Correlation Induced Metallic, Half-metallic and Superconducting Phases in Strongly Correlated ***Band Insulators***

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*Work Done in collaboration with
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Phys. Rev. B **91**, 235108 (2015); Phys Rev. B **99**, 155127 (2019)
Arxiv **1909.03893**; and manuscript in preparation

Motivation

- Well known that strong electron-electron interactions can drastically affect band-metals.
- Inducement of spin or charge density wave gaps at the Fermi surface at half (or commensurate) filling (even at weak interactions for nested Fermi surfaces)
- the Mott metal-insulator transition, even in the paramagnetic state of a half-filled band.
- High temperature superconductivity, anomalous normal state, Pseudo-gap phase, etc., upon doping (away from half-filling) of Mott (or SDW) insulators
- Work-horse model: The Hubbard Model

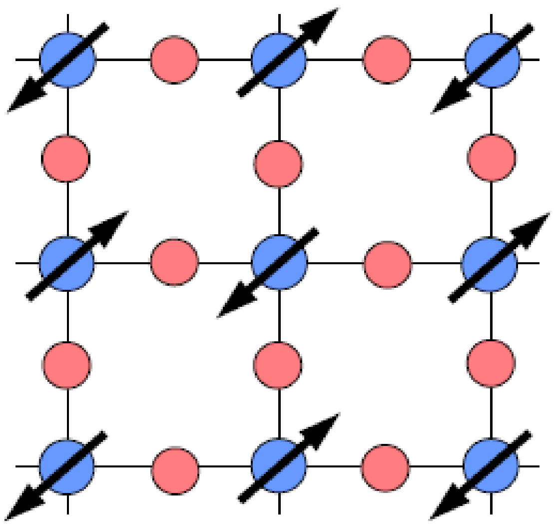
Anderson’s Remarkable suggestion

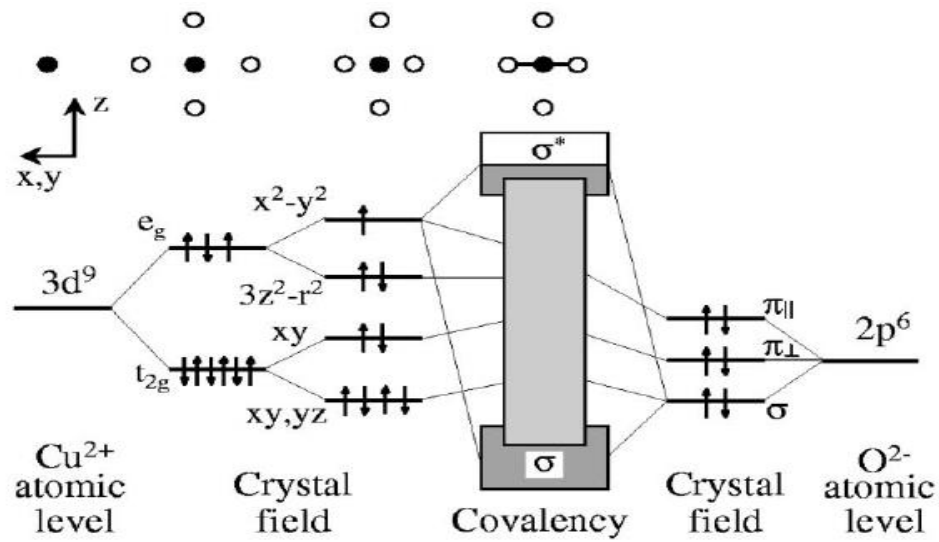
P.W. Anderson, Science *235, 1196 (1987),* **cond-mat/0201429**

2-d Hubbard model away from half filling

– appropriate minimal model for Cuprate superconductors!

$$\mathcal{H} = -t \sum_{\langle ij \rangle\, \sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i} n_i$$





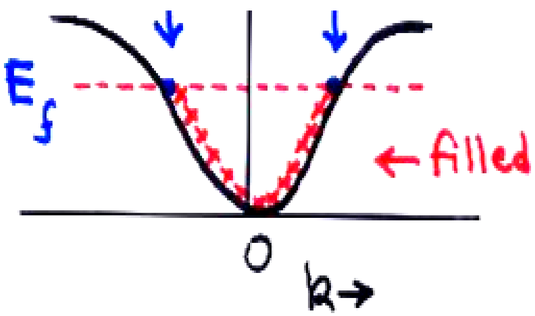
$La_{(2\text{-}x)}Sr_xCuO4$: x=0 → one d(x^2-y^2) electron per Cu site

<u>Band theory</u>

La**2**CuO**4**:

Half-filled

in **k**-space



Ignoring Interactions

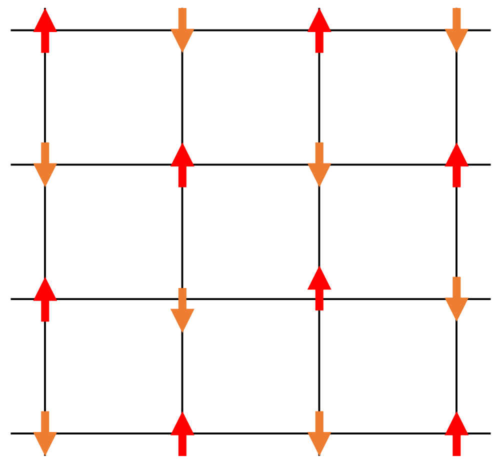
→ metal X

Experiments → La_2CuO_4 Insulator!

Strong Coulomb Interaction

$$U n_{i\uparrow} n_{i\downarrow} \qquad U \gg t$$

Half-filled in **r**-space: one electron/site



Charge→ Mott Insulator

Spin → Antiferromagnet

i.e., La_2CuO_4 is a Mott Insulator, and Cuprate Superconductors are doped Mott Insulators!

How Do Strong Electron Correlations Affect **Band Insulators?!**

- It might seem, at first sight, that nothing dramatic is likely.
  - *U* promotes localization of electrons and insulating behavior, but the system is already insulating!
  - Doping leads to a small number of carriers in the valence or conduction band, therefore correlation effects would be weak!
- Will show that, actually, dramatic things do happen when U ~ 2Δ, the Insulating band-gap
- Most of the discussion will use what is perhaps the simplest model for a correlated band insulator: the **Ionic Hubbard Model at Half-filling** *(and also a bit with doping)*
- Studies mostly use **Dynamical Mean Field Theory (DMFT),** which maps lattice models to quantum impurity models embedded in self consistent electron baths**, and approximate impurity solvers**
  - Using *Iterated Perturbation Theory (**IPT**) and Continuous Time – Hybridization Expansion-Quantum MonteCarlo (**CTQMC**) techniques*
- Part of the studies use the Strong Coupling Gutzwiller approximation

The Ionic Hubbard Model

Obtained by adding a Local correlation energy *U* to the tight binding model of electrons with a staggered "ionic" potential

$$H = -\sum_{ij} t_{ij}\, \hat{a}^{+}_{i\sigma}\hat{a}_{i\sigma} + U\sum_{i}\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} + \Delta\sum_{i\in A}\hat{n}_{i} - \Delta\sum_{i\in B}\hat{n}_{i} - \mu\sum_{i}\hat{n}_{i}$$

t IHM : $t_{ij} = t$ only for *nn* sites

$t - t'$ *IHM* : $t_{ij} = t$ for *nn* sites

t' for *nnn* sites

"half filling" $\Leftrightarrow$ $\langle \hat{n}_A \rangle + \langle \hat{n}_B \rangle = 2$ $\Leftrightarrow$ $\mu = U/2$ (if $t' = 0$)

t IHM with $U = 0$: Simplest Model of a Band Insulator, with gap 2 *Δ*

Does anything interesting happen as *U* is increased?

$t - U$ - Δ Ionic Hubbard Model : Simple Limits

- For *$U = 0$* Hamiltonian can be diagonalized exactly by transforming to ***k*** space $\Rightarrow$ Two bands (in half the BZ of the square lattice) with energy dispersions given by

$$E^{\pm}_{\mathbf{k}} = \pm\sqrt{(\varepsilon_{\mathbf{k}})^2 + \Delta^2}\ ;$$

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

- At "half filling" $\Leftrightarrow$ $\langle \hat{n}_A \rangle + \langle \hat{n}_B \rangle = 2$, Lower band is full and upper band is empty $\Rightarrow$ Paramagnetic band Insulator with *charge gap* of Δ (from the chemical potential, at 0) for electron or hole excitations of either spin

- $\Delta = 0$: Standard Hubbard Model $\Rightarrow$ Metal for *$U = 0$,* and also in *Restricted Hartree-Fock* (RHF) approximation for finite *U*
- However, Unrestricted HF analysis leads to an AF - Insulating state with a charge *gap* of $Um_s / 2$ where

$$m_s \equiv [(\langle n_{A\uparrow} \rangle - \langle n_{A\downarrow} \rangle) - (\langle n_{B\uparrow} \rangle - \langle n_{B\downarrow} \rangle)] / 2$$

  is the staggered magnetization.
- Gap is *the same* for both spins

$t - U - \Delta$ Ionic Hubbard Model : Simple Limits

(Restricted or Paramagnetic) Hartree-Fock results

$$\Sigma_\alpha = U \langle n_\alpha \rangle / 2 \qquad \alpha = A, B$$

The Staggered Charge $\delta n \equiv (\langle n_B \rangle - \langle n_A \rangle) / 2$

Obeys the Self Consistent equation

$$\delta n = \left| \Delta - U\, \delta n / 2 \right| \sum_{\mathbf{k}} \left| \tilde{E}_{\mathbf{k}}^{-} \right|^{-1}$$

With $\tilde{E}_{\mathbf{k}}^{\pm} = \pm \sqrt{(\varepsilon_{\mathbf{k}})^2 + (\Delta - U\, \delta n / 2)^2}$

Effective Gap = $\left| (\Delta - U\, \delta n / 2) \right|$, decreases as U increases, but never vanishes!

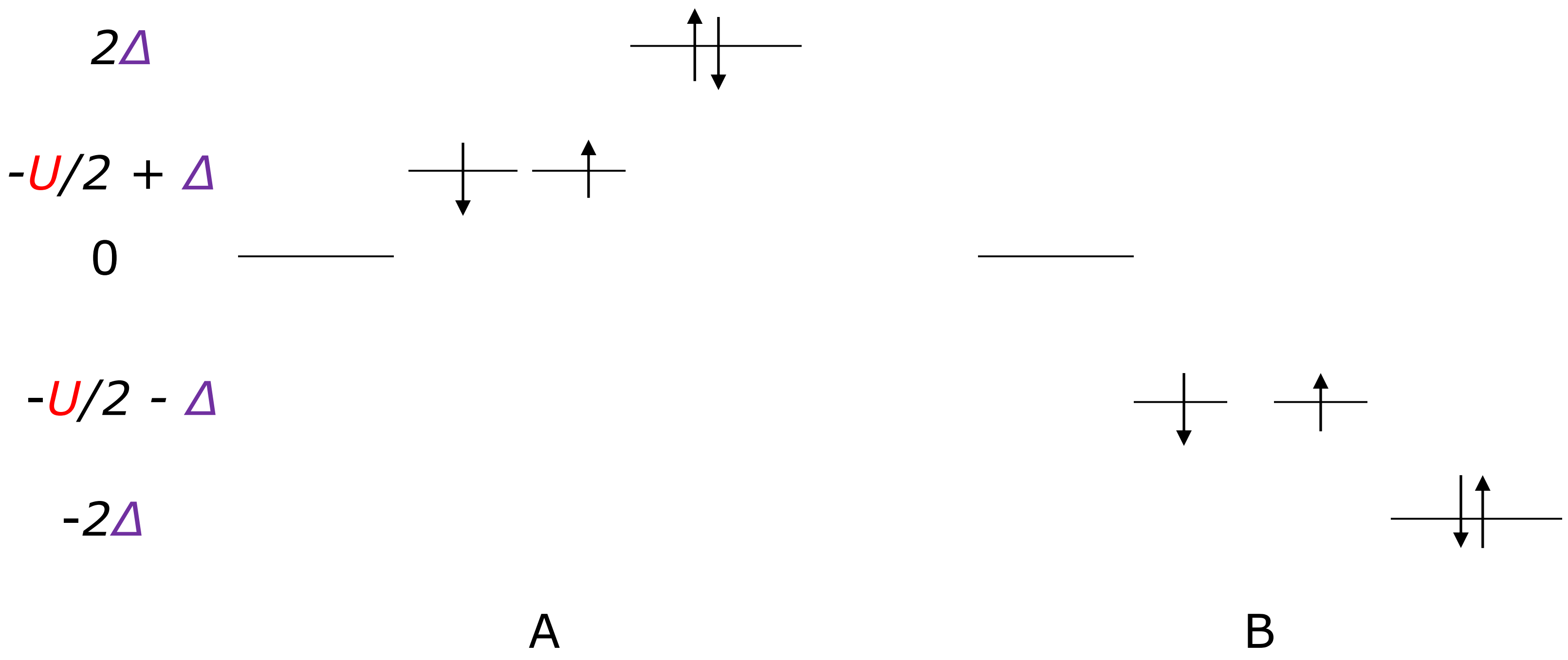
Once Δ is non-zero, System is an Insulator for all U

But interesting, new possibilities arise when one uses methods that work better for large U, e.g., DMFT!

$t - U - \Delta$ Ionic Hubbard Model : Simple Limits

Atomic ($t=0$) Limit of the model

for $U < 2\Delta$: "Band Insulator" , with $n_A = 0$, $n_B = 2$,
Charge Gap = $\Delta - U/2$.
Also characterizable as "ionic", A^+B^-



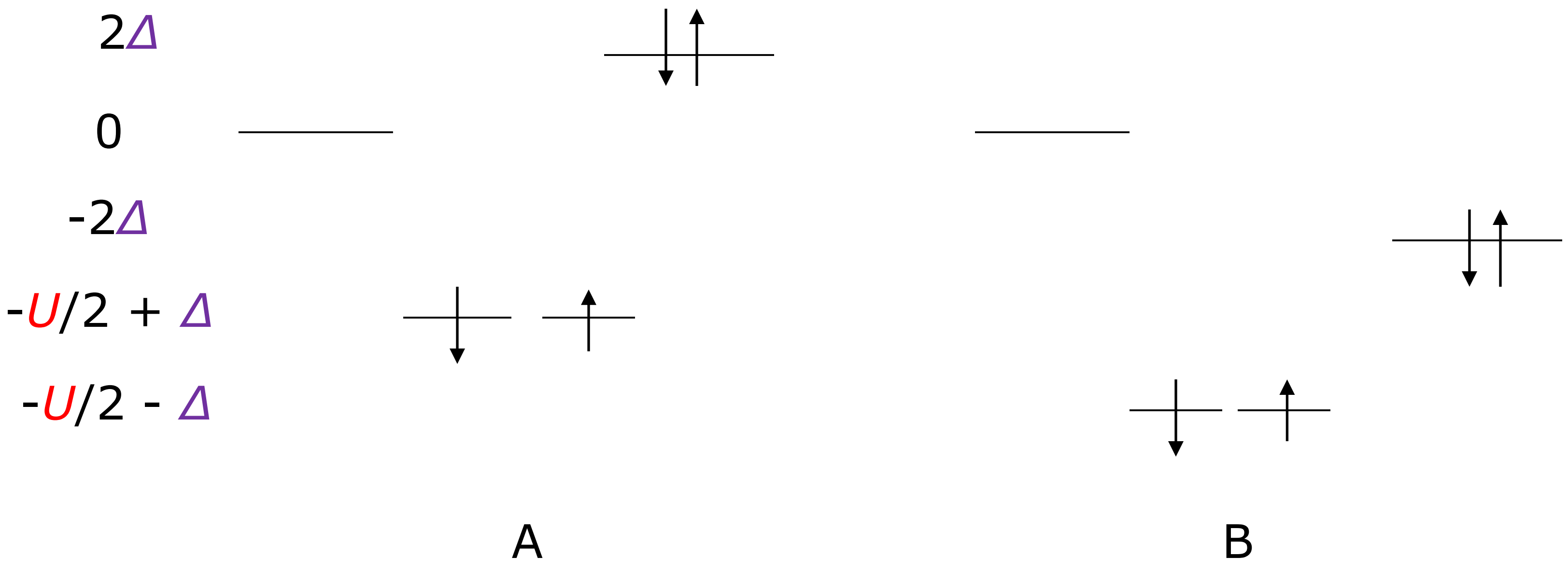
$t - U$ - Δ Ionic Hubbard Model : Simple Limits

Atomic (t=0) Limit of the model

for $U > 2\,\Delta$: "Mott Insulator" with $n_A = n_B = 1$,

Charge Gap = $U/2 - \Delta$ + *Local moments*

Also characterizable as "neutral"



"metal" with local moments for $U = 2\,\Delta$?!

Novel Results I : Correlation Induced Metallicity in the Paramagnetic Phases of IHB!

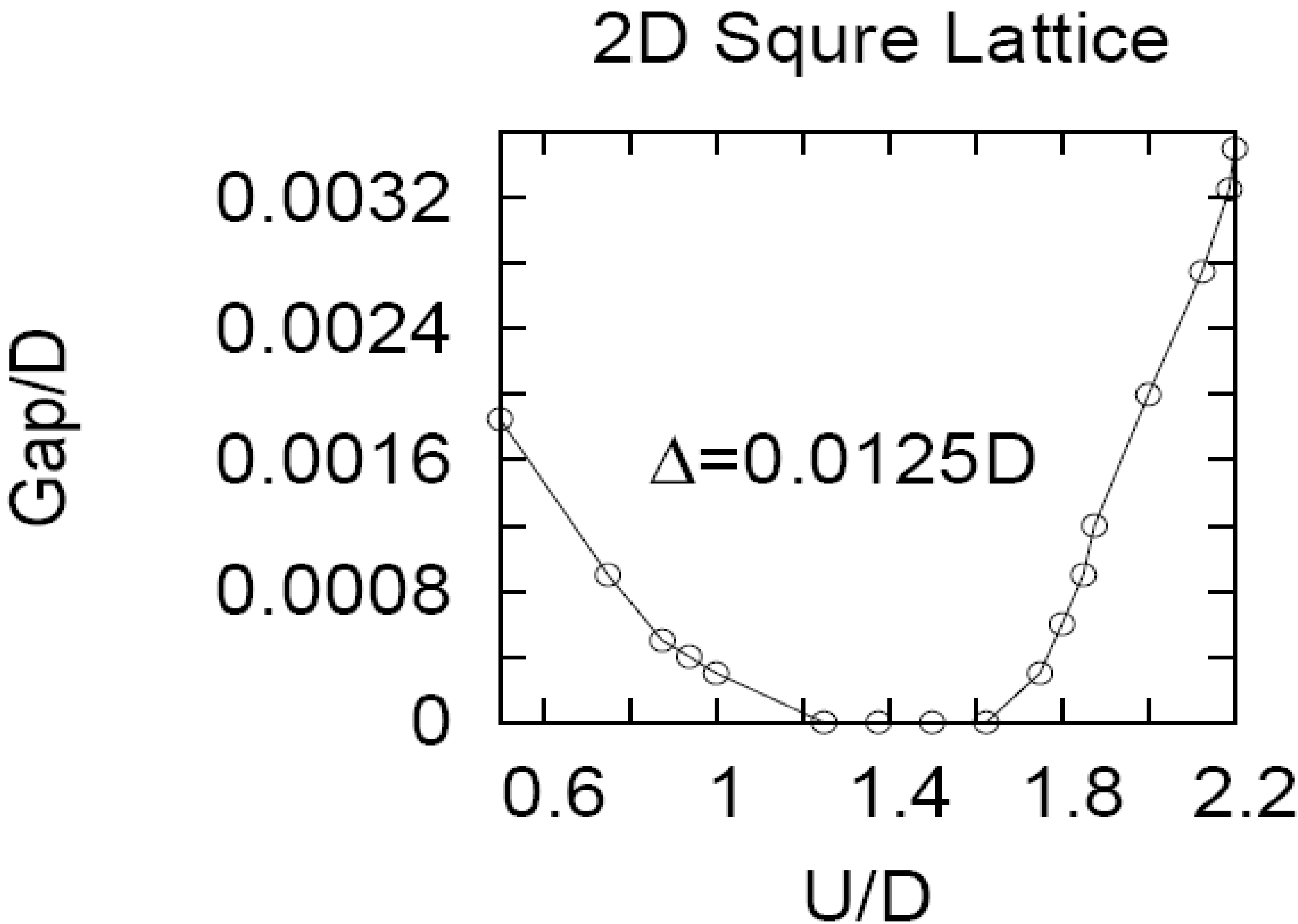
(At half filling and $T=0$)

[Garg, HRK, Randeria - PRL **97,** 046403(2006)]

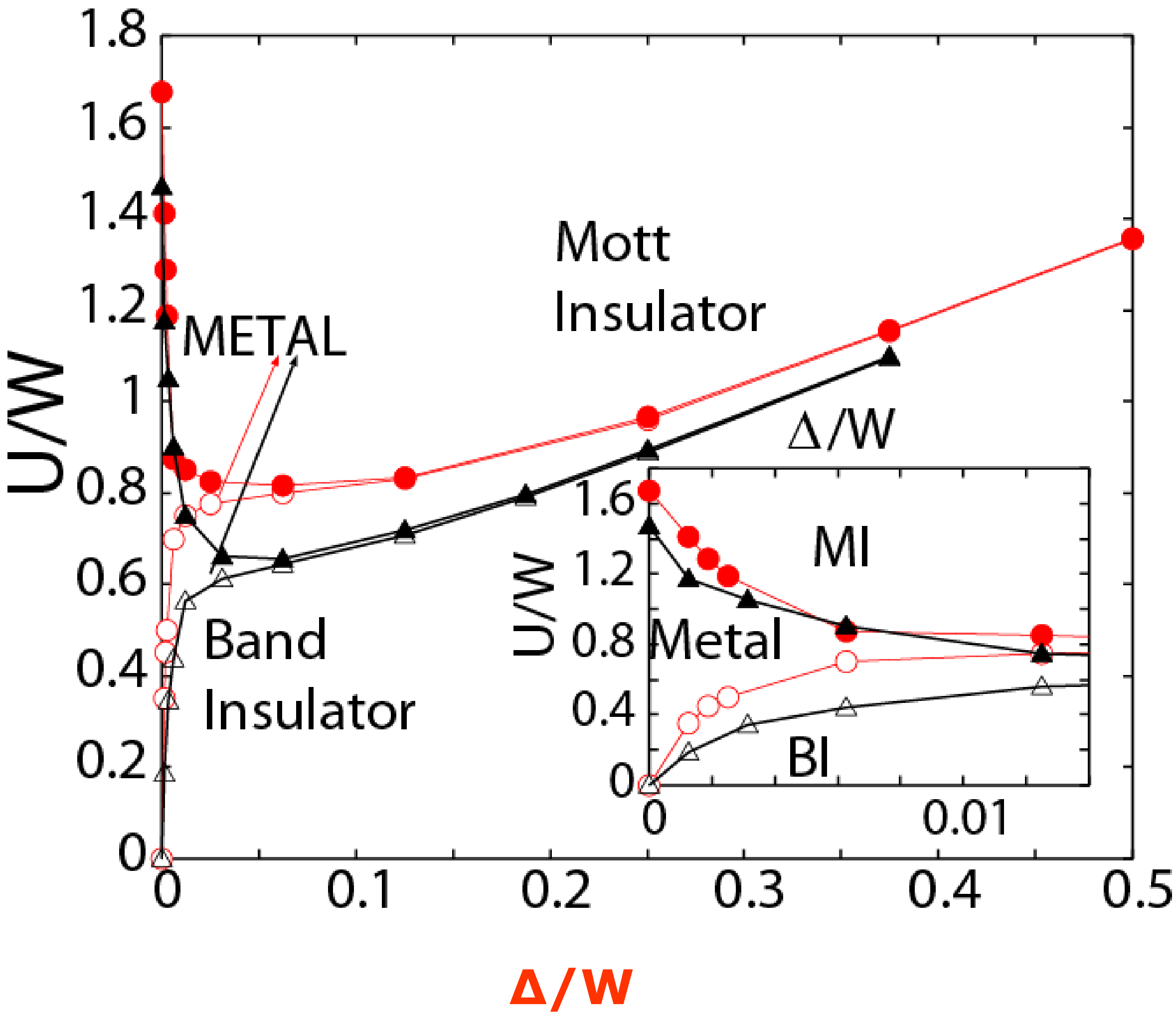
- In the (enforced) paramagnetic state (or in models with sufficient frustration eg., on non-bipartite lattices,) *turning on correlations reduces the Band insulating gap, which vanishes at a finite* U_{c1}!

  $\Rightarrow$ Correlation Induced Quantum Phase Transition (QPT) from **Band Insulator** to a **metallic phase!**
- **Metallic phase stable for a narrow range of *U***
- Gap becomes non-zero again ($U>U_{c2}$), and increases as U increases $\Rightarrow$ Mott Insulator for larger U

Gap in Single Particle Spectrum (DMFT+IPT)



T=0 Phase Diagram of IHB at Half Filling (With Enforced Para-magnetism, IPT)



Black :

2-d Square lattice

Δ : U_{c1}

▲ : U_{c2}

W = 8t

Red :

Bethe lattice

($z \rightarrow \infty$)

o : Uc1

● : Uc2

W= 4t

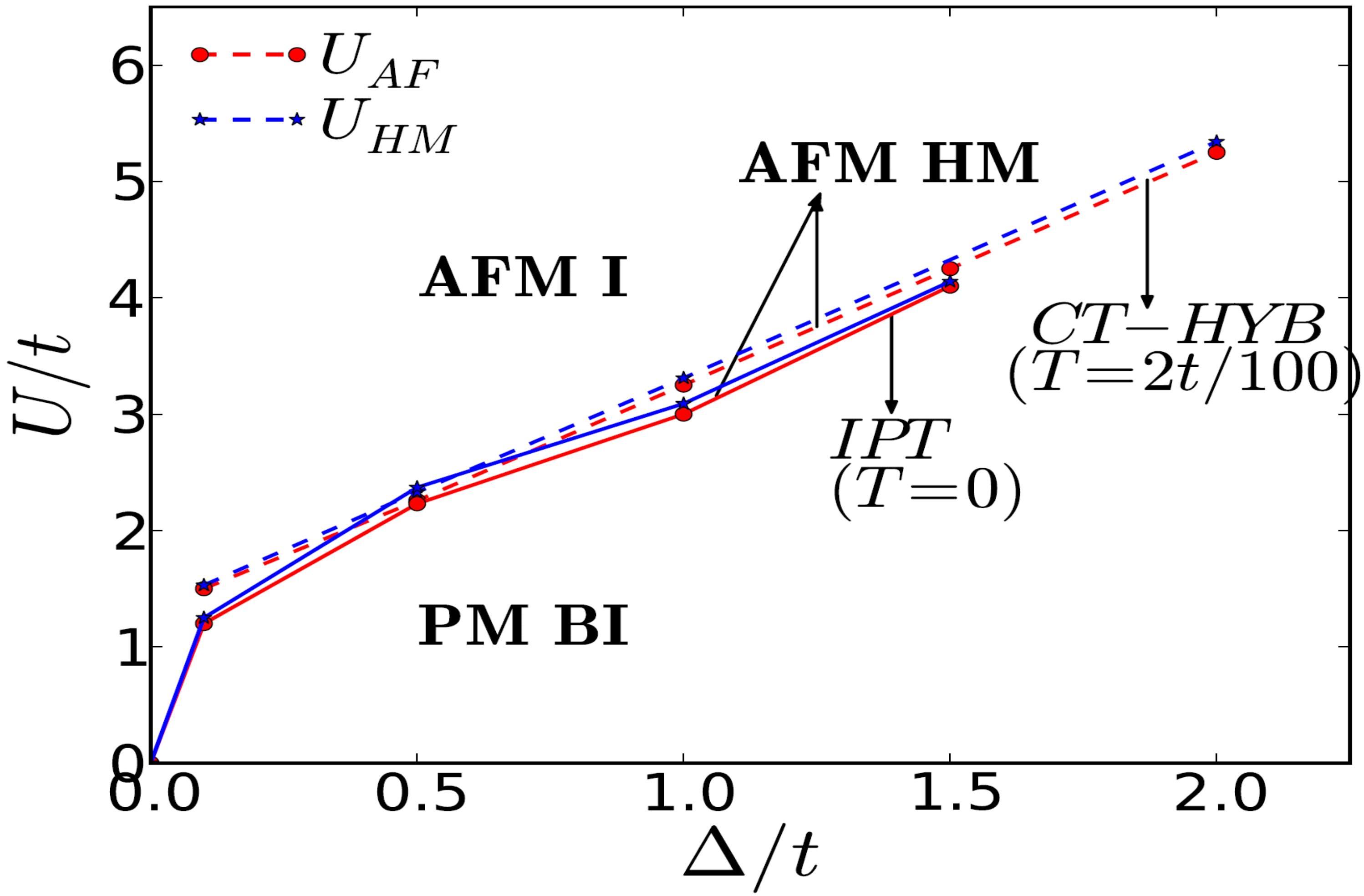
Novel Results II : Antiferromagnetic Phases and phase transitions in the half filled IHB

[Bag, Garg, HRK - Phys. Rev. B **91**, 235108 (2015)]

- Bipartite or non frustrated lattices
  - *first order* quantum phase transition (QPT) at $U=U_{AF}(\Delta)$ to an Antiferromagnetic Insulating (AFM-I) phase
  - Preempts QPT into paramagnetic metallic phase
- For nonzero *T,*
  - thermal transition from AFM-I to the paramagnetic [Band Insulator (BI)] phase is *first order* for weak to intermediate U, but *continuous* for large U
  - *Line of tri-critical points* separates the surfaces of first order and continuous transitions in the 3-d (U, Δ, T) *space*

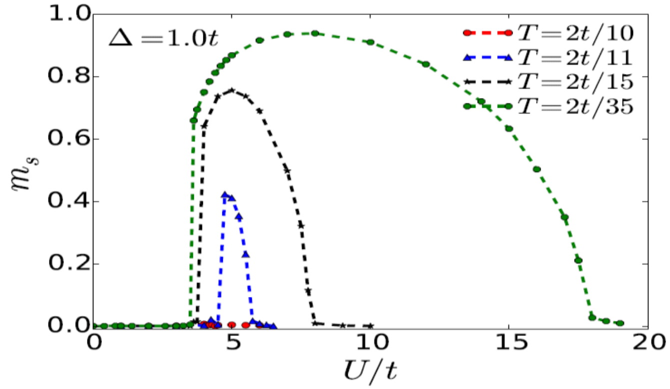
T=0 Phase Diagram of IHB at Half Filling

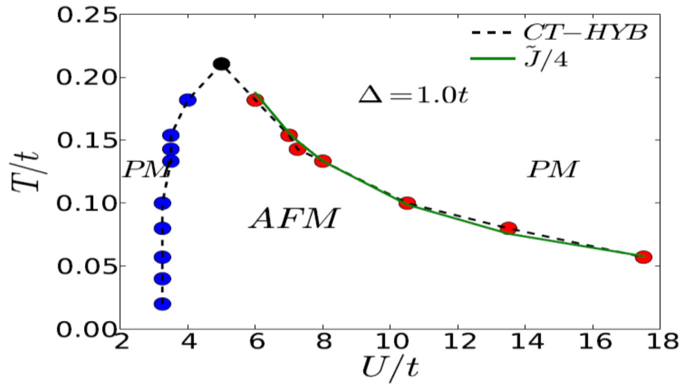
(Bethe Lattice, allowing for Antiferromagnetism)

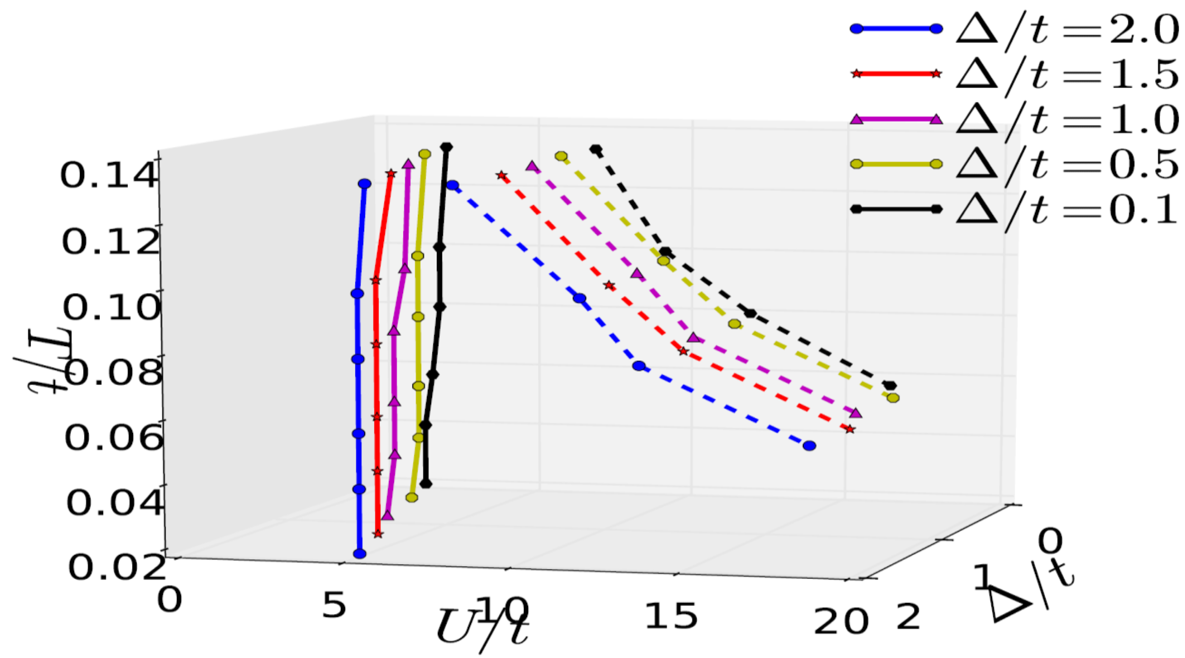


T≠0 Phase Diagram of IHB at Half Filling

(Bethe Lattice, permitting Antiferromagnetism, CTQMC)







Novel Results III :

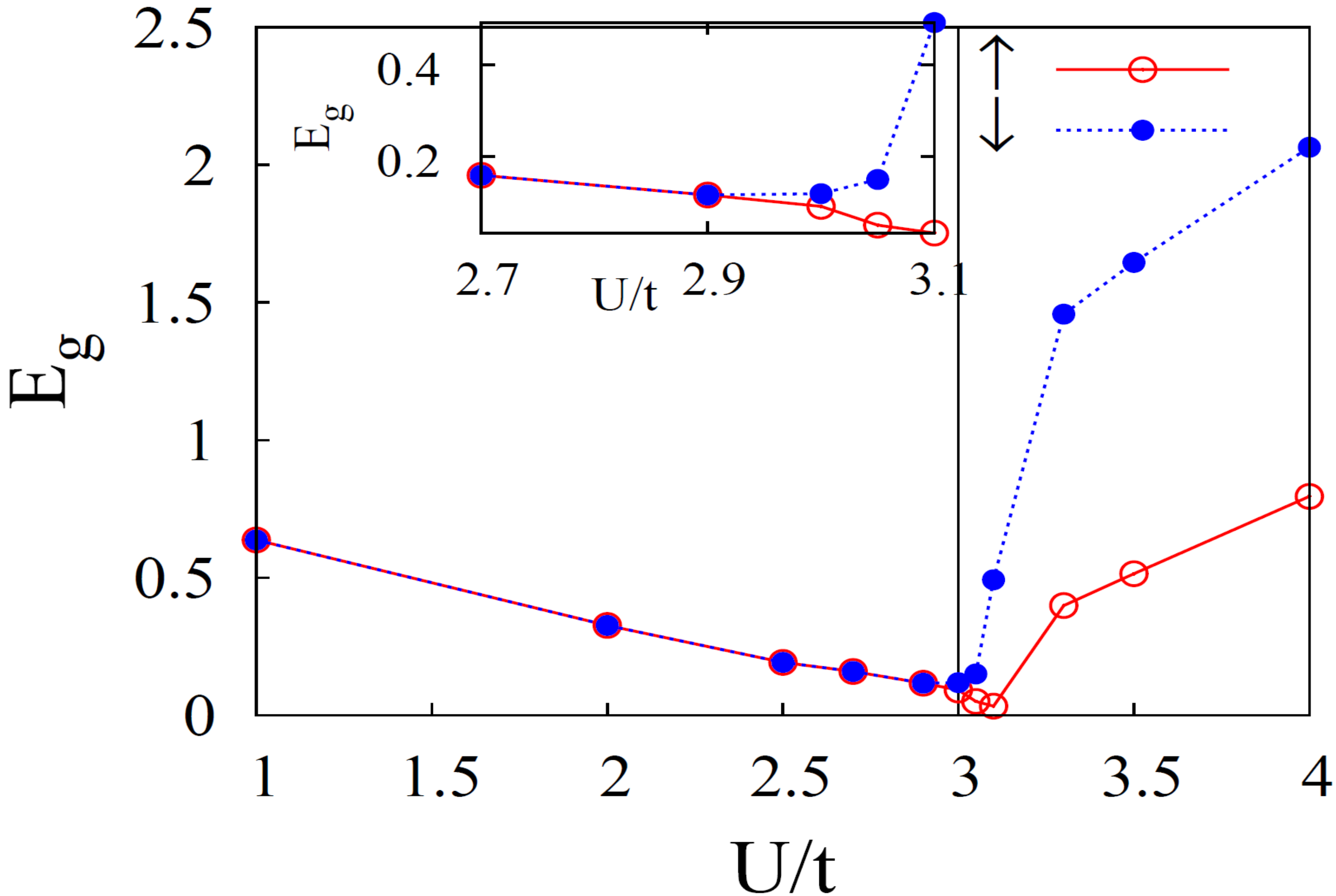
Half metallic phases in the IHB at *T=0!*

[Garg, HRK, Randeria – PRL **112**, 106406 (2014)]

- In the AFI state, *up and down spin particles (or holes) have different gaps*
- There is a range of U in which one (up) spin gap increases with increasing U while the other (down) spin gap decreases!
- $\Rightarrow$ There is a critical U where one (down) spin gap vanishes $\Rightarrow$ Correlation induced, Antiferromagnetic Half Metal along a Quantum Critical line in the phase diagram!
- In this regime of U, a small amount of doping leads to a Ferrimagnetic half metal (FHM) phase $\Rightarrow$ entirely new mechanism for obtaining FHM
- Of value for Spintronics?!

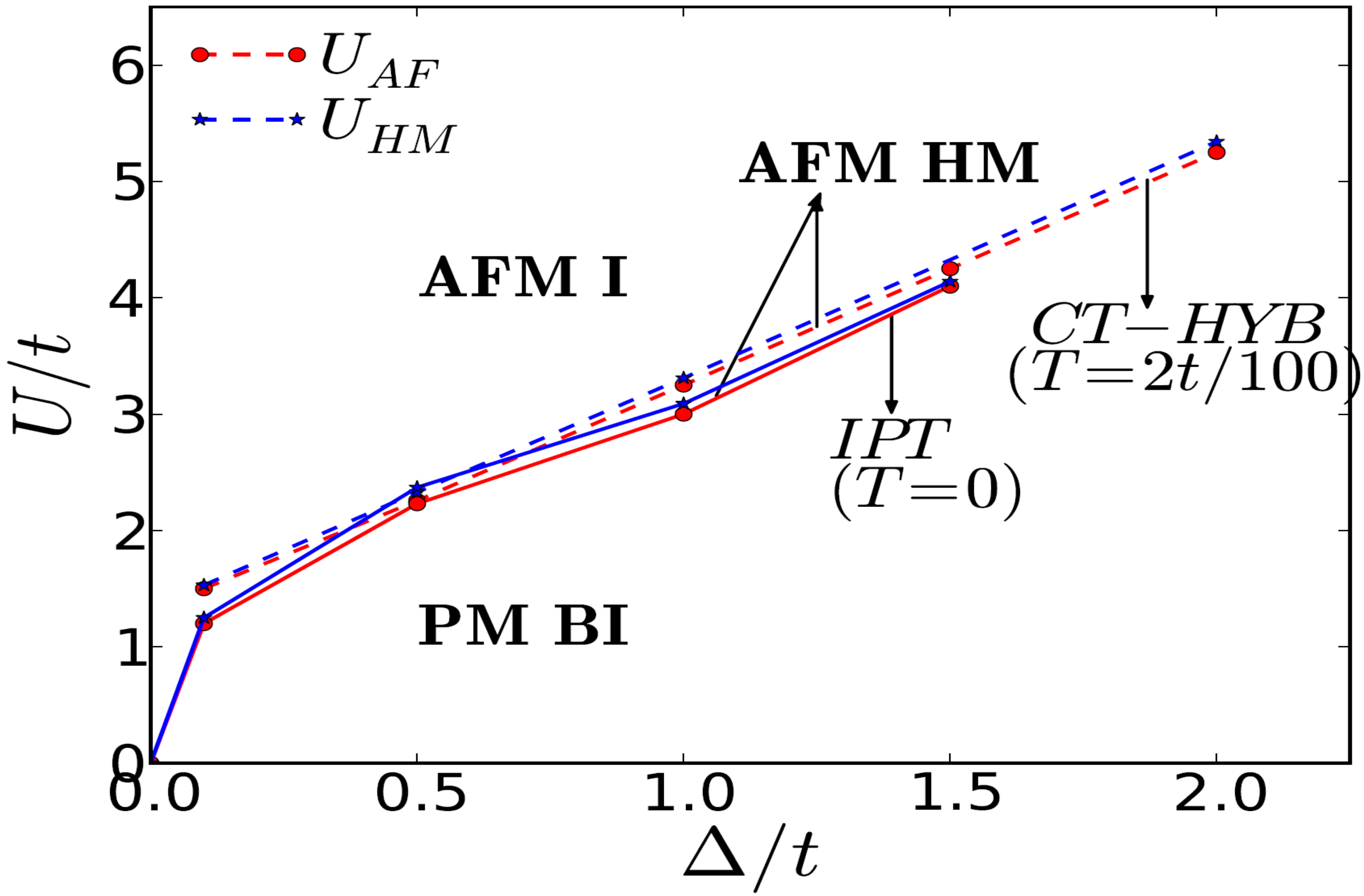
Single Particle Gaps versus U (IPT)

(n=1, Δ/t = 1.0, Bethe Lattice)

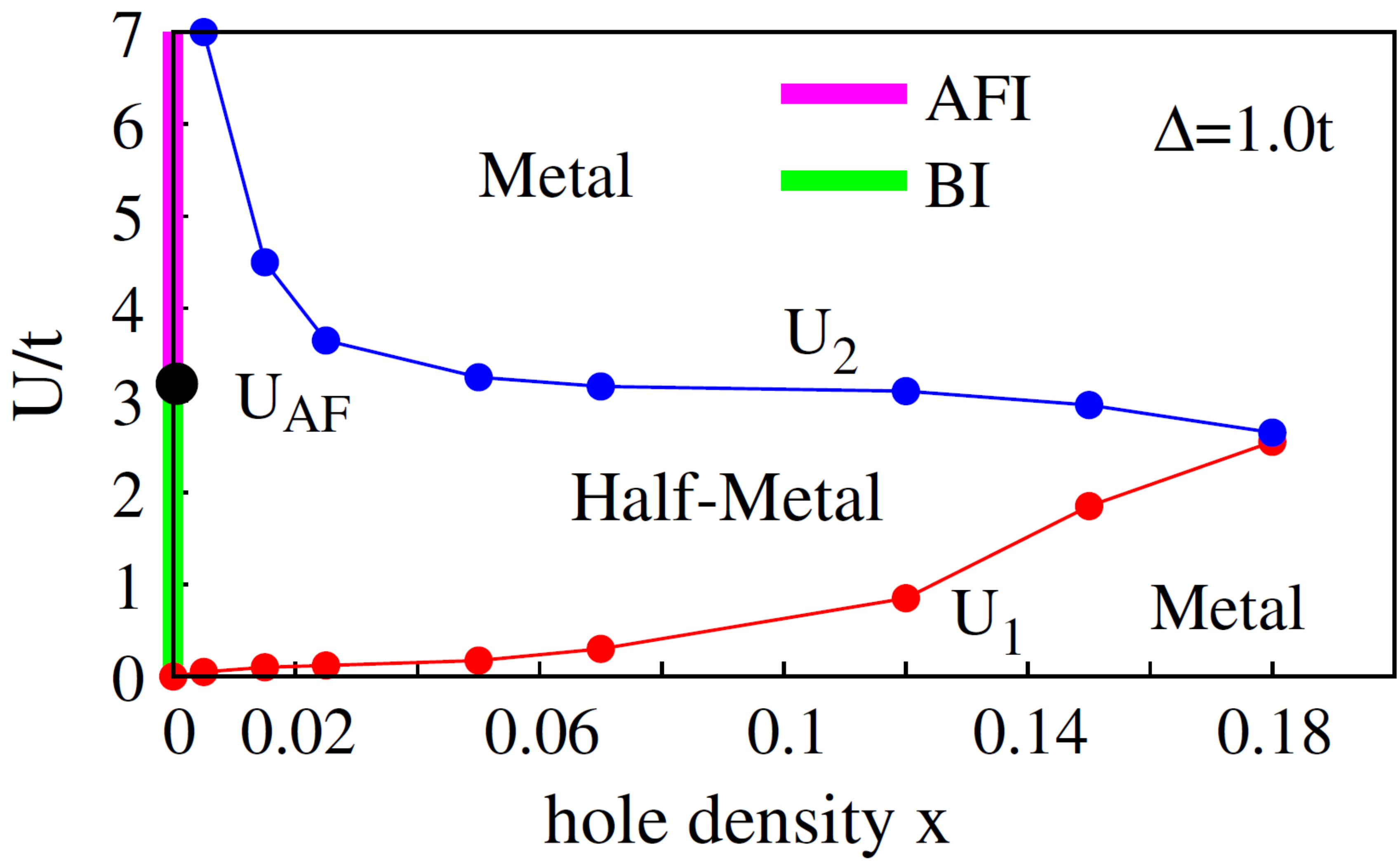


T=0 Phase Diagram of IHB at Half Filling

(Bethe Lattice, allowing for Antiferromagnetism)



Phase diagram with doping (IPT)



$t - t'$ Ionic Hubbard Model, with Frustration

$$H = -\sum_{\langle ij \rangle} t_{ij}\, \hat{a}^{+}_{i\sigma} \hat{a}_{j\sigma} + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

$$+ \Delta \sum_{i \in A} \hat{n}_i - \Delta \sum_{i \in B} \hat{n}_i - \mu \sum_i \hat{n}_i$$

$t - t'$ IHM : $t_{ij} = t$ for *nn* sites

t' for *nnn* sites

"half filling" $\Leftrightarrow$ $\langle \hat{n}_A \rangle + \langle \hat{n}_B \rangle = 2$

For large U, this maps to a Heisenberg model with frustration

$$H = \sum_{ij} J_{ij}\, \vec{S}_i \cdot \vec{S}_j$$

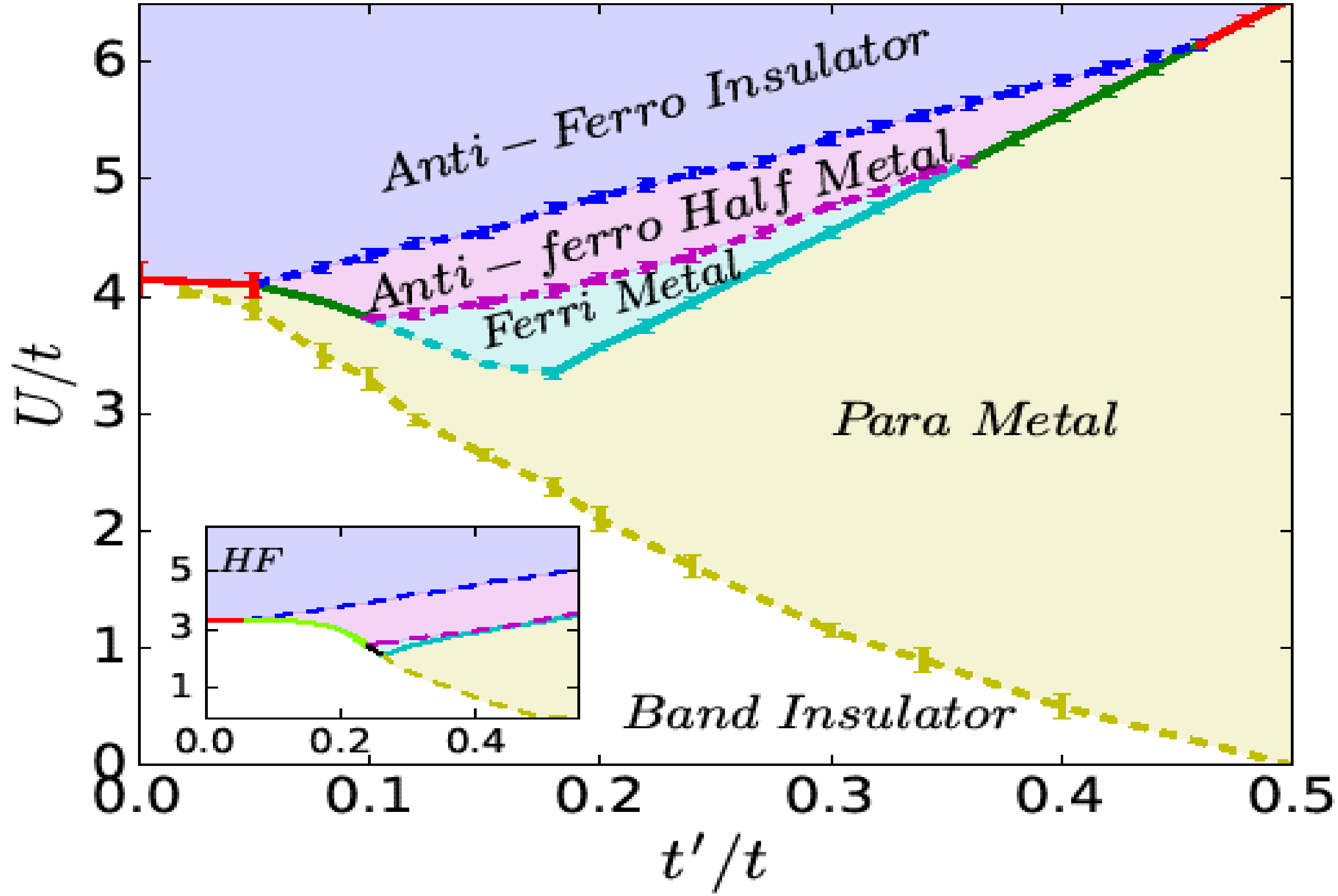
$J_{ij} = J = 4t^2/U$ for *nn* sites

$J' = 4t'^2/U$ for *nnn* sites

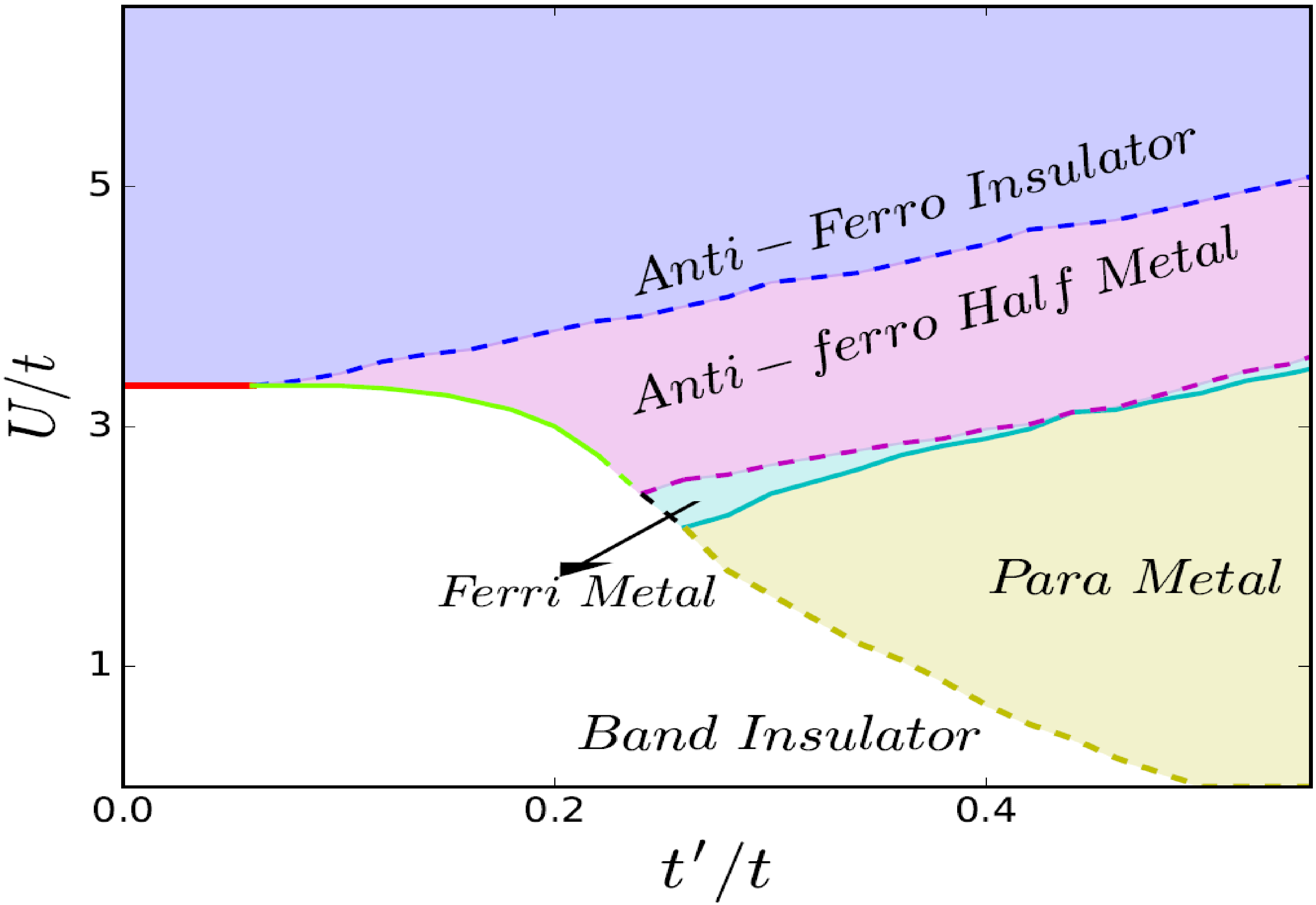
Can this suppress AFM enough to allow formation of PMM phase?

