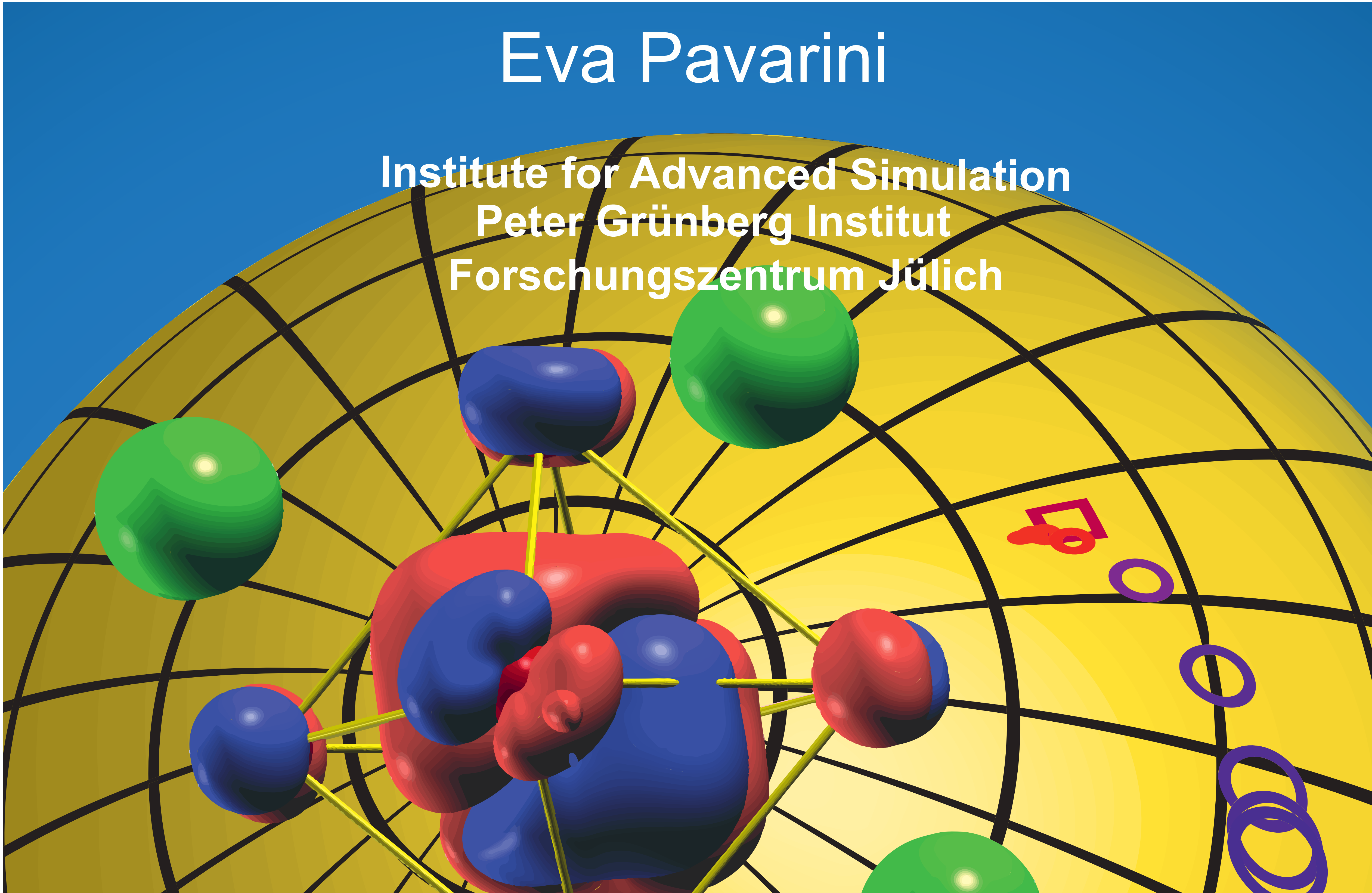
DMFT for Linear Response Functions



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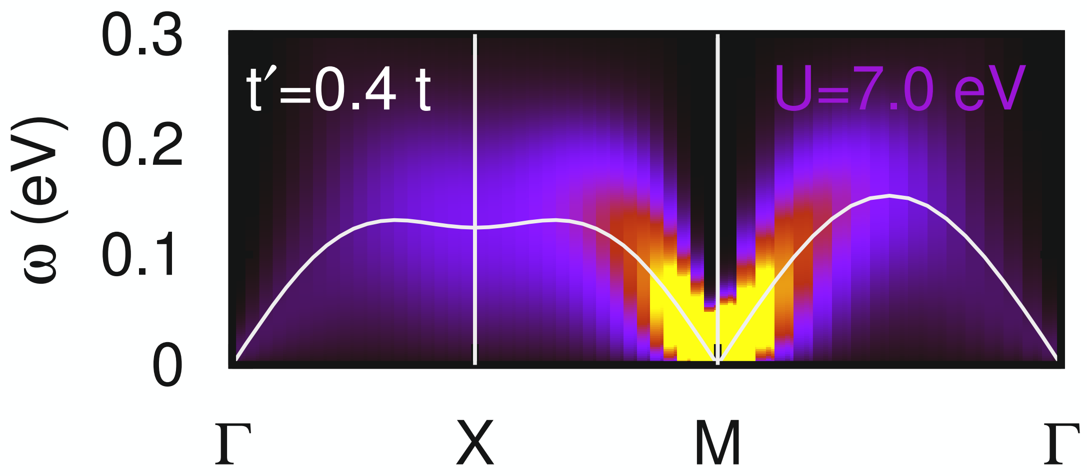
scheme of the lecture

$$\chi(\boldsymbol{q};\omega)$$



I. DMFT and LDA+DMFT

II. linear response functions

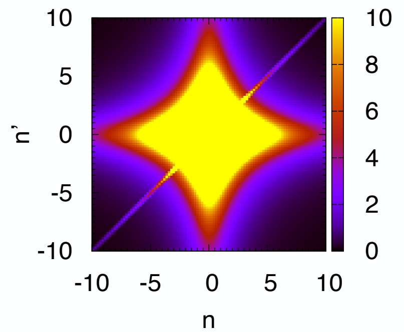
III. magnetic response for the Hubbard model

IV. linear response in DMFT and LDA+DMFT

J. Musshoff, G. Zhang, E. Koch, E. Pavarini
Phys. Rev. B **100**, 045116 (2019)

J. Musshoff, A. Kiani, and E. Pavarini,
Phys. Rev. B 103, 075136 (2021)

E. Pavarini, E. *Riv. Nuovo Cim.* **44**, 597–640 (2021).
https://doi.org/10.1007/s40766-021-00025-8



I: DMFT and LDA+DMFT

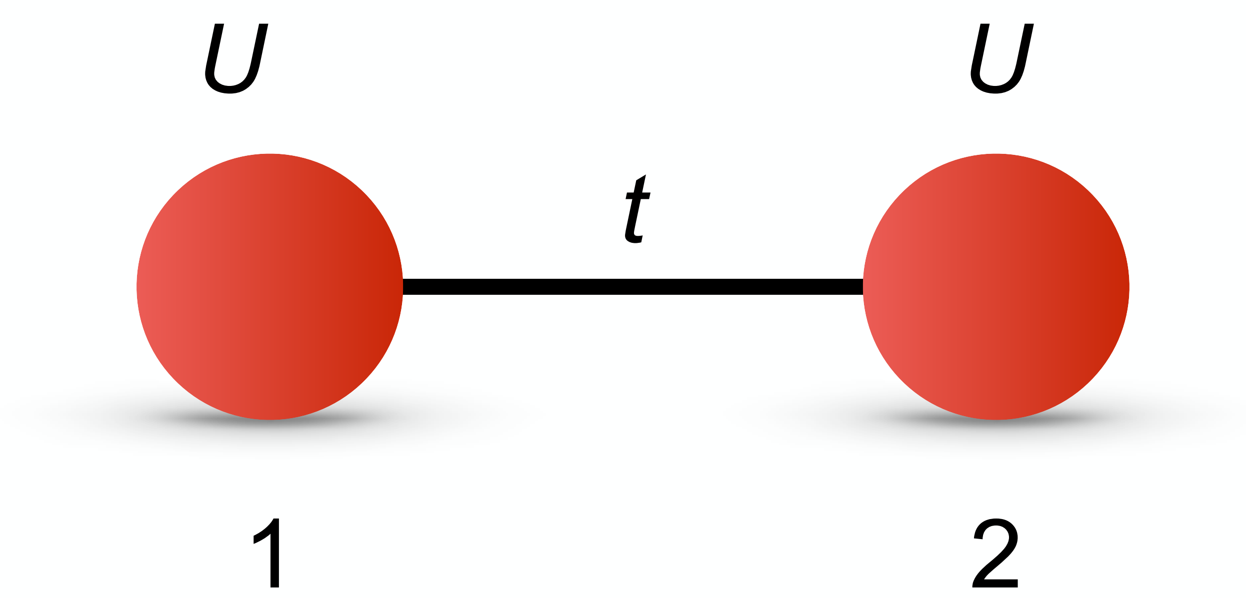
DMFT for the Hubbard dimer

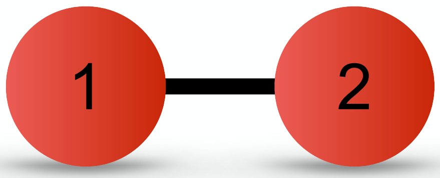
this is a **toy** model: coordination number is one

DMFT is exact for *t=0*, *U=0, for a single correlated site* and in the **infinite dimension** limit

the Hubbard dimer

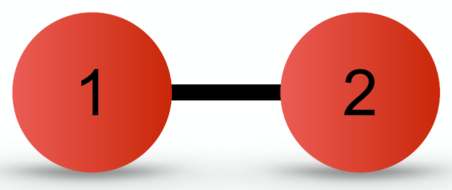
$$\hat{H} = \varepsilon_d \sum_{i\sigma} \hat{n}_{i\sigma} - t \sum_{\sigma} \left(c^{\dagger}_{1\sigma} c_{2\sigma} + c^{\dagger}_{2\sigma} c_{1\sigma} \right) + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$





t=0: exact diagonalization

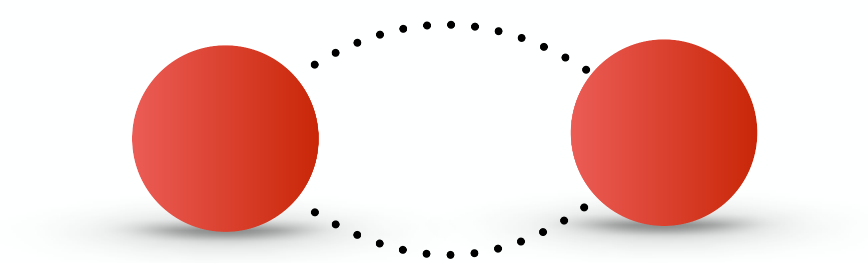
$\|N,S,S_z\rangle$			N	S	$E(N,S)$
$\|0,0,0\rangle$	$=$	$\|0\rangle$	0	0	0
$\|1,1/2,\sigma\rangle_1$	$=$	$c^\dagger_{1\sigma}\|0\rangle$	1	$1/2$	ε_d
$\|1,1/2,\sigma\rangle_2$	$=$	$c^\dagger_{2\sigma}\|0\rangle$	1	$1/2$	ε_d
$\|2,1,1\rangle$	$=$	$c^\dagger_{2\uparrow}c^\dagger_{1\uparrow}\|0\rangle$	2	1	$2\varepsilon_d$
$\|2,1,-1\rangle$	$=$	$c^\dagger_{2\downarrow}c^\dagger_{1\downarrow}\|0\rangle$	2	1	$2\varepsilon_d$
$\|2,1,0\rangle$	$=$	$\frac{1}{\sqrt{2}}\left[c^\dagger_{1\uparrow}c^\dagger_{2\downarrow}+c^\dagger_{1\downarrow}c^\dagger_{2\uparrow}\right]\|0\rangle$	2	1	$2\varepsilon_d$
$\|2,0,0\rangle_0$	$=$	$\frac{1}{\sqrt{2}}\left[c^\dagger_{1\uparrow}c^\dagger_{2\downarrow}-c^\dagger_{1\downarrow}c^\dagger_{2\uparrow}\right]\|0\rangle$	2	0	$2\varepsilon_d$
$\|2,0,0\rangle_1$	$=$	$c^\dagger_{1\uparrow}c^\dagger_{1\downarrow}\|0\rangle$	2	0	$2\varepsilon_d+U$
$\|2,0,0\rangle_2$	$=$	$c^\dagger_{2\uparrow}c^\dagger_{2\downarrow}\|0\rangle$	2	0	$2\varepsilon_d+U$
$\|3,1/2,\sigma\rangle_1$	$=$	$c^\dagger_{1\sigma}c^\dagger_{2\uparrow}c^\dagger_{2\downarrow}\|0\rangle$	3	$1/2$	$3\varepsilon_d+U$
$\|3,1/2,\sigma\rangle_2$	$=$	$c^\dagger_{2\sigma}c^\dagger_{1\uparrow}c^\dagger_{1\downarrow}\|0\rangle$	3	$1/2$	$3\varepsilon_d+U$
$\|4,0,0\rangle$	$=$	$c^\dagger_{1\uparrow}c^\dagger_{1\downarrow}c^\dagger_{2\uparrow}c^\dagger_{2\downarrow}\|0\rangle$	4	0	$4\varepsilon_d+2U$

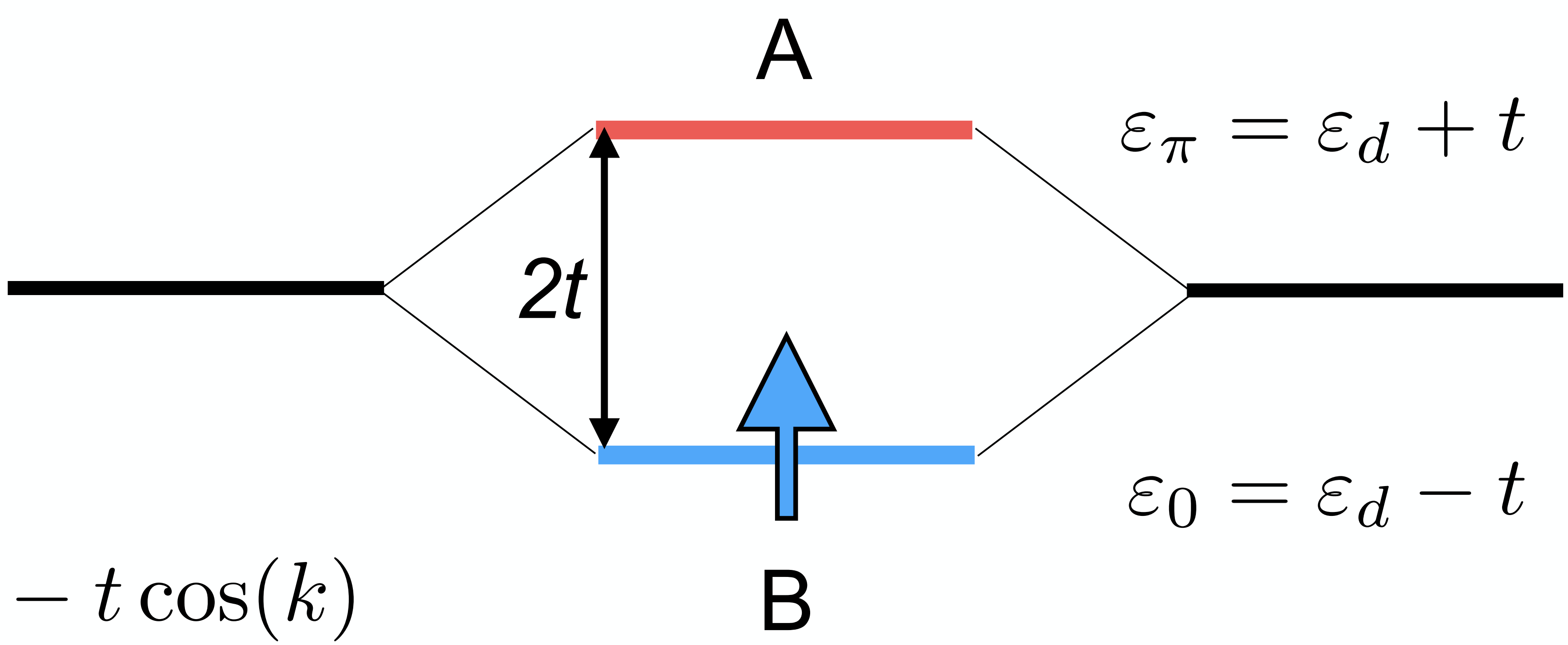


finite *t*: exact diagonalization

N=1

$\|1,S,S_z\rangle_\alpha$	$E_\alpha(1,S)$	$d_\alpha(1,S)$
$\|1,1/2,\sigma\rangle_+ = \frac{1}{\sqrt{2}}\left(\|1,1/2,\sigma\rangle_1 - \|1,1/2,\sigma\rangle_2\right)$	$\varepsilon_d + t$	2
$\|1,1/2,\sigma\rangle_- = \frac{1}{\sqrt{2}}\left(\|1,1/2,\sigma\rangle_1 + \|1,1/2,\sigma\rangle_2\right)$	$\varepsilon_d - t$	2

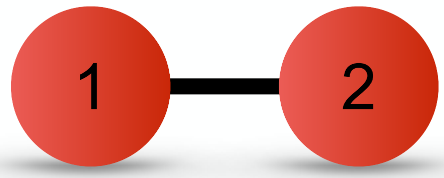




$$\varepsilon_\pi = \varepsilon_d + t$$ **k=π**

$$\varepsilon_0 = \varepsilon_d - t$$ **k=0**

$$\varepsilon_k = \varepsilon_d - t\cos(k)$$



exact diagonalization

S=1 states | S=0 states | half filling (N=2)

$$
\hat{H}_2(\varepsilon_d, U, t) = \begin{pmatrix}
2\varepsilon_d & 0 & 0 & 0 & 0 & 0 \\
0 & 2\varepsilon_d & 0 & 0 & 0 & 0 \\
0 & 0 & 2\varepsilon_d & 0 & 0 & 0 \\
0 & 0 & 0 & 2\varepsilon_d & -\sqrt{2}t & -\sqrt{2}t \\
0 & 0 & 0 & -\sqrt{2}t & 2\varepsilon_d + U & 0 \\
0 & 0 & 0 & -\sqrt{2}t & 0 & 2\varepsilon_d + U
\end{pmatrix}
$$

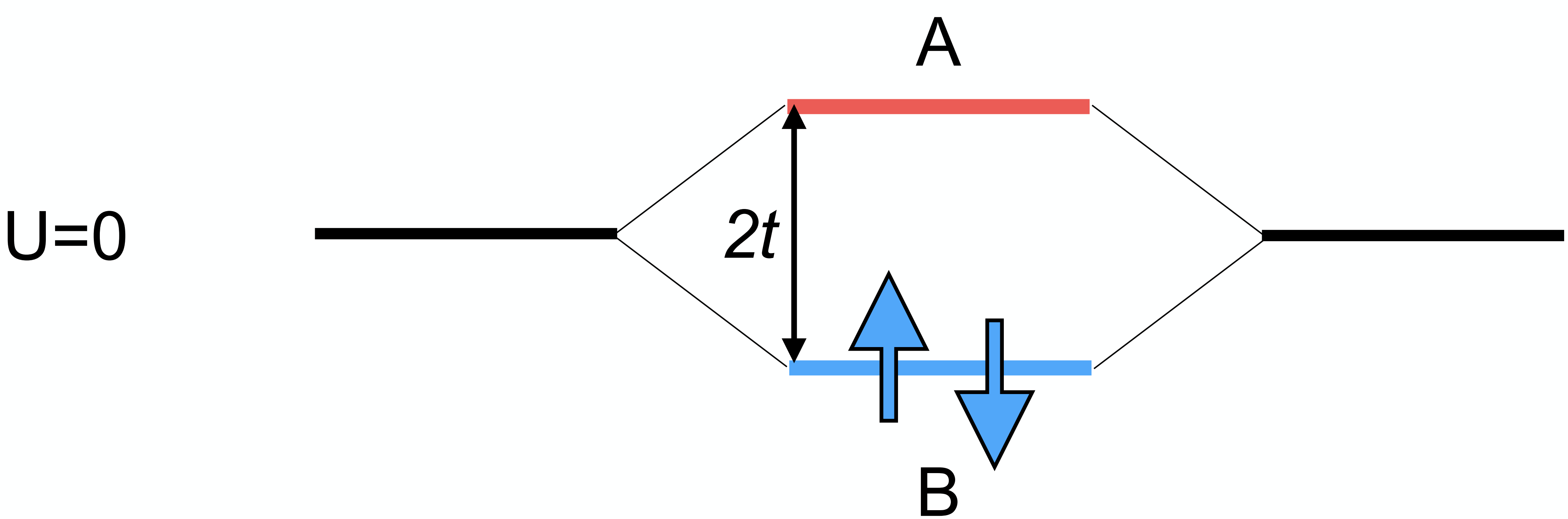
$\lvert 2,1,1\rangle$	$=$	$c^\dagger_{2\uparrow} c^\dagger_{1\uparrow} \lvert 0\rangle$	2	1	$2\varepsilon_d$
$\lvert 2,1,-1\rangle$	$=$	$c^\dagger_{2\downarrow} c^\dagger_{1\downarrow} \lvert 0\rangle$	2	1	$2\varepsilon_d$
$\lvert 2,1,0\rangle$	$=$	$\frac{1}{\sqrt{2}} \left[c^\dagger_{1\uparrow} c^\dagger_{2\downarrow} + c^\dagger_{1\downarrow} c^\dagger_{2\uparrow} \right] \lvert 0\rangle$	2	1	$2\varepsilon_d$
$\lvert 2,0,0\rangle_0$	$=$	$\frac{1}{\sqrt{2}} \left[c^\dagger_{1\uparrow} c^\dagger_{2\downarrow} - c^\dagger_{1\downarrow} c^\dagger_{2\uparrow} \right] \lvert 0\rangle$	2	0	$2\varepsilon_d$
$\lvert 2,0,0\rangle_1$	$=$	$c^\dagger_{1\uparrow} c^\dagger_{1\downarrow} \lvert 0\rangle$	2	0	$2\varepsilon_d + U$
$\lvert 2,0,0\rangle_2$	$=$	$c^\dagger_{2\uparrow} c^\dagger_{2\downarrow} \lvert 0\rangle$	2	0	$2\varepsilon_d + U$

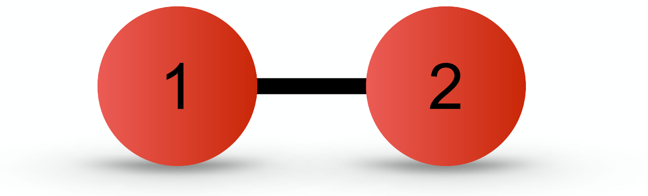
finite t: exact diagonalization

half filling (N=2)

$\|2,S,S_z\rangle_\alpha$	$E_\alpha(2,S)$	$d_\alpha(2,S)$
$\|2,0,0\rangle_+ = a_1\|2,0,0\rangle_0 - \frac{a_2}{\sqrt{2}}\big(\|2,0,0\rangle_1 + \|2,0,0\rangle_2\big)$	$2\varepsilon_d + \frac{1}{2}\left(U+\Delta(t,U)\right)$	1
$\|2,0,0\rangle_o = \frac{1}{\sqrt{2}}\big(\|2,0,0\rangle_1 - \|2,0,0\rangle_2\big)$	$2\varepsilon_d + U$	1
$\|2,1,m\rangle_o = \|2,1,m\rangle$	$2\varepsilon_d$	3
$\|2,0,0\rangle_- = a_2\|2,0,0\rangle_0 + \frac{a_1}{\sqrt{2}}\big(\|2,0,0\rangle_1 + \|2,0,0\rangle_2\big)$	$2\varepsilon_d + \frac{1}{2}\left(U-\Delta(t,U)\right)$	1

$$\Delta(t,U) = \sqrt{U^2 + 16t^2}$$





the ground state (N=2)

$$|G\rangle_H = \frac{a_2(t,U)}{\sqrt{2}} \left(c^\dagger_{1\uparrow} c^\dagger_{2\downarrow} - c^\dagger_{1\downarrow} c^\dagger_{2\uparrow} \right) |0\rangle + \frac{a_1(t,U)}{\sqrt{2}} \left(c^\dagger_{1\uparrow} c^\dagger_{1\downarrow} + c^\dagger_{2\uparrow} c^\dagger_{2\downarrow} \right) |0\rangle$$

$$a_1^2(t,U) = \frac{1}{\Delta(t,U)} \frac{\Delta(t,U) - U}{2}, \qquad a_2^2(t,U) = \frac{4t^2}{\Delta(t,U)} \frac{2}{\Delta(t,U) - U},$$

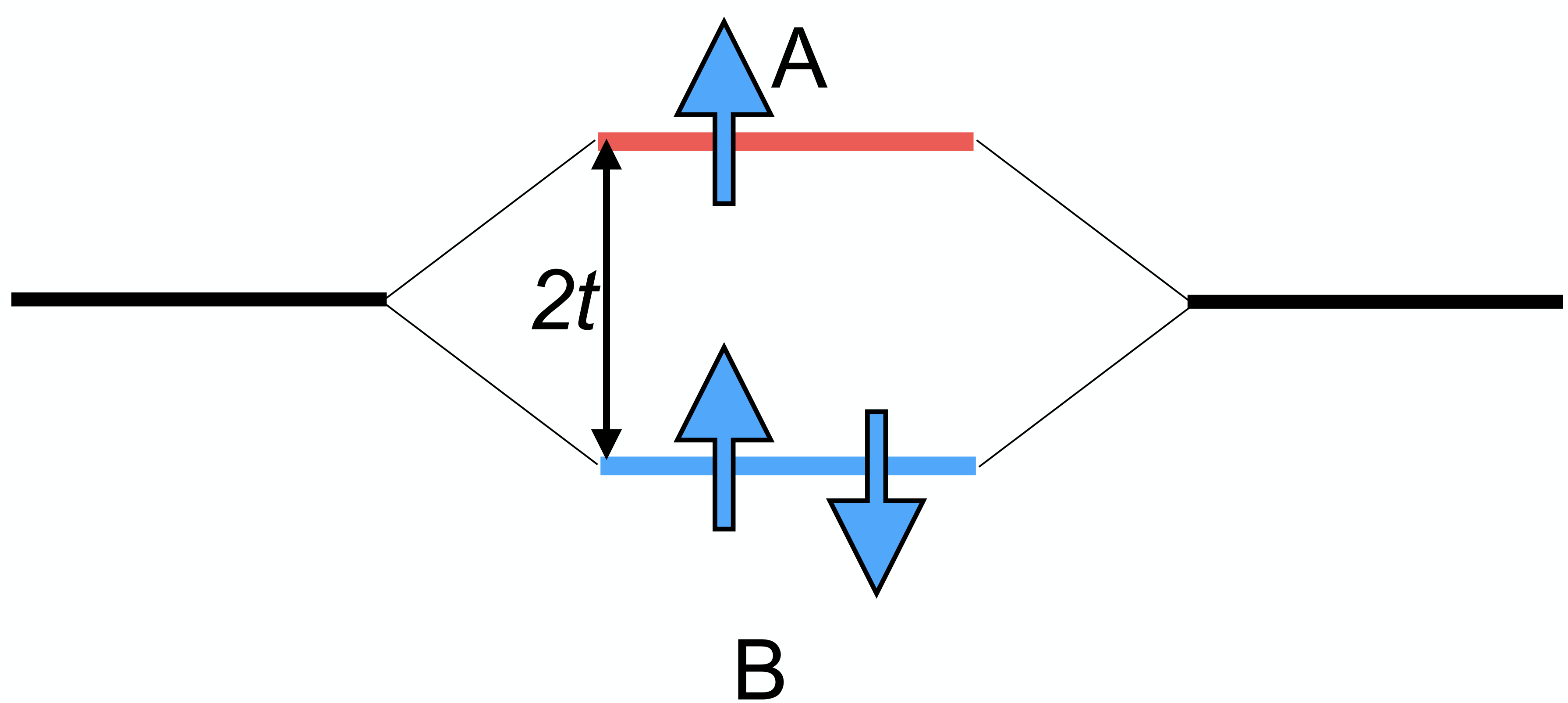
$$\Delta(t,U) = \sqrt{U^2 + 16t^2}$$

$$E_0(2) = 2\varepsilon_d + \frac{1}{2}\left(U - \Delta(t,U)\right)$$

finite t: exact diagonalization

N=3

$\lvert 3,S,S_z\rangle_\alpha$	$E_\alpha(3)$	$d_\alpha(3,S)$
$\lvert 3,1/2,\sigma\rangle_+ = \frac{1}{\sqrt{2}}\left(\lvert 1,1/2,\sigma\rangle_1 + \lvert 1,1/2,\sigma\rangle_2\right)$	$3\varepsilon_d + U + t$	2
$\lvert 3,1/2,\sigma\rangle_- = \frac{1}{\sqrt{2}}\left(\lvert 1,1/2,\sigma\rangle_1 - \lvert 1,1/2,\sigma\rangle_2\right)$	$3\varepsilon_d + U - t$	2



