

# Effects of Su-Schrieffer-Heeger coupling in single band Hubbard square lattice

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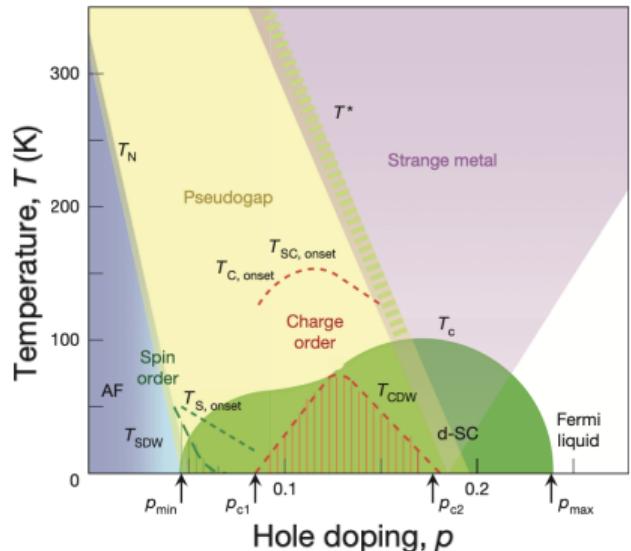
06 March, 2024



\*This work is supported by the U.S. Department of Energy,  
under award DE-SC0022311



# Cuprate & Hubbard Model



Cuprate Phase diagram

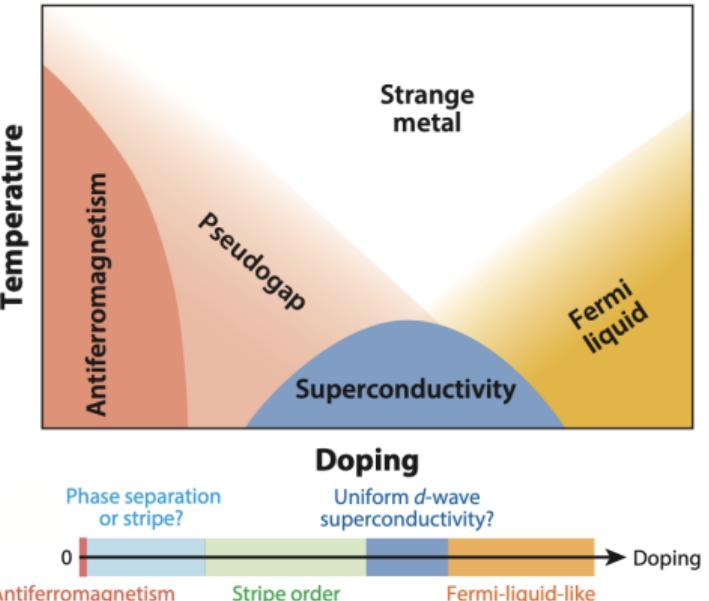
B. Keimer et. al., Nature 518, pages 179–186 (2015)

Mai, P. et. al. Nat Commun 14 2889 (2023)

Huang, W. E. et al., Science 358, 1161–1164 (2017)

Zheng, B.-X. et al. Science 358, 1155–1160 (2017)

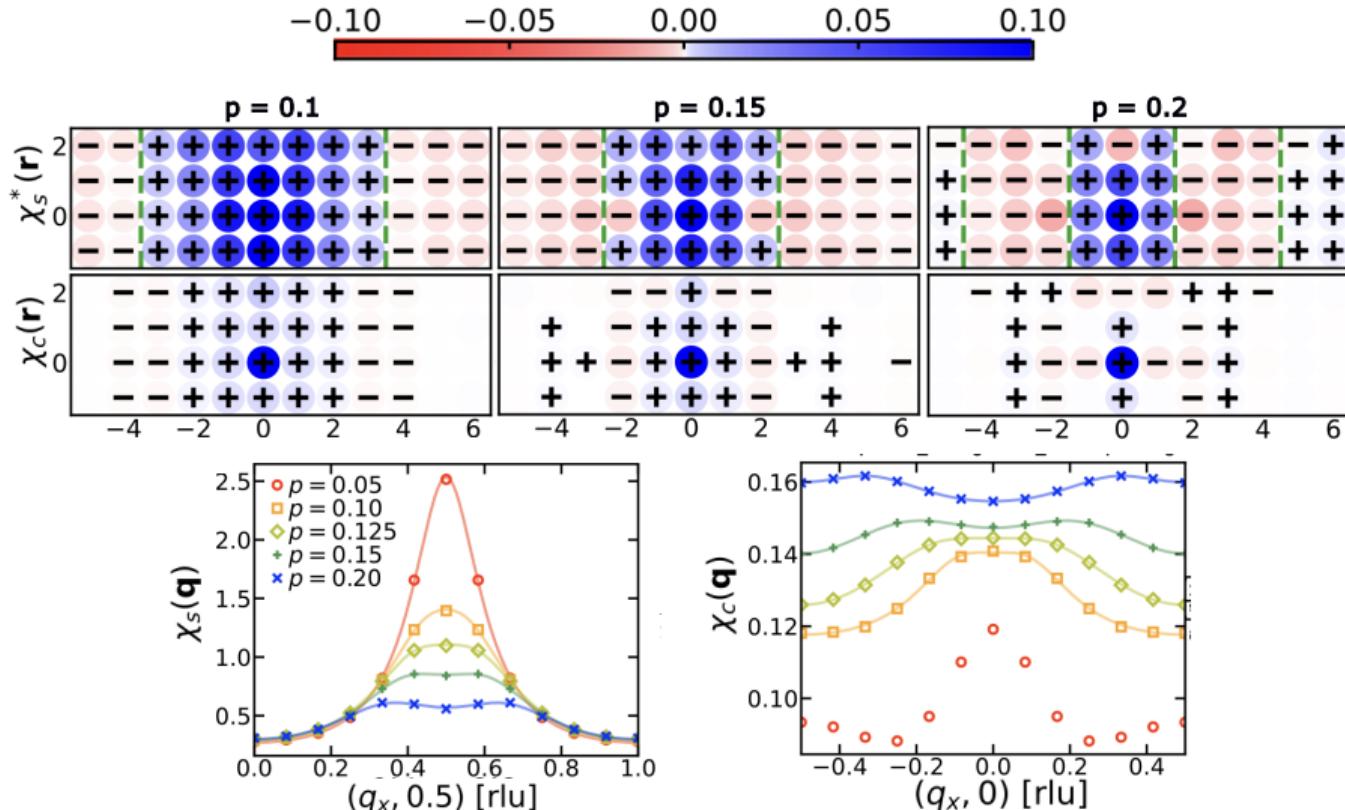
White, S. R. et. al. Phys. Rev. Lett. 80, 1272 (1998)