$t - t'$- U - Δ IHB at Half-filling

DMFT+CTQMC Phase Diagram



$t - t'$- U - Δ IHB at Half-filling
Unrestricted Hartree-Fock (UHF) Phase Diagram



$t - t'$- U - Δ IHB at Half-filling
Unrestricted Hartree-Fock (UHF) Theory

Two (spin dependent) lower bands and two (spin dependent) upper bands (in half the BZ of the square lattice) with energy dispersions given by

$$\xi^{\pm}_{\mathbf{k}\sigma} = -4t' \cos k_x \cos k_y + U(1-\sigma m_f)/2 \pm E_{\mathbf{k}\sigma}$$

$$E_{\mathbf{k}\sigma} \equiv \sqrt{(\gamma_{\mathbf{k}})^2 + [\Delta - U(\delta n + \sigma m_s)/2]^2} \;;$$

$$\gamma_{\mathbf{k}} \equiv -2t[\cos(k_x) + \cos(k_y)]$$

$$m_s \equiv [(\langle n_{A\uparrow}\rangle - \langle n_{A\downarrow}\rangle) - (\langle n_{B\uparrow}\rangle - \langle n_{B\downarrow}\rangle)]/2$$

$$m_f \equiv [(\langle n_{A\uparrow}\rangle - \langle n_{A\downarrow}\rangle) + (\langle n_{B\uparrow}\rangle - \langle n_{B\downarrow}\rangle)]/2$$

$$\delta n \equiv (\langle n_B\rangle - \langle n_A\rangle)/2$$

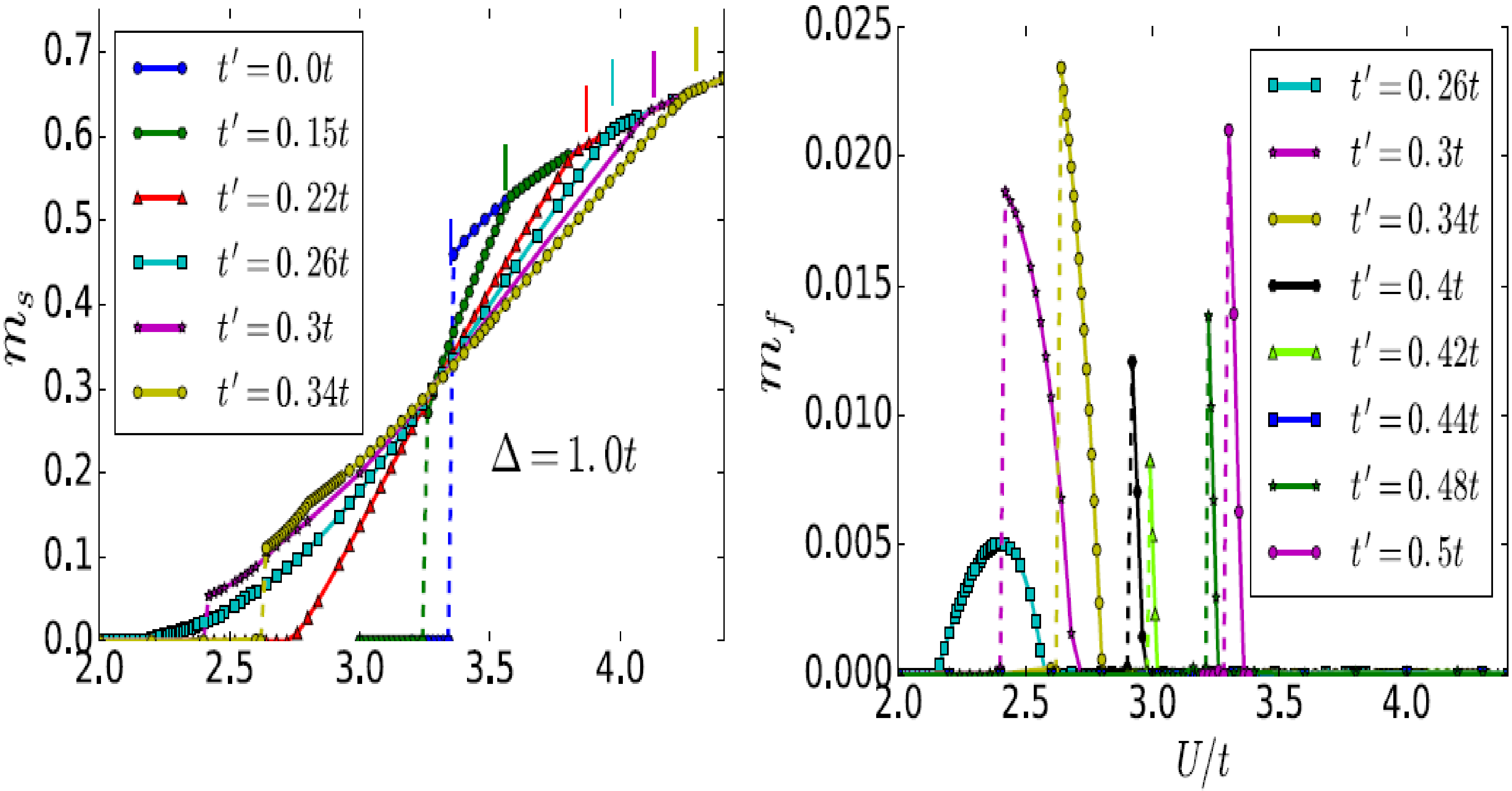
Upper band minima at $\mathbf{K} \equiv (\pm\pi/2, \pm\pi/2)$

$$\xi^{+}_{\mathbf{K}\sigma} = |\Delta - U(\delta n + \sigma m_s)/2|$$

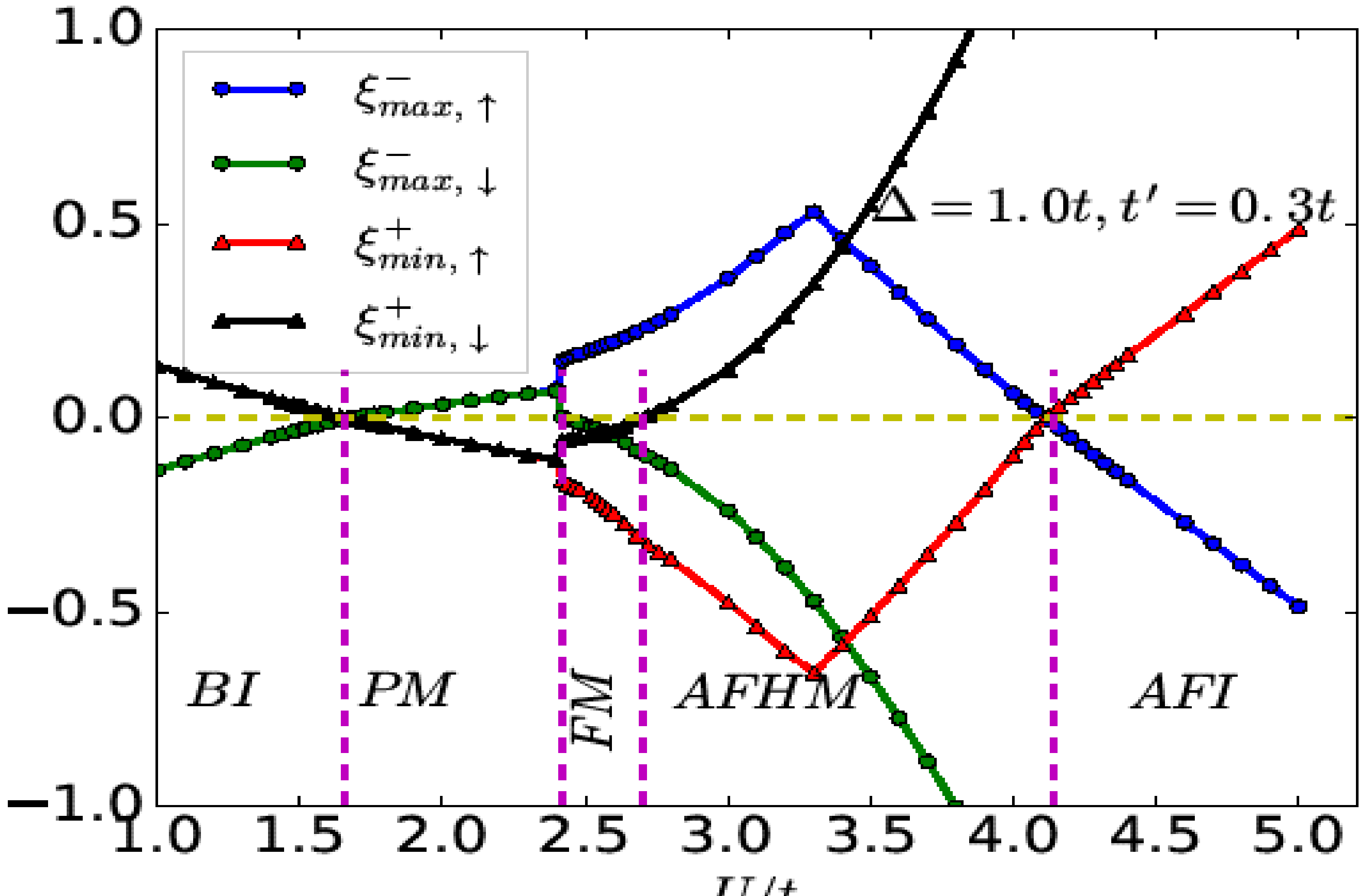
Lower band maxima at $\mathbf{K}' \equiv (\pm\pi, 0)$, $(0, \pm\pi)$

$$\xi^{-}_{\mathbf{K}'\sigma} = 4t' + U(1-\sigma m_f)/2 - |\Delta - U(\delta n + \sigma m_s)/2|$$

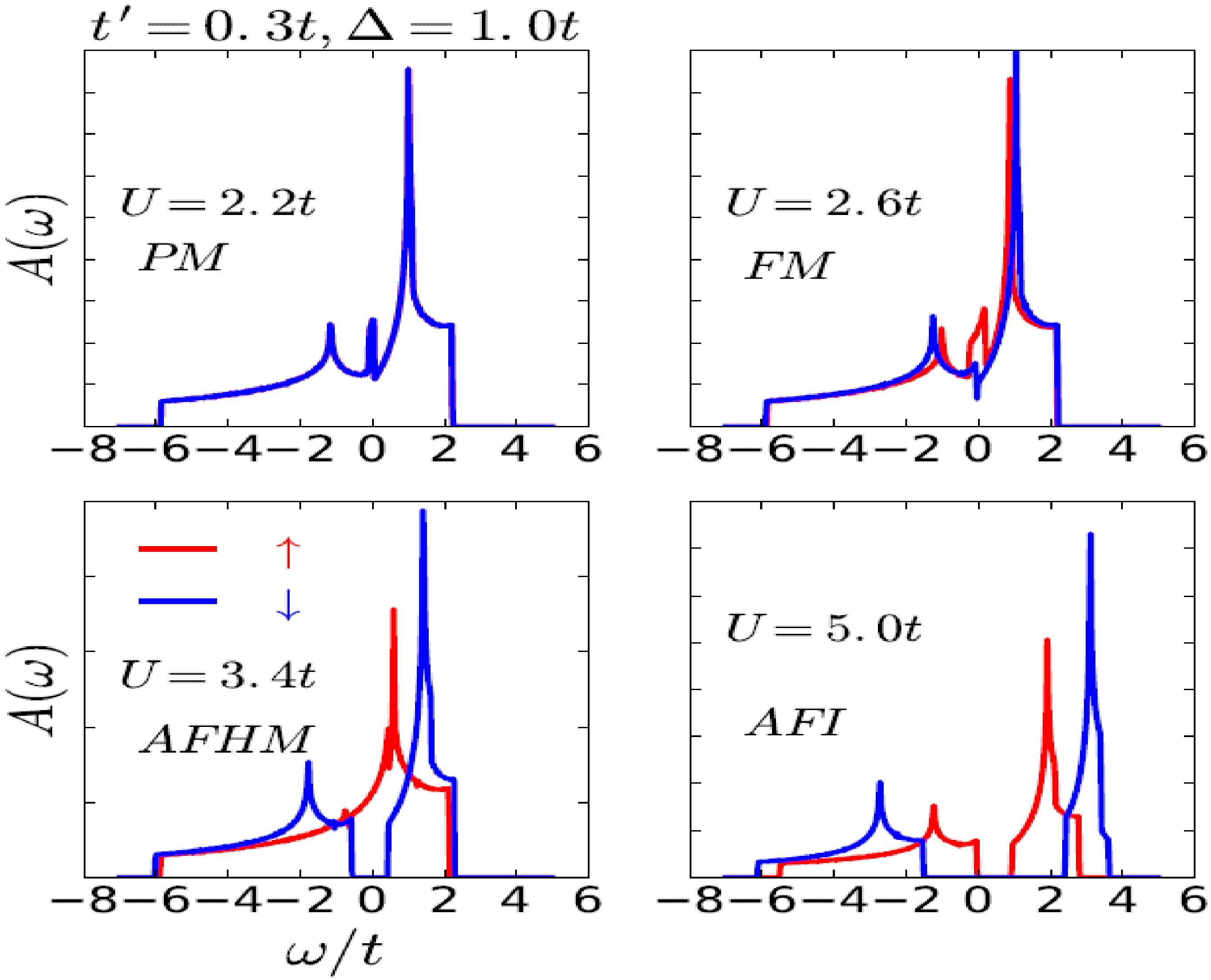
$t - t'$- U - Δ IHB at Half-filling
Unrestricted Hartree-Fock (UHF) Theory
Magnetic Transitions



$t - t'$- U - Δ IHB at Half-filling
Unrestricted Hartree-Fock (UHF) Theory
Upper Band Minima and Lower Band Maxima

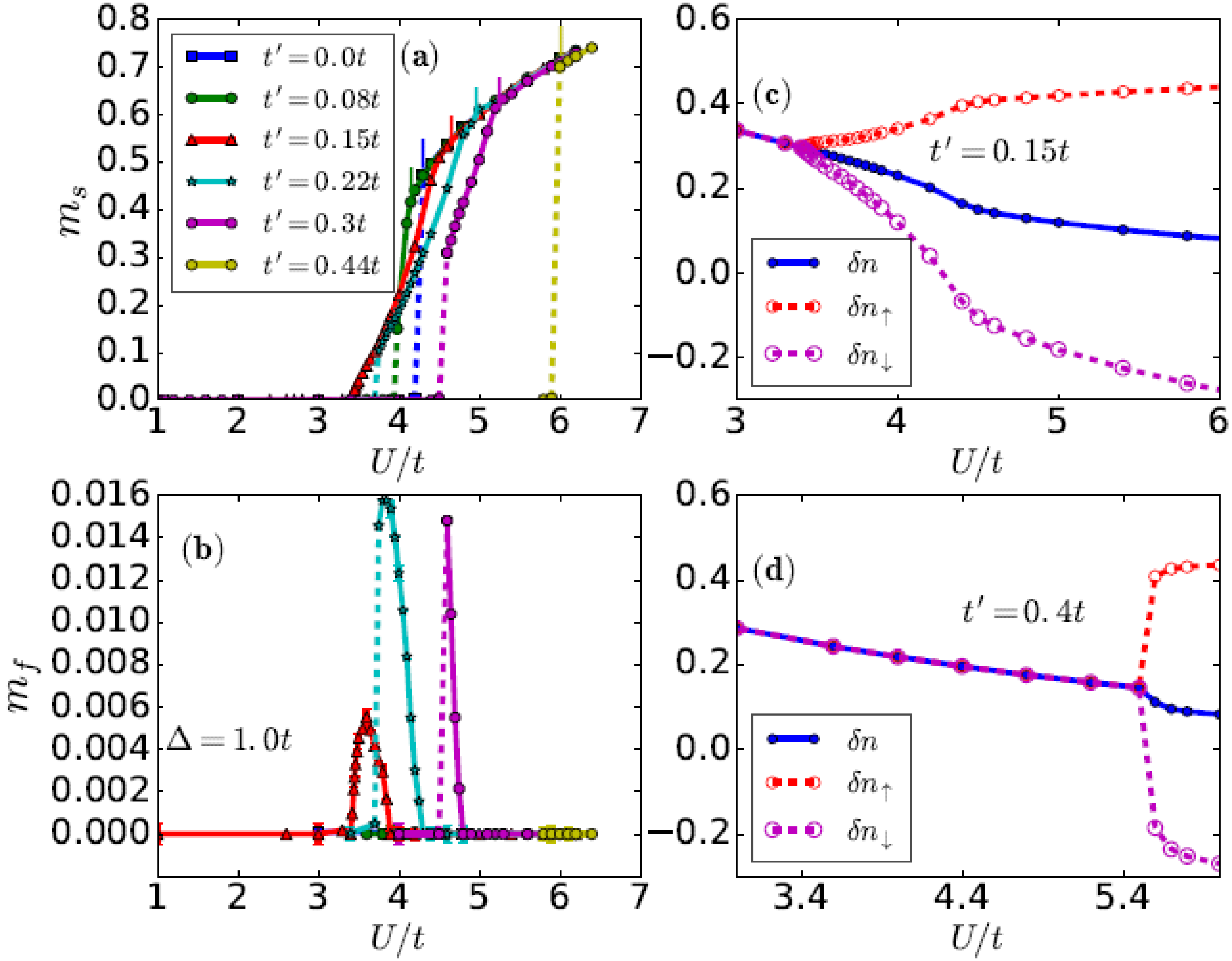


$t - t'$- U - Δ IHB at Half-filling
Unrestricted Hartree-Fock (UHF) Theory
Spin resolved Spectral Functions



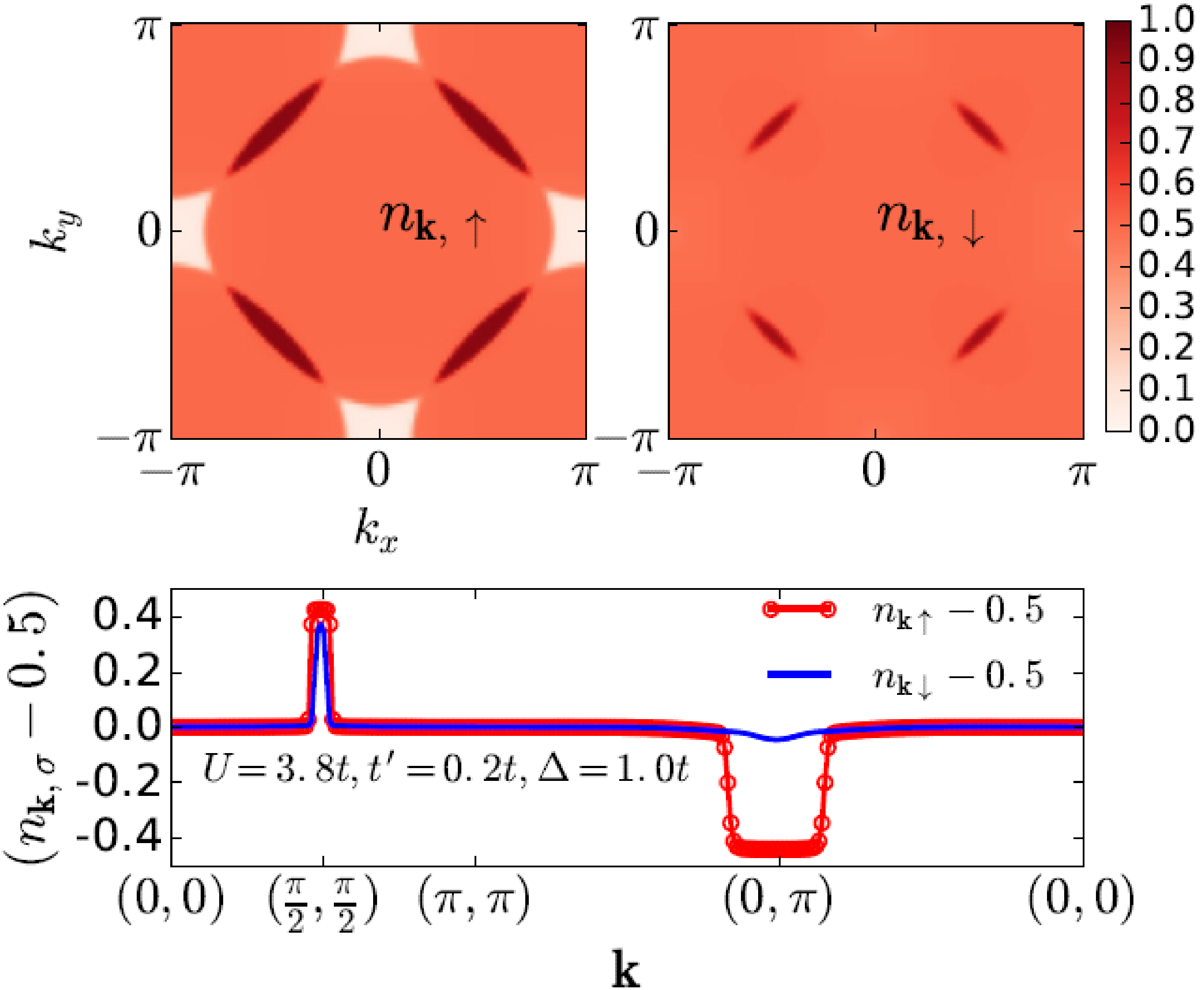
$t - t'$- U - Δ IHB at Half-filling

DMFT+CTQMC Magnetic Transitions

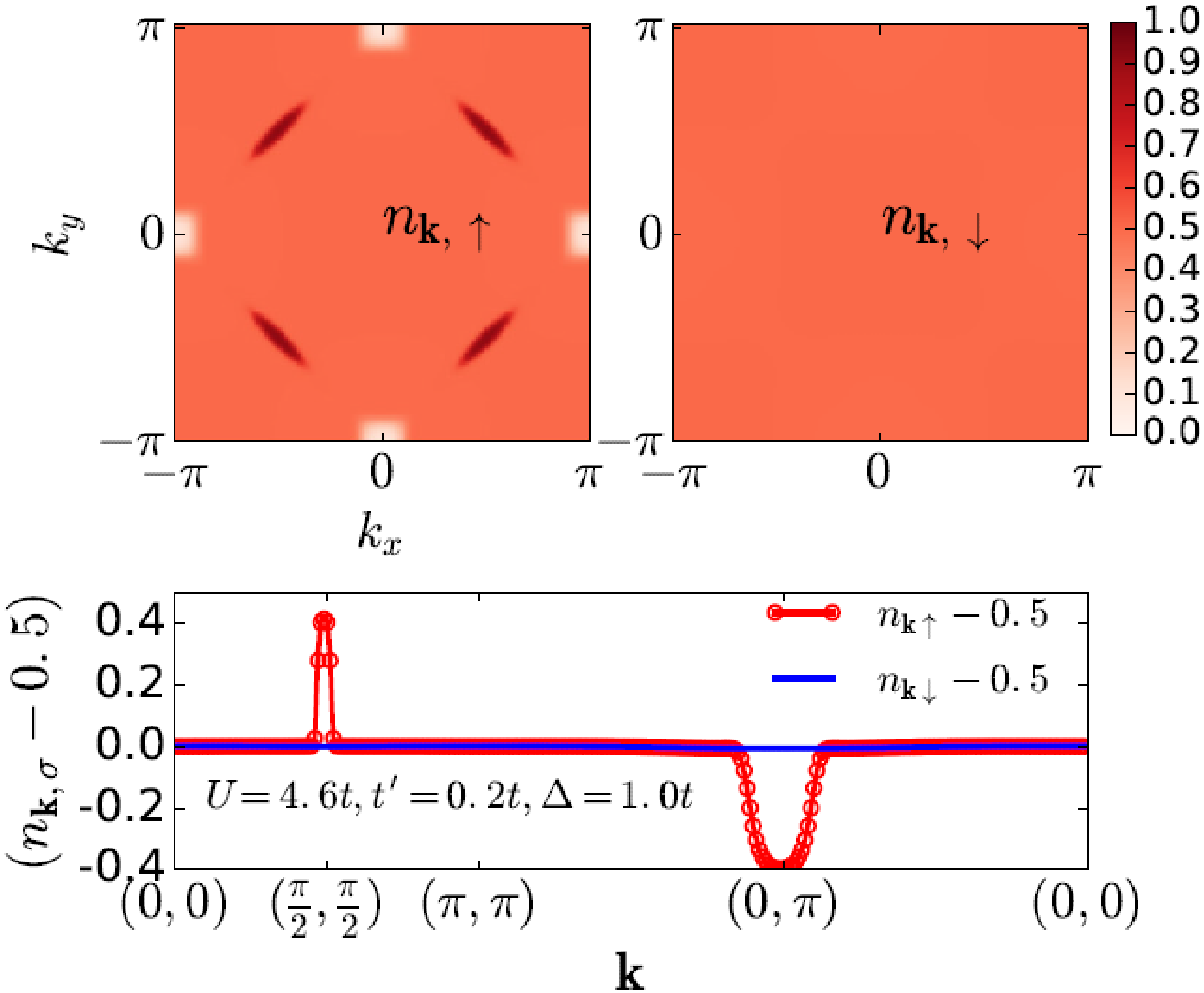


$t - t'$- U - Δ IHB at Half-filling DMFT+CTQMC

MDF – Ferrimagnetic Metal (FM) Phase

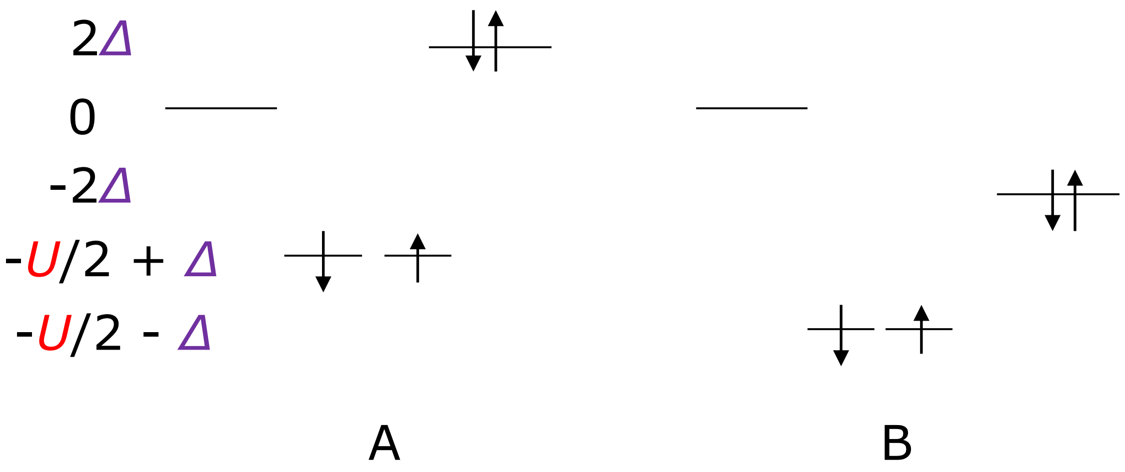


$t - t'$- U - Δ IHB at Half-filling DMFT+CTQMC
MDF – Anti Ferromagnetic Half Metal (AFHM) Phase



Possibility of High Tc Superconductivity in the (very strongly correlated) half filled IHM!

Superconductivity in the half filled
t – *U* - *Δ* Ionic Hubbard Model for *U, Δ >> t, U - 2Δ < t ?!*



In this limit, doublons on A sites and holons on B sites are too high in energy and get projected out

Effective Low energy Hamiltonian (Samanta & Sensarma PRB **94**, 224517 (2016))

$$\tilde{H} = \sum_i \mu_i^d n_{iA}^d + \mu_i^h n_{iB}^h + \mu_{iA}^f n_{iA}^f + \mu_{iB}^f n_{iB}^f$$
$$-t \sum_{\langle ij \rangle \sigma} \sigma f_{jB\bar{\sigma}} f_{iA\sigma} d_{iA}^\dagger h_{jB}^\dagger + \text{H.c.}$$
$$+ \frac{2t^2}{U+V} \sum_{\langle ij \rangle} \left[\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} n_i^f n_j^f \right] + \frac{2t^2}{V} \sum_{\langle ij \rangle} n_{iA}^d n_{jB}^h ,$$

$$V \equiv 2\Delta,$$
$$\mu_i^d = U - 2\Delta - 2\mu - \mu_i^A$$
$$\mu_{iA}^f = -\Delta - \mu - \mu_i^A$$
$$\mu_{iB}^f = \Delta - \mu - \mu_i^B$$
$$\mu_i^h = -\mu_i^B$$

μ_i^A and μ_i^B are Lagrange multipliers required to impose the local constraints:

$$d_{iA}^\dagger d_{iA} + \sum_\sigma f_{iA\sigma}^\dagger f_{iA\sigma} = 1 \text{ and } h_{iB}^\dagger h_{iB} + \sum_\sigma f_{iB\sigma}^\dagger f_{iB\sigma} = 1$$

Slave Boson Mean field Theory showing Superconductivity in the half-filled t – U - Δ IHM for U, Δ >> t, U - 2Δ < t

(From Samanta &Sensarma, PRB94, 224517 (2016))

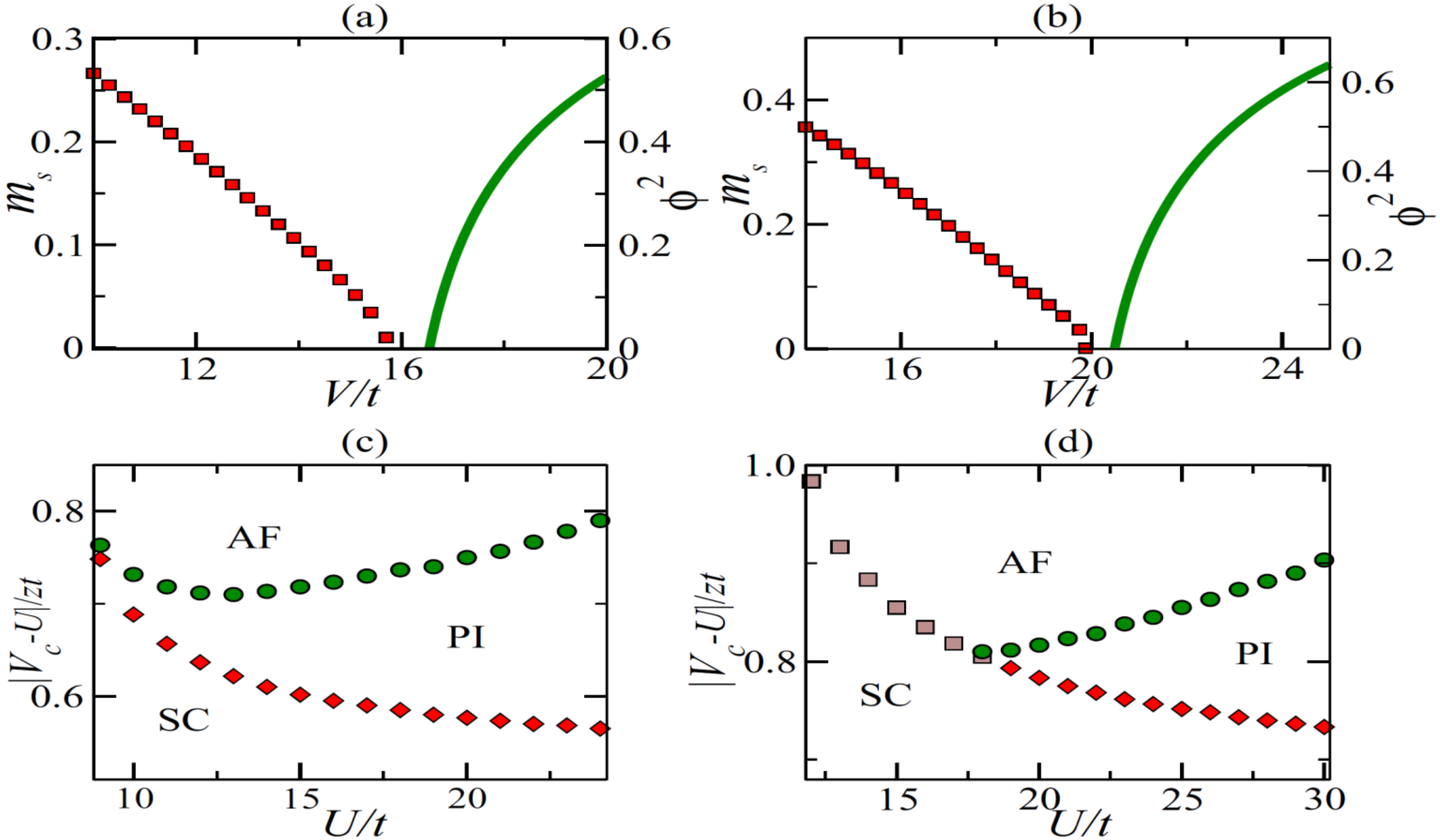
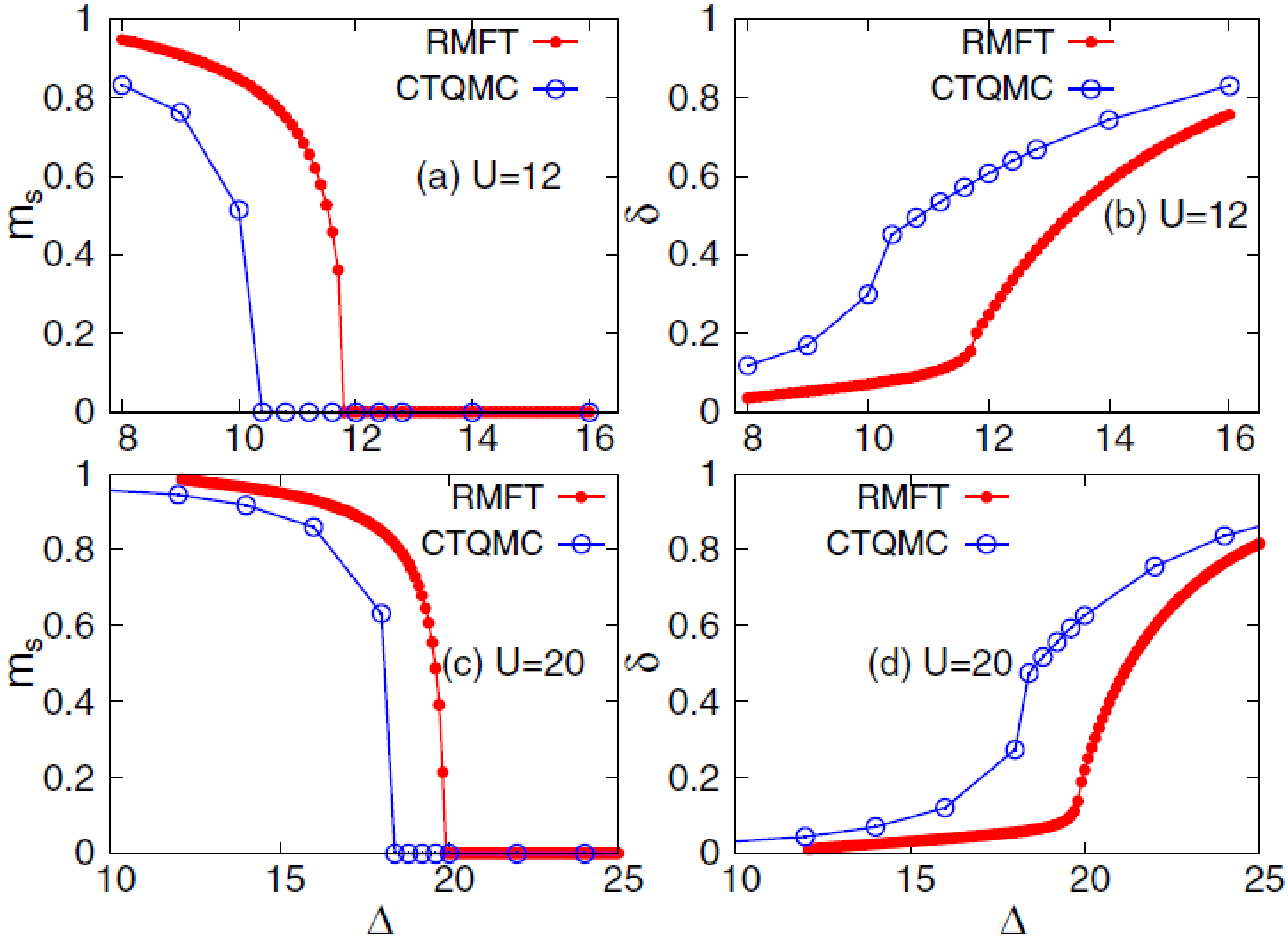
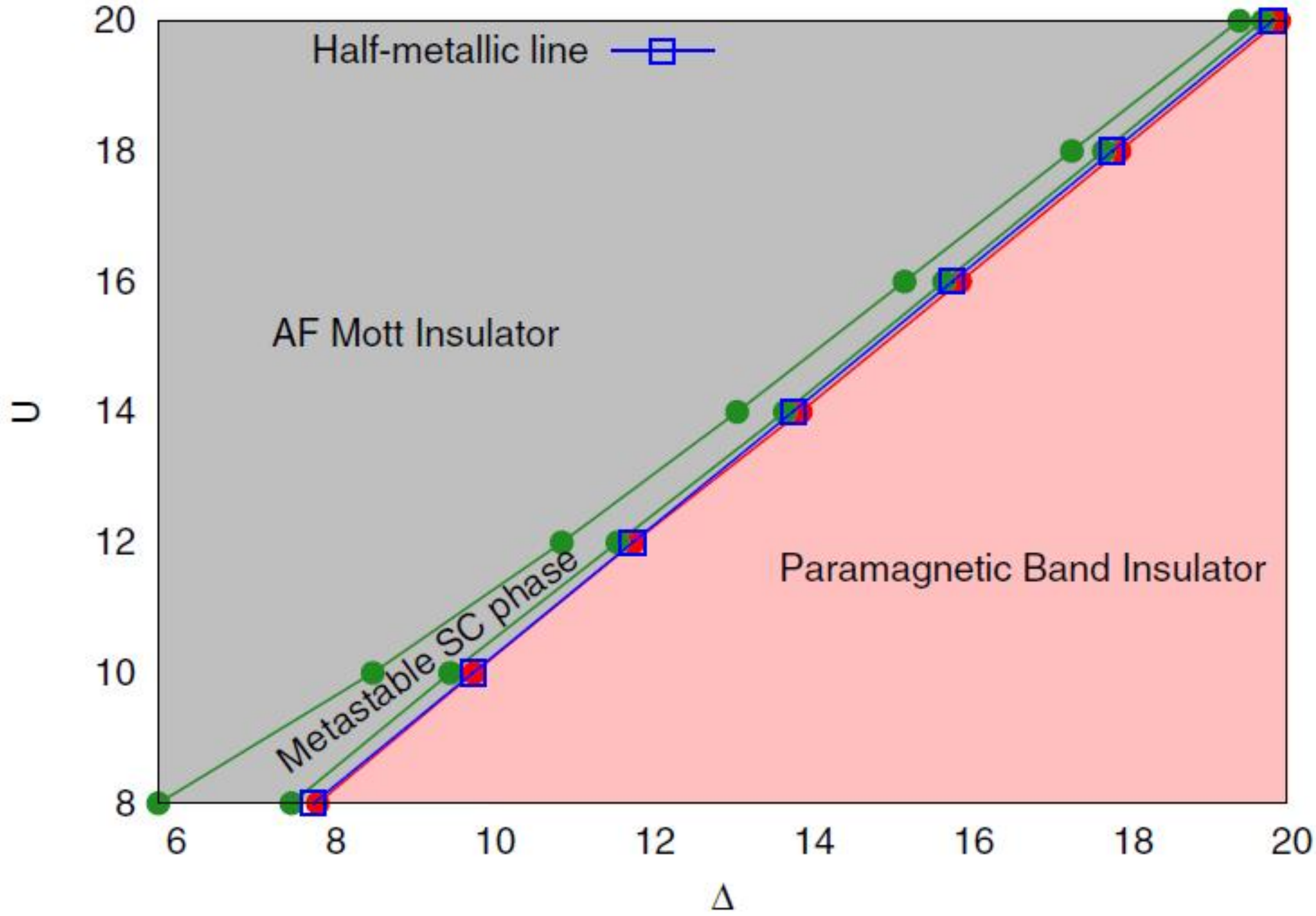


FIG. 1. The staggered magnetization m_s and the condensate fraction of the doublons (holons) ϕ^2 as a function of the ionic potential V for (a) a square lattice with $U = 20t$ and (b) a cubic lattice with $U = 25t$. The phase diagram in the U-V plane for (c) a square lattice and (d) a cubic lattice.

