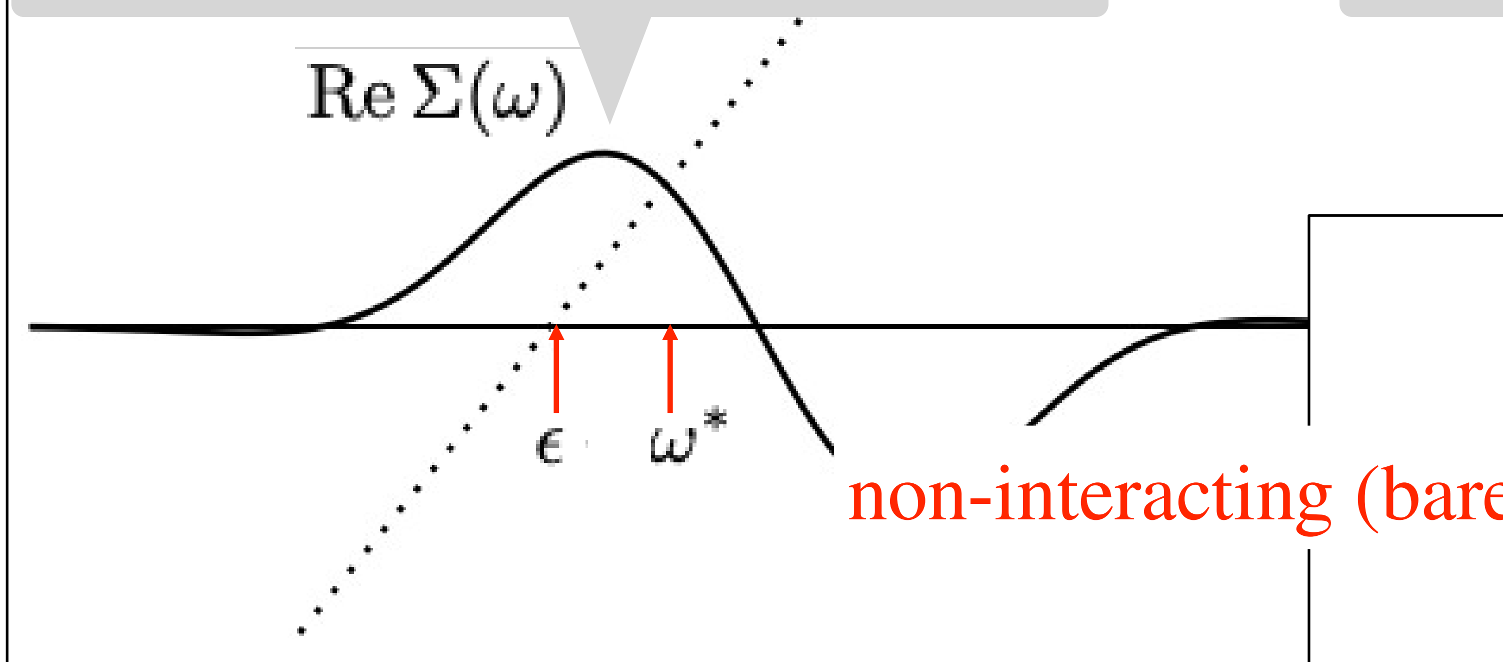
exp:

the:

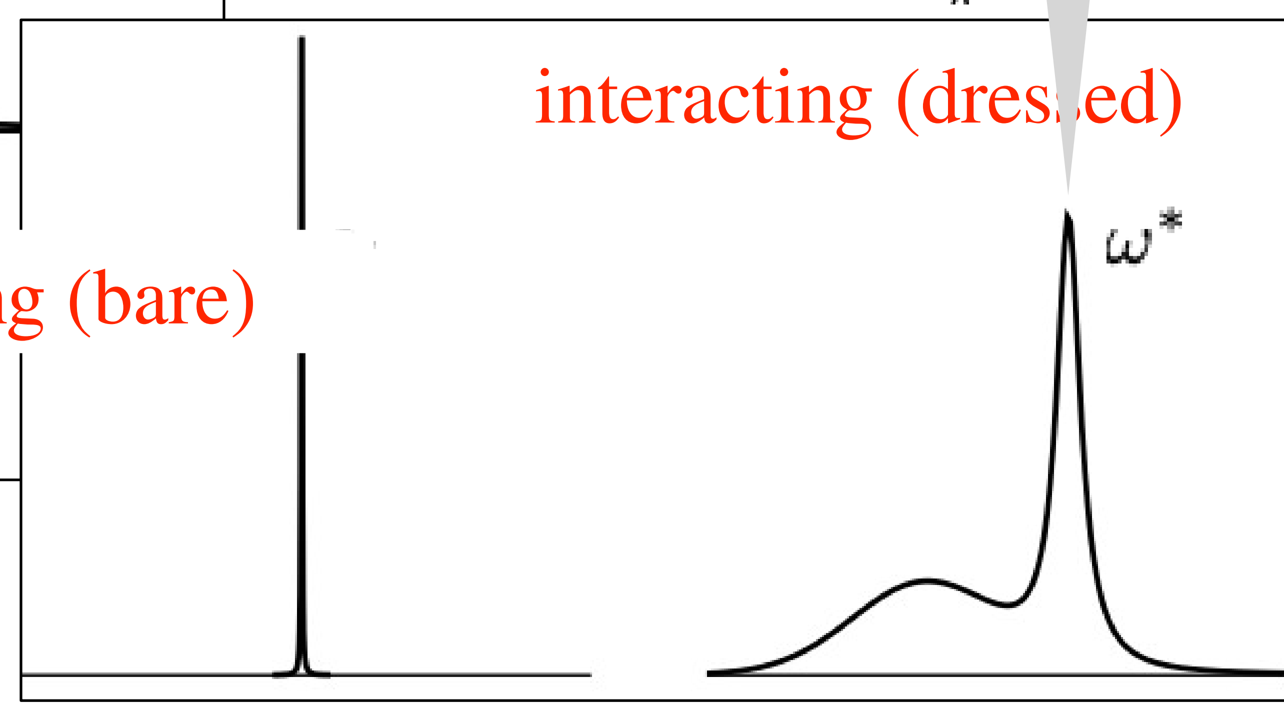


FL regime

* with a li



$A(\omega) = -\frac{1}{\pi}\,\mathrm{Im}\,G(\omega)$

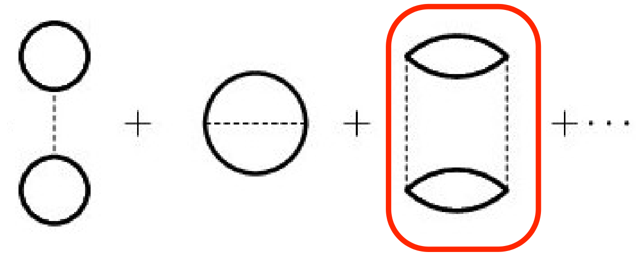


interacting (dressed)

non-interacting (bare)

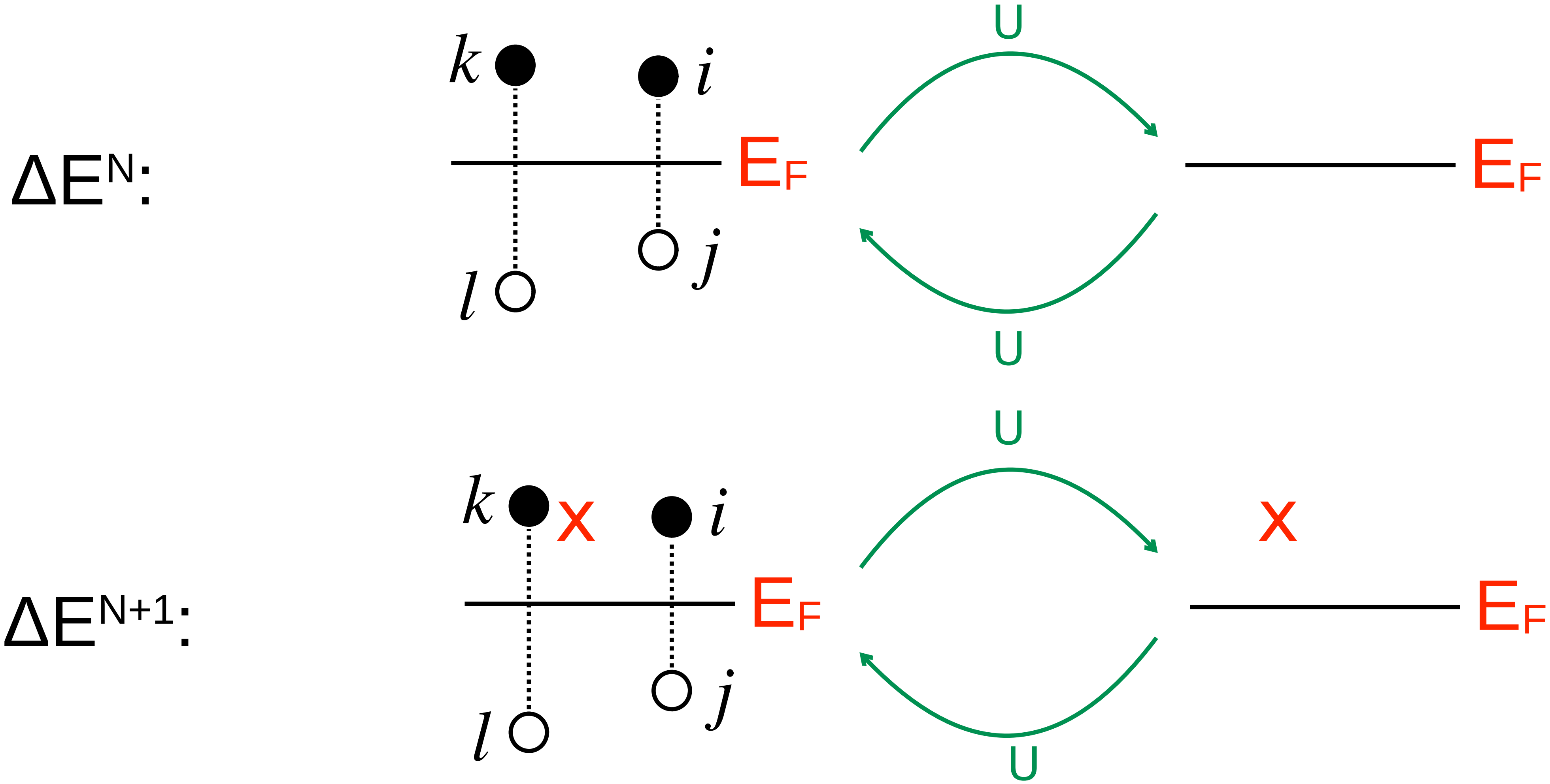
2nd order perturbation theory (small U)

$$\Delta E^N = -\frac{U^2}{V^3}\sum_{i,j,k,l}\frac{(1-n_i)n_j(1-n_k)n_l}{\epsilon_i-\epsilon_j+\epsilon_k-\epsilon_l}$$



