The photoemission spectra for Mott insulating surfaces

Adolfo Trumper and Luis Manuel

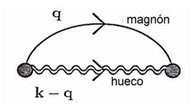
Instituto de Física Rosario and Universidad Nacional de Rosario (Argentina)

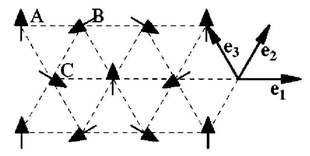
Abstract

We show theoretically the fingerprints of short-range spiral magnetic correlations in the photoemission spectra of the Mott insulating ground states realized in the $\sqrt{3}\times\sqrt{3}$ triangular silicon surfaces K/Si(111)–B and SiC(0001). The calculated spectra present low-energy features of magnetic origin with a reduced dispersion ∼10–40 meV compared with the centre-of-mass spectra bandwidth ∼0.2–0.3 eV. Remarkably, we find that the quasiparticle (QP) signal survives only around the magnetic Goldstone modes. Our findings position these silicon surfaces as new candidates for investigation in the search for non-conventional QP excitations.

Effective Hamiltonian Spinless fermions + magnons

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



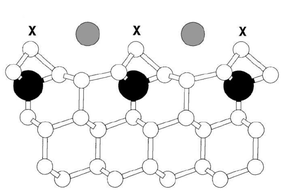


$$\Sigma_{\mathbf{k}}(\omega)=\frac{3t^2}{N_s}\sum_{\mathbf{q}}\frac{|\ M_{\mathbf{kq}}\ |^2}{\omega-\omega_{\mathbf{q}}-\epsilon_{\mathbf{k}-\mathbf{q}}-\Sigma_{\mathbf{k}-\mathbf{q}}(\omega-\omega_{\mathbf{q}})}$$

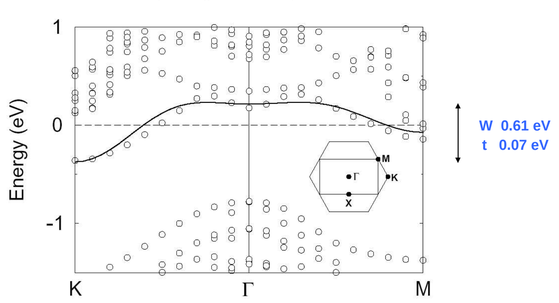
Surfaces are ideal to look for Mott states → reconstruction lowers t; → low coordination

√3 x √3 – K/Si(111)-B

Side view

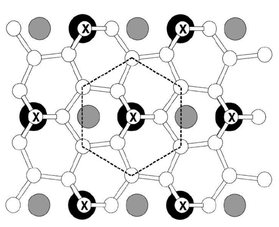


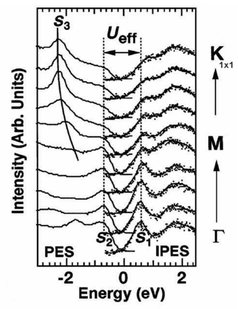
LDA calculation
(Hellberg et al, PRL'99)



Photoemission
(Weitering et al, PRL '97)

Top view

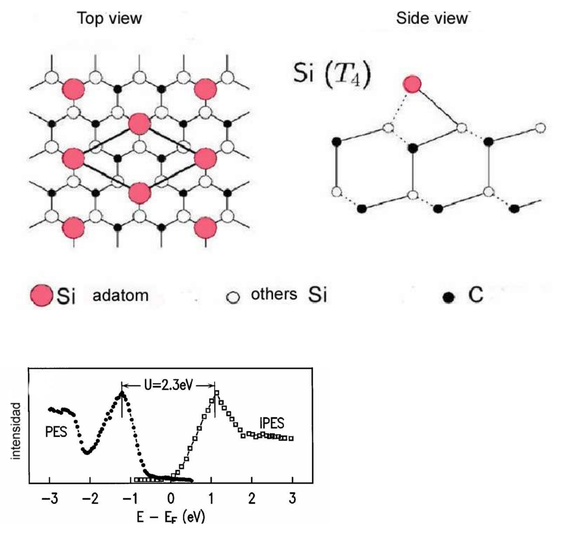


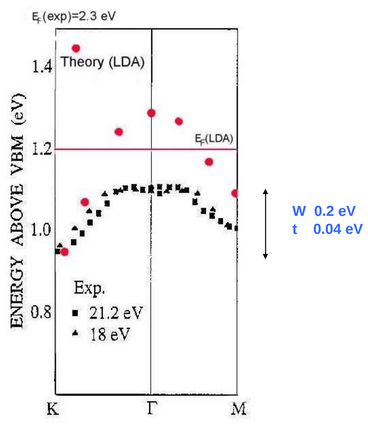


Ueff 1-2 eV

Motivation it has also been argued that K/Si–B is the first experimental realization of a triangular Heisenberg spin-1/2 model with a 120° Néel order. However, standard density-functional methods combined with exact diagonalization (ED) studies suggest a Mott insulator with a non-magnetic ground state [5]. In addition, it was speculated that the reconstructed triangular surface SiC(0001)-($\sqrt{3}\times\sqrt{3}$) [2] (hereafter SiC) also presents a 120° Néel ordered ground state [3]. Since direct measurements of magnetic order in such surfaces are difficult to implement, the magnetic properties of these MI ground states still remain to be established [3].

