Photoemission spectra in Mott Insulating Surfaces

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CORPES05

Outline

- **Mott state in Silicon triangular surfaces**
  - **Magnetic properties**

    ¿Can be detected 120° Néel order in these surfaces?
  - **Spectroscopic fingerprints of the magnetic order**
    - **Model and methods used**
- **Conclusions and perspectives**

Silicon surfaces are ideal to look for Mott states

Although Coulomb potential U is not so large (1eV)

Electrons can localize due to

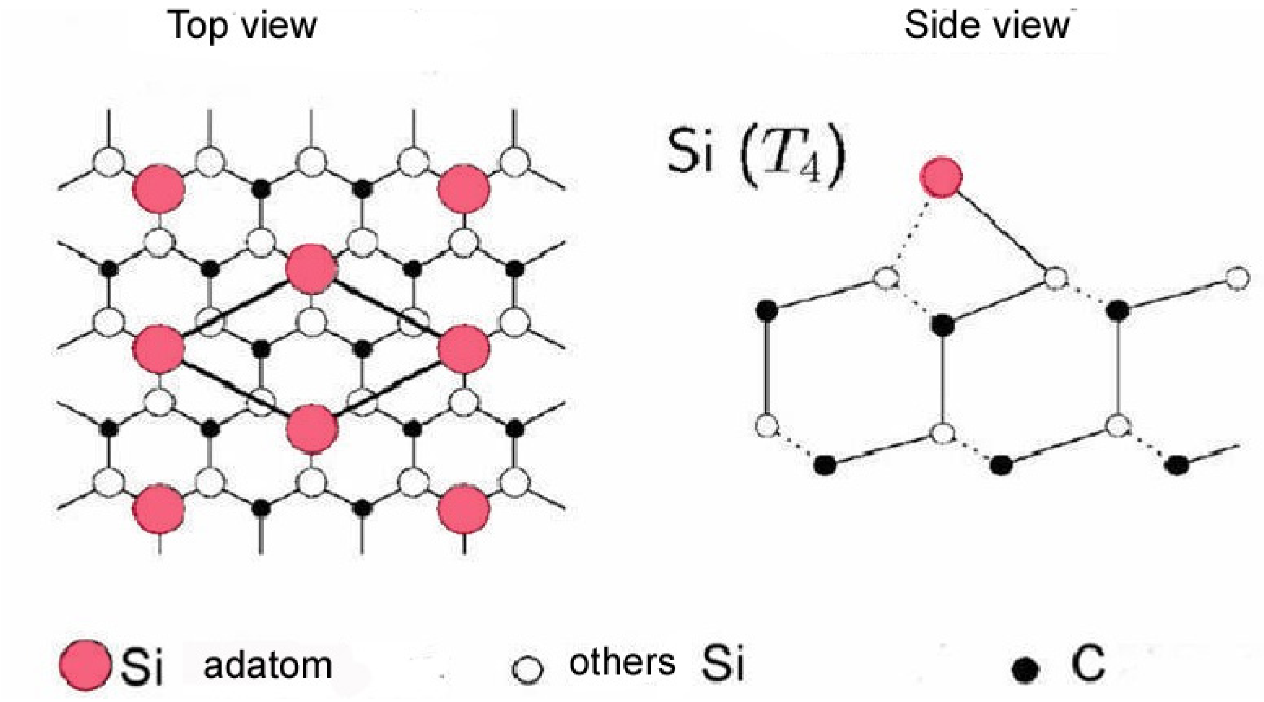
- **Atoms at surfaces have lower coordination than in the bulk**
- **reconstruction yields much larger interorbital spacing in the bulk → lower t**

↓

$U / W > 1$ strong correlation without transition metal ions

Surface SiC (0001)

- LEED and STM → *triangular* **√3 x √3** reconstruction
- First principles total energy calculation
  (Northrup et al, PRB ‘95)