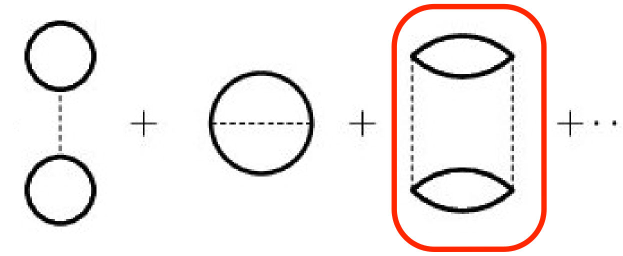
$$\Delta E^{N+1}-\Delta E^N = -\frac{U^2}{V^3}\sum_{i,j,k}(1-n_i)n_j\left[\frac{(1-n_k)}{\epsilon_i-\epsilon_j+\epsilon_k-\epsilon}-\frac{n_k}{\epsilon_i-\epsilon_j+\epsilon-\epsilon_k}\right]$$

2nd order 0th order (non-interacting)



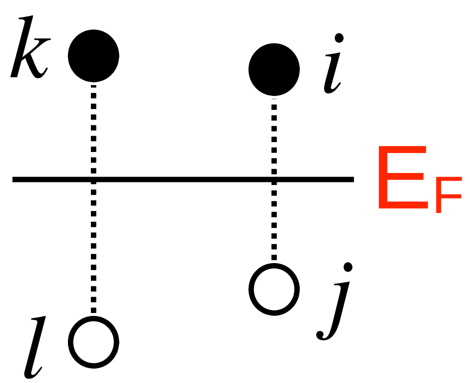
2nd order perturbation theory (small U)

$$\Delta E^N = -\frac{U^2}{V^3}\sum_{i,j,k,l}\frac{(1-n_i)n_j(1-n_k)n_l}{\epsilon_i-\epsilon_j+\epsilon_k-\epsilon_l}$$

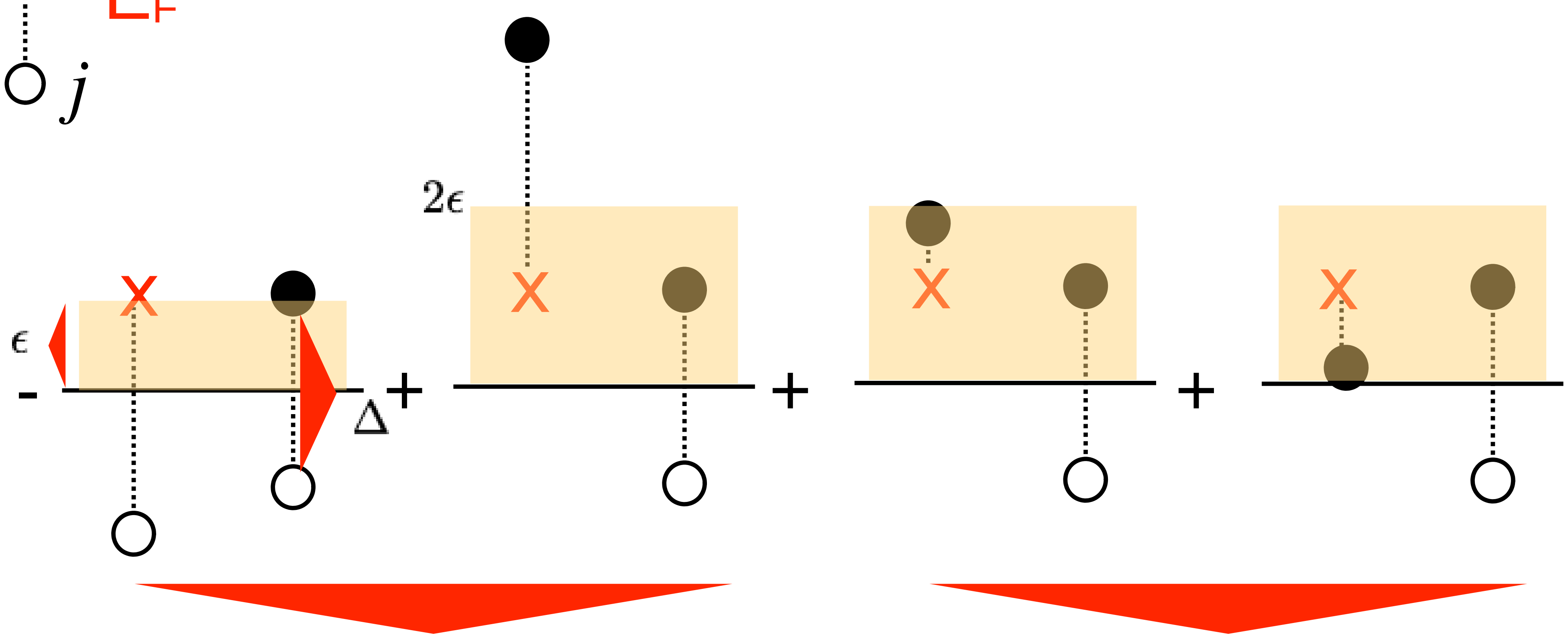


$$\Delta E^{N+1}-\Delta E^N = -\frac{U^2}{V^3}\sum_{i,j,k}(1-n_i)n_j\left[\frac{(1-n_k)}{\epsilon_i-\epsilon_j+\epsilon_k-\epsilon}-\frac{n_k}{\epsilon_i-\epsilon_j+\epsilon-\epsilon_k}\right]$$

ΔE^N:



ΔE^{N+1}-ΔE^N:

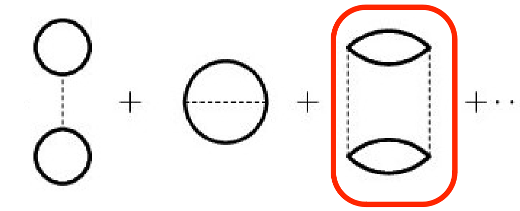


0

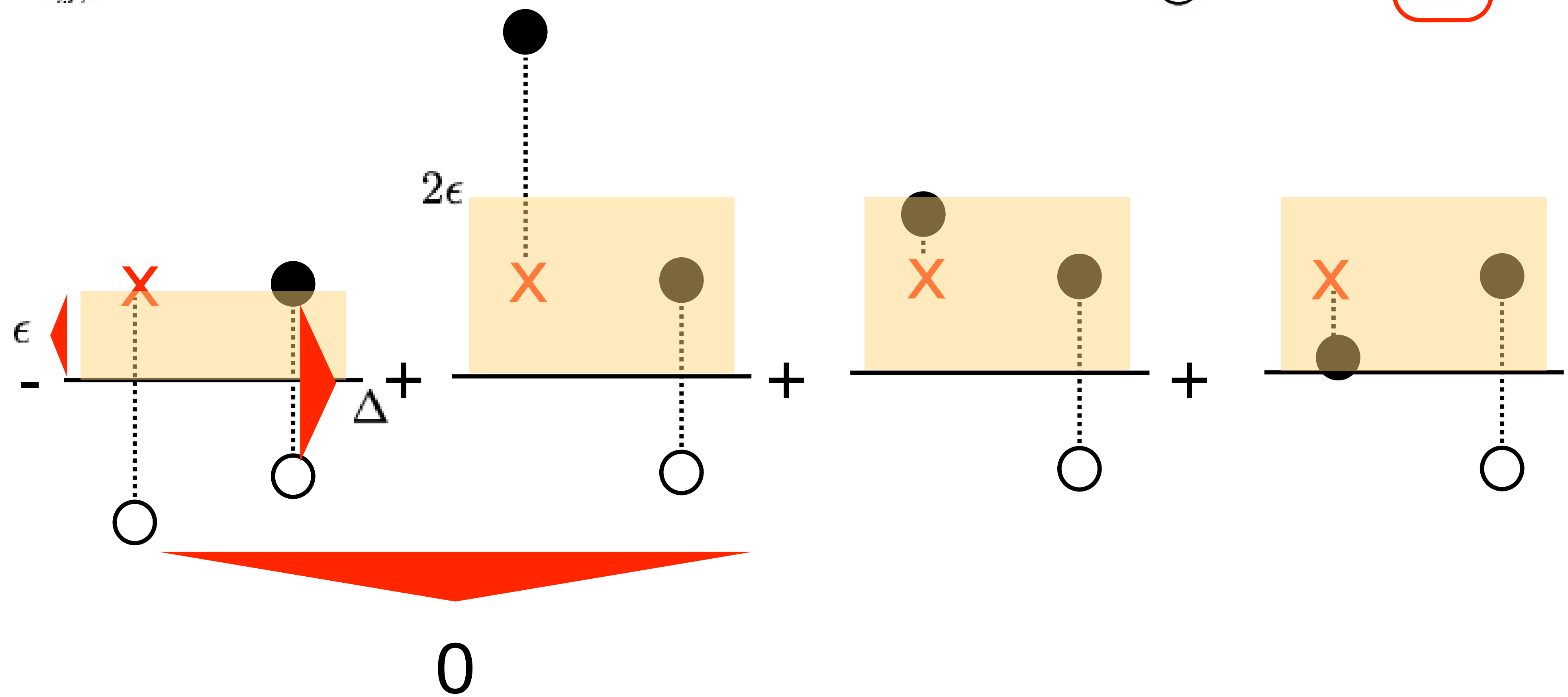
$$\sim \int_0^{\epsilon} dx\left(\frac{1}{\Delta+x}+\frac{1}{\Delta-x}\right) = 2\,\mathrm{th}^{-1}\left(\frac{\epsilon}{\Delta}\right) \sim \epsilon$$

