Exciton Condensation in Doped Hubbard Bilayers: A Sign-Free Quantum Monte Carlo Study

Xuxin Huang[1,3], Martin Claassen[2], Brian Moritz[3], Thomas. P. Devereaux[3]

[1]Department of Applied Physics, Stanford University, [2]Flatiron Institute, Simons Foundation [3]SLAC National Accelerator Laboratory

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I. Introduction

- Exciton Condensation
  - Bound electron-hole quasiparticles can condense like any other boson
  - Recombination limits lifetime. Spatial separation may suppress recombination.
- Bilayer Hubbard model

$$\hat{H} = -t \sum_{\langle i,j\rangle,\alpha,\sigma} (\hat{c}^\dagger_{i\alpha\sigma}\hat{c}_{j\alpha\sigma} + h.c.) - \Delta \sum_{i\sigma}(\hat{n}_{iA\sigma} - \hat{n}_{iB\sigma}) + U\sum_{i\alpha}(\hat{n}_{i\alpha\uparrow} - \tfrac{1}{2})(\hat{n}_{i\alpha\downarrow} - \tfrac{1}{2}) + V\sum_{i\sigma\sigma'}(\hat{n}_{iA\sigma} - \tfrac{1}{2})(\hat{n}_{iB\sigma'} - \tfrac{1}{2})$$

References:

[1] J. M. Blatt *et al.*, Phys. Rev. 126, 1691 (1962).

[2] Y. E. Lozovik *et al.*, Zh. Eksp. i Teor. Fiz 71, 738 (1976).

II. Method

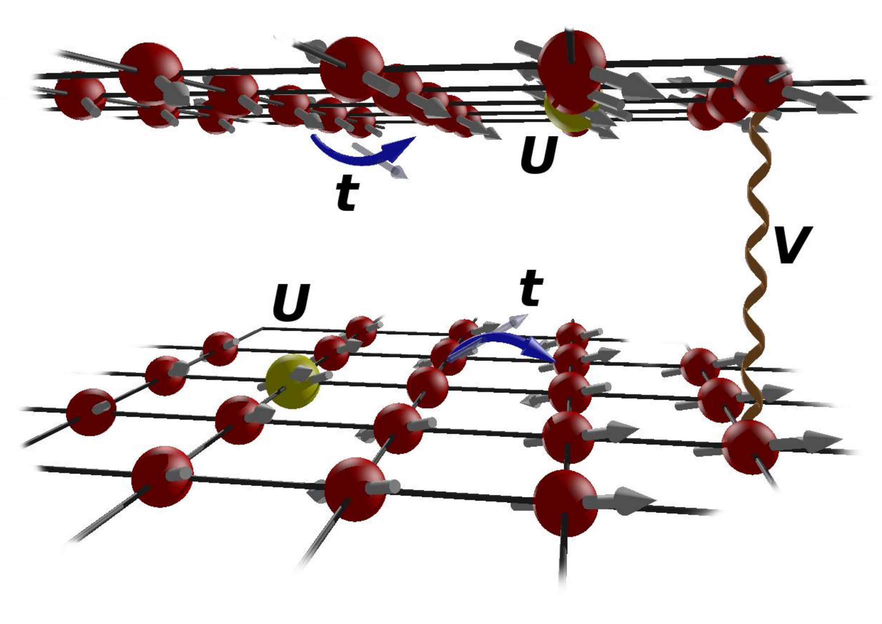

Fig. 1: Schematic for the bilayer Hubbard model.

- Definition of excitonic correlation function:

$$\langle b^\dagger_q b_q\rangle,\ b^\dagger_q = \sum_{k\sigma\sigma'} c^\dagger_{k+qA\sigma} c_{kB\sigma'}$$

- Determinant Quantum Monte Carlo(DQMC)
  - Numerically exact; finite temperatures
  - Limited by fermion sign problem
  - Exploit symmetry for a sign-free scheme

References:

[1] R. Blankenbecler *et al.*, Phys. Rev. D 24, 2278 (1981).