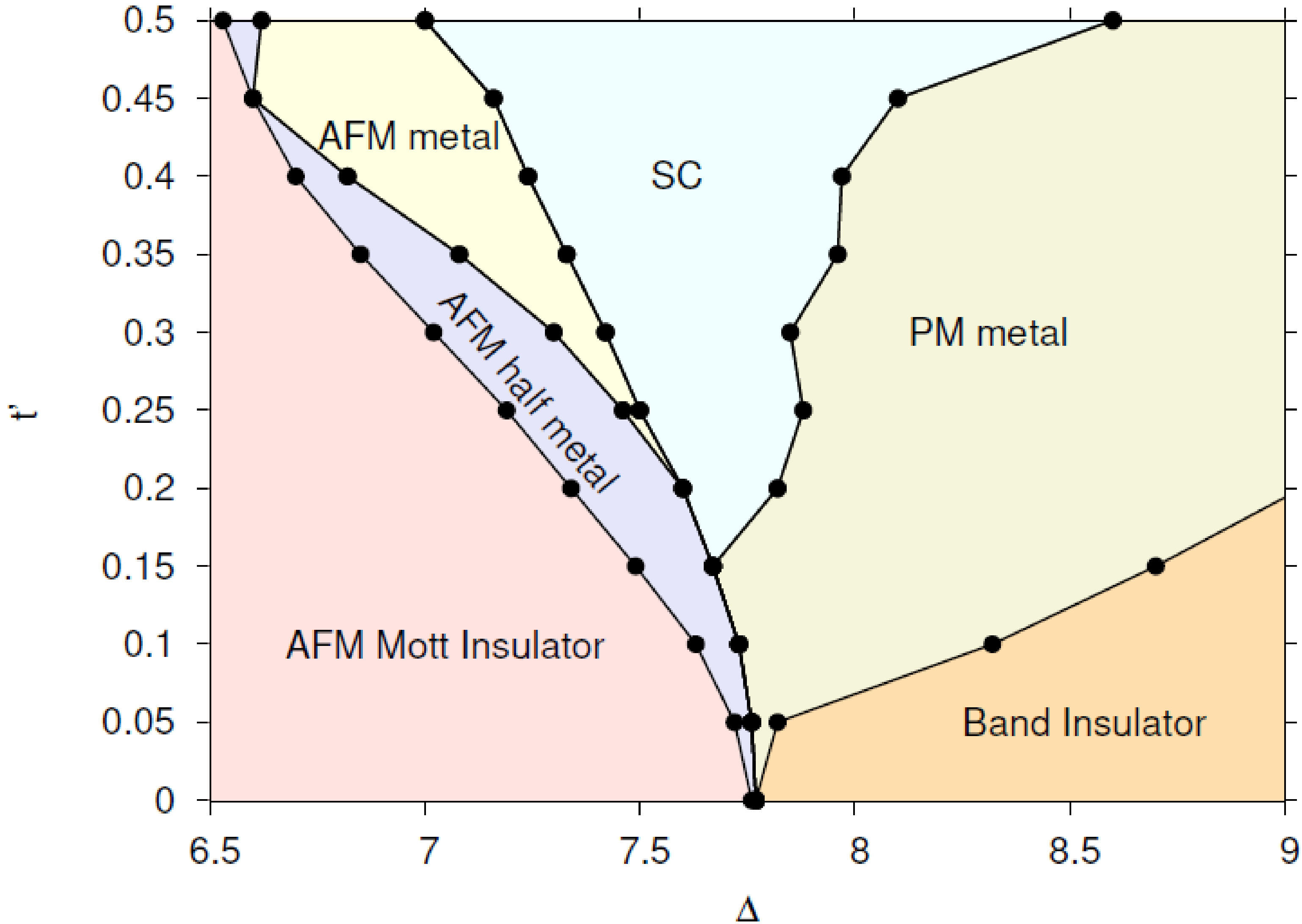
t – *U* - *Δ* Ionic Hubbard Model
Gutzwiller-Renormalized Mean Field Theory



$t - U$ - Δ Ionic Hubbard Model
Gutzwiller-Renormalized Mean Field Theory



t –*t'*- *U* - *Δ* Ionic Hubbard Model
Gutzwiller-Renormalized Mean Field Theory



Concluding comments - I

Lots of Novel and Fascinating possibilities in the Ionic Hubbard Model!

Results raise lots of open questions!

- Generic to all Strongly Correlated Band Insulators with two (or more) inequivalent correletaed sites per unit cell ?
- Will the effects found in DMFT survive in more accurate theories? Will other phases (BOND-ORDERED PHASE) intrude? (Such effects not included in Single-site DMFT, but can be explored in cluster DMFT)
- What is the nature of the QPT between the insulating and metallic phases? Is there one QPT or 2 QPTs?
- What are the properties of the paramagnetic metallic phase? Is it a non-fermi-liquid?
- What about the antiferromagnetic and ferrimagnetic half metal phases? What kinds of metals are they?

Concluding comments – II – Is it for Real?

- Can one find/make materials where the AFM spin-ordering is suppressed enough to yield such correlation induced metallic, half metallic and superconducting phase without doping?
- How will one identify such a metallic phase experimentally?
  - Pressure will drive it (band) insulating !
  - …
- Antiferromagnetic half metallic phase is tantalizing from the stand-point of spintronics
  - Can be looked for by first using DFT to identify materials that are in the appropriate range of parameters, and then experimentally.

Concluding Comments - III

- Can doping strongly correlated band insulators lead to other exotic phases?
    - superconducting phases with higher Tc than cuprates?
    - Pseudo-gap phases?
    - …?
- What possibilities are there with the inclusion of spin-orbit coupling and topological effects?
- What about non-equilibrium phenomena involving the IHM?

Thank You for your attention

Plan of the rest of the talk

- **DMFT and "Impurity" Solvers**
- Results with Para-magnetism enforced
  - Bethe lattice in infinite dimensions
  - 2-d square lattice
- Results allowing for Anti-ferromagnetism
  - Half filling and the AFHM line
  - Finite Temperature transitions
  - Ferrimagnetic Half Metallic phase with doping
- Some More recent results
  - Model with frustration
  - Superconductivity at Half filling?!
  - Quenching in the IHM
- Concluding Comments

The Dynamical Mean Field Theory (DMFT)

A.Georges, G. Kotliar, W.Kranth & M.J.Rozenberg, Rev. Mod Phys <u>68</u>, 13 (1996)

Better called Dynamical Effective Medium Theory?

Extension to correlated electronic models of

Curie-Weiss MFT for Heisenberg Model

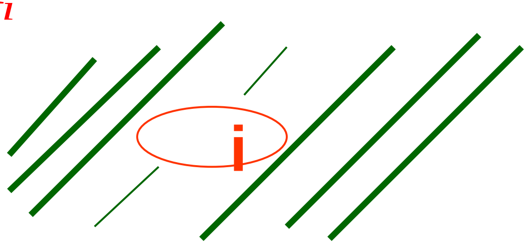
Coherent Potential Approximation (CPA) for disordered systems

Exact in infinite dimensions

<u>Curie-Weiss MFT for Heisenberg Model on “d” dimensional lattice</u>

$$H = J\sum_{ij}\vec{S}_i\cdot\vec{S}_j = \sum_i \vec{S}_i\cdot\left(J\sum_j \vec{S}_j\right) \equiv \sum_i \vec{S}_i\cdot\vec{h}_i$$

$\vec{h}_i$: Molecular field or Effective medium due to other sites



Self Consistency condition: $\Downarrow$

$$H_{eff} \approx \sum_i \vec{S}_i\cdot\vec{h}_i \;,\; \vec{h}_i \approx J\times 2d\times\langle\vec{S}_j\rangle$$

Approximation is exact if $J = J^*/(2d)$ and $d\to\infty$

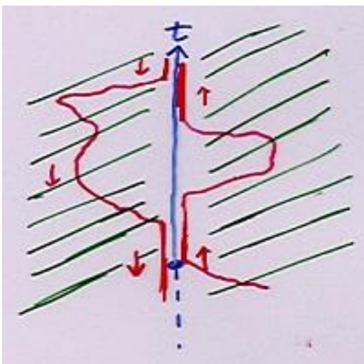
$$\vec{h}_i = \frac{J^*}{2d}\sum_{d=1}^{2d}\vec{S}_j$$

is *NON-FLUCTUATING*

Dynamical Mean Field Theory (DMFT)

Dynamical Mean Field or Effective medium Approximation for Hubbard model on a “d” dimensional lattice

Site variables : Electrons of either spin which move in and out of a site i and interact with each other on site i:



Effective medium representing other sites :

$\Rightarrow$ “free electron bath” which site i electrons leak into and out of

i.e., with which they “hybridize” :

$$H_{eff} \cong -\mu\, a^{+}_{i\sigma} a_{i\sigma} + U n_{i\uparrow} n_{i\downarrow}$$

$$+\sum_{k} \tilde{\varepsilon}_{k\sigma} c^{+}_{k\sigma} c_{k\sigma} + \sum_{k} V(\tilde{\varepsilon}_{k})[c^{+}_{k\sigma} a_{i\sigma} + a^{+}_{i\sigma} c_{k\sigma}]$$

i.e : The Anderson Impurity Problem !

Dynamical Mean Field Theory (DMFT)

Time dependent amplitude $G_h(t\text{-}t')$ for electrons at site i to leave site at time t and return at at time t' from effective medium :

$$\mathrm{G_h}^{-1}(\omega) = \omega + \mu - \int_k \frac{\left(V(\tilde{\varepsilon}_k)\right)^2}{\omega - \tilde{\varepsilon}_k}$$

"Host or Medium (Inverse) propagator"

Self Consistency condition comes from the condition that the impurity self energy arising from Collisions between electrons of opposite spins at site i

$\Rightarrow$ the (local) self energy $\Sigma(\omega)$ for the lattice problem

Total time dependent propagator for electrons at site i: $G(t\text{-}t')$

$$G(\omega) = \sum_{\vec{k}} \frac{1}{\mu + \omega - \varepsilon_{\vec{k}} - \Sigma(\omega)}$$

$$= \int \frac{D(\varepsilon_{\vec{k}})d\varepsilon_{\vec{k}}}{\omega + \mu - \varepsilon_{\vec{k}} - \Sigma(\omega)}$$

$$= [G_h^{-1}(\omega) - \Sigma(\omega)]^{-1}$$

Dynamical Mean Field Theory (DMFT)
The Triangle of Self Consistency

Local Self Energy

$$\Sigma_{ii}(i\omega)$$

Impurity problem !
Hard!

$$G_{ii}(\omega) = \int \frac{D(\varepsilon_{\vec{k}})\, d\varepsilon_{\vec{k}}}{\omega + \mu - \varepsilon_k - \Sigma_{ii}(i\omega)}$$

Band DOS dependent.

Local Propagator

Host Propagator

$$G_{h,ii}^{-1}(\omega) = [G_{ii}^{-1}(\omega) + \Sigma_{ii}(\omega)]$$

$$= \omega - \varepsilon_d - \int_{\varepsilon} \frac{|V(\varepsilon)|^2\, d\varepsilon}{\omega - \varepsilon}$$

Reverse Dyson Equation

d level

hybridization

DMFT Scheme for the IHM

Need to work with Matrix Green Functions

$$\mathbf{G}^{\sigma}(\vec{k},\omega)=\begin{pmatrix}\mu+\omega-\Delta-\Sigma_{A\sigma}(\omega) & -\varepsilon_{\vec{k}} \\ -\varepsilon_{\vec{k}} & \mu+\omega+\Delta-\Sigma_{B\sigma}(\omega)\end{pmatrix}^{-1}\equiv\begin{pmatrix}\zeta_{A\sigma} & -\varepsilon_{\vec{k}} \\ -\varepsilon_{\vec{k}} & \zeta_{B\sigma}\end{pmatrix}^{-1}$$

Local Green functions $\mathbf{G}^{\sigma}(\omega)=\sum_{\vec{k}}\mathbf{G}^{\sigma}(\vec{k},\omega)$

Given by $\mathbf{G}^{\sigma}(\omega)=\int d\varepsilon_{\vec{k}}\,\frac{\rho_0(\varepsilon_{\vec{k}})}{\zeta_{A\sigma}\zeta_{B\sigma}-(\varepsilon_{\vec{k}})^2}\begin{pmatrix}\zeta_{B\sigma} & \varepsilon_{\vec{k}} \\ \varepsilon_{\vec{k}} & \zeta_{A\sigma}\end{pmatrix}$

Exploit Symmetry Properties at Half filling:

$$G_A(i\omega_n)=-G_B(-i\omega_n) \qquad \Sigma_A(i\omega_n)=U-\Sigma_B(-i\omega_n)$$

$$\mathbf{G}_A{}^{\sigma}(\omega)=-\mathbf{G}_B{}^{\bar{\sigma}}(-\omega) \qquad \Sigma_A{}^{\sigma}(\omega)=U-\Sigma_B{}^{\bar{\sigma}}(-\omega)$$

Iterated Perturbation Theory (IPT) Scheme

Georges & Kotliar PRB 45, 6479 (92), Georges & Krauth PRB 48, 7167 (93)

Bottleneck in DMFT: *$\Sigma(G_h)$* for the impurity problem is hard to calculate.

Iterated Perturbation Theory : Prescription for an approximation for *Σ*

with the following Properties:

- Good for *U/t* << 1
- Exact in the atomic, *t*=0, limit (i.e., for very large U)!
- Exact in the high frequency limit for all *U/t*, which imposes various exact sum rules
- reasonable and interesting interpolation for all *U*.

Possible just using the second order self-energy computed in terms of the Hartree Corrected Host Green Function

$$\tilde{\mathcal{G}}_{0\alpha}^{-1}(\omega^+) = \mathcal{G}_{0\alpha}^{-1}(\omega^+) - \Sigma_\alpha^{HF}$$

IPT for the Half filled Ionic Hubbard Model

$$\Sigma_\alpha^{IPT}(\omega^+) = \Sigma_\alpha^{HF} + A_\alpha \Sigma_\alpha^{(2)}(\omega^+)$$

$$A_\alpha = n_\alpha(1 - n_\alpha/2)/\left[n_{0\alpha}(1 - n_{0\alpha}/2)\right]$$

$$n_\alpha = -2\int_{-\infty}^{0} \mathrm{Im}\ G_\alpha(\omega^+) d\omega/\pi$$

$$n_{0\alpha} = -2\int_{-\infty}^{0} \mathrm{Im}\tilde{\mathcal{G}}_{0\alpha}(\omega^+) d\omega/\pi$$

$$\Sigma_\alpha^{(2)}(\omega^+) = U^2 \int_{-\infty}^{\infty} \prod_{i=1}^{3} \left[d\epsilon_i \tilde{\rho}_\alpha(\epsilon_i)\right] \frac{N(\epsilon_1, \epsilon_2, \epsilon_3)}{\omega^+ - \epsilon_1 + \epsilon_2 - \epsilon_3}$$

$$N(\epsilon_1, \epsilon_2, \epsilon_3) = f(\epsilon_1)f(-\epsilon_2)f(\epsilon_3) + f(-\epsilon_1)f(\epsilon_2)f(-\epsilon_3)$$

CTQMC/CT-HYB Impurity Solver

- Implemented using the TRIQS package

  (Parcollet et.al. arxiv:1504.01952)

- Evaluates the partition function as a perturbation expansion in the hybridization by sampling

$$\frac{Z_\alpha}{Z_{0\alpha}} = \prod_\sigma \sum_{k_\sigma=0}^{\infty} \frac{1}{k_\sigma!^2} \int_0^\beta d\tau_1^\sigma \ldots d\tau_{k_\sigma}^\sigma \int_0^\beta d\tau'^\sigma_1 \ldots d\tau'^\sigma_{k_\sigma}$$

$$det \boldsymbol{\Delta}_{\alpha\sigma} \langle \mathbf{T}_\tau \mathbf{c}_{0\alpha\sigma}(\tau_1^\sigma) \mathbf{c}^\dagger_{0\alpha\sigma}(\tau'^\sigma_1) \ldots \mathbf{c}_{0\alpha\sigma}(\tau^\sigma_{\mathbf{k}}) \mathbf{c}^\dagger_{0\alpha\sigma}(\tau'^\sigma_{\mathbf{k}_\sigma}) \rangle_{\mathbf{S}^\alpha_{\mathbf{loc}}} (16)$$

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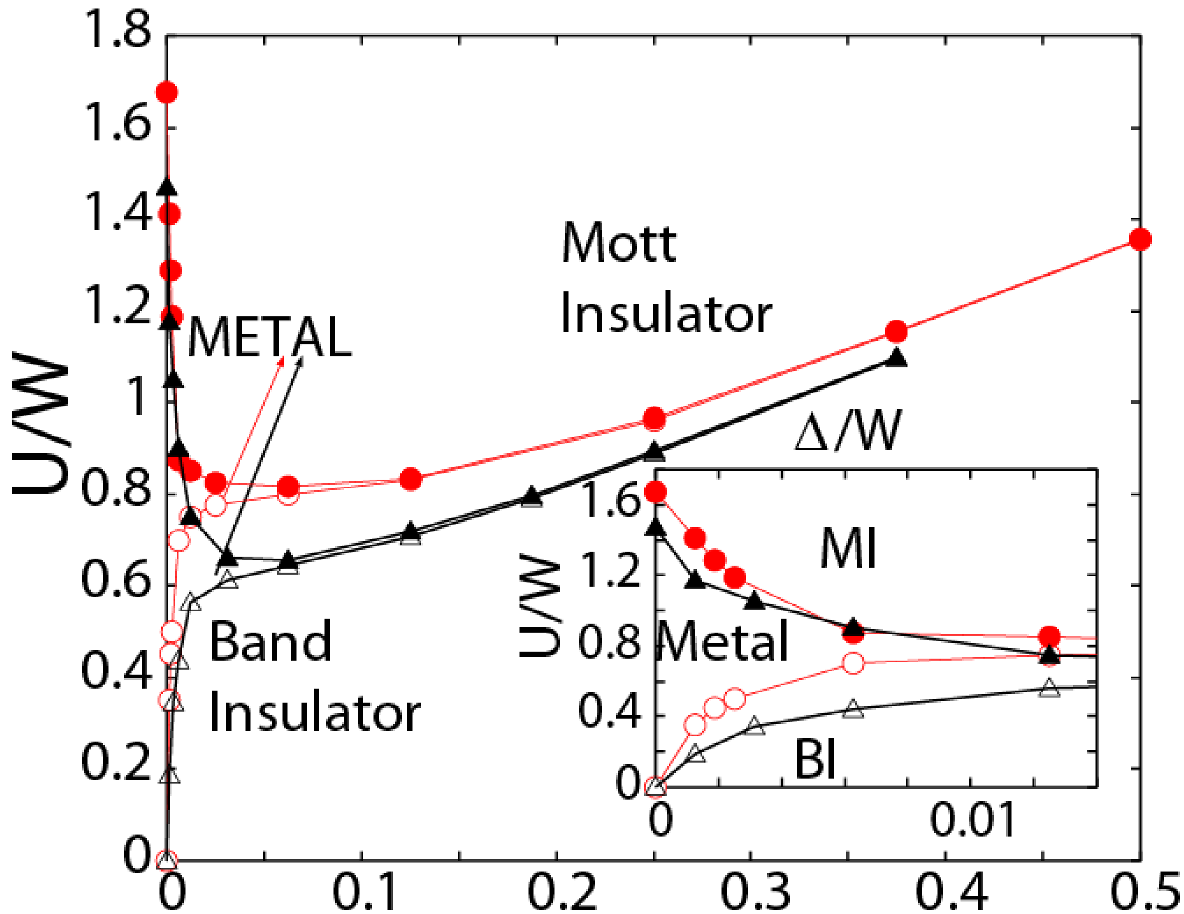
T=0 Phase Diagram of IHB at Half Filling (With Enforced Para-magnetism, IPT)



Δ/W

Black :

2-d Square lattice

Δ : U_{c1}

▲ : U_{c2}

W = 8t

Red :

Bethe lattice

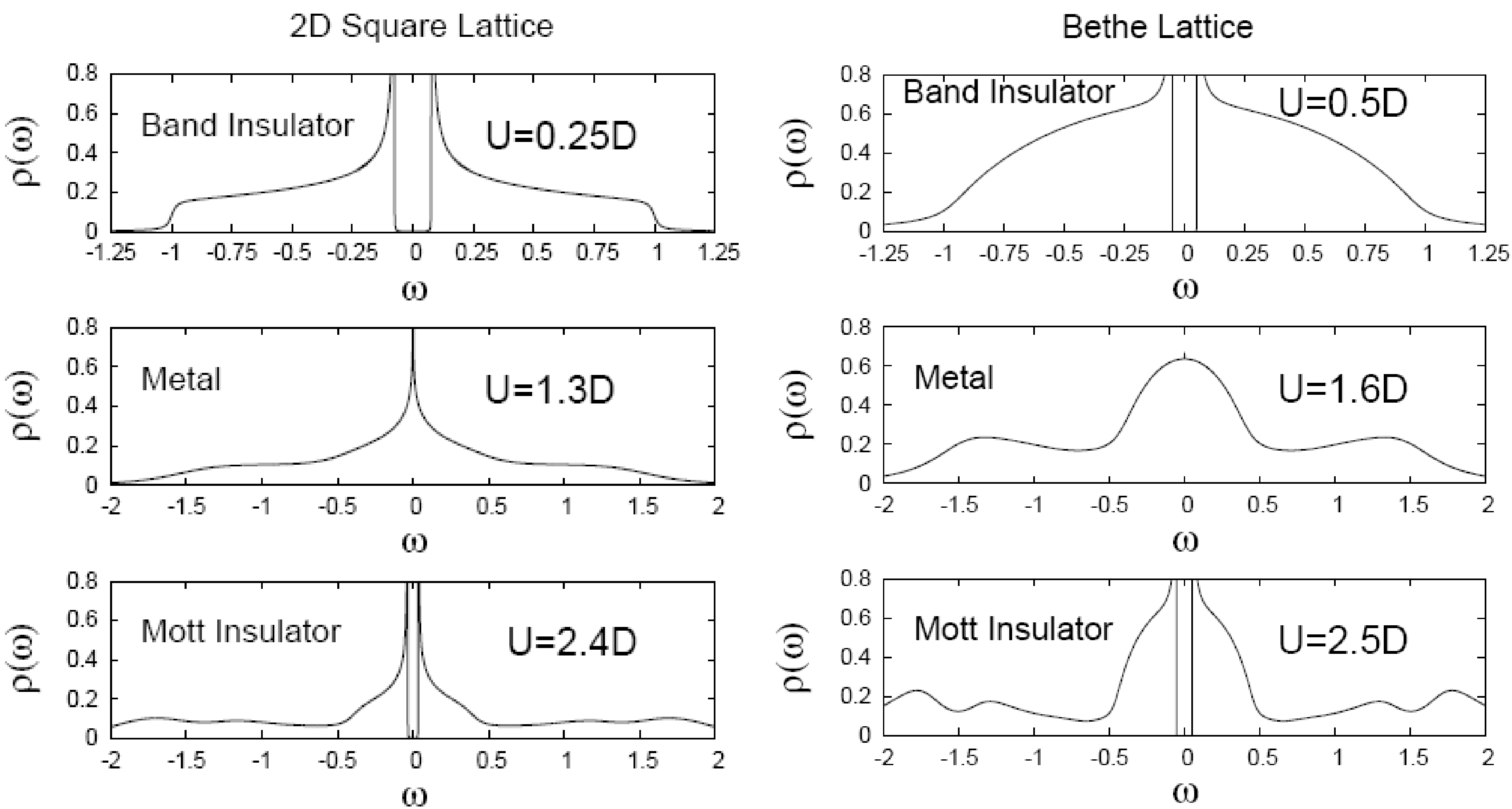
(z −>∞)

o : Uc1

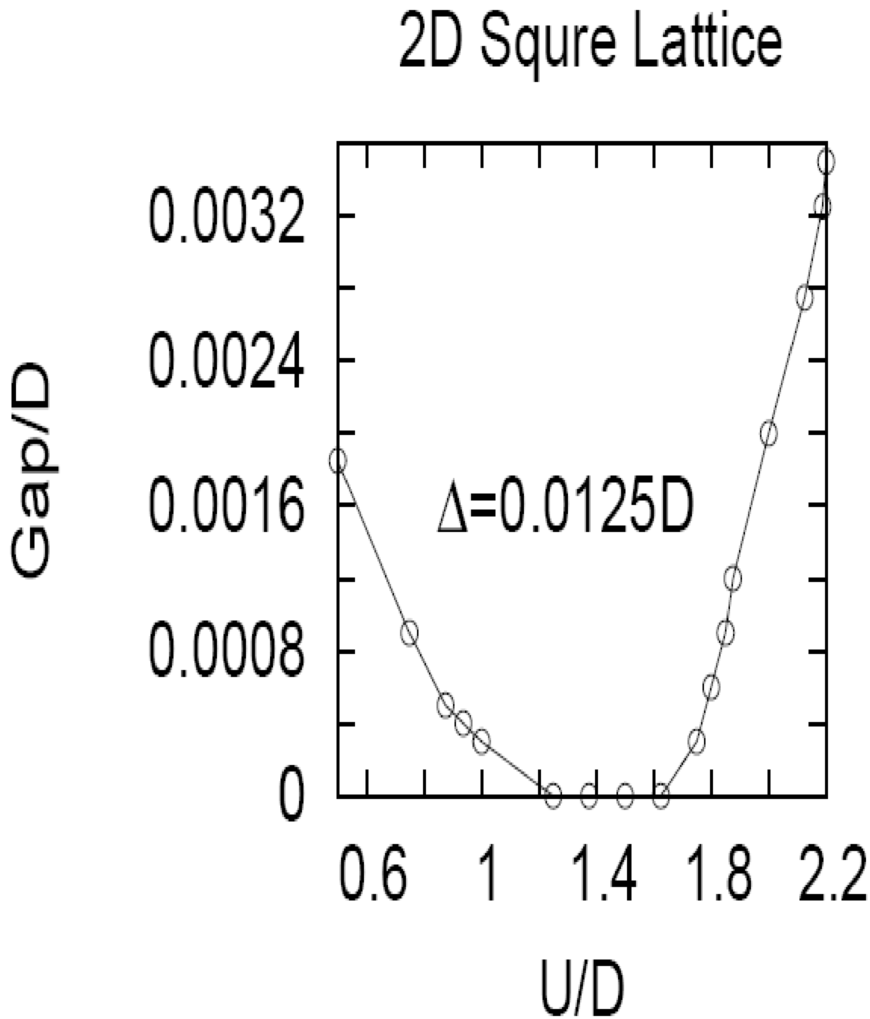
● : Uc2

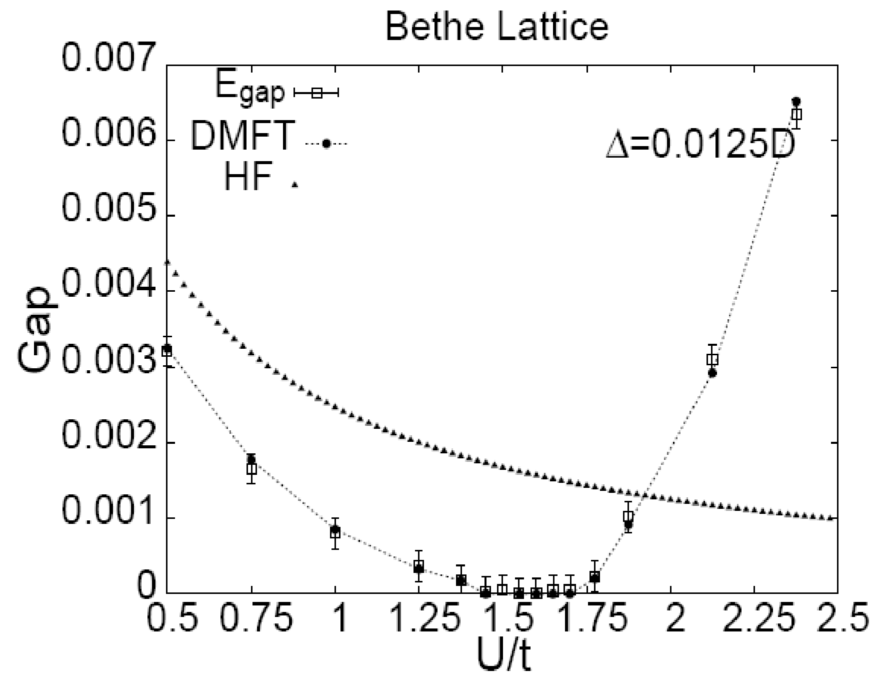
W= 4t

Density of States



Gap in Single Particle Spectrum

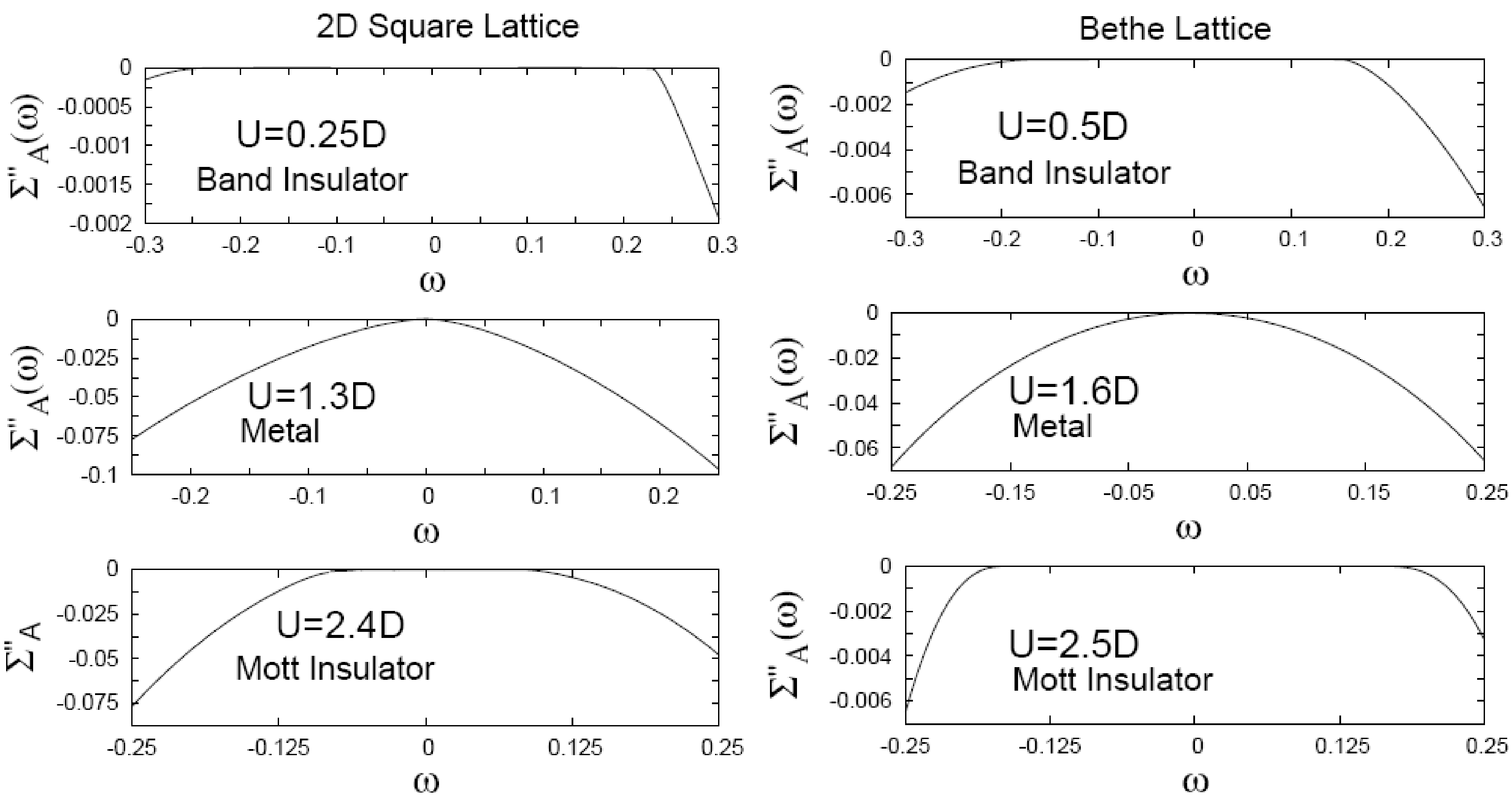




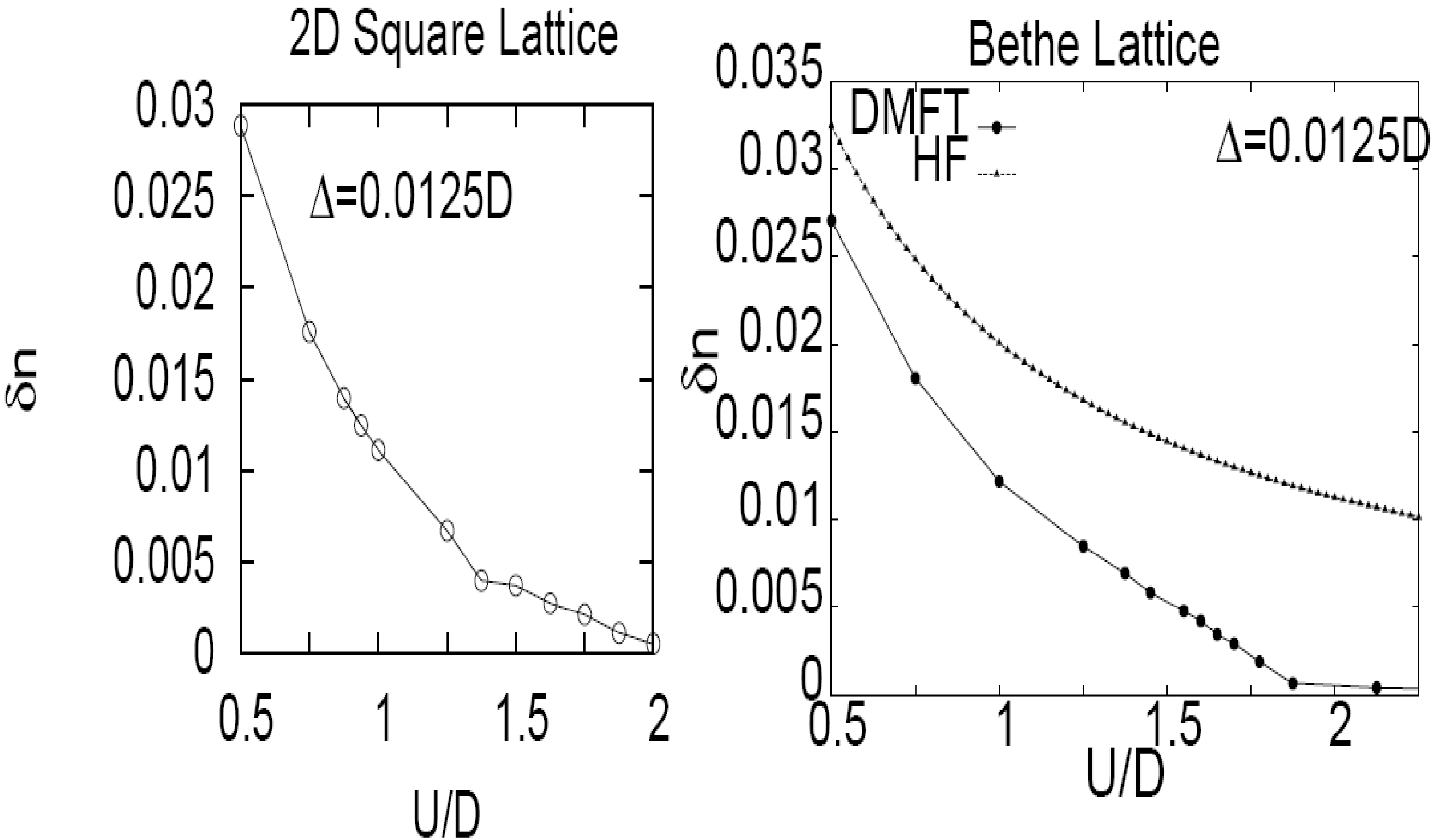
$$\Sigma'_\alpha(\omega) = \Sigma'_\alpha(0) + (1 - Z^{-1})\omega + \dots$$

$$E_{gap} = Z\left|\Delta - \frac{U\delta n}{2} + P\int_{-\infty}^{\infty} d\omega \frac{\Sigma''_A(\omega)}{\pi\omega}\right|$$

Imaginary Part of the Self-Energy



Difference in Filling of sub-lattices



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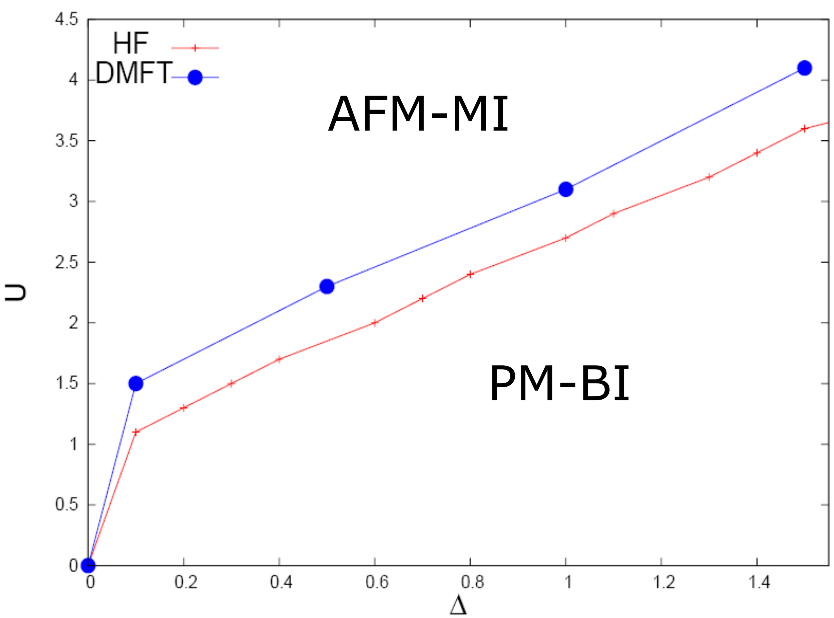
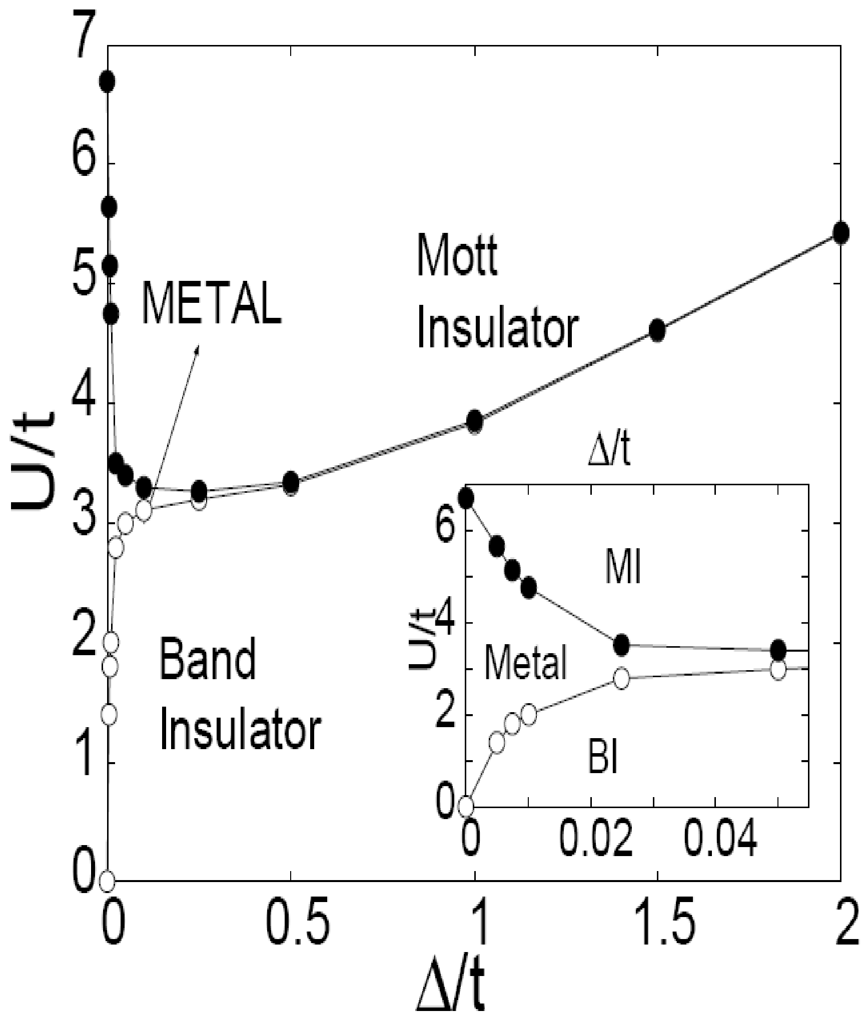
Phase Diagram of the IHM Allowing for Anti-ferromagnetism (AFM)

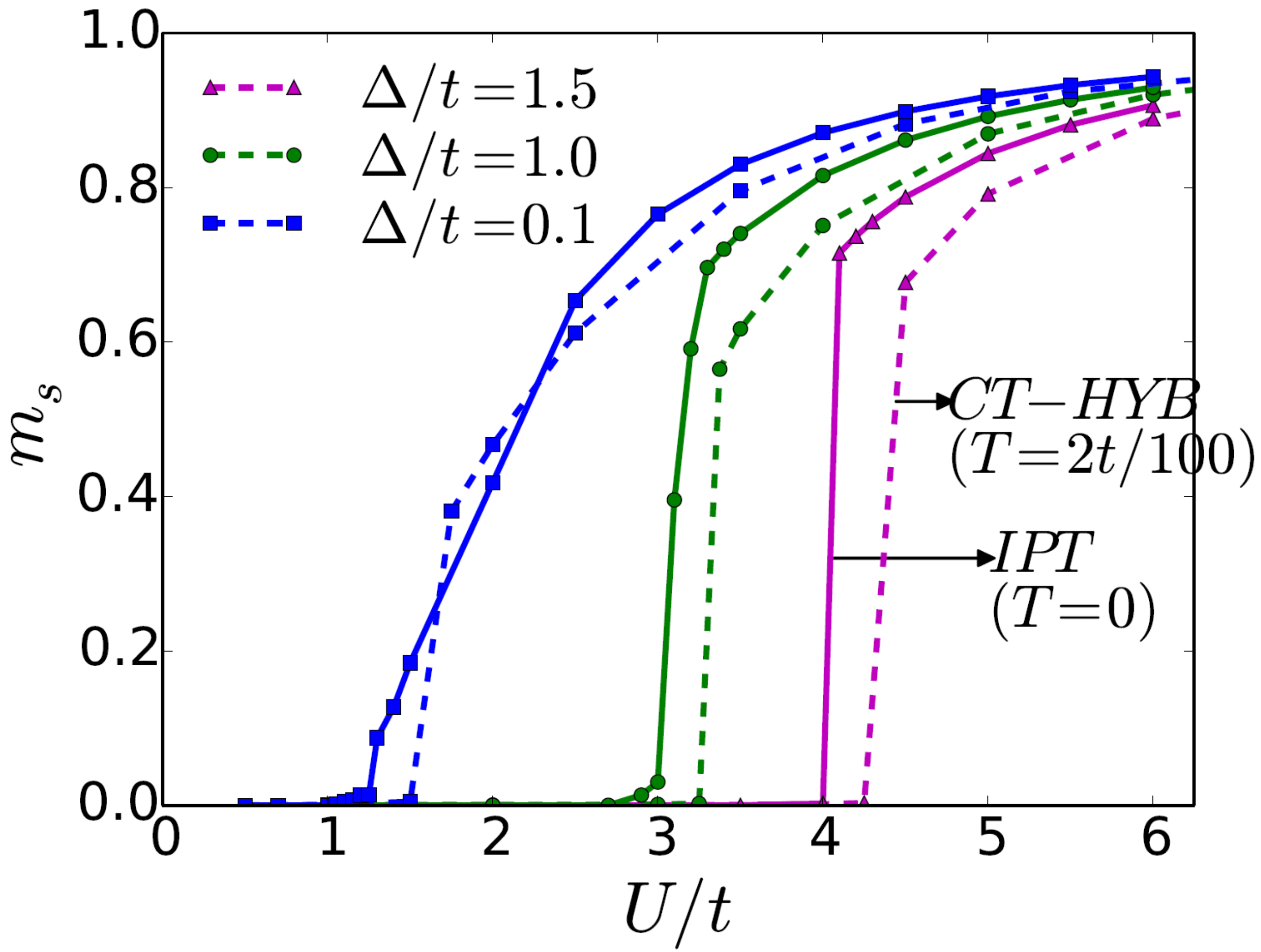
PM-BI to AFM-MI Transition preempts
the PM-BI to PM-M Transition!