2nd order perturbation theory (small U)

$$\Delta E^{N+1} - \Delta E^{N} = -\frac{U^2}{V^3}\sum_{i,j,k}(1-n_i)n_j\left[\frac{(1-n_k)}{\epsilon_i-\epsilon_j+\epsilon_k-\epsilon} - \frac{n_k}{\epsilon_i-\epsilon_j+\epsilon-\epsilon_k}\right]$$



ΔE^{N+1}-ΔE^{N}:



$$\sim \int_0^C d\Delta \int_0^\epsilon dx\left(\frac{\Delta}{\Delta+x}+\frac{\Delta}{\Delta-x}\right) =$$

$$= 2\int_0^C d\Delta\int_0^\epsilon dx + \int_0^C d\Delta\int_0^\epsilon dx\,\frac{2x^2}{(\Delta-x)(\Delta+x)} =$$

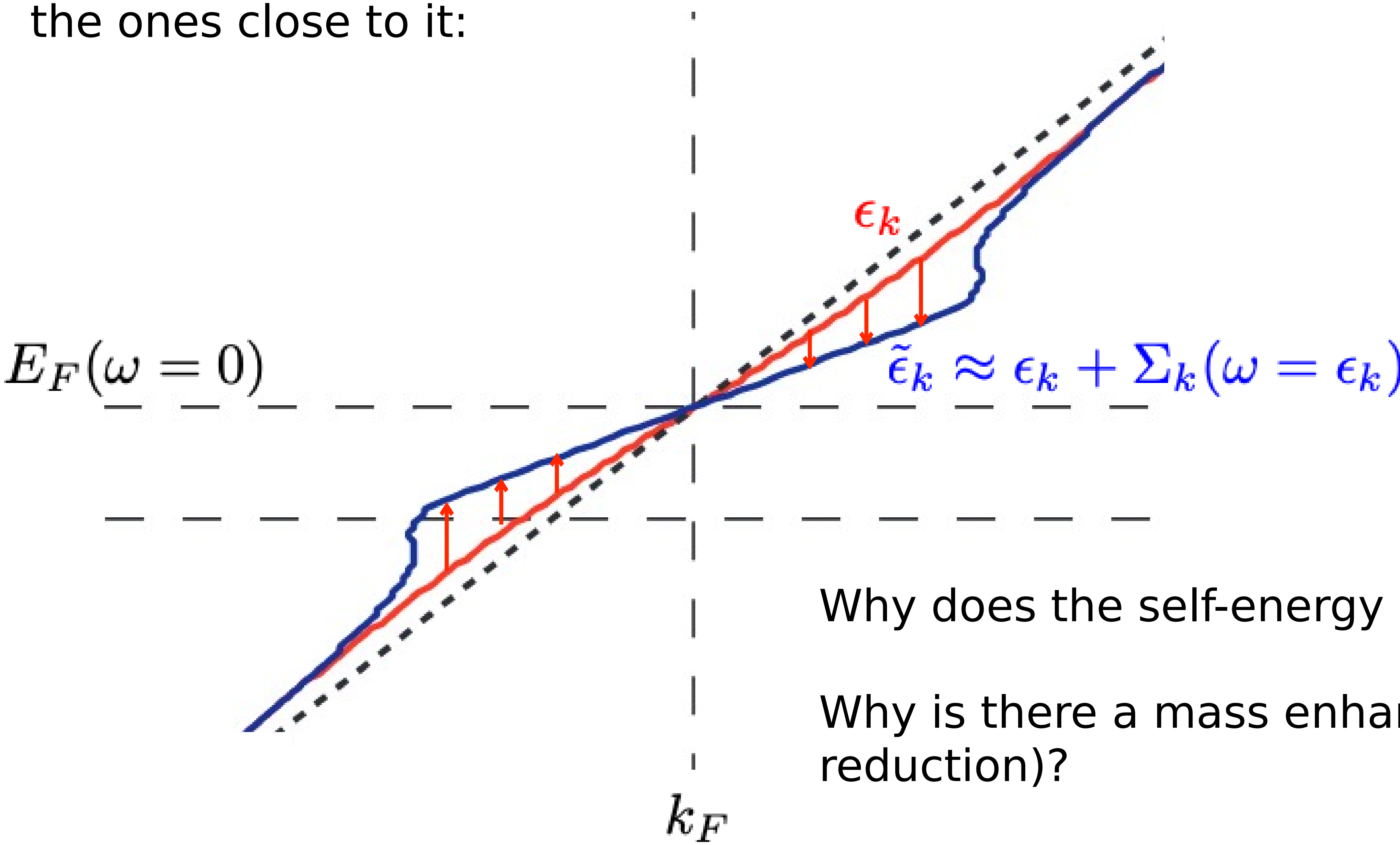
$$= 2C\epsilon + \int_0^\epsilon dx\int_{-C}^{C} d\Delta\,\frac{x^2}{(\Delta-x)(\Delta+x)}$$

$$= 2C\epsilon + \int_0^\epsilon dx\left[\int_{-\infty}^{\infty} d\Delta\,\frac{x^2}{(\Delta-x)(\Delta+x)} - 2\int_C^\infty d\Delta\,\frac{x^2}{(\Delta-x)(\Delta+x)}\right]$$

$$\approx 2C\epsilon - 2\int_0^\epsilon\int_C^\infty \frac{x^2}{\Delta^2} = \boxed{2C\epsilon - \frac{2}{3C}\epsilon^3}$$

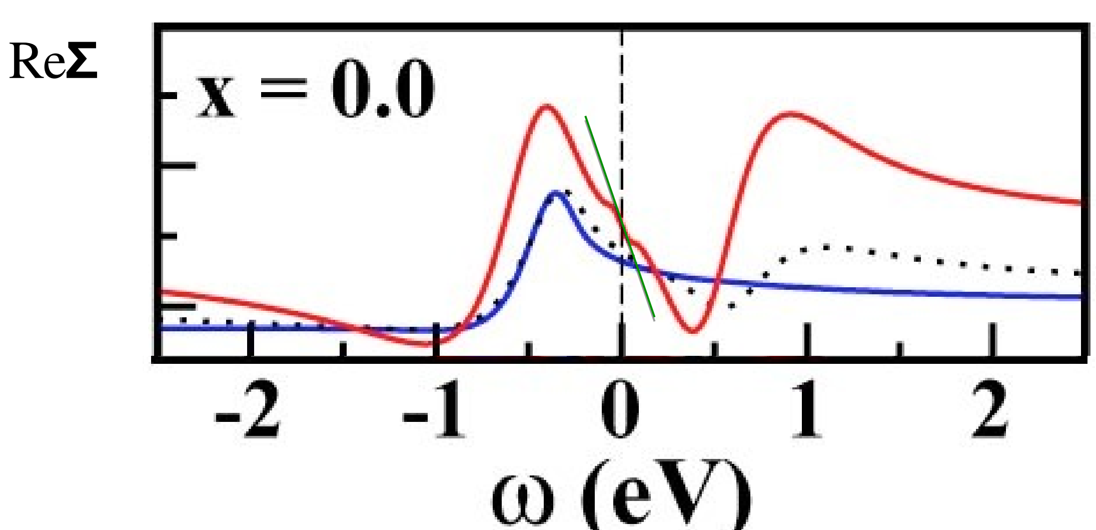
Electron mass enhancement

Electronic energies further from the Fermi level are renormalized (**reduced**) more than the ones close to it:



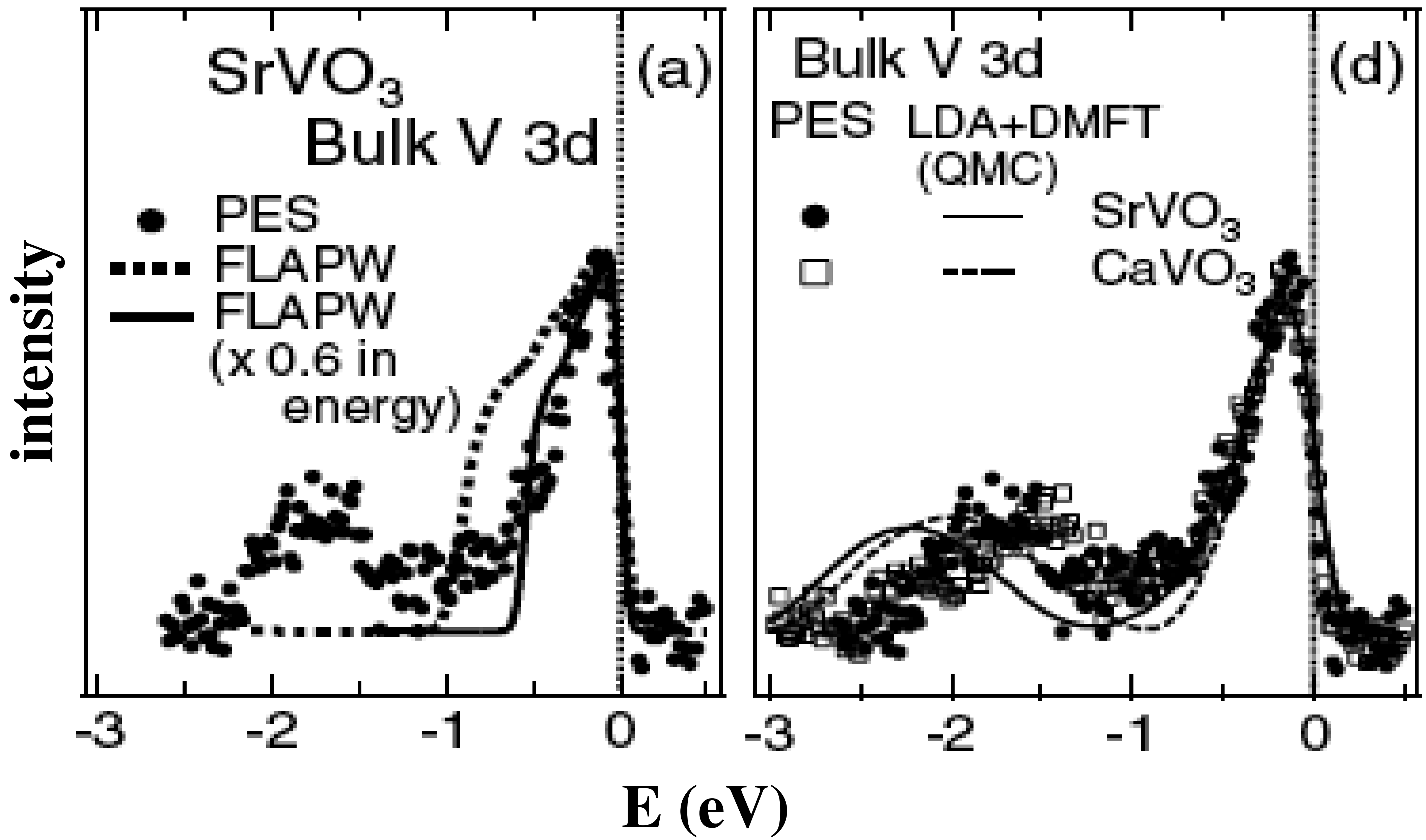
Why does the self-energy change sign at E_F?

Why is there a mass enhancement (and not reduction)?



Comparison to experiment

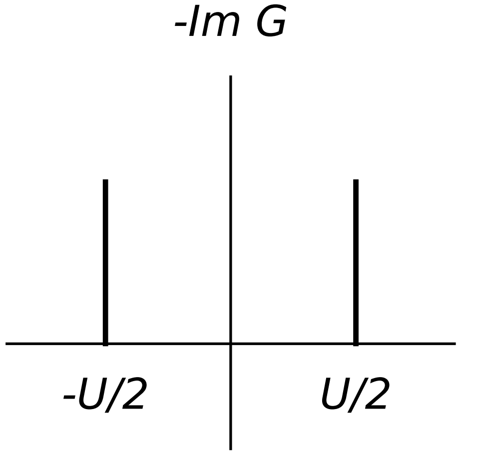
Photoemission spectroscopy vs LDA+DMFT



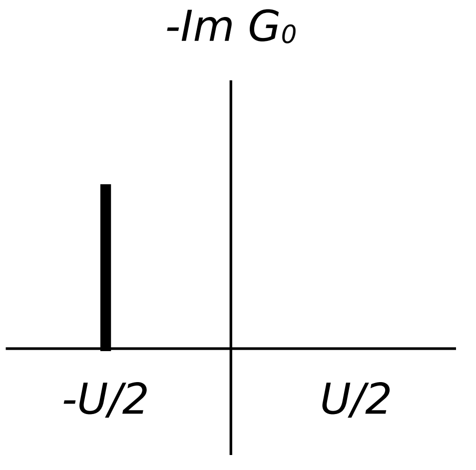
Sekiyama, PRL ***93****, 156402 (2004)*

Atomic limit n=1 (large U)

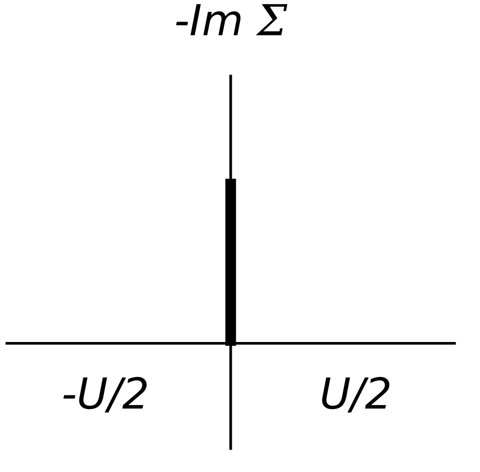
$$G(\omega) = \frac{1}{2}\left(\frac{1}{\omega + U/2} + \frac{1}{\omega - U/2}\right) = \frac{\omega}{\omega^2 - (U/2)^2}$$



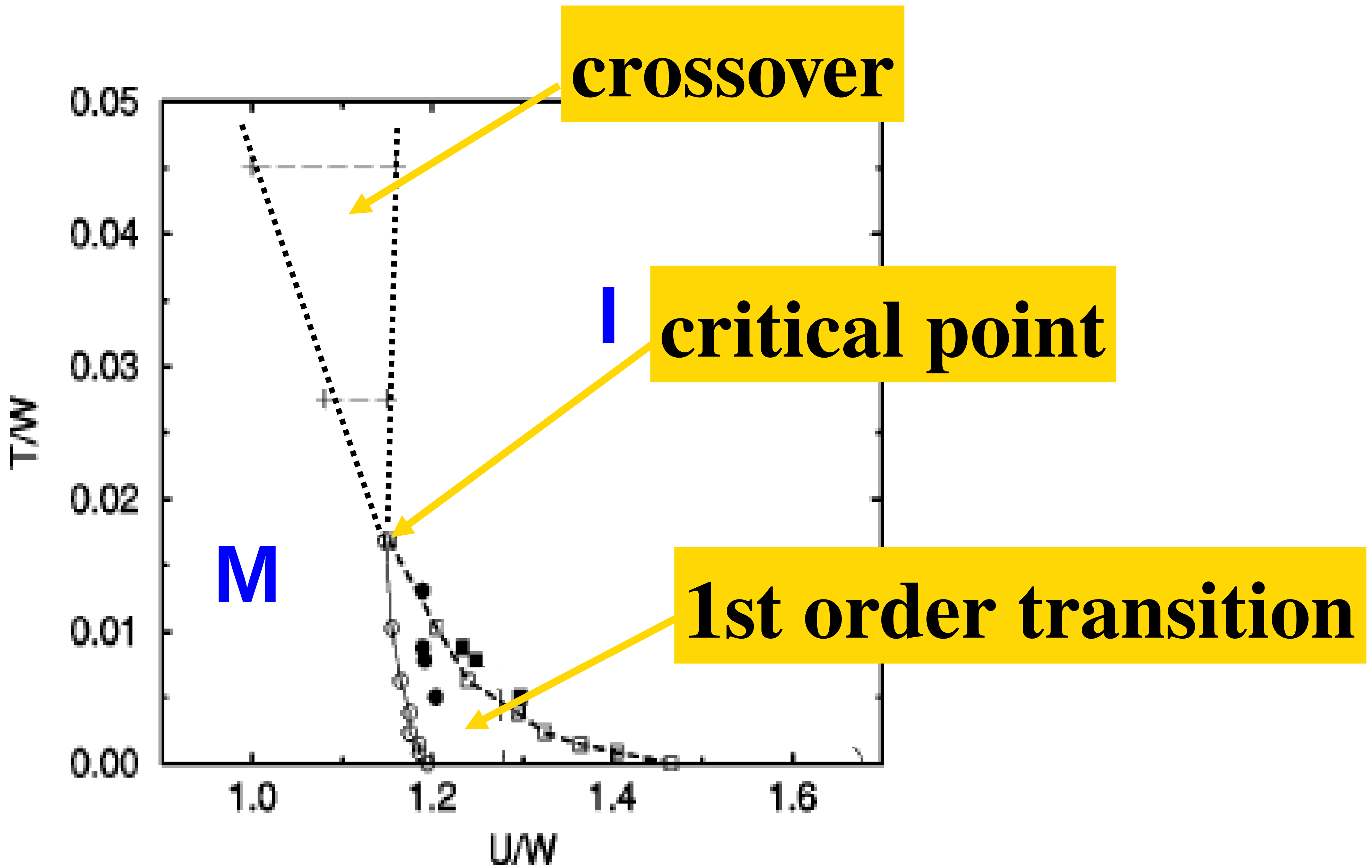
$$G_0(\omega) = \frac{1}{\omega + U/2}$$



$$\Sigma(\omega) = G_0^{-1}(\omega) - G^{-1}(\omega) = U/2 + \frac{(U/2)^2}{\omega}$$