Lehmann representation

$$G^{\sigma}_{i,i}(i\nu_n) = -\int_0^{\beta} d\tau \, e^{i\nu_n \tau} \langle \mathcal{T} c_{i\sigma}(\tau) c^{\dagger}_{i\sigma}(0) \rangle,$$

fermionic
Matsubara frequency

imaginary time

$$G^{\sigma}_{i,i}(i\nu_n) = \frac{1}{Z} \sum_{ll'NN'} \frac{e^{-\Delta E_{l'}(N')\beta} + e^{-\Delta E_l(N)\beta}}{i\nu_n + \Delta E_l(N) - \Delta E_{l'}(N')} \left| \langle N'_{l'} | c^{\dagger}_{i\sigma} | N_l \rangle \right|^2.$$

$$\Delta E_l(N) = E_l(N) - \mu N$$

the local Green function

using Lehmann representation

$$\mu = \varepsilon_d + \frac{U}{2}$$

d¹ ➡ d⁰

$$|\langle 1|c_\sigma|2\rangle|^2$$

$$G^\sigma_{i,i}(i\nu_n) = \frac{1}{4}\Bigg(\frac{1+w(t,U)}{i\nu_n - (E_0(2) - \varepsilon_d + t - \mu)} + \frac{1-w(t,U)}{i\nu_n - \big(E_0(2) - \varepsilon_d - t - \mu\big)}$$

E(2)-E(1)

$$|\langle 3|c^\dagger_\sigma|2\rangle|^2$$

$$+ \frac{1-w(t,U)}{i\nu_n - \big(-E_0(2) + U + 3\varepsilon_d + t - \mu\big)} + \frac{1+w(t,U)}{i\nu_n - \big(-E_0(2) + U + 3\varepsilon_d - t - \mu\big)}\Bigg)$$

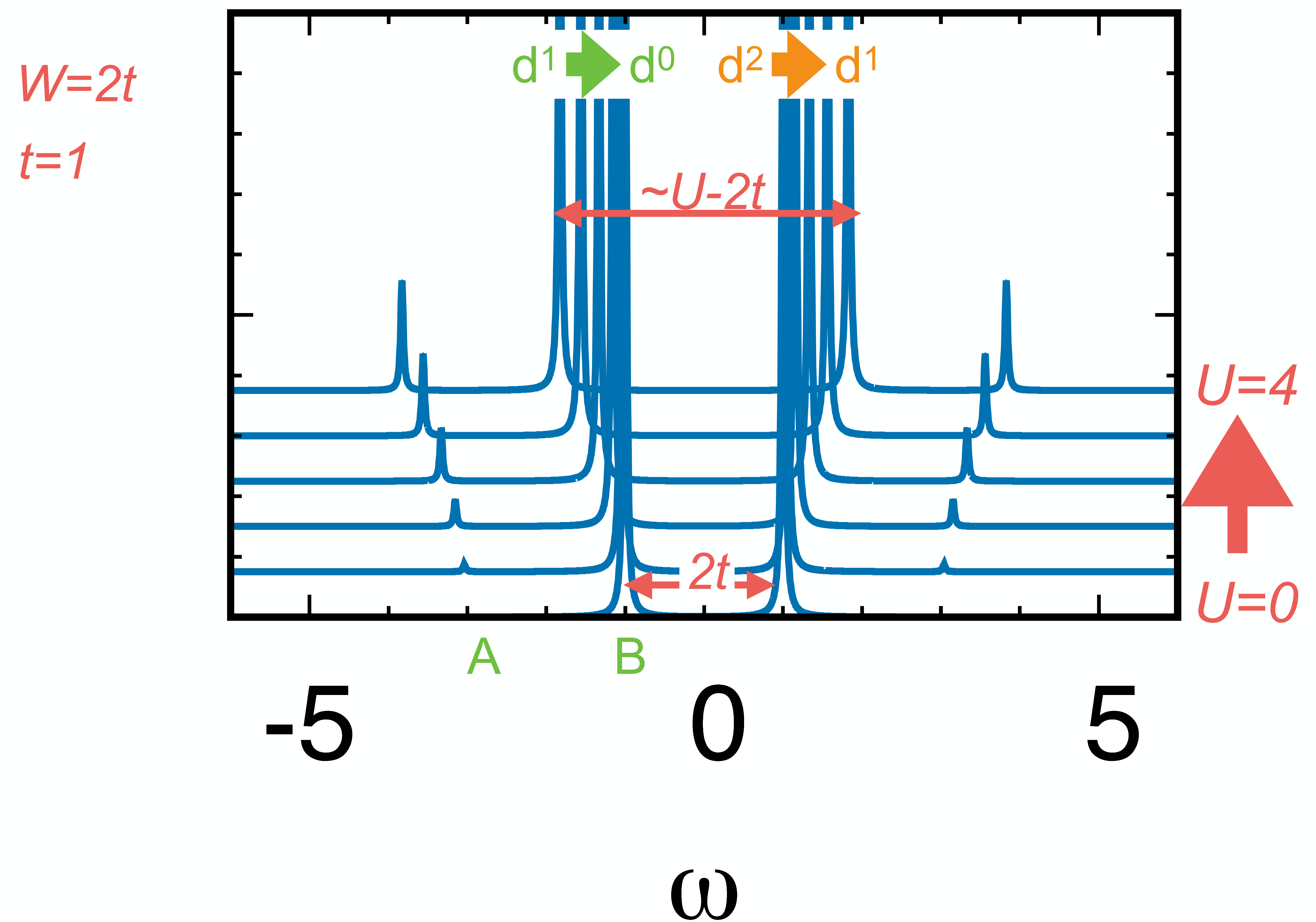
E(3)-E(2)

d² ➡ d¹

U=0: $E(2) = 2\varepsilon_d - 2t$

t=0: $E(2) = 2\varepsilon_d$

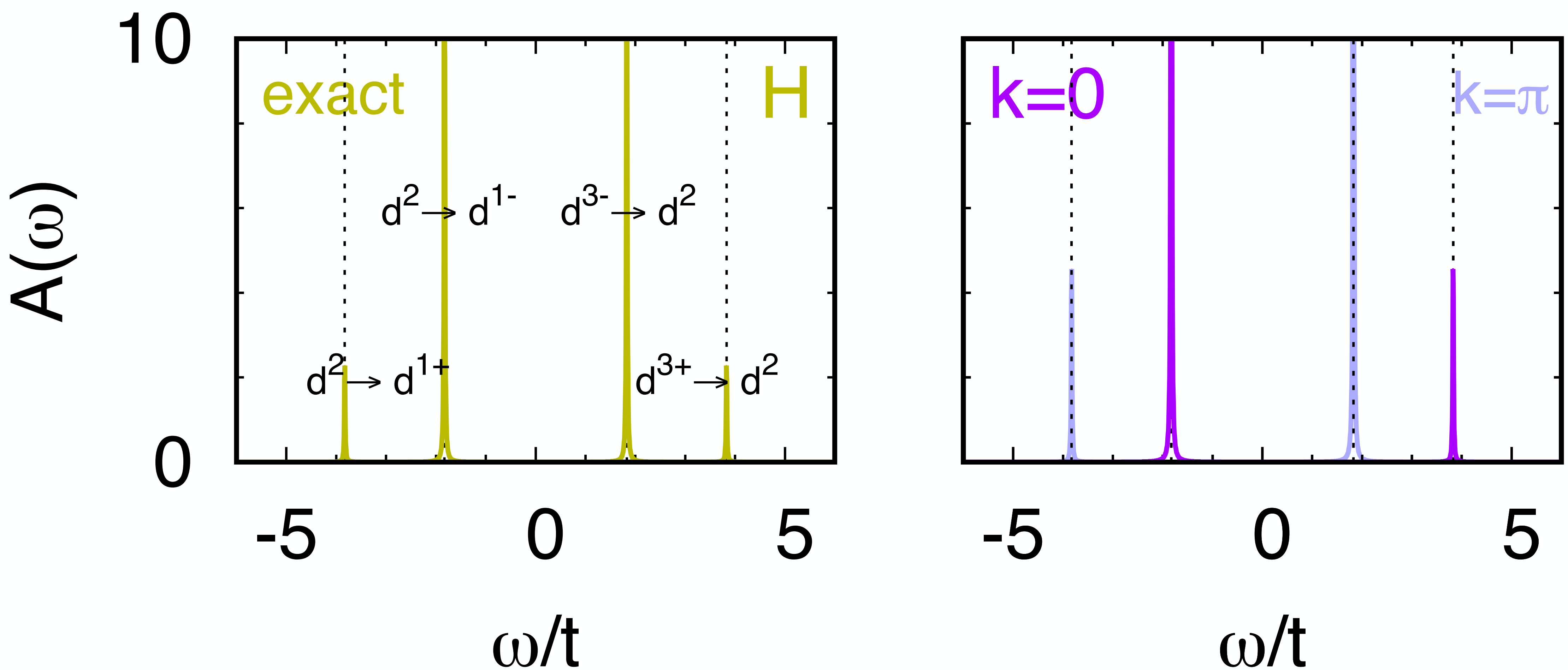
the local spectral function

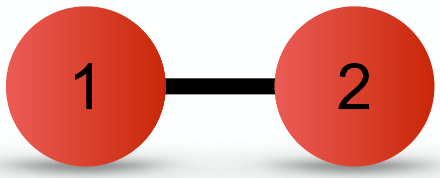


the local Green function

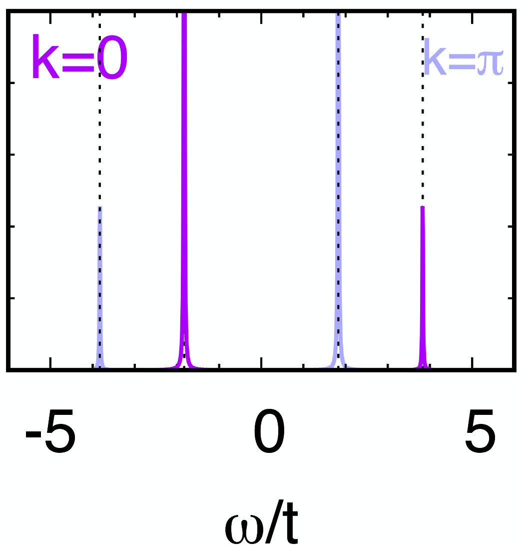
change from **site** to ***k*** representation

$$c_{k\sigma} = \frac{1}{\sqrt{2}}\left(c_{1\uparrow} \mp c_{2\uparrow}\right)$$





the local Green function



sum two terms together

k=0

$$G^{\sigma}_{i,i}(i\nu_n) = \frac{1}{4}\left(\frac{1+w(t,U)}{i\nu_n - (E_0(2) - \varepsilon_d + t - \mu)} + \frac{1-w(t,U)}{i\nu_n - \big(E_0(2) - \varepsilon_d - t - \mu\big)}\right.$$

$$\left. + \frac{1-w(t,U)}{i\nu_n - \big(-E_0(2) + U + 3\varepsilon_d + t - \mu\big)} + \frac{1+w(t,U)}{i\nu_n - \big(-E_0(2) + U + 3\varepsilon_d - t - \mu\big)}\right)$$

k=pi

$d^1 \rightarrow d^0$

E(2)-E(1)

E(3)-E(2)

$d^2 \rightarrow d^1$

the local Green function

change from site to *k* representation

$$G^{\sigma}_{i,i}(i\nu_n) = \frac{1}{2}\Bigg(\underbrace{\frac{1}{i\nu_n + \mu - \varepsilon_d + t - \Sigma^{\sigma}(0, i\nu_n)}}_{G^{\sigma}(0, i\nu_n)} + \underbrace{\frac{1}{i\nu_n + \mu - \varepsilon_d - t - \Sigma^{\sigma}(\pi, i\nu_n)}}_{G^{\sigma}(\pi, i\nu_n)} \Bigg)$$

$$\Sigma^{\sigma}(k, i\nu_n) = \frac{U}{2} + \frac{U^2}{4} \frac{1}{i\nu_n + \mu - \varepsilon_d - \frac{U}{2} - \; e^{ik} \, 3t}.$$

$$\varepsilon_k = -t\cos(k)$$

local Green function

U=0 vs finite *U*

$$G_{11}^{0\sigma}(i\nu_n) = \frac{1}{2}\sum_k \frac{1}{i\nu_n - (\varepsilon_k - \mu)} = \frac{1}{i\nu_n - (\varepsilon_d + F^0(i\nu_n) - \mu)},$$

$$G_{11}^{\sigma}(i\nu_n) = \frac{1}{2}\sum_k \frac{1}{i\nu_n - (\varepsilon_k + \Sigma^\sigma(k, i\nu_n) - \mu)} = \frac{1}{i\nu_n - (\varepsilon_d + \Sigma_l^\sigma(i\nu_n) + F^\sigma(i\nu_n) - \mu)}$$

$$\varepsilon_k = \varepsilon_d - t\cos(k)$$

local self-energy plus modified hybridization function

the local Green function

energy level

$$\varepsilon_d$$

modified energy level

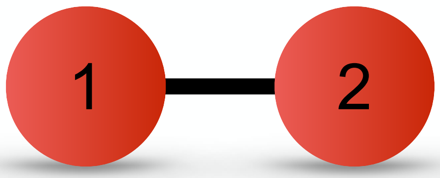
$$\varepsilon_d + \Sigma_l^\sigma(i\nu_n)$$

local self-energy

$$\Sigma_l^\sigma(i\nu_n) = \frac{1}{2}\left(\Sigma^\sigma(\pi, i\nu_n) + \Sigma^\sigma(0, i\nu_n)\right) = \frac{U}{2} + \frac{U^2}{4}\,\frac{i\nu_n + \mu - \varepsilon_d - \frac{U}{2}}{(i\nu_n + \mu - \varepsilon_d - \frac{U}{2})^2 - (3t)^2}$$

second order in U!

it is a function! → **more poles**



the local Green function

hybridization function

$$F^0(i\nu_n) = \frac{t^2}{i\nu_n - (\varepsilon_d - \mu)}$$

modified **hybridization function**

$$F^\sigma(i\nu_n) = \frac{(t + \Delta\Sigma_l(i\nu_n))^2}{i\nu_n - (\varepsilon_d - \mu + \Sigma_l^\sigma(i\nu_n))}$$

non-local self-energy

$$\Delta\Sigma_l^\sigma(i\nu_n) = \frac{1}{2}\Big(\Sigma^\sigma(\pi, i\nu_n) - \Sigma^\sigma(0, i\nu_n)\Big) = -\frac{U^2}{4}\,\frac{3t}{(i\nu_n + \mu - \varepsilon_d - \frac{U}{2})^2 - (3t)^2}$$

local Dyson equation

$$\Sigma_l^\sigma(i\nu_n) = \frac{1}{\mathfrak{G}_{i,i}^\sigma(i\nu_n)} - \frac{1}{G_{i,i}^\sigma(i\nu_n)},$$

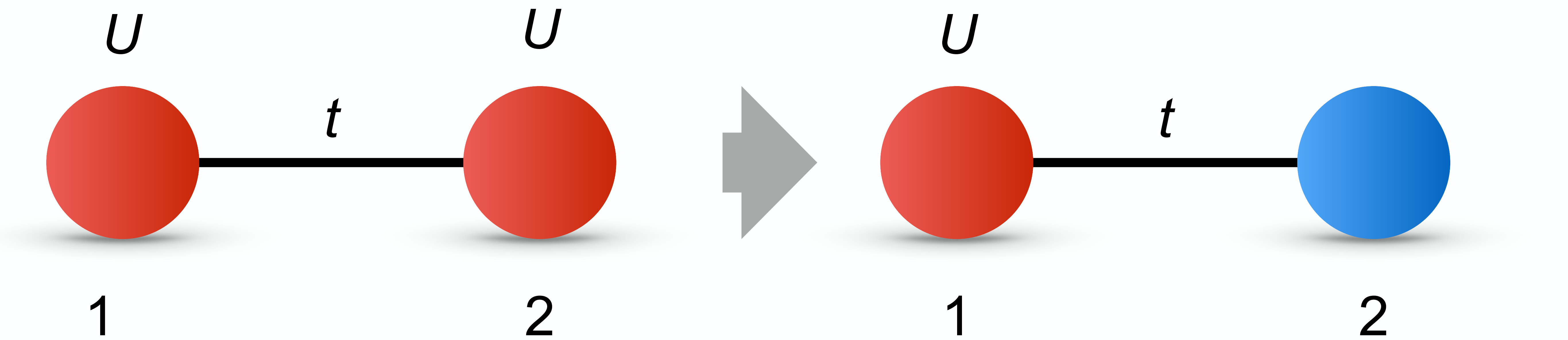
$$\mathfrak{G}_{i,i}^\sigma(i\nu_n) = \frac{1}{i\nu_n + \mu - \varepsilon_d - F^\sigma(i\nu_n)}.$$

similar to quantum impurity Dyson equation

$$\Sigma_A^\sigma(i\nu_n) = \frac{1}{G_{d,d}^{0\sigma}(i\nu_n)} - \frac{1}{G_{d,d}^\sigma(i\nu_n)}$$

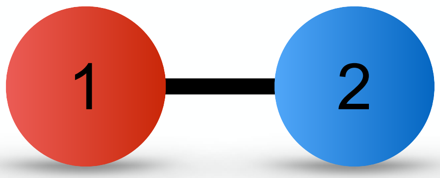
map to a quantum impurity model ?

the Anderson molecule



$$\hat{H}^{\mathrm{A}} = \varepsilon_s \sum_\sigma \hat{n}_{s\sigma} - t \sum_\sigma \left(c^\dagger_{d\sigma} c_{s\sigma} + c^\dagger_{s\sigma} c_{d\sigma} \right) + \varepsilon_d \sum_\sigma \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow}$$

~ same local self-energy and Green-function?



self-consistency

half filling: N=2

Hubbard

$$\hat{H}_2(\varepsilon_d, U, t) = \begin{pmatrix} 2\varepsilon_d & 0 & 0 & 0 & 0 & 0 \\ 0 & 2\varepsilon_d & 0 & 0 & 0 & 0 \\ 0 & 0 & 2\varepsilon_d & 0 & 0 & 0 \\ 0 & 0 & 0 & 2\varepsilon_d & -\sqrt{2}t & -\sqrt{2}t \\ 0 & 0 & 0 & -\sqrt{2}t & 2\varepsilon_d{+}U & 0 \\ 0 & 0 & 0 & -\sqrt{2}t & 0 & 2\varepsilon_d{+}U \end{pmatrix}$$

Anderson

$$\hat{H}_2^A(\varepsilon_d, U, t; \varepsilon_s) = \begin{pmatrix} \varepsilon_d{+}\varepsilon_s & 0 & 0 & 0 & 0 & 0 \\ 0 & \varepsilon_d{+}\varepsilon_s & 0 & 0 & 0 & 0 \\ 0 & 0 & \varepsilon_d{+}\varepsilon_s & 0 & 0 & 0 \\ 0 & 0 & 0 & \varepsilon_d{+}\varepsilon_s & -\sqrt{2}t & -\sqrt{2}t \\ 0 & 0 & 0 & -\sqrt{2}t & 2\varepsilon_d{+}U & 0 \\ 0 & 0 & 0 & -\sqrt{2}t & 0 & 2\varepsilon_s \end{pmatrix}$$

same occupations of Hubbard dimer

$\varepsilon_s = \varepsilon_d + U/2 = \mu$

solution: Hubbard vs Anderson

Anderson molecule

$$G^{\sigma}_{dd}(i\nu_n) = \frac{1}{i\nu_n - (\varepsilon_d - \mu + \Sigma^{\sigma}_l(i\nu_n) + F^{\sigma}_0(i\nu_n))}$$

Hubbard dimer

$$G^{\sigma}_{11}(i\nu_n) = \frac{1}{i\nu_n - (\varepsilon_d - \mu + \Sigma^{\sigma}_l(i\nu_n) + F^{\sigma}(i\nu_n))}$$

the local self-energies are identical!

let us neglect the **non-local** self-energy in Hubbard model

solution: Hubbard vs Anderson

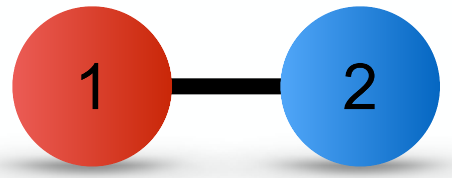
hybridization function

$$F^0(i\nu_n) = \frac{t^2}{i\nu_n - (\varepsilon_d - \mu)},$$

modified **hybridization function**

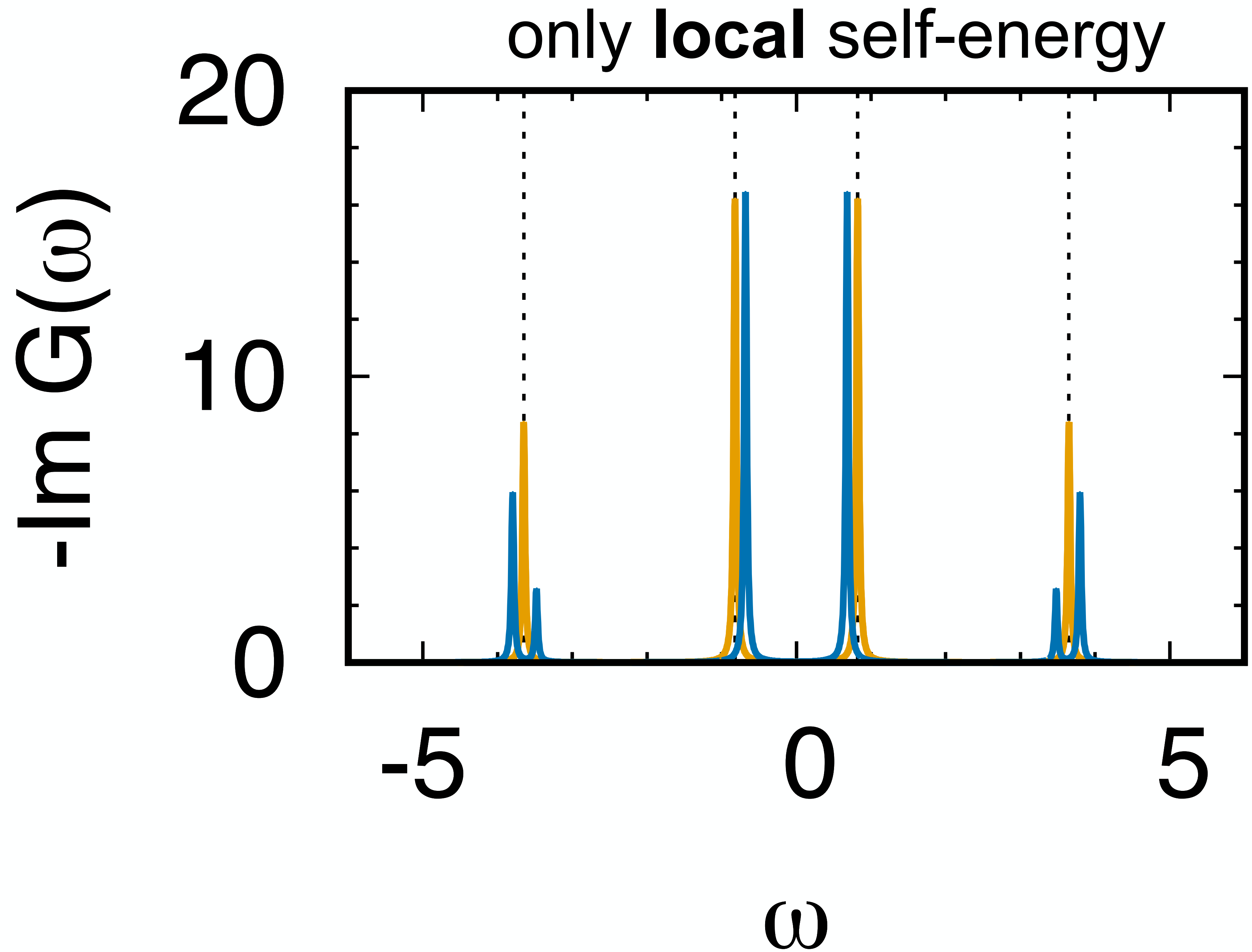
$$F^\sigma(i\nu_n) = \frac{(t + \cancel{\Delta\Sigma_l(i\nu_n)})^2}{i\nu_n - (\varepsilon_d - \mu + \Sigma_l^\sigma(i\nu_n))}.$$

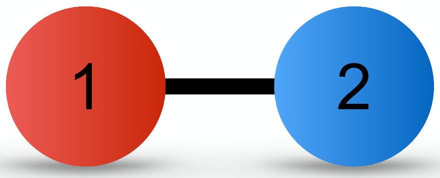
local self-energy approximation



Green function *U=4t*

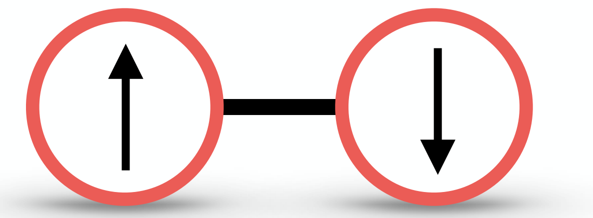
Anderson vs Hubbard (local self-ene approx)





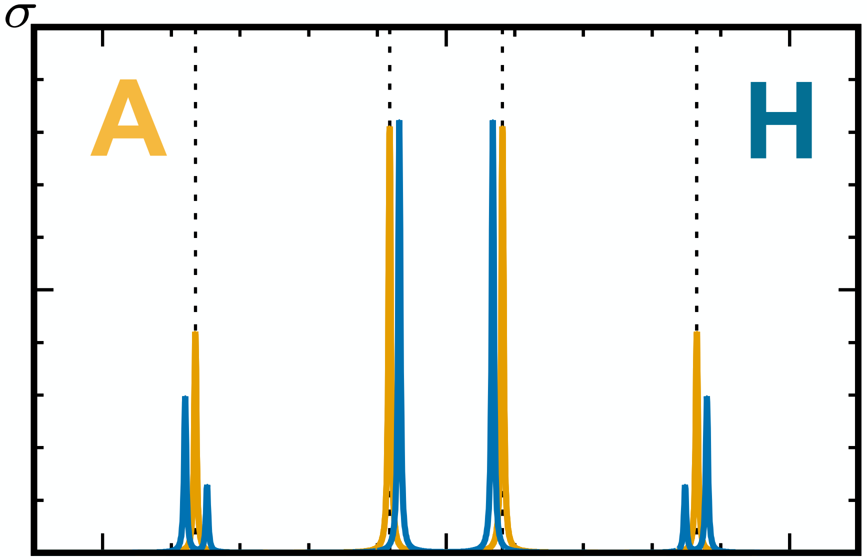
DMFT for the dimer

$$\hat{H} = \varepsilon_d \sum_{i\sigma} \hat{n}_{i\sigma} - t \sum_{\sigma} \left(c^\dagger_{1\sigma} c_{2\sigma} + c^\dagger_{2\sigma} c_{1\sigma} \right) + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$



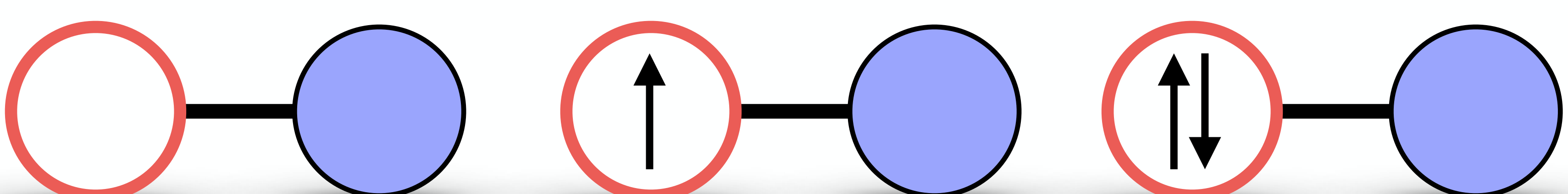
map to quantum impurity model (QIM) in local self-energy approximation

$$\hat{H}^{\mathrm{A}} = \varepsilon_s \sum_{\sigma} \hat{n}_{s\sigma} - t \sum_{\sigma} \left(c^\dagger_{d\sigma} c_{s\sigma} + c^\dagger_{s\sigma} c_{d\sigma} \right) + \varepsilon_d \sum_{\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow}$$