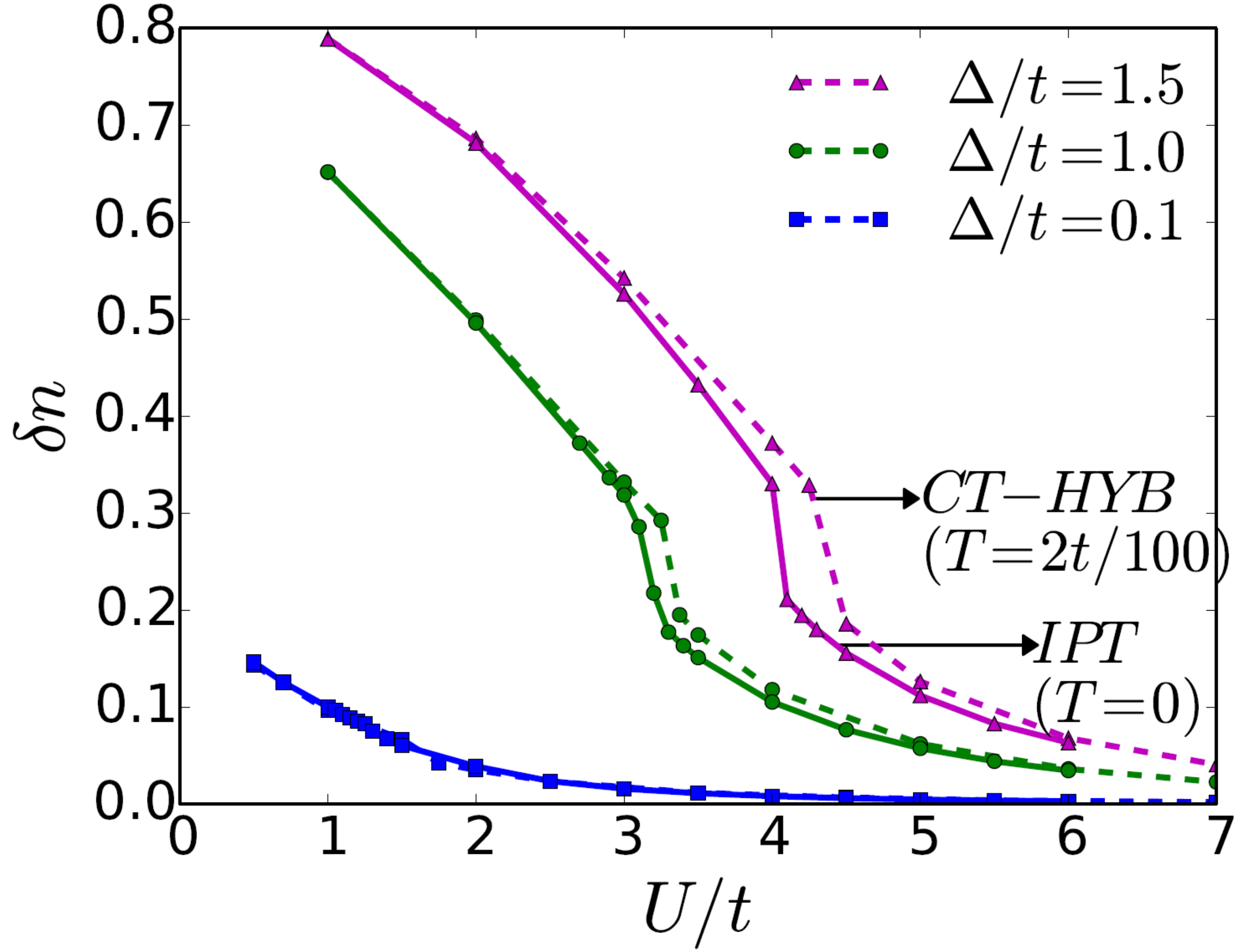


Bethe Lattice

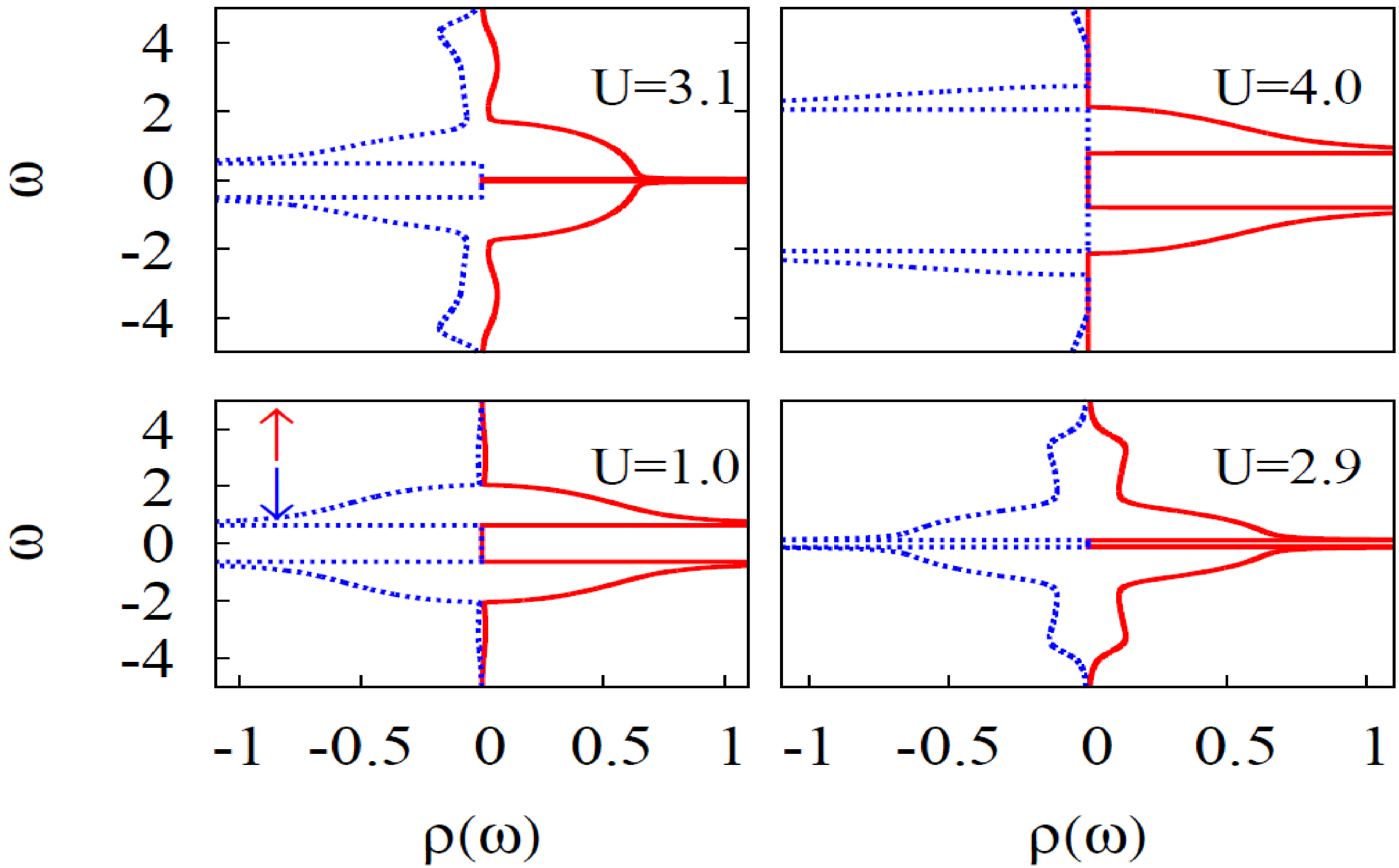
Staggered Magnetization vs. U/t for various values of Δ/t (IPT and CT-HYB)



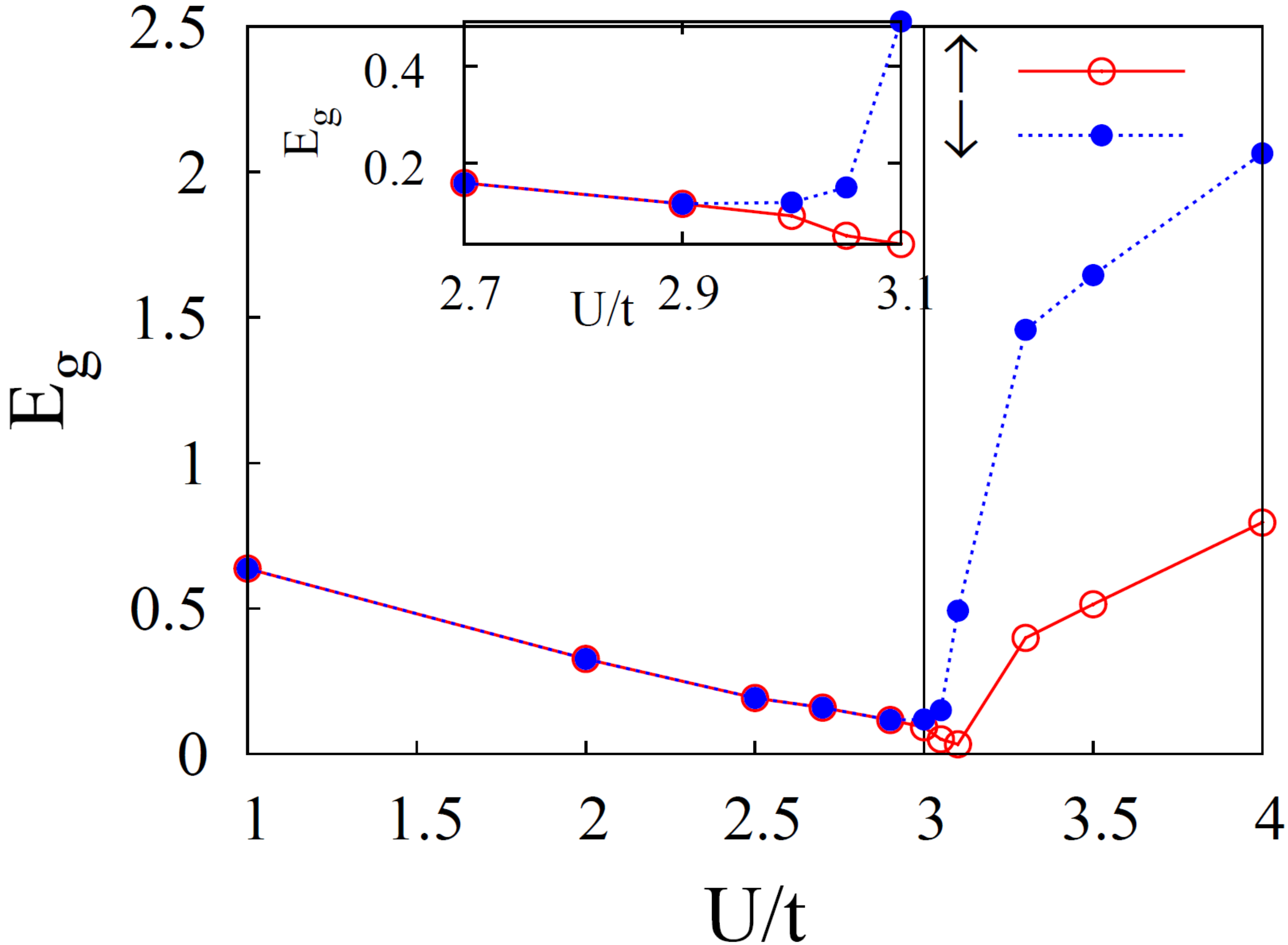
Staggered Charge versus U for various values of Δ/t (IPT and CT-HYB)



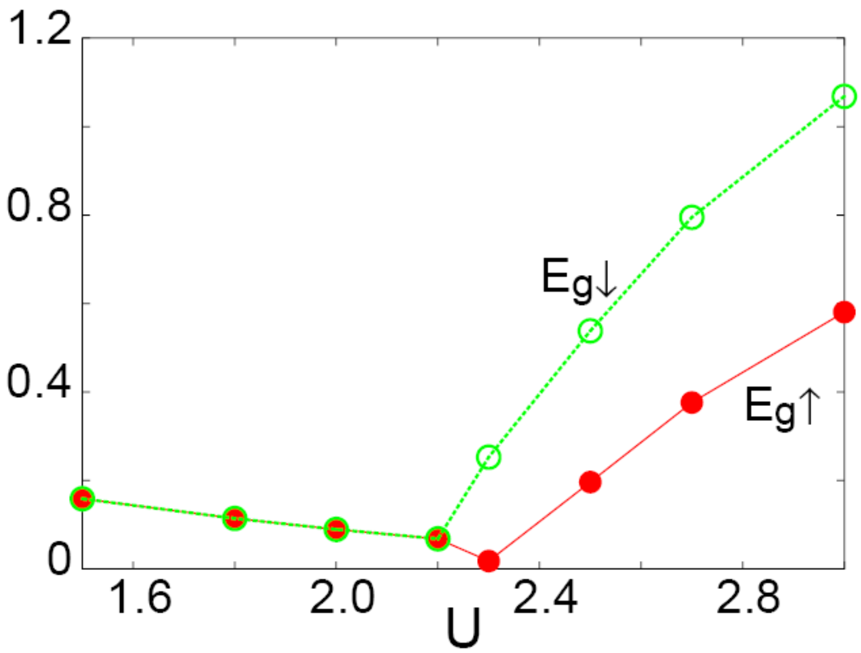
Evolution of single particle DOS with U (n=1, Δ/t = 1.0)-IPT



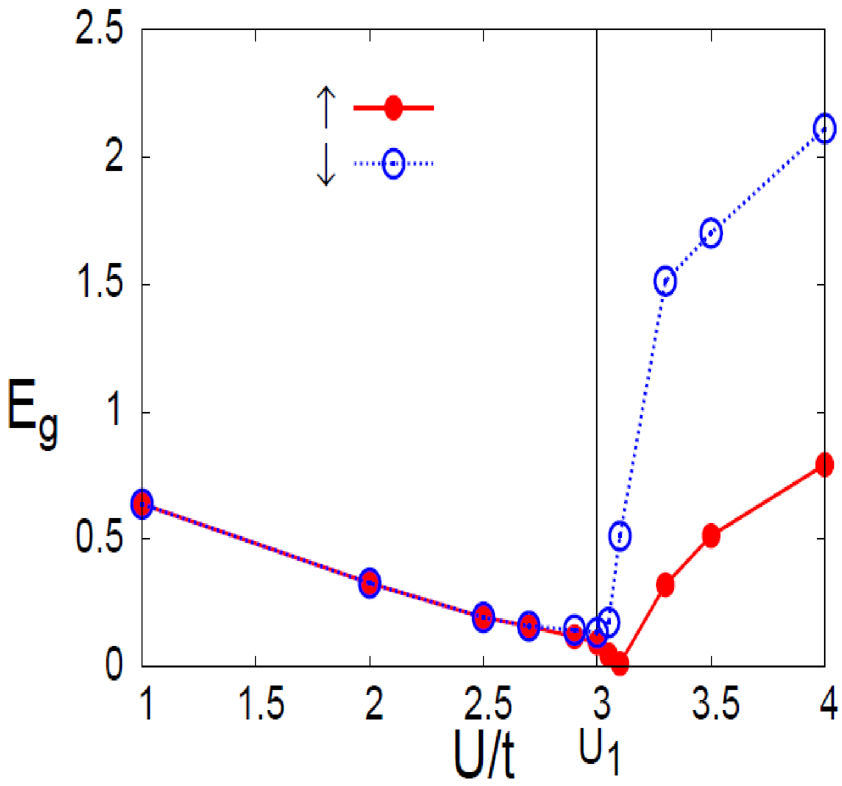
Single Particle Gaps versus U
(n=1, Δ/t = 1.0) - IPT



Single Particle Gaps versus U (n=1, IPT)



Δ/t = 0.5

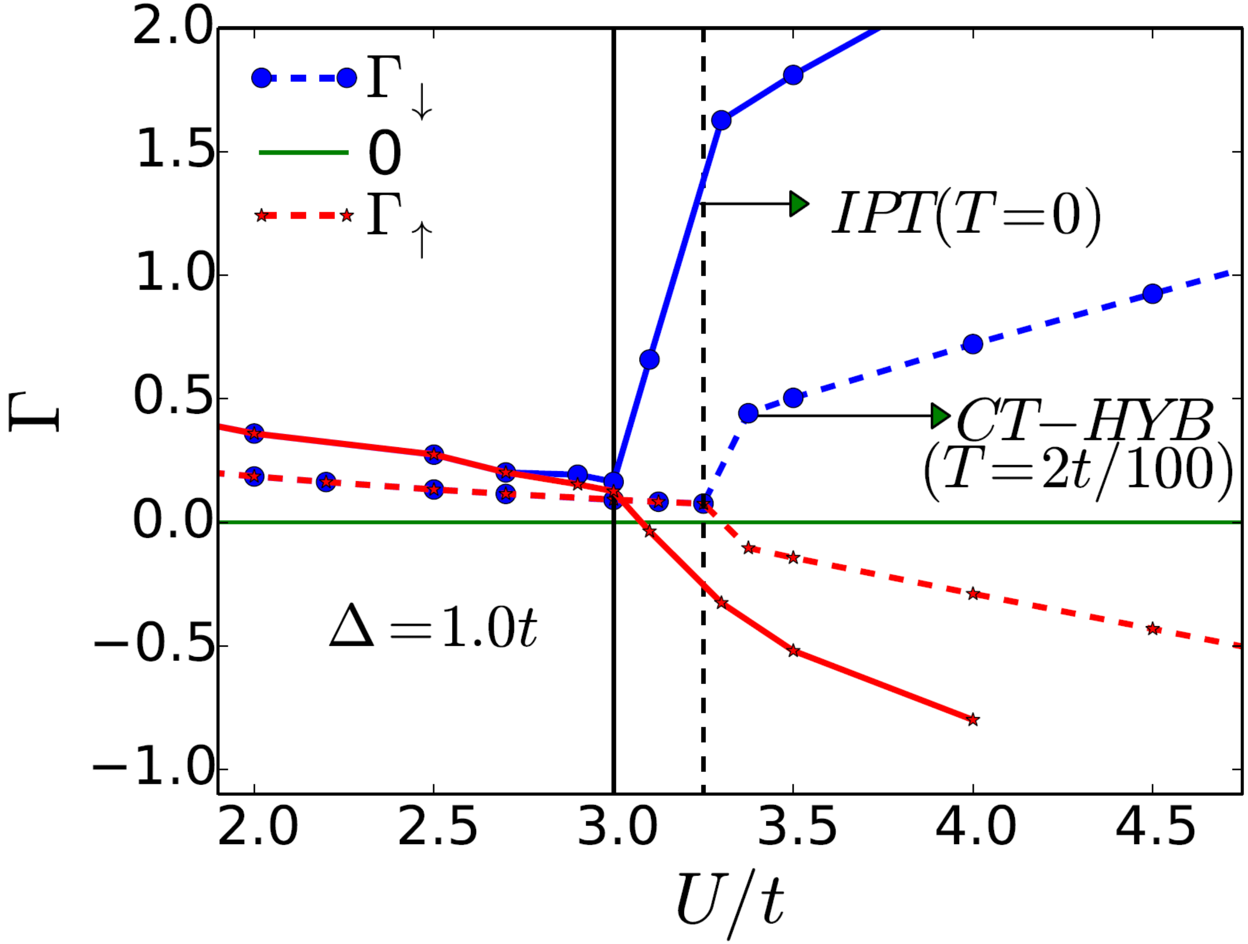


Δ/t = 1.0

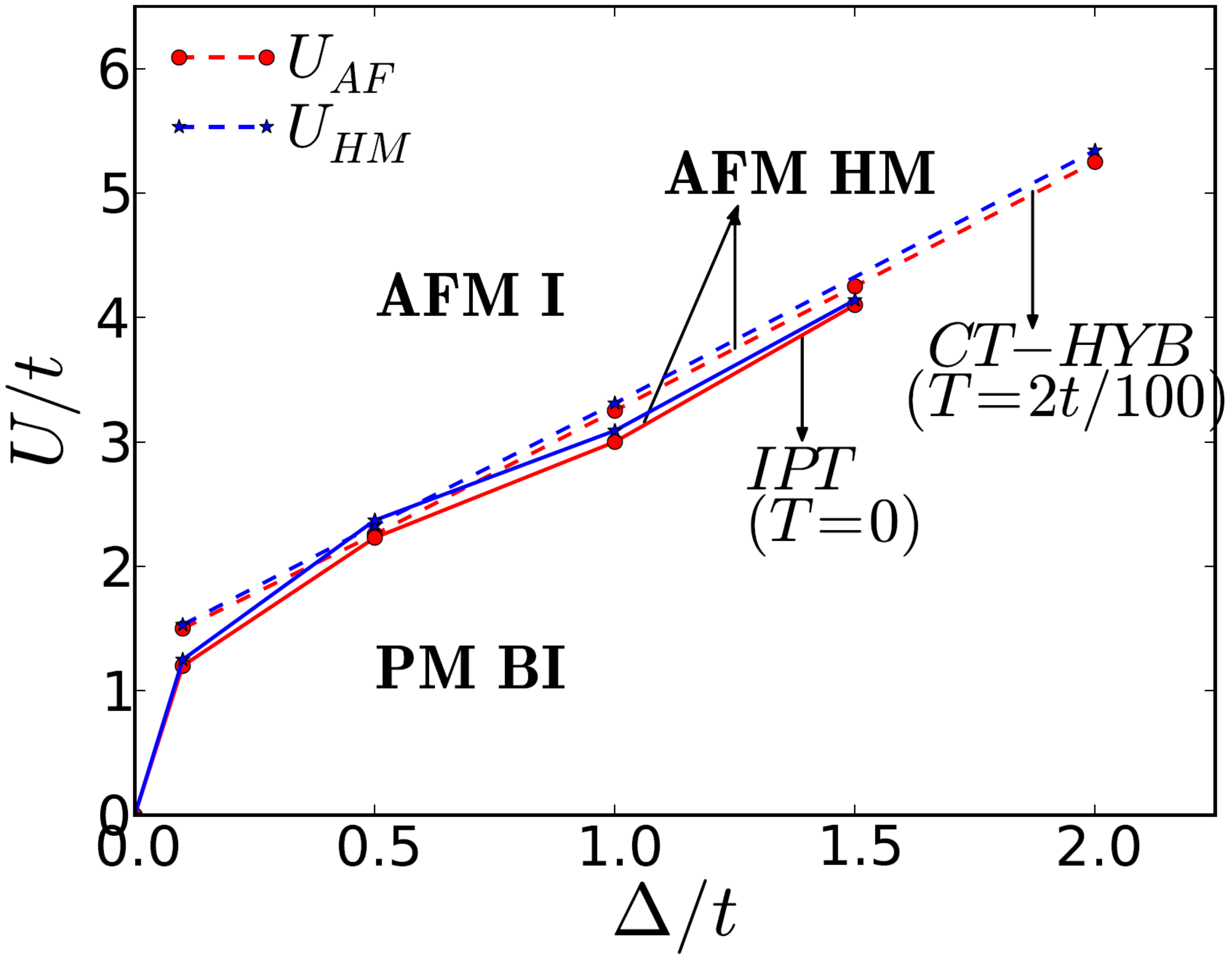
Correlation Induced Half-metal!

Low frequency analysis and the Gaps (IPT and CT-HYB)

$$E_\sigma^{gap} = Z_\sigma \left| \Delta - \frac{U(\delta n + \sigma m_s)}{2} + P \int_{-\infty}^{\infty} d\omega \frac{\Sigma''_{A\sigma}(\omega)}{\pi\omega} \right| \equiv Z_\sigma |\Gamma_\sigma|$$

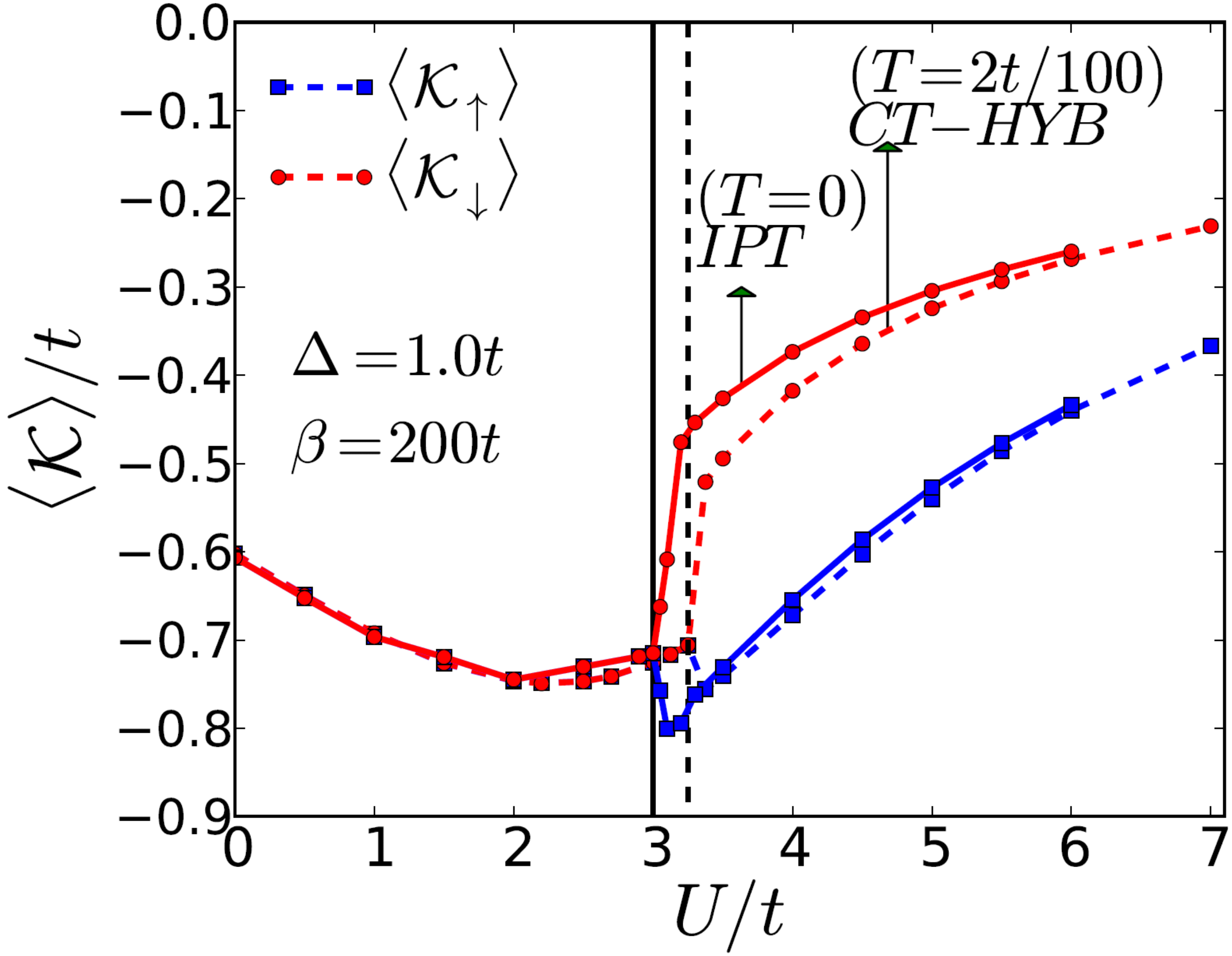


T=0 Phase Diagram of IHB at Half Filling
(Bethe Lattice, allowing for Antiferromagnetism)



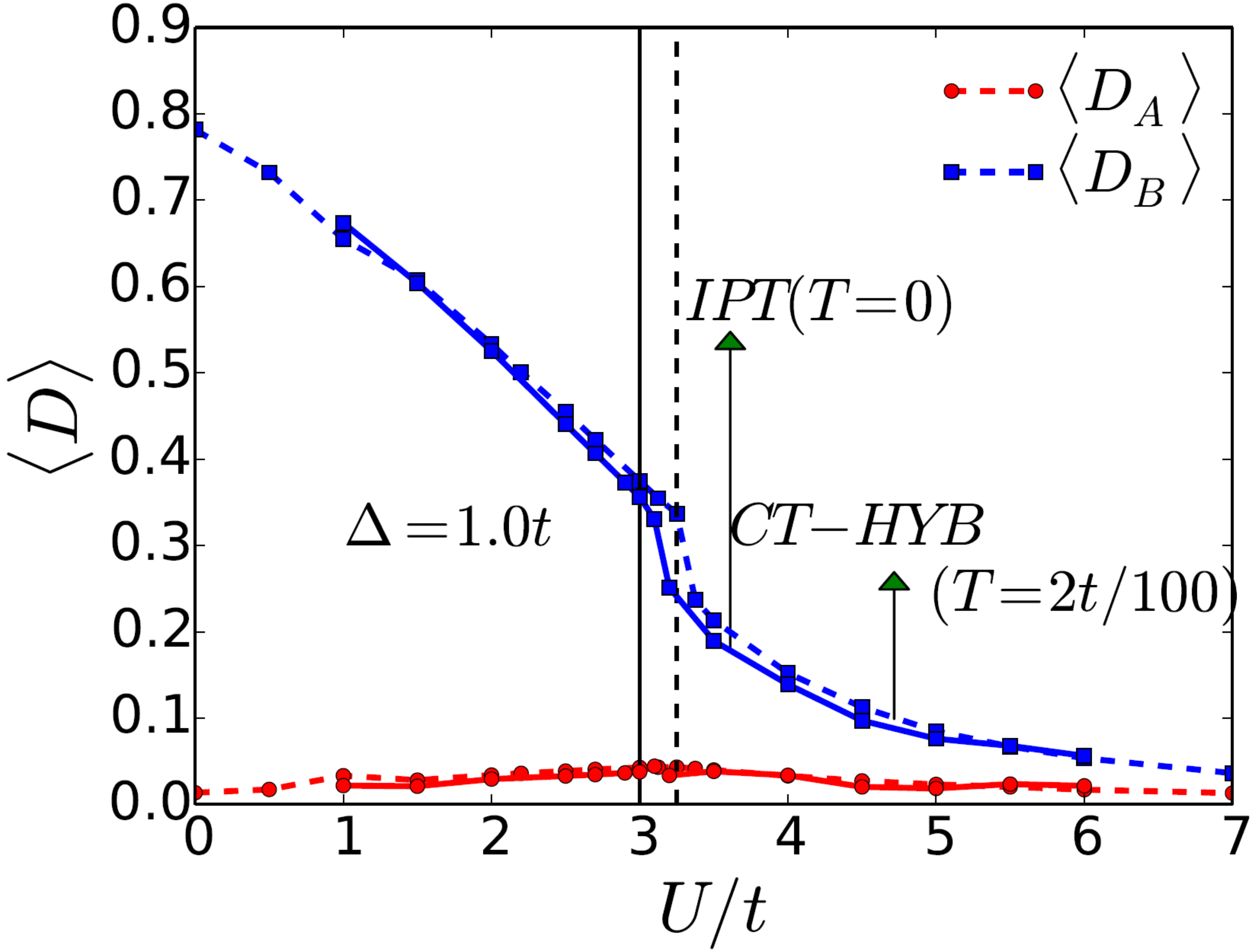
Kinetic Energies of the two spin species versus U/t (Δ/t=1.0)

$$\langle \mathrm{K}_{\sigma} \rangle = 2T \int d\text{ò}\, \rho_0(\text{ò}) \sum_{n} G^{\sigma}_{AB}(\text{ò}, i\omega_n)$$



Average Double Occupancy <D> versus U/t (Δ/t=1.0)

$$\langle D_\alpha \rangle = \langle n_{\alpha\uparrow} n_{\alpha\downarrow} \rangle = \frac{1}{2U}\left[T \sum_{n,\sigma} \mathrm{i}\omega_n G_{\alpha\sigma}(\mathrm{i}\omega_n) + \mu_\alpha n_\alpha - \langle \mathrm{K} \rangle \right]$$



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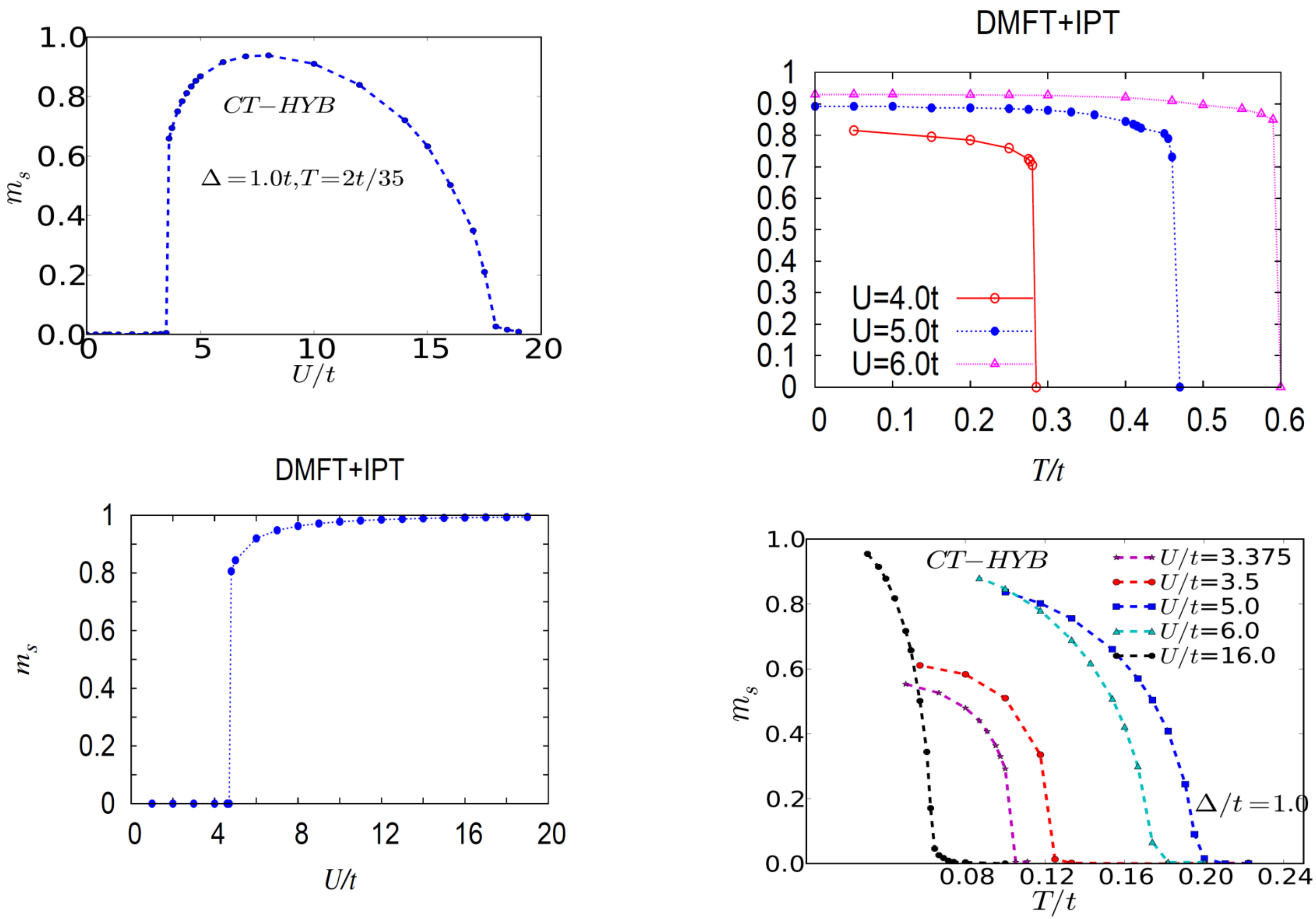
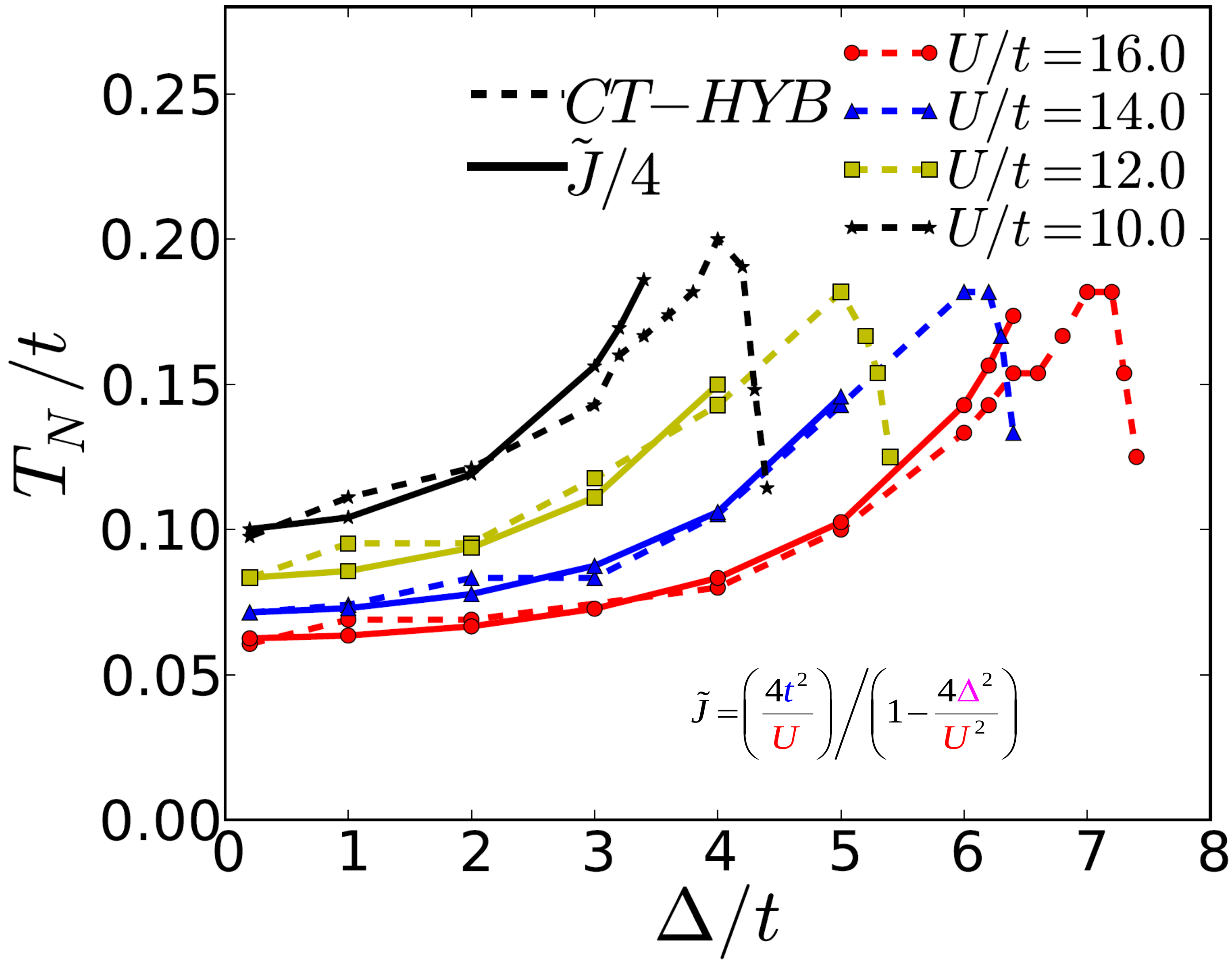
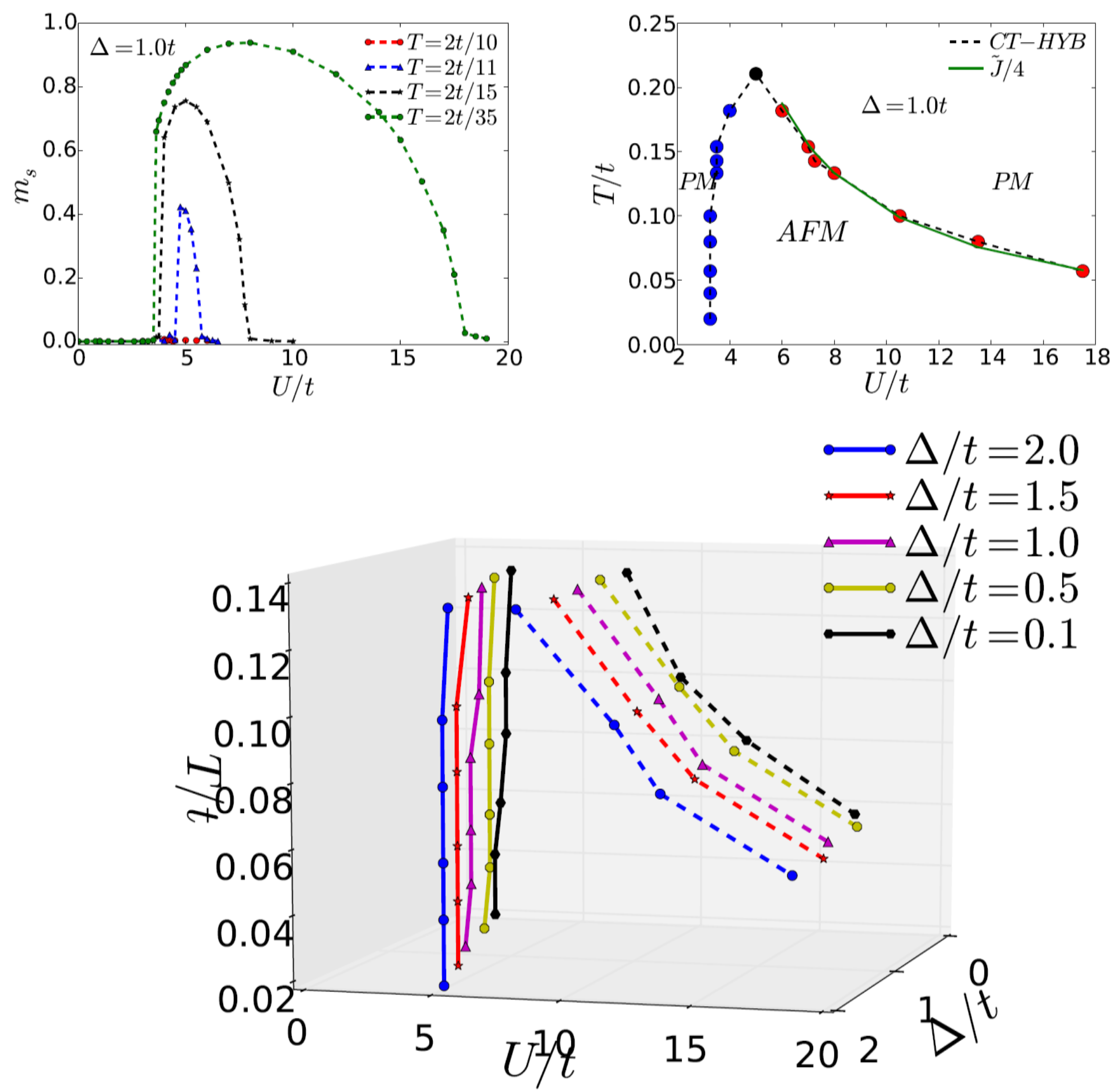
Limitations of IPT and comparison with CT-HYB for large U and finite T



AFM-PM Thermal Transitions



$T \neq 0$ Phase Diagram of IHB at Half Filling (Bethe Lattice, permitting Antiferromagnetism, CTQMC)



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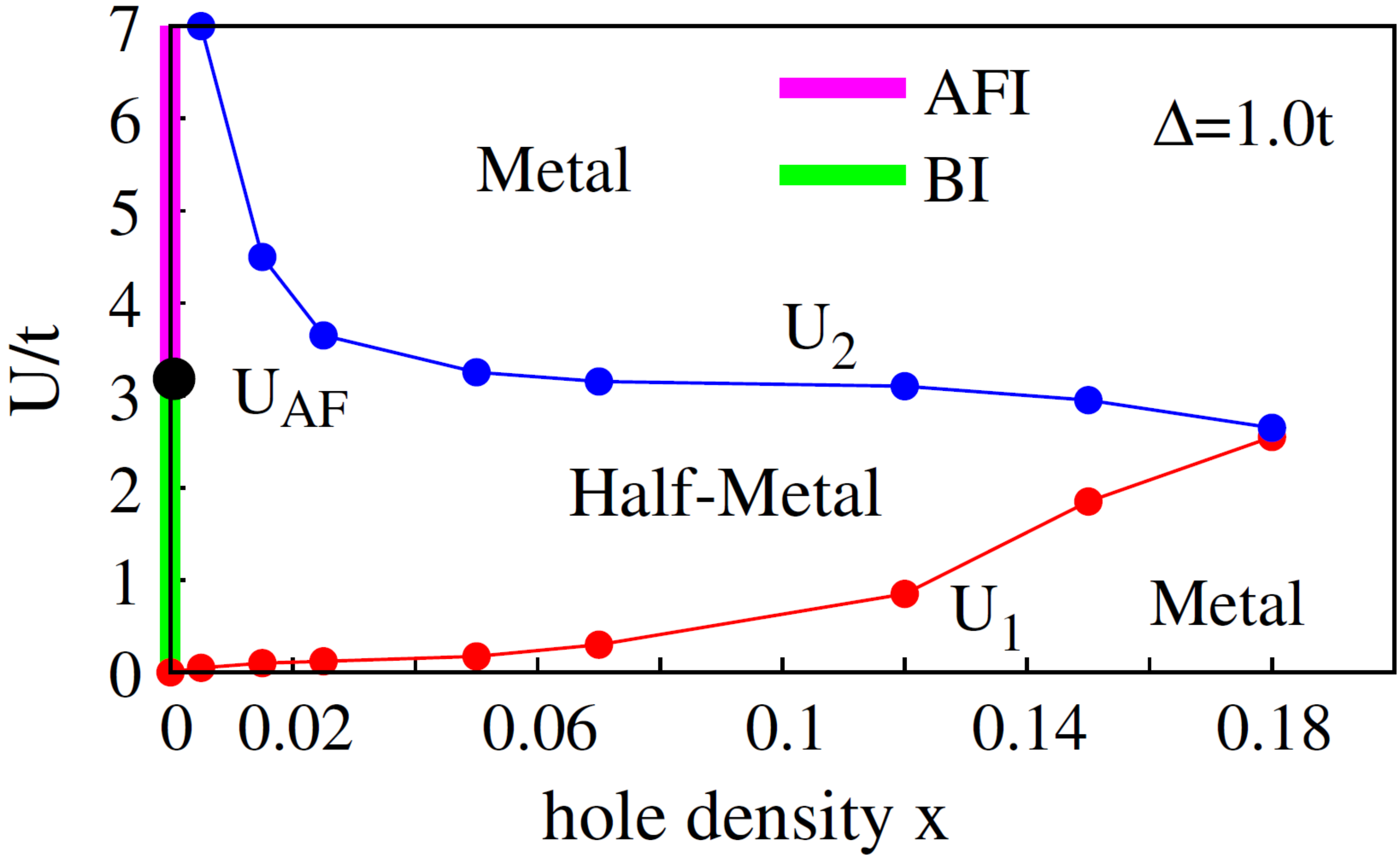
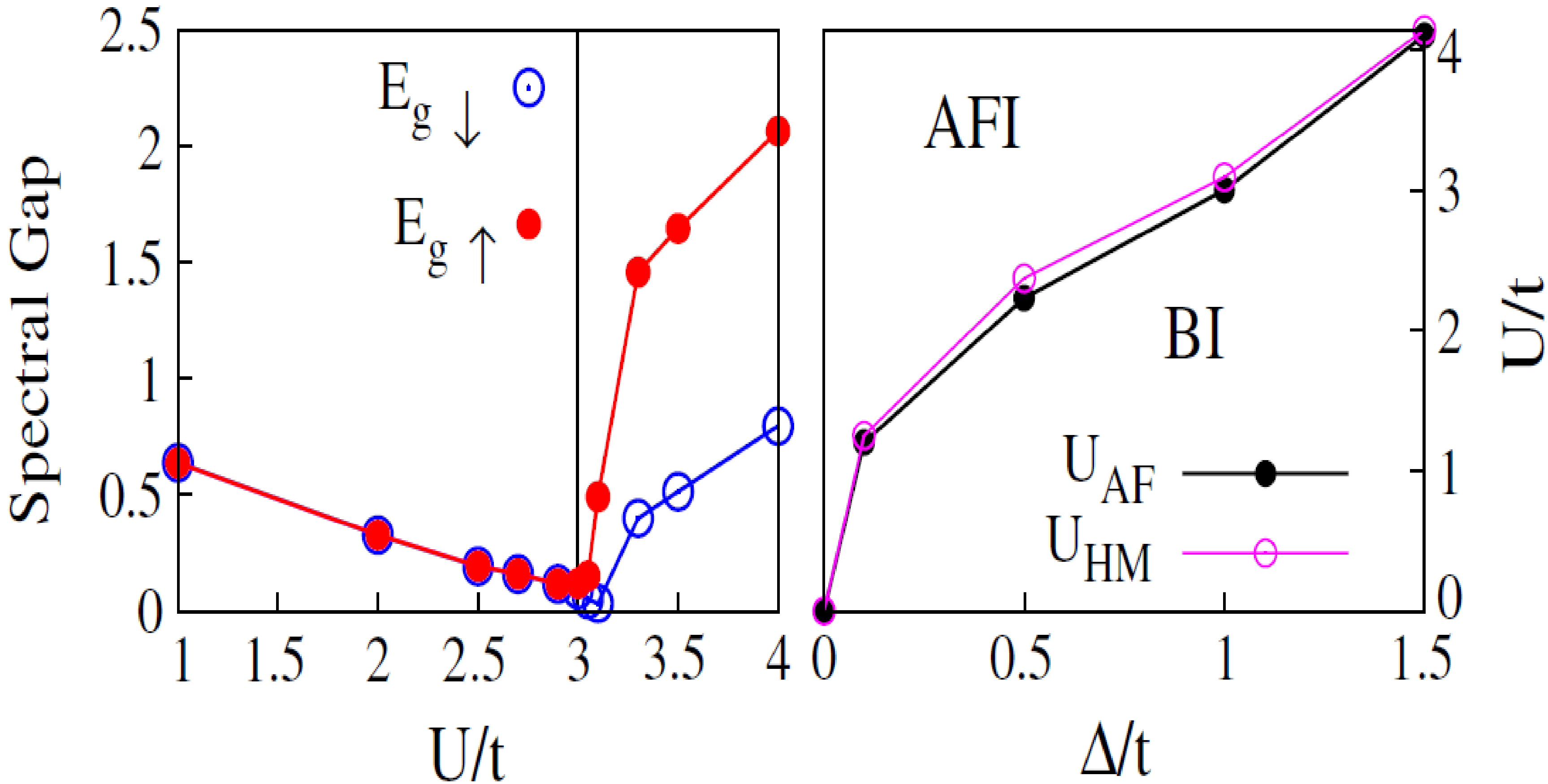
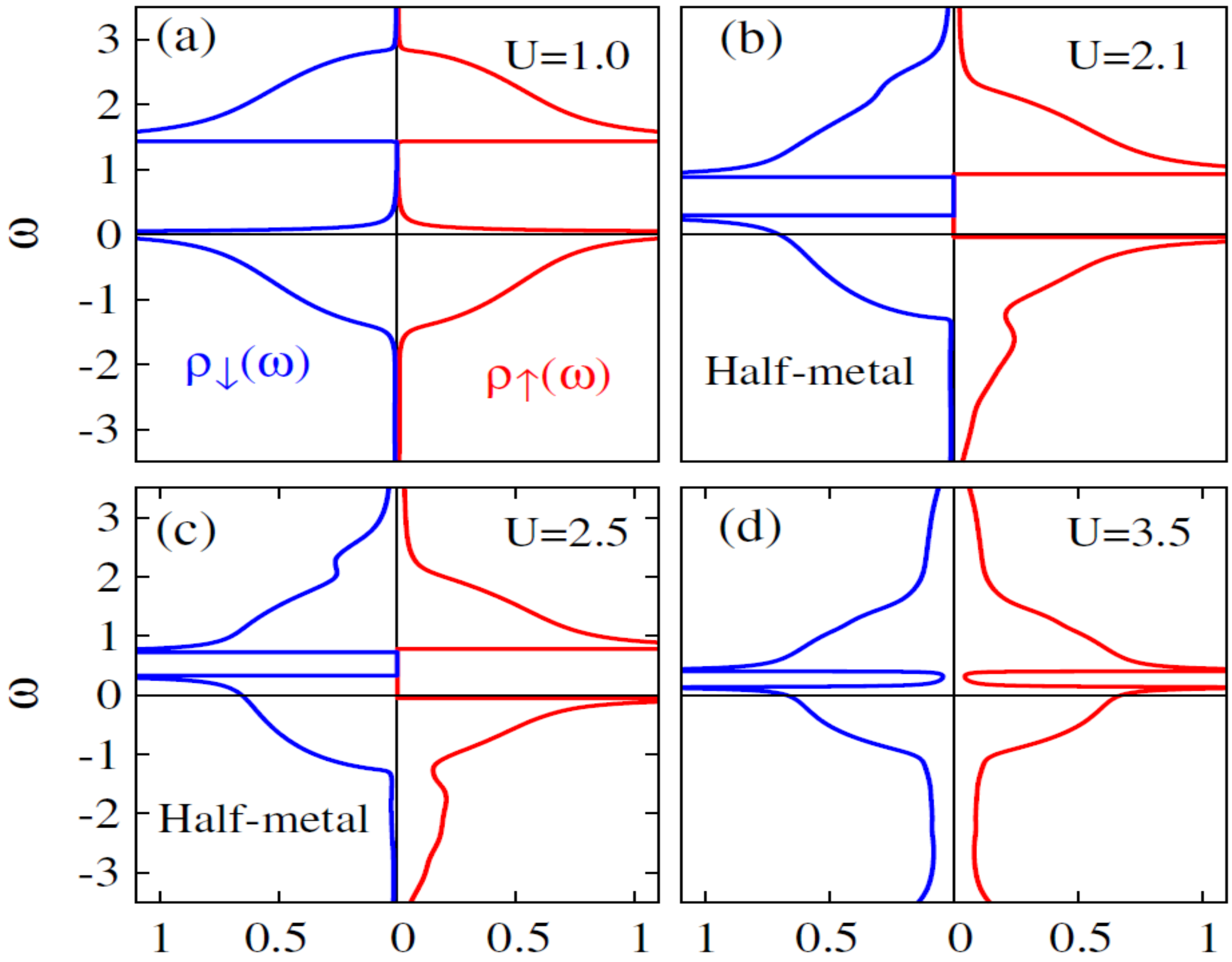
Phase diagram with doping