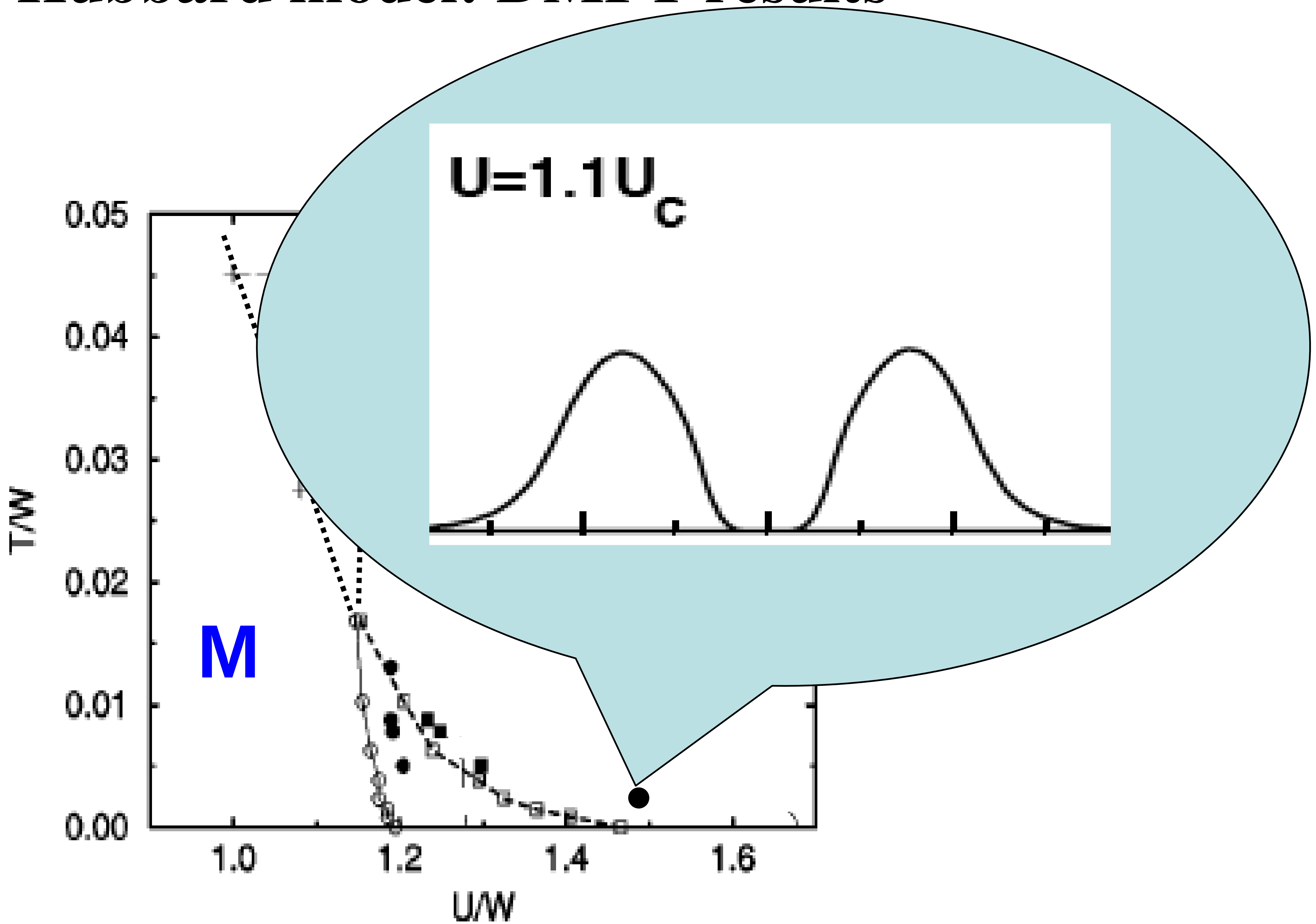


Hubbard model: DMFT results



*Bulla et al. PRB **64**, 045103 (2001)*

Hubbard model: DMFT results



Bulla et al. PRB ***64****, 045103 (2001)*

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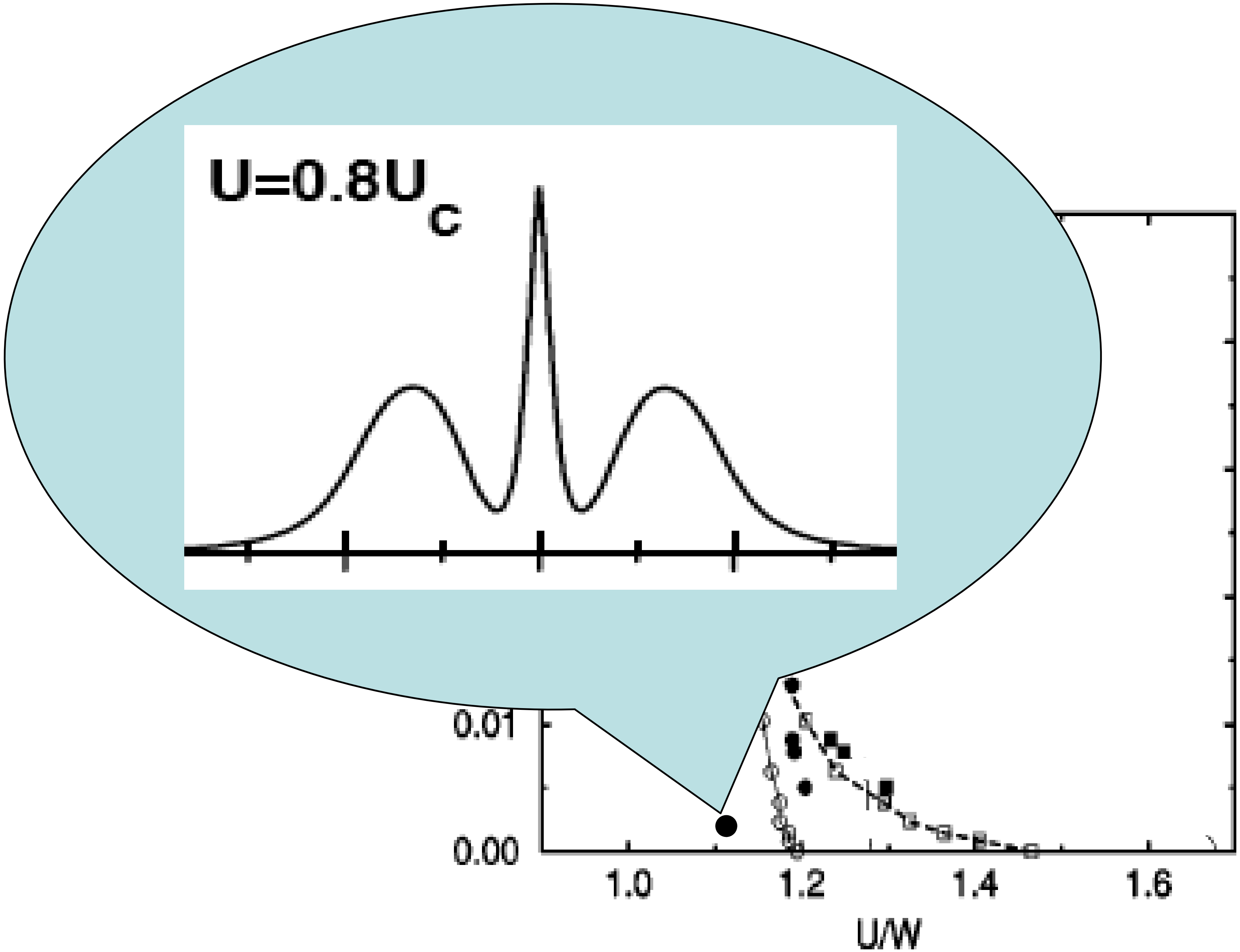
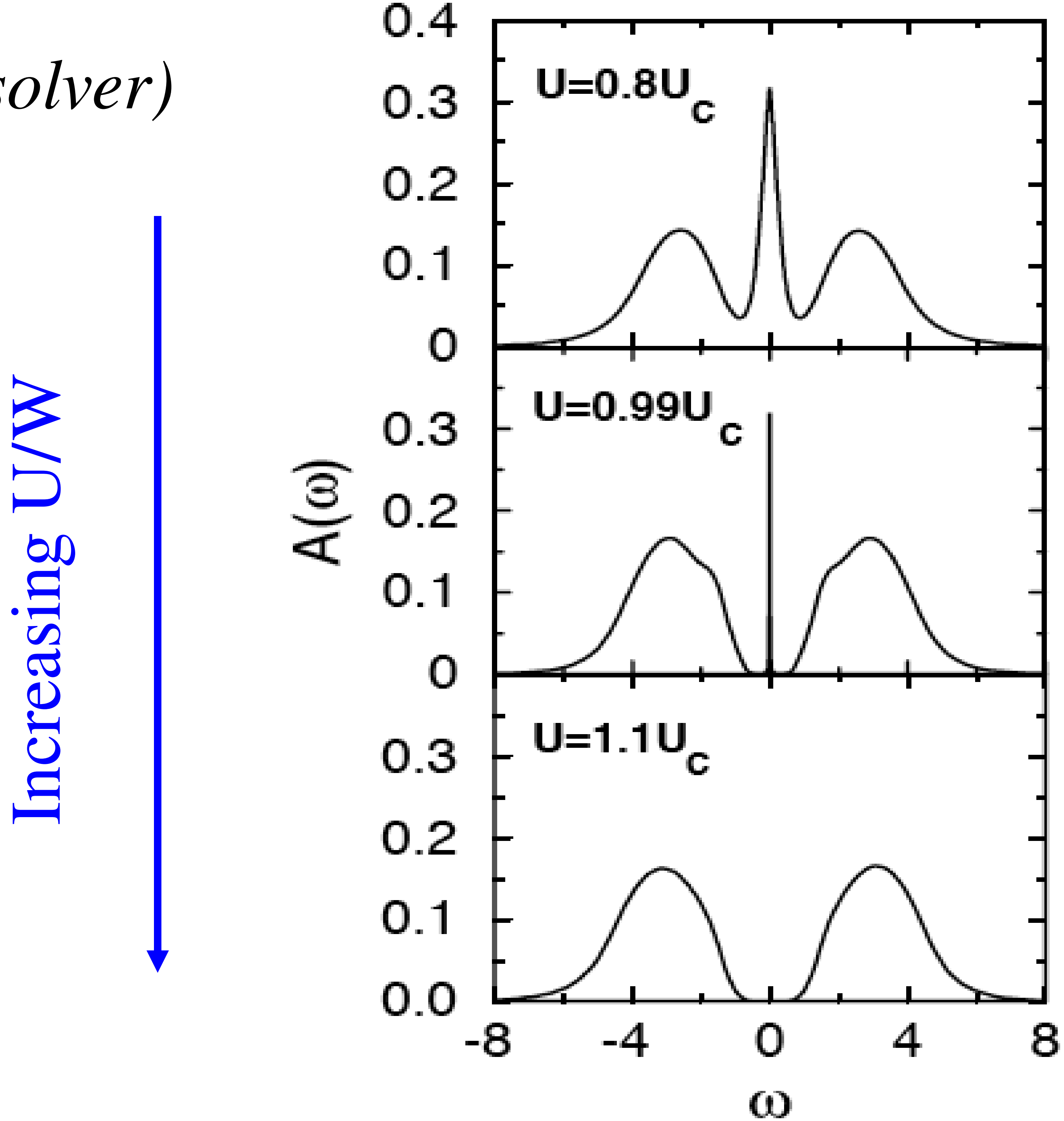