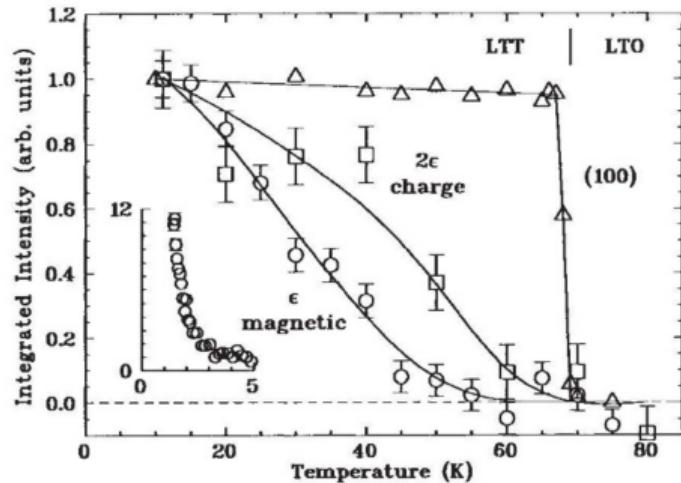
Phase diagram by Hubbard Model

Mingpu Qin et. al., Annu. Rev. Condens. Matter Phys. 2022 13:1, 275-302

# Fluctuating Intertwined Stripes at finite T

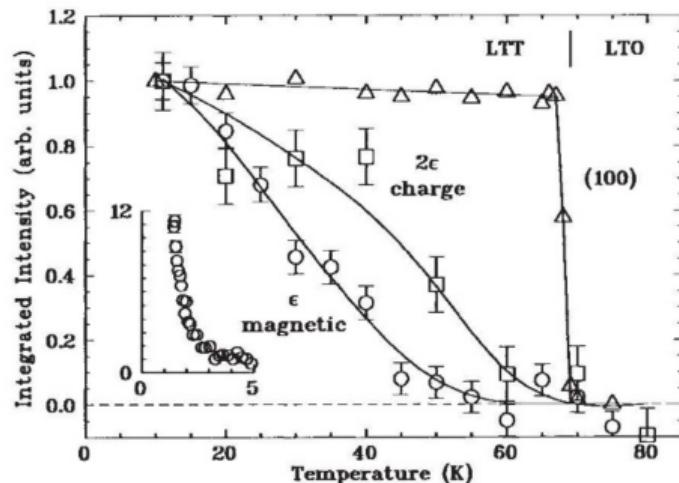


# Disparity of Stripes

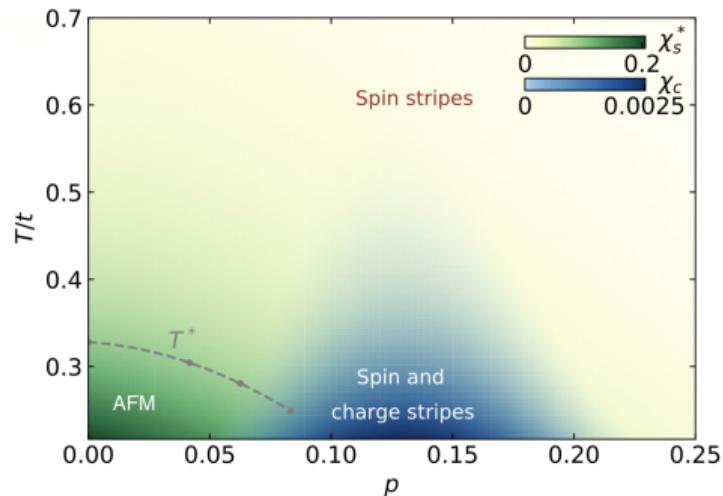


Exp. peaks for SDW and CDW vs T  
Tranquada, J. et al, Nature 375, 561–563 (1995)

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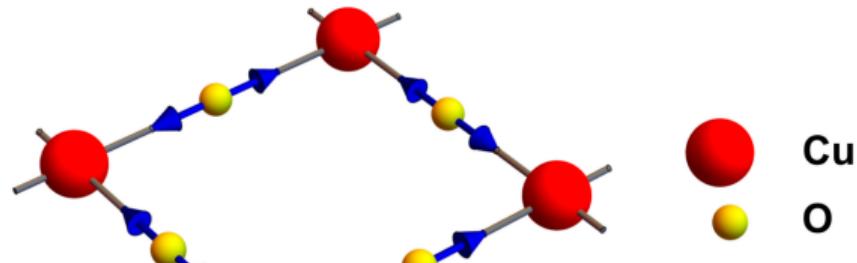
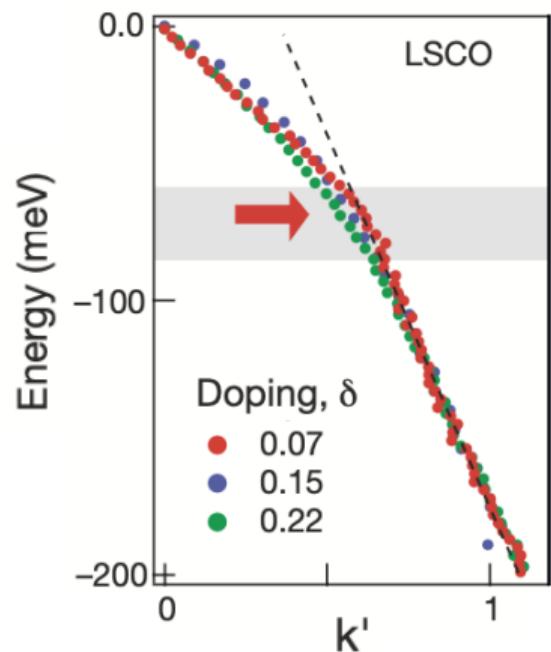
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Spin & Charge stripe intensities: Hubbard Model