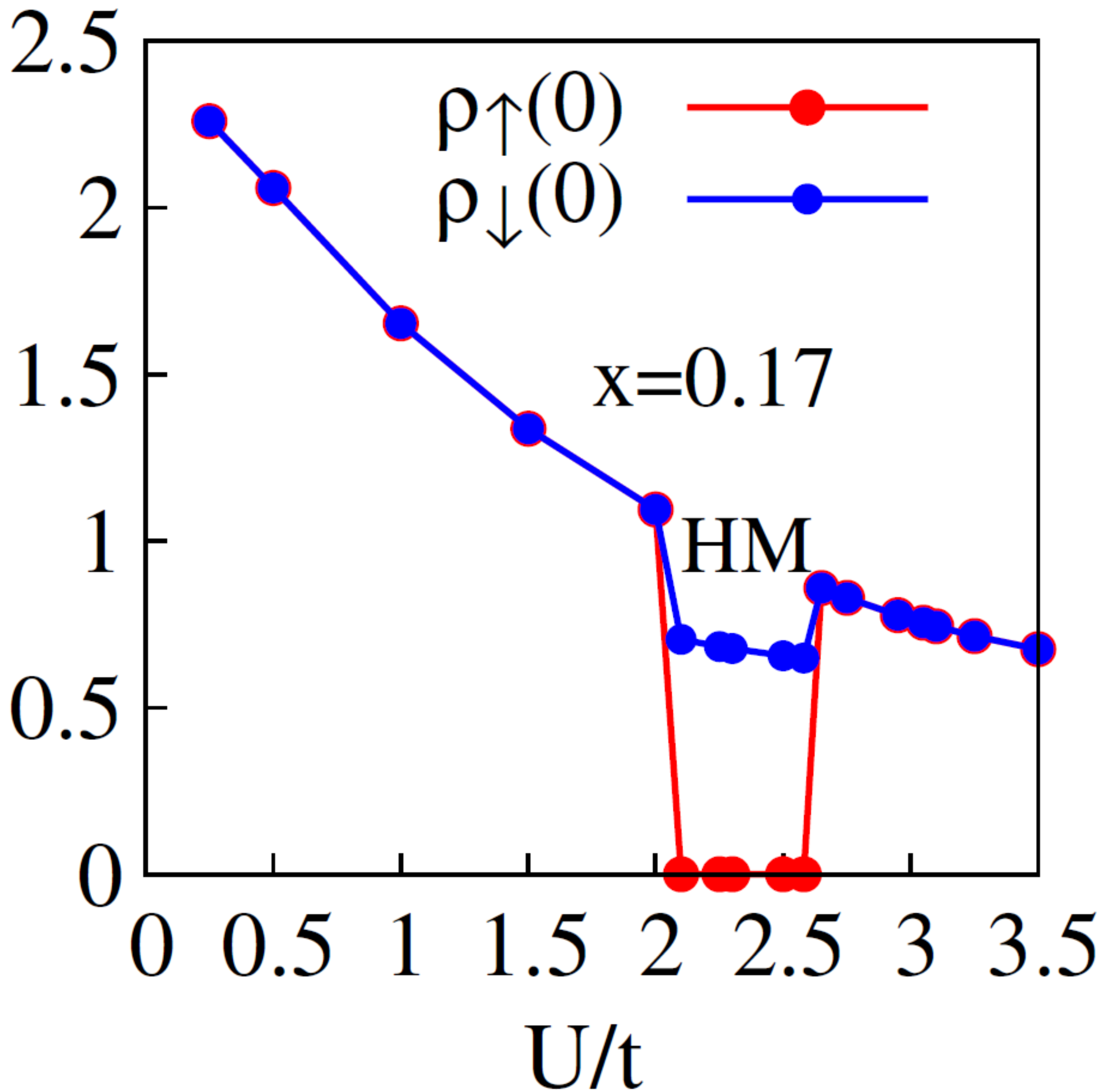
Evolution of spin gaps and half-metallicity in the half-filled IHB



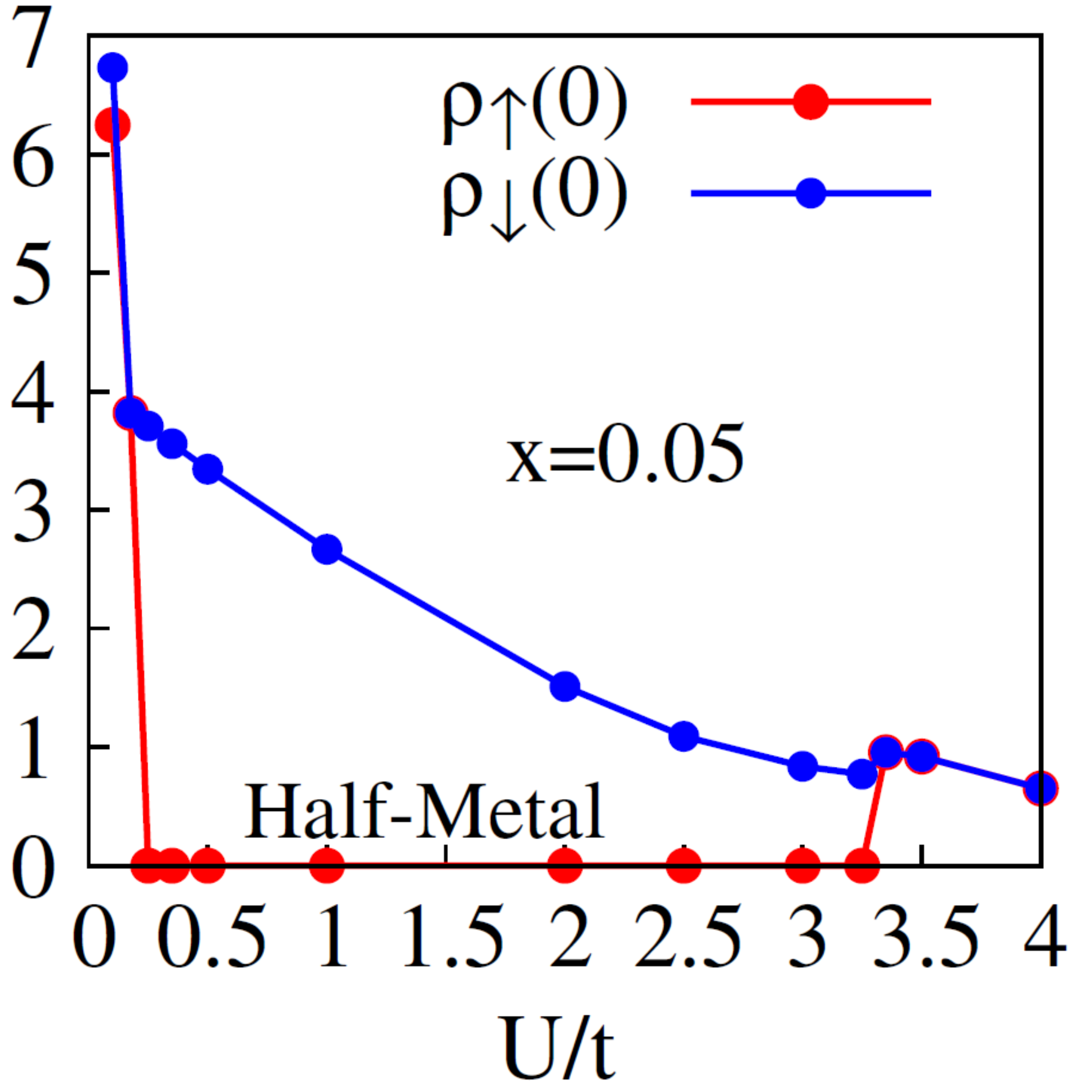
Spin Resolved DOS of hole-doped IHB for x=0.17 and Δ/t = 1.0



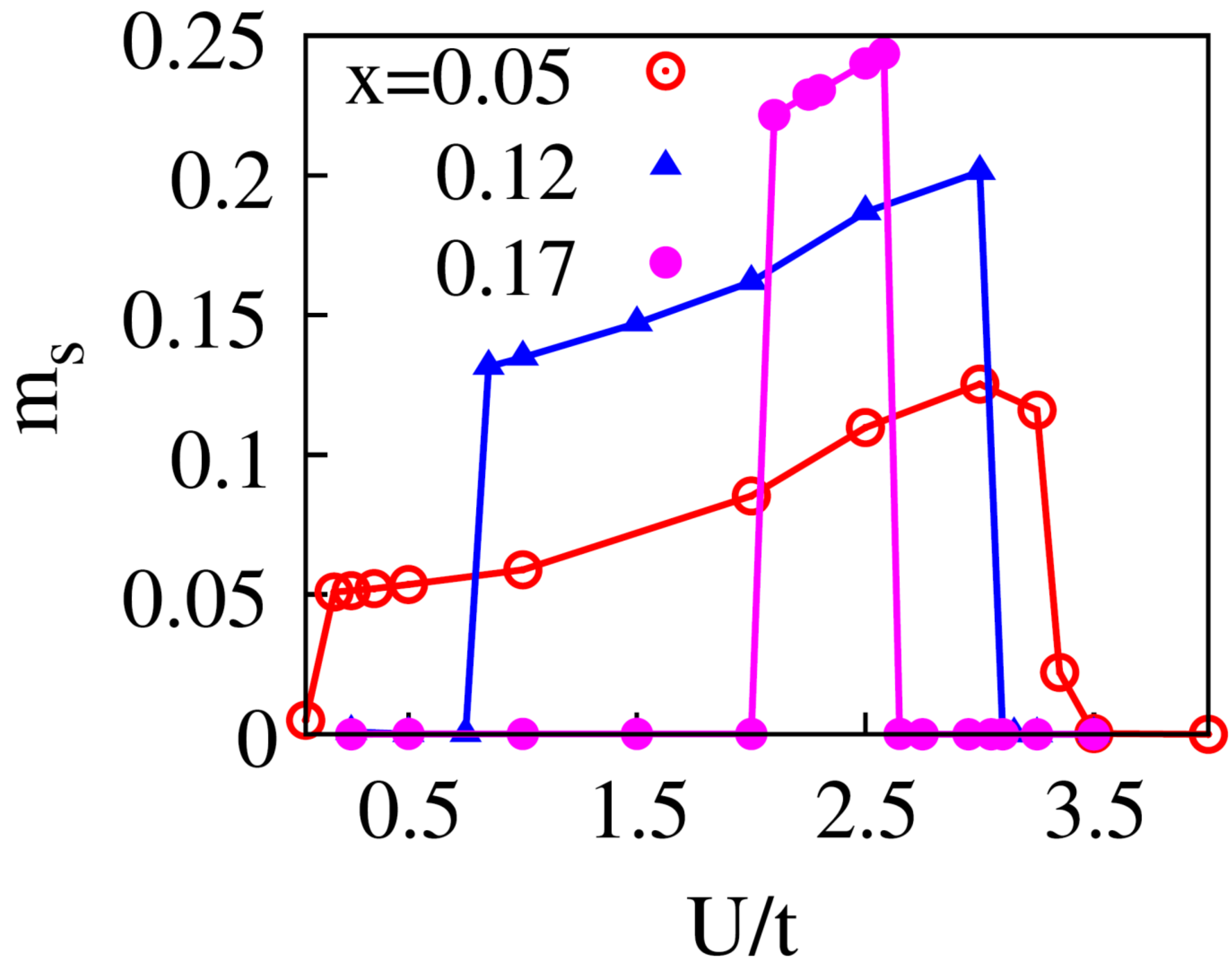
Single Particle DOS vs. U ($\Delta/t = 1.0$)



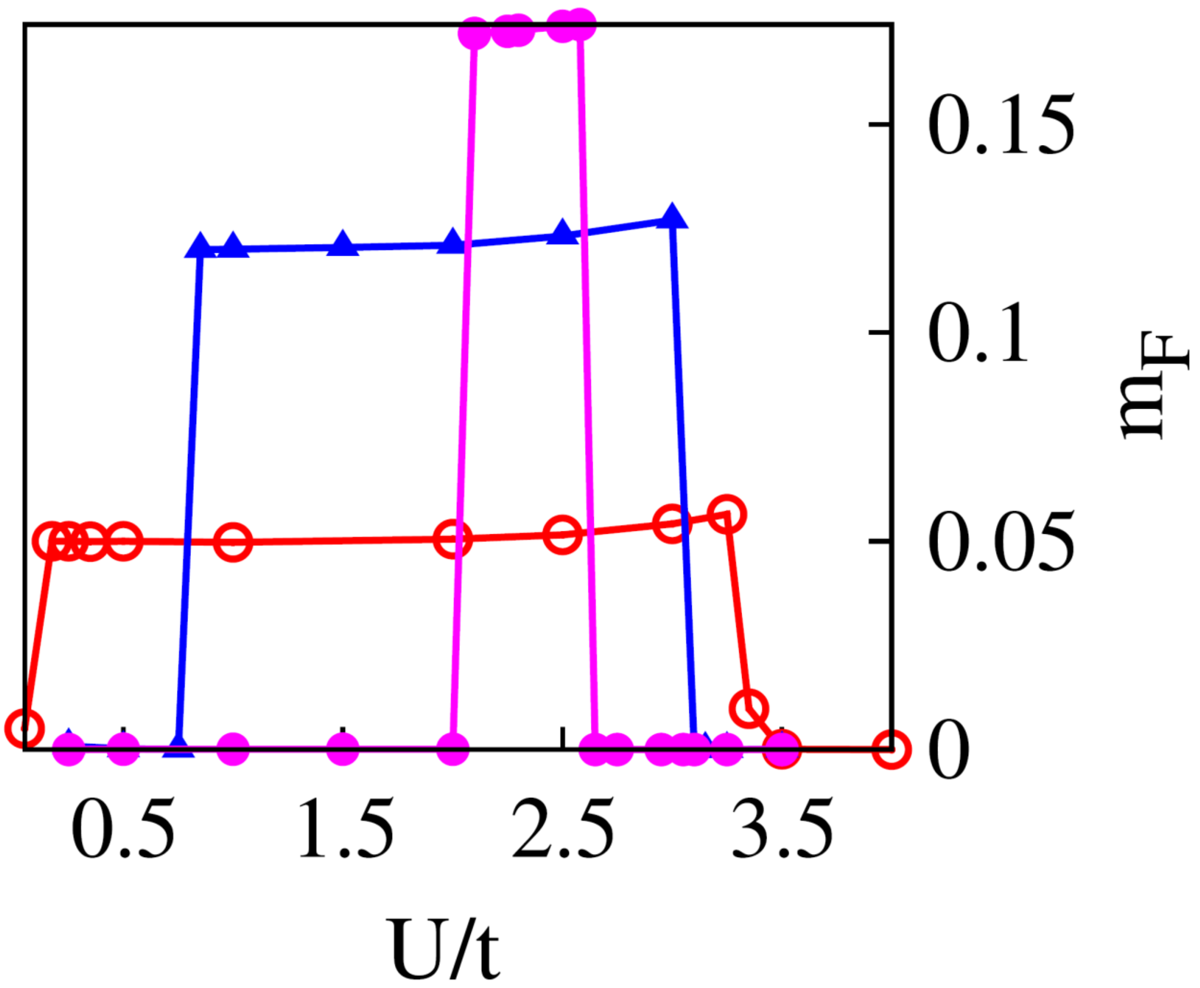
Single Particle DOS vs. U ($\Delta/t = 1.0$)



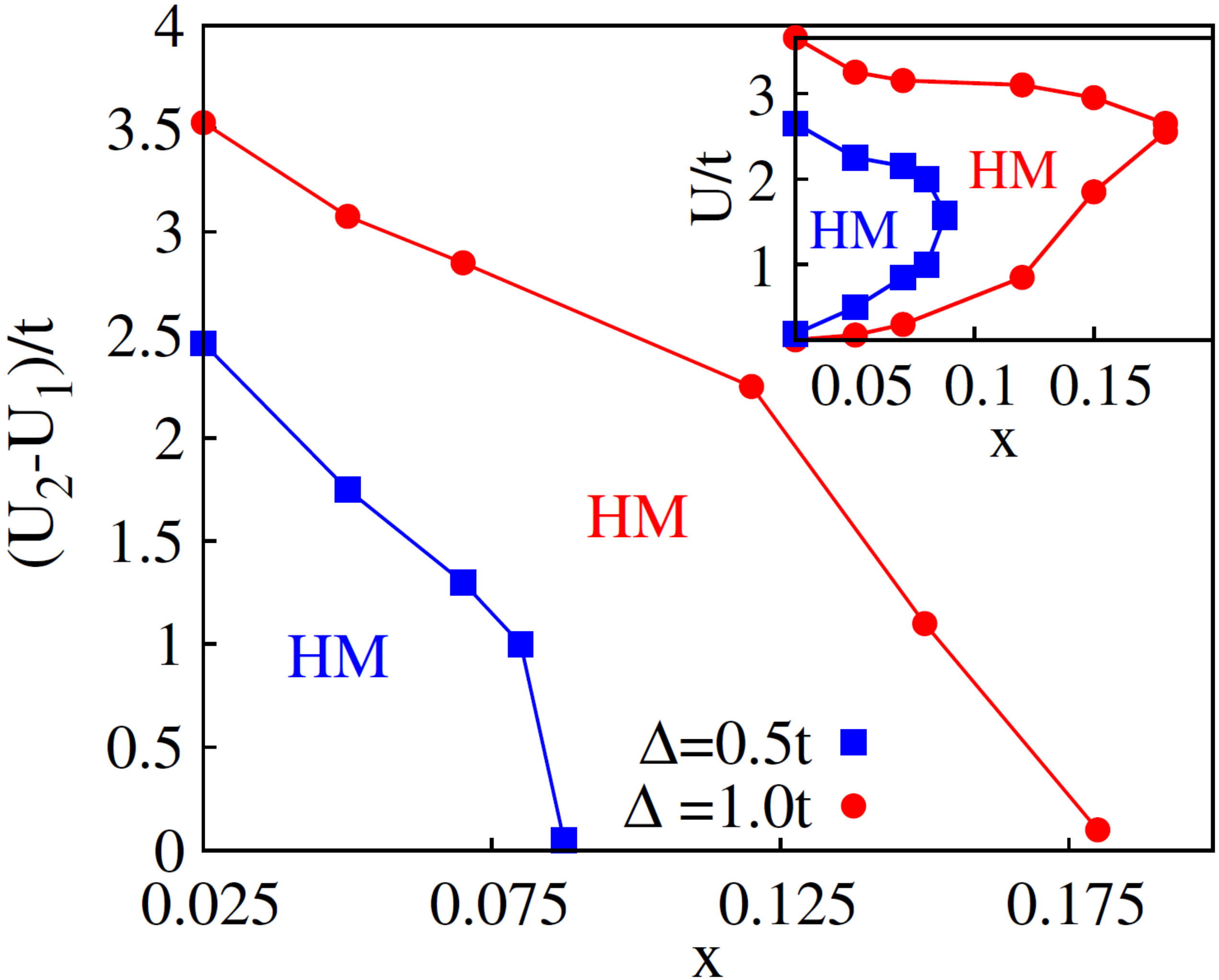
Staggered magnetization vs. U (Δ/t = 1.0) for different values of filling



Net magnetization vs. U ($\Delta/t = 1.0$) for different values of filling



Half metal phase shrinks with increasing doping or decreasing bandgap



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  - Model with frustration-DMFT+CT-HYB-QMC
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  - Quenching in the IHM
- Concluding Comments – Is it for Real?

Ionic Hubbard Model with Frustration

$$H = -\sum_{\langle ij \rangle} t_{ij}\, \hat{a}^{+}_{i\sigma} \hat{a}_{j\sigma} + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

$$+ \Delta \sum_{i \in A} \hat{n}_i - \Delta \sum_{i \in B} \hat{n}_i - \mu \sum_i \hat{n}_i$$

$t - t'$ IHM : $t_{ij} = t$ for *nn* sites

t' for *nnn* sites

"half filling" $\Leftrightarrow$ $\langle \hat{n}_A \rangle + \langle \hat{n}_B \rangle = 2$

For large U, this maps to a Heisenberg model with frustration

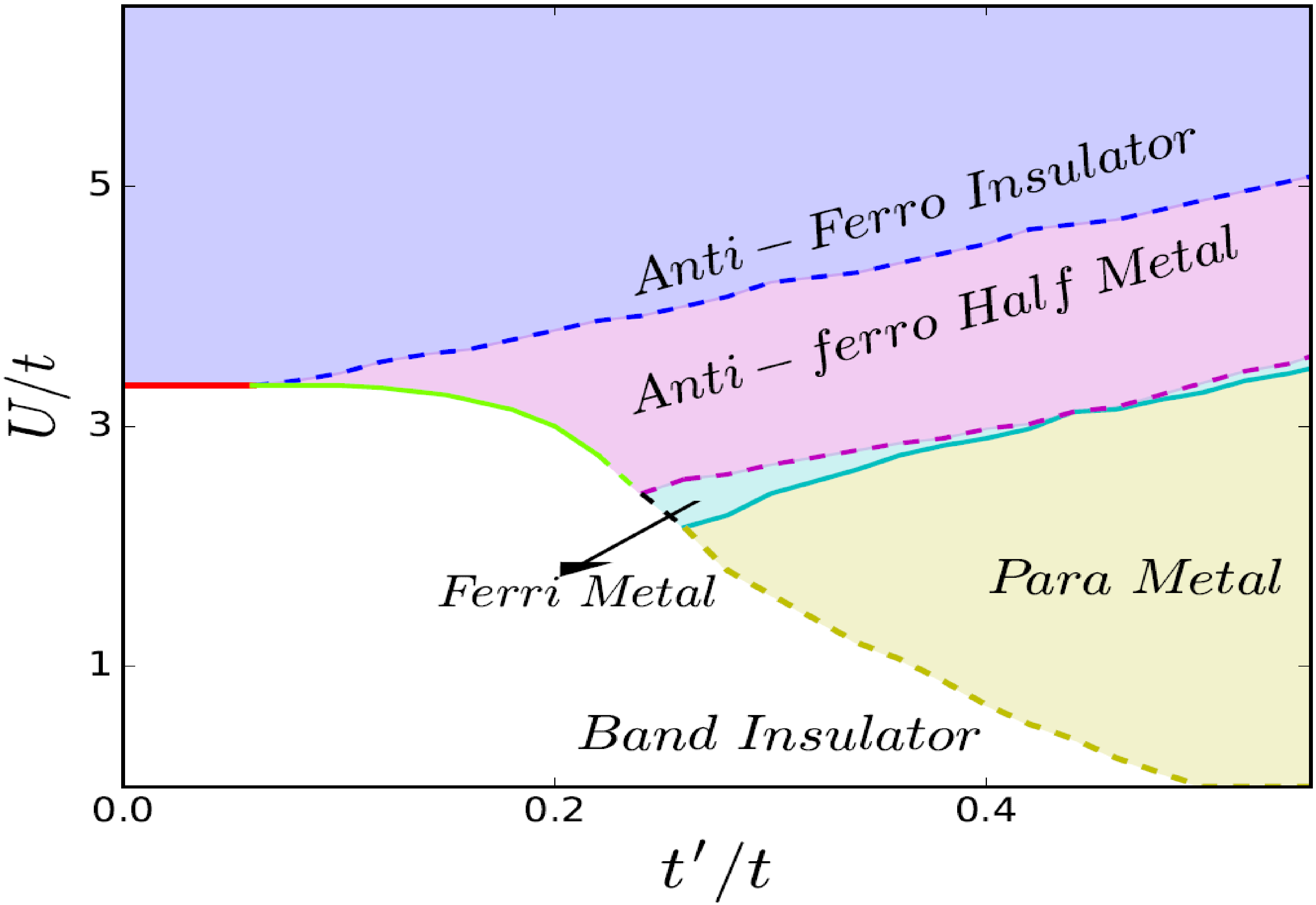
$$H = \sum_{ij} J_{ij}\, \vec{S}_i \cdot \vec{S}_j$$

$J_{ij} = J = 4t^2/U$ for *nn* sites

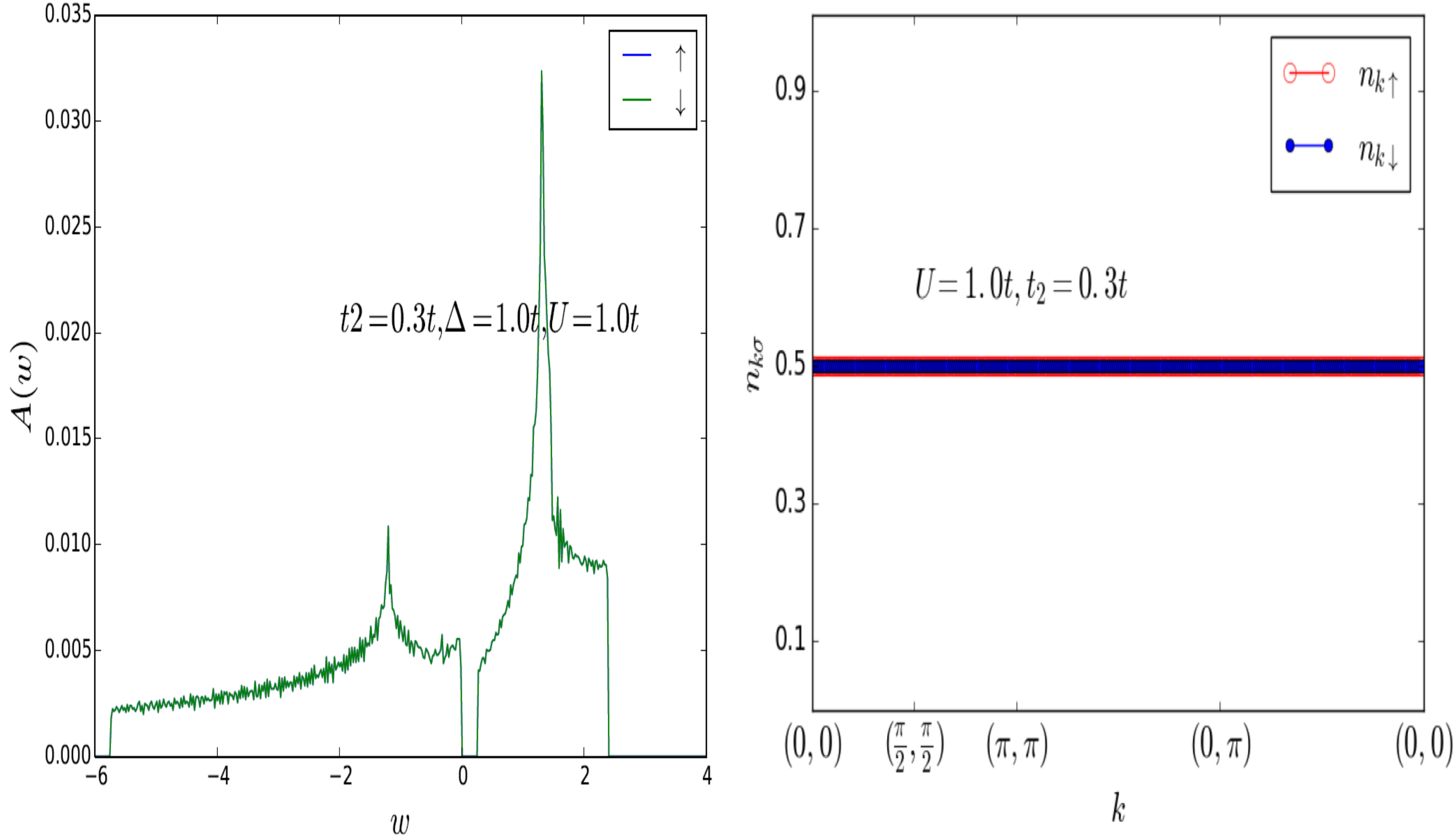
$J' = 4t'^2/U$ for *nnn* sites

Can this suppress AFM enough to allow formation of PMM phase?

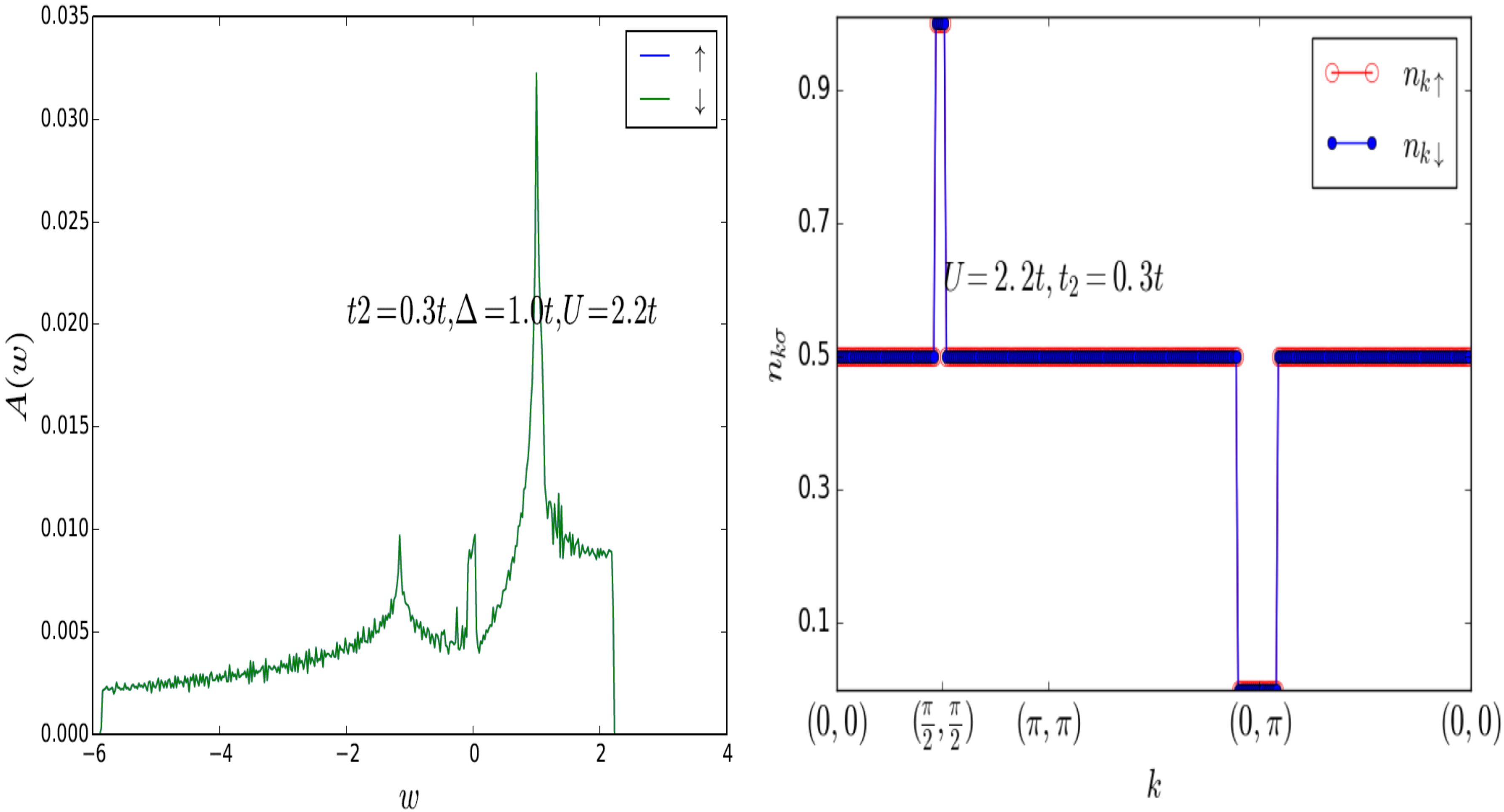
$t - t'$- U - Δ IHB at Half-filling
Unrestricted Hartree-Fock (UHF) Phase Diagram



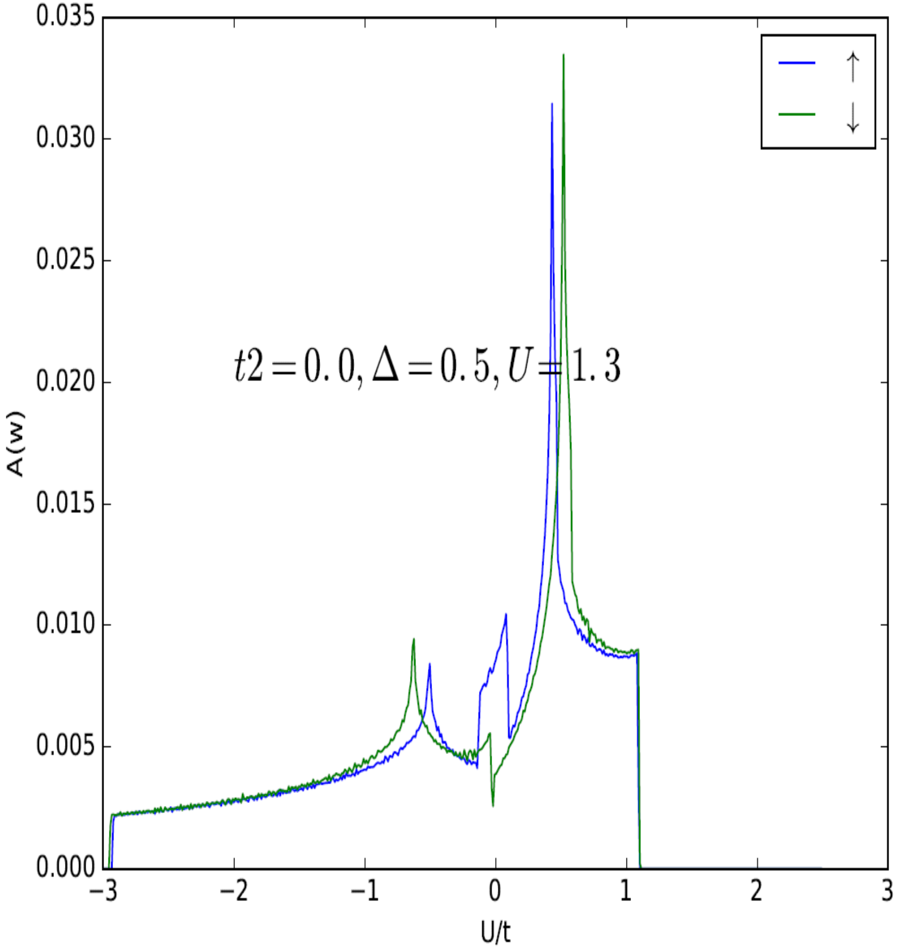
Evolution of (UHF) Spectral and Momentum distribution functions with U: Band Insulator

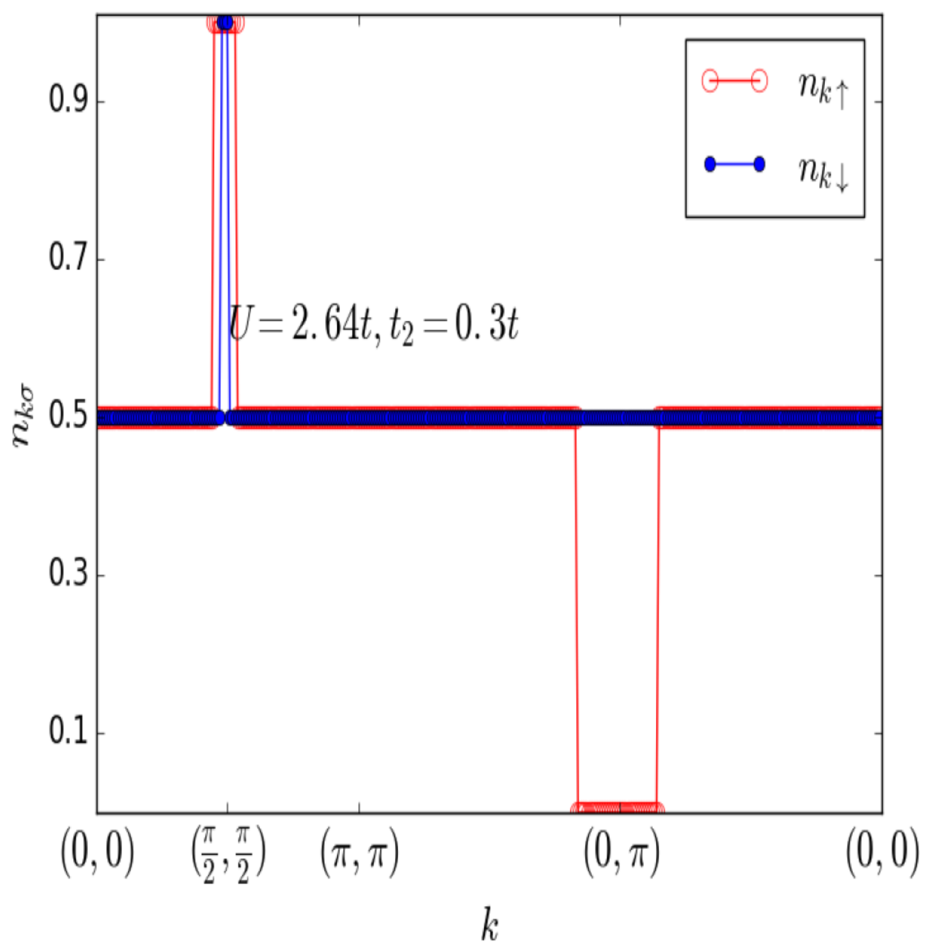


Evolution of (UHF) Spectral and Momentum distribution functions with U: Paramagnetic metal

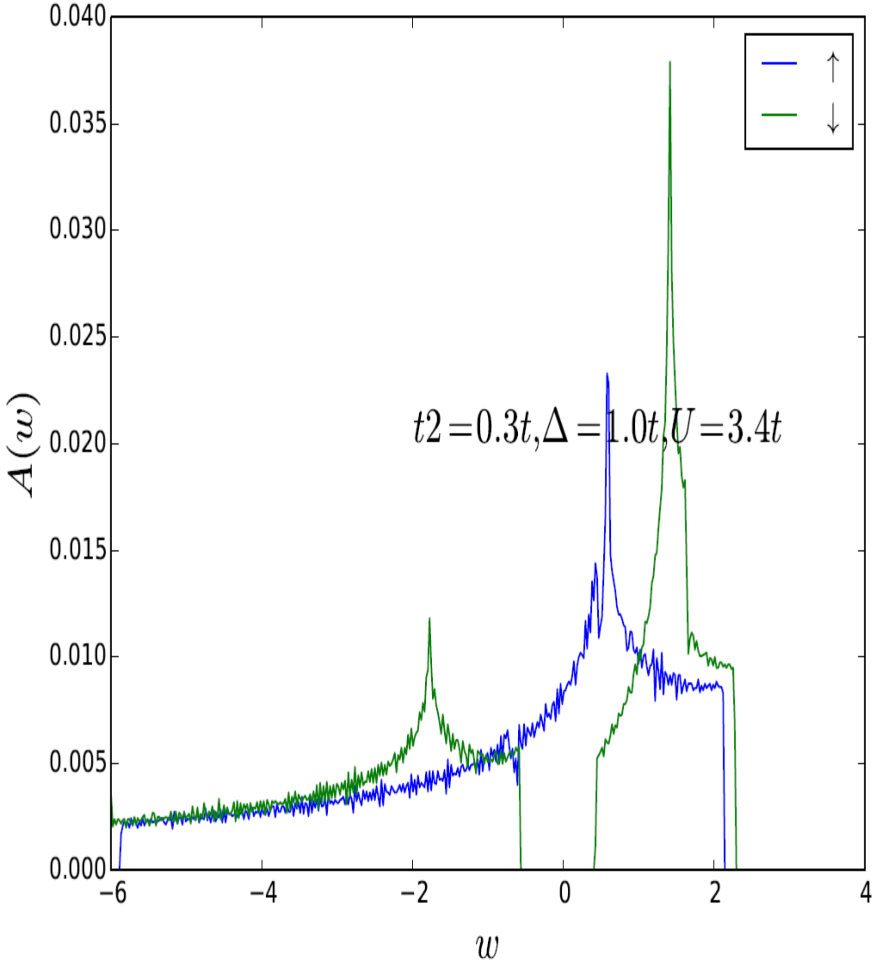


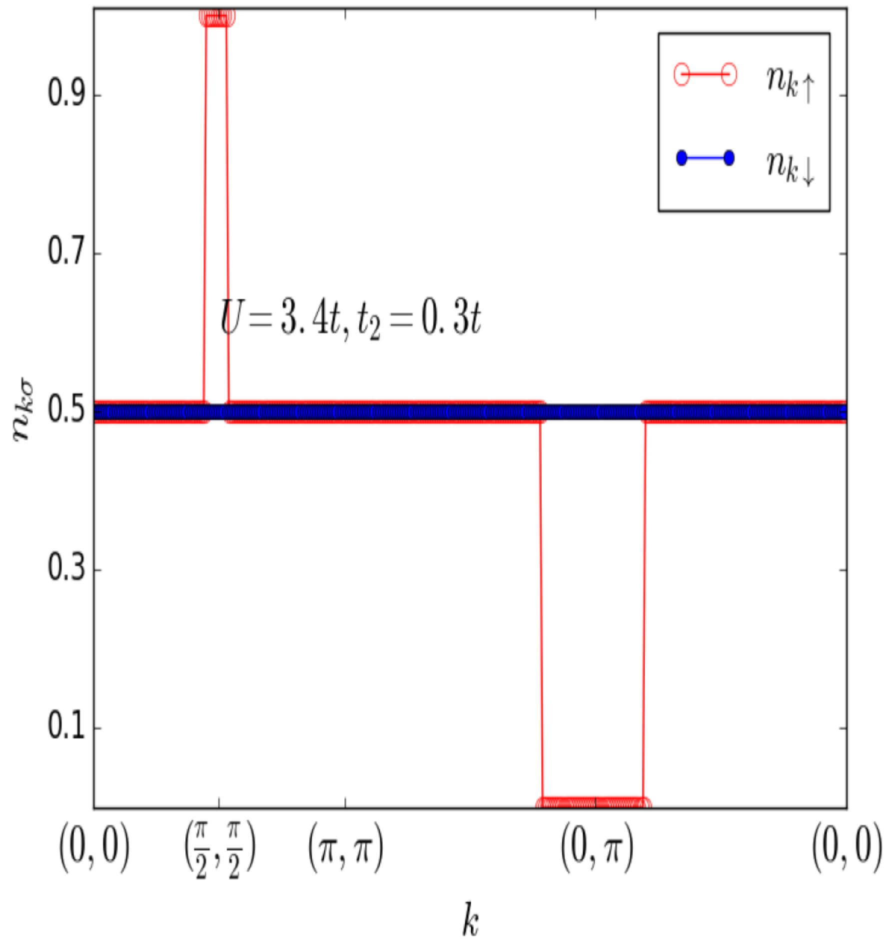
Evolution of (UHF) Spectral and Momentum distribution functions with U: Ferri-magnetic metal



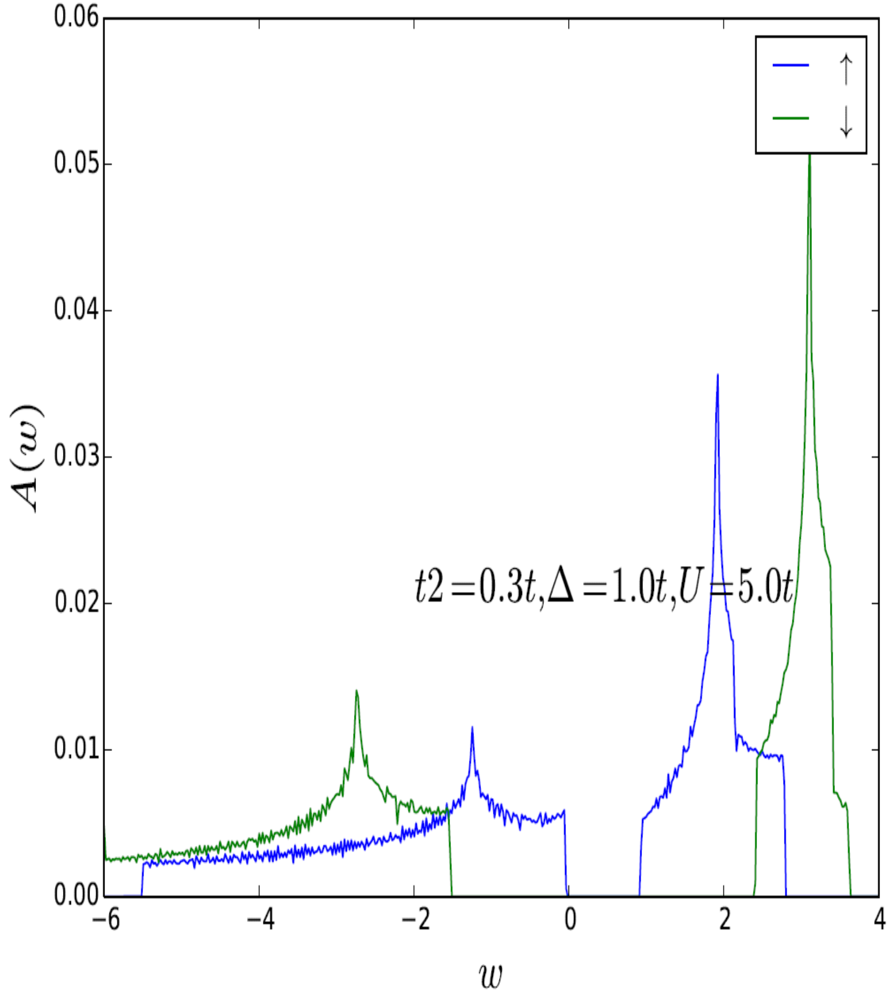


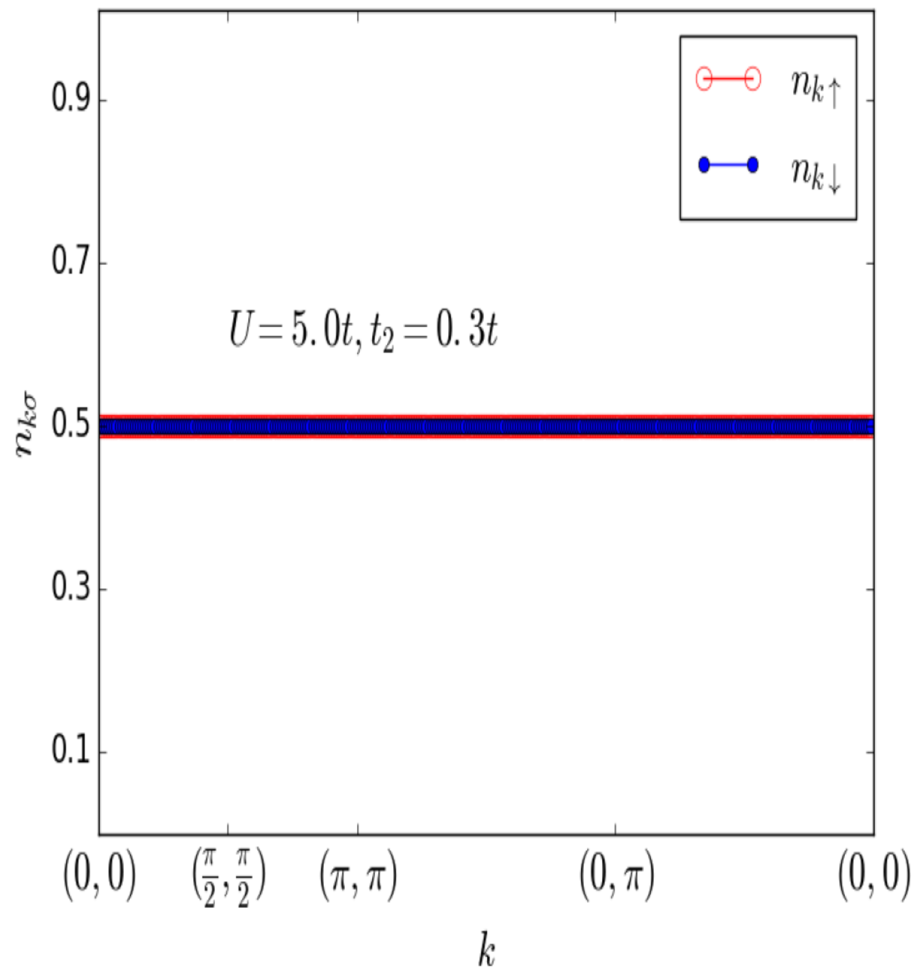
Evolution of (UHF) Spectral and Momentum distribution functions with U: Antiferromagnetic Half metal