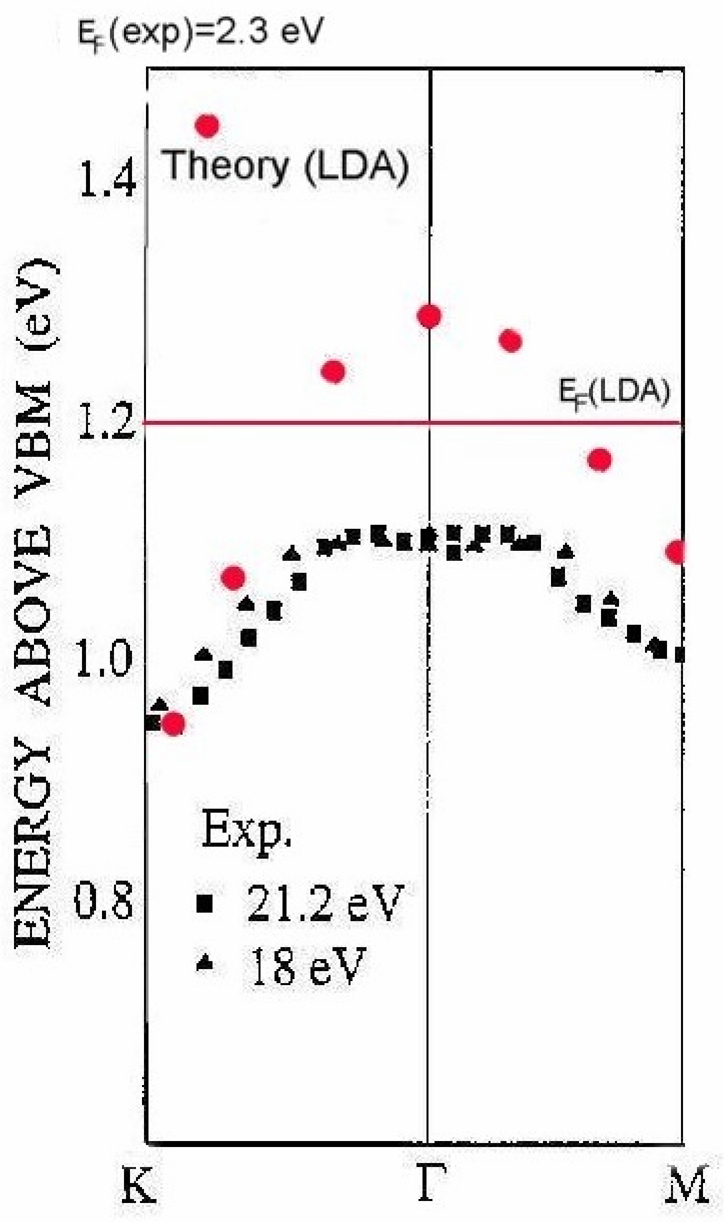
A non-saturated sate per absorbed Si →

LDA predicts a half-filled metallic surface band

W = 0.35 eV **t = 0.04 eV**

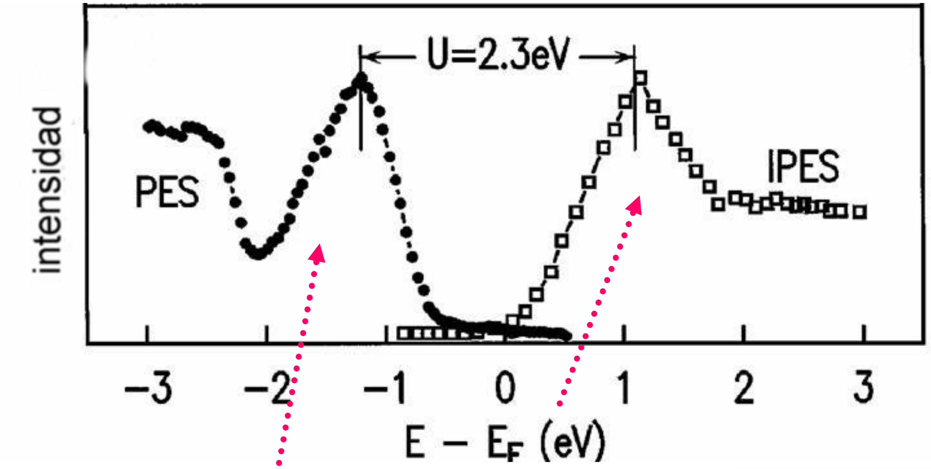
Experimentally, it is found a similar band ... but completely filled

W = 0.20 eV



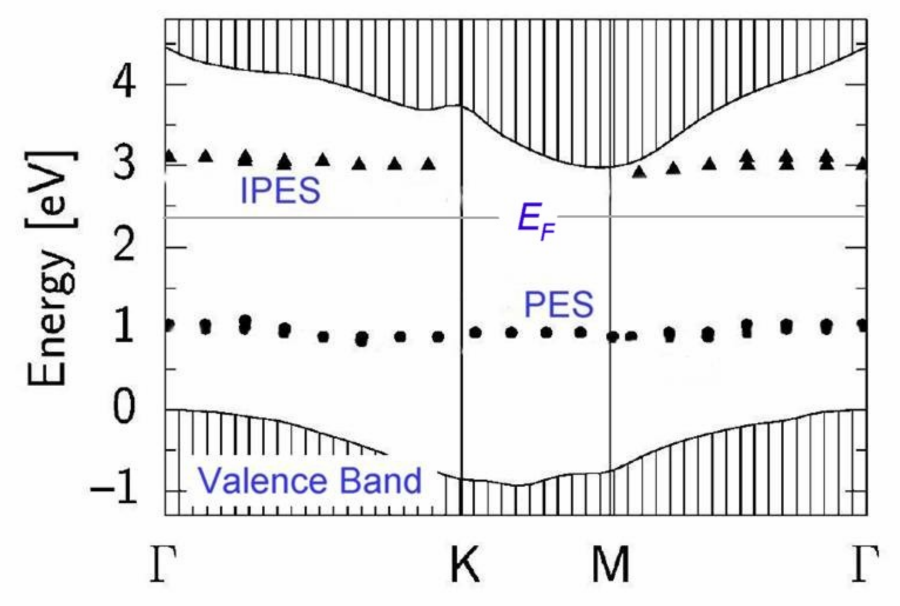
Photoemission: inverse and direct

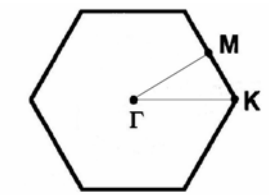
(Johansson *et al*, Surf. Sci. ’96)



U >> W →
surface Mott state

surface states



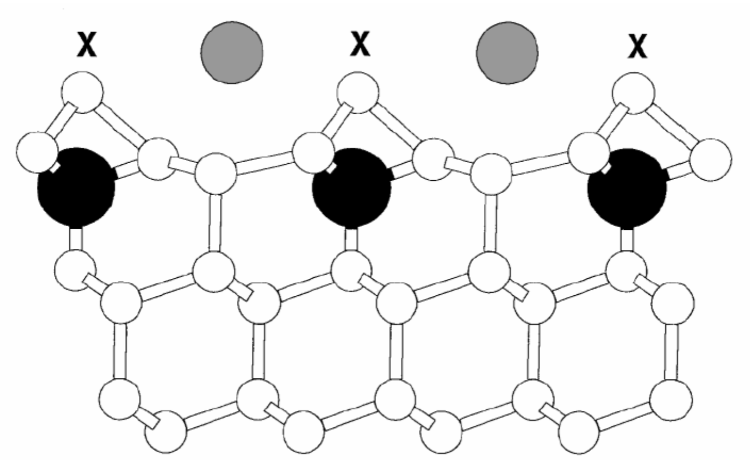


√3 x √3 – K/Si(111)-B

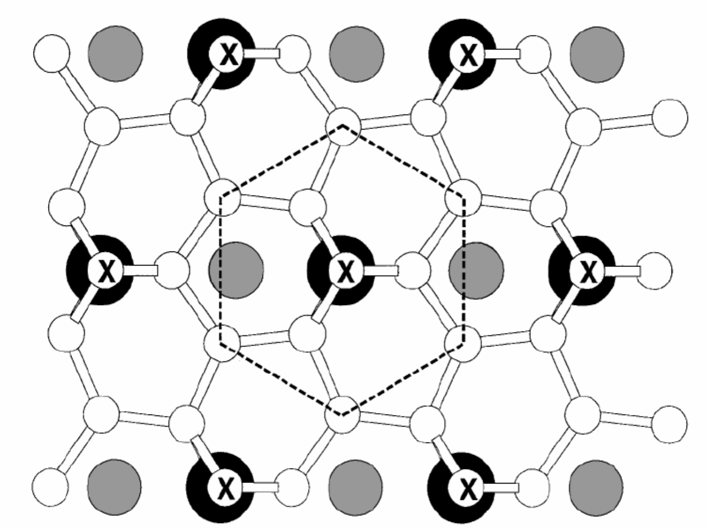
- LEED → *triangular* **√3 x √3** reconstruction
- First principles total energy calculation

(Y. Ma et al PRL’90)