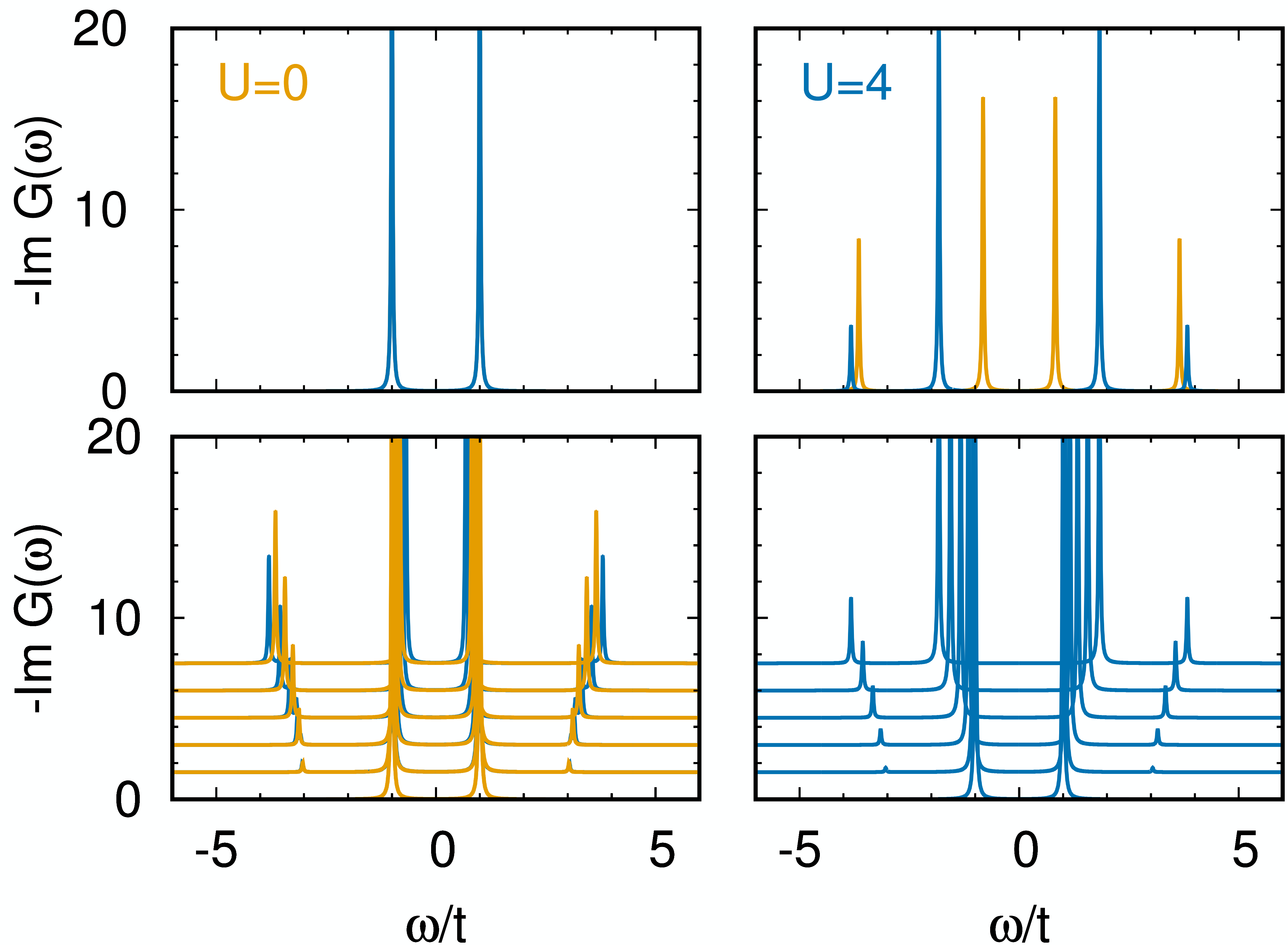


QIM solver

self-consistency loop



DMFT for the Hubbard dimer



DMFT for the one-band Hubbard model

$$H = \varepsilon_d \sum_i \sum_\sigma c_{i\sigma}^\dagger c_{i\sigma} - t \sum_{\langle ii' \rangle} \sum_\sigma c_{i\sigma}^\dagger c_{i'\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

self-consistency loop

$$H = \varepsilon_d \sum_i \sum_\sigma c^\dagger_{i\sigma} c_{i\sigma} - t \sum_{\langle ii' \rangle} \sum_\sigma c^\dagger_{i\sigma} c_{i'\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

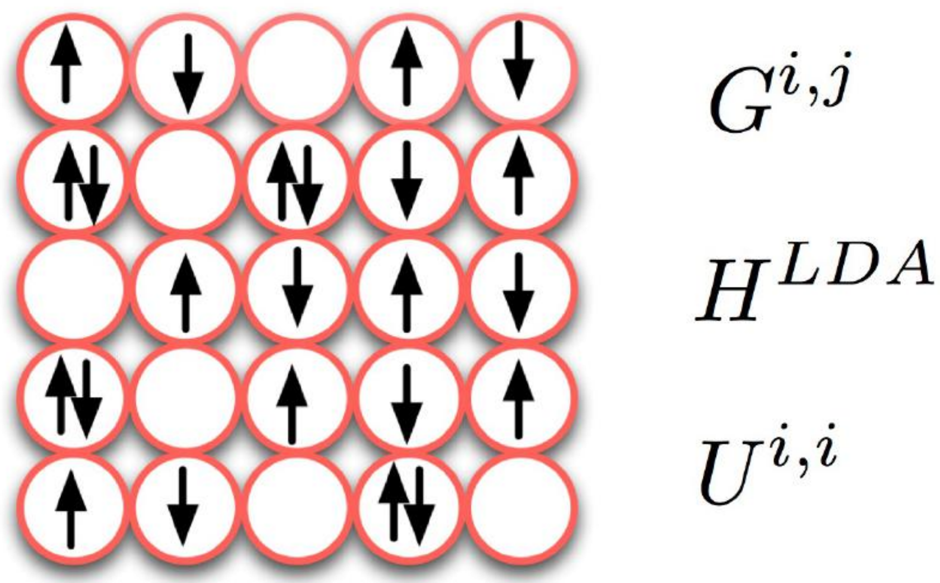
quantum impurity model (QIM)

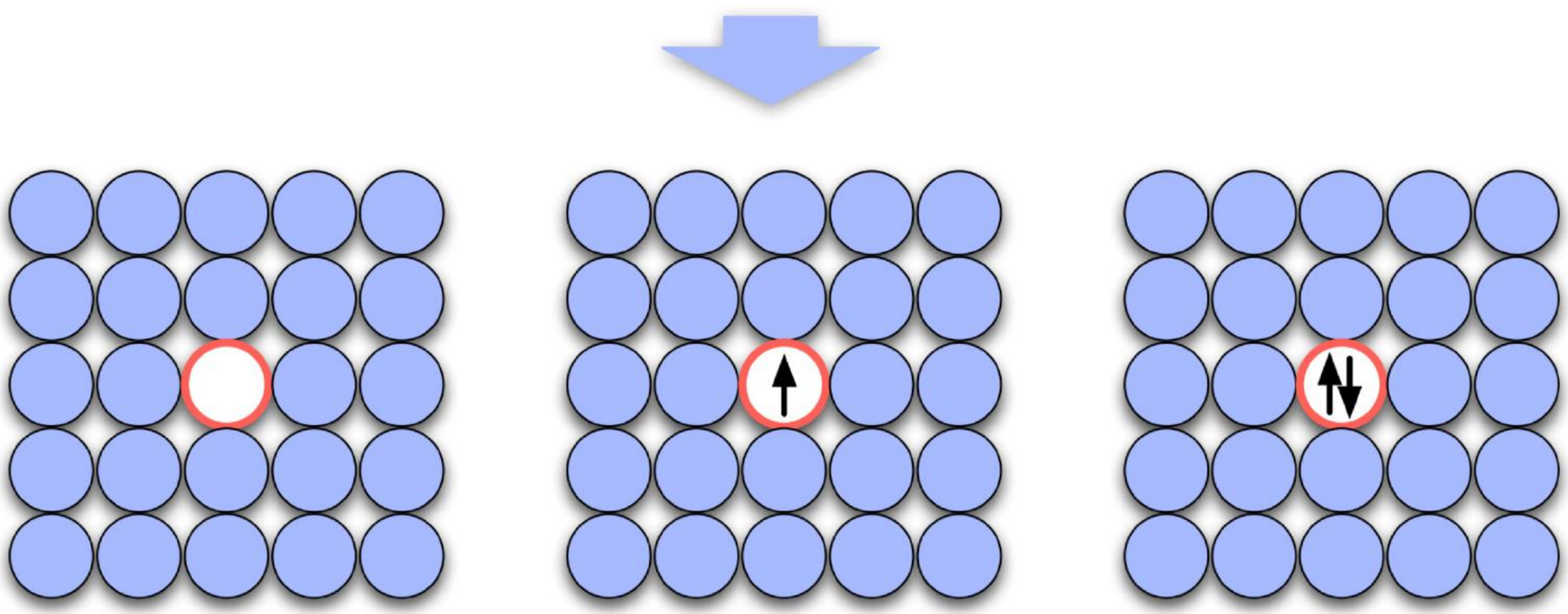
$$\hat{H}^A = \underbrace{\sum_{\boldsymbol{k}\sigma} \varepsilon^s_{\boldsymbol{k}} \hat{n}_{\boldsymbol{k}\sigma}}_{\hat{H}_{\text{bath}}} + \underbrace{\sum_{\boldsymbol{k}\sigma} \left(V^s_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}\sigma} c_{d\sigma} + \text{h.c.} \right)}_{\hat{H}_{\text{hyb}}} + \underbrace{\varepsilon_d \sum_\sigma \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow}}_{\hat{H}_{\text{imp}}}$$

QIM solver: **QMC**, ED, NRG, DMRG,…

self-consistency loop ***$G_{dd}=G_{ii}$***

dynamical mean-field theory

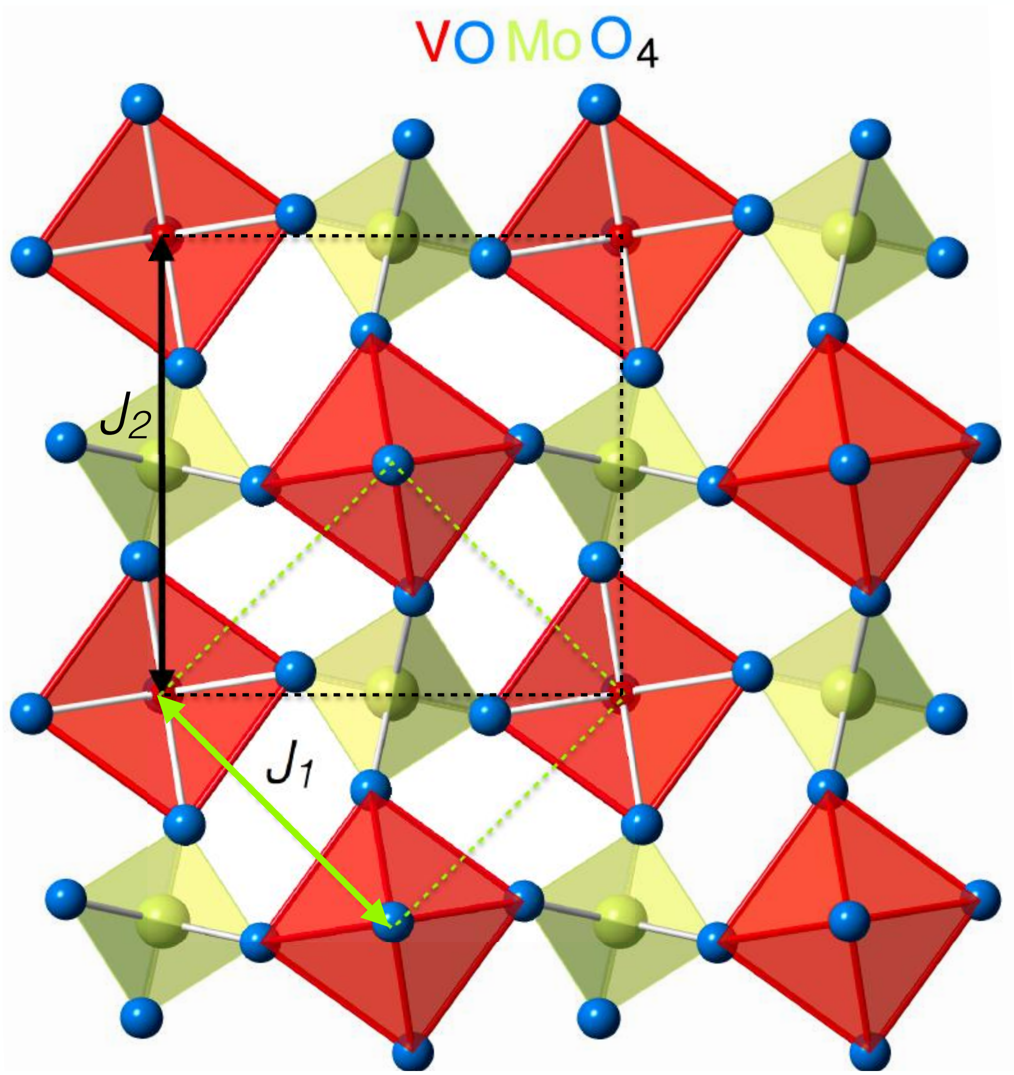


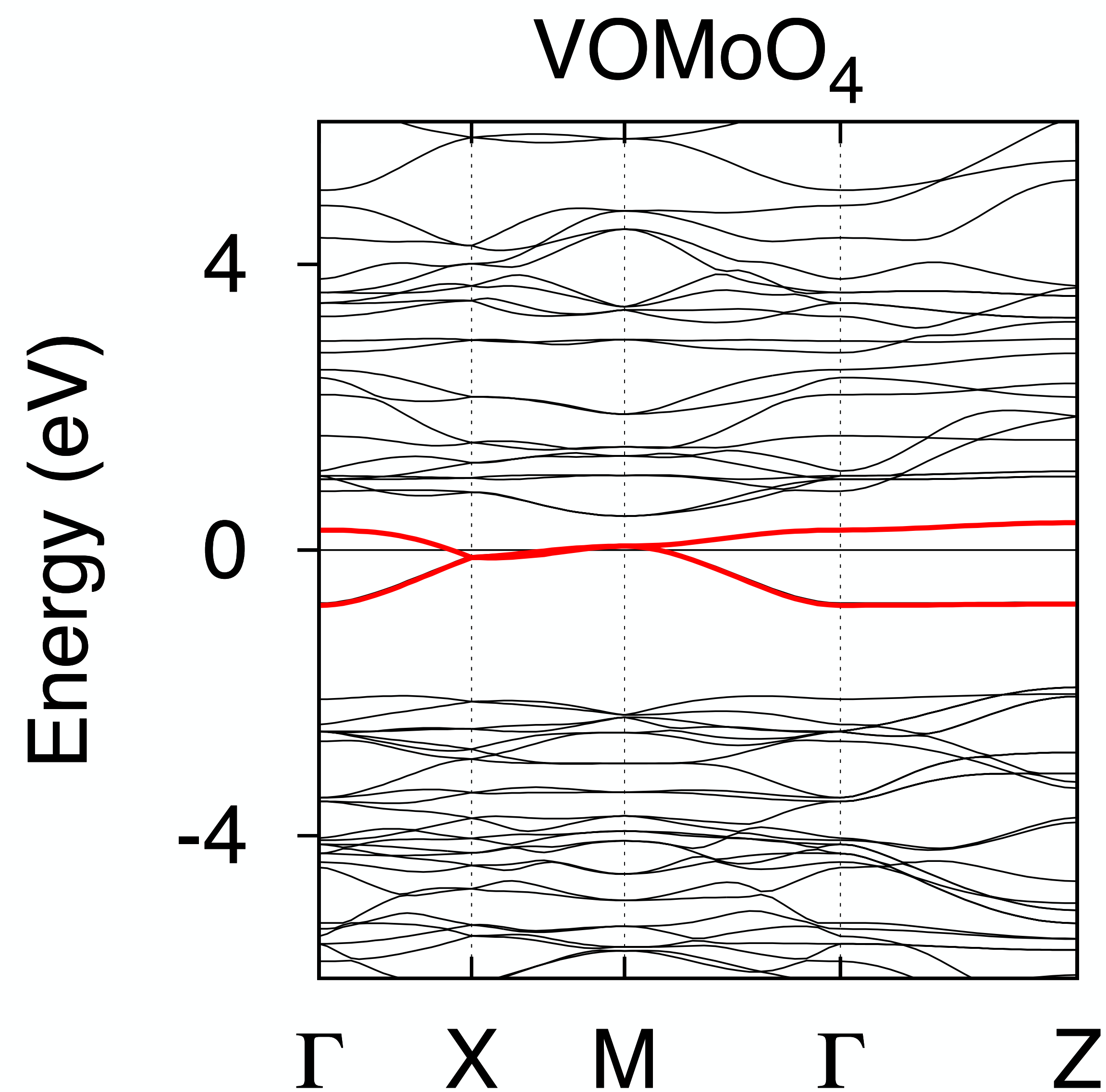


$$\mathcal{G}^{-1} = G^{-1} + \Sigma$$
$$G = G^{i,i}$$

Metzner and Vollhardt, PRL **62**, 324 (1989); Georges and Kotliar, PRB **45,** 6479 (1992)

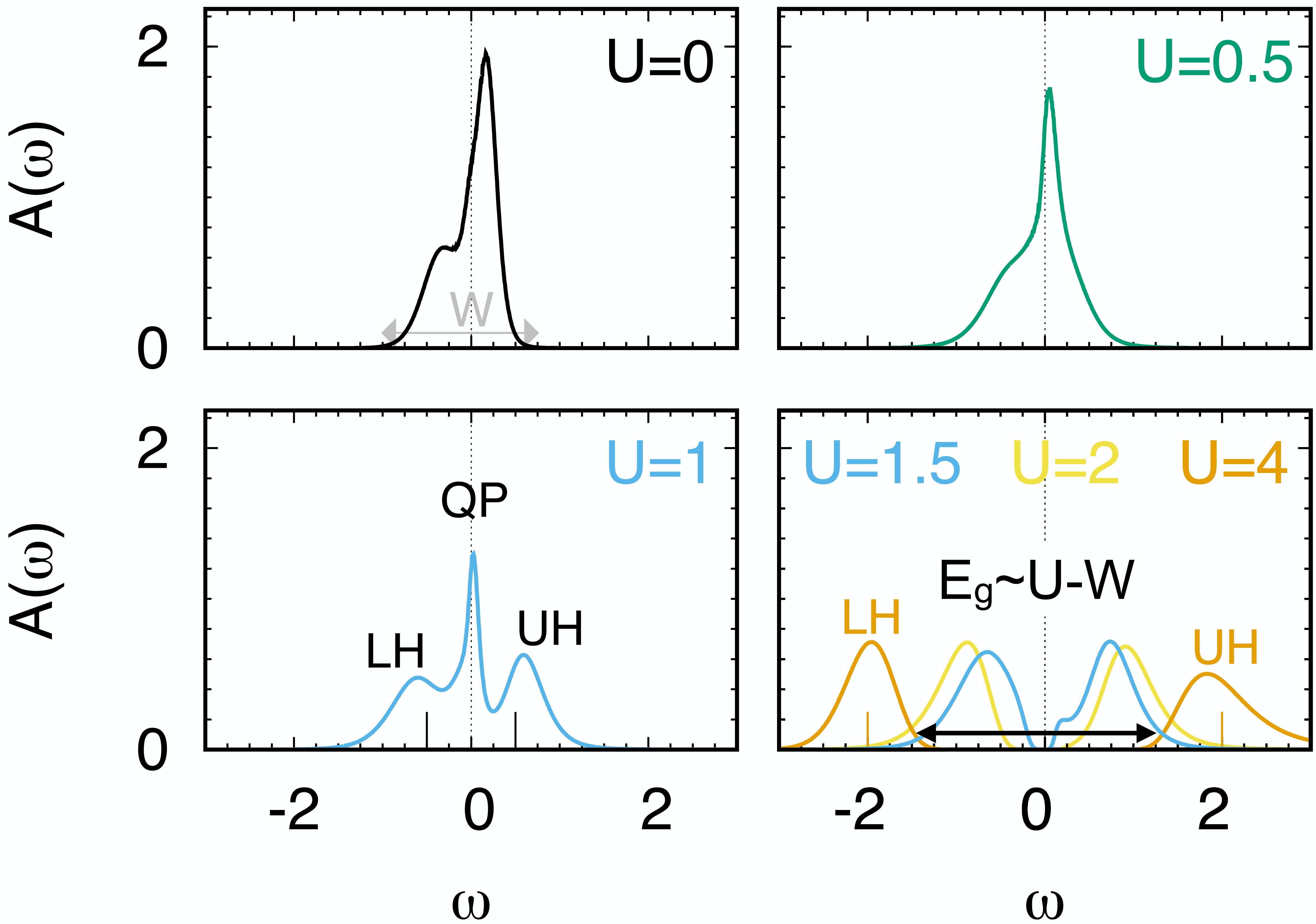
a real-system case: $VOMoO_4$





Amin Kiani and Eva Pavarini, Phys. Rev. B **94**, 075112 (2016)

a real-system: $VOMoO_4$

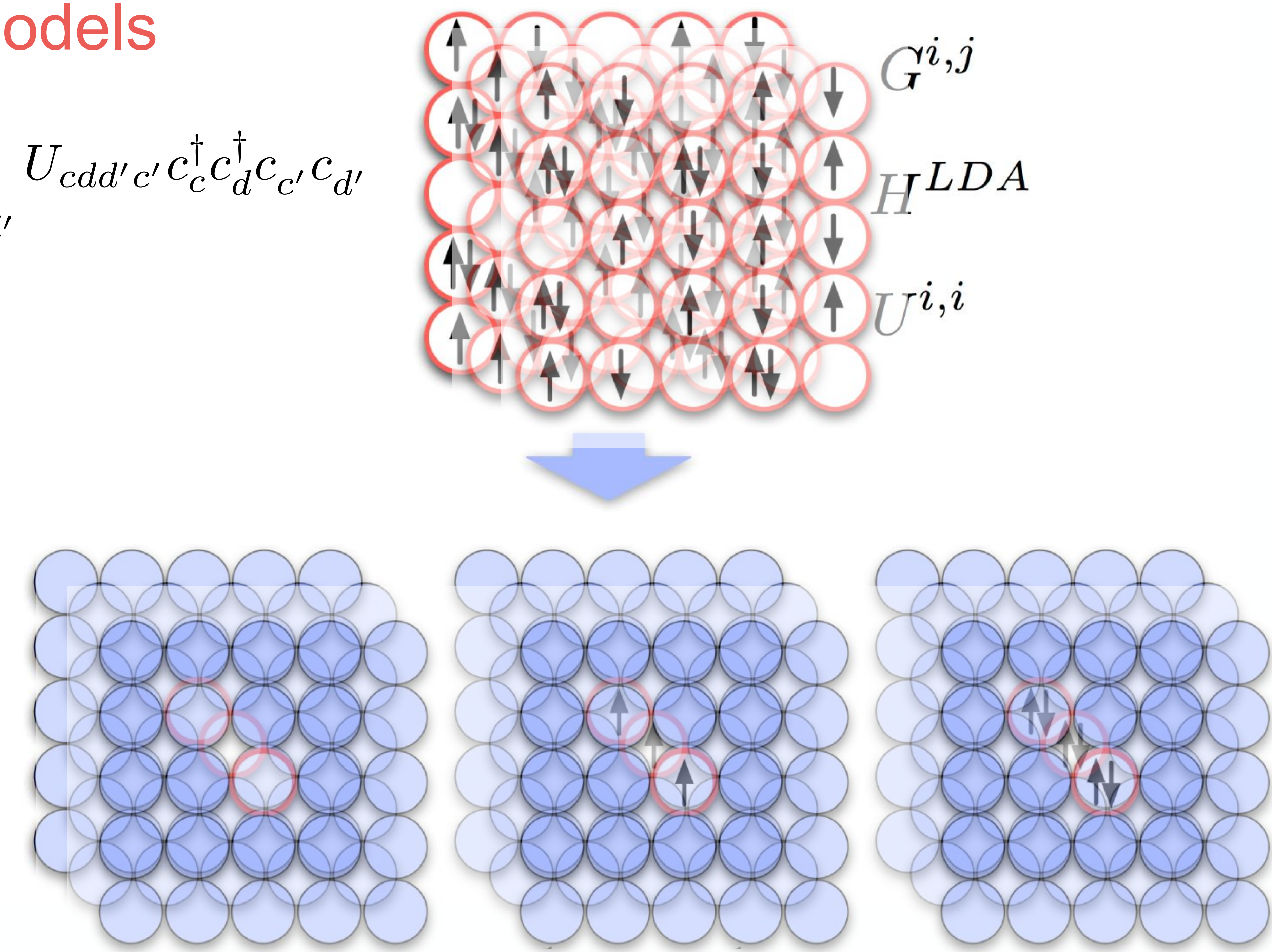


DMFT for materials

DMFT for real materials

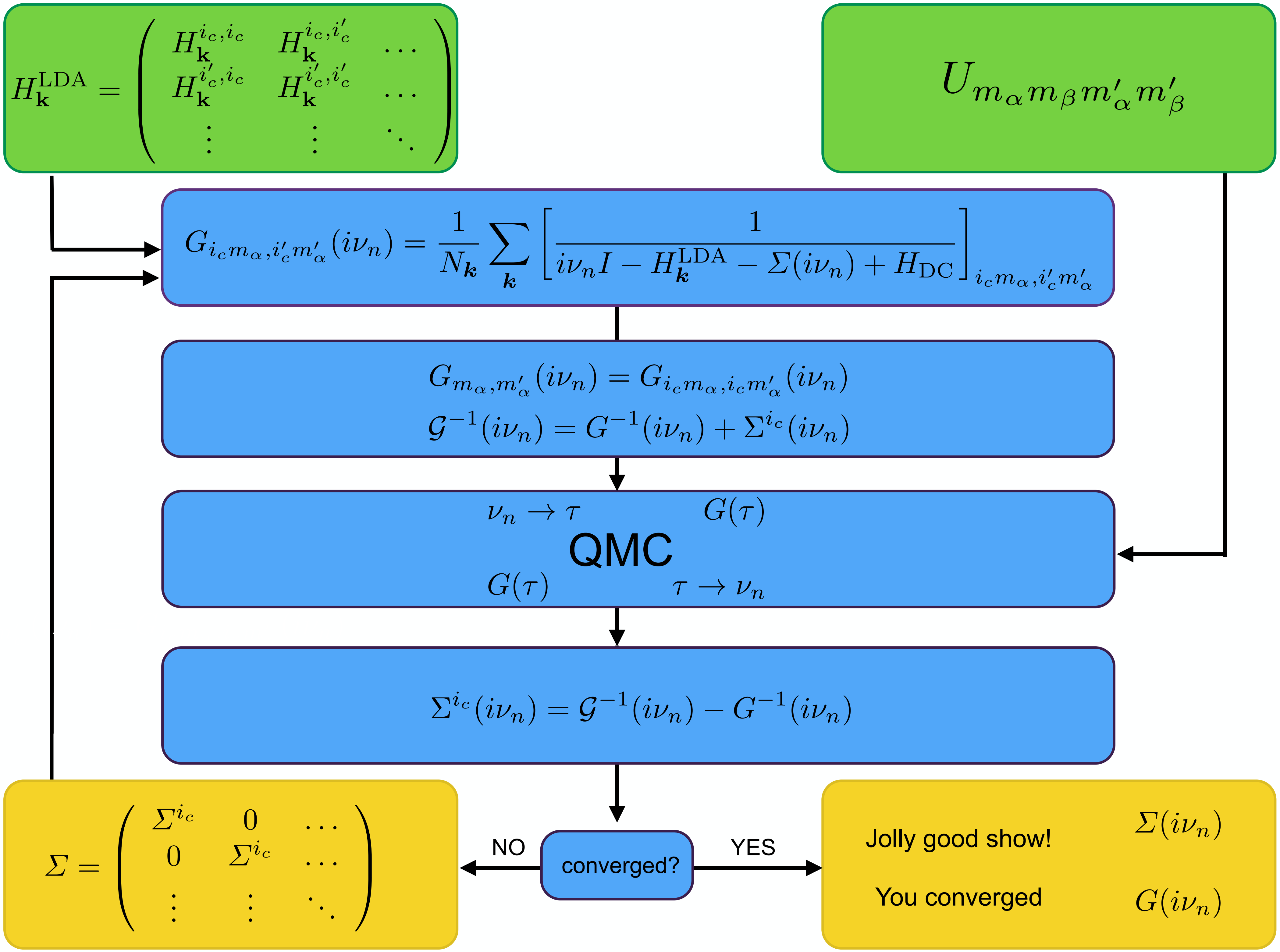
realistic models

$$\hat{H}_e = \sum_{ab} t_{ab} c_a^\dagger c_b + \frac{1}{2} \sum_{cdc'd'} U_{cdd'c'} c_c^\dagger c_d^\dagger c_{c'} c_{d'}$$



realistic self-consistent quantum-impurity (QI) model

in theory, more indices



in practice, QMC-based solvers

computational time

limited number of orbitals/site

finite temperature

sign problem

some *interactions* are worse than others

some *bases* are worse than others

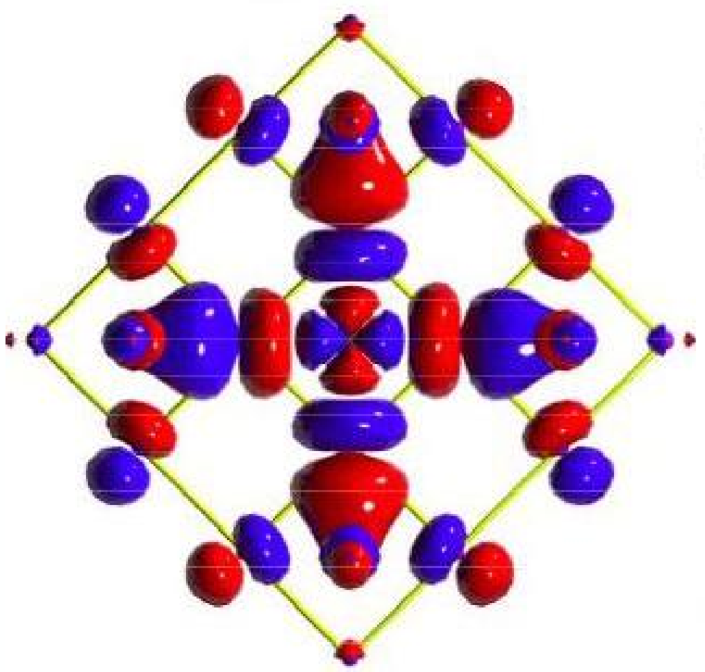
we need **minimal** material-specific models

minimal material-specific models

$$\hat{H}_e = \sum_i \hat{H}_i^0 + \sum_{i \neq i'} \frac{1}{|\mathbf{r}_i - \mathbf{r}_{i'}|} \quad \Rightarrow \quad \hat{H}_e = \sum_{ab} t_{ab} c_a^\dagger c_b + \frac{1}{2} \sum_{cdc'd'} U_{cdd'c'} c_c^\dagger c_d^\dagger c_{c'} c_{d'}$$

chose the one-electron basis in a *smart* way — minimal models

idea: DFT-based Wannier functions



- span full Hamiltonian
- good electron density
- very good description of weakly correlated states
- average and long-range Coulomb included
- information on lattice and chemistry
- allow energy- and symmetry-based downfolding

E. Pavarini *et al.*, PRL **87**, 047003 (2001); PRL **92**, 176403 (2004); New J. Phys. **7**, 188 (2005)

details matter!