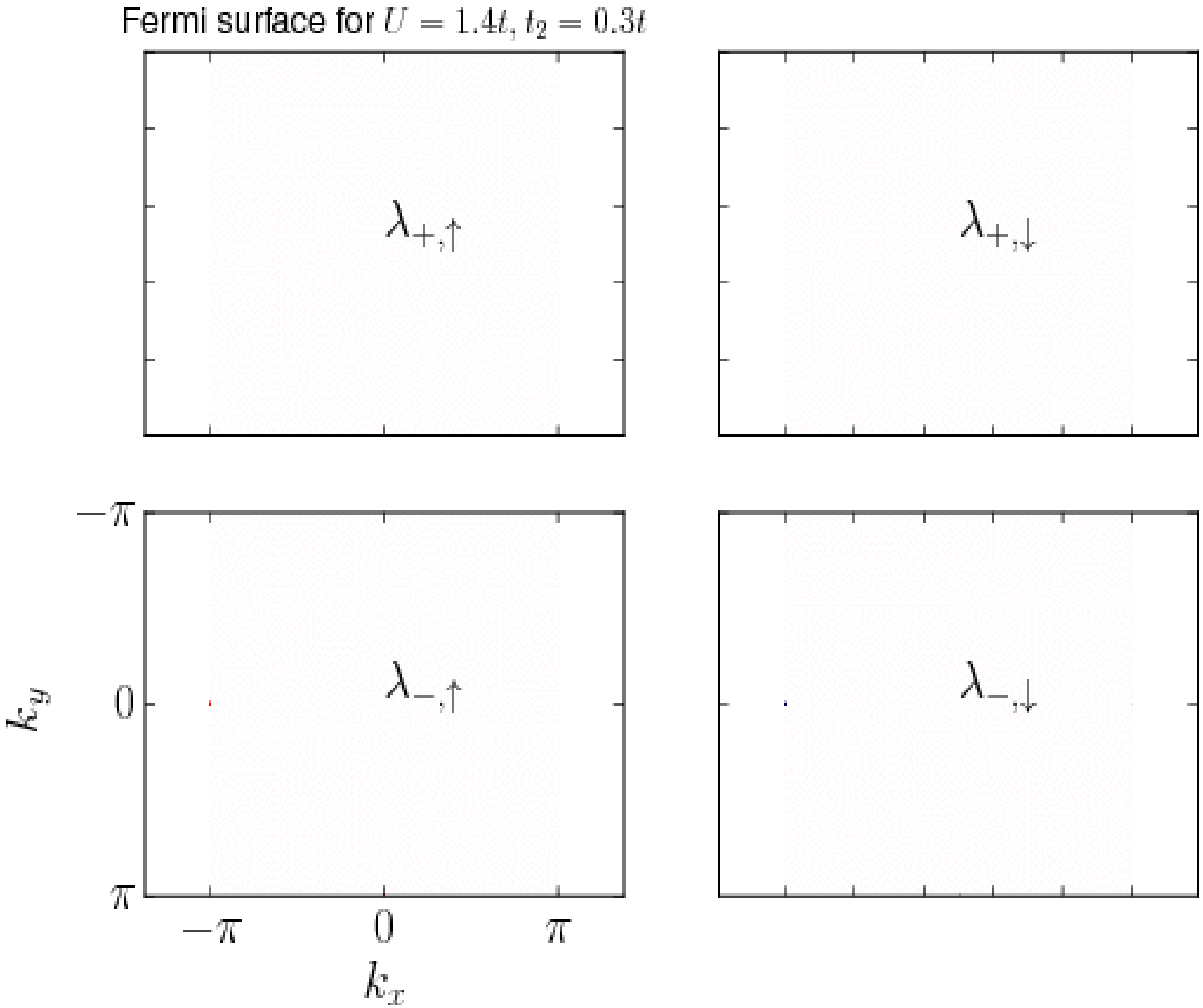


Evolution of (UHF) Spectral and Momentum distribution functions with U: Antiferromagnetic Insulator

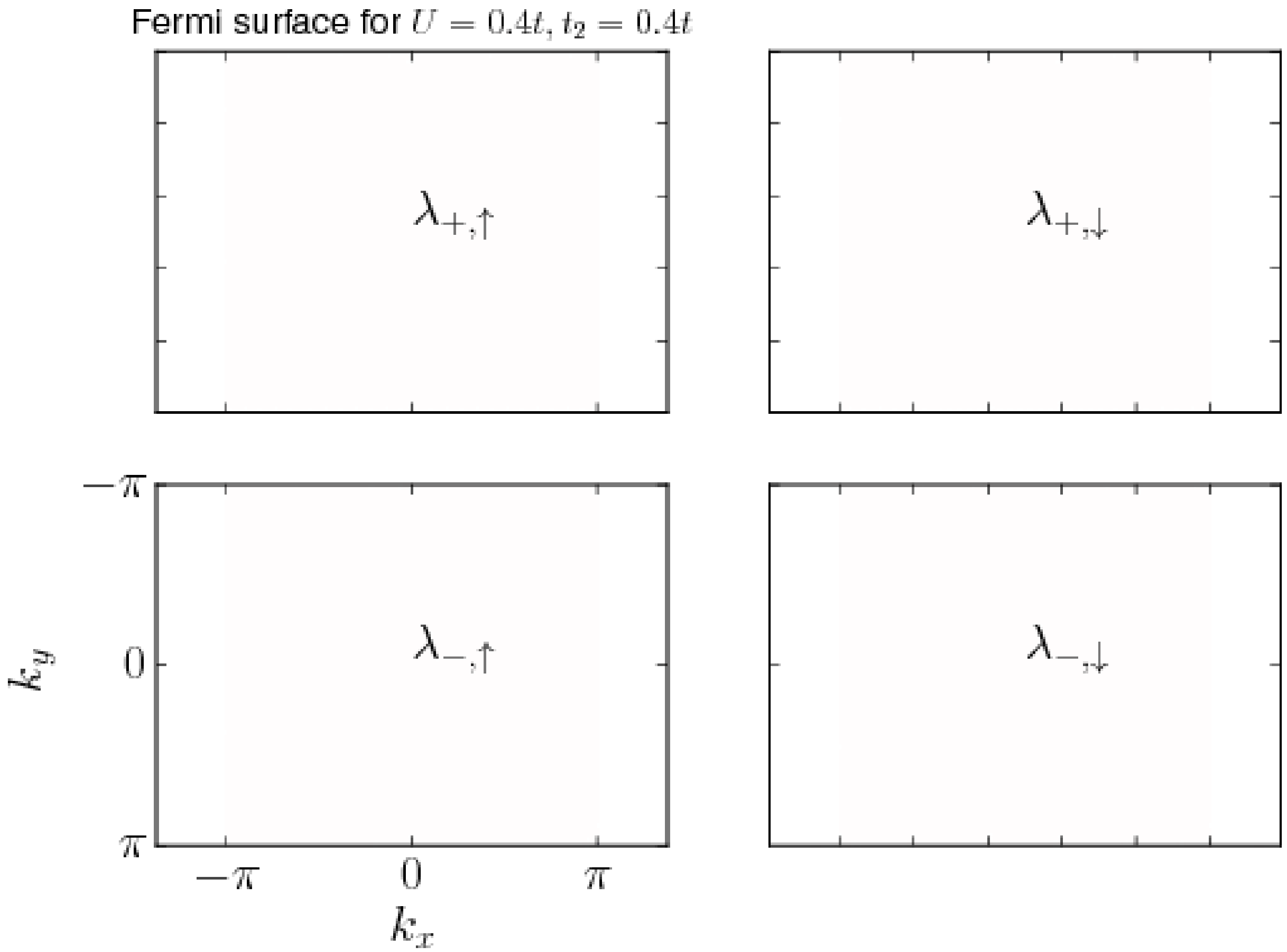




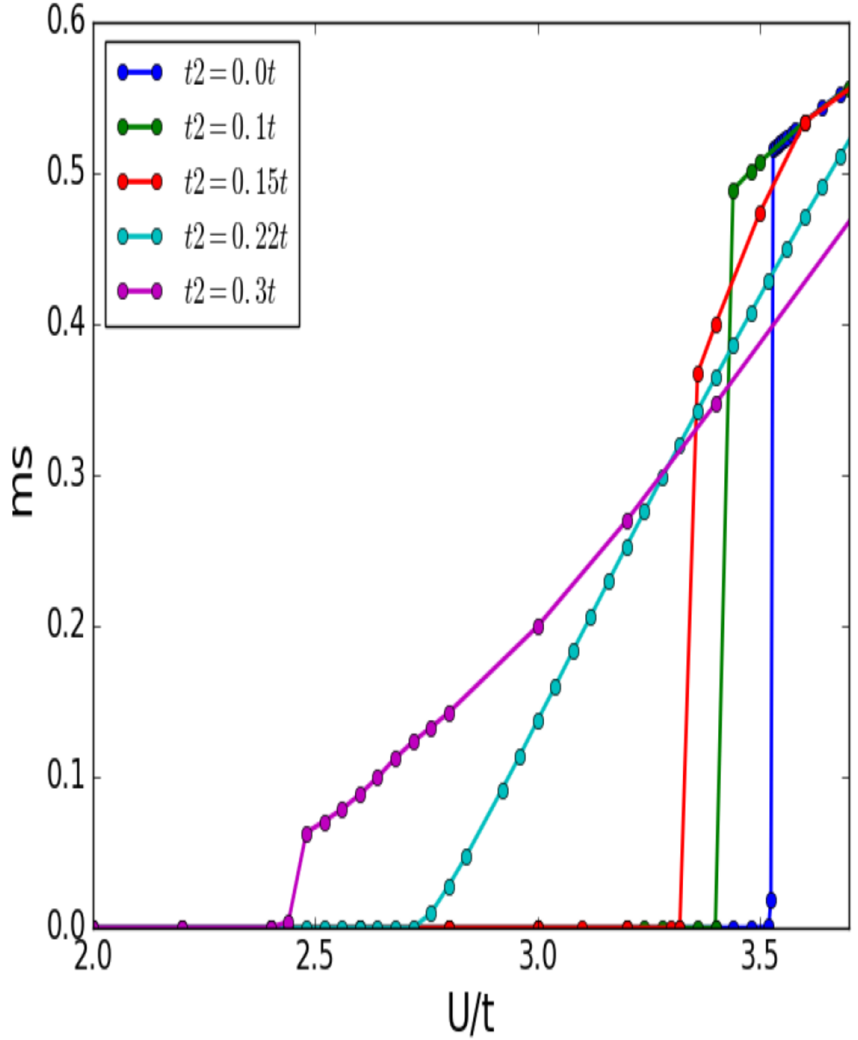
Evolution of (UHF) Fermi-Surface with U ($t'=0.3t$):

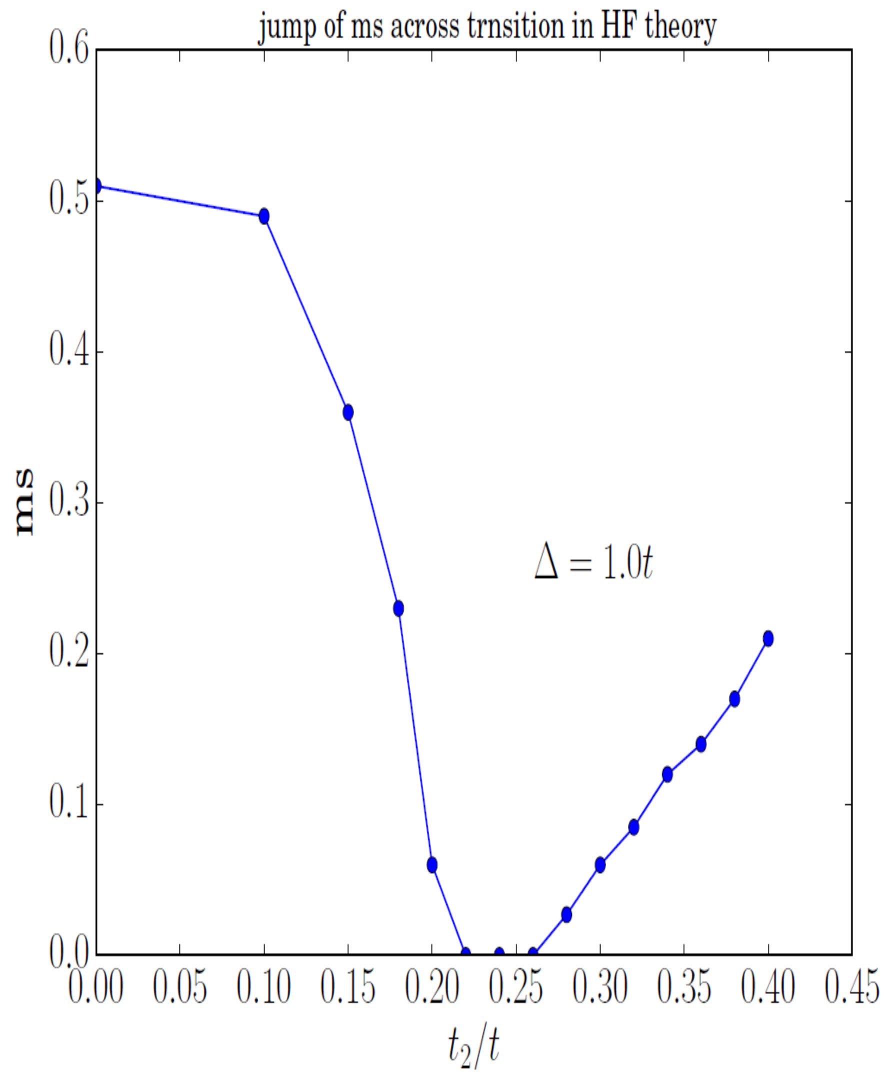


Evolution of (UHF) Fermi-Surface with U (t'=0.4t):

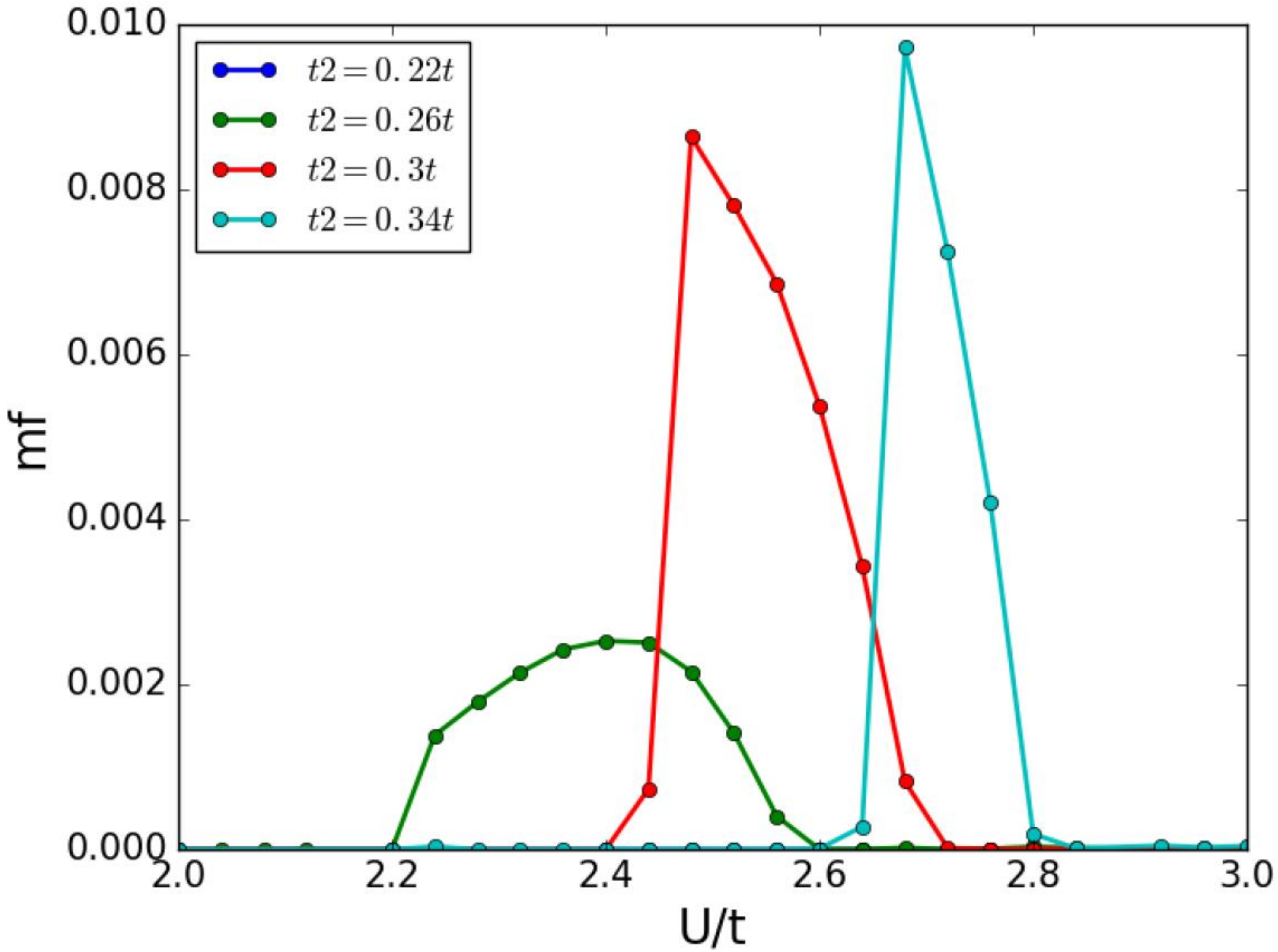


(UHF) Staggered magnetization vs U and t_2





(UHF) Net (Ferro) magnetization vs U and t_2



Plan of the rest of the talk

- DMFT and “Impurity” Solvers
- Results with Para-magnetism enforced
  - Bethe lattice in infinite dimensions
  - 2-d square lattice
- Results allowing for Anti-ferromagnetism
  - Half filling and the AFHM line
  - Finite Temperature transitions
  - Ferrimagnetic Half Metallic phase with doping
- **Some more recent results**
  - Model with frustration-UHF
  - **Model with frustration-DMFT+CT-HYB-QMC**
  - Superconductivity at Half filling?!
  - Quenching in the IHM
- Concluding Comments – Is it for Real?

$t - t_2$- U - Δ IHB at Half-filling

DMFT+CT-HYB-QMC Matsubara Green Functions

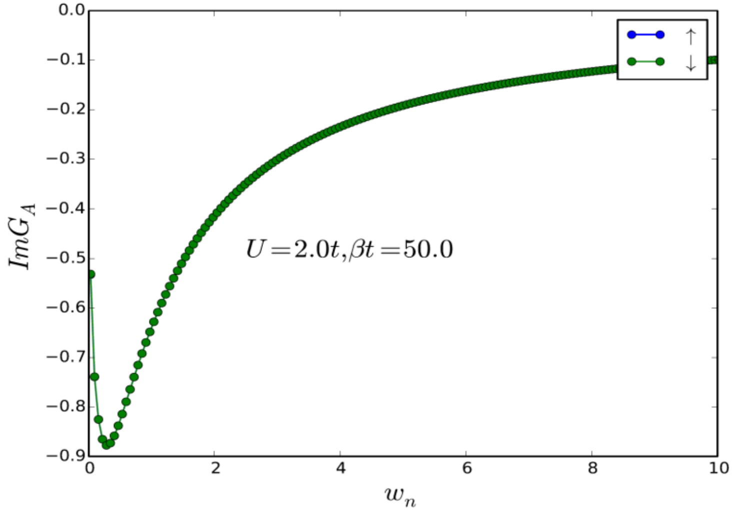


Figure 5: $U = 2.0t_1$, Paramagnetic Band insulator

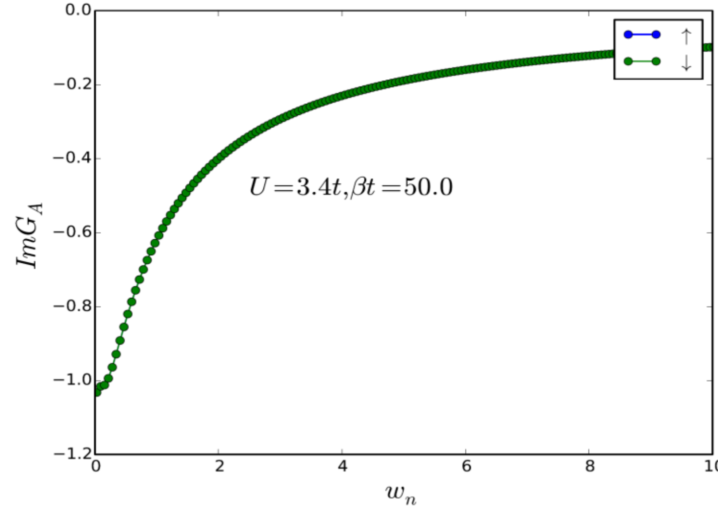


Figure 6: $U = 3.4t_1$, Metallic Phase

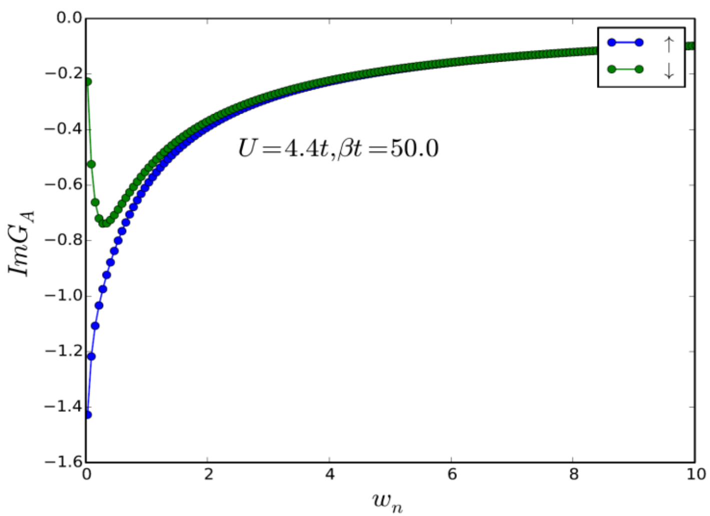


Figure 7: $U = 4.4t_1$, Half Metallic Phase

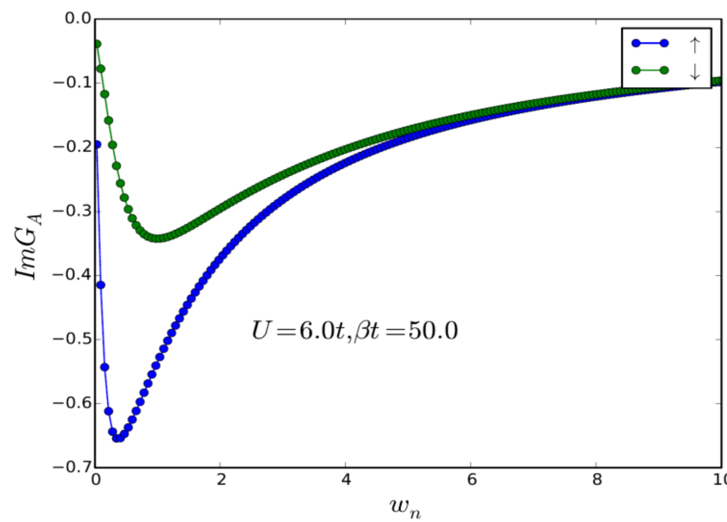
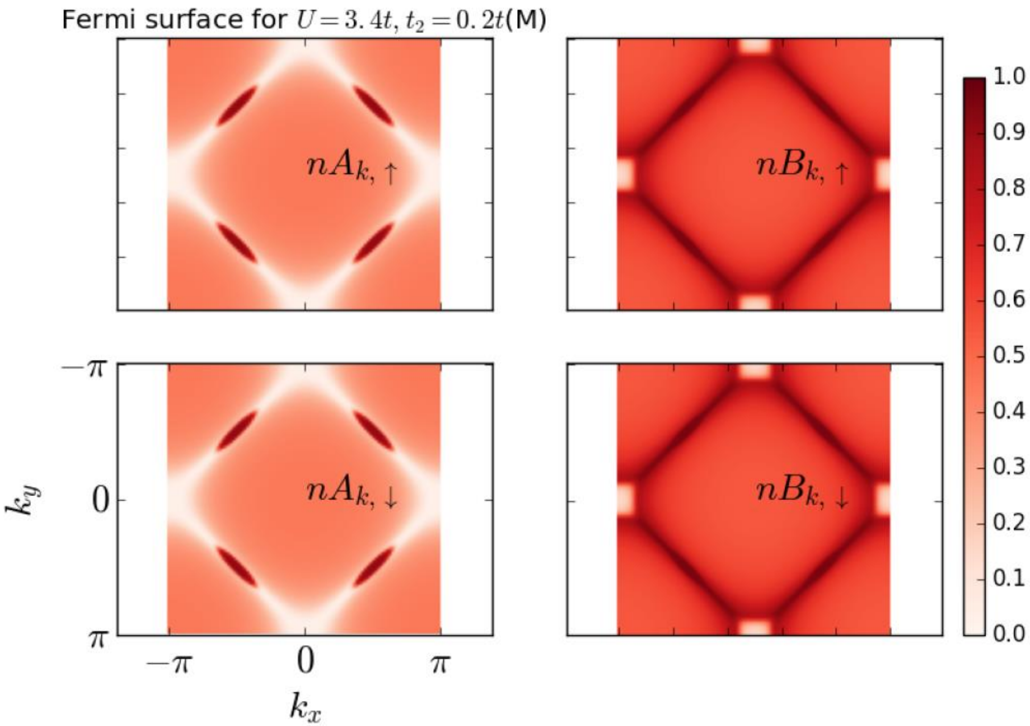


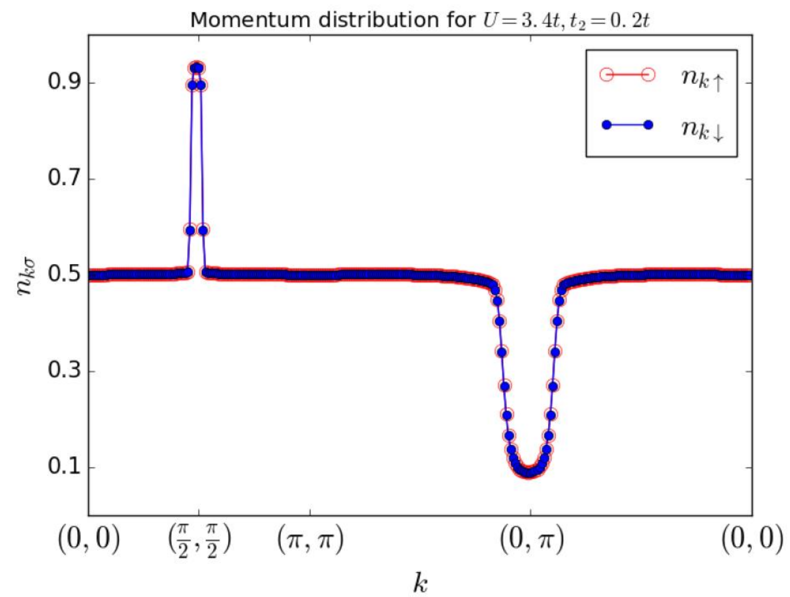
Figure 8: $U = 6.0t_1$, AFM insulating phase

Evolution of DMFT+CTQMC Momentum distribution functions with U:

Paramagnetic Metal

n = 1.000, m_s=0.000 m_f=0.000

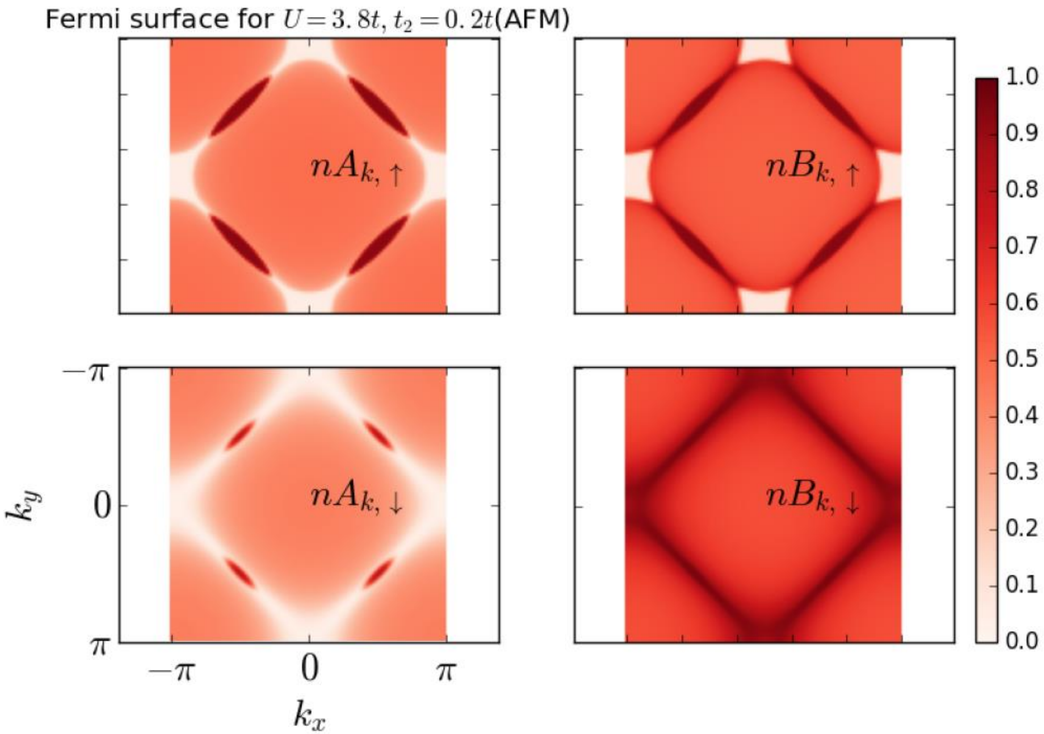


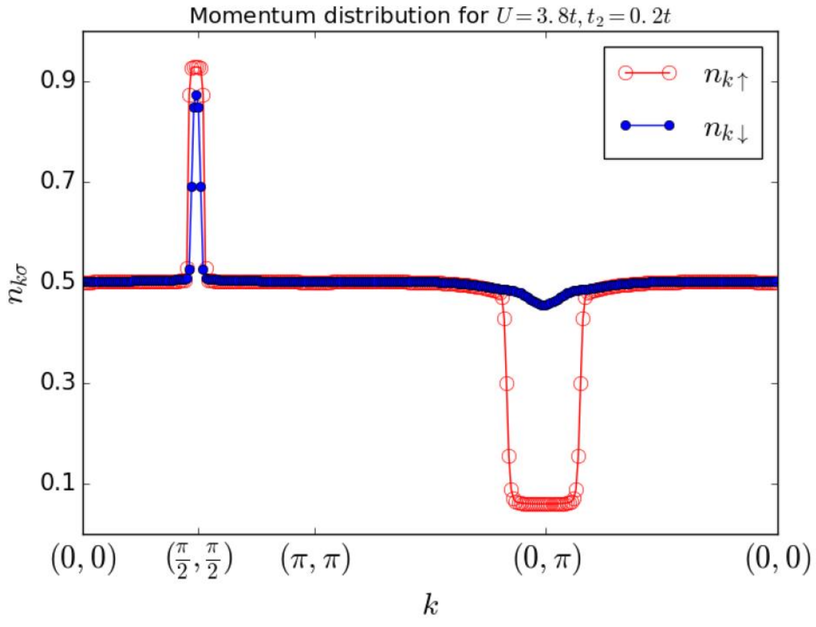


Evolution of DMFT+CTQMC Momentum distribution functions with U:

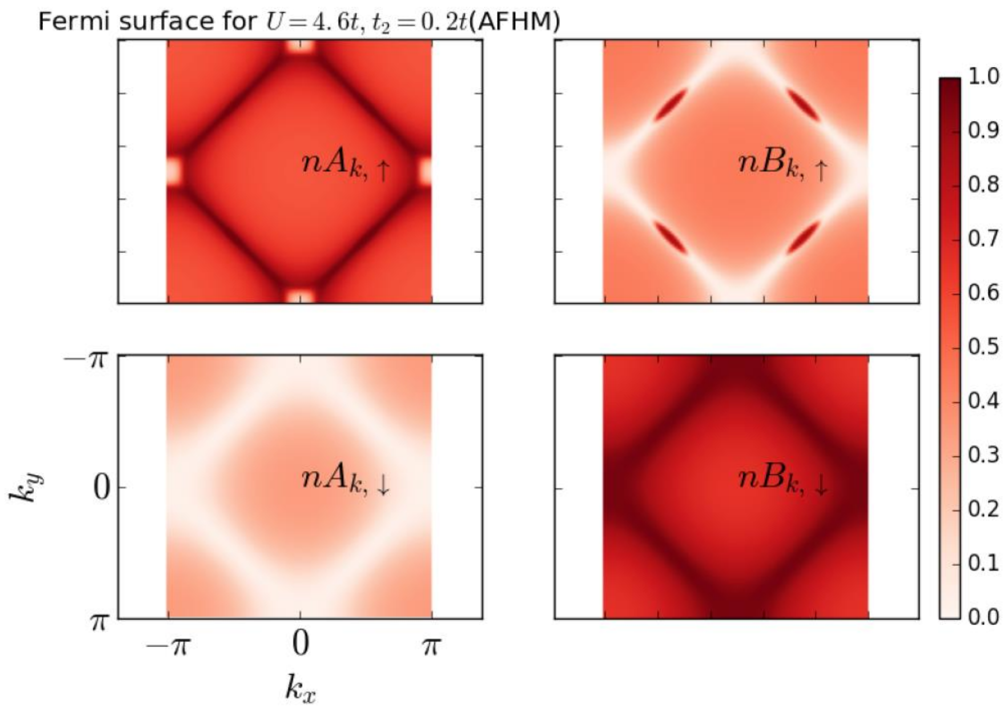
Ferri-magnetic Metal

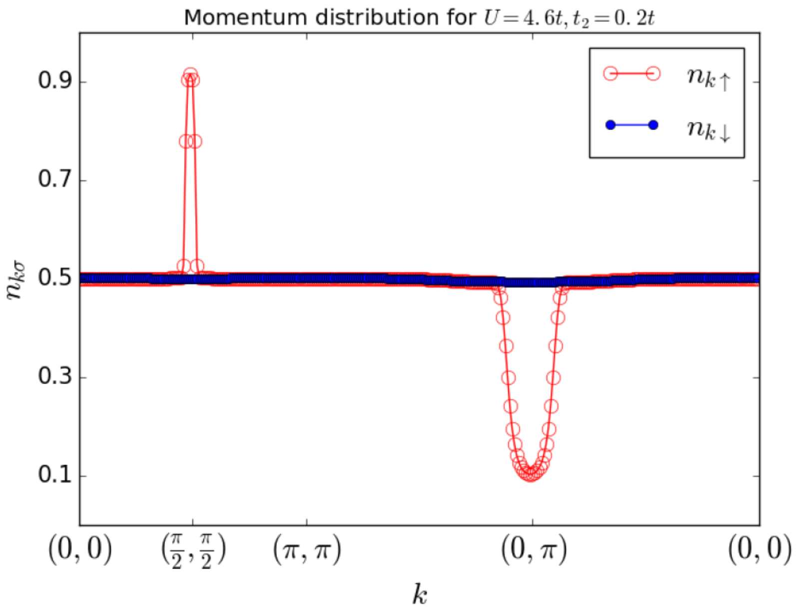
n = 0.998, m_s=0.141 m_f=0.013





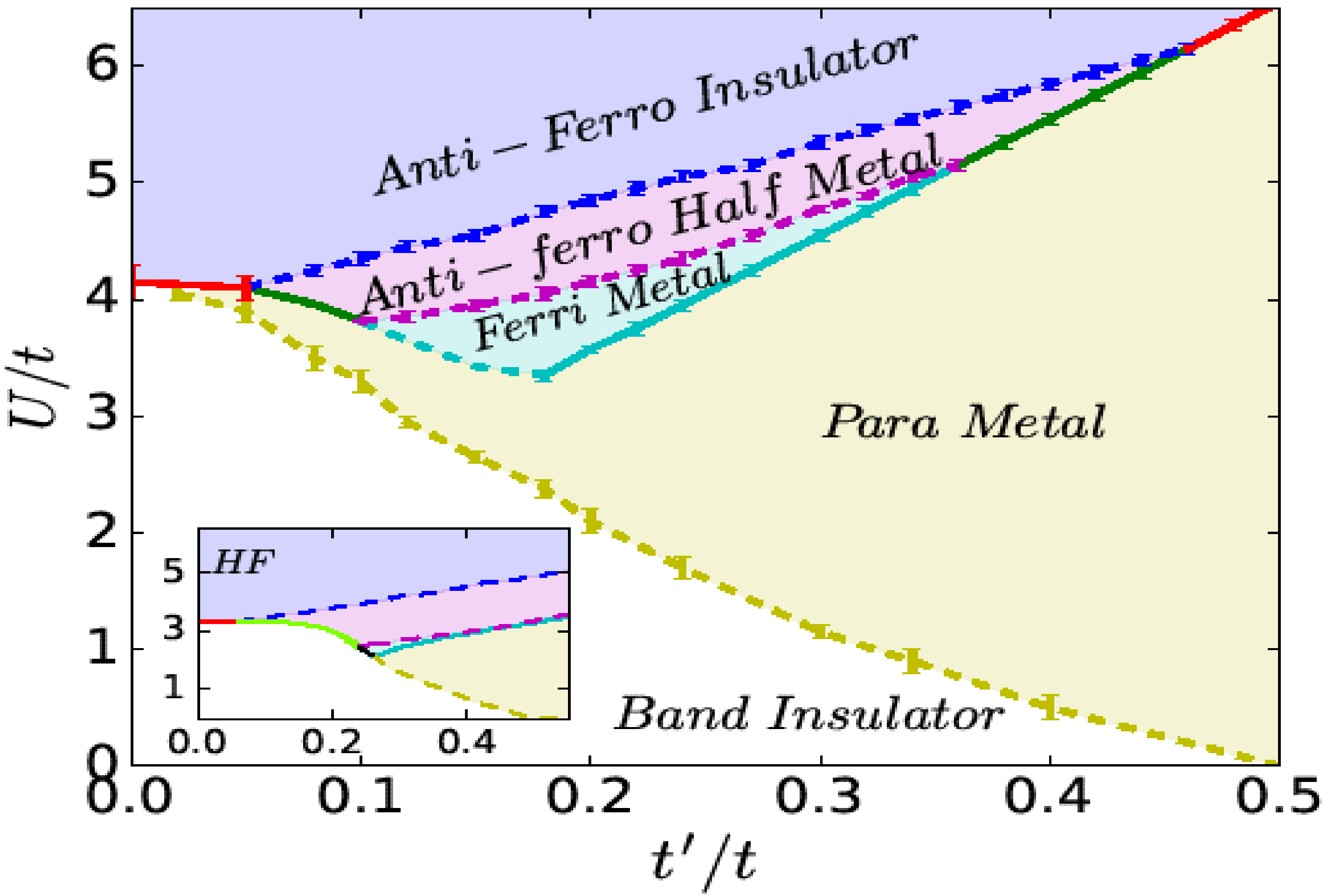
Evolution of DMFT+CTQMC Momentum distribution functions with U:
Antiferromagnetic Half Metal
n = 1.000, m_s=0.286 m_f=0.000





$t - t'$- U - Δ IHB at Half-filling

DMFT+CT-HYB-QMC Phase Diagram

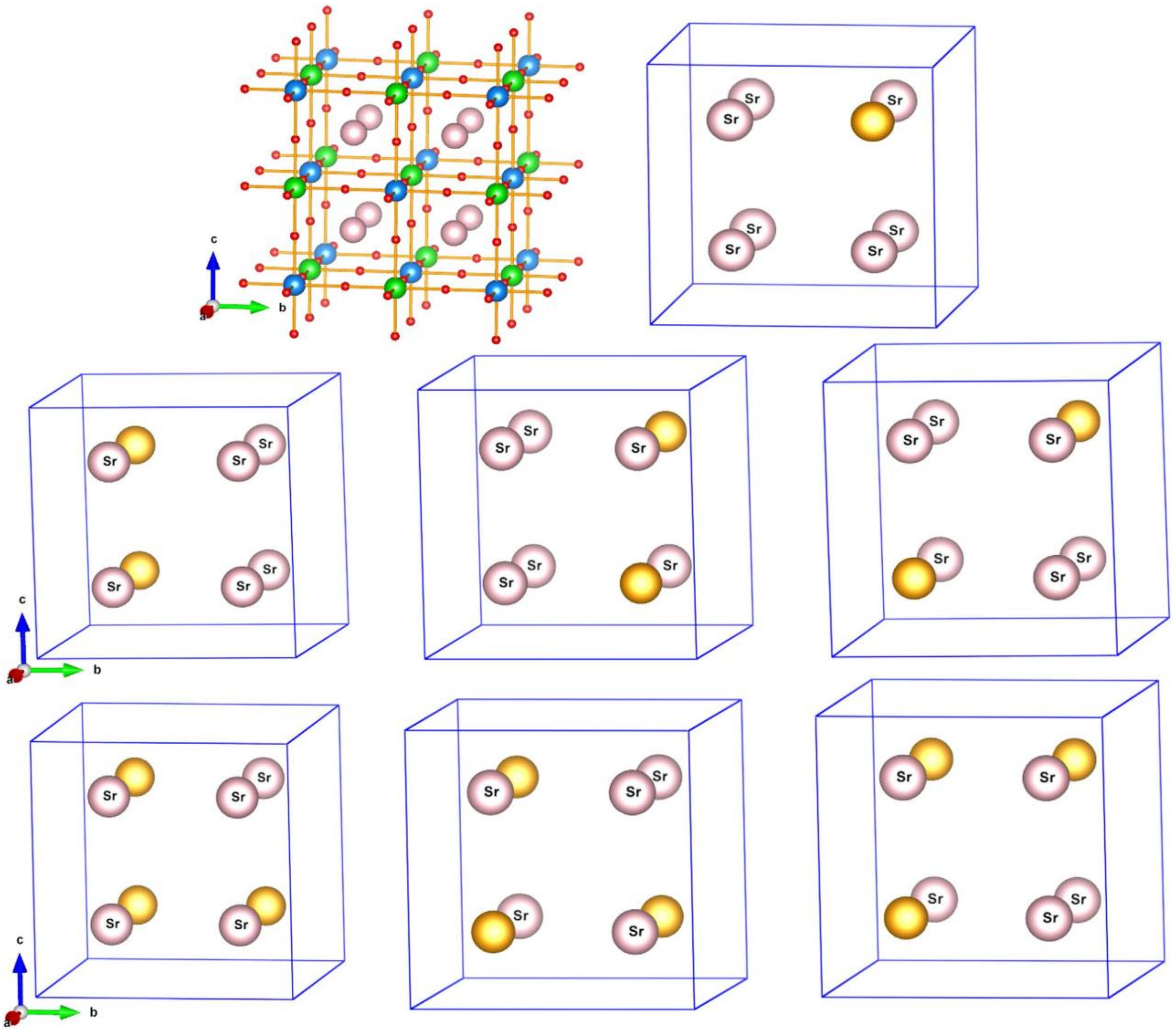


Possibility in La and Na Doped Sr_2CrOsO_6 Double Perovskite?