Edwin W. Huang et al(2023), PRB107, 085126  
Peizhi Mai, et. al.(2022) PNAS 119 (7) e2112806119

# Electron-phonon coupling



O(yellow) motion affecting  $t$  for Cu-Cu(red) bond

$$\mathcal{H}_{e-ph} = \alpha \sum_{i,j,\nu} \hat{X}_{i,\nu} (c_i^\dagger c_j + h.c.)$$

Kink due to e-ph coupling  
A. Lanzara, Nature volume 412, 510–514 (2001)

# Model : Hubbard SSH

$$\mathcal{H} = \mathcal{H}_U + \mathcal{H}_{ph} + \mathcal{H}_{e-ph}$$

$$\mathcal{H}_U = -t \sum_{i,j,\sigma}^{NN} (c_i^\dagger c_j + h.c.) - t' \sum_{i,j,\sigma}^{NNN} (c_i^\dagger c_j + h.c.) + U \sum_i n_{i,\uparrow} n_{i,\downarrow} - \mu \sum_i n_i$$

$$\mathcal{H}_{ph} = \sum_{i,\nu} \left( \frac{\hat{P}_{i,\nu}^2}{2M} + \frac{1}{2} K \hat{X}_{i,\nu}^2 \right)$$

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In cuprates,  
 $t \sim 0.3 \text{ eV} = 300 \text{ meV};$   
 $\Omega \sim 70 - 100 \text{ meV}$

$$\therefore \Omega(\max) \approx t/3$$

$\Omega = t/2 = 200 \text{ meV}$ : still very high, lower  $\Omega$  unexplored.

J. Liu et. al. arXiv:2309.13868  
Karakuzu, S., et. al. Commun Phys 5, 311 (2022)

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SmoQyDQMC.jl\* (arXiv:2311.09395) → access lower  $\Omega$

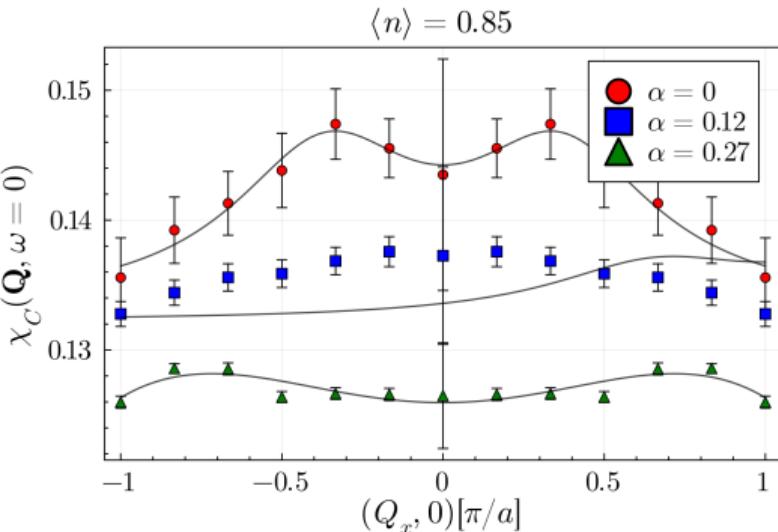
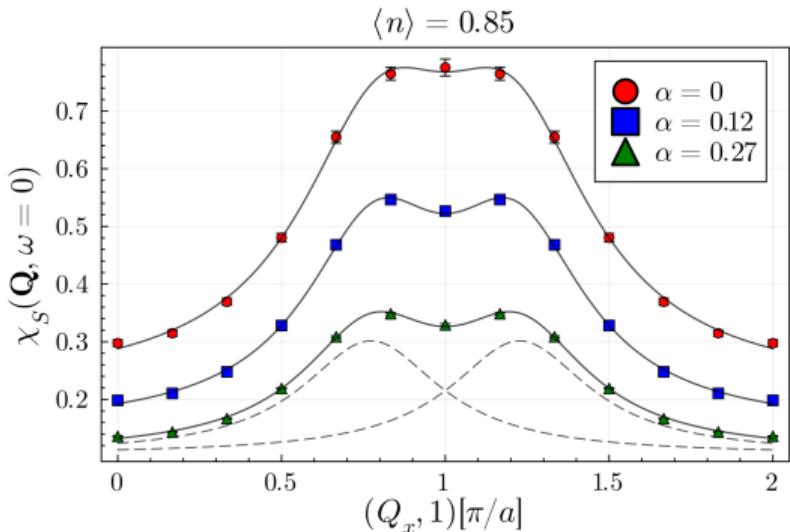
$$t = 1; \quad t' = -0.25t; \quad \Omega = 0.3t; \quad M = 1$$