*Bulla et al. PRB **64**, 045103 (2001)*

Single-band Hubbard model D=∞

T=0   *(NRG solver)*

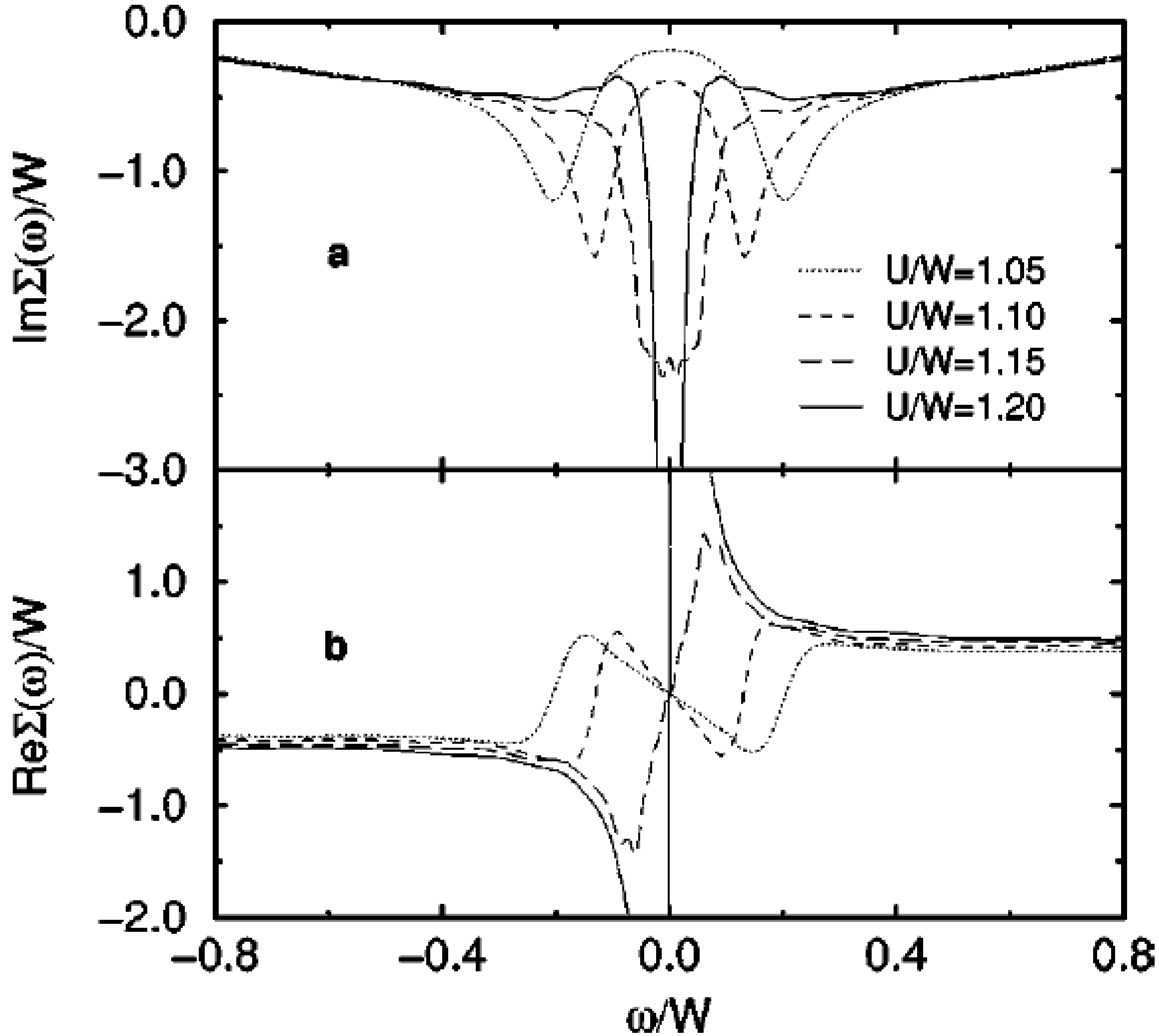


Bulla, PRL ***83****, 136 (1999)*

Hubbard model: metal-insulator transition

$$G_{\mathbf{k}}^{-1}(\omega) = \frac{1}{\omega - \varepsilon - \Sigma(\omega)}$$

self-energy:



- with increasing U quasiparticles become heavier ($m^* \to \infty$)
- in Mott insulator $\Sigma(\omega)$ develops pole inside the band
- in DMFT the gaps opens due to self-consistency

*Bulla et al. PRB **64**, 045103 (2001)*

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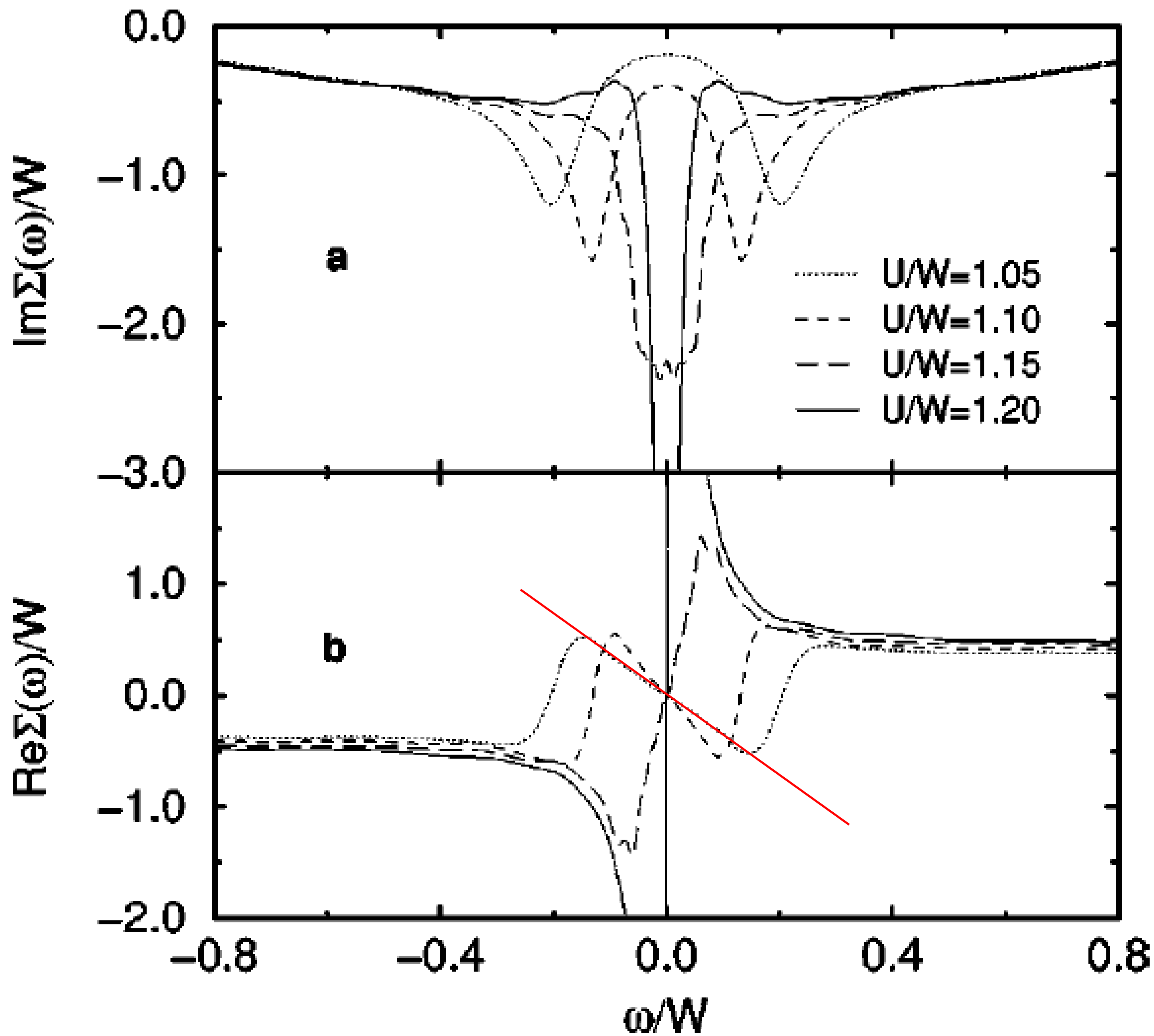