[2] S. R. White *et al.*, Phys. Rev. B 40, 506 (1989).

[3] S. E. Koonin *et al.*, *Physics reports* 278, 1 (1997).

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[5] T. Grover, Phys. Rev. Lett. 111, 130402 (2013).

- Exploit anti-unitary symmetry

$$\hat{\mathcal{P}} = \sum_{i\sigma} [|i,\sigma,A\rangle\langle i,\sigma,B| - |i,\sigma,B\rangle\langle i,\sigma,A|]\ \hat{\mathcal{K}} \qquad \hat{\mathcal{P}}^2 = -1 \qquad \hat{\mathcal{P}}^{-1} = -\hat{\mathcal{P}}$$

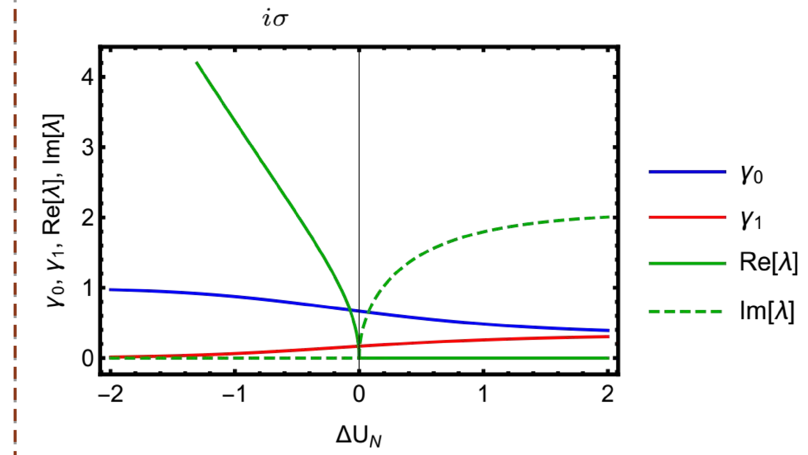

Fig. 2: Decoupling parameters for density and inter-layer Ising interactions. $U_M > 0$, $U_N < 0$ in the sign problem-free regime.

- Change variables after Trotterizing

$$U\sum_{i\alpha}\hat{n}_{i\alpha\uparrow}\hat{n}_{i\alpha\downarrow} - V\sum_{i\sigma\sigma'}\hat{n}_{iA\sigma}\hat{n}_{iB\sigma'} \sim$$

$$\sim \sum_i \left[\left(\frac{U-V}{4}\right)\left(\hat{N}_i\right)^2 + \left(\frac{U+V}{4}\right)\left(\hat{M}_i\right)^2\right]$$

- Continuous HS transformation

$$\hat{\mathcal{P}}^{-1}\sqrt{-\beta\frac{U-V}{4}}\hat{N}\ \hat{\mathcal{P}} = \left[\sqrt{-\beta\frac{U-V}{4}}\right]^\star \hat{N}$$

$$\hat{\mathcal{P}}^{-1}\sqrt{-\beta\frac{U+V}{4}}\hat{M}\ \hat{\mathcal{P}} = -\left[\sqrt{-\beta\frac{U+V}{4}}\right]^\star \hat{M}$$

III. Results and Discussion

- SU(4) symmetry
  - U = V = 6t, **Δ** = 0
  - With SU(4) symmetry, the Hamiltonian H is invariant under transformation Q:

$$\hat{Q} : \downarrow A \rightarrow \uparrow B, \uparrow B \rightarrow \downarrow A$$

  - Excitonic correlation function and static spin structure factor are equivalent:

$$\sum \hat{c}^\dagger_{k+q\uparrow A}\hat{c}_{k\uparrow B}\hat{c}^\dagger_{k'-q\uparrow B}\hat{c}_{k'\uparrow A} \xrightarrow{\hat{Q}} \sum \hat{c}^\dagger_{k+q\downarrow A}\hat{c}_{k\uparrow A}\hat{c}^\dagger_{k'-q\uparrow A}\hat{c}_{k'\downarrow A}$$