$$U = 6t; \quad \beta t = 3.5$$

$\alpha$  : variable

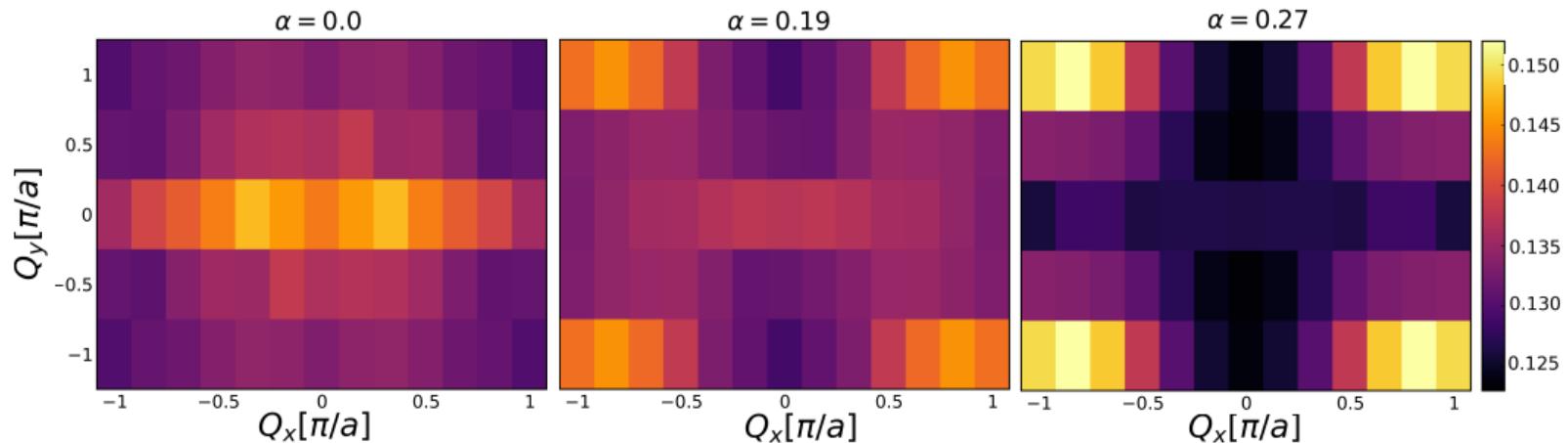
\*For more details, talk by B. C. Stead today @ 3 p.m (205D)

# Spin & charge susceptibility



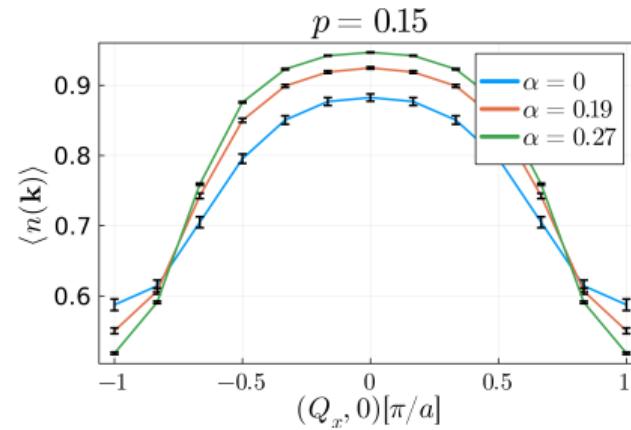
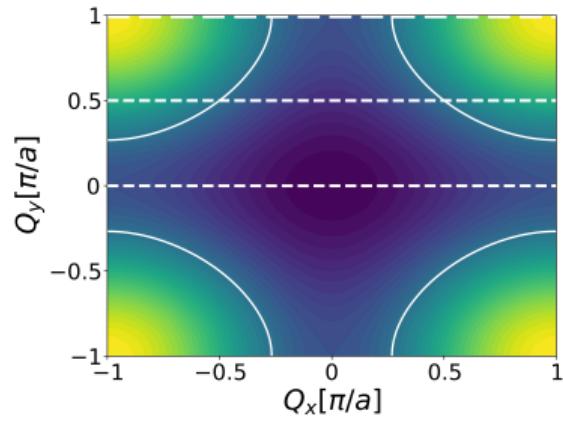
\*errorbars in the plots are  $2\sigma$ ,  
systems simulated using SmoQyDQMC.jl, arXiv:2311.09395

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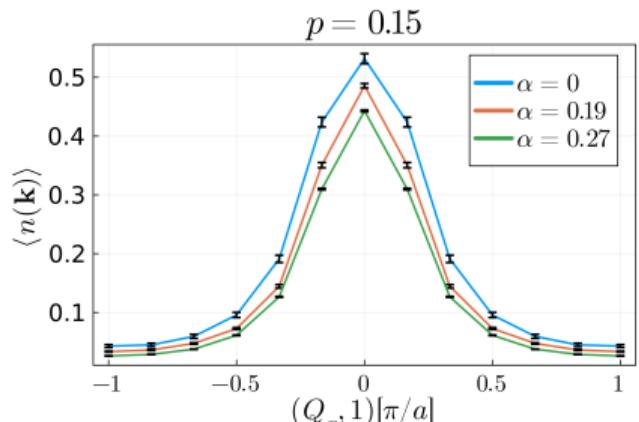
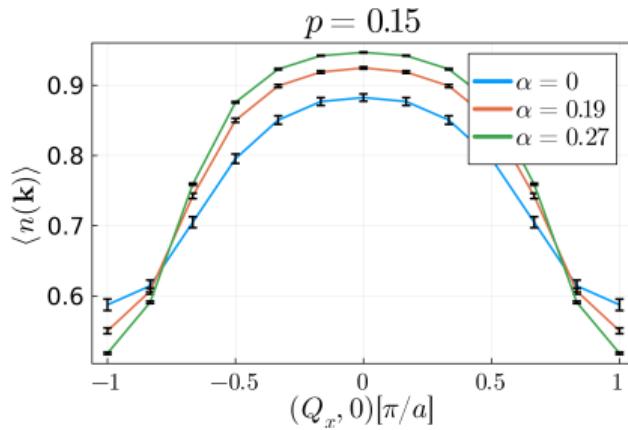
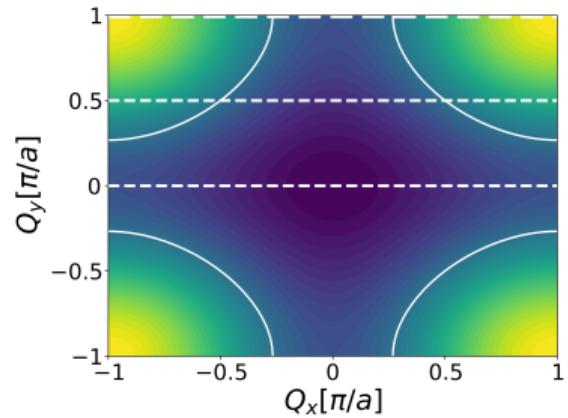