Side view



Top view



○ Si ● B ● K

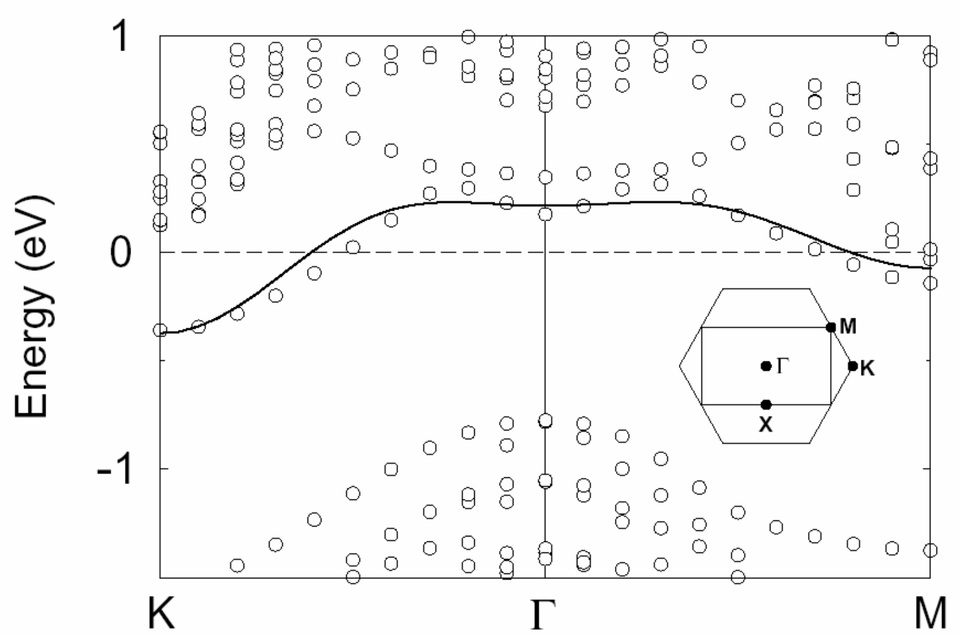
X Si dangling bond

Theory vs Experiments

√3 x √3 – K/Si(111)-B

LDA calculation

(Hellberg et al, PRL'99)



$$\varepsilon(\mathbf{k}) = 2t_1[\cos(k_y) + 2\cos(k_x\sqrt{3}/2)\cos(k_y/2)] + 2t_2[\cos(k_x\sqrt{3}) + 2\cos(k_x\sqrt{3}/2)\cos(3k_y/2)].$$

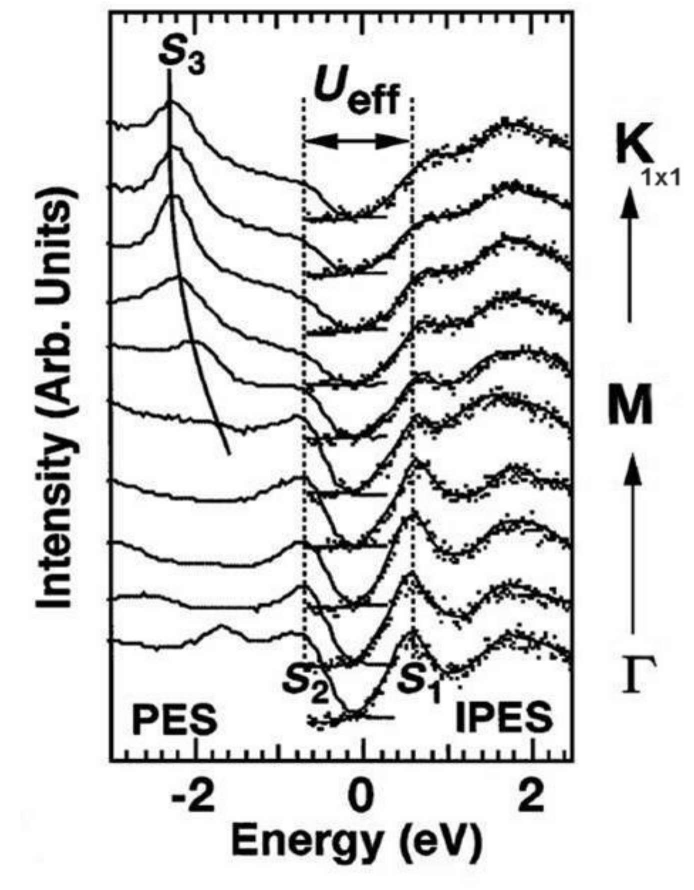
$t_1 = 0.07$ eV

$t_2 = -0.03$ ev

$U_{eff} = 1$ eV

Photoemission

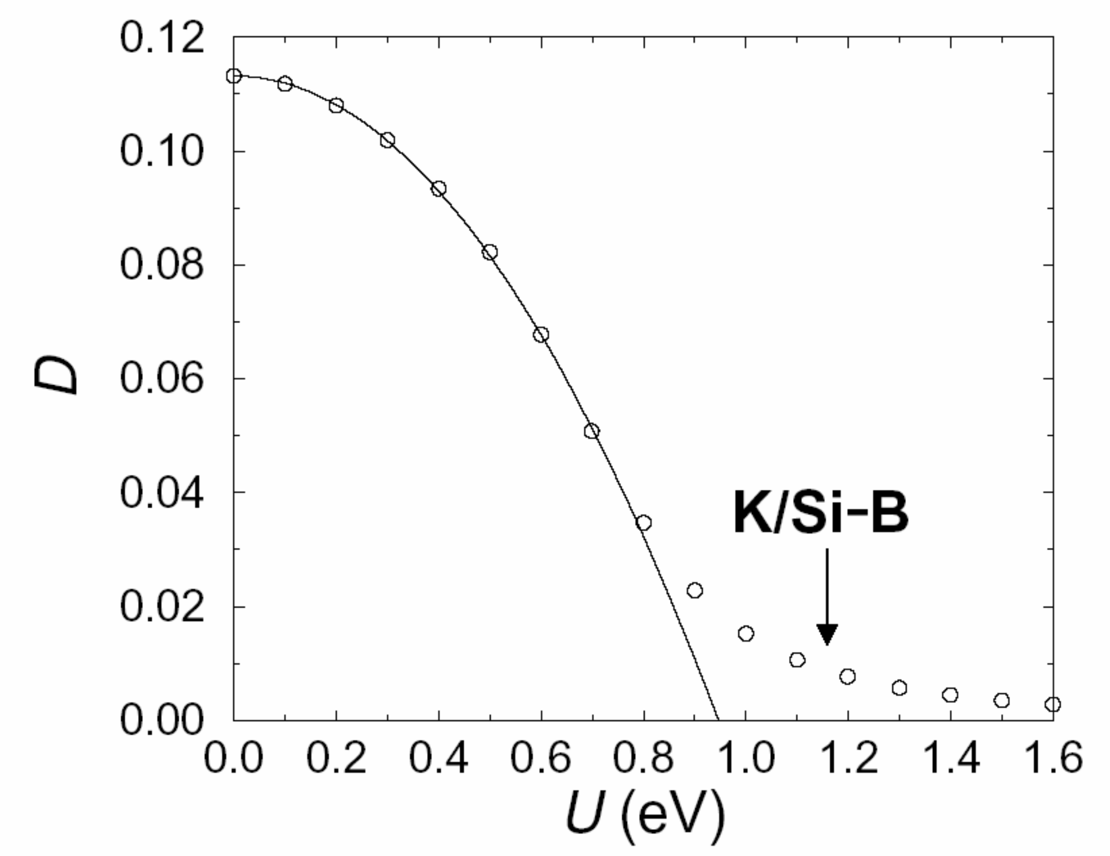
(Weitering et al, PRL '97)