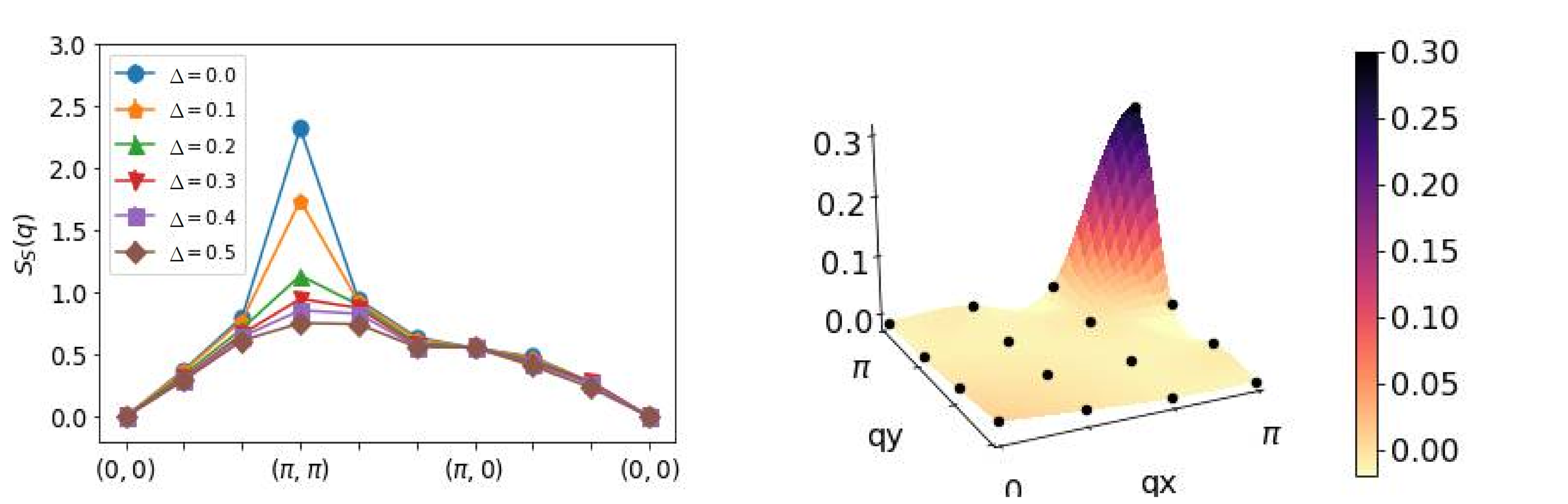

Fig. 3: Left: Static spin structure factor for U=V=6t and various **Δ**. The blue line shows SU(4) symmetric result. Right: Density plot of background subtracted excitonic correlation function at the SU(4) symmetry point.