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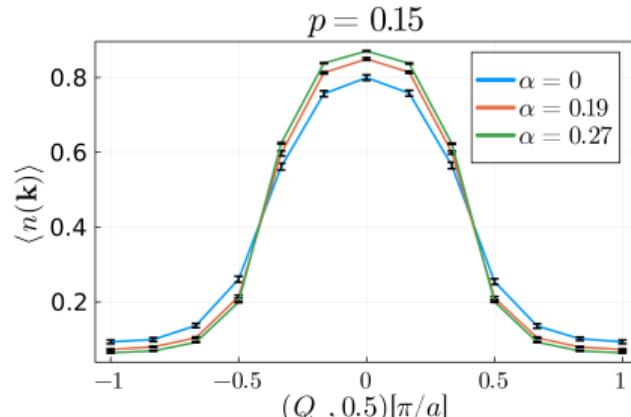
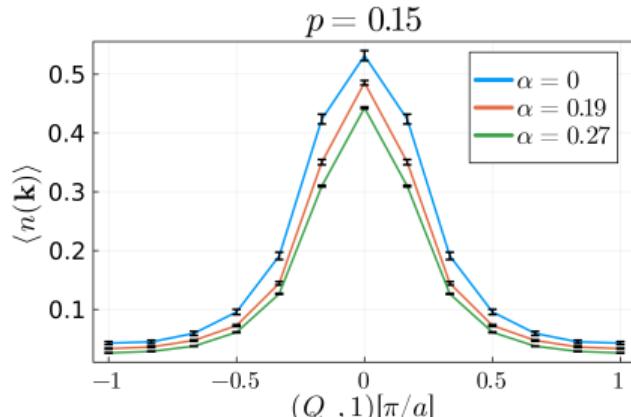
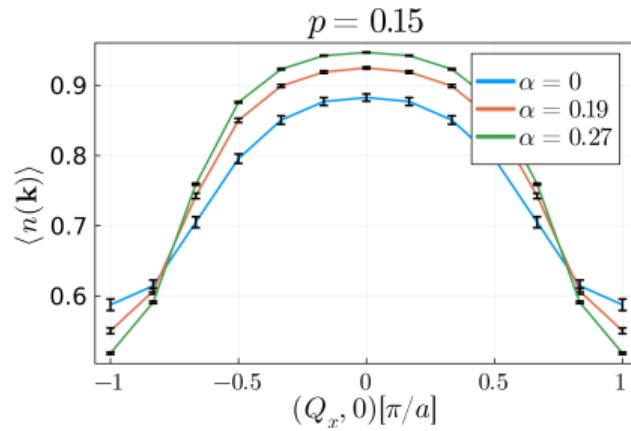
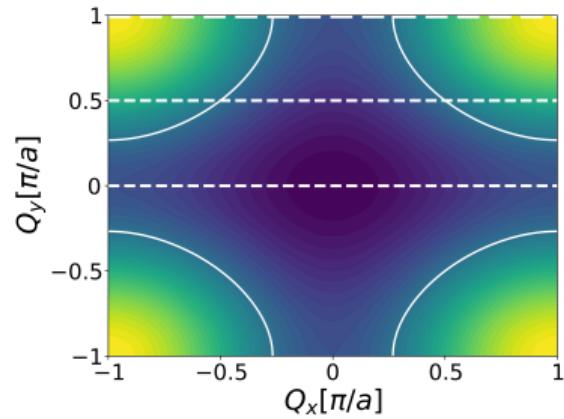
# Renormalization of spectral weight



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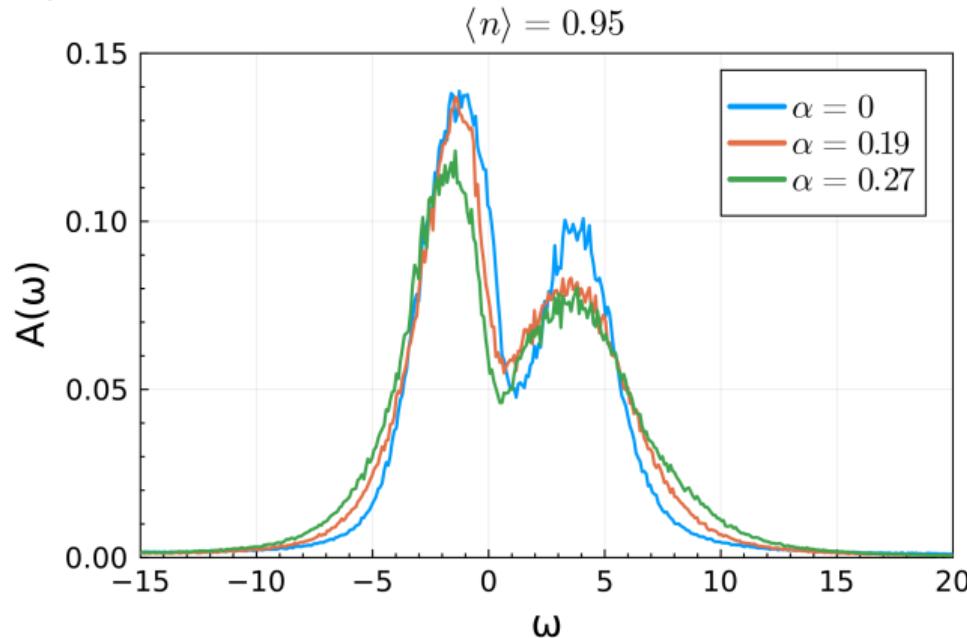
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## Caveat: Bonds contract

