

Supplementary Materials for Stripe order from the perspective of the Hubbard model

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I. SQUARE GEOMETRY SIMULATIONS

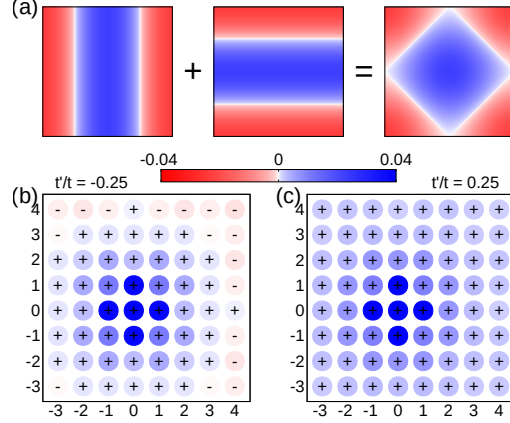


FIG. S1. (a) Illustration of expected staggered spin correlation functions for a superposition of horizontal and vertical stripes. (b) and (c) Staggered spin correlation functions calculated by DQMC for parameters $U/t = 6, t'/t = \pm 0.25, T/t = 0.22, p = 0.125$.

To ensure that our results are robust against variations in cluster geometry, we perform DQMC calculations on a 8×8 square cluster. Our findings are summarized in Fig. S1. Assuming the presence of the same stripes as demonstrated in the main text, but without breaking of C_4 rotational symmetry, the square cluster's spin correlations should appear as an equal superposition of correlations from horizontal and vertical stripes (Fig. S1a). The predicted diamond pattern from such a superposition is observed in Fig. S1b for the parameters $U/t = 6, t'/t = -0.25, T/t = 0.22, p = 0.125$, which for the rectangular geometry we have observed period-5 stripes (Fig. 1). We note that the rough shape of the diamond is most likely related to the imperfect compatibility of period-5 stripes with the 8×8 period cluster. Unfortunately, the severity of the fermion sign problem (~ 0.01 for the 8×8 clusters) prevents us from characterizing any larger clusters. Nevertheless, the qualitative behavior of the correlations and their distinction from the purely commensurate antiferromagnetism in Fig. S1c ($t'/t = +0.25$) provide a picture of stripes consistent with our results for the rectangular cluster.

II. EFFECT OF VARYING t'/t FROM DMRG

In addition to our DQMC results in Fig. 2, the dependence of stripe behavior on t' can be studied by DMRG. Fig. S2 displays the spin correlations and charge density profiles from our DMRG simulations for parameters $p = 0.125, U/t = 6$ and $t'/t = -0.25, 0.0, +0.25$. As in Fig. 2, the spin stripes roughly double in period going from $t'/t = -0.25$ to 0.0 , and are absent for $t'/t = +0.25$. At $t'/t = -0.25$ and 0.0 , charge stripes are locked to the spin stripes, with maxima in the hole occupancy aligned to spin antiphase domain walls. For $t'/t = +0.25$, while the spin structure is purely antiferromagnetic, charge stripes with period 4 are present. We note that in electron-doped cuprates, recent X-ray scattering experiments have observed a signal at momentum transfer $q \sim (0.25, 0)$ in r.l.u., possibly arising from

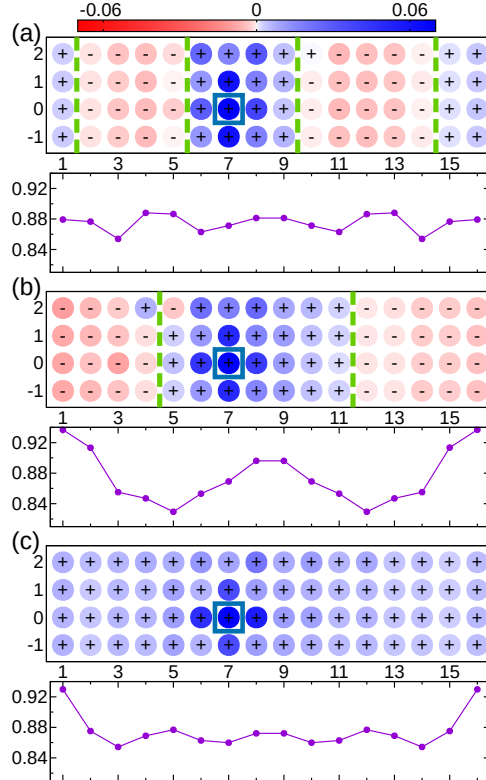


FIG. S2. (a-c) Staggered spin correlation functions (top) and charge density profiles (bottom) from DMRG simulations with parameters $U/t = 6, T/t = 0, p = 0.125$ and at $t'/t = -0.25$ (a), 0.0 (b), and 0.25 (c).

period 4 charge ordering [1–3].

- [1] Eduardo H. da Silva Neto, Riccardo Comin, Feizhou He, Ronny Sutarto, Yeping Jiang, Richard L. Greene, George A. Sawatzky, and Andrea Damascelli, “Charge ordering in the electron-doped superconductor $\text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4$,” *Science* **347**, 282–285 (2015).
- [2] Eduardo H. da Silva Neto, Biqiong Yu, Matteo Minola, Ronny Sutarto, Enrico Schierle, Fabio Boschini, Marta Zonno, Martin Bluschke, Joshua Higgins, Yangmu Li, Guichuan Yu, Eugen Weschke, Feizhou He, Mathieu Le Tacon, Richard L. Greene, Martin Greven, George A. Sawatzky, Bernhard Keimer, and Andrea Damascelli, “Doping-dependent charge order correlations in electron-doped cuprates,” *Science Advances* **2**, e1600782 (2016).
- [3] H. Jang, S. Asano, M. Fujita, M. Hashimoto, D. H. Lu, C. A. Burns, C.-C. Kao, and J.-S. Lee, “Superconductivity-insensitive order at $q \sim 1/4$ in electron-doped cuprates,” *Phys. Rev. X* **7**, 041066 (2017).