- Charge structure factor

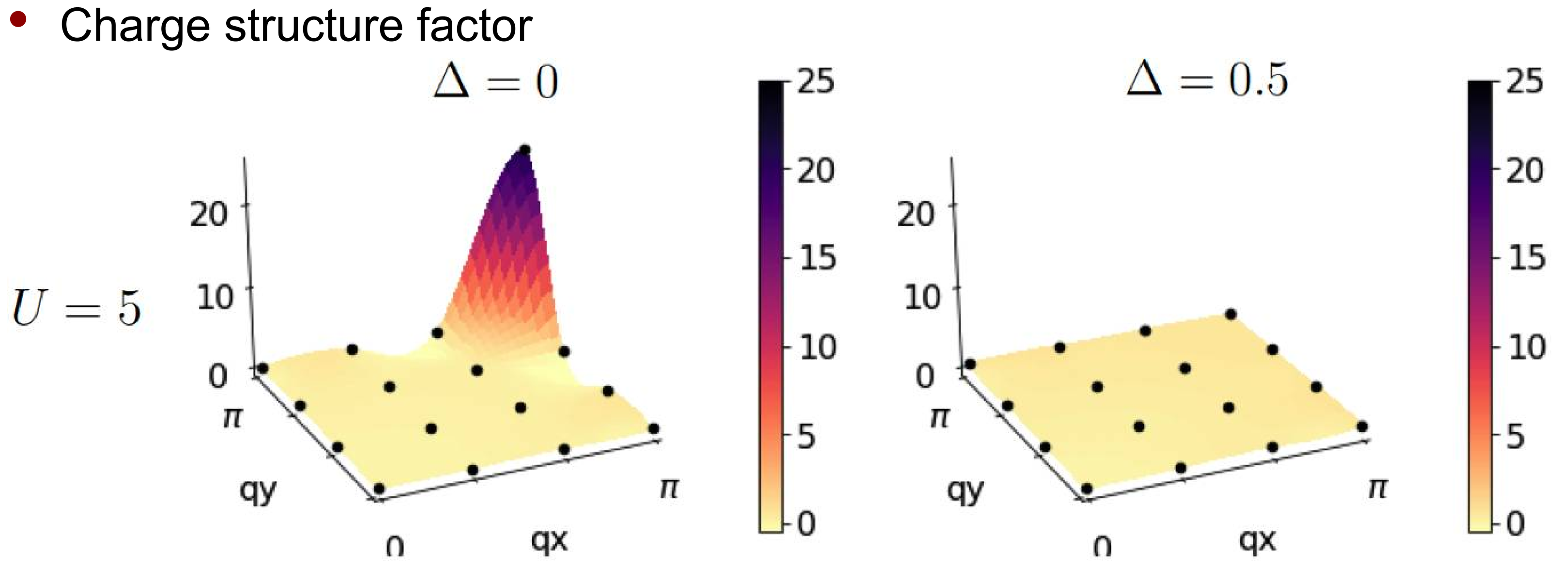

Fig. 4: Static charge structure factor measured at V = 6t.