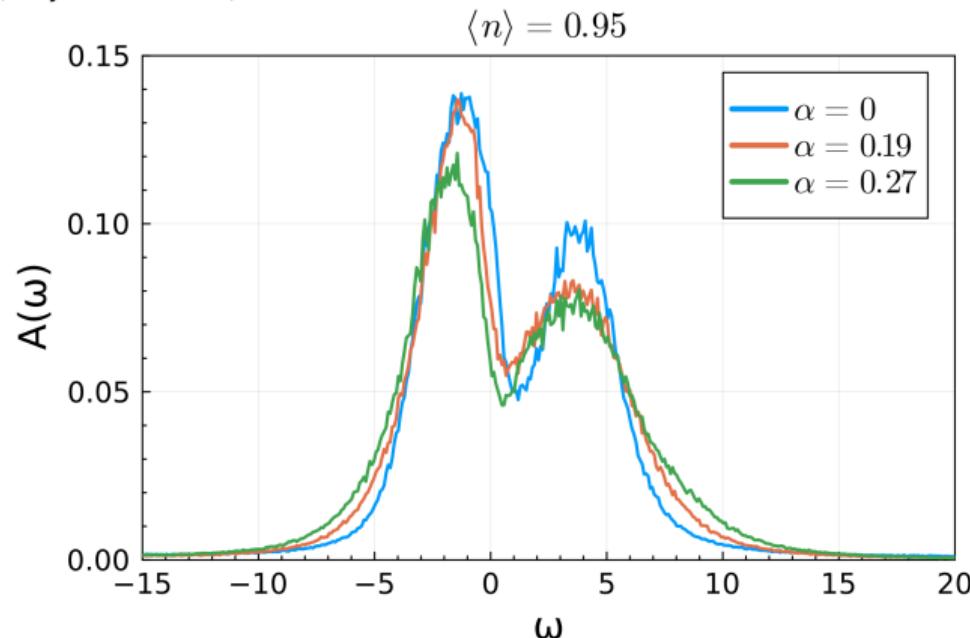
Phonons on the bonds  $\implies \langle \hat{X} \rangle \neq 0$ ; bonds contract  $t_{\text{eff}} \approx t(1 - \alpha \langle \hat{X} \rangle)$   
S. Malkaruge Costa et. al, Phys. Rev. B 108, 165138



\*Spectral function computed using SmoQyDEAC.jl (<https://github.com/SmoQySuite/SmoQyDEAC.jl>)

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Nevertheless, suppression(enhancement) of SDW(CDW) warrants further investigation, esp,  $T = 0$

\*Spectral function computed using SmoQyDEAC.jl (<https://github.com/SmoQySuite/SmoQyDEAC.jl>)

## Acknowledgements/Q&A



Dr. Benjamin  
Cohen-Stead, UTK



Prof. Steve Johnston,  
UTK

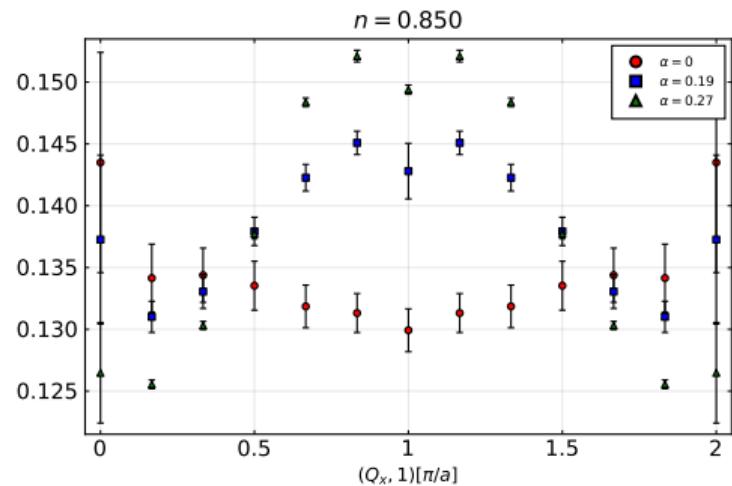
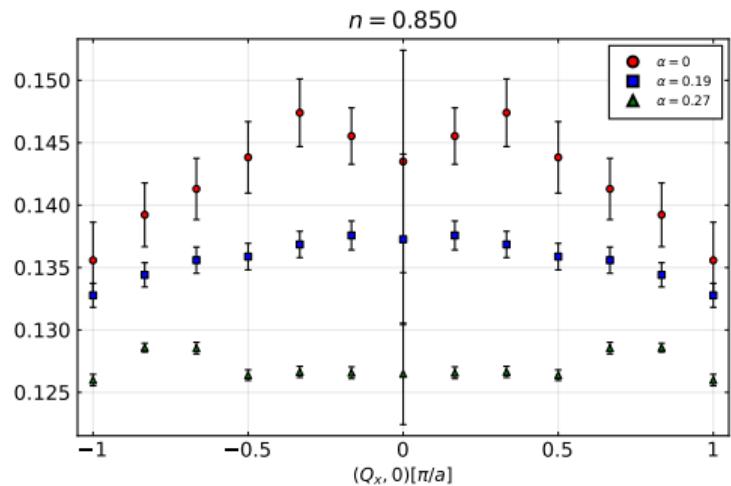


*THANK YOU! Questions?*

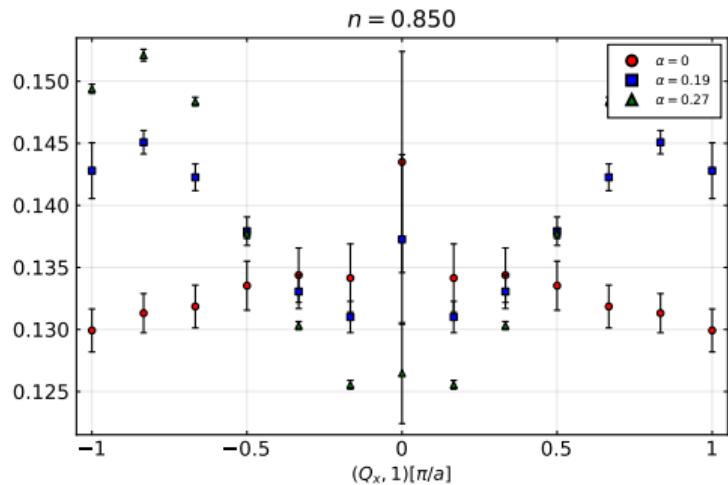
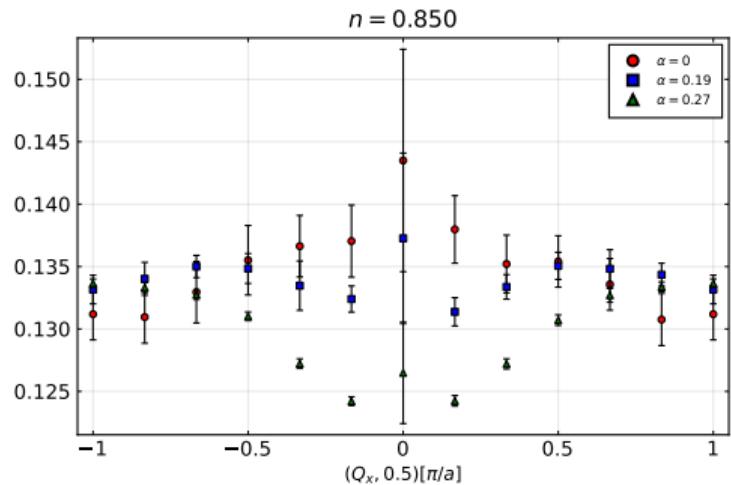
This work is supported by the U.S. Department of Energy, under award DE-SC0022311.