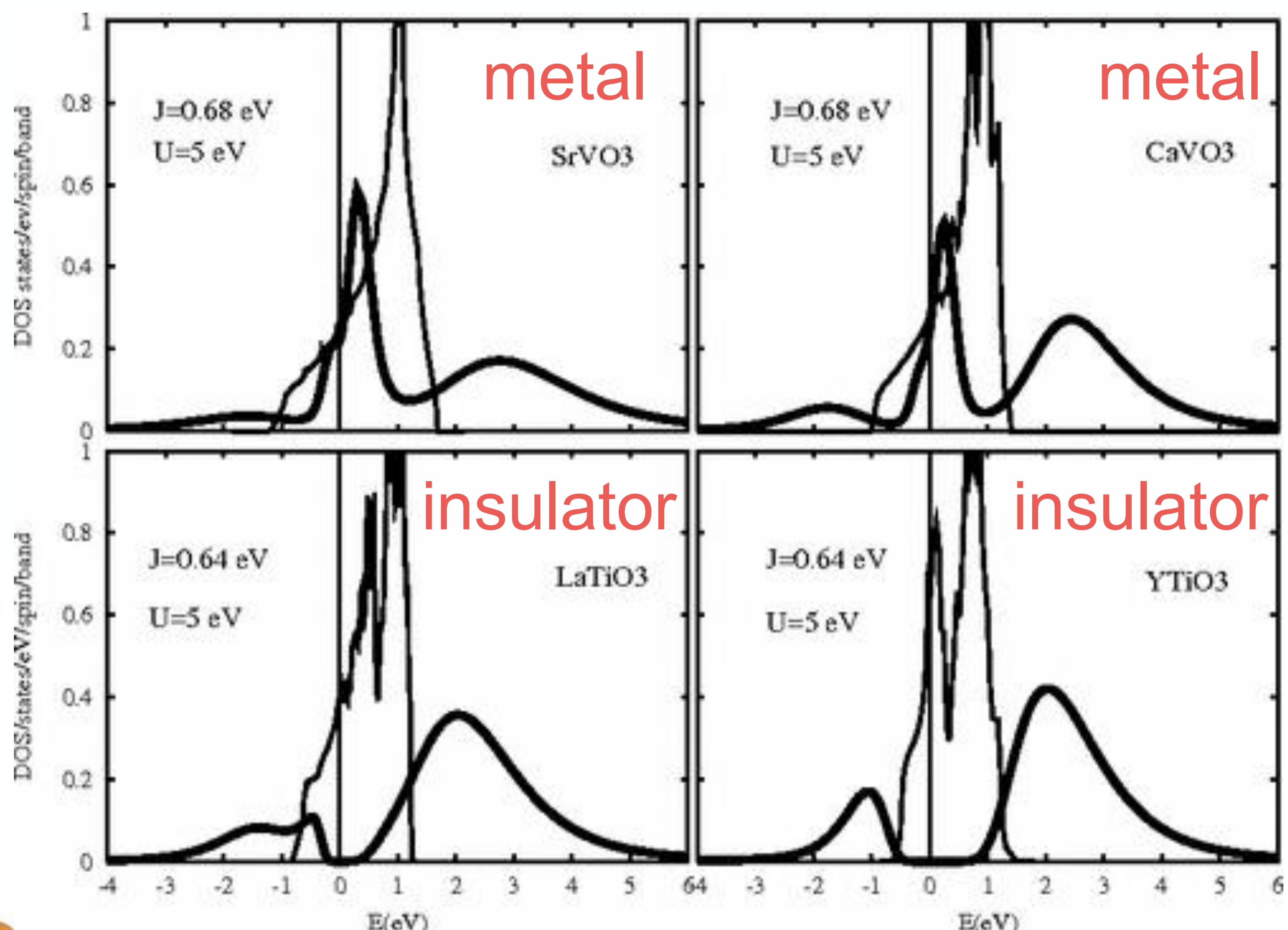
VOLUME 92, NUMBER 17 PHYSICAL REVIEW LETTERS week ending 30 APRIL 2004

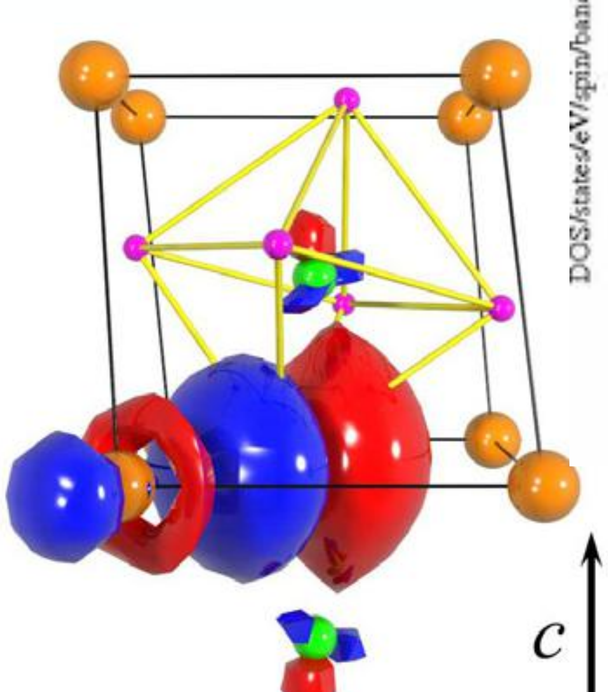
Mott Transition and Suppression of Orbital Fluctuations in Orthorhombic $3d^1$ Perovskites

E. Pavarini,[1] S. Biermann,[2] A. Poteryaev,[3] A. I. Lichtenstein,[3] A. Georges,[2] and O. K. Andersen[4]

$SrVO_3$ $CaVO_3$

$LaTiO_3$ $YTiO_3$



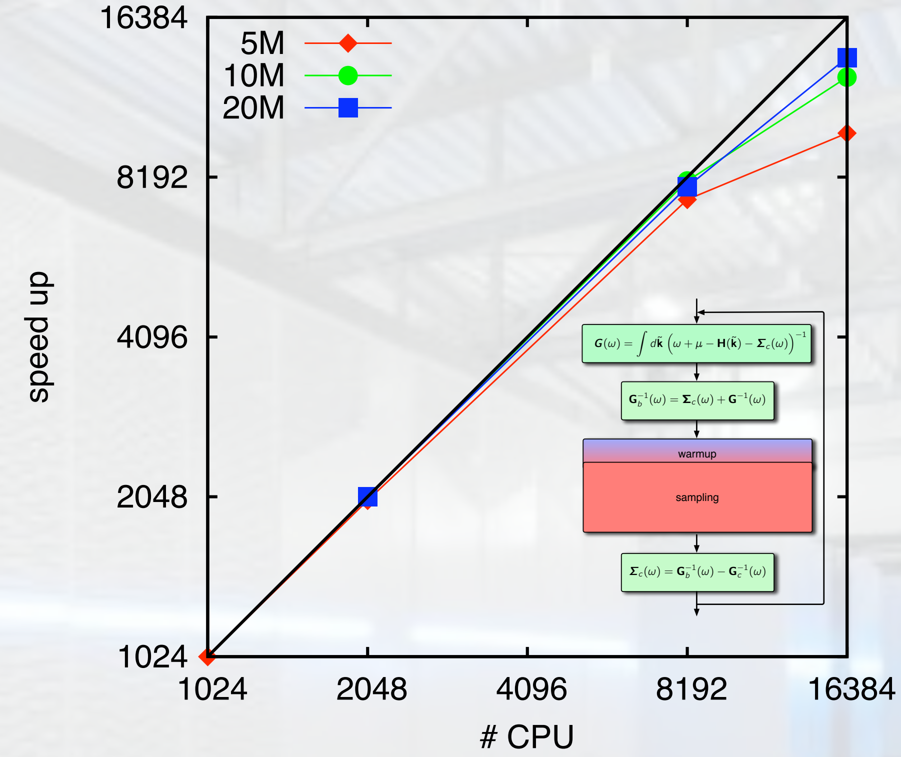


770 K

flexible and efficient solvers

$$H = -\sum_{ii'}\sum_{mm'}\sum_{\sigma} t^{ii'}_{mm'} c^{\dagger}_{im\sigma} c_{i'm'\sigma} + U\sum_{im} n_{im\uparrow} n_{im\downarrow} + \frac{1}{2}\sum_{im\neq m'\sigma\sigma'} (U - 2J - J\delta_{\sigma\sigma'}) n_{im\sigma} n_{im'\sigma'} - J\sum_{m\neq m'} (c^{\dagger}_{m\uparrow} c^{\dagger}_{m'\downarrow} c_{m'\uparrow} c_{m\downarrow} + c^{\dagger}_{m\uparrow} c^{\dagger}_{m\downarrow} c_{m'\uparrow} c_{m'\downarrow})$$

self-energy matrix in spin-orbital space



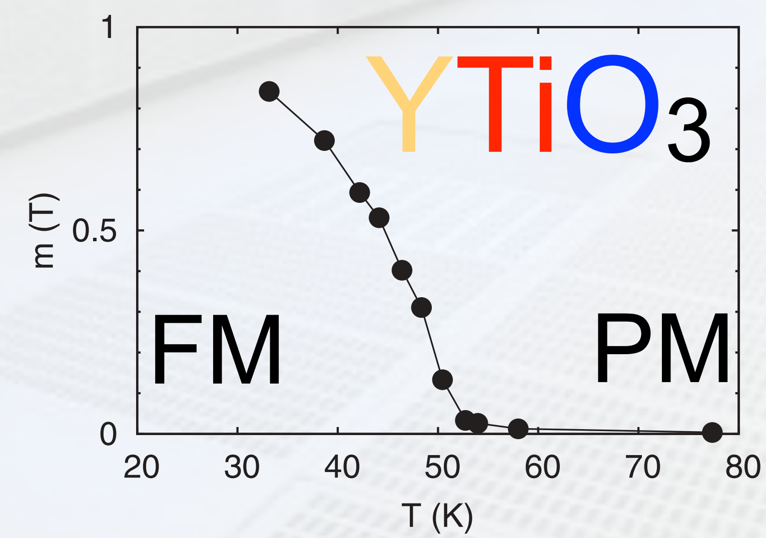
DMFT and cDMFT

generalized quantum impurity solvers:

general HF QMC

general CT-INT QMC

general CT-HYB QMC



- ✦ CT-HYB: A. Flesch, E. Gorelov, E. Koch and E. Pavarini Phys. Rev. B **87**, 195141 (2013)
- ✦ CT-INT: E. Gorelov et al, PRL 104, 226410 (2010)
- ✦ CT-INT+SO: G. Zhang, E. Gorelov, E. Sarvestani, and E. Pavarini, Phys. Rev. Lett. 116, 106402 (2016)

sign problem: smart adapted basis choice

II: Linear response functions

linear-response functions

in short

$$\langle m \rangle \sim \chi \, h$$

with more in detail

a **small** space- and time-dependent perturbation *H_1*

$$\hat{H} \quad \rightarrow \hat{H} + \int d\boldsymbol{r}\, \hat{H}_1(\boldsymbol{r};t) + \dots$$

$$\hat{H}_1(\boldsymbol{r};t) \quad = -\sum_\nu \hat{O}_\nu(\boldsymbol{r};t) h_\nu(\boldsymbol{r};t),$$

property of the system external field

$$\hat{O}_\nu(\boldsymbol{r};t) = e^{i(\hat{H}-\mu\hat{N})t}\hat{O}_\nu(\boldsymbol{r})e^{-i(\hat{H}-\mu\hat{N})t},$$

$$\langle\hat{A}\rangle_0 = \frac{\mathrm{Tr}\left(e^{-\beta(\hat{H}-\mu\hat{N})}\hat{A}\right)}{\mathrm{Tr}\left(e^{-\beta(\hat{H}-\mu\hat{N})}\right)}$$

$\beta=1/k_BT$

$$\Delta\hat{A}(\boldsymbol{r};t) = \hat{A}(\boldsymbol{r};t) - \langle\hat{A}(\boldsymbol{r})\rangle_0$$

difference wrt unperturbed equilibrium case

with more details

linear effect on some property P

$$\langle \hat{P}_\nu(\boldsymbol{r};t) \rangle = \langle \hat{P}_\nu(\boldsymbol{r}) \rangle_0 + \langle \delta \hat{P}_\nu(\boldsymbol{r};t) \rangle_0,$$

$$\langle \delta \hat{P}_\nu(\boldsymbol{r};t) \rangle_0 = -i \int d\boldsymbol{r}' \int_{-\infty}^{t} dt' \left\langle \left[\Delta \hat{P}_\nu(\boldsymbol{r};t), \Delta \hat{H}_1(\boldsymbol{r}';t') \right] \right\rangle_0 .$$

replacing H_1 with its expression

$$\langle \delta \hat{P}_\nu(\boldsymbol{r};t) \rangle_0 = -i \sum_{\nu'} \int d\boldsymbol{r}' \int_{-\infty}^{t} dt' \left\langle \left[\Delta \hat{P}_\nu(\boldsymbol{r};t), \Delta \hat{O}_{\nu'}(\boldsymbol{r}';t') \right] \right\rangle_0 h_{\nu'}(\boldsymbol{r}';t')$$

linear response function

$$\chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\boldsymbol{r}, \boldsymbol{r}'; t, t') = i \left\langle \left[\Delta\hat{P}_\nu(\boldsymbol{r}; t), \Delta\hat{O}_{\nu'}(\boldsymbol{r}'; t') \right] \right\rangle_0 \Theta(t - t')$$

Fourier transform

$$\langle \delta\hat{P}_\nu(\boldsymbol{q}; \omega) \rangle_0 = \sum_{\nu'} \chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\boldsymbol{q}; \omega) h_{\nu'}(\boldsymbol{q}; \omega)$$

example: magnetic susceptibility

$$\chi_{\hat{S}_z \hat{S}_z}(\boldsymbol{q}; \omega) = i \int dt\, e^{i\omega t} \left\langle \left[\hat{S}_z(\boldsymbol{q}; t), \hat{S}_z(-\boldsymbol{q}; 0) \right] \right\rangle_0 \Theta(t).$$

linear response function

$$\chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\boldsymbol{r}, \boldsymbol{r}'; t, t') = i \left\langle \left[\Delta\hat{P}_\nu(\boldsymbol{r}; t), \Delta\hat{O}_{\nu'}(\boldsymbol{r}'; t') \right] \right\rangle_0 \Theta(t - t')$$

Fourier transform

$$\langle \delta\hat{P}_\nu(\boldsymbol{q}; \omega) \rangle_0 = \sum_{\nu'} \chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\boldsymbol{q}; \omega) h_{\nu'}(\boldsymbol{q}; \omega)$$

example: magnetic susceptibility

$$\chi_{\hat{S}_z \hat{S}_z}(\boldsymbol{q}; \omega) = i \int dt\, e^{i\omega t} \left\langle \left[\hat{S}_z(\boldsymbol{q}; t), \hat{S}_z(-\boldsymbol{q}; 0) \right] \right\rangle_0 \Theta(t).$$

in imaginary time and frequency

$$\hat{S}^i_\nu(\tau_1,\tau_2) \quad = \quad \sum_{\boldsymbol{\alpha}} p^\nu_{\boldsymbol{\alpha}}\, c^\dagger_{i\alpha'}(\tau_2)c_{i\alpha}(\tau_1) \qquad\qquad p^\nu_{\boldsymbol{\alpha}} = -g\mu_B\langle\sigma'|\hat{\sigma}_\nu|\sigma'\rangle,$$

$$\chi_{\hat{S}^i_\nu\ \hat{S}^{i'}_{\nu'}}(\tau) \quad = \quad \langle\mathcal{T}\Delta\hat{S}^i_\nu(\tau,\tau)\Delta\hat{S}^{i'}_{\nu'}(0,0)\rangle_0,$$

$$\chi_{\hat{S}^i_\nu\ \hat{S}^{i'}_{\nu'}}(i\omega_m) = \int d\tau e^{i\omega_m\tau}\chi_{\hat{S}^i_\nu\ \hat{S}^{i'}_{\nu'}}(\tau)$$

↑

bosonic Matsubara frequency $\qquad \omega_m = \frac{\pi}{\beta}2m$

let's make it more complicated

$$\chi_{\hat{S}^{i}_{\nu}\,\hat{S}^{i'}_{\nu'}}(\boldsymbol{\tau}) \quad = \quad \langle \mathcal{T} \Delta \hat{S}^{i}_{\nu}(\tau_1, \tau_2) \Delta \hat{S}^{i'}_{\nu'}(\tau_3, \tau_4) \rangle_0,$$

3 independent times

$$\tau_{ll'} = \tau_l - \tau_{l'}$$

$$\tau_{12}, \underline{\tau_{23},} \tau_{34}$$

let's make it more complicated

Fourier transform

$$\tau_{12}, \tau_{23}, \tau_{34}$$

$$(\tau_1, \tau_2, \tau_3, \tau_4) \Rightarrow \boldsymbol{\nu} = (\nu_n, -\nu_n - \omega_m, \nu_{n'} + \omega_m, -\nu_{n'})$$

3 independent frequencies

$$\chi_{\hat{S}^i_\nu \; \hat{S}^{i'}_{\nu'}}(\boldsymbol{\nu})$$

fermionic

$$\nu_n = \frac{\pi}{\beta}(2n+1)$$

bosonic

$$\omega_m = \frac{\pi}{\beta} 2m$$

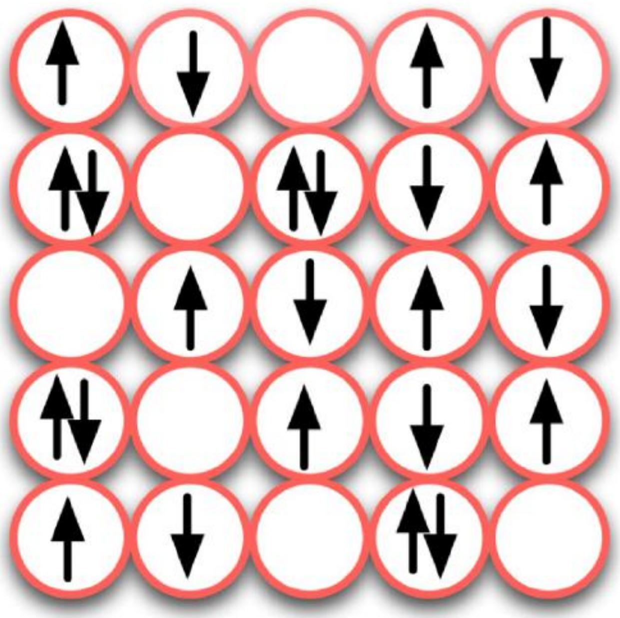
$$\chi_{\hat{S}^i_\nu \; \hat{S}^{i'}_{\nu'}}(i\omega_m) = \frac{1}{\beta^2} \sum_{n,n'} \chi_{\hat{S}^i_\nu \; \hat{S}^{i'}_{\nu'}}(\boldsymbol{\nu})$$

III: magnetic response for the Hubbard model

Hubbard model

atomic hoppings atomic

$$\hat{H} = \varepsilon_d \sum_i \sum_\sigma c^\dagger_{i\sigma} c_{i\sigma} - t \sum_{\langle ii' \rangle} \sum_\sigma c^\dagger_{i\sigma} c_{i'\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} = \hat{H}_d + \hat{H}_T + \hat{H}_U$$



at half filling:

1. *t=0*: collection of atoms, **insulator**
2. *U=0*: half-filled band, **metal**

$$\hat{M}_z(\boldsymbol{q}) = -\frac{g\mu_B}{2} \sum_{\boldsymbol{k}} \sum_\sigma s_\sigma c^\dagger_{\boldsymbol{k}+\boldsymbol{q}\sigma} c_{\boldsymbol{k}\sigma}$$

$$\chi_{zz}(\boldsymbol{q}; i\omega_m) = \langle \hat{M}_z(\boldsymbol{q}; \omega_m) \hat{M}_z(-\boldsymbol{q}; 0) \rangle_0 - \langle \hat{M}_z(\boldsymbol{q}) \rangle_0 \langle \hat{M}_z(-\boldsymbol{q}) \rangle_0,$$

magnetic susceptibility 3-times

$\tau_{ij} = \tau_i - \tau_j$

$$\chi_{zz}(\boldsymbol{q};\boldsymbol{\tau}) = (g\mu_B)^2 \frac{1}{4} \sum_{\sigma\sigma'} s_\sigma s_{\sigma'} \underbrace{\frac{1}{\beta} \frac{1}{N_{\boldsymbol{k}}^2} \sum_{\boldsymbol{k}\boldsymbol{k}'} [\chi(\boldsymbol{q};\boldsymbol{\tau})]_{\boldsymbol{k}\sigma,\boldsymbol{k}'\sigma'}}_{\chi_{\sigma\sigma\sigma'\sigma'}(\boldsymbol{q};\boldsymbol{\tau})}$$

$$\begin{aligned}[\chi(\boldsymbol{q};\boldsymbol{\tau})]_{\boldsymbol{k}\sigma,\boldsymbol{k}'\sigma'} &= \left\langle \mathcal{T} c_{\boldsymbol{k}\sigma}(\tau_1) c^\dagger_{\boldsymbol{k}+\boldsymbol{q}\sigma}(\tau_2) c_{\boldsymbol{k}'+\boldsymbol{q}\sigma'}(\tau_3) c^\dagger_{\boldsymbol{k}'\sigma'}(\tau_4) \right\rangle_0 \\ &\quad - \left\langle \mathcal{T} c_{\boldsymbol{k}\sigma}(\tau_1) c^\dagger_{\boldsymbol{k}+\boldsymbol{q}\sigma}(\tau_2) \right\rangle_0 \left\langle \mathcal{T} c_{\boldsymbol{k}'+\boldsymbol{q}\sigma'}(\tau_3) c^\dagger_{\boldsymbol{k}'\sigma'}(\tau_4) \right\rangle_0\end{aligned}$$

$$\chi_{zz}(\boldsymbol{q};i\omega_m) = (g\mu_B)^2 \frac{1}{4} \sum_{\sigma\sigma'} s_\sigma s_{\sigma'} \frac{1}{\beta^2} \sum_{nn'} \chi^{n,n'}_{\sigma\sigma\sigma'\sigma'}(\boldsymbol{q};i\omega_m),$$

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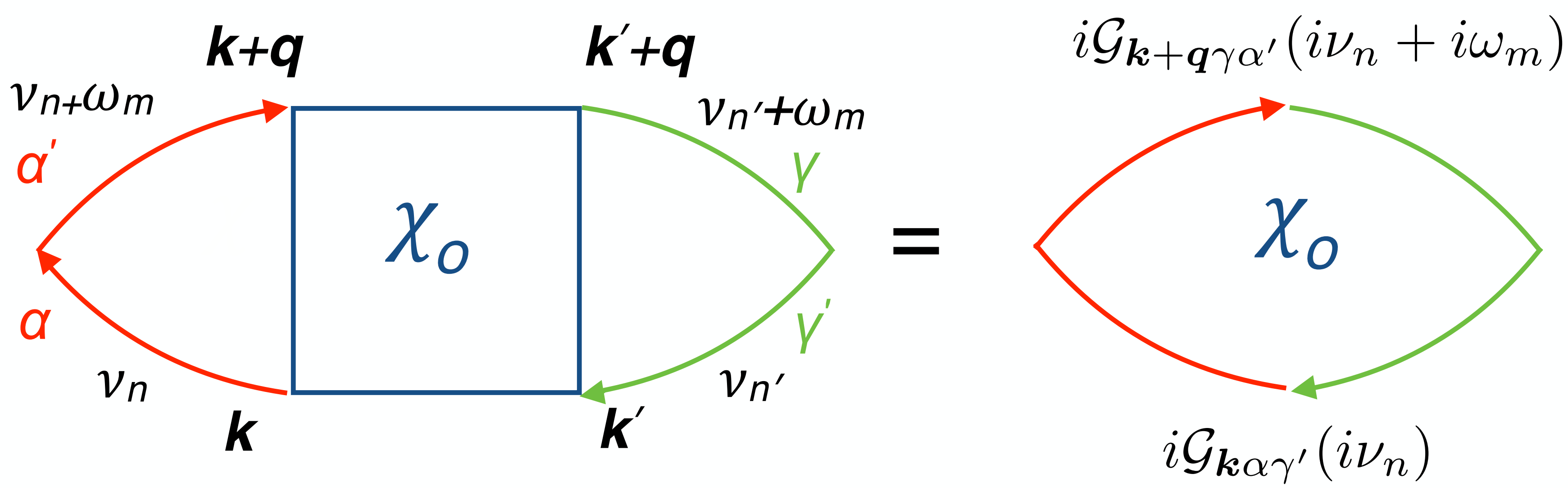
non-interacting limit

Matsubara formalism and Wick theorem

$$[\chi(\boldsymbol{q};\boldsymbol{\tau})]_{\boldsymbol{k}\sigma,\boldsymbol{k}'\sigma'} = \langle \mathcal{T} c_{\boldsymbol{k}\sigma}(\tau_1) c^\dagger_{\boldsymbol{k}+\boldsymbol{q}\sigma}(\tau_2) c_{\boldsymbol{k}'+\boldsymbol{q}\sigma'}(\tau_3) c^\dagger_{\boldsymbol{k}'\sigma'}(\tau_4)\rangle_0$$

$$- \langle \mathcal{T} c_{\boldsymbol{k}\sigma}(\tau_1) c^\dagger_{\boldsymbol{k}+\boldsymbol{q}\sigma}(\tau_2)\rangle_0 \langle \mathcal{T} c_{\boldsymbol{k}'+\boldsymbol{q}\sigma'}(\tau_3) c^\dagger_{\boldsymbol{k}'\sigma'}(\tau_4)\rangle_0$$



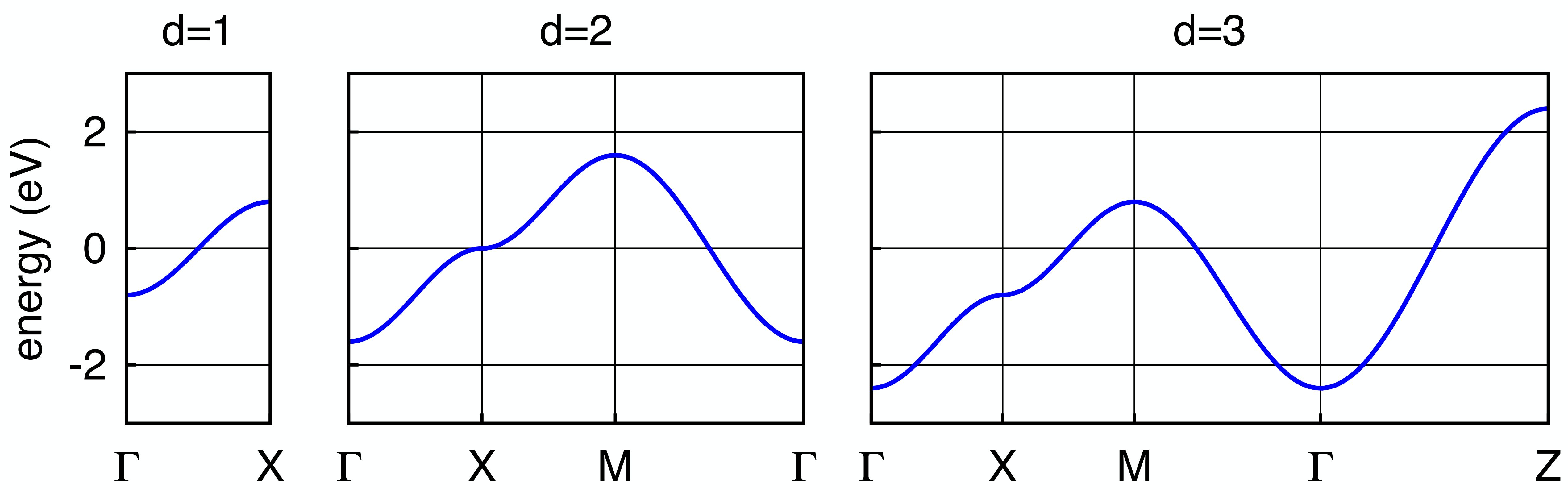
$$[\chi_0(\boldsymbol{q};i\omega_m)]_{\boldsymbol{k}L_\alpha,\boldsymbol{k}'L_\gamma} = -\beta N_{\boldsymbol{k}} \mathcal{G}_{\boldsymbol{k}\alpha\gamma'}(i\nu_n) \mathcal{G}_{\boldsymbol{k}'+\boldsymbol{q}\alpha'\gamma}(i\nu_{n'} + i\omega_m)\delta_{n,n'}\delta_{\boldsymbol{k},\boldsymbol{k}'}$$