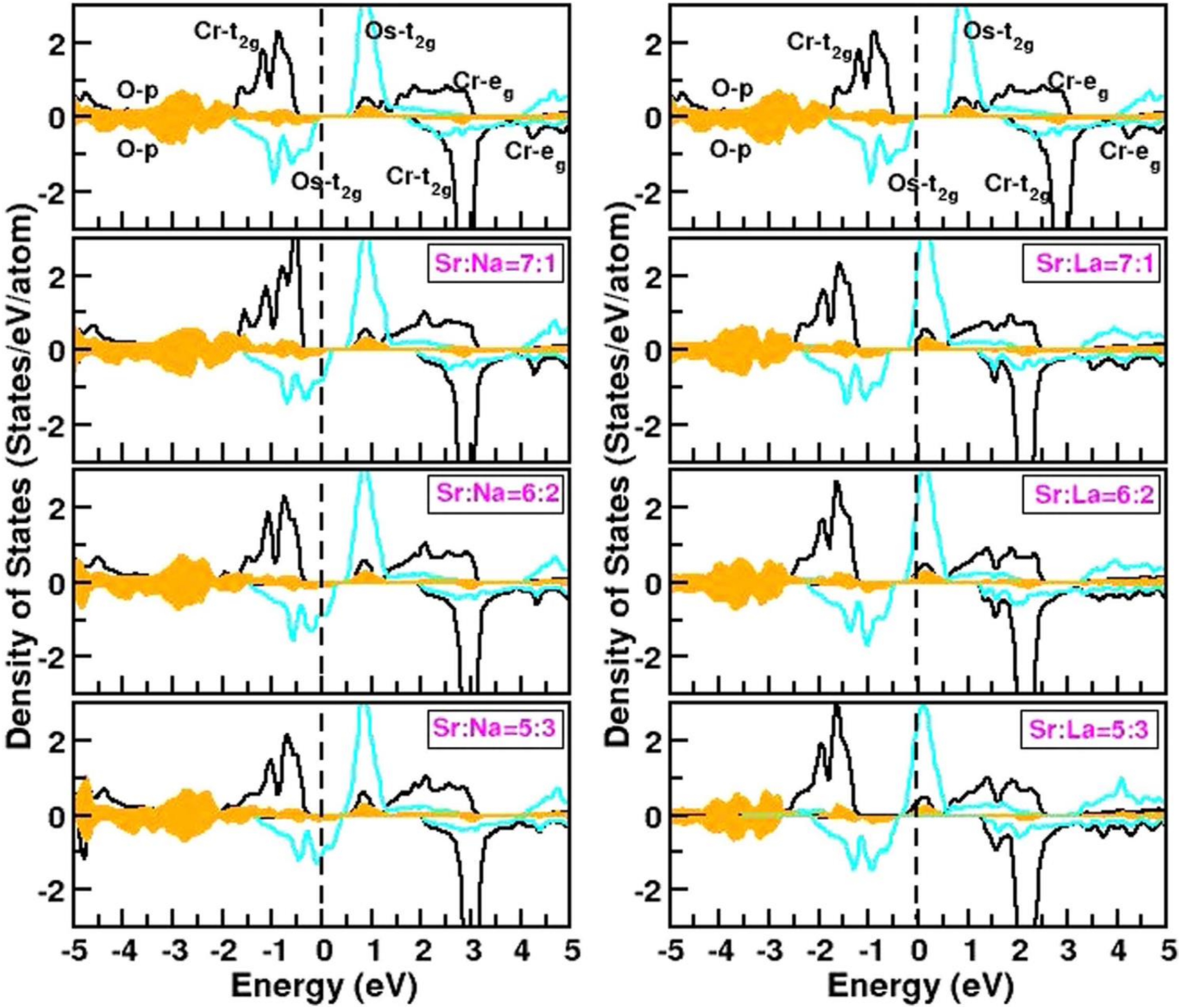
(K Samanta, P Sanyal & T Saha-Dasgupta, *Sci. Rep.* **5**, 15010 (2015))

- Sr_2CrOsO_6, is a known ferrimagnetic insulator with transition temperature (T_c) of 725 K, highest ever known in the oxide family
- In the above work, six different doped compounds :

  $Sr_{1.875}La_{0.125}CrOsO_6$, $Sr_{1.75}La_{0.25}CrOsO_6$, $Sr_{1.625}La_{0.375}CrOsO_6$, $Sr_{1.875}Na_{0.125}CrOsO_6$, $Sr_{1.75}Na_{0.25}CrOsO_6$, $Sr_{1.625}Na_{0.375}CrOsO_6$.
  were studied using *first-principles density functional theory* (DFT) based calculations together with *exact diagonalization of Cr-Os model Hamiltonian* constructed in a first-principles derived Wannier function basis
- Half-metallic, ferrimagnetic state seen with reasonably large net magnetic moment of ≈ 0.5–1.0 μ_B and magnetic transition temperature nearly as high as the parent compound



Top row, left panel: The cubic double perovskite structure of Sr_2CrOsO_6 . The large shaded brown, medium green, medium blue and small red balls represent Sr, Cr, Os and O atoms respectively.
Top row, right panel: The *A* sublattice with one out of eight Sr atoms substituted by Na/La. The substituted atom is shown as yellow ball. **Middle row:** The *A* sublattice with two out of eight Sr atoms substituted by Na/La, in various inequivalent positions. **Bottom row:** The *A* sublattice with three out of eight Sr atoms substituted by Na/La, in various inequivalent positions.

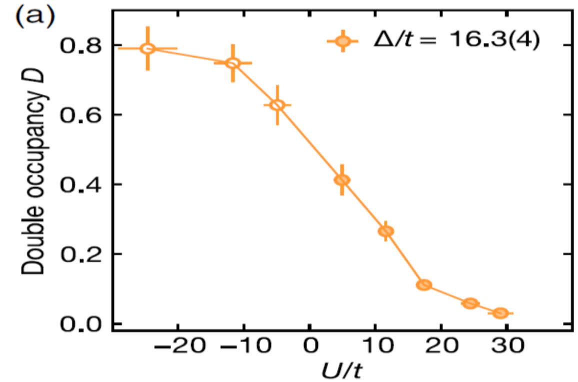


GGA + *U* + SOC density of states of the parent compound, and the Na and Sr doped compounds. The black, cyan, yellow shaded area represent the states projected to Cr *d*, Os *d* and O *p* states, respectively. The dashed, vertical lines in each panel mark the positions of Fermi level.

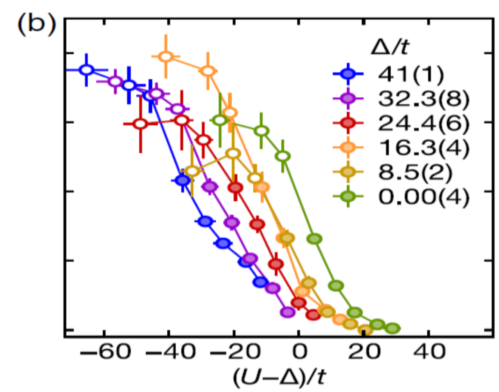
Ultra-Cold Atom Emulator of IHB

[Messer et al, PRL 115, 115303(2015)]

- System emulates the IHB on a honeycomb lattice
- Measurements:
  - noise correlation data from absorption images of the atomic momentum distribution as a measure of CDW order
  - Average double occupancy using Interaction dependent rf spectroscopy
  - Lattice modulation spectroscopy

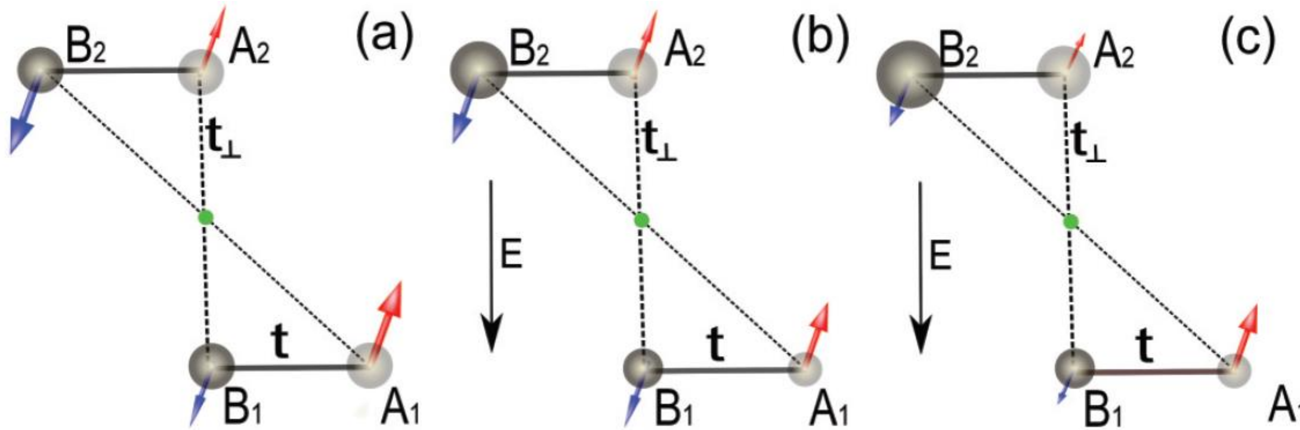


- Consistent with increasing U supressing CDW order (e.g. not seen when U=25.3 and 2 Δ = 20.3)
- Yet to address existence of BOI



Half metallic phase in Bilayer Graphene?!

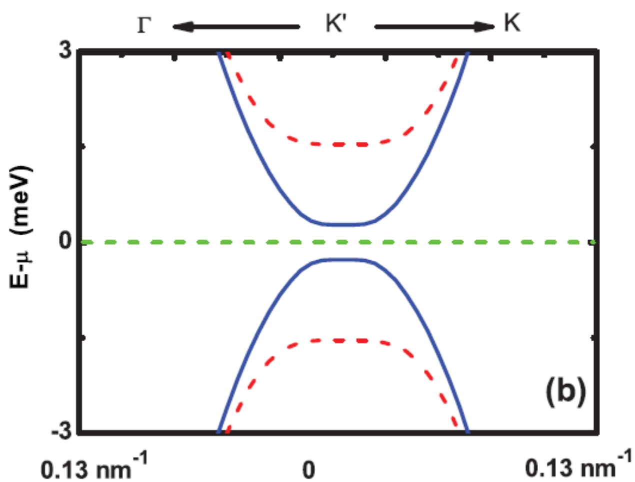
[Yuan et al Phys. Rev. B 88, 201109(R) (2013)]

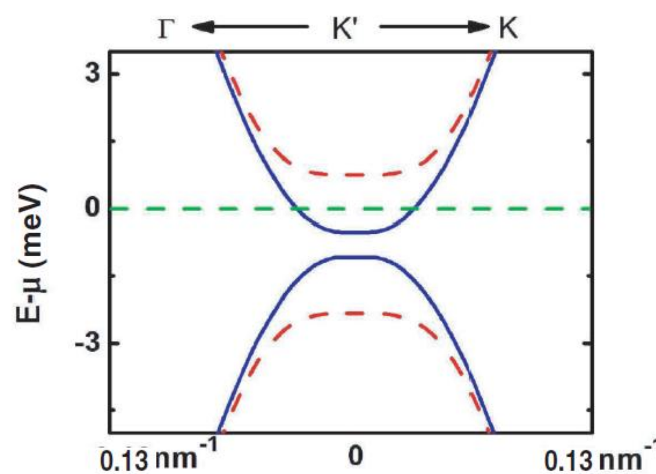


E=0 LAFI

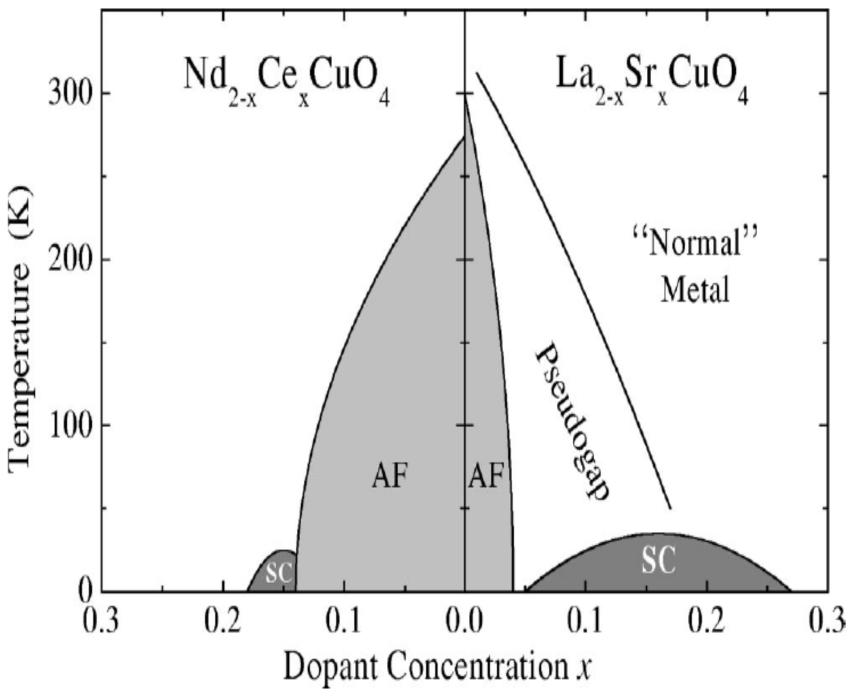
Finite E LAFI

Doped FHM





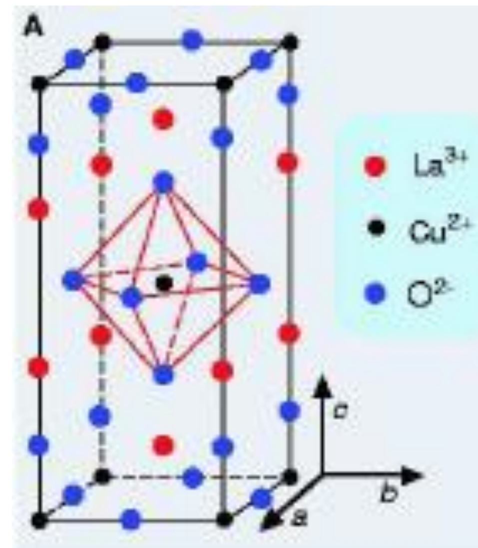
High Tc Cuprate Superconductors



← Electron doping

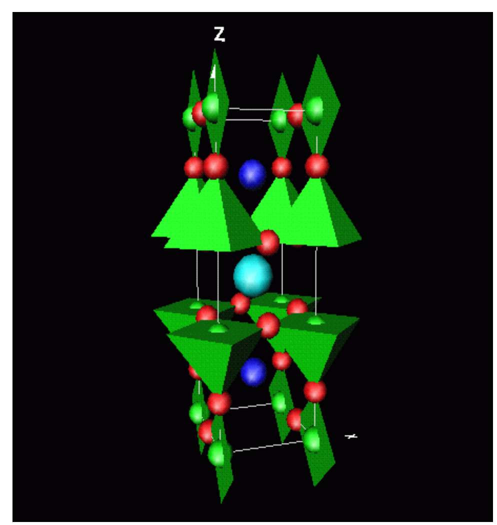
Mott insulator

→ Hole doping



$La_{(2-x)}Sr_xCuO4$

Max Super-conducting Tc ≈ 40K

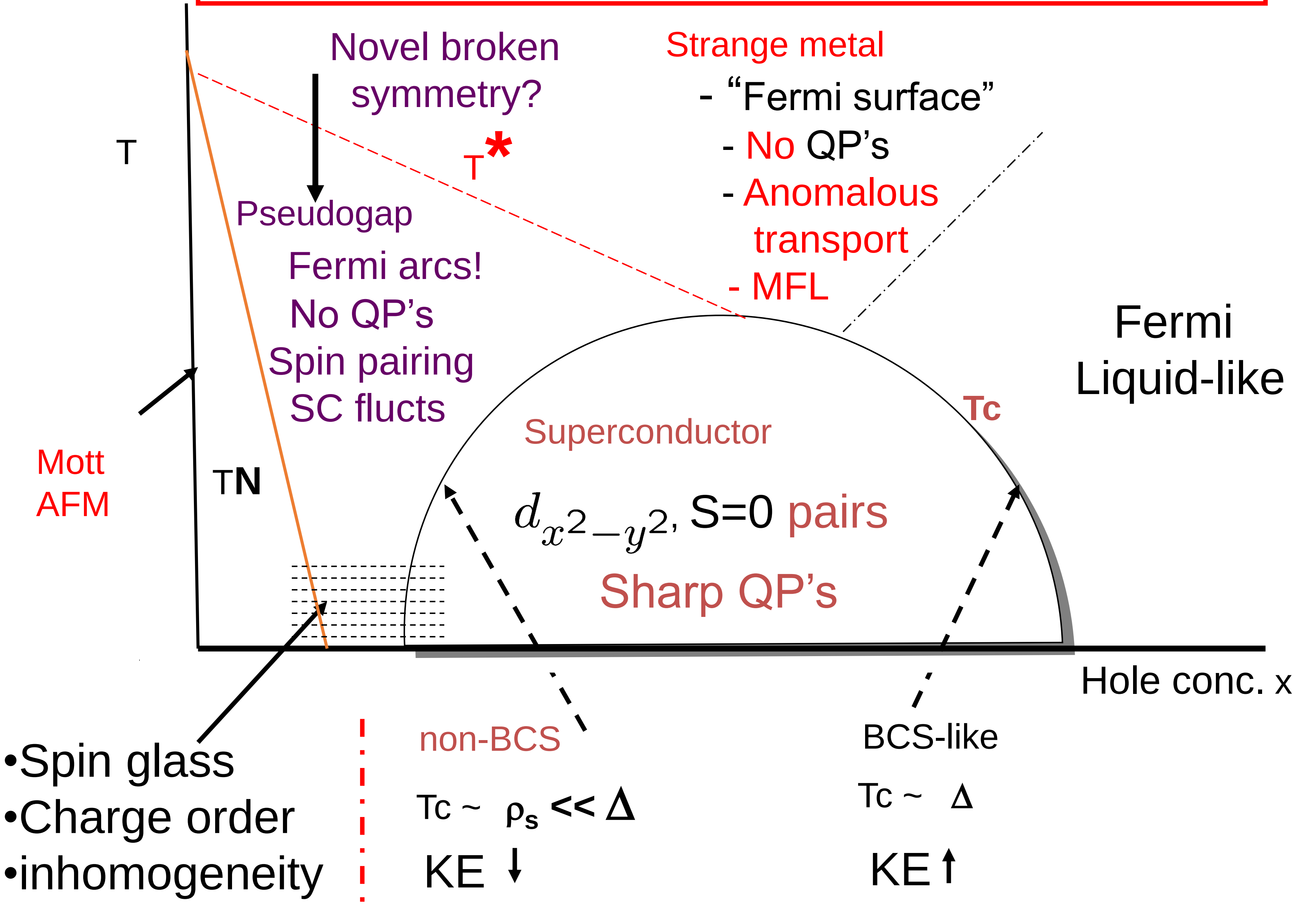


$YBa_2Cu_3O_7$

Super-conducting Tc ≈ 90K

20 years of Experiments on the hole-doped Cuprates

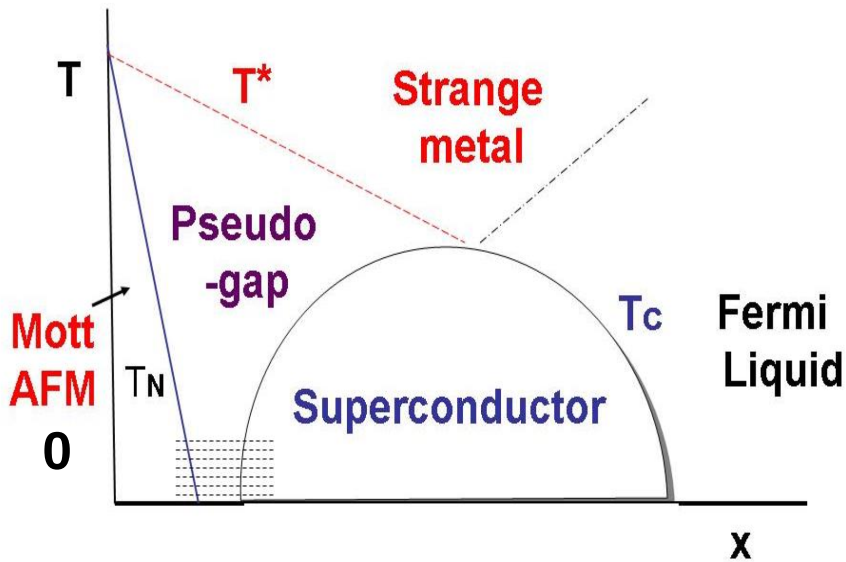
(Slide courtesy M Randeria)



Failure of (at least) three central paradigms of 20^{th} Century Solid State Physics

(Slide courtesy M Randeria)

(1) Band theory fails for $x = 0$ parent insulator



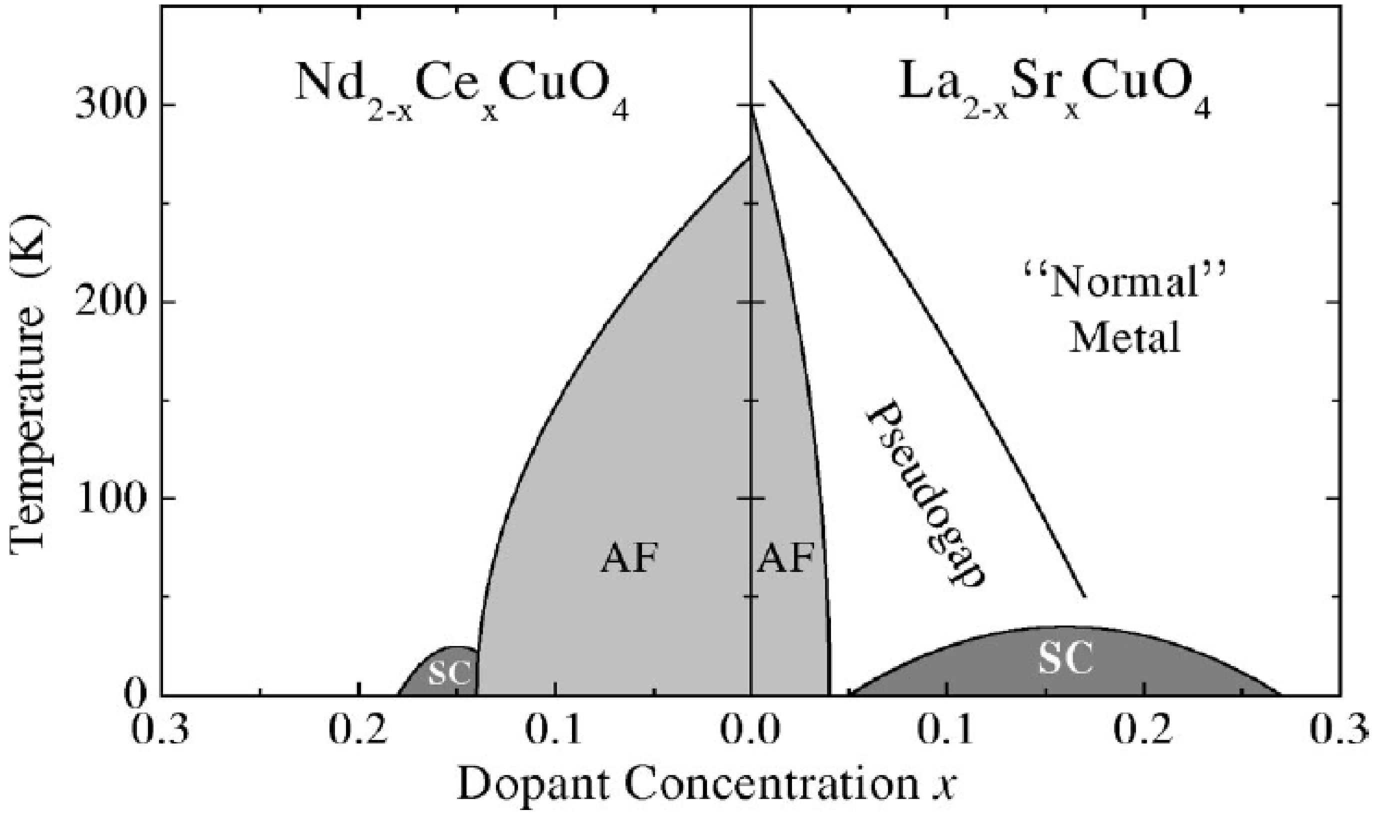
(2) Landau's Fermi liquid theory fails for **strange metal** and **pseudogap regimes**

(3) BCS theory fails for **Unconventional SC** particularly for $x \ll 1$

Competing orders:
Antiferromagnetism;
Charge ordering;
Circulating currents

Hidden **Quantum Critical Point** under the dome**?**

Phase Diagram of High Tc Cuprate Superconductors



← Electron doping | Hole doping →

Mott insulator

Strange Metal regime:

"Marginal Fermi Liquid" Phenomenology

C. M. Varma et al, PRL (1989)

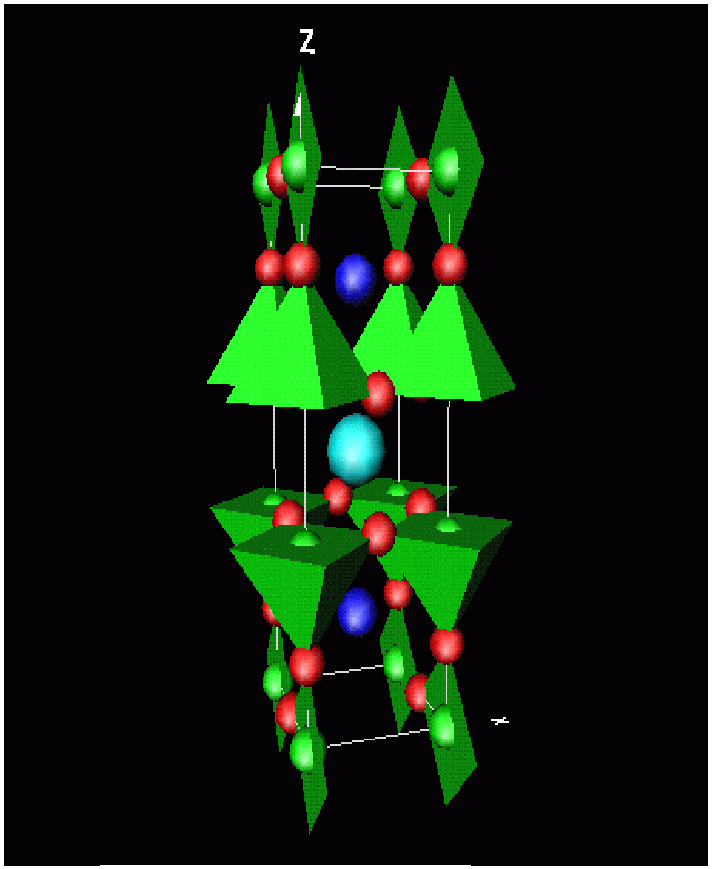
- No energy scale like (E_f, Θ_D)
- Only energy scale is T or ω
- Both single-particle and transport scattering rates $1/\tau \simeq \max(\omega, T)$
- ω/T scaling of response functions
- no scaling in q-space

Microscopic origin?

Quantum Critical Point under the SC dome ?

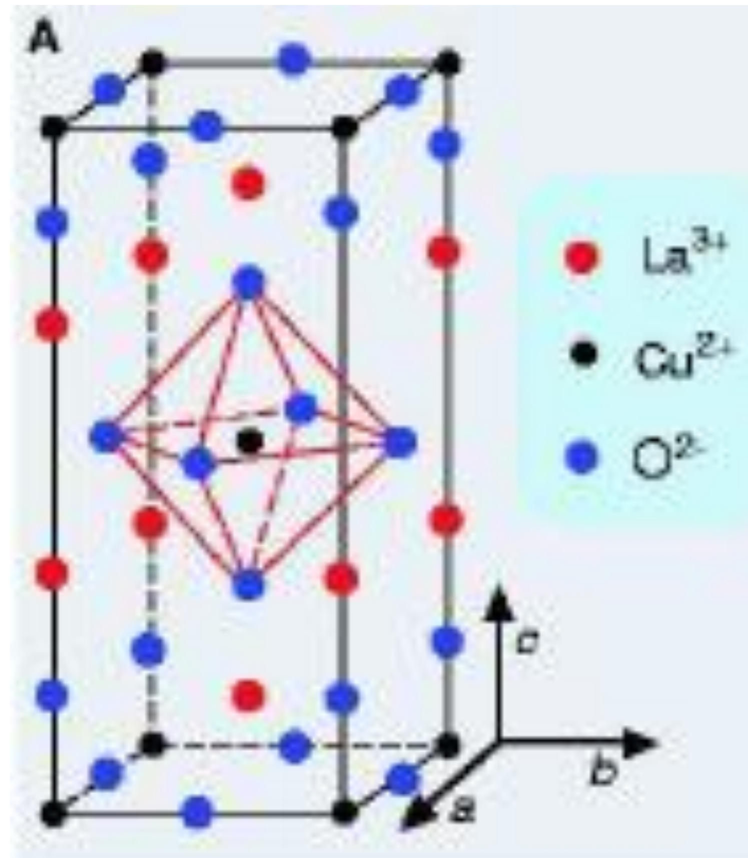
Structure of Cuprate Superconductors

The Ubiquitous CuO2 planes



$YBa_2Cu_3O_7$

Superconducting Tc ≈ 90K



$La_{(2-x)}Sr_xCuO4$

Superconducting Tc ≈ 40K

A Brief History of the IHB

- Essentially proposed by Hubbard and Torrance [PRL 47, 1750 (1981)] to provide a heuristic explanation for the (then) recently observed "transformation" in some organic solids (eg. TTF-Chloranil) from neutral to ionic states when cooled (seen via changes in the optical, Raman and infrared spectra, and in the lattice constants over a broad temperature range from 84 K down to ~50 K)
- Egami et. al., Science 261, 1307 (1993) studied the 1-d IHB numerically by exact diagonalization.

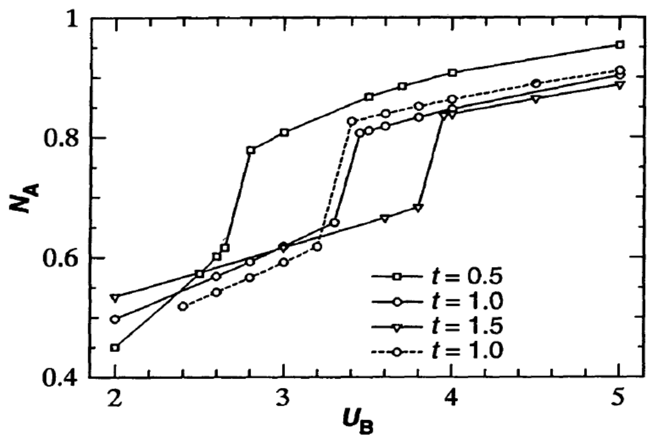


Fig. 2. Dependence of N_A on U_B for $\Delta = 2$ and $U_A = 5$ for various values of t. Results are shown for both the 4A + 4B system (solid lines) and the 3A + 3B system (dashed line).

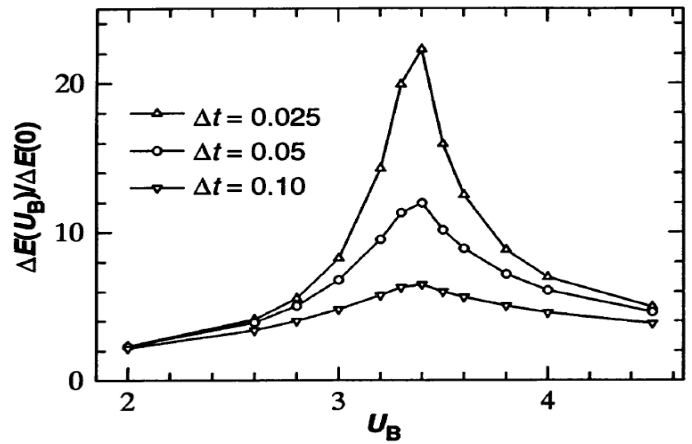
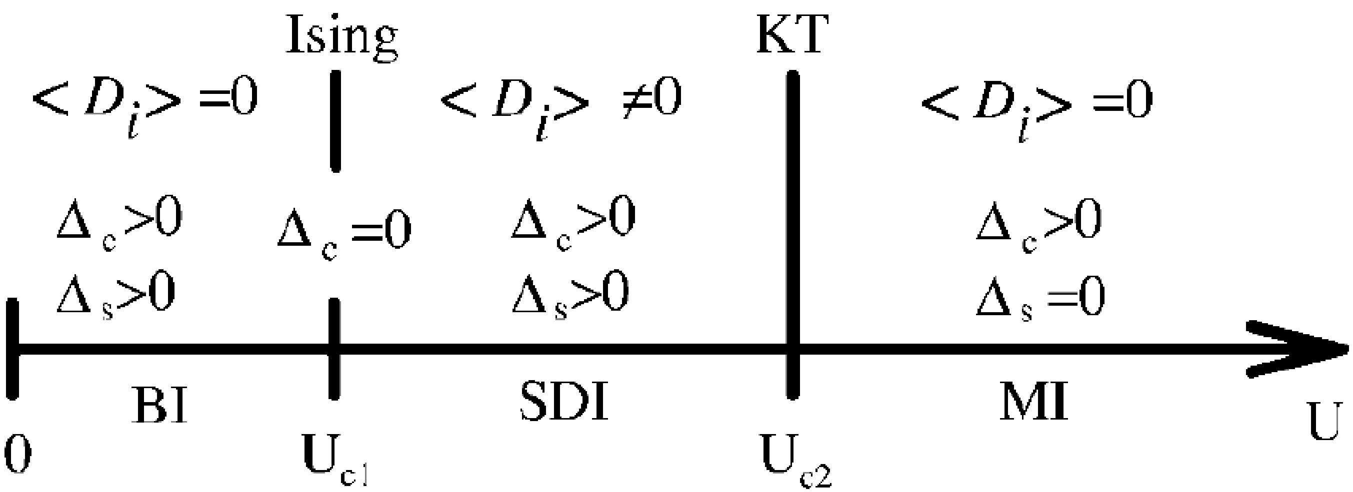


Fig. 3. Change in the ground-state energy, $\Delta E(U_B)$, of the Hamiltonian (Eq. 1) as a result of dimerization, normalized to the value for $U_B = 0$ for various values of Δt. We assumed $t = 1$ and $U_A = 5$.

A Brief History of the IHB

- Fabrizio *et al* [PRL 83, 2014 (1999)] used bosonization techniques to infer a T=0 phase diagram for the 1-d IHB as a function of U (fixed Δ):



- SDI: Spontaneously dimerized (or Bond-Ordered) Insulating state with non-zero expectation value of the dimerization operator

$$\mathcal{D} = \sum_{i,\sigma} (-1)^i \left[c^\dagger_{i\sigma} c_{i+1\sigma} + \text{H.c.} \right]$$

- Initial efforts to verify these using other methods (Different QMC methods, exact diagonalization, DMRG, Slave Boson…) inconclusive and controversial. Perhaps the most careful study, using DMRG, by Manmana *et al* [PR B 70, 155115 (2004)] Broadly in agreement.

A Brief History of the IHB

- Batista and Aligia, PhysRevLett.92.246405 (2004) : U, Δ >> t Limit
- Derive effective Hamiltonian excluding doublons on A sites and holons on B sites
- When U=2 Δ, can find one exactly soluble parameter set (including nearest neighbor Repulsion V) for which BOI is the Ground state

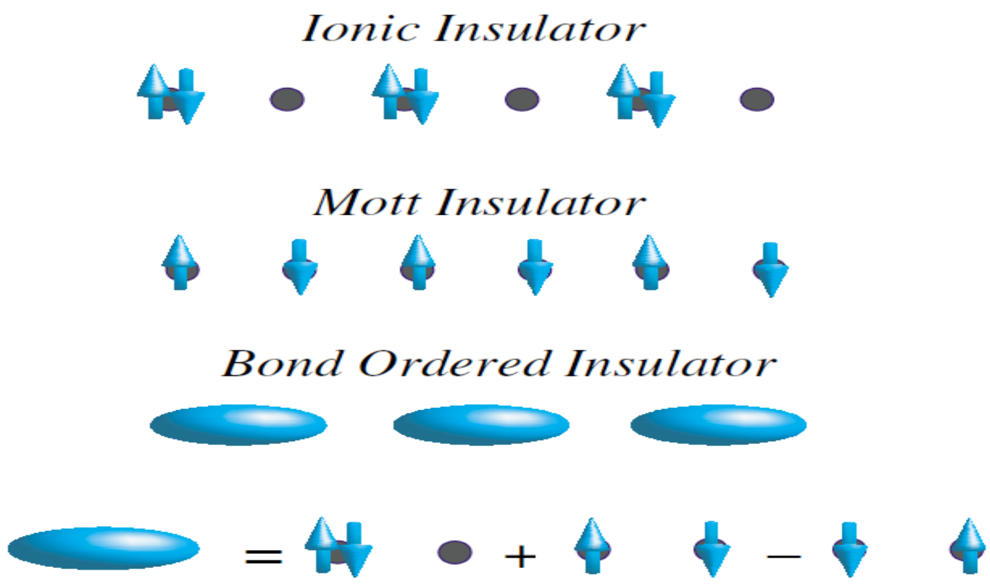
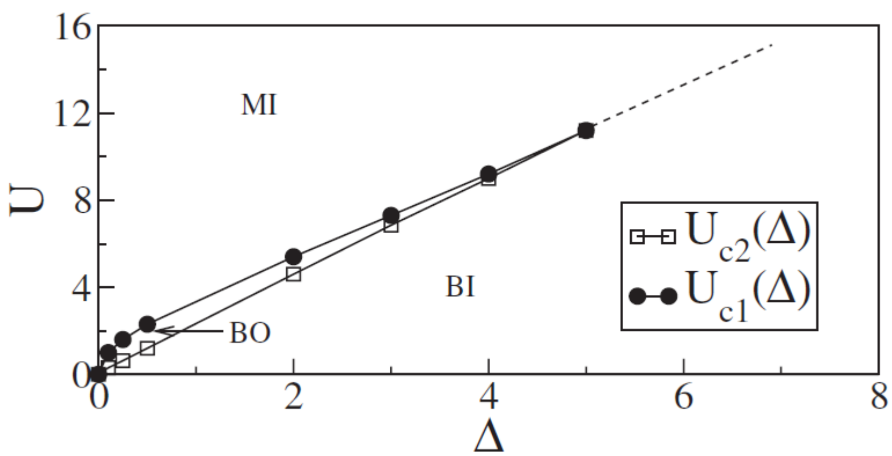


FIG. 1 (color online). Schematic plot of the different ground states of H_{eff}.

Cluster-DMFT results for 2-d IHB at Half-filling

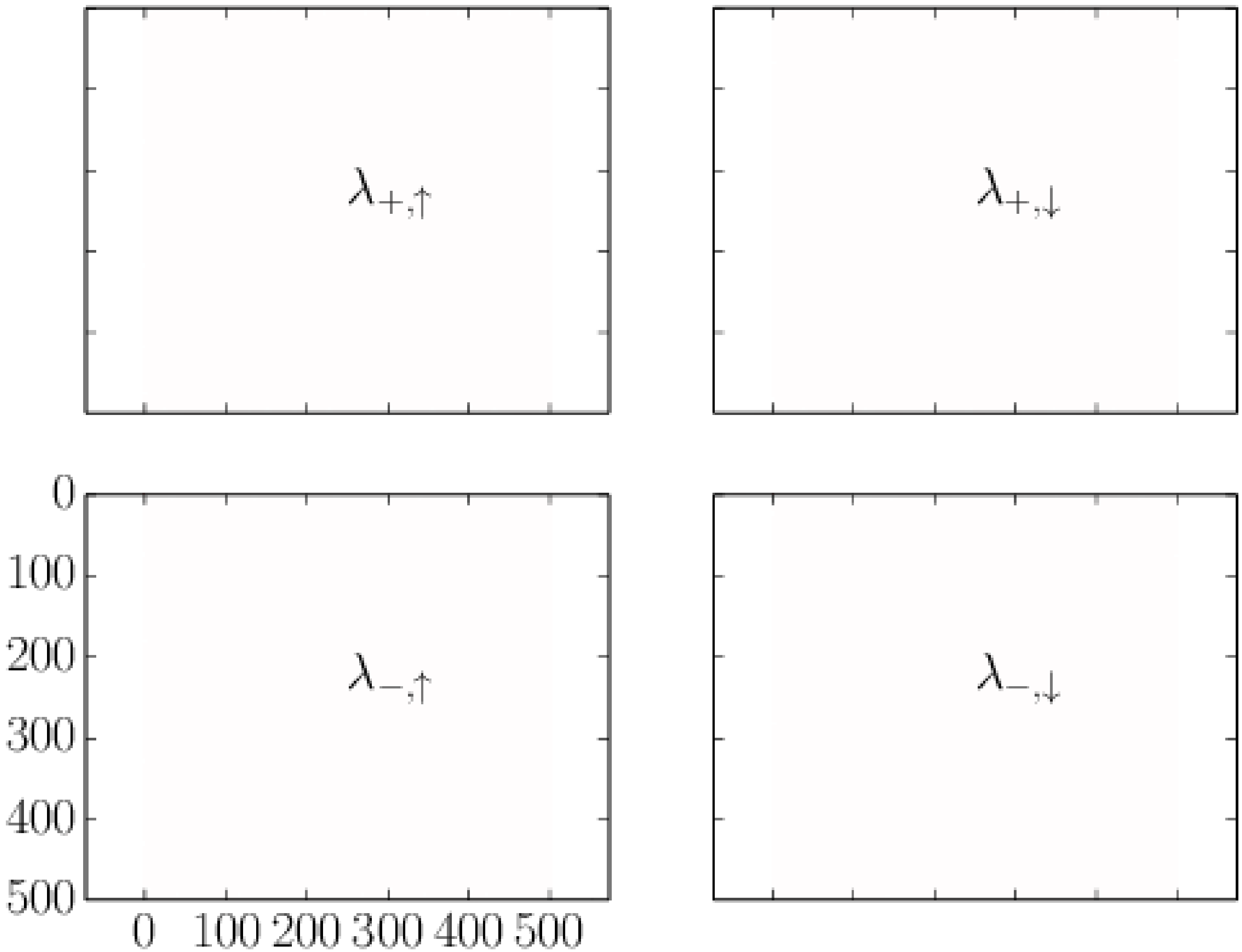
[Kancharla and Dagotto, PRL **98**, 016402 (2007)]

- Cluster-DMFT with 4 cluster sites and 8 bath sites



- Charge gap closes at $U_{c1}(\Delta)$, whereas in 1-d only the excitonic (or optical) gap closes at $U_{c2}(\Delta)$! .
- Antiferromagnetic order in MI and BO phases, Nonzero CDW order for all U
- Only Metallic quantum critical *line* at the MI-BOI transition (for *$\Delta < \Delta c$ ~4.5),* and at the MI-BI transition (for *$\Delta > \Delta c$*)

Fermi surface for $U = 0.4t, t_2 = 0.4t$



Dynamical Mean Field Theory (DMFT)

DMFT **Exact if ..** $t \square \frac{t^*}{\sqrt{2d}}, d \to \infty$

Dependence on the band DOS :

- **In general obtained numerically**
- **Particularly simple for semi-circular DOS (Bethe Lattice in infinite d):**

$$D(\varepsilon) = \frac{2}{\pi}\sqrt{D^2 - \varepsilon^2}$$

$$G(i\omega_n) = 2\left[z_n + \sqrt{z_n^2 - D^2}\,\right]^{-1},$$
$$z_n \equiv i\omega_n + \mu - \Sigma(i\omega_n).$$

$$V_\omega^2 \square A(\omega) \equiv -\frac{1}{\pi}\mathrm{Im}\left[G(\omega^+)\right]$$

The "Renormalised" DOS

The d=∞ or local Approximation [Metzner & Vollhardt, PRL 62, 324(81)]

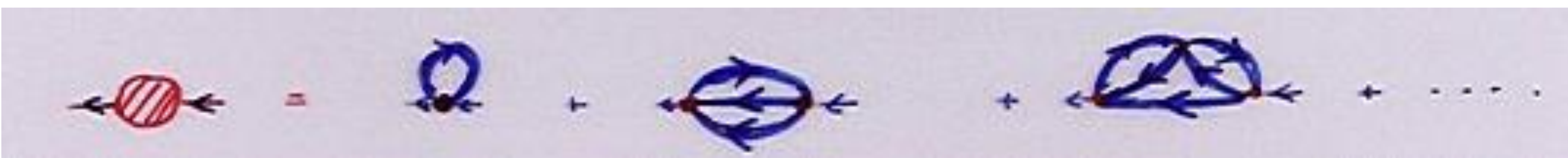
Scale $t_{ij} \square \frac{t^*}{\sqrt{d}} \Longrightarrow$ $\text{for large d,}\ G_{ij} \square \frac{1}{\sqrt{d}} \square\ G_{ii}$

In the d→∞ limit, $\left\{ \begin{matrix} \text{Self Energy } \Sigma \\ \text{Vertex parts } \Gamma \end{matrix} \right\}$ are purely local.

Can also be regarded as "local approximation" in finite d.

Skeleton graph expansion for the local self energy $\Sigma(i\omega_n)$

In terms of $G_{ii} = \int_{-D}^{D} \frac{D(\varepsilon_k)d\varepsilon_k}{\mu + i\omega_n - \varepsilon_k - \Sigma(i\omega_n)}$ and **U**



Is exactly the same as for a single site or "impurity" problem

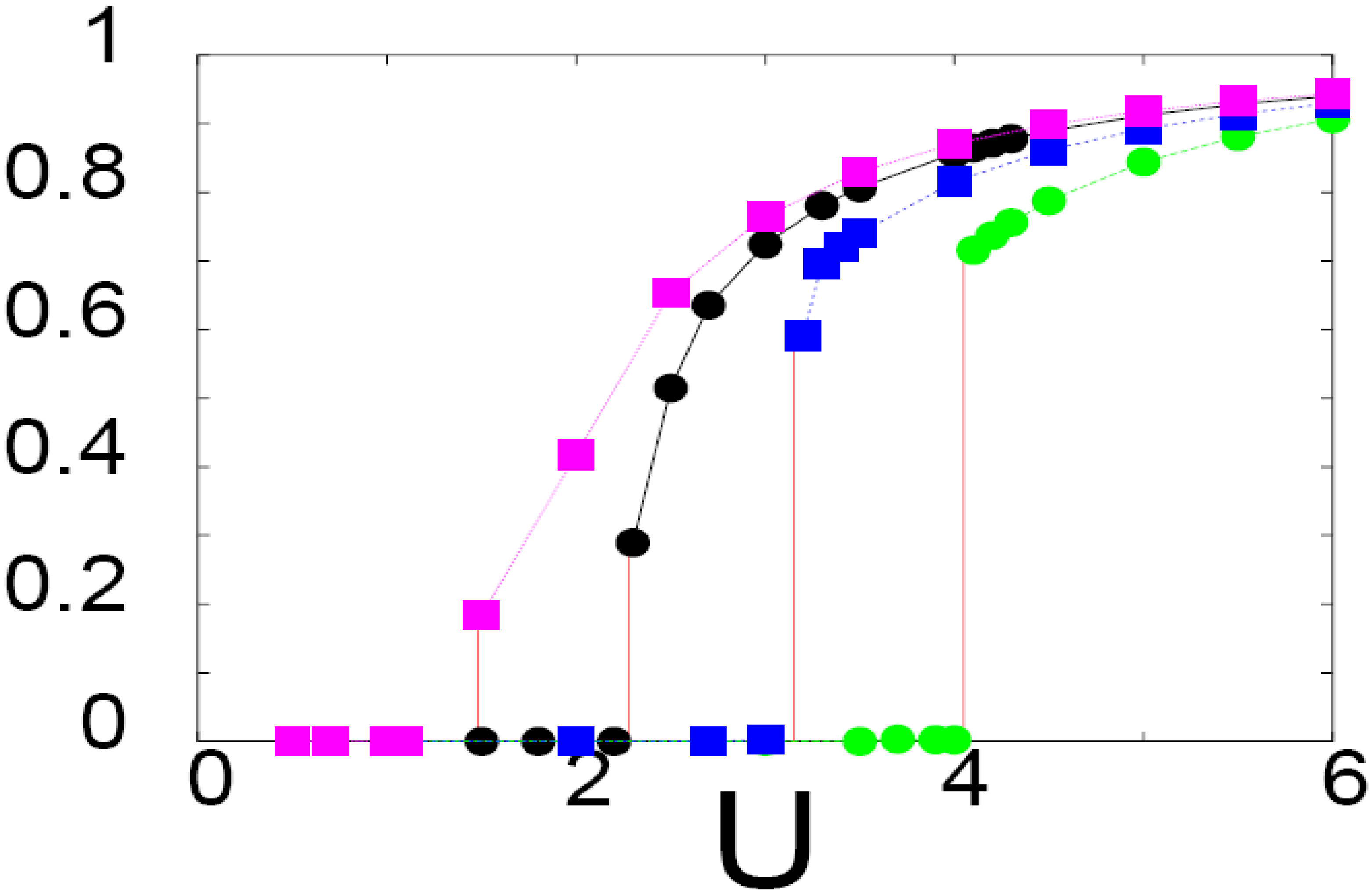
with a local "host" propagator G_h such that

$$G_{ii}^{-1} = G_{h,ii}^{-1} - \Sigma \qquad \Rightarrow \qquad \boxed{G_{h,ii} = [G_{ii}^{-1} + \Sigma]^{-1}}$$

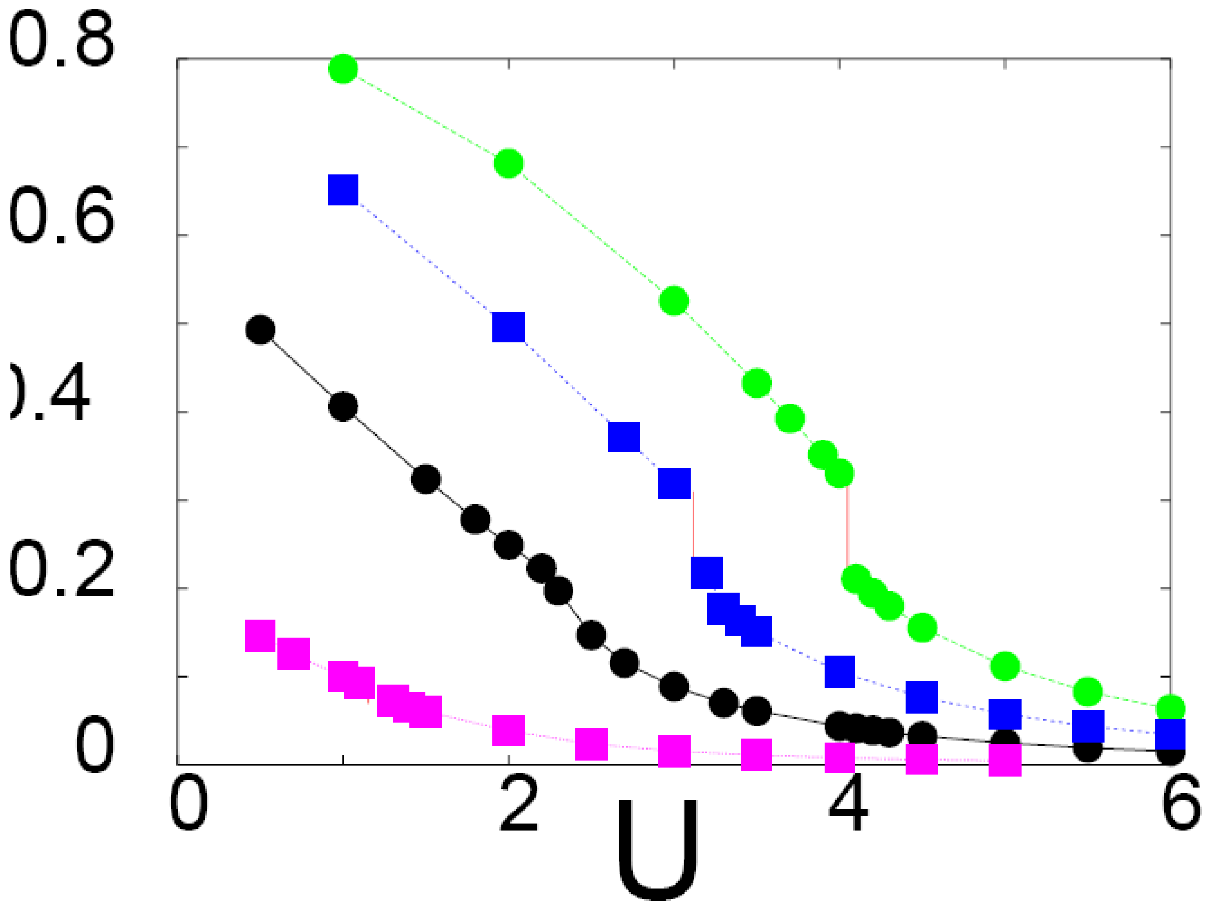
Is determined by the solution of the impurity problem given G_h or G_{ii}

"self consistent embedding" which closes the equations.