Hubbard model realistic parameters

$$D = \partial^2 E / \partial \phi^2$$

Zero frequency conductivity or Drude weight



K/Si-B insulator

(Hellberg PRL 99’)

What about the magnetic ground states of these surfaces?

Hubbard model
triangular lattice →

No perfect nesting
Critical value U/t
magnetic order

$(U/t)_{\mathrm{SiC}} = 20$, $(U/t)_{\mathrm{K/Si\text{-}B}} = 40 > (U/t)_{\mathrm{crit}} = 12$ (Cappone PRB, 2001)

SiC and K/Si-B **seems to be located at AF phase**

Low energy physics of a Mott insulator: dominated by spin fluctuations

↓

Heisenberg model (localized spins)

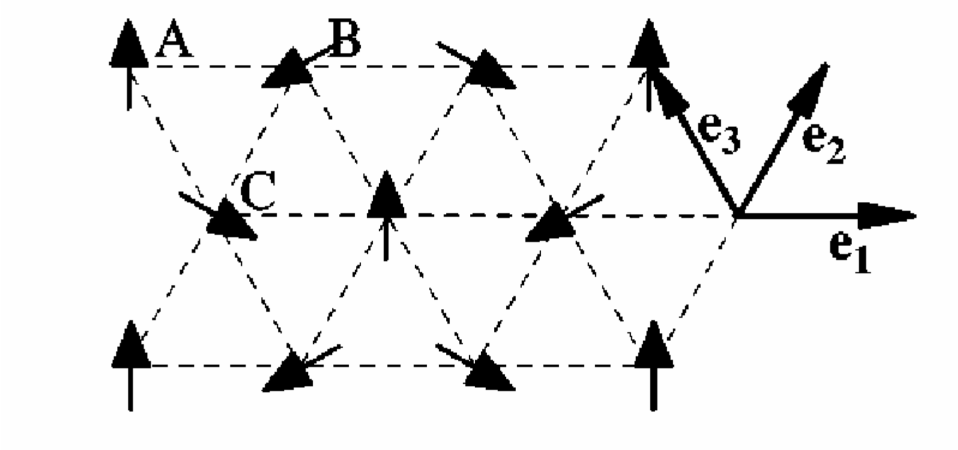
$$H = \sum_{<ij>} J_{ij} \mathbf{S_i} . \mathbf{S_j}$$

$$J_{ij} = \frac{4t_{ij}^2}{U}$$

SiC(0001) and K/Si(111)-B: first experimental realization of the Heisenberg model on triangular lattice

Theory: **120° Néel oder ground state**

(Capriotti Trumper Sorella, PRL ’99)
(Bernu et al PRL’92)



Experiments?

*¿ Can be detected **120 ° Néel order** in these surfaces?*

- **Usual LRO techniques are difficult to implement**
- **Nowadays, high-resolution (~10 meV) ARPES experiments are possible**
- **Is it possible to obtain *Spectroscopic Fingerprints* of 120° Néel Order ?**

↓

We study the hole-dynamic in 120° Néel order on triangular lattice

For realistic parameters of ***K/Si(111)-B- √3X √3***
SiC(0001)- √3X √3

Model and techniques used

t-J model

$$H = -t \sum_{\langle ij\rangle\sigma} (\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + \hat{c}^{\dagger}_{j\sigma}\hat{c}_{i\sigma}) + J\sum_{\langle ij\rangle}\left(\mathbf{S}_i\mathbf{S}_j - \frac{n_i n_j}{4}\right)$$

Once magnetic order is assumed, spinless fermion and Holstein-Primakov

$$\hat{c}_{i\uparrow} = h^{\dagger}_i \qquad \hat{c}^{\dagger}_{i\downarrow} = h_i S^-_i$$

$$S^x_i \sim \frac{1}{2}(a^{\dagger}_i + a_i) \qquad S^y_i \sim \frac{i}{2}(a^{\dagger}_i - a_i) \qquad S^z_i = \frac{1}{2} - a^{\dagger}_i a_i$$

Effective Hamiltonian

$$H = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} h^{\dagger}_{\mathbf{k}} h_{\mathbf{k}} + \sum_{\mathbf{q}} \omega_{\mathbf{q}} \alpha^{\dagger}_{\mathbf{q}} \alpha_{\mathbf{q}} - t\sqrt{\frac{3}{N_s}} \sum_{\mathbf{k},\mathbf{q}} \left[M_{\mathbf{k}\mathbf{q}} h^{\dagger}_{\mathbf{k}} h_{\mathbf{k}-\mathbf{q}} \alpha_{\mathbf{q}} + h.c.\right]$$

Free hole energy

Free magnon energy

hole-magnon vertex

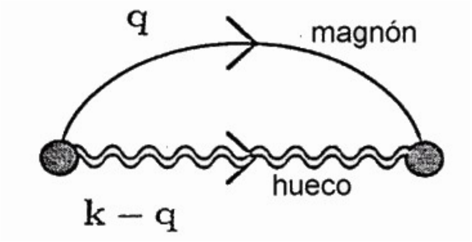
Self-consistent Born approximation (SCBA)

We calculate the hole **spectral function**

$$A_{\mathbf{k}}(\omega) = -\frac{1}{\pi} Im G^h_{\mathbf{k}}(\omega)$$

$$G^h_{\mathbf{k}}(\omega) = \langle AF | h_{\mathbf{k}} \frac{1}{(\omega + i\eta^+ - H)} h^\dagger_{\mathbf{k}} | AF \rangle$$