**The End**

# Charge Susceptibility



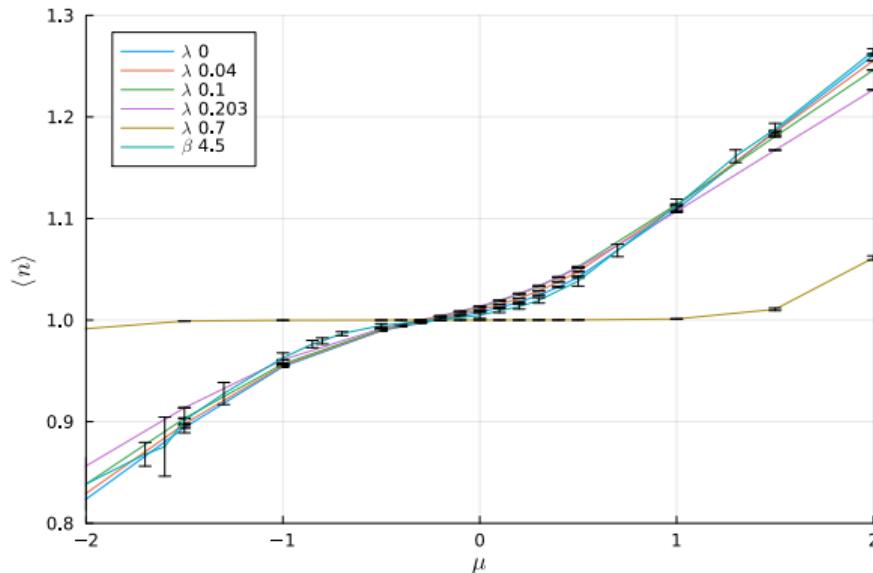
# Charge Susceptibility



## Summary

- Disparity for charge & magnetic stripes among theory & experiments for Cuprates
- Electron-phonon coupling significant, model by SSH mechanism for realistic freq.
- Suppressed(enhanced) spin(charge) susceptibility
- Need further investigation, esp  $T = 0$