$\alpha = \sigma, \gamma' = \sigma'$ $\qquad$ $\alpha' = \sigma, \gamma = \sigma'$

non-interacting limit

hypercubic lattice

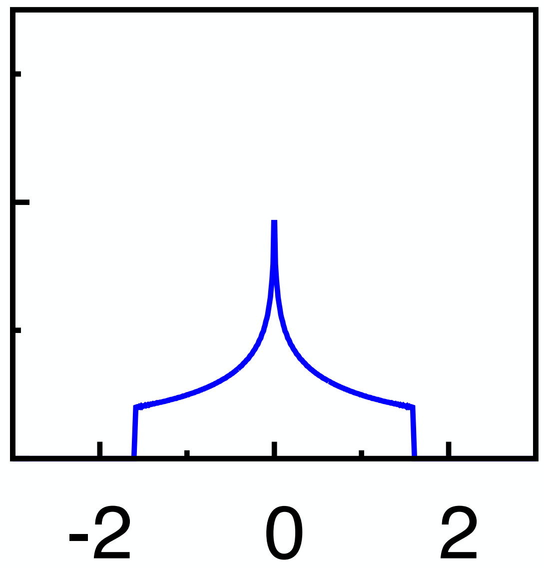
$$\varepsilon_{\boldsymbol{k}} = -2t \sum_{\nu=1}^{d} \cos(k_{r_\nu} a)$$



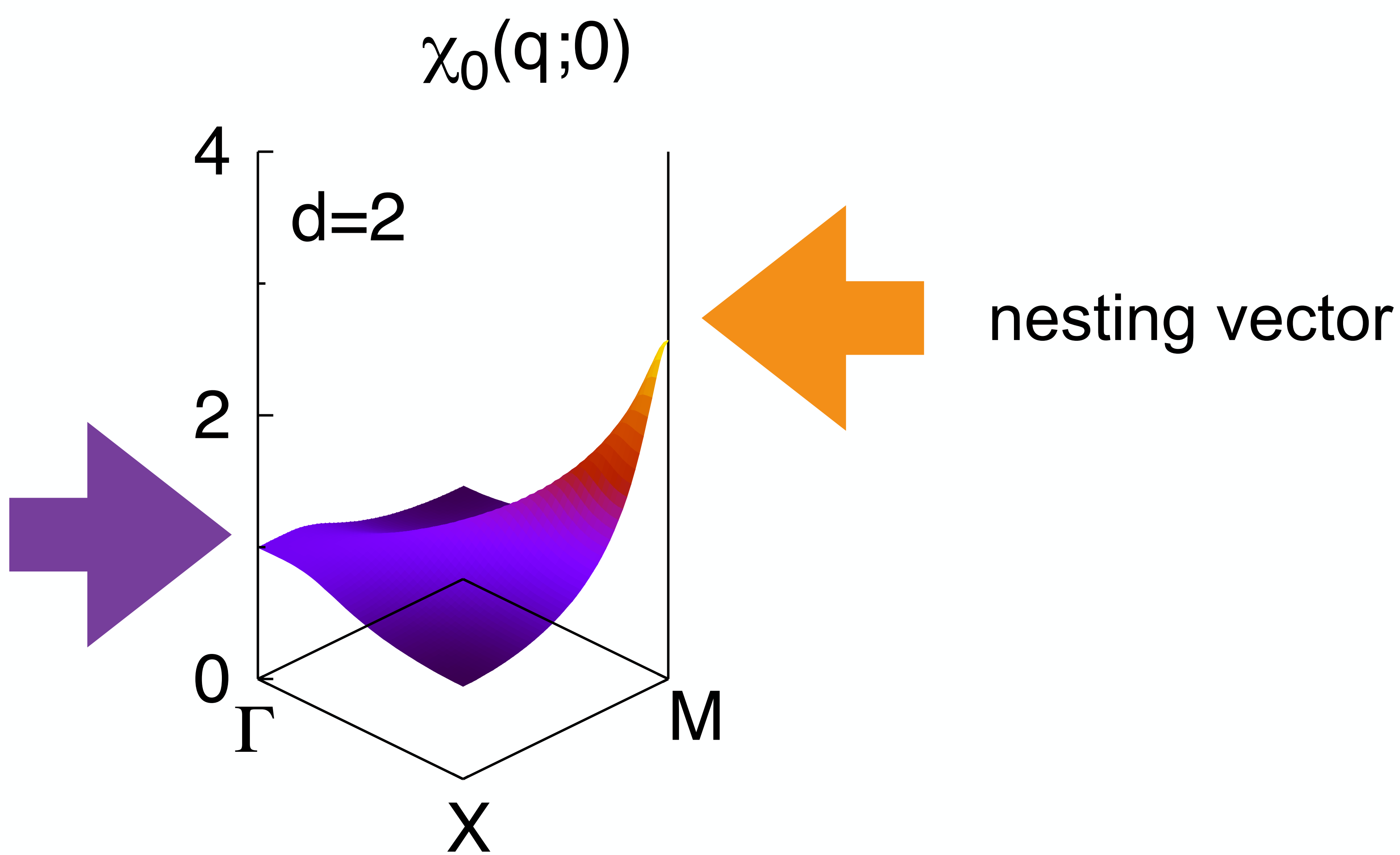
Hubbard model, U=0, n=1, d=2

$$\varepsilon_{\boldsymbol{k}} = -2t[\cos(k_x a) + \cos(k_y a)]$$

T ~ 350 K

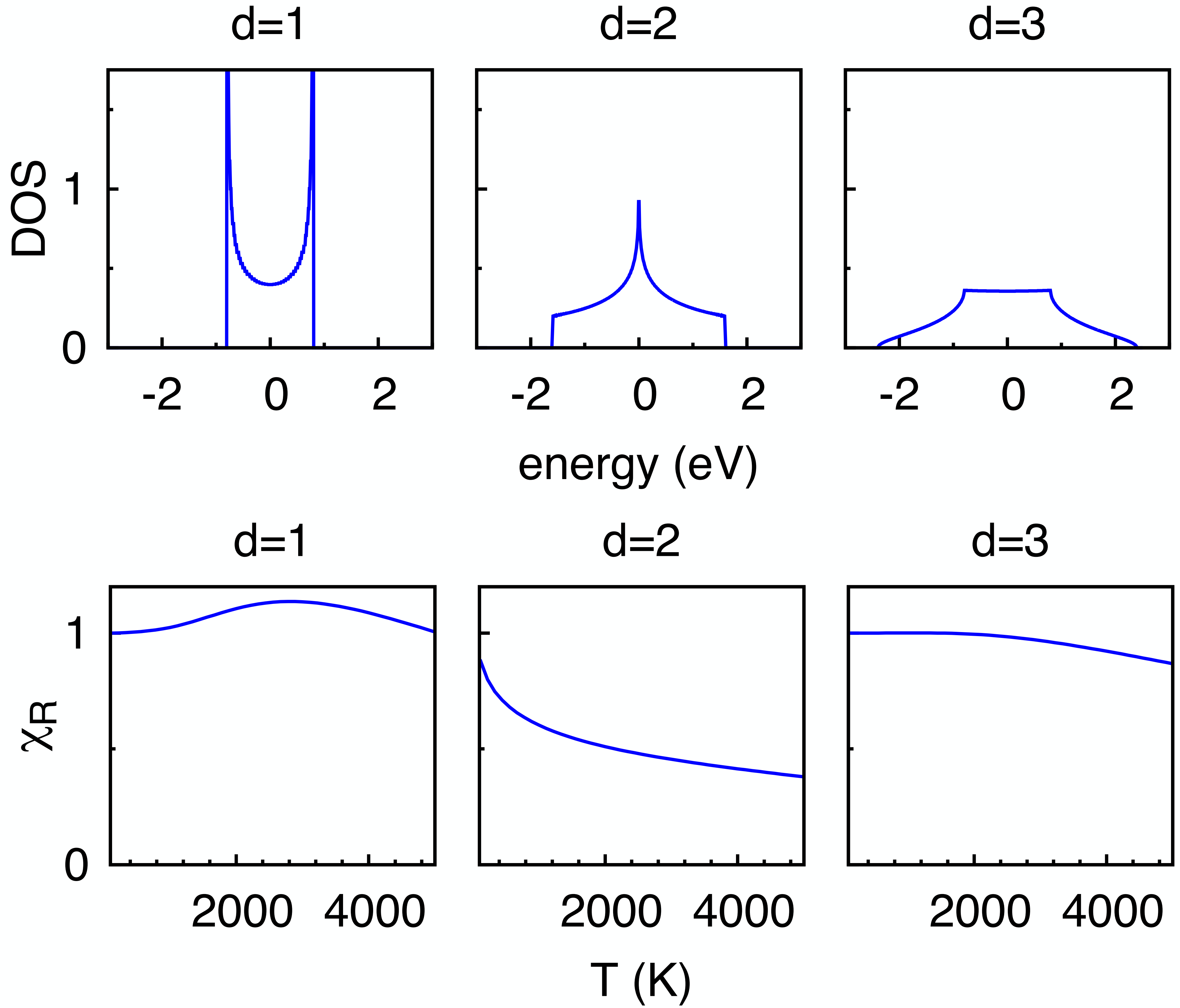


proportional to
density of states
(Pauli)



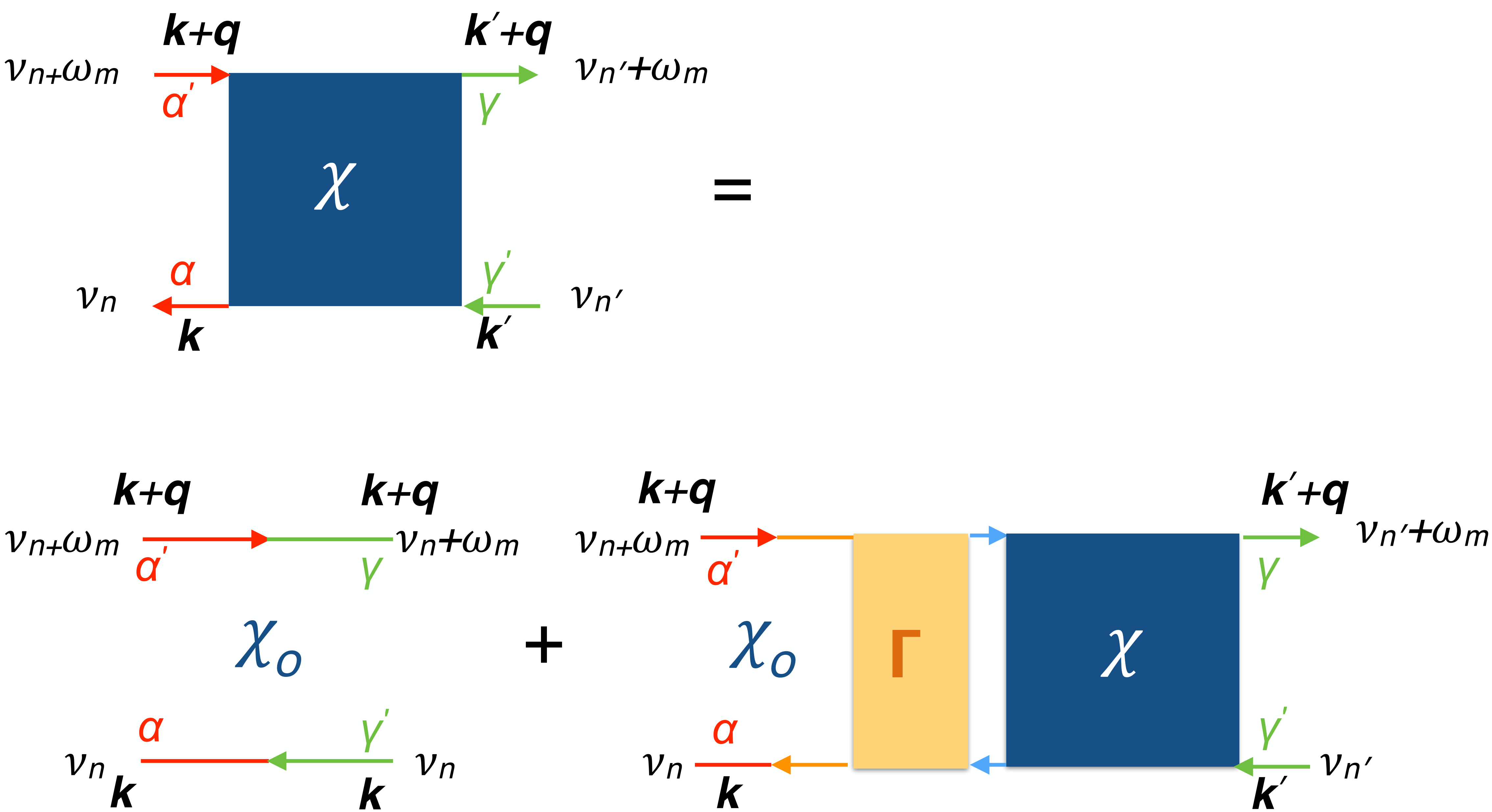
weakly T dependent (except close to van-Hove singularities/divergencies)

q=0, finite temperature



let us switch on U…

Bethe-Salpeter equation



an exact solution: the atomic limit

atomic limit (*t*=*0*) & half filling

$\lvert N,S,S_z\rangle$			N	S	$E(N)$
$\lvert 0,0,0\rangle$	$=$	$\lvert 0\rangle$	0	0	0
$\lvert 1,\frac{1}{2},\uparrow\rangle$	$=$	$c^\dagger_{i\uparrow}\lvert 0\rangle$	1	$1/2$	ε_d
$\lvert 1,\frac{1}{2},\downarrow\rangle$	$=$	$c^\dagger_{i\downarrow}\lvert 0\rangle$	1	$1/2$	ε_d
$\lvert 2,0,0\rangle$	$=$	$c^\dagger_{i\uparrow}c^\dagger_{i\downarrow}\lvert 0\rangle$	2	0	$2\varepsilon_d+U$

$$G_\sigma(i\nu_n)=\frac{1}{2}\left[\frac{1}{i\nu_n+U/2}+\frac{1}{i\nu_n-U/2}\right]$$

static magnetic local susceptibility

$$\chi_{zz}(0) \sim \frac{(g\mu_B)^2}{k_B T} \left\{ \frac{\mathrm{Tr}\left[e^{-\beta(H_i-\mu N_i)} \left(S_z^i\right)^2\right]}{\mathrm{Tr}\left[e^{-\beta(H_i-\mu N_i)}\right]} - \left[\frac{\mathrm{Tr}\left[e^{-\beta(H_i-\mu N_i)} S_z^i\right]}{\mathrm{Tr}\left[e^{-\beta(H_i-\mu N_i)}\right]}\right]^2 \right\}$$

$$= \frac{C_{1/2}}{T} \frac{e^{\beta U/2}}{1+e^{\beta U/2}}$$

large U: Curie form

$$\chi_{zz}(0) = (g\mu_B S)^2 \frac{1}{k_B T} = \frac{C_{1/2}}{T}$$

imaginary time and frequency

$$\chi_{zz}(\boldsymbol{\tau}) = (g\mu_B)^2 \frac{1}{4} \sum_{\sigma\sigma'} s_\sigma s_{\sigma'} \underbrace{\frac{1}{\beta} [\chi(\boldsymbol{\tau})]_{\sigma,\sigma'}}_{\chi_{\sigma\sigma\sigma'\sigma'}(\boldsymbol{\tau})}$$

$$[\chi(\boldsymbol{\tau})]_{\sigma,\sigma'} = \langle \mathcal{T} c_{i\sigma}(\tau_1) c^\dagger_{i\sigma}(\tau_2) c_{i\sigma'}(\tau_3) c^\dagger_{i\sigma'}(\tau_4) \rangle_0 - \langle \mathcal{T} c_{i\sigma}(\tau_1) c^\dagger_{i\sigma}(\tau_2) \rangle_0 \langle \mathcal{T} c_{i\sigma'}(\tau_3) c^\dagger_{i\sigma'}(\tau_4) \rangle_0$$

$$\chi_{zz}(i\omega_m) = (g\mu_B)^2 \frac{1}{4} \sum_{\sigma\sigma'} s_\sigma s_{\sigma'} \frac{1}{\beta^2} \sum_{nn'} \chi^{n,n'}_{\sigma\sigma\sigma'\sigma'}(i\omega_m),$$

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Matsubara formalism, no Wick theorem

$$-\beta < \tau_i < \beta$$

symmetries: six independent sectors

$$\tau_{ij} = \tau_i - \tau_j$$

sector E, τ^+: $\tau_i > 0$

$$\chi_{i\sigma\sigma,i\sigma'\sigma'}(\boldsymbol{\tau}^+) = \frac{e^{\tau_{12}U/2+\tau_{34}U/2} + \delta_{\sigma\sigma'} e^{(\beta-\tau_{12})U/2-\tau_{34}U/2}}{2(1+e^{\beta U/2})} - G^{\sigma}_{i,i}(\tau_{12})\, G^{\sigma'}_{i,i}(\tau_{34}).$$

The mean-field terms $G^{\sigma}_{i,i}(\tau_{12})\, G^{\sigma'}_{i,i}(\tau_{34})$ cancel out in the actual magnetic linear response function, so here we do not give their form explicitly and we will neglect them in the rest of the calculations. For a single atom, the contribution of the $\boldsymbol{\tau}^+$ sector to the imaginary-time magnetic susceptibility is

$$\chi_{zz}(\boldsymbol{\tau}^+) = (g\mu_B)^2 \frac{1}{4}\frac{1}{\beta} \sum_{\sigma\sigma'} s_\sigma s_{\sigma'} \chi_{i\sigma\sigma,i\sigma'\sigma'}(\boldsymbol{\tau}^+) = \frac{(g\mu_B)^2}{4\beta} \frac{1}{(1+e^{\beta U/2})} e^{(\beta-\tau_{12}-\tau_{34})U/2}.$$

Fourier transform: 6 integrals

$$[\chi_{zz}]_{nn'}(i\omega_m) = \beta \frac{1}{4}(g\mu_B)^2 \sum_P \mathrm{sign}(P) f_P$$

$$f_P(i\omega_{P_1}, i\omega_{P_2}, i\omega_{P_3}) = \int_0^\beta d\tau_{14} \int_0^{\tau_{14}} d\tau_{24} \int_0^{\tau_{24}} d\tau_{34}\; e^{i\omega_{P_1}\tau_{14} + i\omega_{P_2}\tau_{24} + i\omega_{P_3}\tau_{34}} f_P(\tau_{14}, \tau_{24}, \tau_{34})$$

$$f_E(\tau_{14}, \tau_{24}, \tau_{34}) = \frac{1}{(1+e^{\beta U/2})}\, e^{\beta U/2}\, e^{-(\tau_{12}+\tau_{34})U/2} = \frac{1}{(1+e^{\beta U/2})}\, g_E(\tau_{14}, \tau_{24}, \tau_{34}).$$

	ω_{P_1}	ω_{P_2}	ω_{P_3}	$g_P(\tau_{14}, \tau_{24}, \tau_{34})$	$\mathrm{sign}(P)$
$E(123)$	ν_n	$-\omega_m - \nu_n$	$\omega_m + \nu_{n'}$	$e^{\beta U/2}\, e^{-(\tau_{12}+\tau_{34})U/2}$	$+$
$A(231)$	$-\omega_m - \nu_n$	$\omega_m + \nu_{n'}$	ν_n	$e^{\beta U/2}\, e^{-(\tau_{12}+\tau_{34})U/2}$	$+$
$B(312)$	$\omega_m + \nu_{n'}$	ν_n	$-\omega_m - \nu_n$	$-e^{+(\tau_{12}+\tau_{34})U/2}$	$+$
$C(213)$	$-\omega_m - \nu_n$	ν_n	$\omega_m + \nu_{n'}$	$-e^{\beta U/2} e^{-(\tau_{12}+\tau_{34})U/2}$	$-$
$D(132)$	ν_n	$\omega_m + \nu_{n'}$	$-\omega_m - \nu_n$	$e^{+(\tau_{12}+\tau_{34})U/2}$	$-$
$F(321)$	$\omega_m + \nu_{n'}$	$-\omega_m - \nu_n$	ν_n	$e^{+(\tau_{12}+\tau_{34})U/2}$	$-$

calculating the integral

$$I_P(x,-x,x;i\omega_{P_1},i\omega_{P_2},i\omega_{P_3}) = \int_0^\beta d\tau_{14} \int_0^{\tau_{14}} d\tau_{24} \int_0^{\tau_{24}} d\tau_{34}\ e^{i\omega_{P_1}\tau_{14}+i\omega_{P_2}\tau_{24}+i\omega_{P_3}\tau_{34}} e^{x(\tau_{14}-\tau_{24}+\tau_{34}}$$

$$= + \int_0^\beta d\tau_{14} \int_0^{\tau_{14}} d\tau\ \int_0^{\tau_{14}-\tau} d\tau'\ e^{(i\omega_{P_1}+i\omega_{P_2}+i\omega_{P_3}+x)\tau_{14}-i(\omega_{P_2}+\omega_{P_3})\tau} e^{-(i\omega_{P_3}+x)\tau'}$$

$$= + \frac{1}{i\omega_{P_3}+x}\frac{1}{-i\omega_{P_2}+x}\left[\frac{1}{i\omega_{P_1}+x}\ \frac{1}{n(x)} + \beta\delta_{\omega_{P_1}+\omega_{P_2}}\right]$$

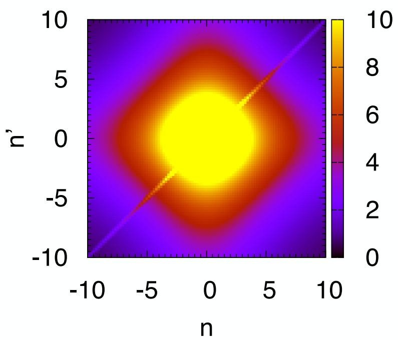
$$+ \frac{1}{i\omega_{P_3}+x}\frac{1-\delta_{\omega_{P_2}+\omega_{P_3}}}{i(\omega_{P_2}+\omega_{P_3})}\left[\frac{1}{i\omega_{P_1}+x} - \frac{1}{i(\omega_{P_1}+\omega_{P_2}+\omega_{P_3})+x}\right]\frac{1}{n(x)}$$

$$+ \delta_{\omega_{P_2}+\omega_{P_3}}\frac{1}{i\omega_{P_3}+x}\left\{\left[\frac{1}{(i\omega_{P_1}+x)}\right]^2\frac{1}{n(x)} - \beta\left[\frac{1}{(i\omega_{P_1}+x)}\right]\frac{1-n(x)}{n(x)}\right\}.$$

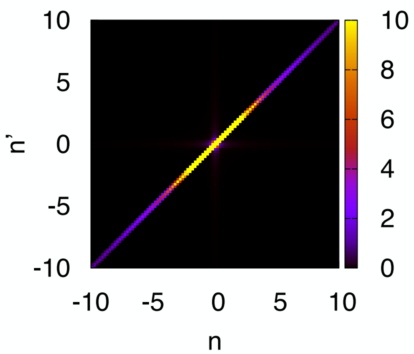
static case: y=U/2

$$\sum_{\sigma\sigma'} \sigma\sigma' \, \chi^{n,n'}_{i\sigma\sigma,i\sigma'\sigma'}(0) = M_{n'} \frac{dM_n}{dy} + M_n \frac{dM_{n'}}{dy} - \beta n(y) \left[\delta_{n,n'} + \delta_{n,-n'} \right] \frac{dM_n}{dy} + \beta n(-y) M_n M_{n'}$$
$$- \frac{1}{y} \left\{ M_{n'} - \beta \left[n(y) \delta_{n,-n'} - n(-y) \delta_{n,n'} \right] \right\} M_n$$

$$n(y) = \frac{1}{1+e^{\beta y}} \qquad M_n = \frac{1}{i\nu_n - y} - \frac{1}{i\nu_n + y}.$$



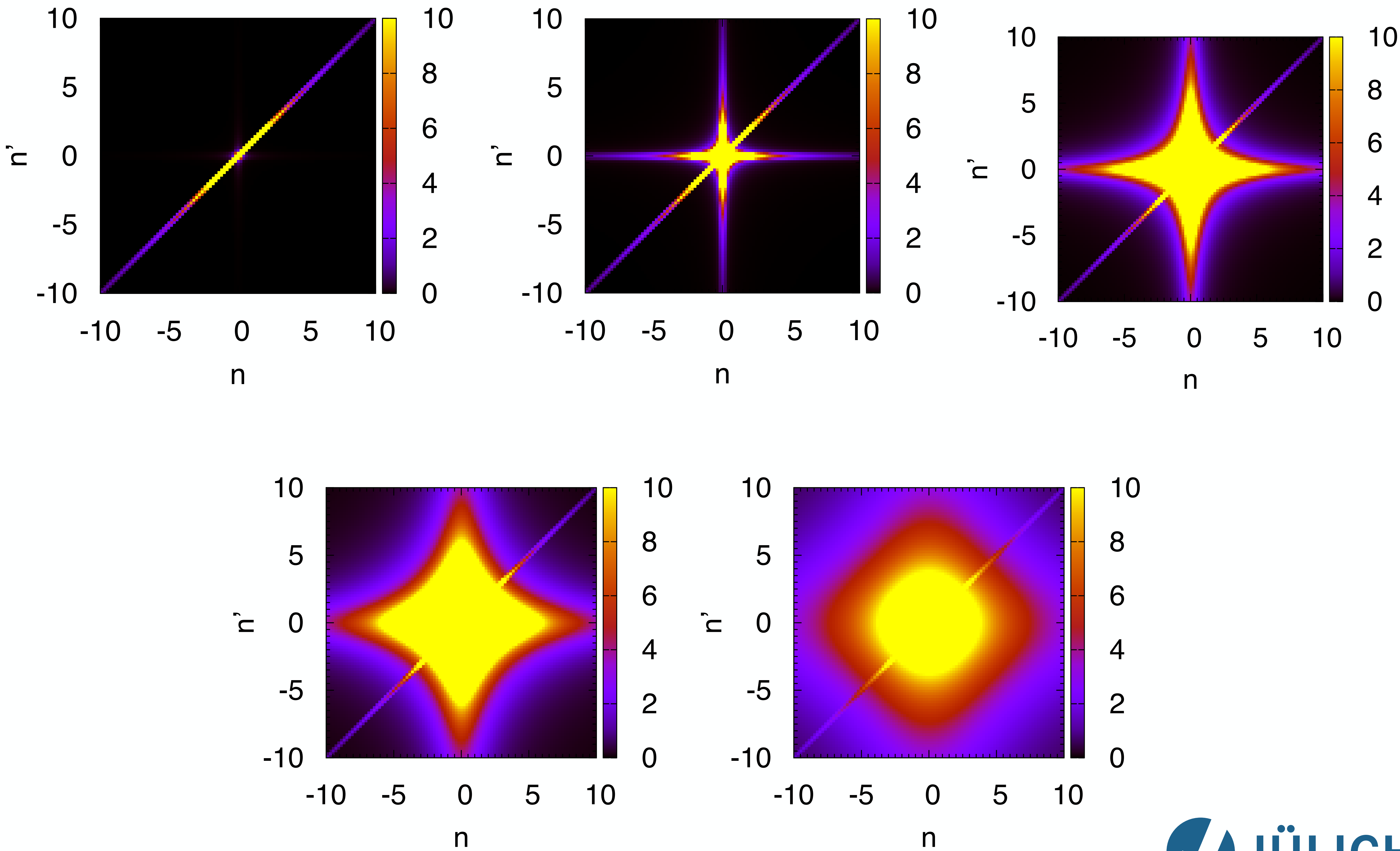
U=0 $$\sum_{\sigma\sigma'} \sigma\sigma' \, \chi^{n,n'}_{i\sigma\sigma,i\sigma'\sigma'}(0) = -\beta \delta_{n,n'} \frac{dM_n}{dy} = -\beta \delta_{n,n'} \frac{2}{(i\nu_n)^2}$$



and after Matsubara sums

$$\chi_{zz}(0) = (g\mu_B)^2 \frac{1}{4k_BT} \frac{e^{\beta U/2}}{1+e^{\beta U/2}}$$

increasing U, low T



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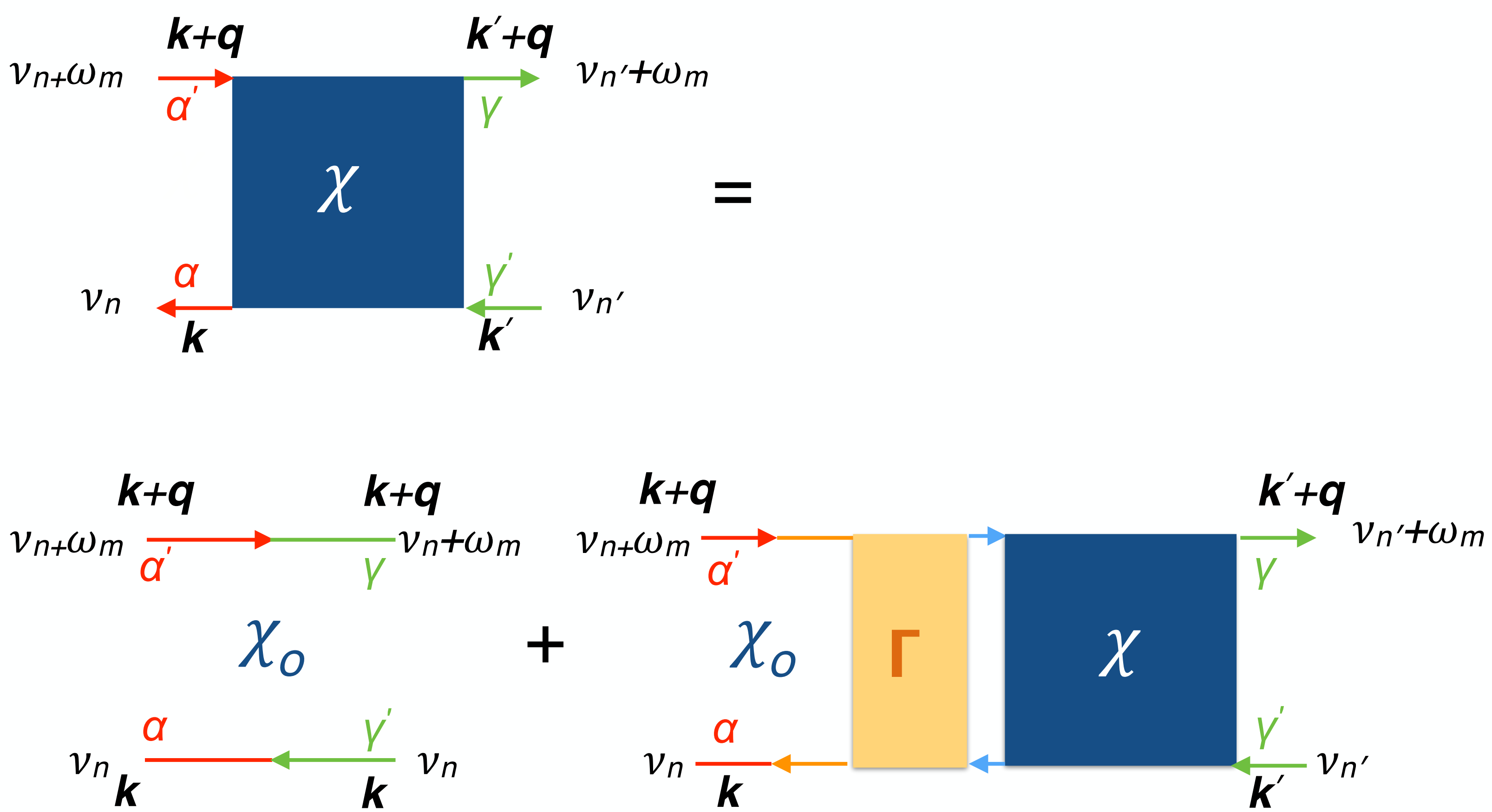
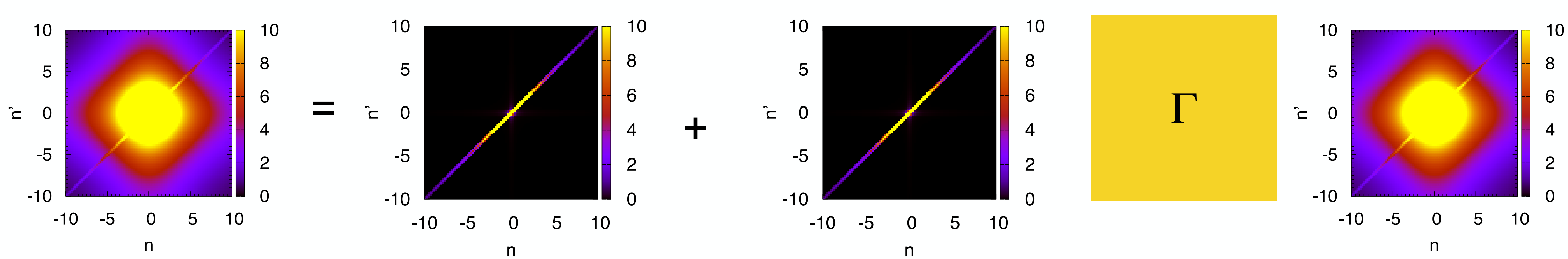
Bethe-Salpeter equation