Solving the self-consistent eqn for self-energy



$$\Sigma_{\mathbf{k}}(\omega) = \frac{3t^2}{N_s} \sum_{\mathbf{q}} \frac{| M_{\mathbf{kq}} |^2}{\omega - \omega_{\mathbf{q}} - \epsilon_{\mathbf{k}-\mathbf{q}} - \Sigma_{\mathbf{k}-\mathbf{q}}(\omega - \omega_{\mathbf{q}})}$$

Quasiparticle weight

$$z_{\mathbf{k}} = \left(1 - \frac{\partial \Sigma_{\mathbf{k}}(\omega)}{\partial \omega}\right)^{-1} \Big|_{\ E_{\mathbf{k}} = \Sigma_{\mathbf{k}}(E_{\mathbf{k}})}$$

Two mechanisms for hole-motion

$$\sum_{k,q}[M_{kq}h_k^\dagger h_{k-q}\alpha_q + \text{h.c.}]$$

Magnon assisted hopping

Spin-polaron origin in
non-frustrates AF

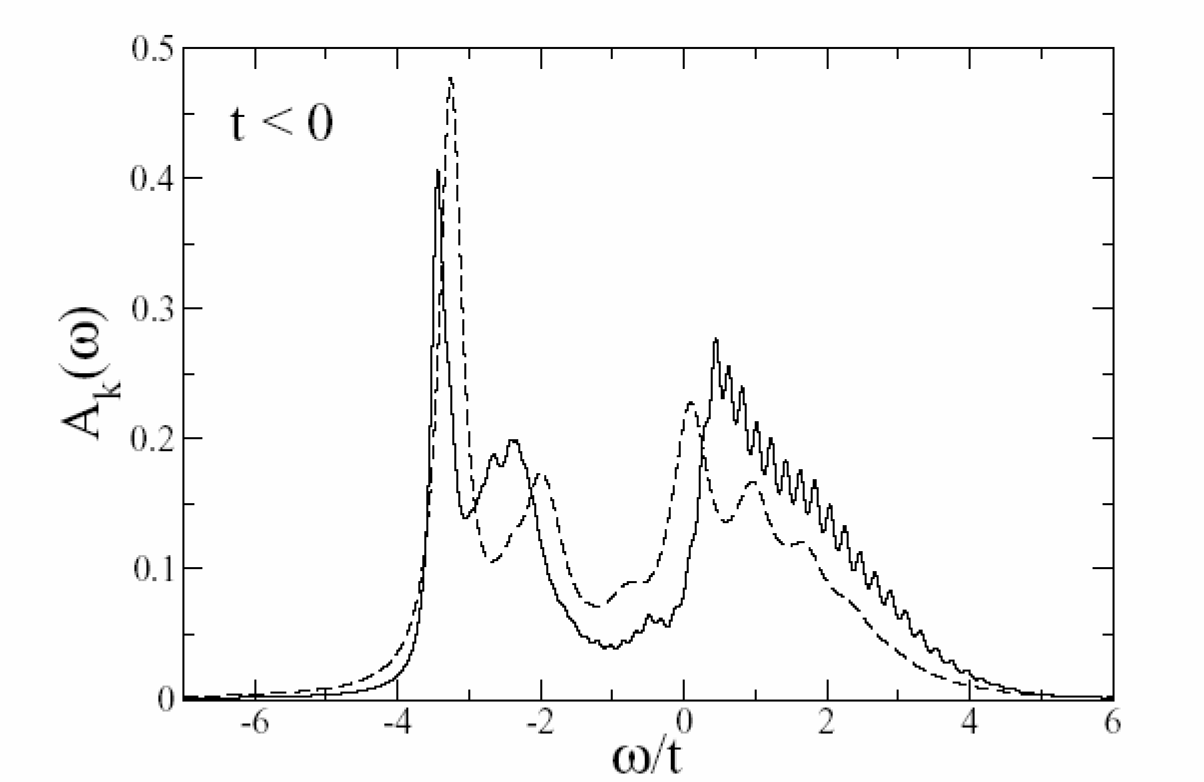
$$\sum_k \epsilon_k h_k^\dagger h_k$$

Free hopping: no absorption or emission of magnons (due to non-collinearity)

Both mechanisms interfere !
Quasiparticle survives?

Comparison SCBA vs exact results : Spectral function

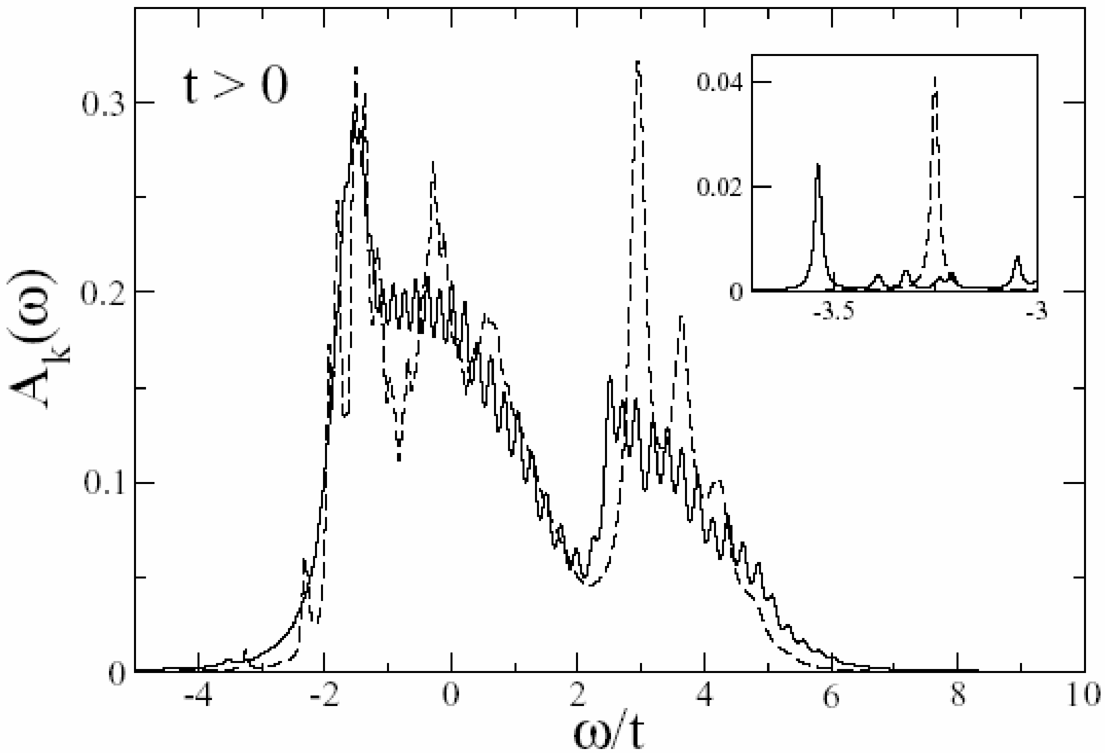
- **Cluster of 21 sites**
- **J =0.4 |t|**
- **t < 0**