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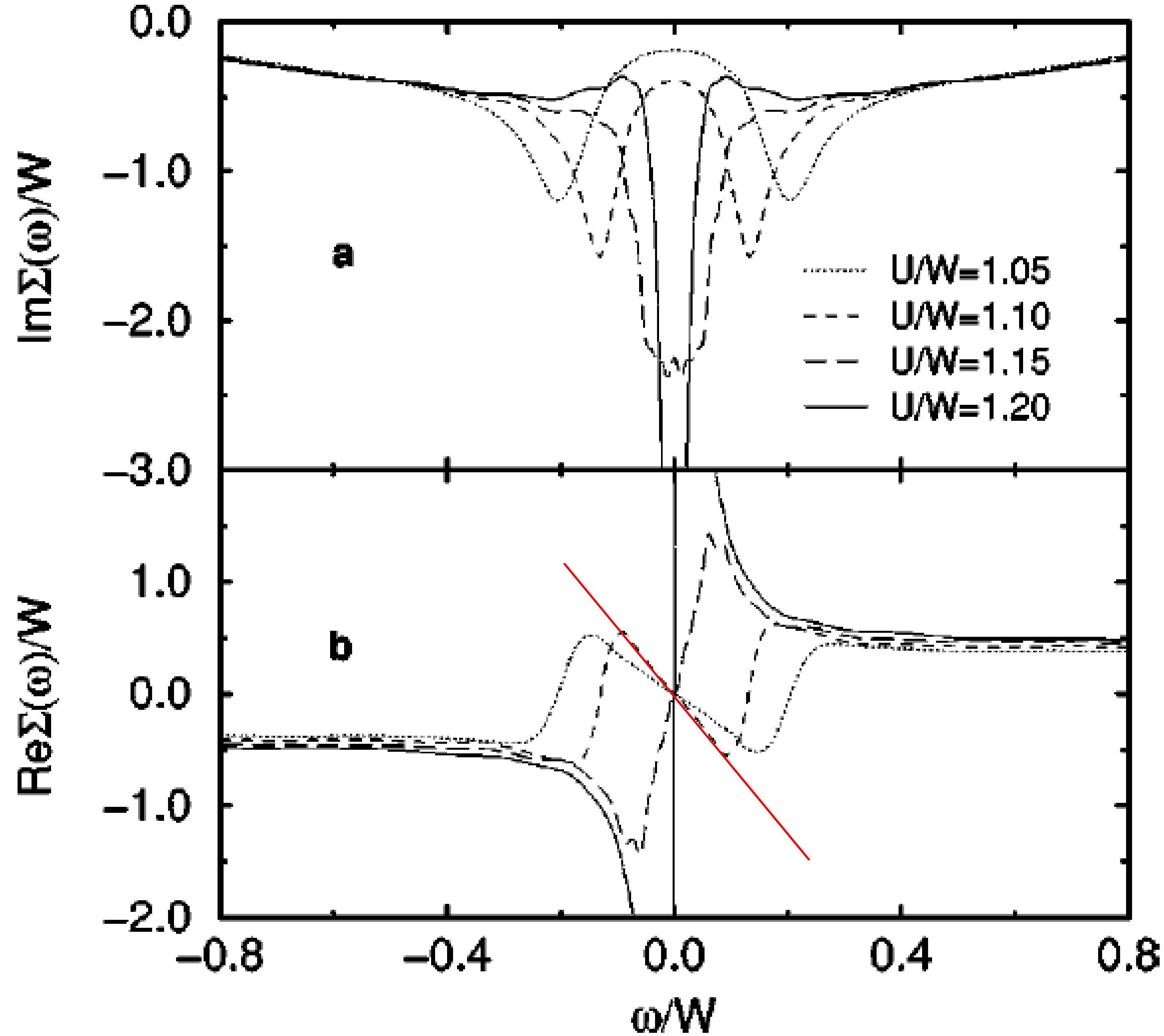

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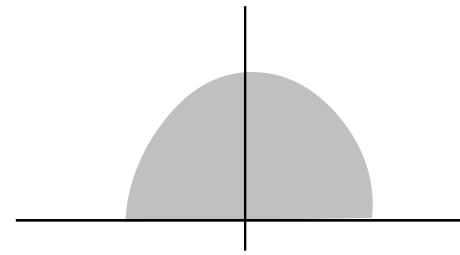
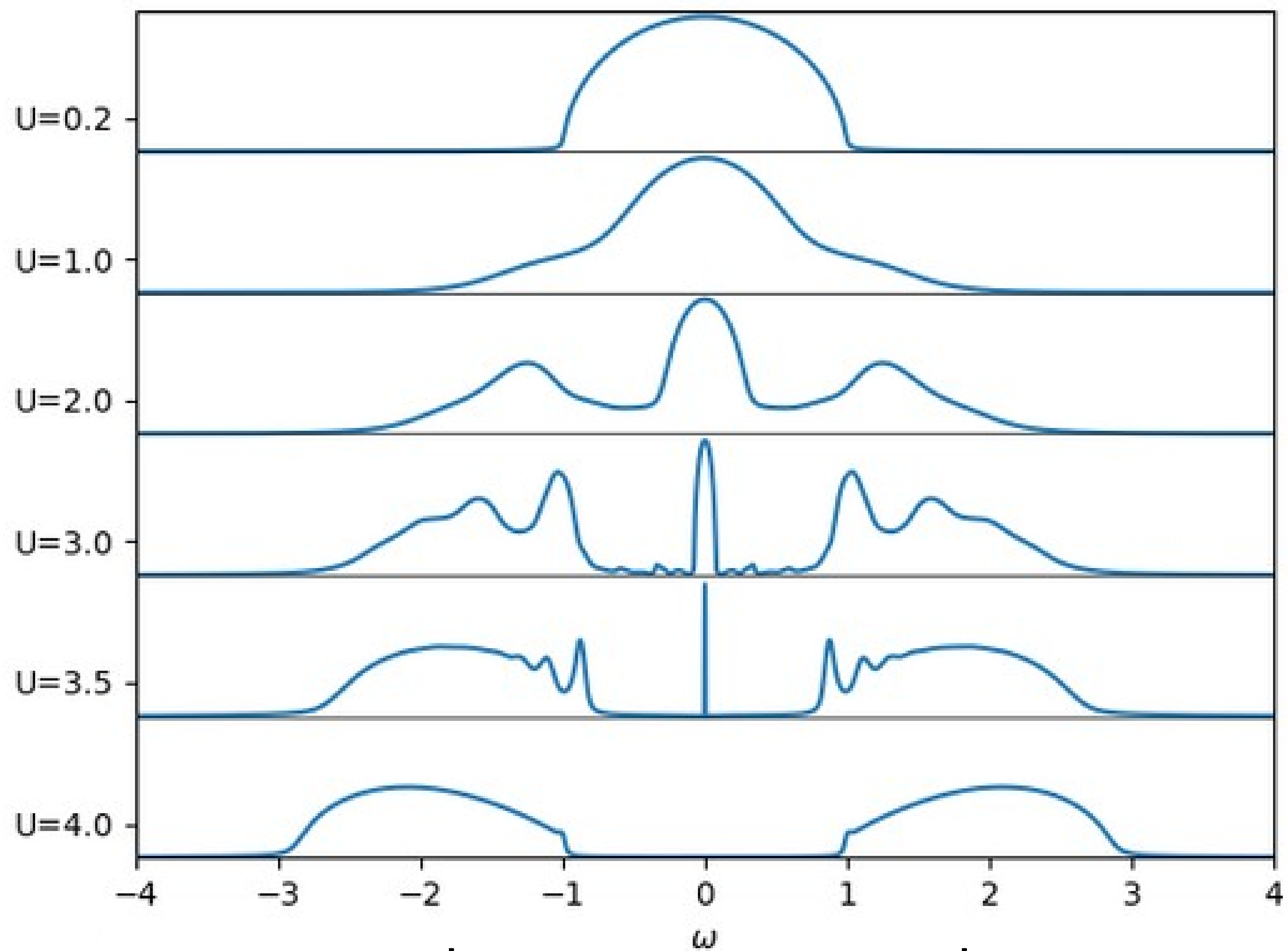
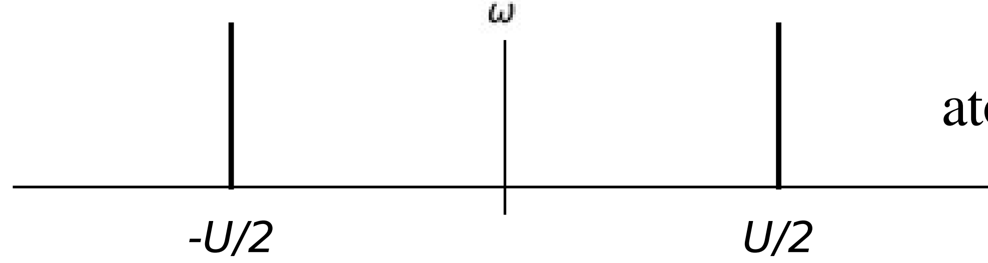