$\omega_m = 0$



vertex in the small U limit

Γ

$$M_n = -\frac{2y}{\nu_n^2 + y^2} \sim -\frac{2y}{\nu_n^2}$$

$$\sum_{\sigma\sigma'} \sigma\sigma' \, \chi^{n,n'}_{i\sigma\sigma, i\sigma'\sigma'}(0) \sim \frac{d}{dy} M_n M_{n'} + \beta M_n M_{n'} - \frac{1}{y}\left\{ M_{n'} M_n + \beta \delta_{n,n'} M_n \right\}$$

$$\sum_{\sigma\sigma'} \sigma\sigma' \, \chi^{n,n'}_{i\sigma\sigma, i\sigma'\sigma'}(0) \sim +\beta\delta_{n,n'} \frac{2}{\nu_n^2} + \frac{4y}{\nu_n^2 \nu_{n'}^2}$$

with normalizations: $\quad \mathit{\Gamma} \sim \frac{2}{(g\mu_B)^2} U$

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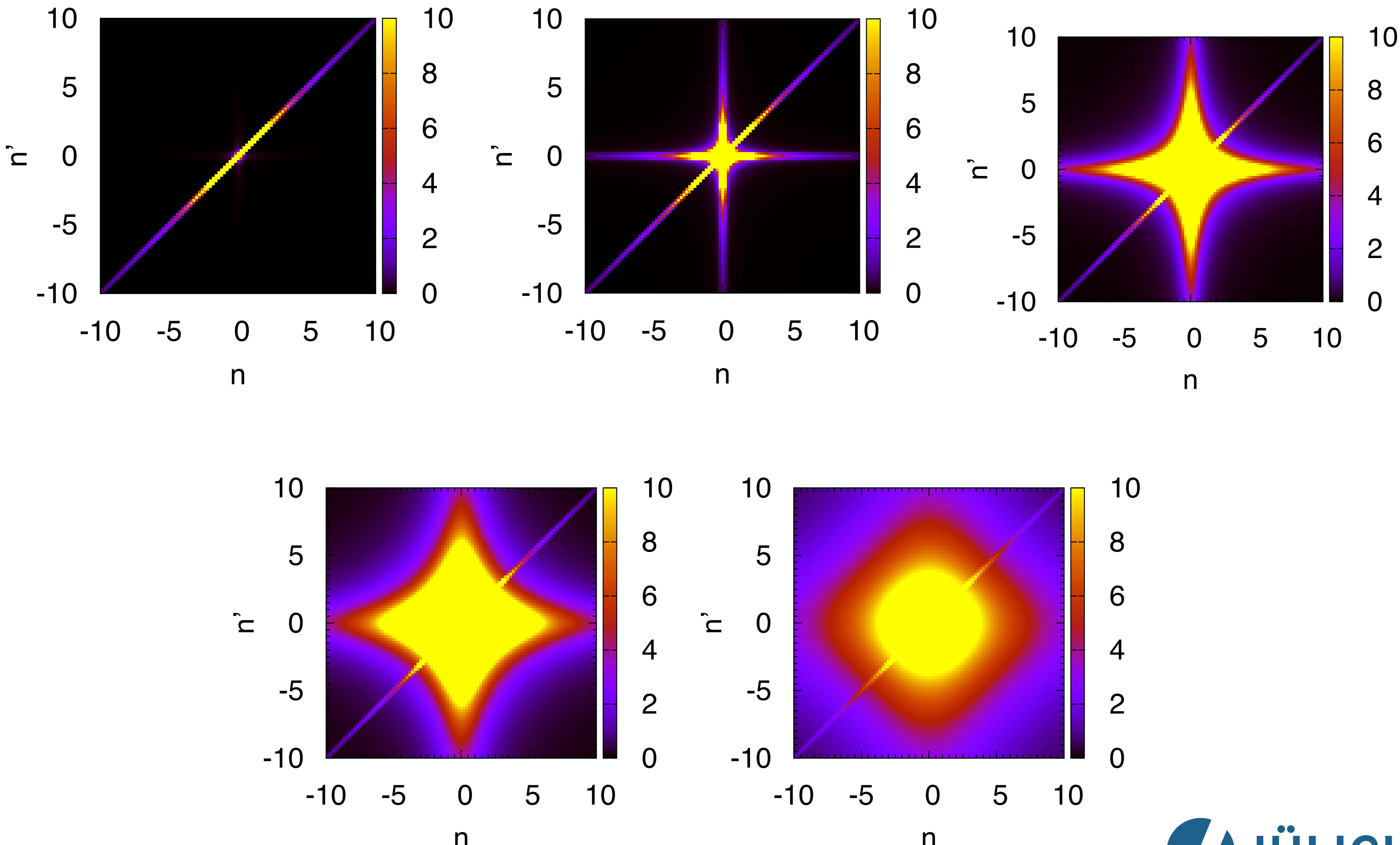
increasing U, low T



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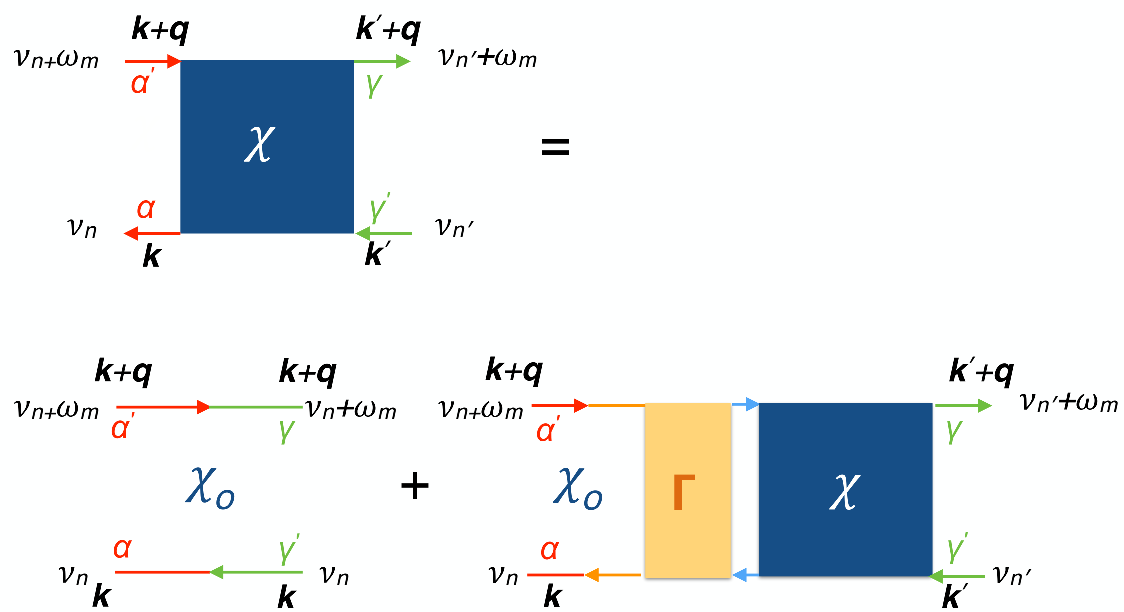
Bethe Salpeter equation

$$\chi_{zz}(\boldsymbol{q};0) = (g\mu_B)^2 \frac{1}{4k_BT}\frac{e^{\beta U/2}}{1+e^{\beta U/2}}$$

$$\Gamma = \frac{1}{\chi^0_{zz}(\boldsymbol{q};0)} - \frac{1}{\chi_{zz}(\boldsymbol{q};0)}$$



small U $\quad \Gamma \sim \frac{2}{(g\mu_B)^2}U$

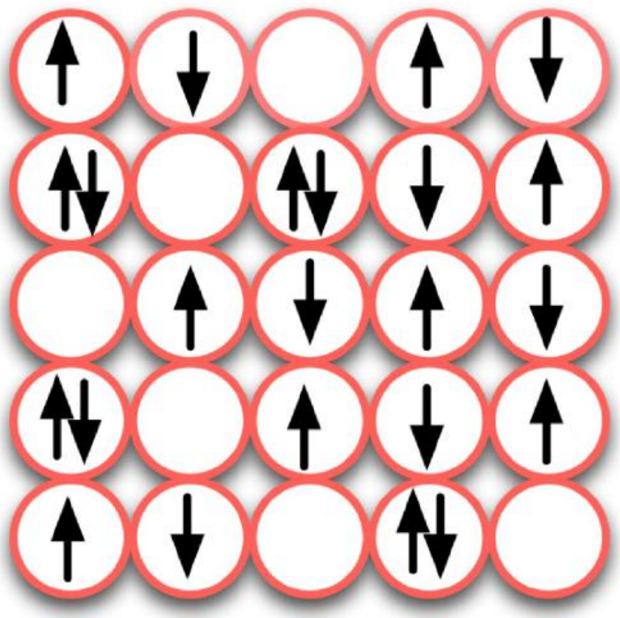
$$\Gamma = \frac{4k_BT}{(g\mu_B)^2}\frac{e^{\beta U/2}-1}{e^{\beta U/2}}$$

large U $\quad \Gamma \sim \frac{4k_BT}{(g\mu_B)^2}$

Hubbard model

atomic — hoppings — atomic

$$\hat{H} = \varepsilon_d \sum_i \sum_\sigma c^\dagger_{i\sigma} c_{i\sigma} - t \sum_{\langle ii' \rangle} \sum_\sigma c^\dagger_{i\sigma} c_{i'\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} = \hat{H}_d + \hat{H}_T + \hat{H}_U$$



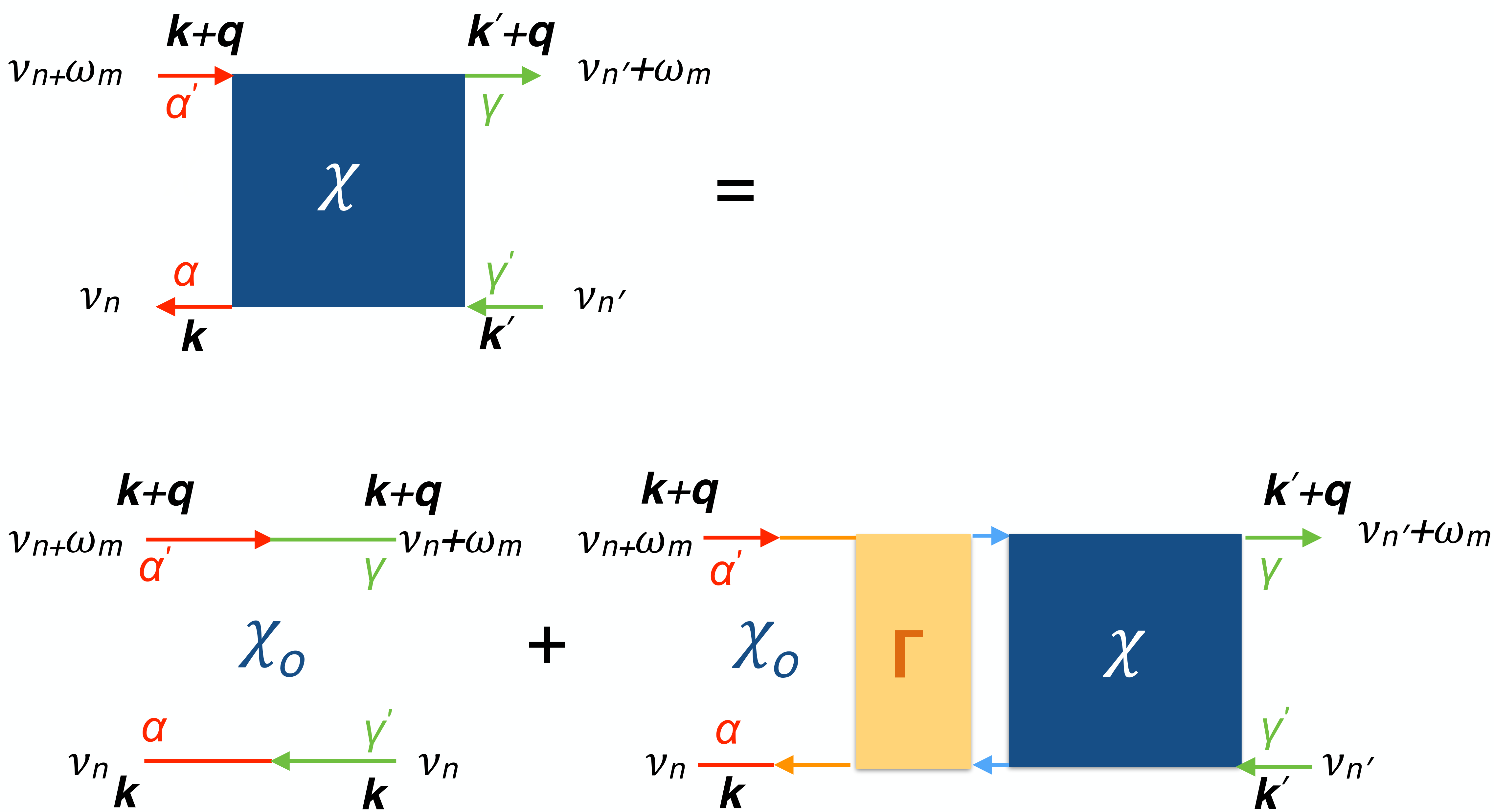
at half filling:

1. *t=0*: collection of atoms, **insulator**
2. *U=0*: half-filled band, **metal**

$$\hat{M}_z(\boldsymbol{q}) = -\frac{g\mu_B}{2} \sum_{\boldsymbol{k}} \sum_\sigma s_\sigma c^\dagger_{\boldsymbol{k}+\boldsymbol{q}\sigma} c_{\boldsymbol{k}\sigma}$$

$$\chi_{zz}(\boldsymbol{q}; i\omega_m) = \langle \hat{M}_z(\boldsymbol{q};\omega_m) \hat{M}_z(-\boldsymbol{q};0) \rangle_0 - \langle \hat{M}_z(\boldsymbol{q}) \rangle_0 \langle \hat{M}_z(-\boldsymbol{q}) \rangle_0,$$

Bethe-Salpeter equation



the small *U/t* limit

Hartree-Fock: perturbation in U

$$U\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} \longrightarrow U\left(\bar{n}_{i\uparrow}\hat{n}_{i\downarrow} + \hat{n}_{i\uparrow}\bar{n}_{i\downarrow} - \bar{n}_{i\uparrow}\bar{n}_{i\downarrow}\right)$$

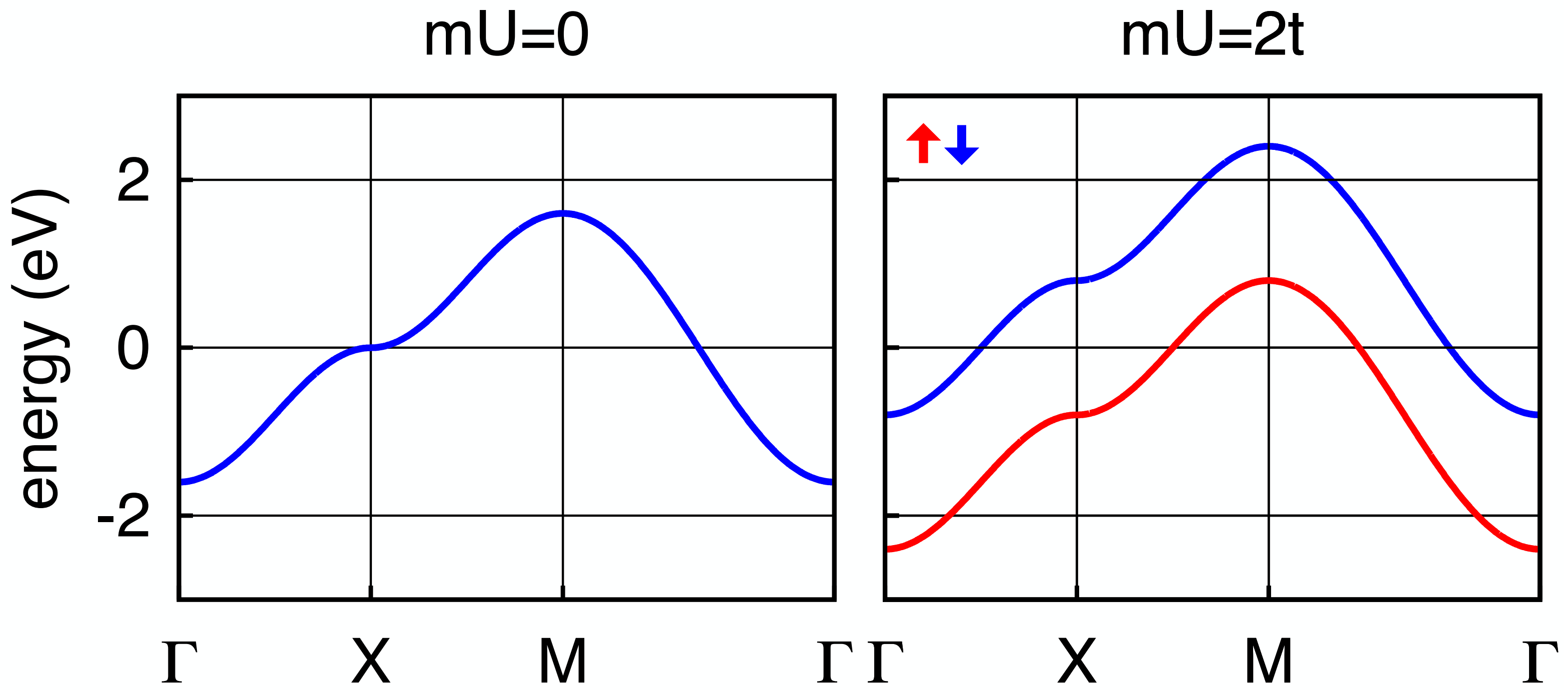
simplest version: expectation value site independent

$$\hat{H}_{\mathrm{MF}} = \sum_{\boldsymbol{k}\sigma}\left[\varepsilon_{\boldsymbol{k}} + U\left(\frac{1}{2} - \sigma m\right)\right]\hat{n}_{\boldsymbol{k}\sigma}$$

m: magnetization

$m \neq 0$ ferromagnetic solution

Hartree-Fock: perturbation in U



$$h_{\text{eff}}(\boldsymbol{q}) = 2m(\boldsymbol{q})U$$

$$m \sim \chi(h + h_{eff}) = \chi(h + 2mU)$$

$$\chi(\boldsymbol{q};0) = \frac{\chi_0(\boldsymbol{q};0)}{1 - \Gamma\chi_0(\boldsymbol{q};0)}, \qquad \Gamma \sim \frac{2}{(g\mu_B)^2}U$$

the small *t/U* limit, half filling

$$H = \varepsilon_d \sum_i \sum_\sigma c^\dagger_{i\sigma} c_{i\sigma} - t \sum_{\langle ii' \rangle} \sum_\sigma c^\dagger_{i\sigma} c_{i'\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} = H_d + H_T + H_U$$

idea: divide Hilbert space into $n_D=0$ and $n_D>0$ sector

n_D = number of doubly occupied sites

next perturbation in U high energy $n_D>0$ sector

$$H_S = \frac{1}{2} \Gamma \sum_{\langle ii' \rangle} \left[\boldsymbol{S}_i \cdot \boldsymbol{S}_{i'} - \frac{1}{4} n_i n_{i'} \right] \qquad \Gamma = \frac{4t^2}{U}$$

static mean-field theory: perturbation in Γ

$$H_S = \frac{1}{2}\Gamma \sum_{\langle ii' \rangle} \left[\boldsymbol{S}_i \cdot \boldsymbol{S}_{i'} - \frac{1}{4} n_i n_{i'} \right] \longrightarrow \Gamma \sum_{\langle ii' \rangle} \left[\boldsymbol{S}_i \cdot \langle \boldsymbol{S}_{i'} \rangle - \frac{1}{4} n_i n_{i'} \right]$$

$$\Gamma_{\boldsymbol{q}} = -\Gamma \sum_{\langle ij \rangle} e^{i\boldsymbol{q}\cdot(\boldsymbol{T}_i + \boldsymbol{R}_j)}$$

$$\langle S^z_{j+i} \rangle = -g\mu_B m(\boldsymbol{q}) = -\mu_B \, m \, \cos(\boldsymbol{q} \cdot \boldsymbol{R}_j)$$

$$m(\boldsymbol{q}) \sim \chi_{\rm at}(h + h_{\rm eff}(\boldsymbol{q})) \sim \chi_{\rm at}(h + \Gamma_{\boldsymbol{q}} m(\boldsymbol{q}))$$

$$\chi_{\rm at} = \frac{C_{1/2}}{T}$$

Curie-Weiss susceptibility

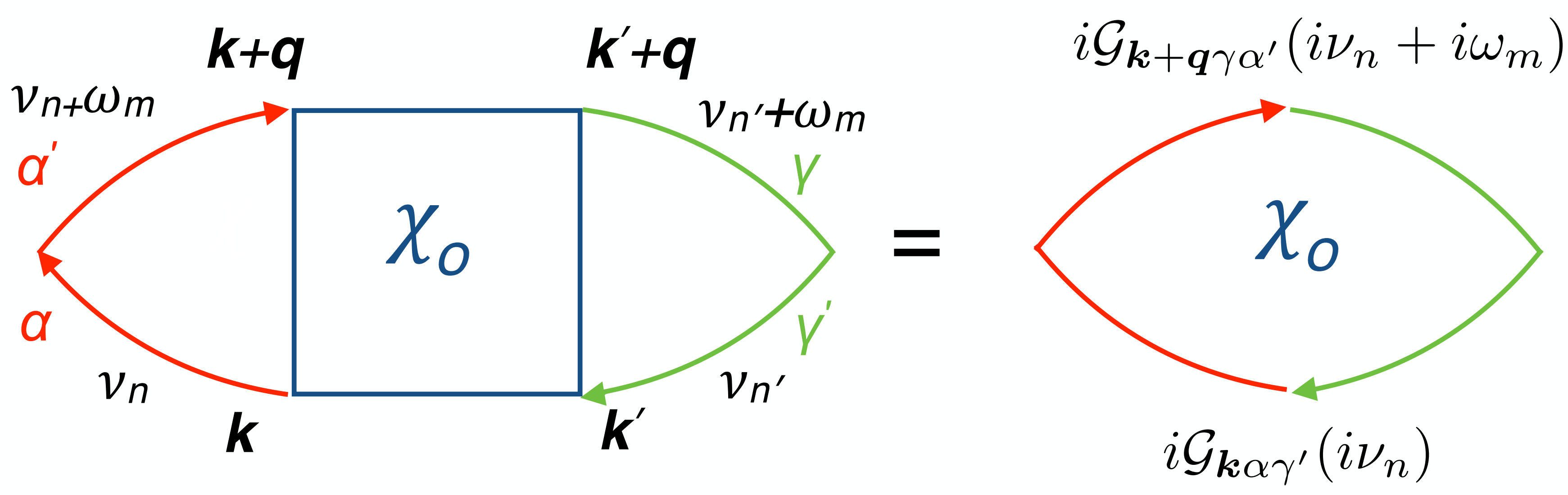
$$\chi_{zz}(\boldsymbol{q};0) = \frac{C_{1/2}}{T - T_{\boldsymbol{q}}} \qquad k_B T_{\boldsymbol{q}} = C_{1/2} \Gamma_{\boldsymbol{q}}$$

IV: Linear response in DMFT and LDA+DMFT

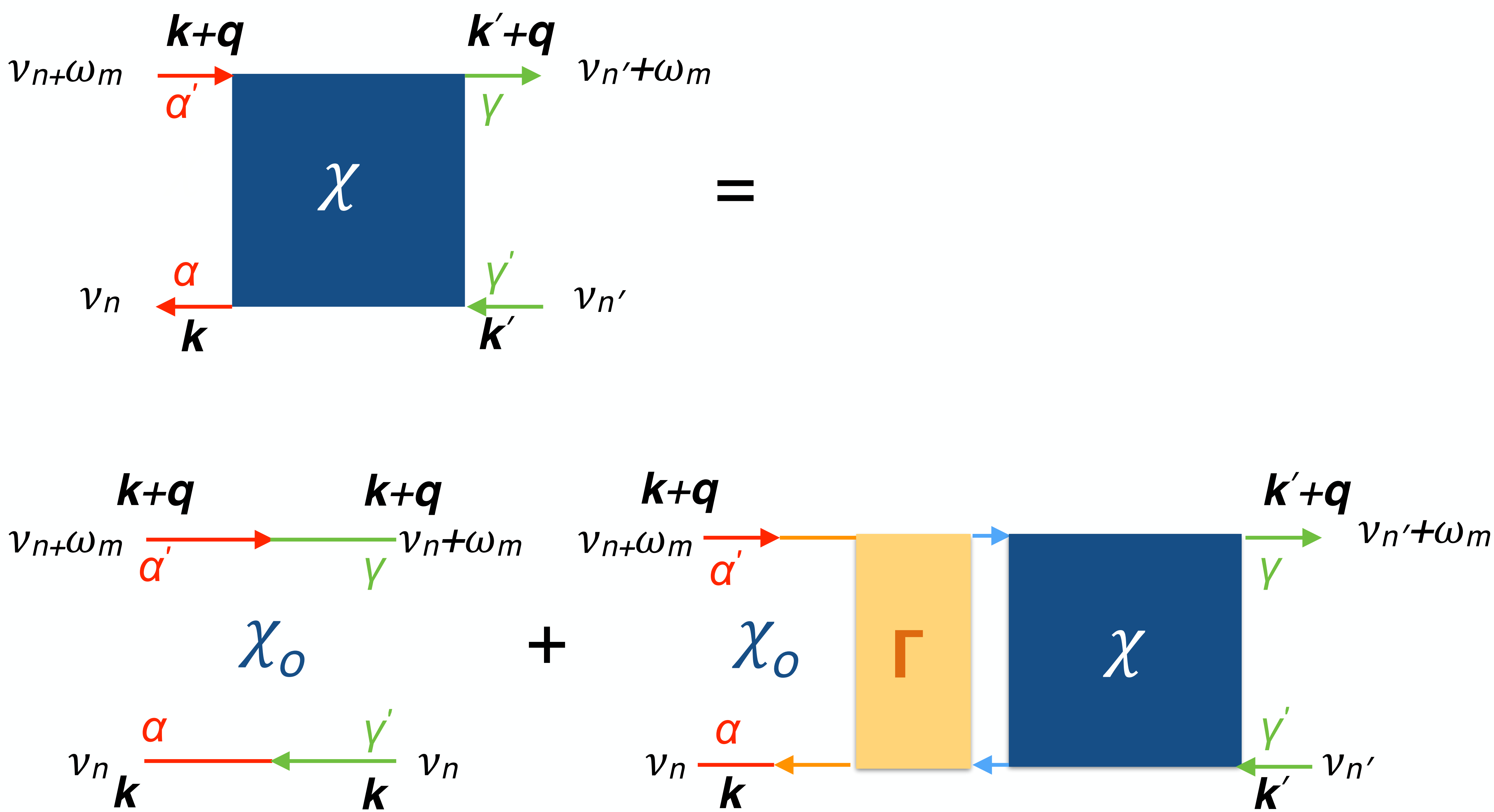
susceptibility in DMFT

1. perturbation around DMFT solution

$$[\chi_0(\boldsymbol{q};i\omega_m)]_{L_\alpha,L_\gamma} = -\beta\delta_{nn'}\frac{1}{N_{\boldsymbol{k}}}\sum_{\boldsymbol{k}} G^{\rm DMFT}_{\alpha\gamma'}(\boldsymbol{k};i\nu_n)G^{\rm DMFT}_{\alpha'\gamma}(\boldsymbol{k}+\boldsymbol{q};i\nu_n+i\omega_m)$$



what about the vertex?