________ Lanczos

_ _ _ _ _ _ _ SCBA

- **Cluster of 21 sites**
- **J =0.4 t**
- **t > 0**



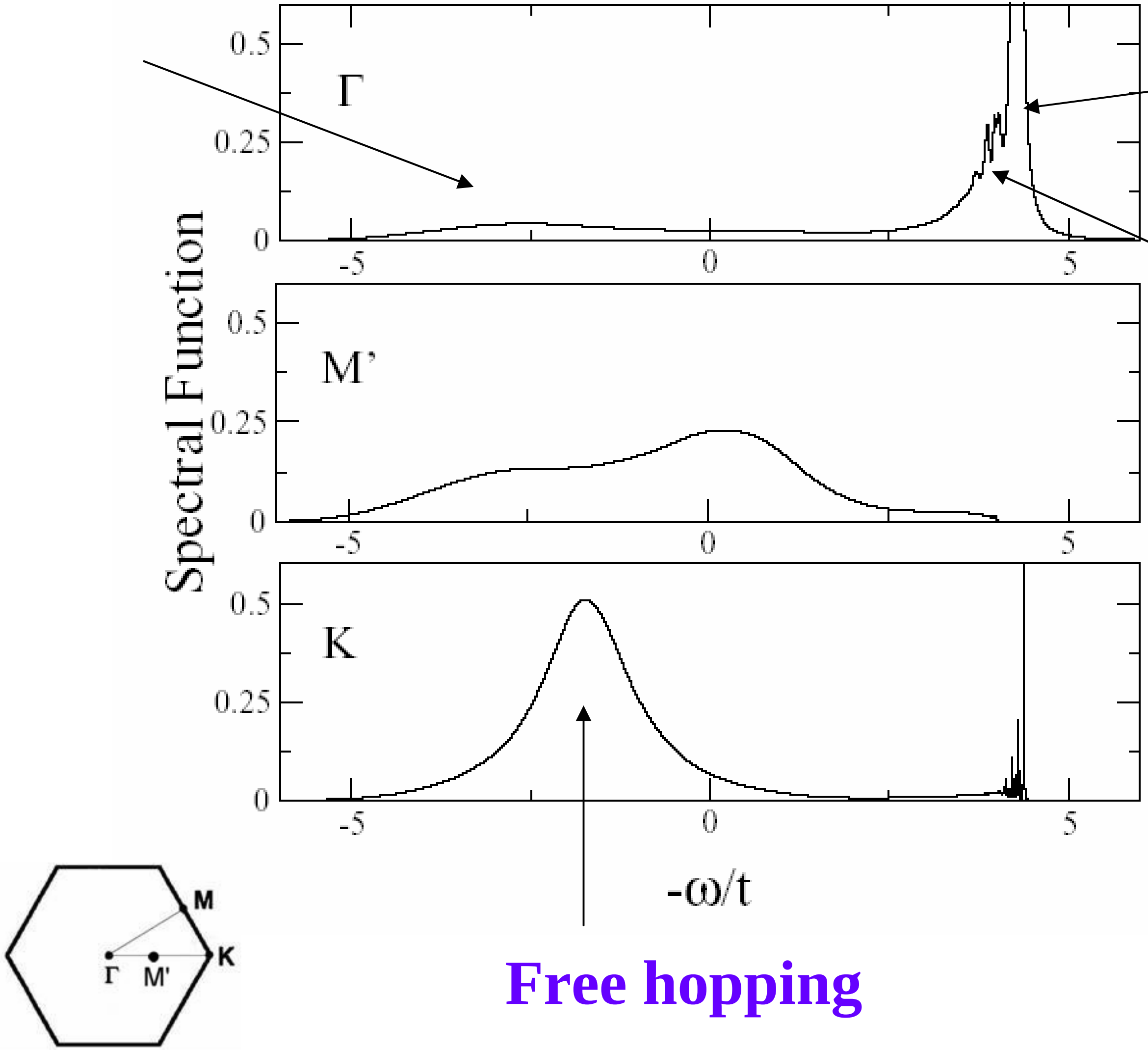
________ Lanczos

_ _ _ _ _ _ _ SCBA

Photoemission spectra (SCBA)