Surface Sic (0001)





On the other hand, nowadays it is possible to perform photoemission experiments with higher resolution than the previous ones, which should allow a detailed analysis of the single-hole properties in these MI ground states. These issues motivated us to study theoretically the single-hole dynamics in a triangular antiferromagnet (AF) with two objectives: (i) to investigate the effect of a frustrated magnetic order on the quasiparticle (QP) behaviour; and (ii) to obtain spectroscopic fingerprints of magnetic order through the photoemission spectra calculated for realistic parameters of the surfaces K/Si–B and SiC. A careful comparison with future higher-resolution spectroscopy experiments could give some information about the underlying short-range magnetic structure.

SCBA vs Lanczos

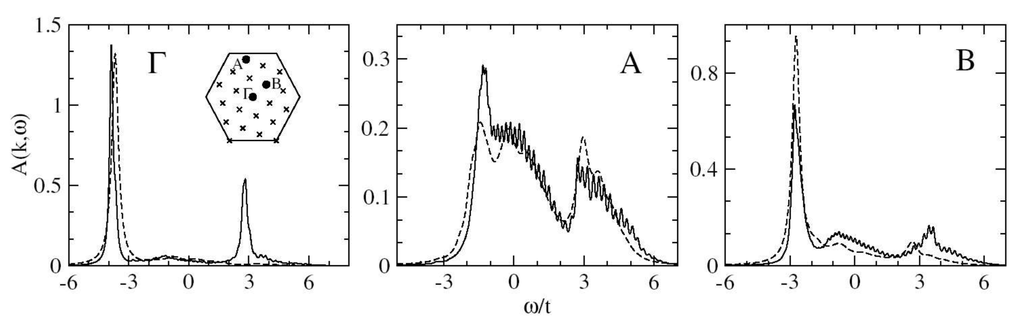


Figure 1. Spectral functions versus frequency for $J/t=0.4$ and $N=21$ corresponding to the momenta at BZ points $\Gamma=(0,0)$, A $=\frac{4\pi}{21}(-1,3\sqrt{3})$, and B $=\frac{4\pi}{21}(2,\sqrt{3})$, shown as filled circles in the inset of the left panel (the crosses represent the other momenta). The solid and dashed curves are the exact and SCBA results, respectively.

Quasiparticle weight

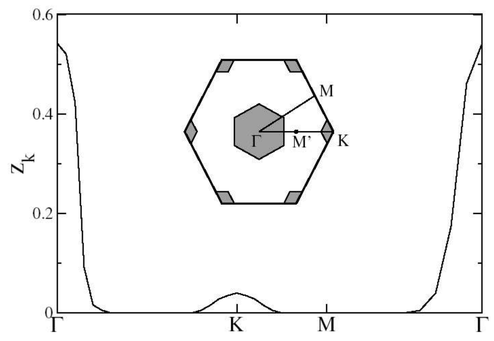


Figure 3. QP intensity along the Γ–K–M–Γ path for $J/t=0.4$. Inset: the $\sqrt{3}\times\sqrt{3}$ BZ. In the shaded areas, the QP weight is finite.

Predicted fingerprints of magnetic order

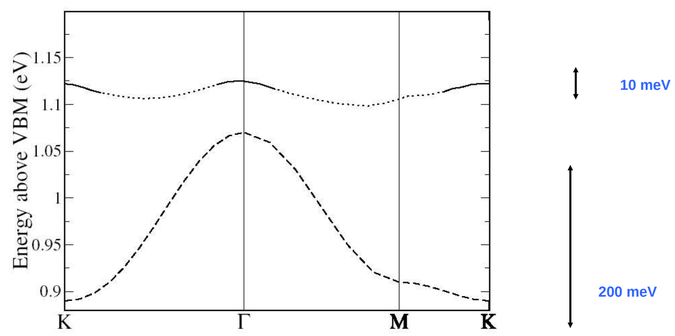


Figure 4. Surface band structure for realistic parameters ($J/t=0.1$, $t=0.04$ eV) of the SiC(0001)-($\sqrt{3}\times\sqrt{3}$) surface. The dotted line is the photothreshold energy, the solid one is the QP dispersion, and the dashed one is the centre-of-mass spectra band. Energies are given relative to the measured bulk valence band maximum (VBM). Experimentally the Fermi level is located at 2.3 eV above the VBM.

Conclusions we have studied theoretically the hole spectral function in the triangular t–J model for realistic parameters relevant for the silicon surfaces SiC(0001)-($\sqrt{3}\times\sqrt{3}$) and K/Si(111)-($\sqrt{3}\times\sqrt{3}$). Assuming the presence of a long-range magnetic Néel order, we have observed the emergence of low-energy features of magnetic origin with a reduced dispersion band. As the photoemission spectrum is not sensitive to the asymptotic low-energy magnetic properties of the system, we speculate however that it could give important information about the presence of short-range magnetic order. We have also obtained an unexpected vanishing of the QP weight for a large region of the BZ for these MI surfaces. Our theoretical predictions could provide a useful basis for the analysis of future improved photoemission experiments. Using a simple and reliable analytical method (SCBA), we have found clear signatures of interesting physics caused by strong electronic correlation on simple silicon surfaces.

References

[3] Santoro G, Scandolo S and Tosatti E 1999 *Phys. Rev.* B **59** 1891
Anisimov V I, Bedin A E, Korotin M A, Santoro G, Scandolo S and Tosatti E 2000 *Phys. Rev.* B **61** 1752

[5] Hellberg C S and Erwin S C 1999 *Phys. Rev. Lett.* **83** 1003