# Decreasing Mott gap

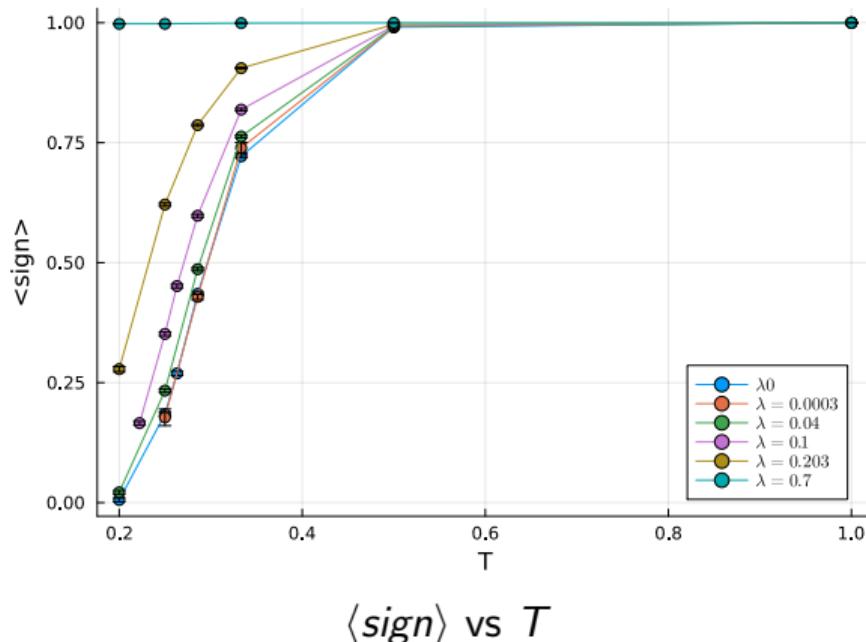


$\langle n \rangle$  vs  $\mu$

$$\lambda = \frac{2\alpha^2}{M\Omega^2 W}; \quad W = 8t$$

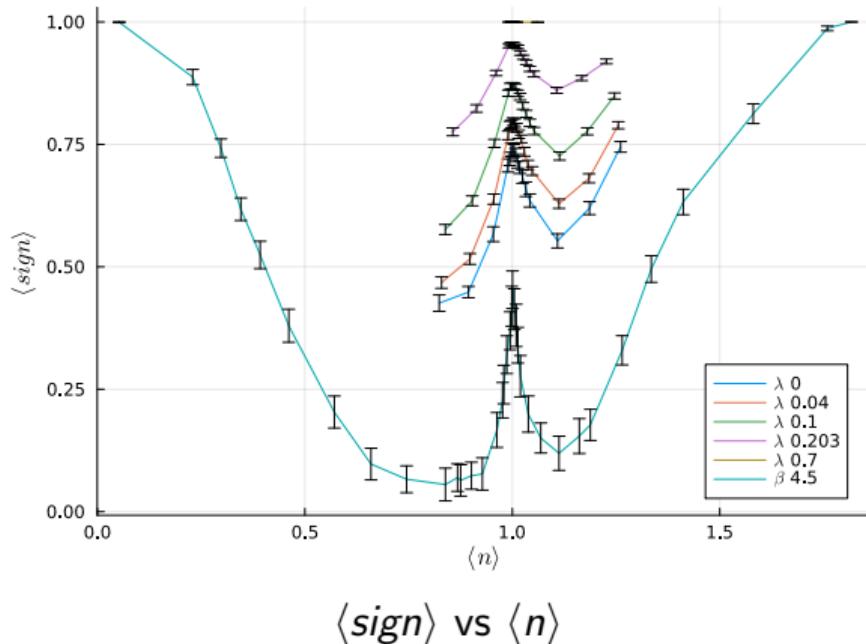
$\beta = 3.5$  unless specified

# Sign problem



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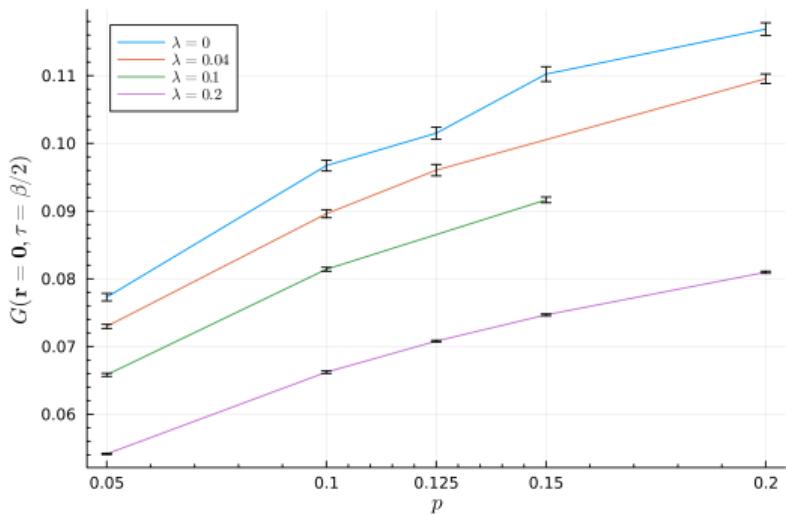
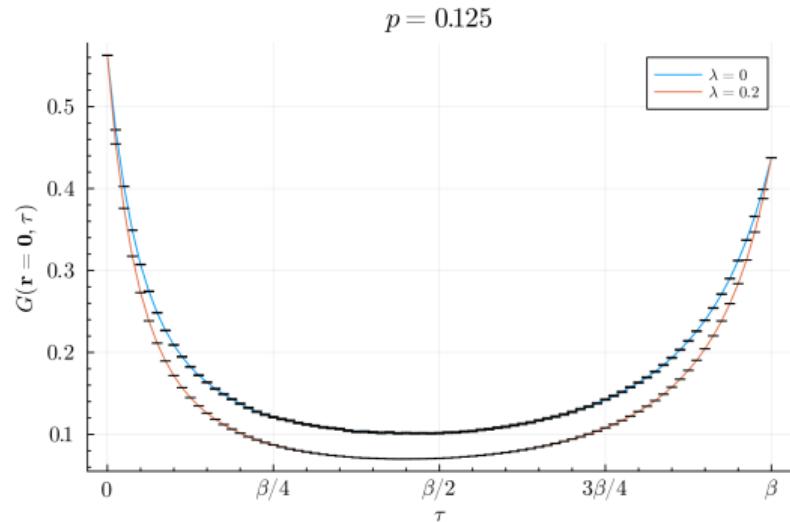
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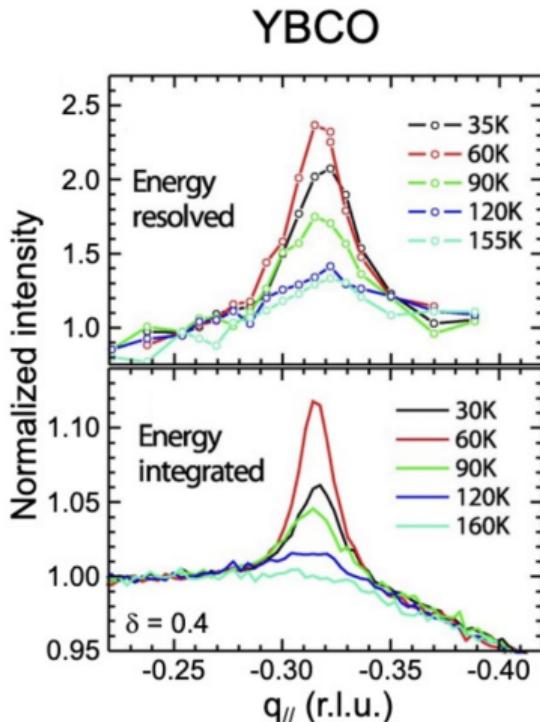
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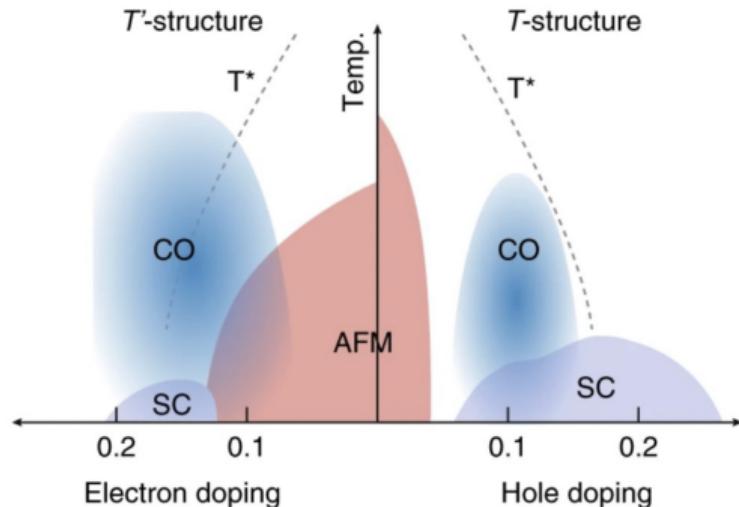
# Drop in spectral weigh for all doping



# Fluctuating CO



# Fluctuating CO at high T



Kang et al., Nature Physics 15, 335(2019)

# Questions?

# Final The End!