thermodynamic limit

incoherent
background

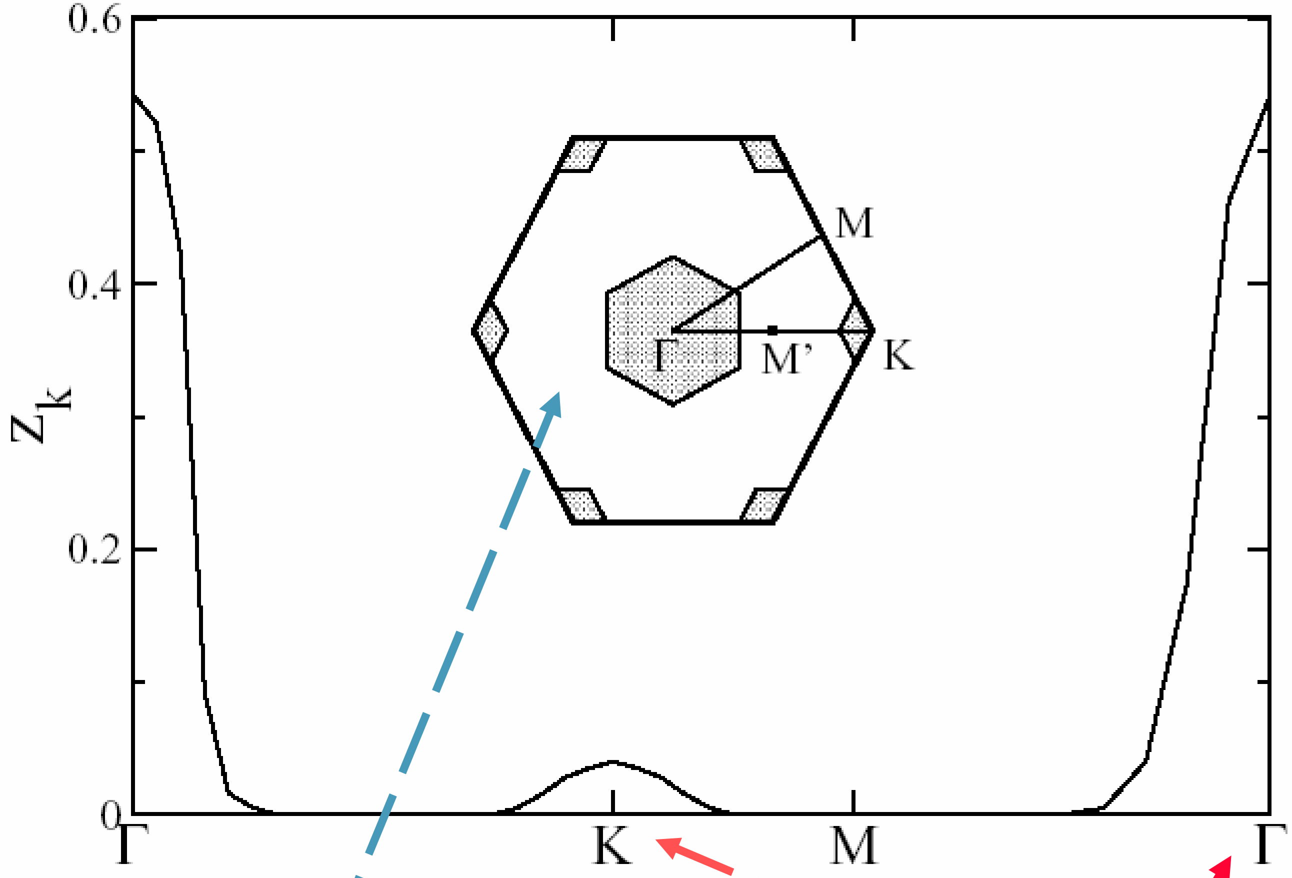


quasiparticle
(spin-polaron)

Magnetic
resonances
string-like

Free hopping

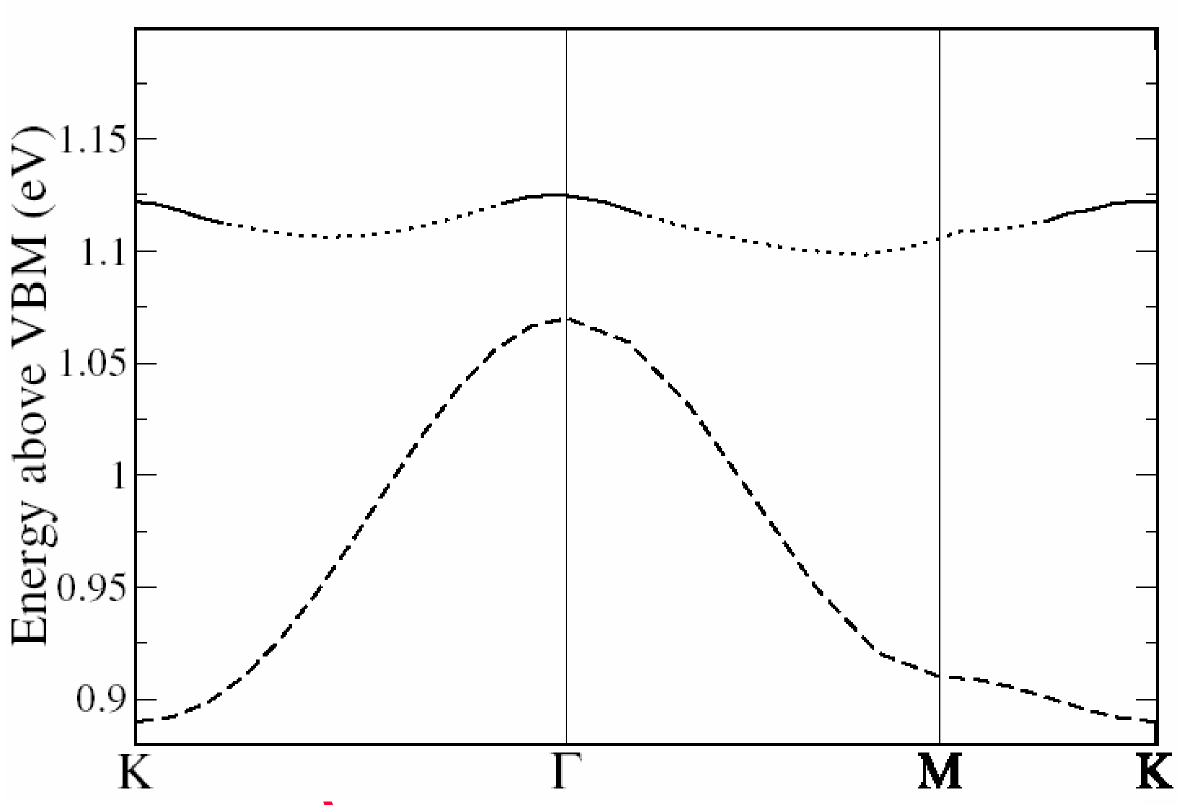
Quasiparticle weight

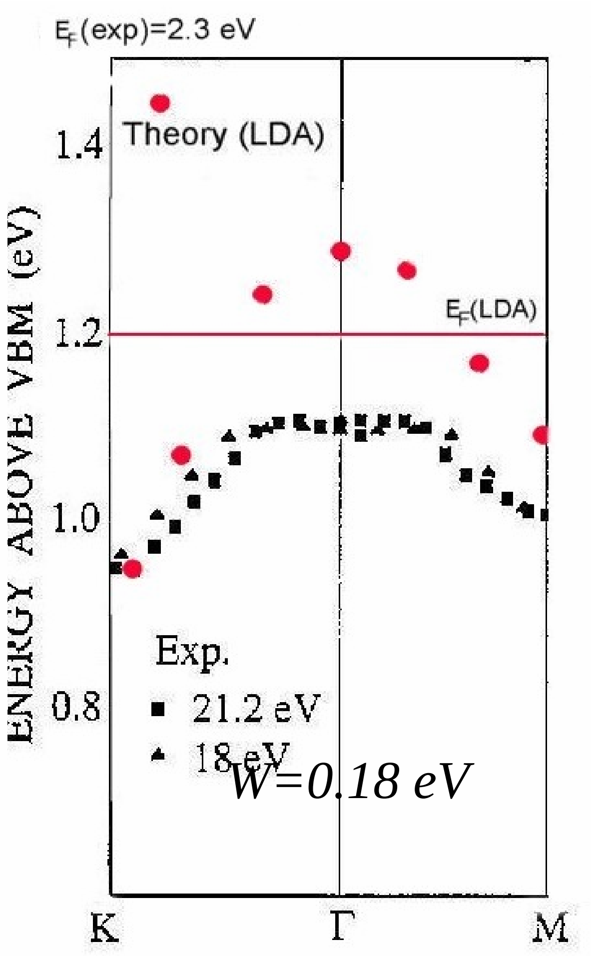


no QP

Goldstone modes

Band structure SiC(0001)