- Away from SU(4) symmetry

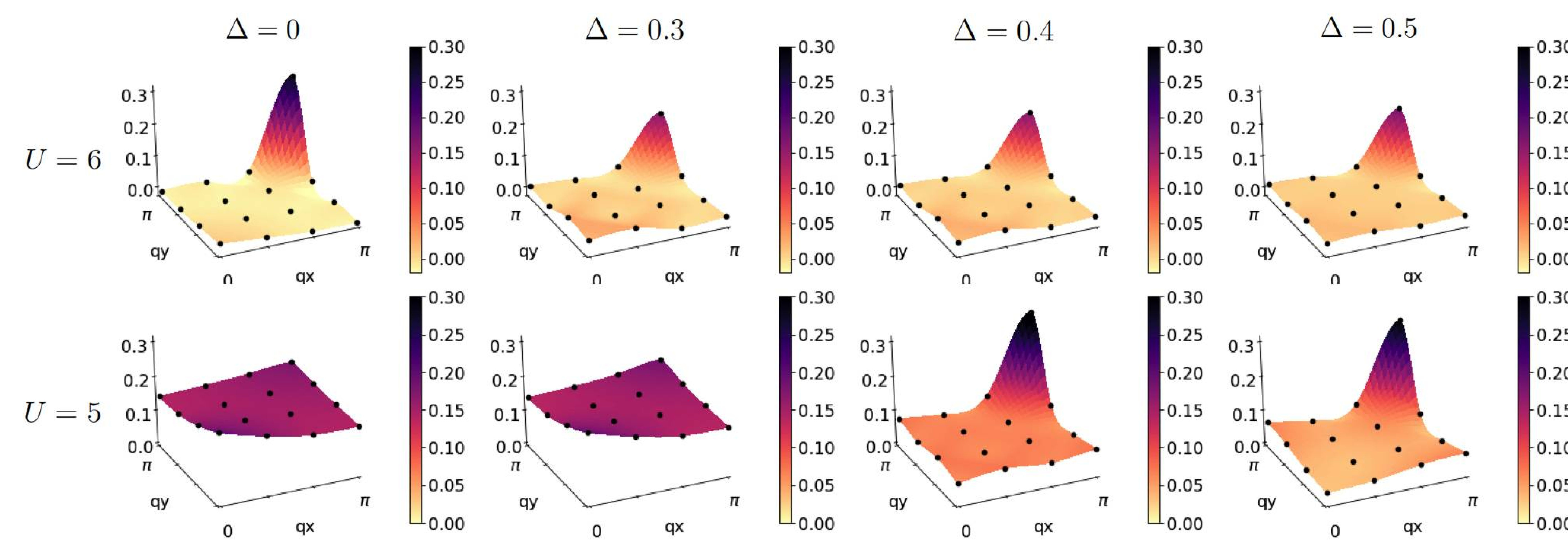

Fig. 5: The excitonic correlation function measured away from SU(4) symmetry. In the first row, interactions are kept at U = V = 6t, while the system is doped away from single-layer half-filling (**Δ** = 0). The peak at (π, π), though slightly suppressed as **Δ** increases, still survives throughout this doping process. In contrast, in the second row where U = 5t and V = 6t, no obvious peak appears in momentum space when **Δ** = 0. However as the doping level increases, the excitonic correlation peak at (π, π) reappears after **Δ** reaches 0.4t.

- Summary of correlation functions

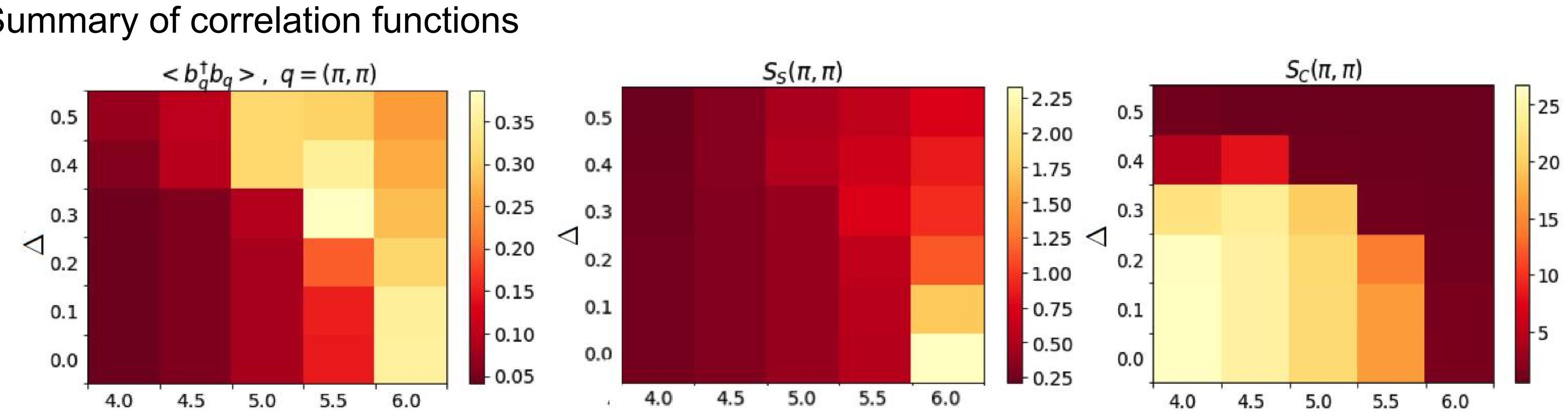

Fig. 6: Excitonic correlation functions and static charge and spin structure factors at (π, π). V is fixed at V = 6t. As U approaches V and for large doping, excitons condense at (π, π), rather than the system forming a charge density wave at (π, π). For smaller values of U and lower doping, the bilayer system tends to form a charge density wave. Strong spin density wave correlations only appear in the vicinity of the SU(4) symmetric point, where there is an equivalence to the excitonic correlation function.

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