DMFT for 1- and 2- particle GFs

Green Function

k-dependent Dyson equation matrix

$$G(\boldsymbol{k}; i\nu_n) = G_0(\boldsymbol{k}; i\nu_n) + G_0(\boldsymbol{k}; i\nu_n)\Sigma(\boldsymbol{k}; i\nu_n)G(\boldsymbol{k}; i\nu_n)$$

local self-energy approximation

$$\Sigma(\boldsymbol{k}; i\nu_n) \to \Sigma(i\nu_n)$$

local Dyson equation

$$G(i\nu_n) = G_0(i\nu_n) + G_0(i\nu_n)\Sigma(i\nu_n)G(i\nu_n)$$

Susceptibility

q-dependent Bethe-Salpeter equation matrix

$$\chi(\boldsymbol{q}; i\omega_m) = \chi_0(\boldsymbol{q}; i\omega_m) + \chi_0(\boldsymbol{q}; i\omega_m)\Gamma(\boldsymbol{q}; i\omega_m)\chi(\boldsymbol{q}; i\omega_m)$$

local vertex approximation

$$\Gamma(\boldsymbol{q}; i\omega_m) \to \Gamma(i\omega_m)$$

local Bethe-Salpeter equation

$$\chi(i\omega_m) = \chi_0(i\omega_m) + \chi_0(i\omega_m)\Gamma(i\omega_m)\chi(i\omega_m)$$

local-vertex approximation

vertex in BS equation local in infinite dimensions

$$[\chi(\boldsymbol{q};i\omega_m)]_{L_\alpha,L_\gamma} = [\chi_0(\boldsymbol{q};\omega_m) + \chi_0(\boldsymbol{q};i\omega_m)\Gamma(i\omega_m)\chi(\boldsymbol{q};i\omega_m)]_{L_\alpha,L_\gamma}$$

define local susceptibilities

$$[\chi_0(i\omega_m)]_{L_\alpha^{ic},L_\gamma^{ic}} = \frac{1}{N_{\boldsymbol{q}}}\sum_{\boldsymbol{q}}[\chi_0(\boldsymbol{q};i\omega_m)]_{L_\alpha^{ic},L_\gamma^{ic}}\,,$$

$$[\chi(i\omega_m)]_{L_\alpha^{ic},L_\gamma^{ic}} = \frac{1}{N_{\boldsymbol{q}}}\sum_{\boldsymbol{q}}[\chi(\boldsymbol{q};i\omega_m)]_{L_\alpha^{ic},L_\gamma^{ic}}$$

$L_\alpha = n \times \alpha$

local-vertex approximation

2. solve local BS equation

$$[\Gamma(i\omega_m)]_{L_\alpha,L_\gamma} = \left[\chi_0^{-1}(i\omega_m)\right]_{L_\alpha,L_\gamma} - \left[\chi^{-1}(i\omega_m)\right]_{L_\alpha,L_\gamma}$$

local susceptibility: from quantum impurity solver

3. solve *q*-dependent BS equation

$$[\chi(\boldsymbol{q};i\omega_m)]_{L_\alpha,L_\gamma} = [\chi_0(\boldsymbol{q};\omega_m) + \chi_0(\boldsymbol{q};i\omega_m)\Gamma(i\omega_m)\chi(\boldsymbol{q};i\omega_m)]_{L_\alpha,L_\gamma}$$

q-dependence here from non-interacting part

Hubbard Model in Infinite Dimensions: A Quantum Monte Carlo Study

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(Received 5 December 1991)

An essentially exact solution of the infinite-dimensional Hubbard model is made possible by a new self-consistent Monte Carlo procedure. Near half filling antiferromagnetism and a pseudogap in the single-particle density of states are found for sufficiently large values of the intrasite Coulomb interaction. At half filling the antiferromagnetic transition temperature obtains its largest value when the intrasite Coulomb interaction $U \approx 3$.

PACS numbers: 75.10.Jm, 71.10.+x, 75.10.Lp, 75.30.Kz

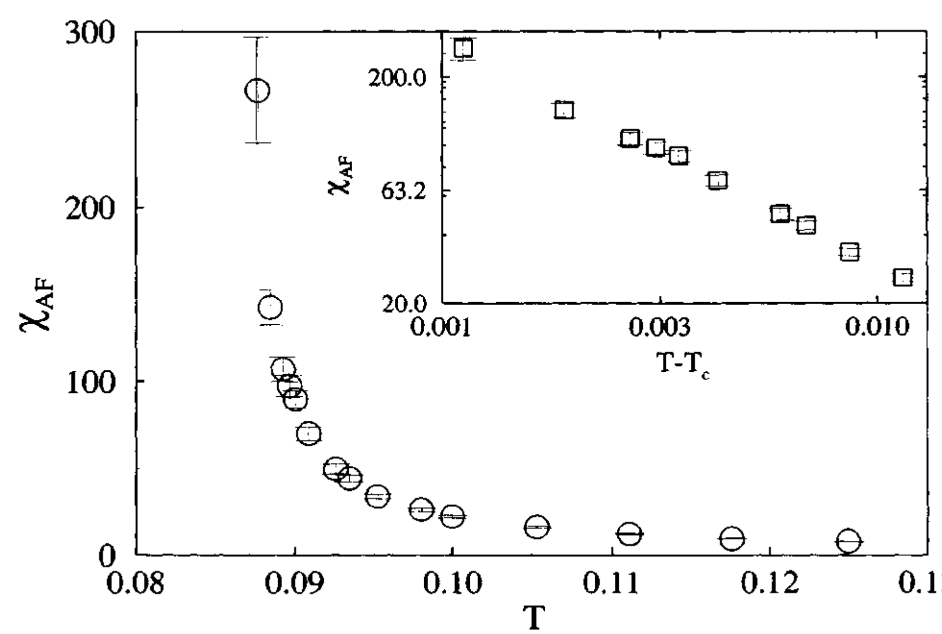
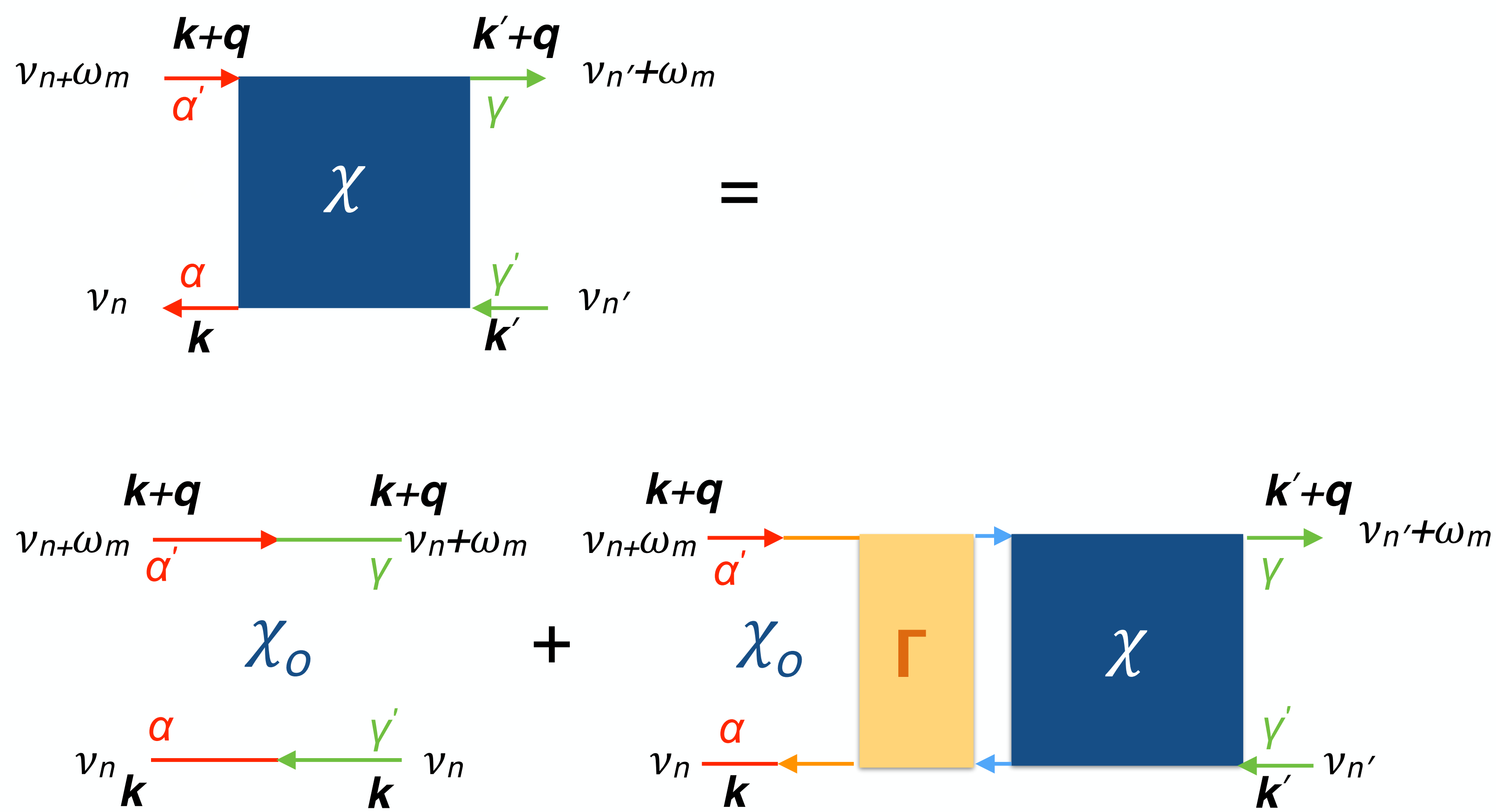
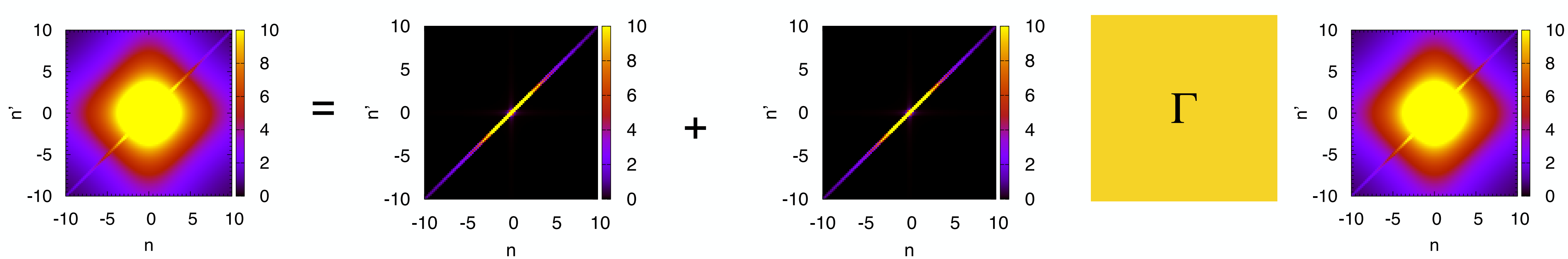


FIG. 3. Antiferromagnetic susceptibility $\chi_{AF}(T)$ vs temperature T when $U=1.5$ and $\epsilon=0.0$. The logarithmic scaling behavior is shown in the inset. The data close to the transition fit the form $\chi_{AF} \propto |T-T_c|^{\nu}$ with $T_c=0.0866\pm0.0003$ and $\nu=-0.99\pm0.05$. The points at $U=0$ reflect exactly known limits.

Bethe-Salpeter equation



$\omega_m = 0$



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alternative representations

(instead of fermionic Matsubara frequencies)

$$f_l^m(\tau) = e^{-i\varphi_m(\tau)} \begin{cases} \sqrt{2l+1}\, p_l(x(\tau)), & \tau > 0 \\ -(-1)^m \sqrt{2l+1}\, p_l(x(\tau+\beta)), & \tau < 0 \end{cases}$$

where $p_l(x(\tau))$ is a Legendre polynomial of degree l, with $x(\tau) = 2\tau/\beta - 1$; here the factor $(-1)^m$ in the second row ensures anti-periodicity for all values of m, which is the index for the bosonic Matsubara frequency ω_m. Via the orthogonality properties of the polynomials we obtain

$$\chi_{\boldsymbol{\alpha\gamma}}(i\omega_m) = \frac{1}{\beta^2} \sum_{ll'} f_l^{-m}(0^+)\, \chi_{\boldsymbol{\alpha\gamma}}^{l,l'}(i\omega_m)\, f_{l'}^{-m}(0^+). \tag{90}$$

The expansion coefficients in Eq. (90) take the form

$$\chi_{\boldsymbol{\alpha\gamma}}^{l,l'}(i\omega_m) = \int_0^\beta d\tau_{23} \int_0^\beta d\tau_{12} \int_0^\beta d\tau_{34}\, e^{-i\omega_m \tau_{23}} f_l^m(\tau_{12}) \chi_{\gamma\gamma'}^{\alpha\alpha'}(\tau_{14}, \tau_{24}, \tau_{34}, 0) f_{l'}^m(\tau_{34}), \tag{91}$$

Example: Hubbard model in small t/U limit

in the *atomic* limit

$$G(i\nu_n) = \frac{1}{i\nu_n + \mu - \Sigma(i\nu_n)} \qquad \Sigma(i\nu_n) = \mu + \frac{U^2}{4}\frac{1}{i\nu_n}$$

small *t/U* limit: approximate form for the self-energy

$$\Sigma(i\nu_n) = \mu + \frac{r_U U^2}{4}\frac{1}{i\nu_n}$$

Example: Hubbard model in small t/U limit

DMFT bubble

$$\chi_0(\boldsymbol{q};0) \sim (g\mu_B)^2 \frac{1}{4\sqrt{r_U}U}\left[1 - \frac{1}{2}\frac{J_{\boldsymbol{0}}}{\sqrt{r_U}U} - \frac{1}{4}\frac{J_{\boldsymbol{q}}}{\sqrt{r_U}U}\right]$$

$$J_{\boldsymbol{q}} = 2J[\cos q_x + \cos q_y], \quad J \propto t^2/U$$

local magnetic susceptibility

$$\chi_{zz}(\boldsymbol{q};0) = (g\mu_B)^2 \frac{1}{4k_BT}\frac{e^{\beta U/2}}{1+e^{\beta U/2}}$$

Bethe-Salpeter equation

$$\Gamma \sim \frac{1}{\chi^0_{zz}(0)} - \frac{1}{\chi_{zz}(0)} \sim \frac{1}{(g\mu_B)^2}\left[4\sqrt{r_U}U\left(1+\frac{1}{2}\frac{J_{\mathbf{0}}}{\sqrt{r_U}U}\right) - 4k_BT\right]$$

local vertex

$$\chi_{zz}(\boldsymbol{q};0) = \frac{1}{[\chi^0_{zz}(\boldsymbol{q};0)]^{-1} - \Gamma} \sim (g\mu_B)^2\frac{1}{4}\frac{1}{k_BT + J_{\boldsymbol{q}}/4} = \frac{(g\mu_B)^2}{k_B}\frac{1}{4}\frac{1}{T - T_{\boldsymbol{q}}}$$

Curie-Weiss behavior

cluster-size evolution

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Quantum cluster theories

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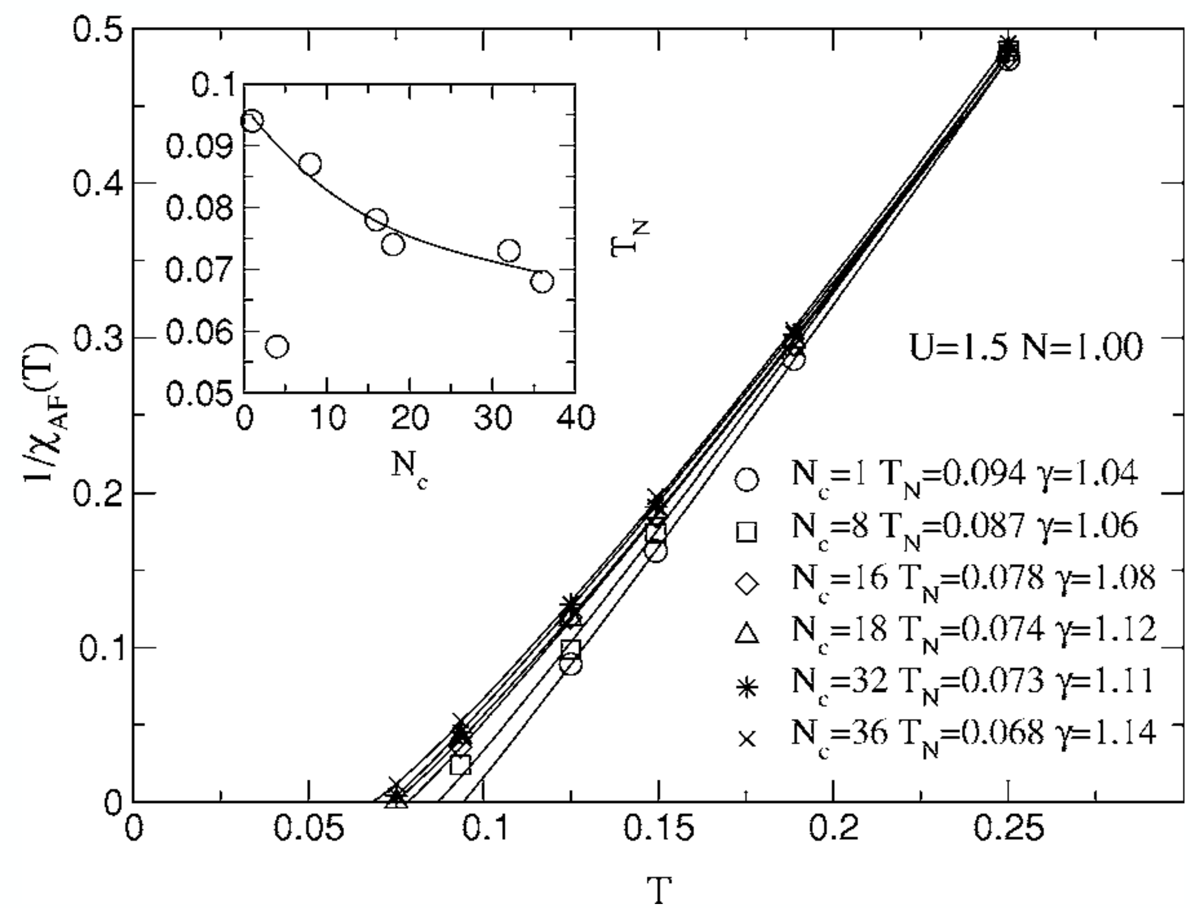

FIG. 26. Inverse antiferromagnetic susceptibility vs temperature in the half-filled 2D Hubbard model calculated with the DCA/QMC method for various cluster sizes N_c when $U=6t$. The lines are fits to the function $(T-T_N)^{\gamma}$. Inset: Corresponding Neél temperatures as a function of the cluster size. Energies are in units of $4t$. From Jarrell, Maier, Huscroft, and Moukouri, 2001.

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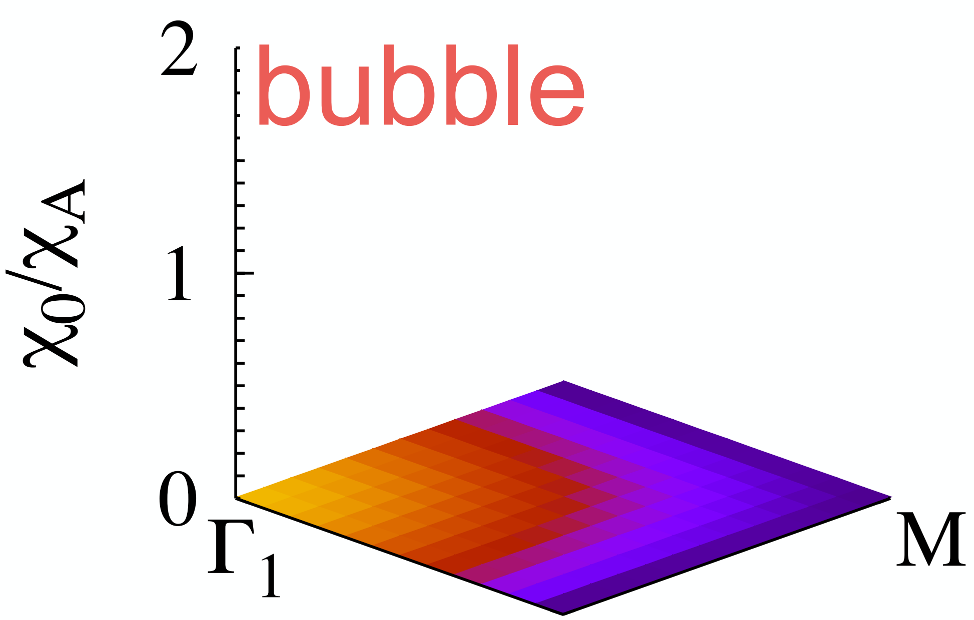
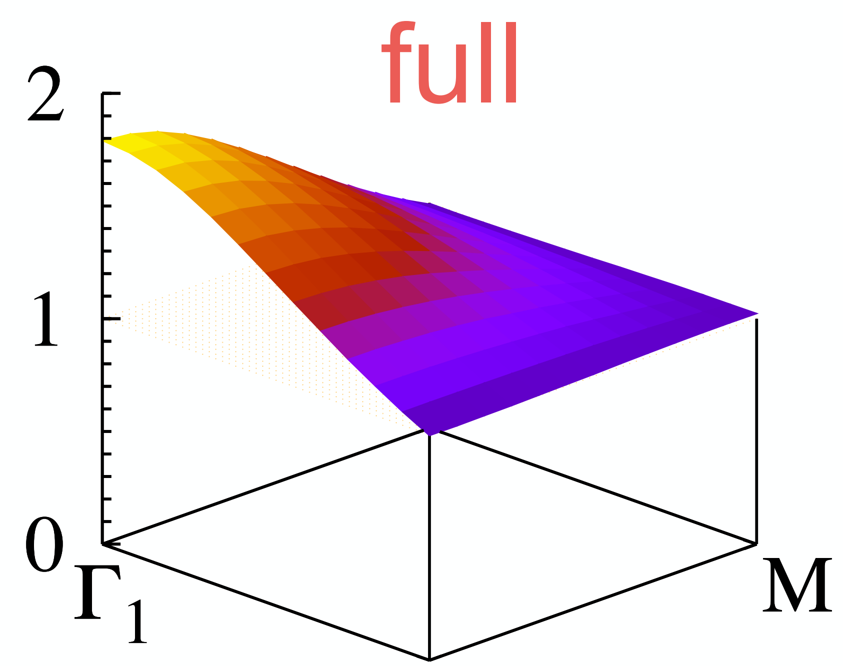
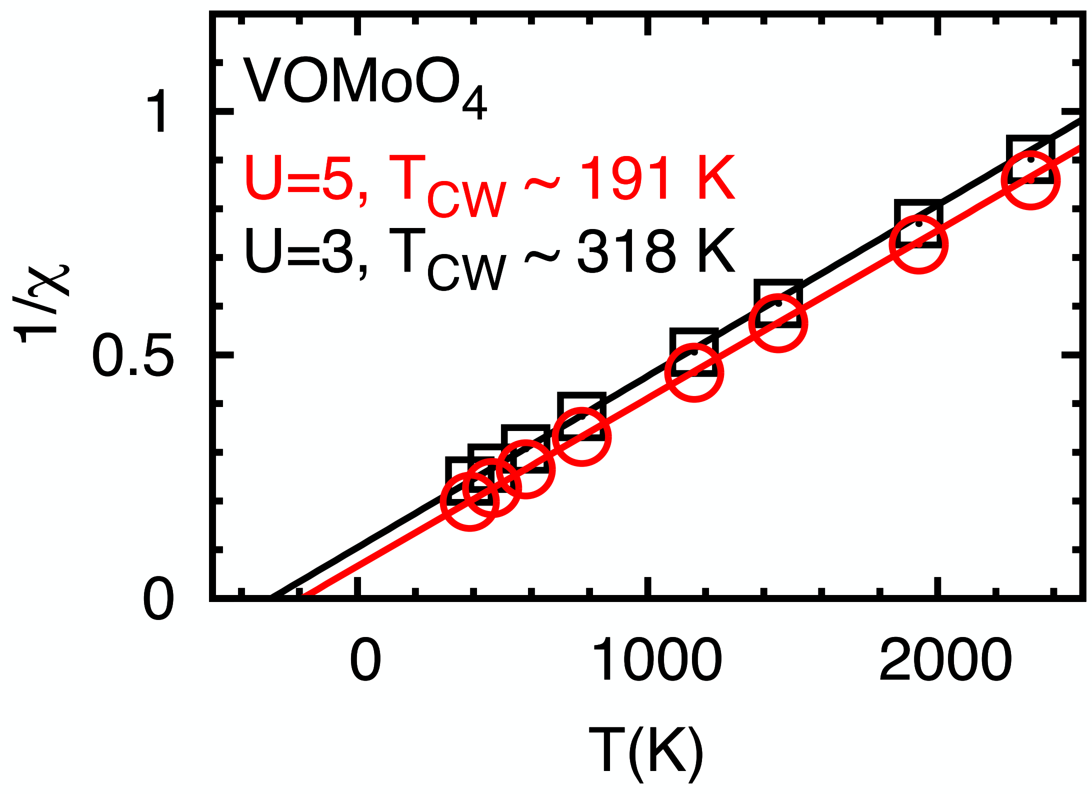
static and dynamical response







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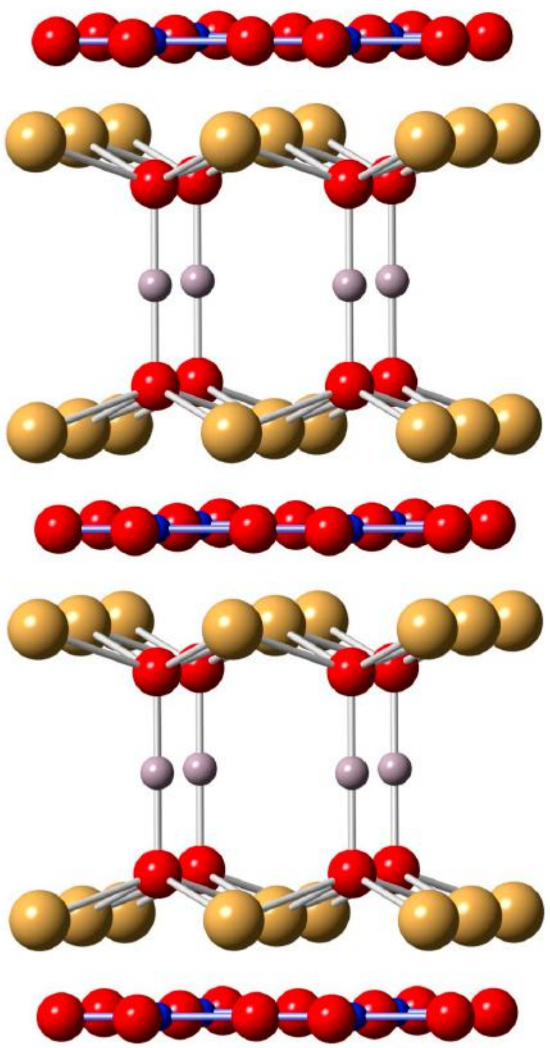
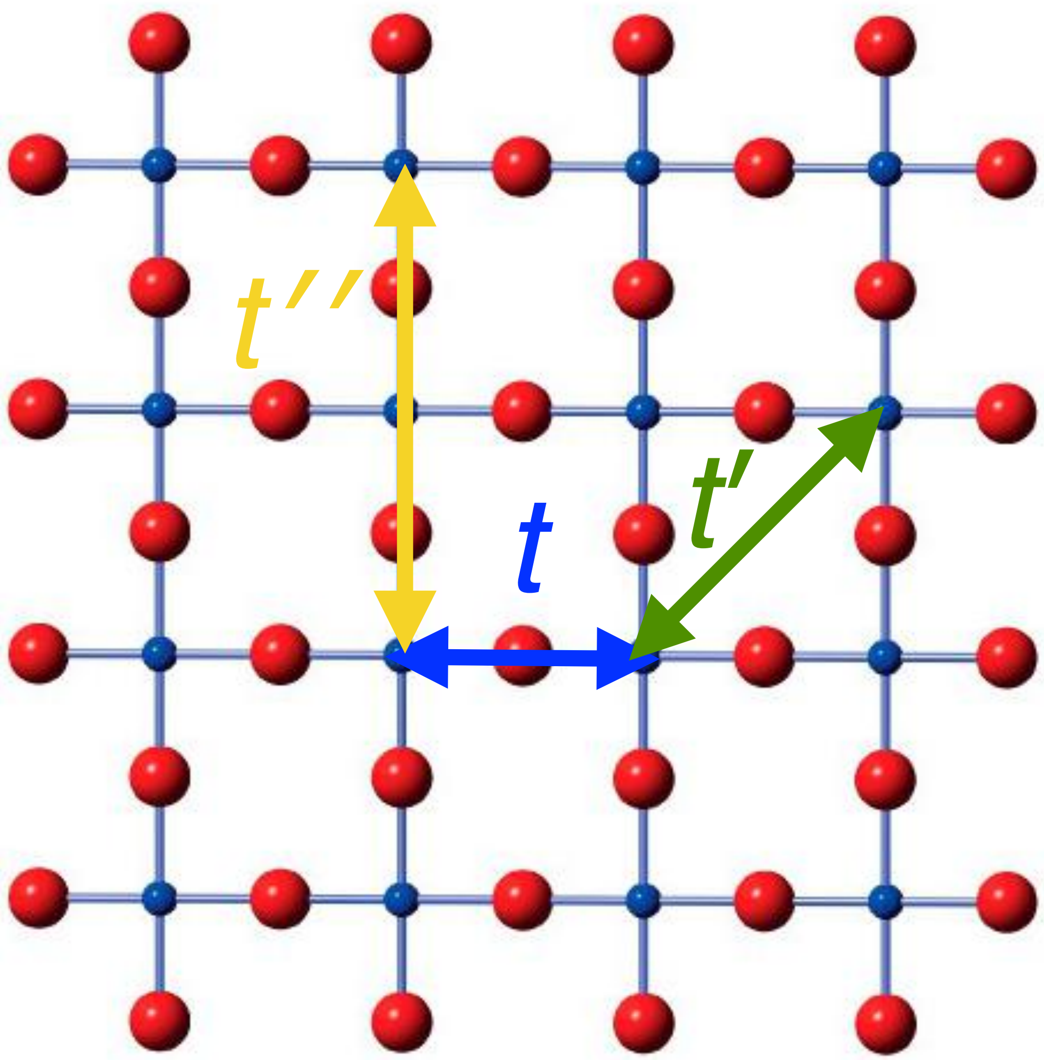
high-T_c superconducting cuprates

$$H = -\sum_{\sigma}\sum_{\langle ii'\rangle} t_{i,i'} c^{\dagger}_{i\sigma} c_{i'\sigma} + \sum_i U n_{i\uparrow} n_{i\downarrow}$$