W=0.18 eV

Center of mass spectrum ***W~0.20 eV***

→ **~ PES experimental band**

Conclusions

➡ We obtained theoretically the spectroscopic fingerprints of the *120° Néel* order in Silicon surfaces

- For SiC(0001) [K/Si(111)-B] photoemission experiment should be done at low temperatures $T < J \sim 40$ K [170 K]

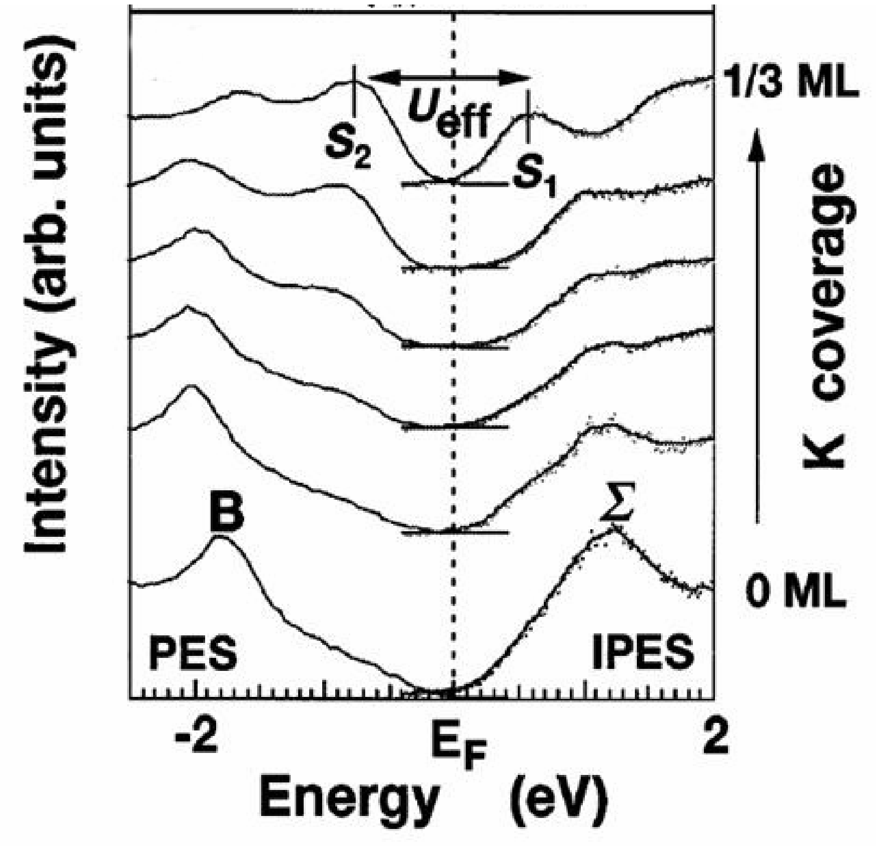
➡ The photo-injected hole does not exist as quasiparticle except for momenta near the magnetic Goldstone modes

➡ In simple silicon surfaces with simple *sp* orbitals there is interesting physics due to correlation effects

Perspectives

- Finite doping? Experimentally it can accomplished by monitoring K coverage in K/Si(111)-B

¿Non conventional excitations at finite doping ?



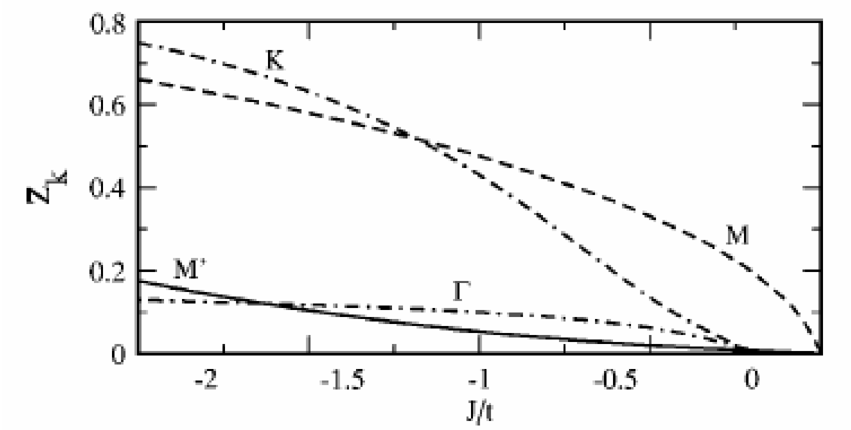
Recently Koretsune and Ogata (PRL sept 2002)
studied the rol played by the particle-hole asymmetry
Δ t-J model

Finite → doping

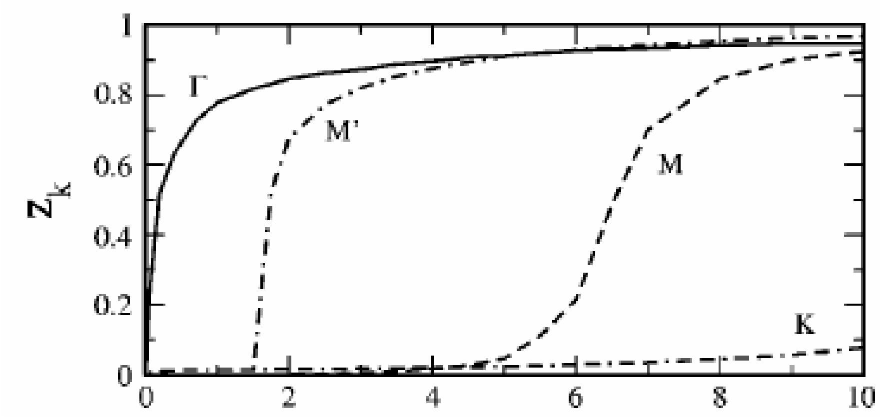
t >0 → RVB magnetic states

t < 0 → Nagaoka's ferromagnetism

For one-hole doping of the 120° Neel order we found



t negative



t positive