non-interacting limit

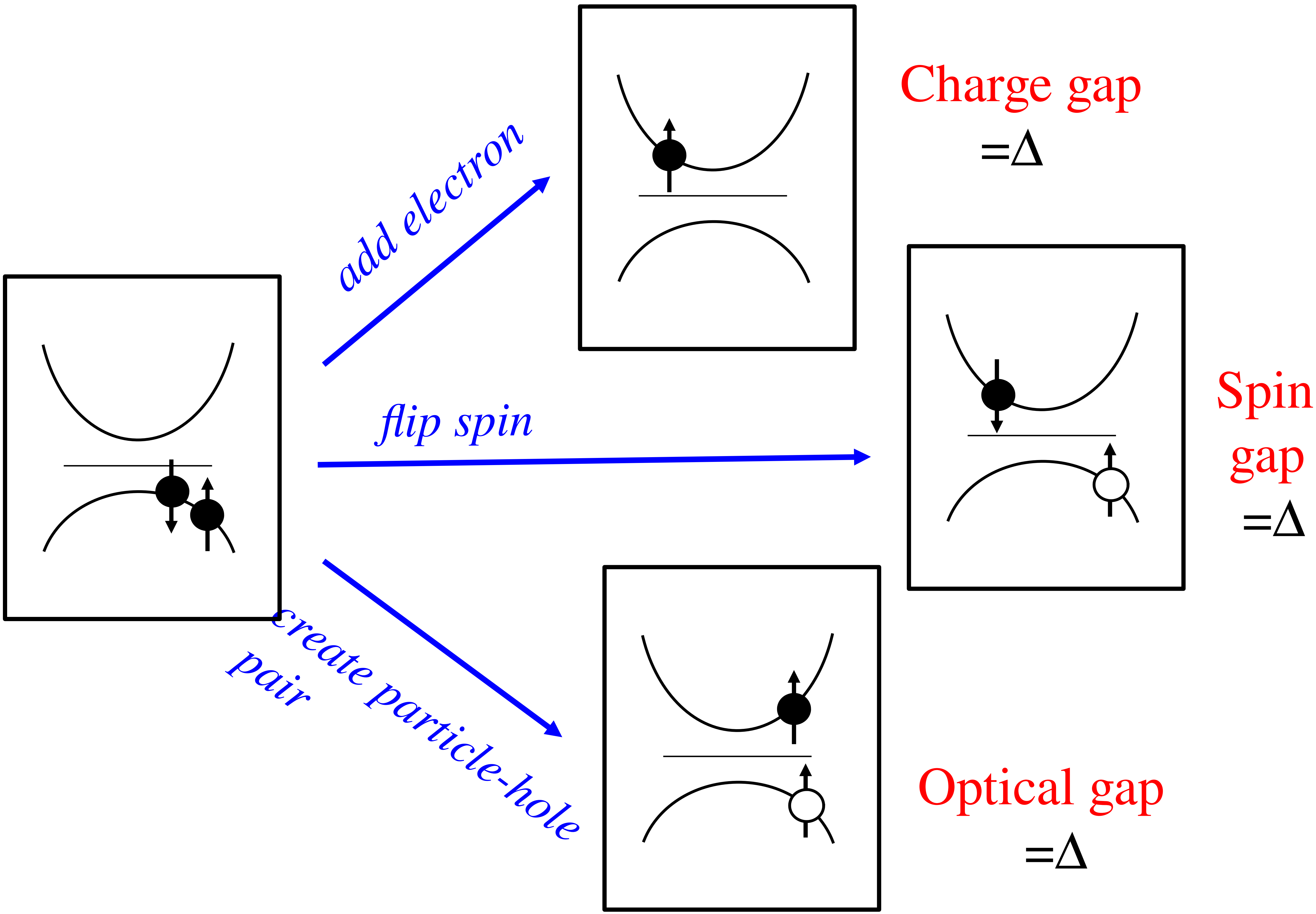




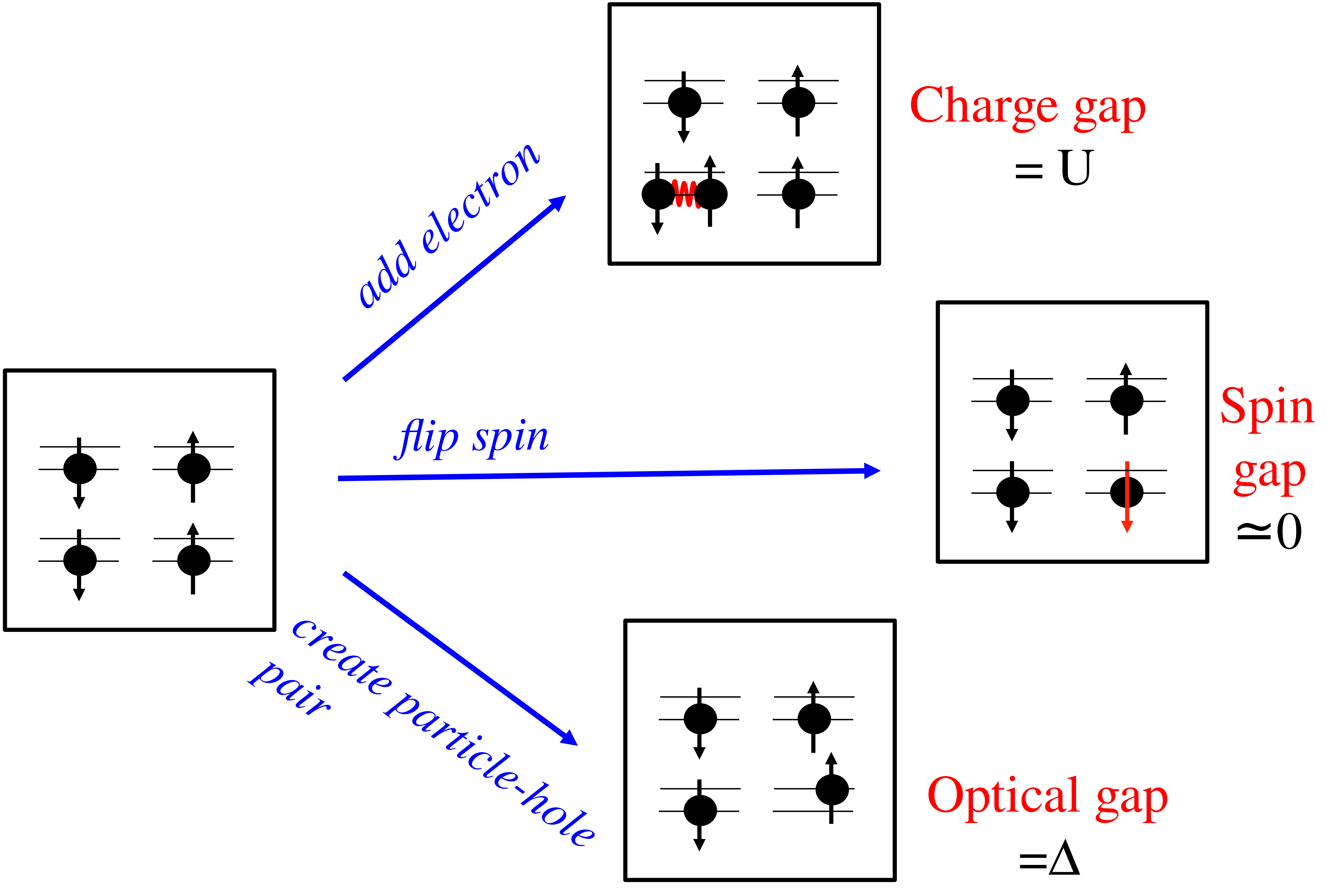
atomic limit

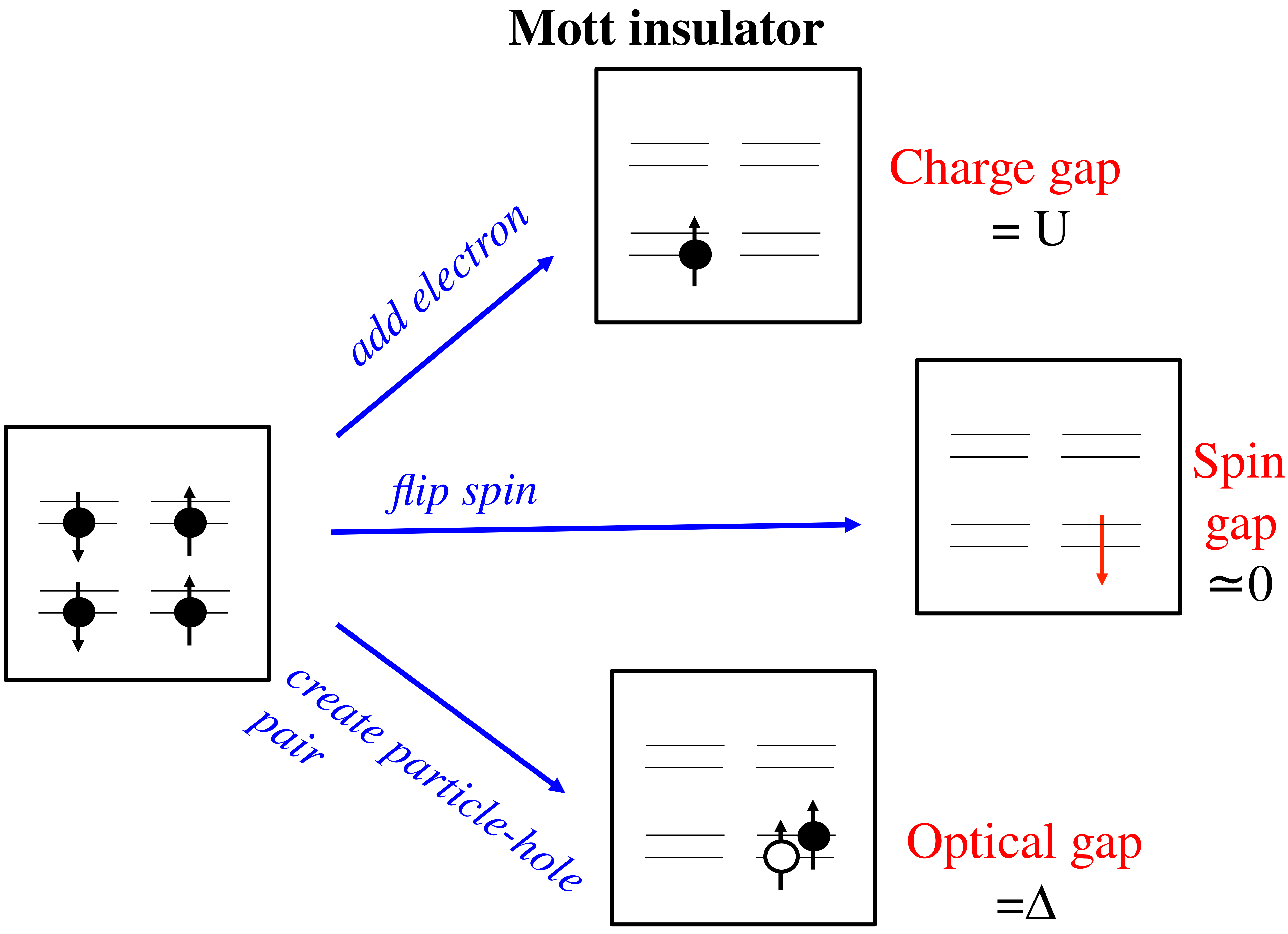
Georges et al., RMP 1996

Band insulator



Mott insulator




Mott insulator
add electron
Charge gap
= U
flip spin
Spin
gap
≃0
create particle-hole
pair
Optical gap
=Δ