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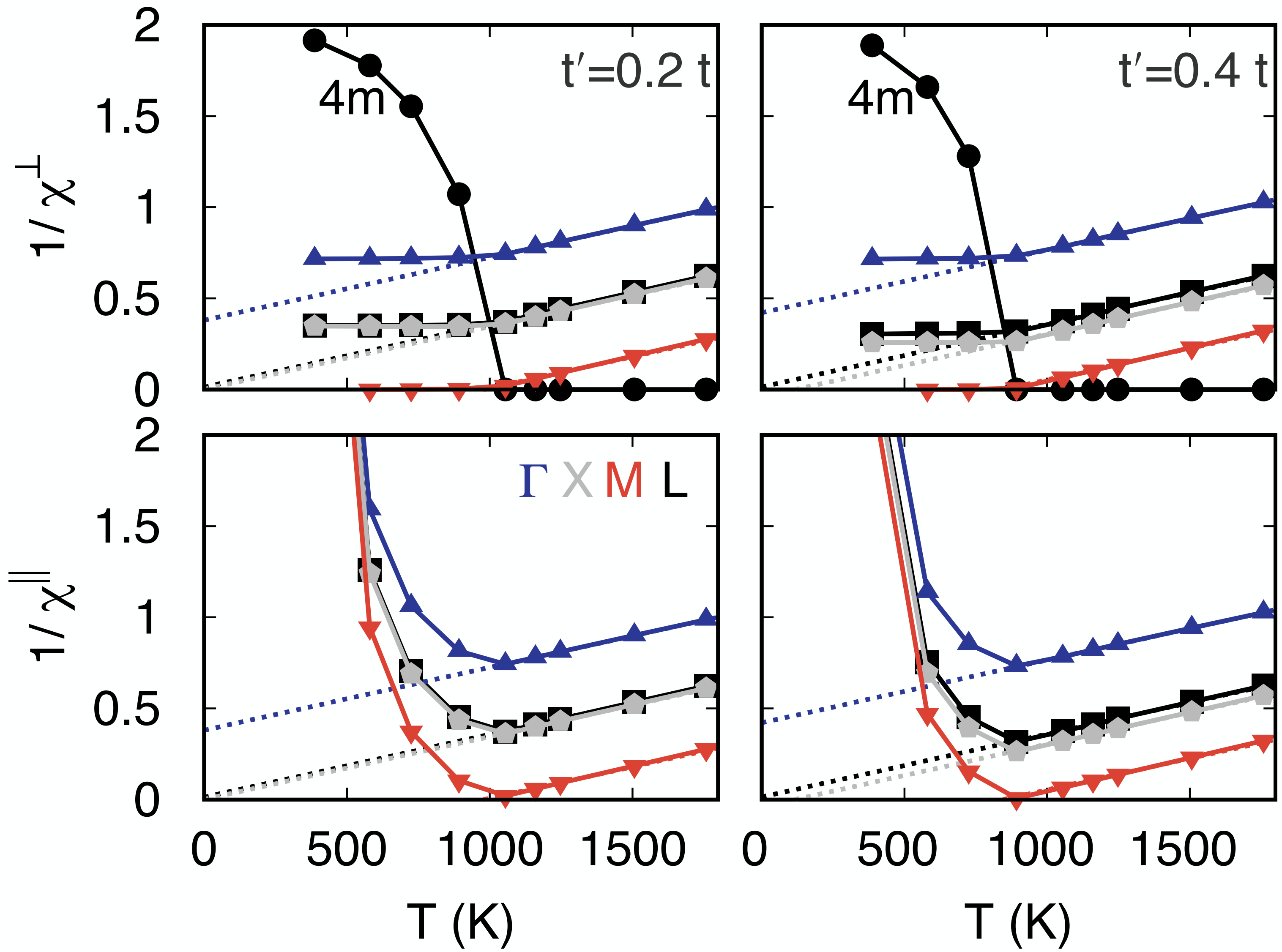
half filling (x=0)



$$\chi_{zz}(\boldsymbol{q};0) = \frac{C_{1/2}(1-\sigma_m^2)}{T-(1-\sigma_m^2)T_{\boldsymbol{q}}}$$

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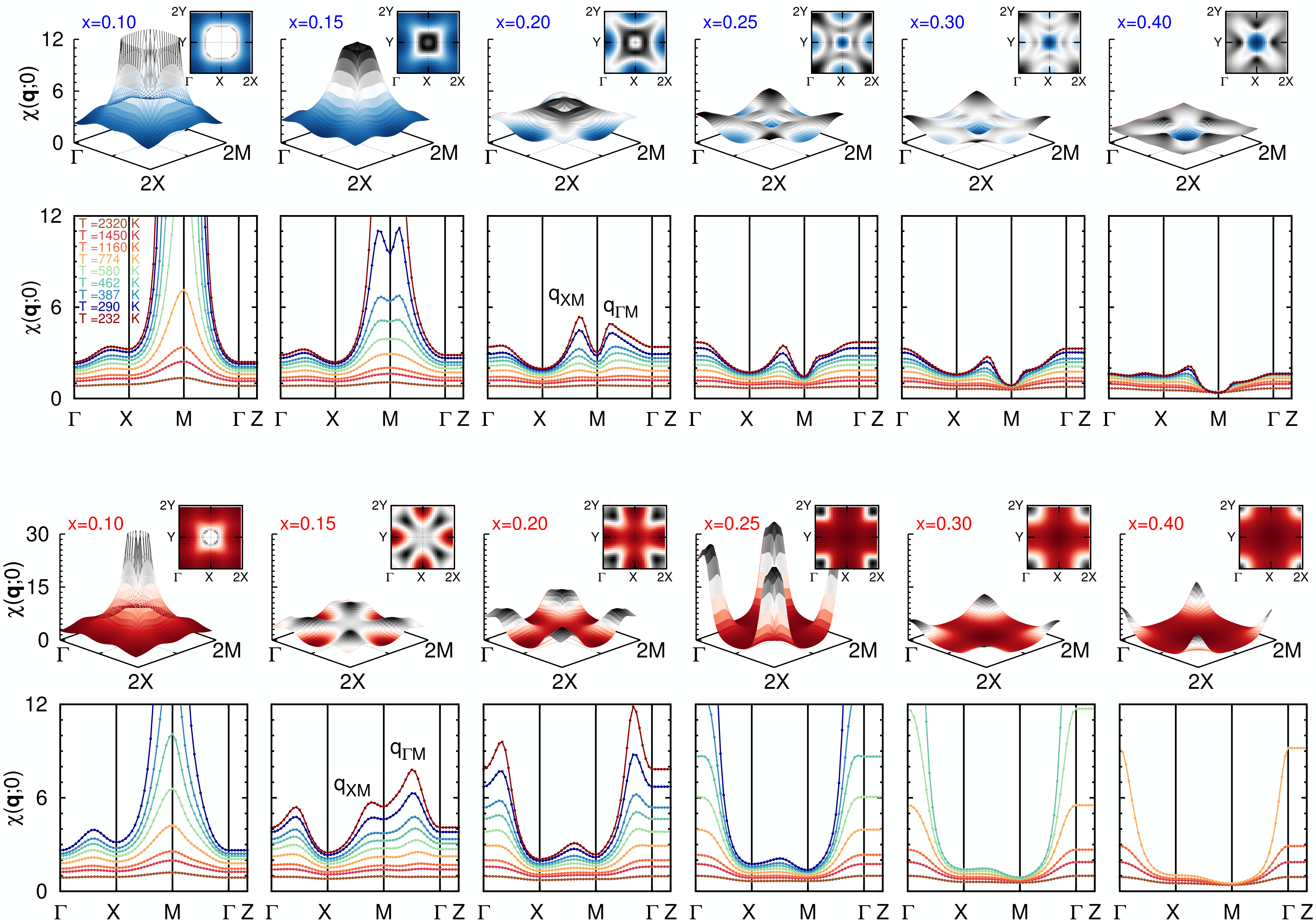
increasing x, finite **q**

t'/t=0.2

t'/t=0.4



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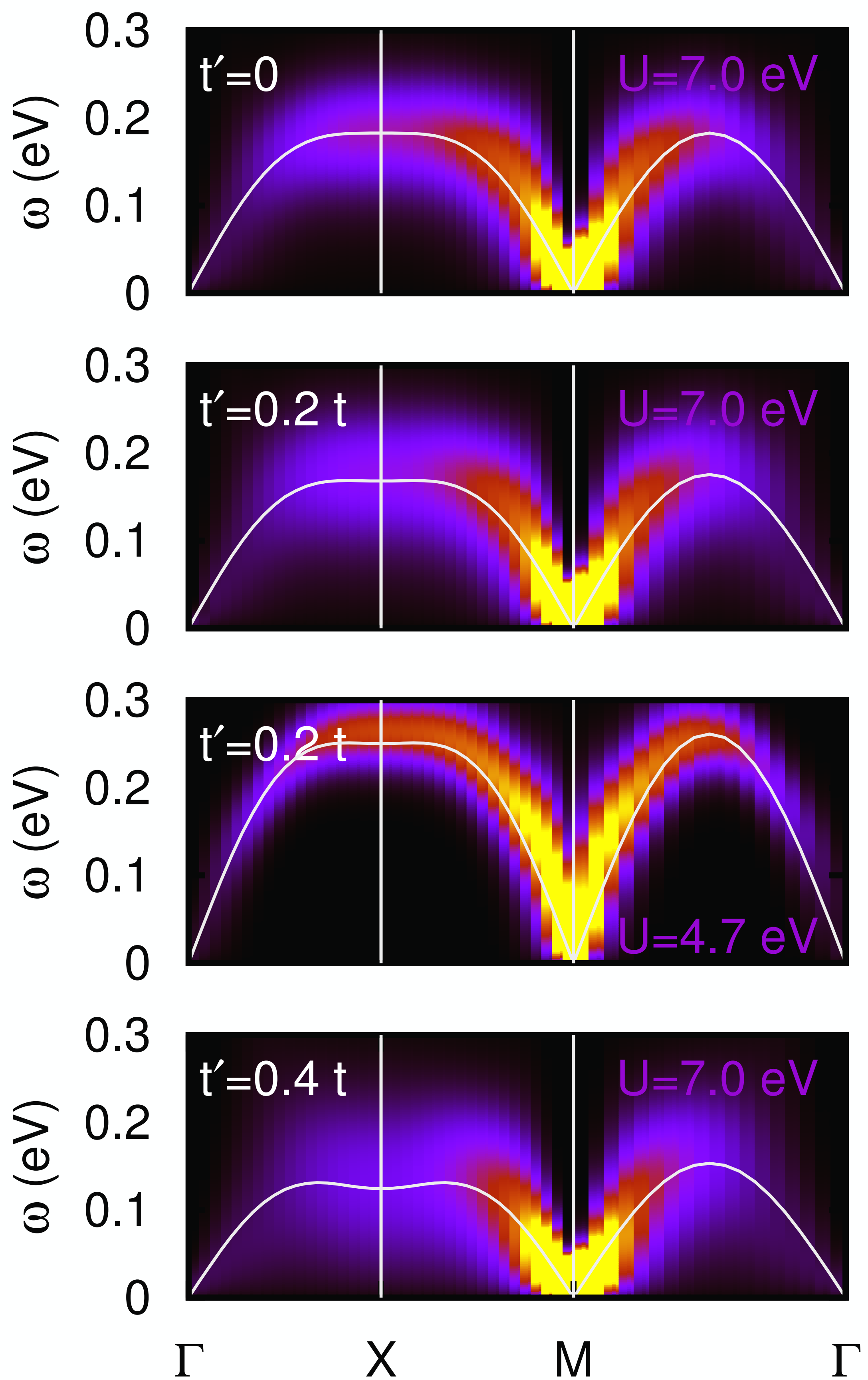
finite frequency: spin waves



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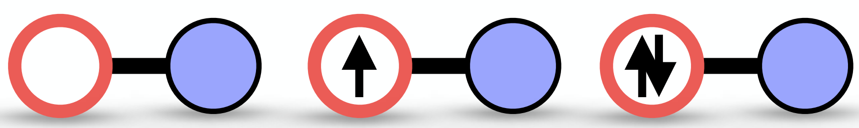
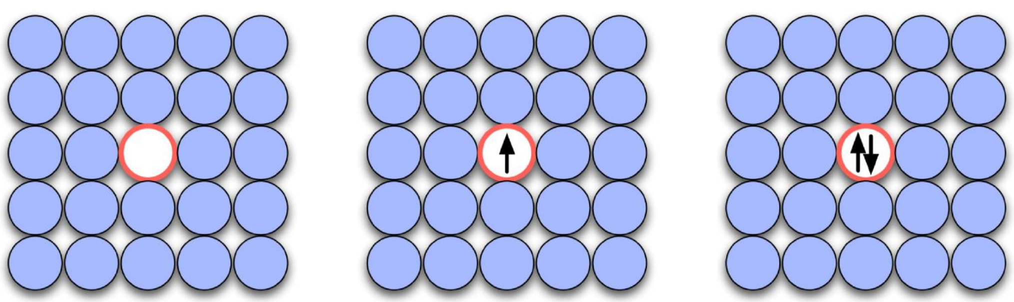
conclusions

DMFT and LDA+DMFT

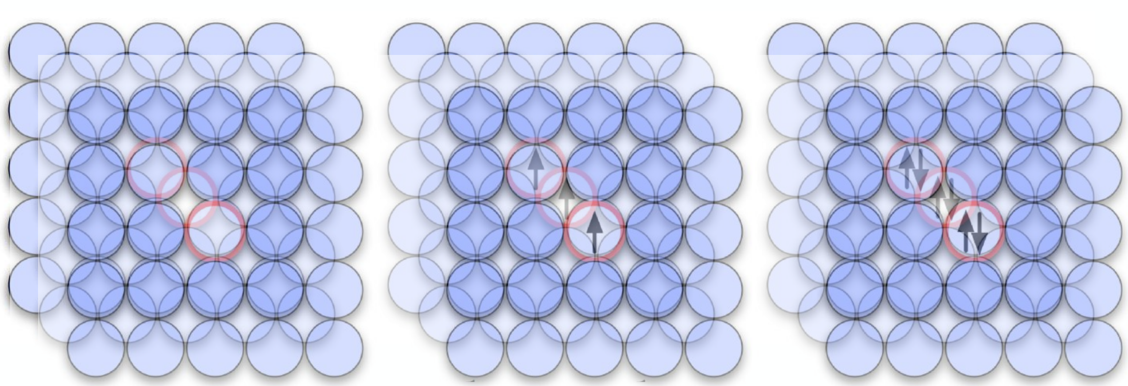
dimer

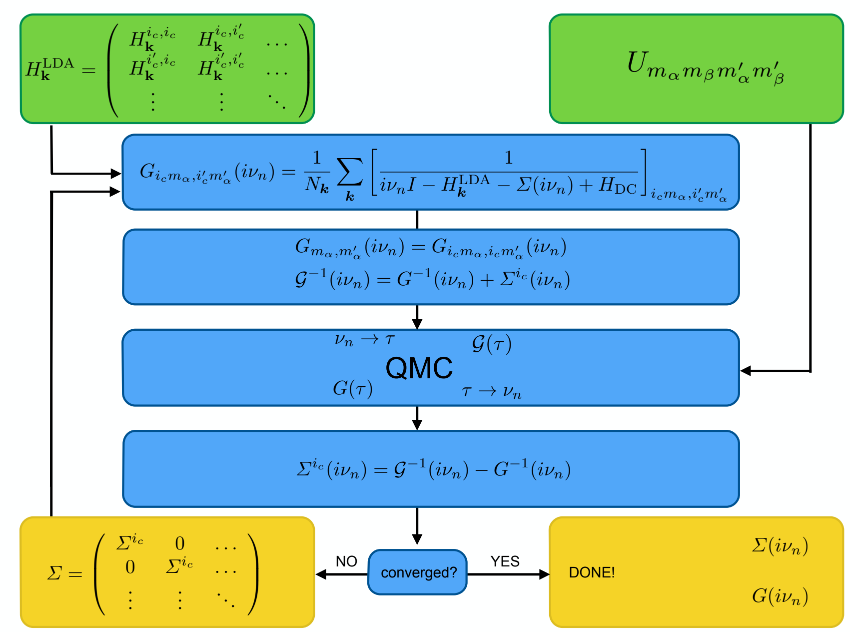


one band



multiband





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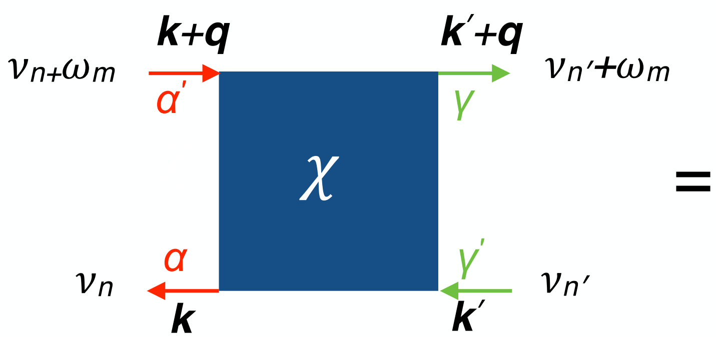
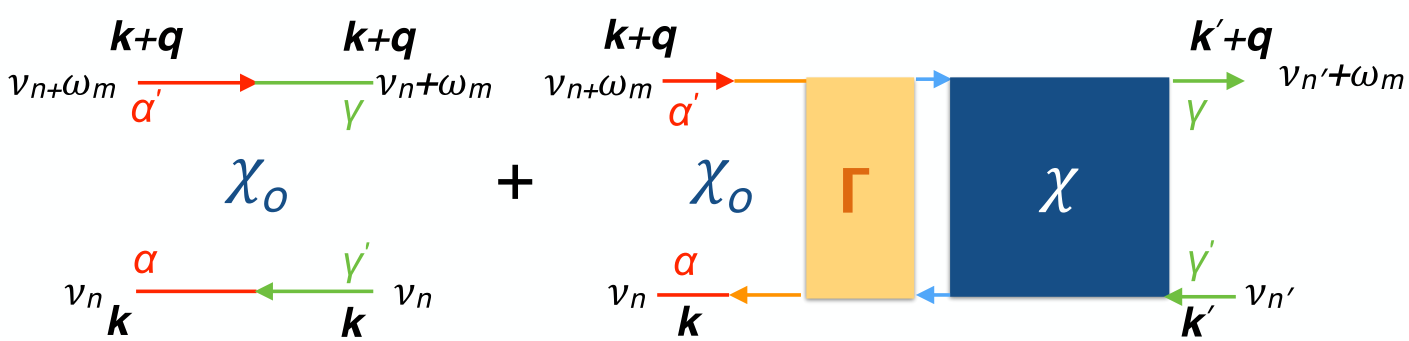
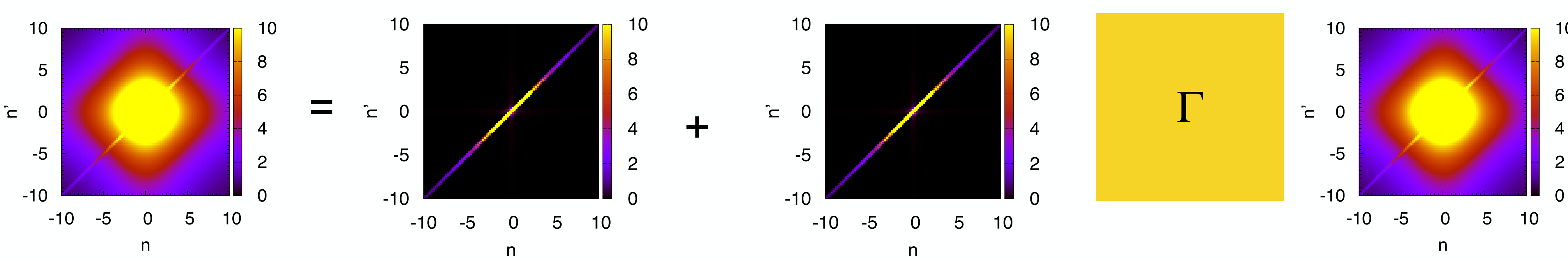
conclusions

linear responses in local vertex approximation







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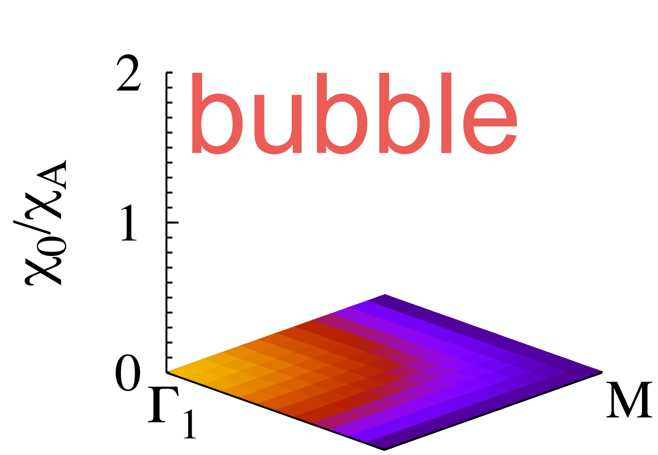
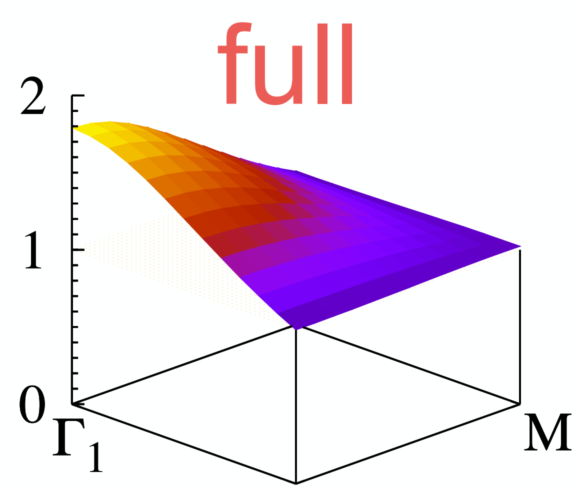
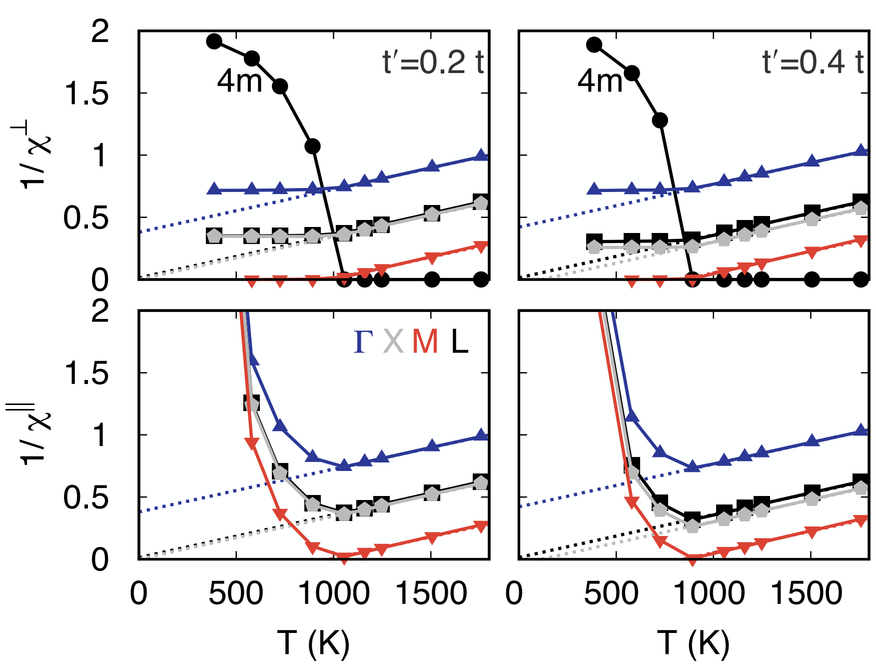
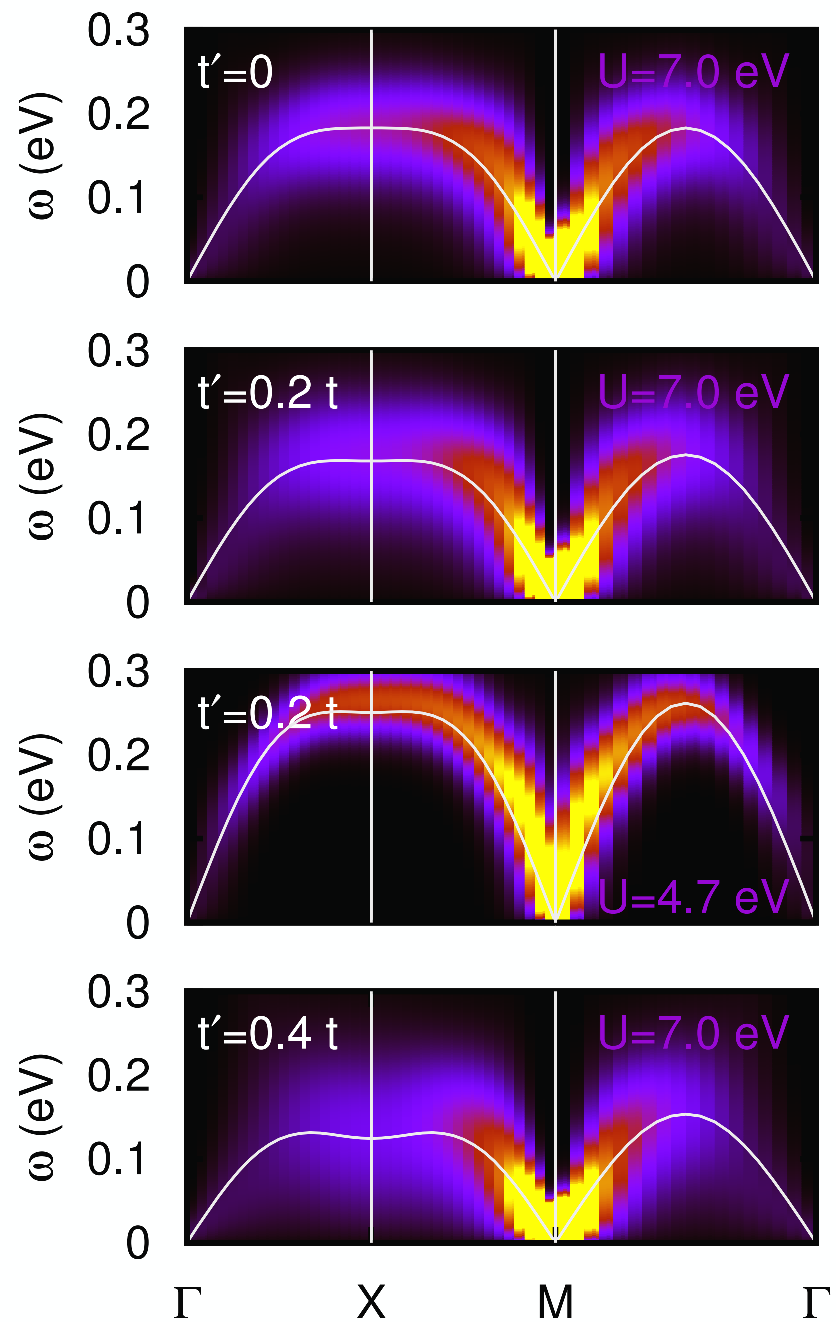
conclusions

linear responses in local vertex approximation









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thank you!