Photoemission spectra in Mott Insulating Surfaces

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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 (1 eV)

Electrons can localize due to

- Atoms at surfaces have lower coordination than in the bulk
- reconstruction yields much larger interorbital spacing in the bulk $\rightarrow$ lower $t$

$U / W > 1$ strong correlation without transition metal ions
Surface SiC (0001)

- LEED and STM $\rightarrow$ triangular $\sqrt{3} \times \sqrt{3}$ reconstruction

- First principles total energy calculation
  (Northrup et al, PRB ‘95)
A non-saturated state per absorbed Si $\rightarrow$
LDA predicts a half-filled metallic surface band
$W = 0.35 \text{ eV}$ $t = 0.04 \text{ eV}$

Experimentally, it is found a similar band ... but completely filled
$W = 0.20 \text{ eV}$
Photoemission: inverse and direct
(Johansson et al, Surf. Sci. ’96)

\[ U \gg W \rightarrow \text{surface Mott state} \]
\[ \sqrt{3} \times \sqrt{3} – \text{K/Si(111)-B} \]

- LEED $\rightarrow$ *triangular* $\sqrt{3} \times \sqrt{3}$ reconstruction
- First principles total energy calculation
  (Y. Ma et al PRL’90)

**Side view**

**Top view**

- $\circ$ Si
- $\bullet$ B
- $\,$ K
- $\,$ Si dangling bond
Theory vs Experiments

\[
\sqrt{3} \times \sqrt{3} - \text{K/Si(111)-B}
\]

LDA calculation
(Hellberg et al, PRL'99)

Photoemission
(Weitering et al, PRL’97)

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

\[t_1 = 0.07 \text{ eV}\]
\[t_2 = -0.03 \text{ ev}\]
\[U_{\text{eff}} = 1 \text{ eV}\]
Hubbard model
realistic parameters

$$D = \frac{\partial^2 E}{\partial \phi^2}$$

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 \[\rightarrow\]
No perfect nesting
Critical value $U/t$
magnetic order

\[(U/t)_{\text{SiC}} = 20, \quad (U/t)_{\text{K/Si-B}} = 40 > (U/t)_{\text{crit}} = 12\]  
(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)

\[ H = \sum_{\langle ij \rangle} J_{ij} S_i S_j \]

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

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

Theory: \textbf{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 $K/Si(111)-B-\sqrt{3}X\sqrt{3}$

$SiC(0001)-\sqrt{3}X\sqrt{3}$
Model and techniques used

**t-J model**

\[
H = -t \sum_{\langle ij \rangle} (\hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} + \hat{c}^\dagger_{j\sigma} \hat{c}_{i\sigma}) + J \sum_{\langle ij \rangle} \left( S_i S_j - \frac{n_i n_j}{4} \right)
\]

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

\[
\hat{c}^\dagger_{i\uparrow} = h^\dagger_i \quad \hat{c}^\dagger_{i\downarrow} = h_i S_i^-
\]

\[
S_i^x \sim \frac{1}{2} (a_i^\dagger + a_i) \quad S_i^y \sim \frac{i}{2} (a_i^\dagger - a_i) \quad S_i^z = \frac{1}{2} - a_i^\dagger a_i
\]

**Effective Hamiltonian**

\[
H = \sum_k \epsilon_k h^\dagger_k h_k + \sum_q \omega_q \alpha^\dagger_q \alpha_q - t \sqrt{\frac{3}{N_s}} \sum_{k,q} \left[ M_{kq} h^\dagger_k h_{k-q} \alpha_q + h.c. \right]
\]

Free hole energy \quad Free magnon energy \quad hole-magnon vertex
Self-consistent Born approximation (SCBA)

We calculate the hole spectral function

\[ A_k(\omega) = -\frac{1}{\pi} \text{Im} G^h_k(\omega) \]

\[ G^h_k(\omega) = \langle AF | h_k \frac{1}{\omega + i\eta^+ - H} h^\dagger_k | AF \rangle \]

Solving the self-consistent eqn for self-energy

\[ \Sigma_k(\omega) = \frac{3t^2}{N_s} \sum_q \frac{|M_{kq}|^2}{\omega - \omega_q - \epsilon_{k-q} - \Sigma_{k-q}(\omega - \omega_q)} \]

Quasiparticle weight

\[ z_k = \left( 1 - \frac{\partial \Sigma_k(\omega)}{\partial \omega} \right)^{-1} \quad | \quad E_k = \Sigma_k(E_k) \]
Two mechanisms for hole-motion

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

Magnon assisted hopping

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

Spin-polaron origin in non-frustrates AF

Both mechanisms interfere!
Quasiparticle survives?
Comparison SCBA vs exact results: Spectral function

- Cluster of 21 sites
- $J = 0.4 \mid t \mid$
- $t < 0$

![Graph showing comparison between Lanczos and SCBA results.](image)
Cluster of 21 sites

\[ J = 0.4 \, t \]

\[ t > 0 \]

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**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)

Center of mass spectrum $W \sim 0.20 \text{ eV}$

$\sim$ PES experimental band

$\Gamma$}

$E_{F}(\text{exp}) = 2.3 \text{ eV}$

Theory (LDA)

Exp.

- $21.2 \text{ eV}$
- $18 \text{ eV}$

$E_{F}(\text{LDA})$

$W = 0.18 \text{ eV}$
We obtained theoretically the spectroscopic fingerprints of the 120° Néel order in Silicon surfaces.

Conclusions

- For SiC(0001) [K/Si(111)-B] photoemission experiment should be done at low temperatures $T < J \sim 40 \text{ K} \ [170 \text{ 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 role played by the particle-hole asymmetry $\Delta$ in the t-J model.

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

Finite doping:
- $t > 0$ $\rightarrow$ RVB magnetic states
- $t < 0$ $\rightarrow$ Nagaoka's ferromagnetism

Finite doping $\rightarrow$ RVB magnetic states

Finite doping $\rightarrow$ Nagaoka’s ferromagnetism