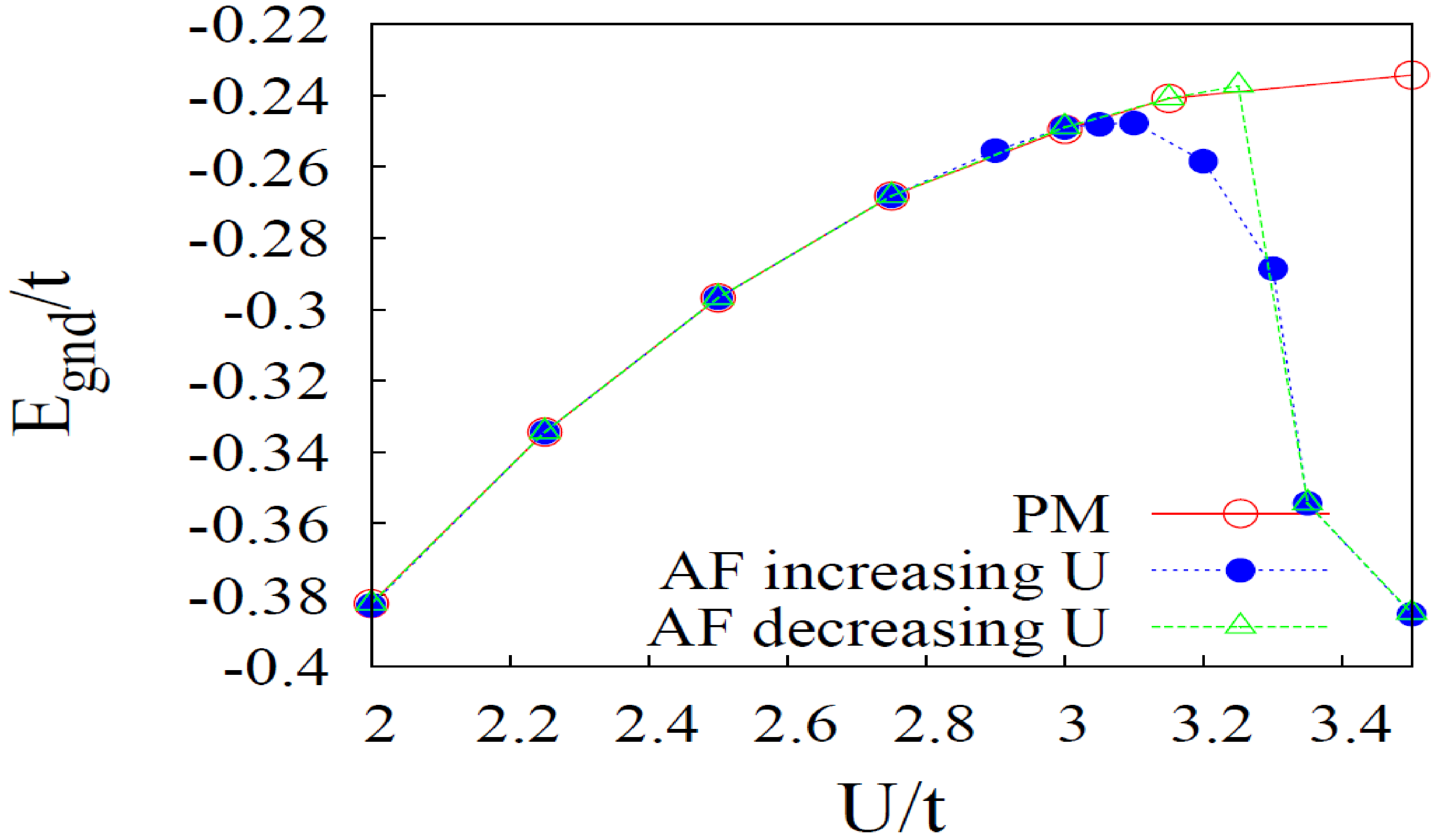
Staggered Magnetization vs. U/t for various values of Δ/t (IPT)



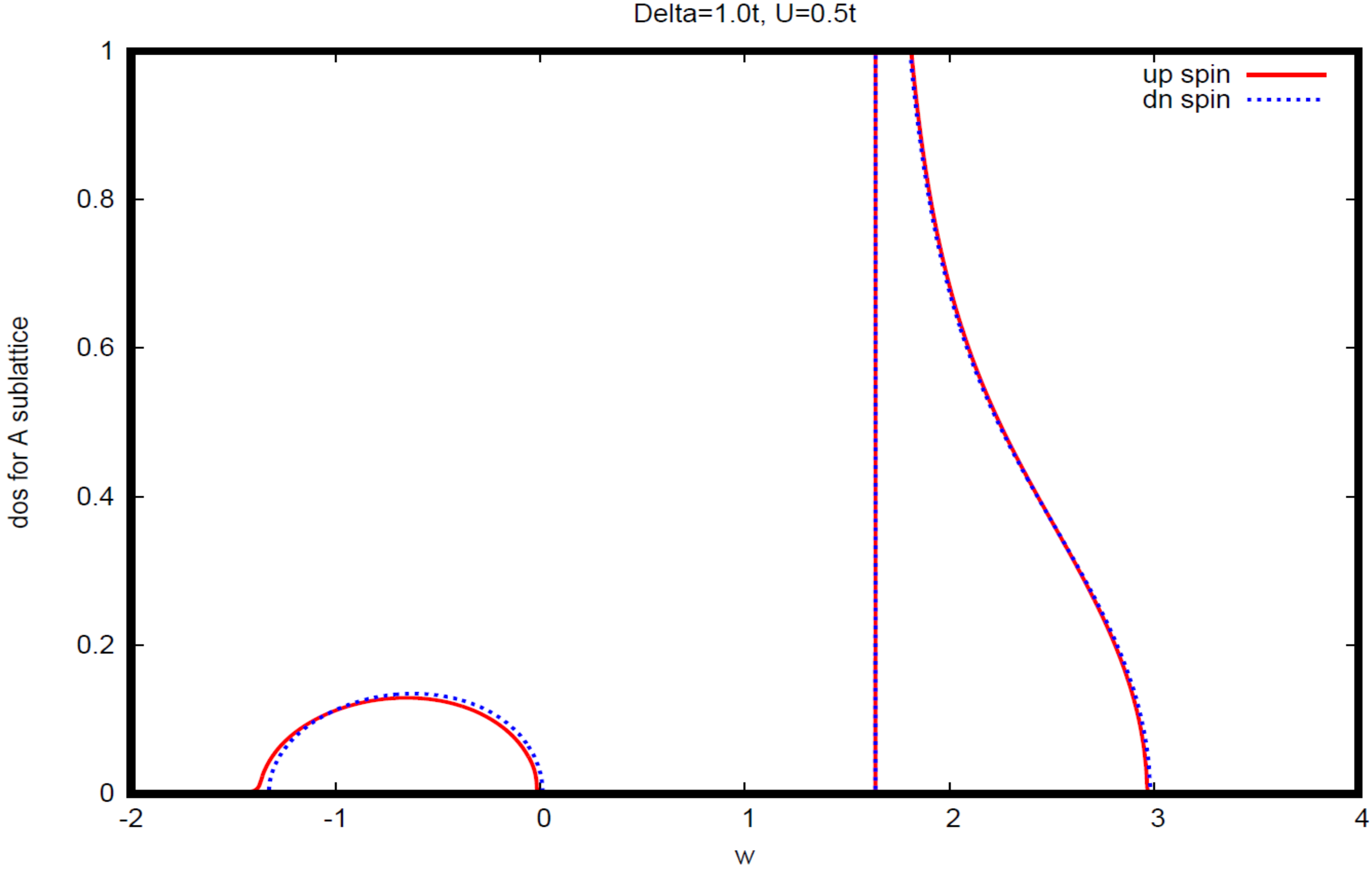
Staggered Charge versus U for various values of Δ/t (IPT)



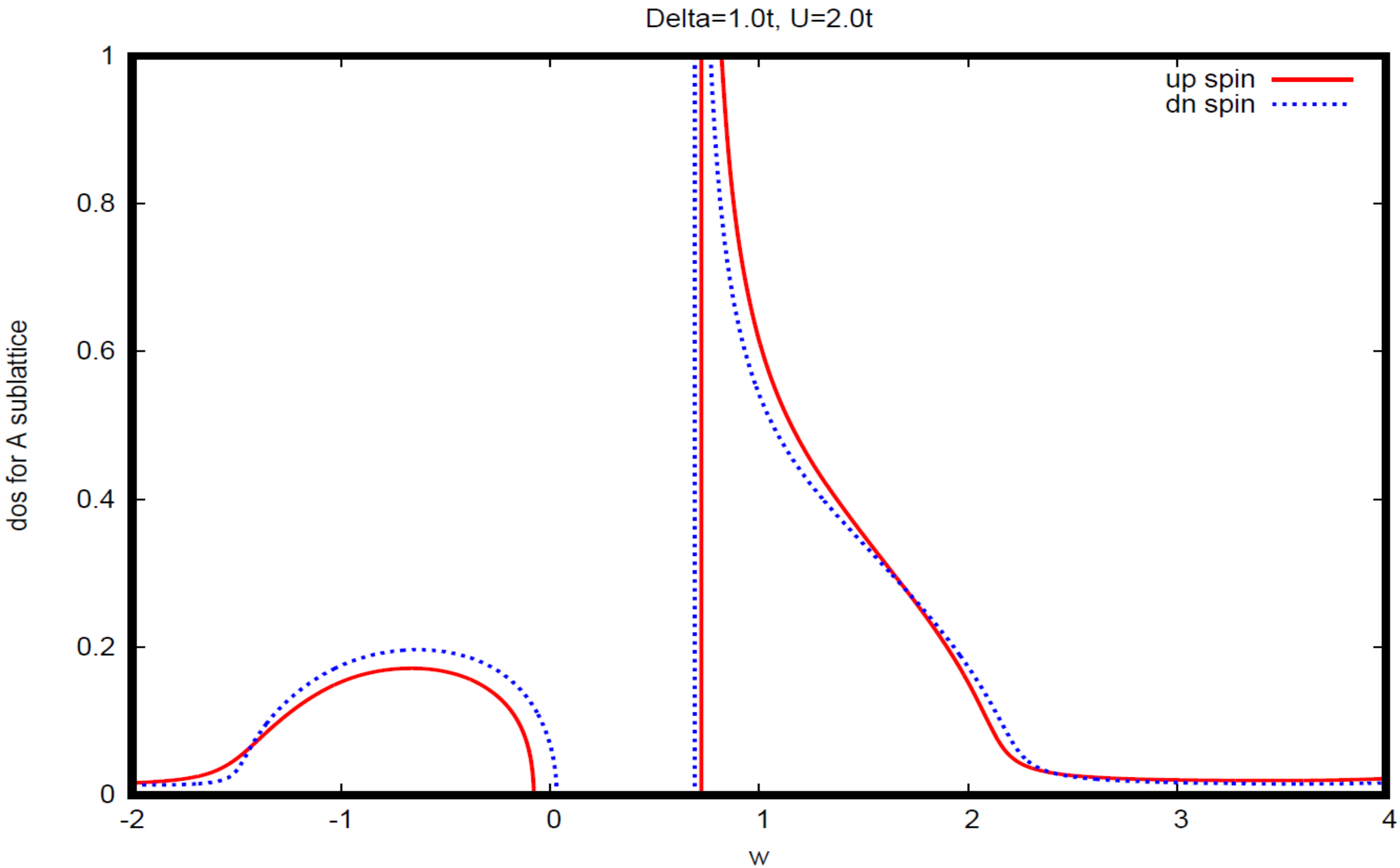
Ground State Energy versus U/t (Δ/t =1.0)



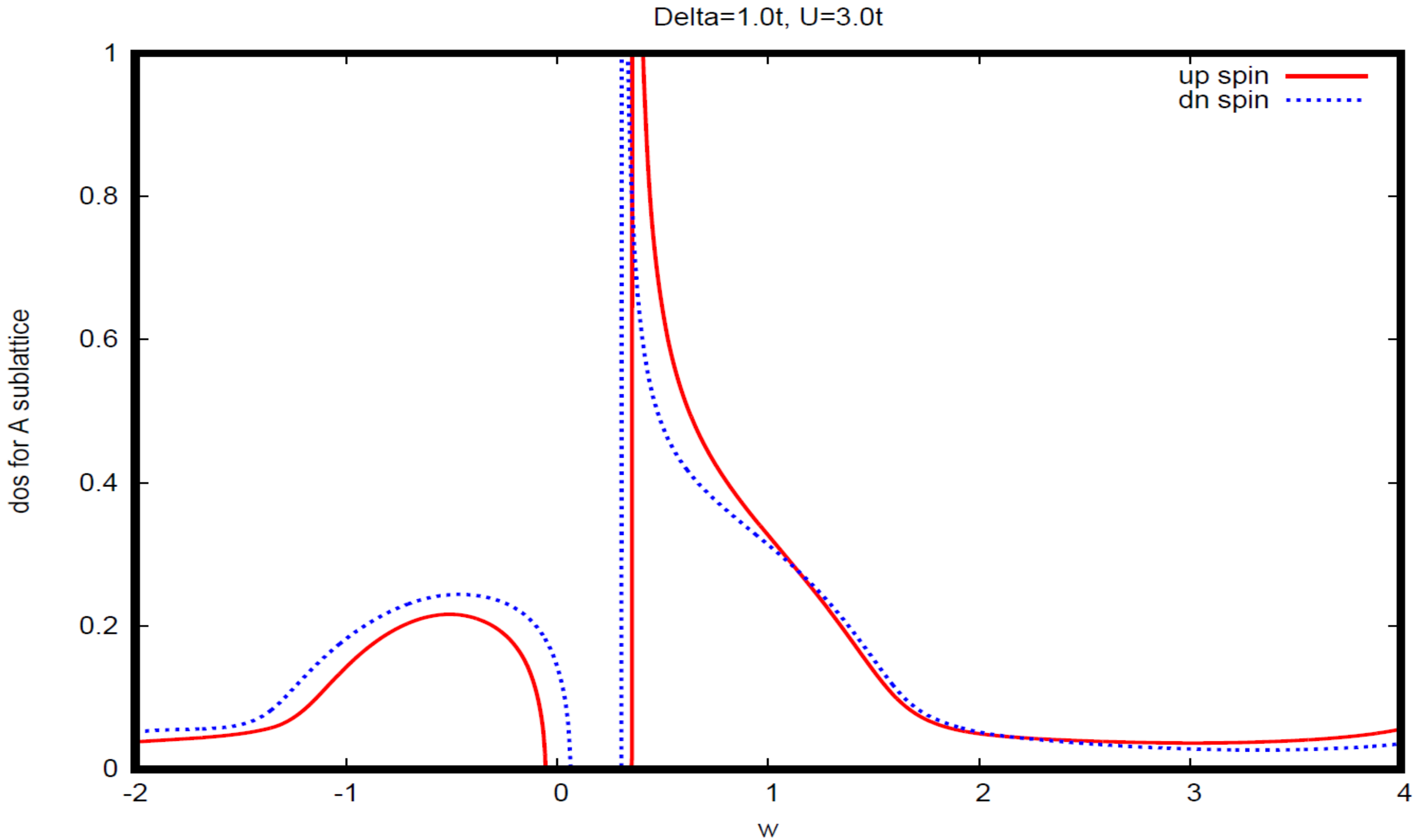
A Sub-lattice DOS for U/t = 0.5 (Δ/t = 1.0, n=0.95)



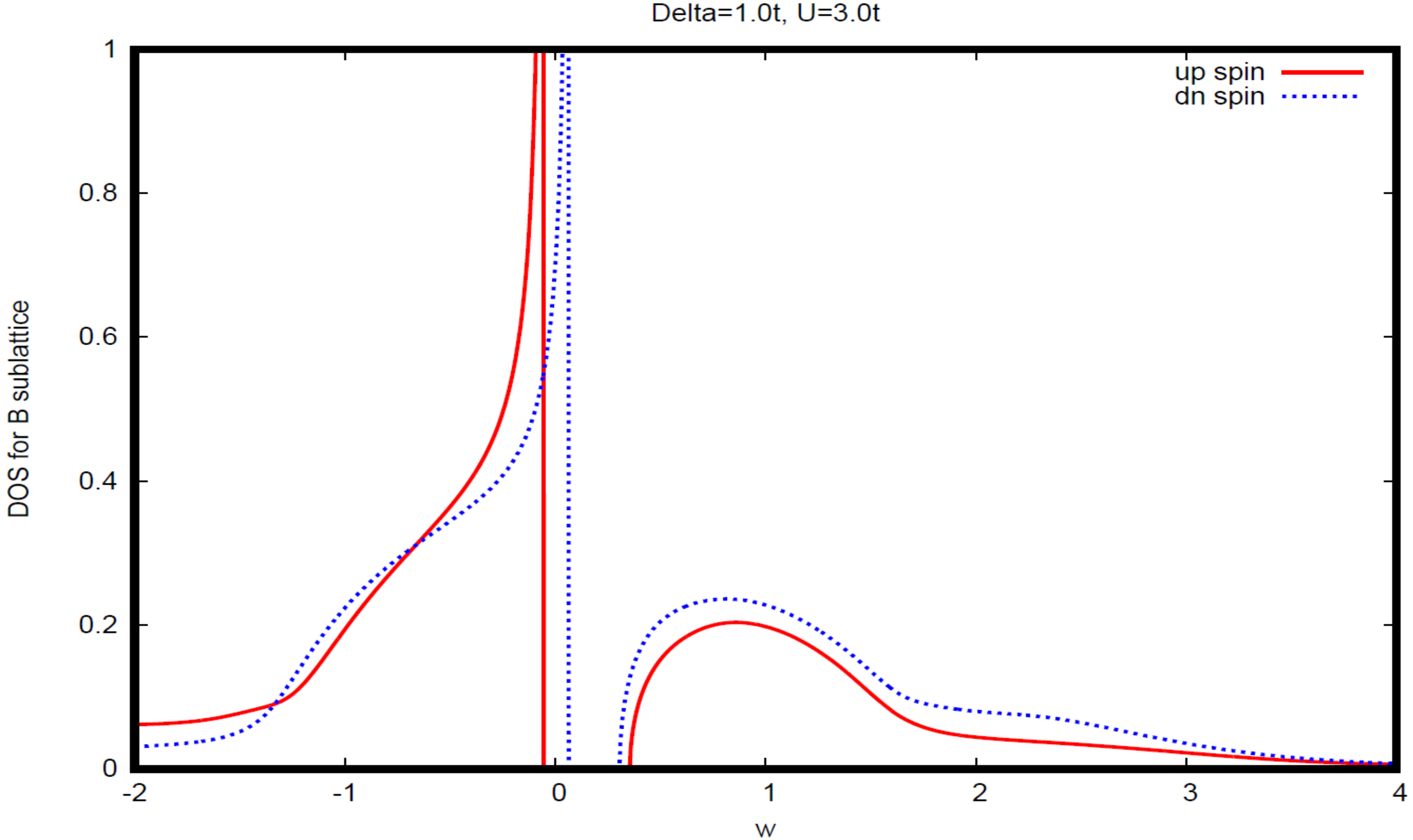
A Sub-lattice DOS for U/t = 2.0 (Δ/t = 1.0, n=0.95)



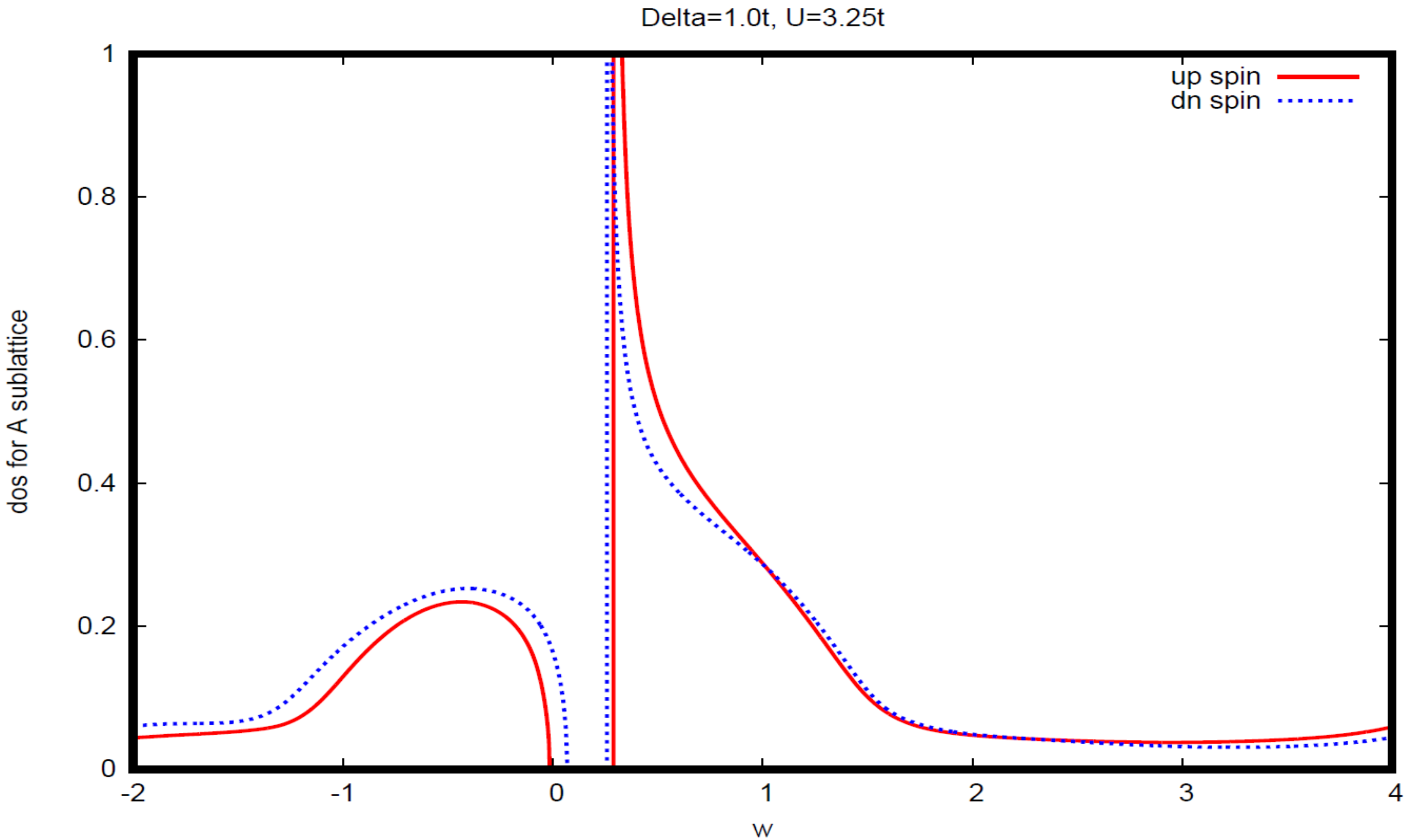
A Sub-lattice DOS for U/t = 3.0 (Δ/t = 1.0, n=0.95)



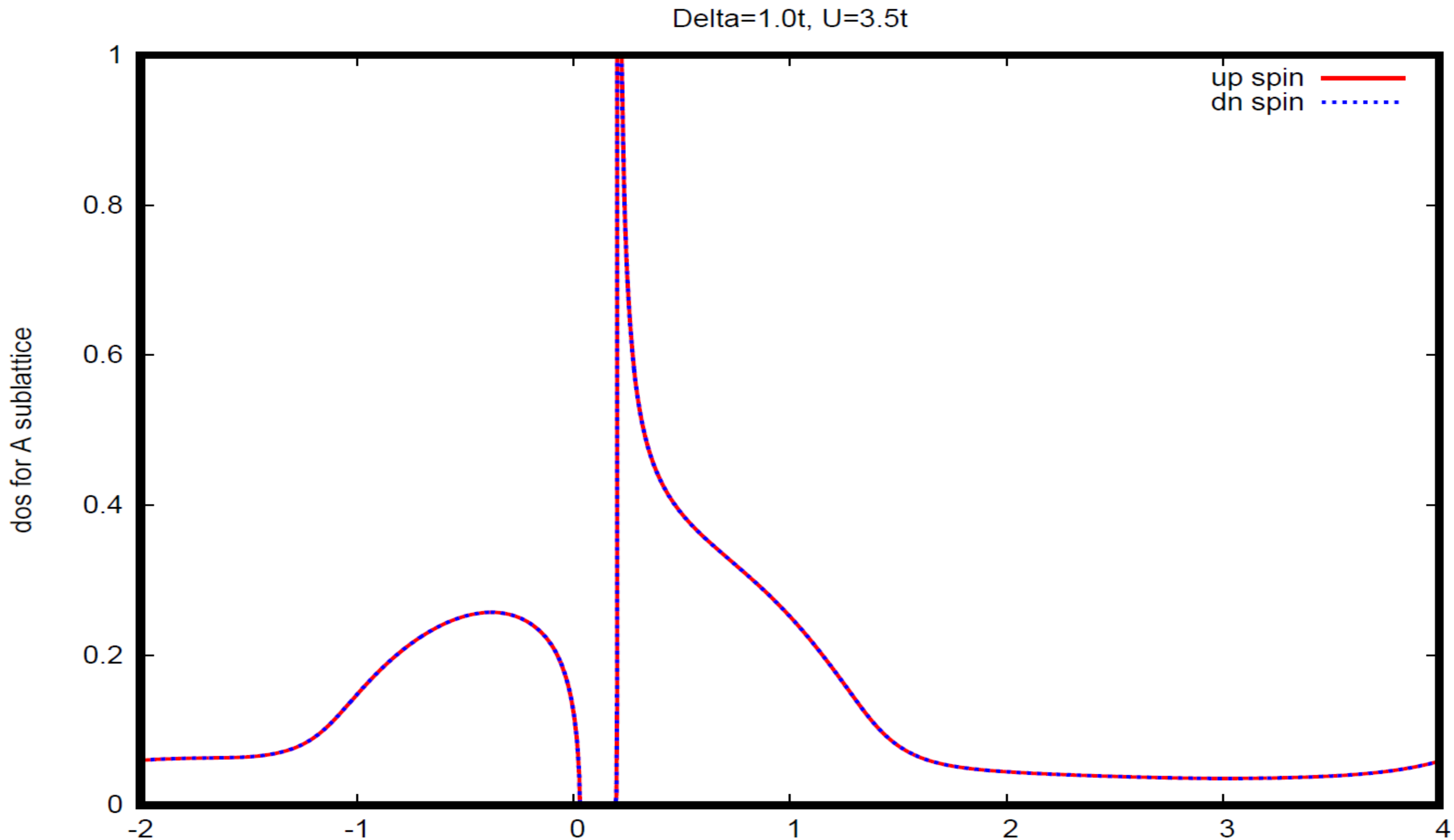
B Sub-lattice DOS for U/t = 3.0 (Δ/t = 1.0, n=0.95)



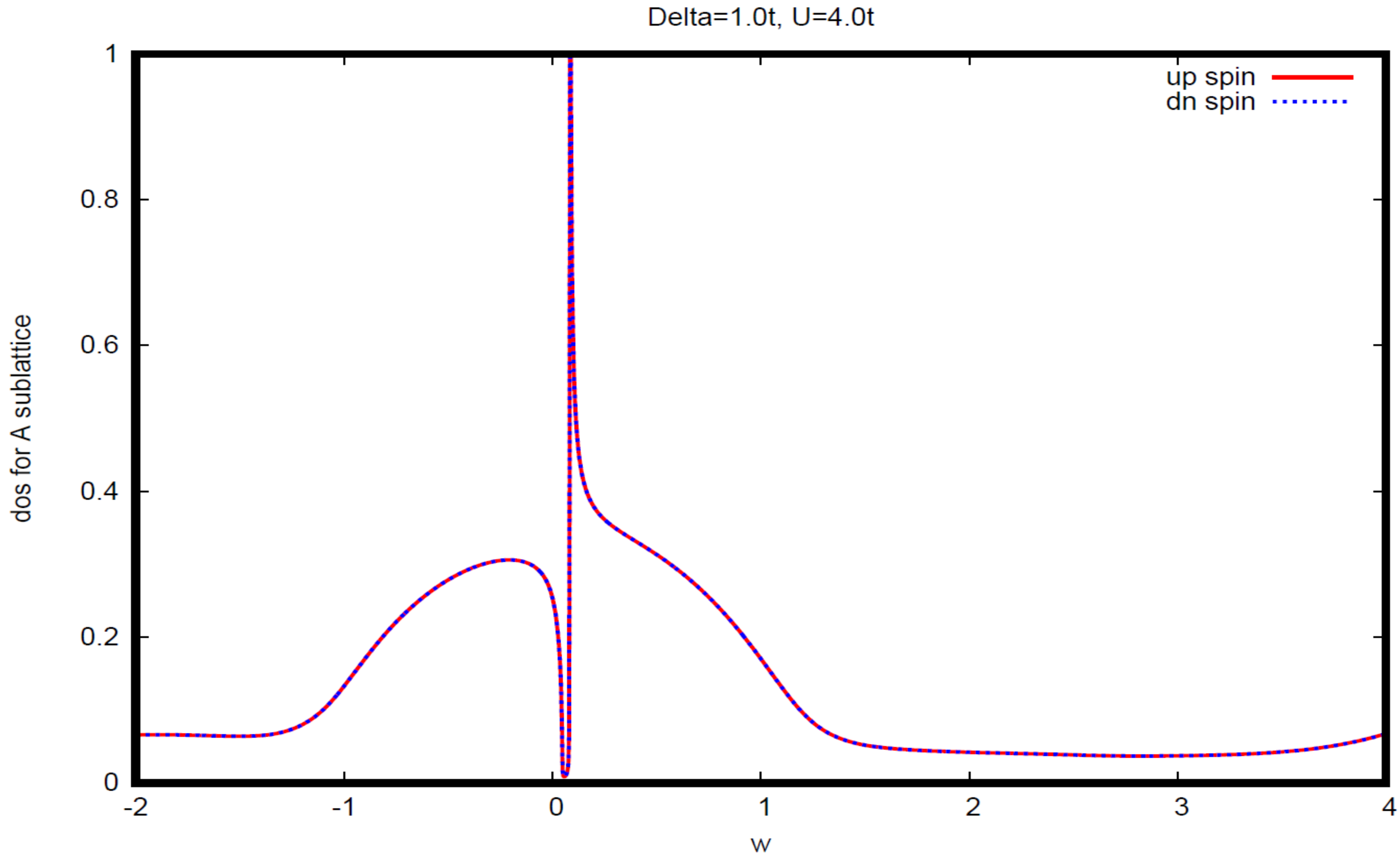
A Sub-lattice DOS for U/t = 3.25 (Δ/t = 1.0, n=0.95)



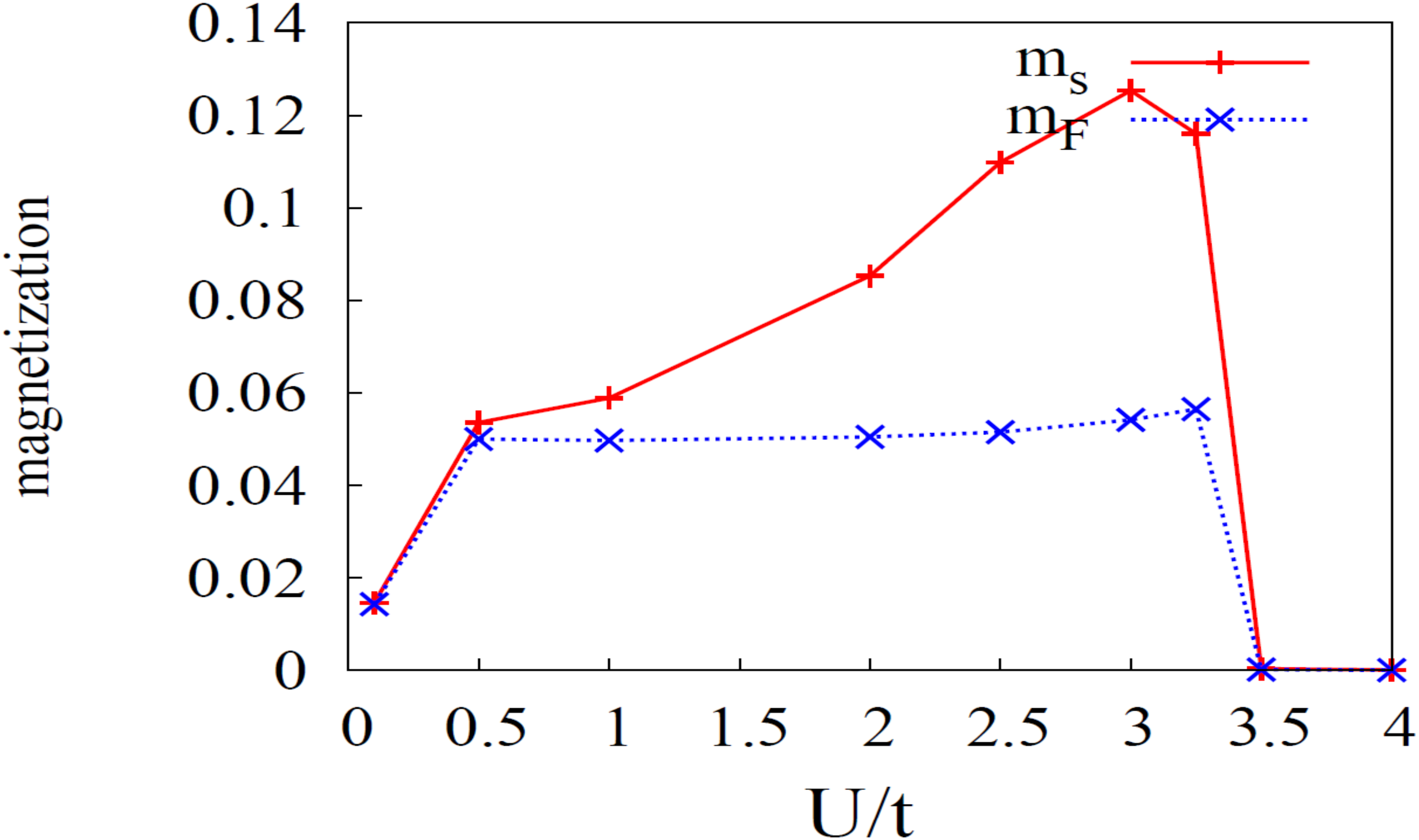
A Sub-lattice DOS for U/t = 3.5 (Δ/t = 1.0, n=0.95)



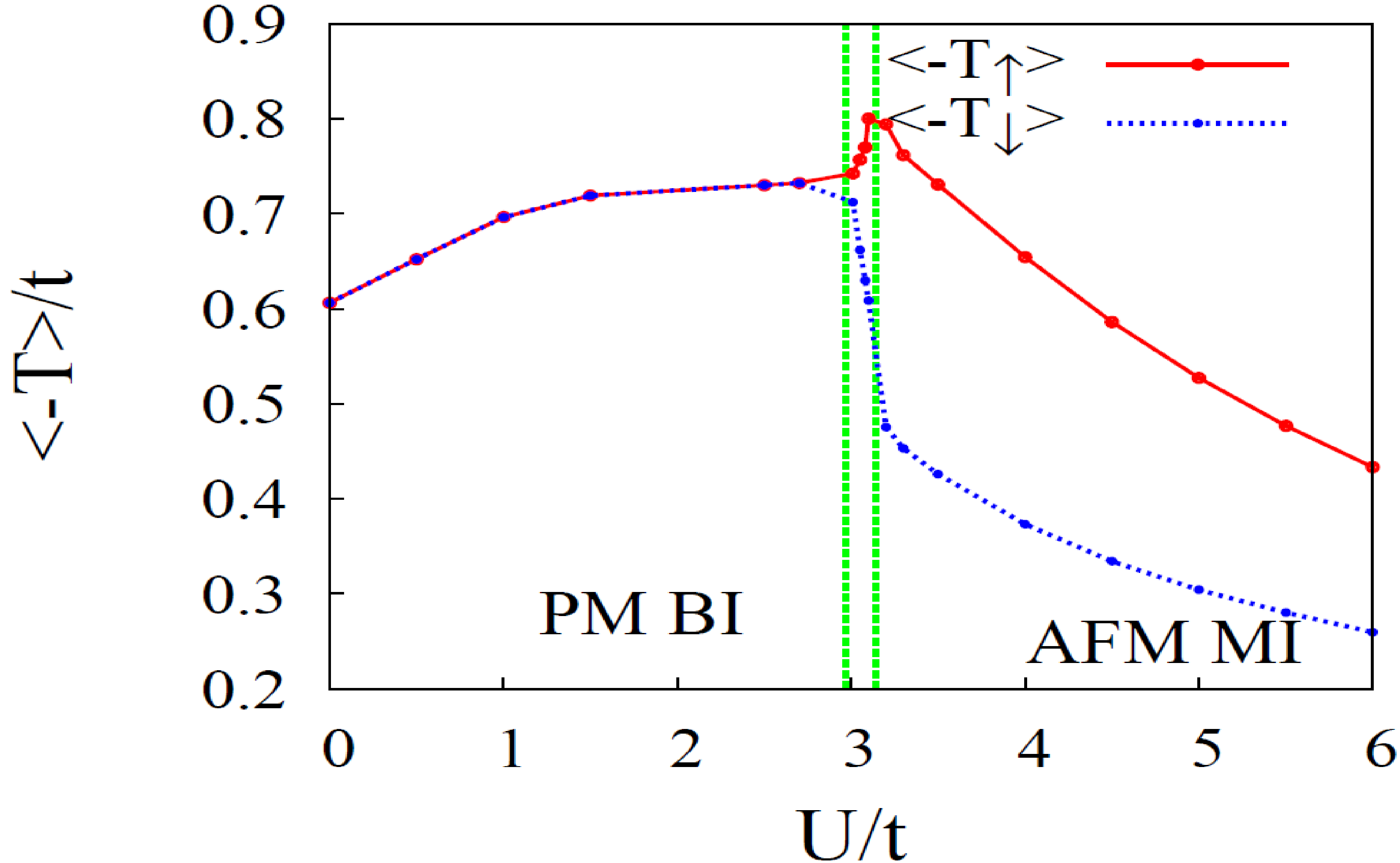
A Sub-lattice DOS for U/t = 4.0 (Δ/t = 1.0, n=0.95)



Staggered magnetization and magnetization vs. U ($\Delta/t = 1.0$, $n=0.95$)



Kinetic Energies of the two spin species versus U/t (Δ/t=1.0)



Quasi Particle weight

$$Z^{-1} = 1 - \frac{\partial \Sigma_{A,B'}(\omega)}{\partial \omega}|_{\omega=0}$$

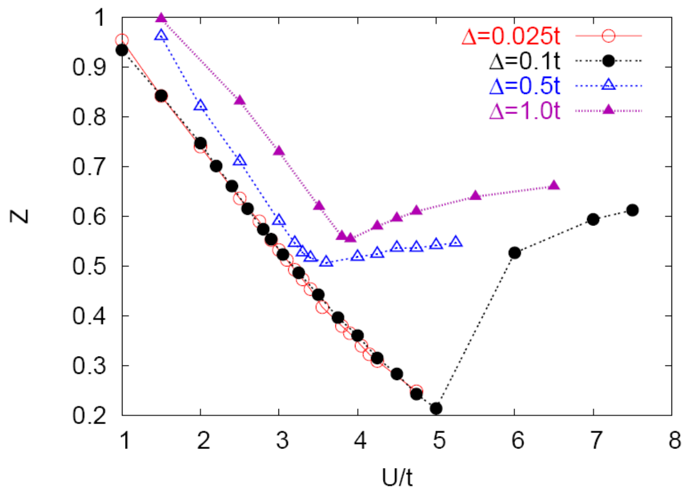
Is well defined in all the phases

In the metallic phase It has the meaning of a quasi-particle residue

$$A(\epsilon, \omega) \approx Z_{QP}\delta(\omega - Z_{QP}\epsilon)$$

With $Z_{QP} = Z$

$Z_{QP} = 0$ in both the insulating phases



An Analysis of the Suppression of the Gap

- In all the three phases, at low frequencies

$$\Sigma'_\alpha(\omega) = \Sigma'_\alpha(0) + (1 - Z^{-1})\,\omega + \ldots,$$

- In the Insulating phases,

$$\Sigma''_\alpha = 0 \ \text{for} \ |\omega| \leq 3E_{\text{gap}}$$

$$\mathcal{A}_{\alpha\alpha}(\epsilon,\omega) = -1/\pi \mathrm{Im} G_{\alpha\alpha}(\epsilon,\omega^+) = \delta(r(\omega) - \epsilon^2)$$

- Gap determined by

$$r(\omega) = (\omega + \mu - \Delta - \Sigma'_A(\omega))(\omega + \mu + \Delta - \Sigma'_B(\omega))$$

$$r\,(E_{\text{gap}}) = 0 \quad \Leftrightarrow \quad E_{\text{gap}} = Z|\Delta - U\delta n/2 + S|$$

$$S = P\int_{-\infty}^{\infty} d\omega \Sigma''_A(\omega)/\pi\omega$$

An Analysis of the Suppression of the Gap

- Correlations "screen" the one –body potential Δ and suppress the Gap via

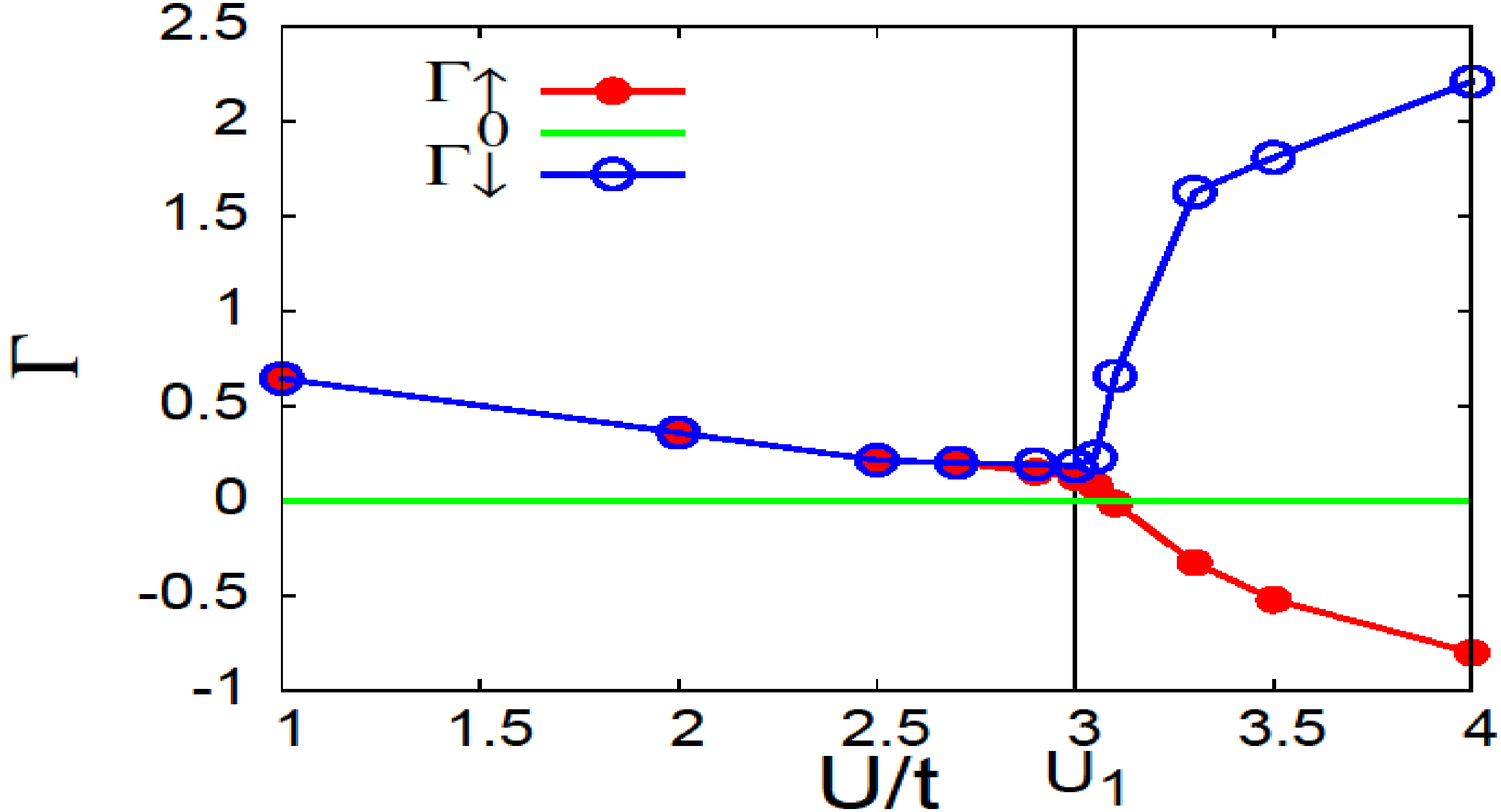
S (< 0) and Z (< 1)

for

$$E_{\text{gap}} = 0 \qquad U = 2|\Delta + S(U)|/\delta n(U)$$

$$U_{c1} \simeq 2\Delta/\delta n(U_{c1}) \geq 2\Delta/\delta n(0) \gg \Delta$$

Low frequency analysis and the Gaps (IPT)



Low frequency analysis and the Gaps (IPT and CT-HYB)