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Antiferromagnetic and bond-order-wave phases in the half-filled 2D optical Su-Schrieffer-Heeger-Hubbard model

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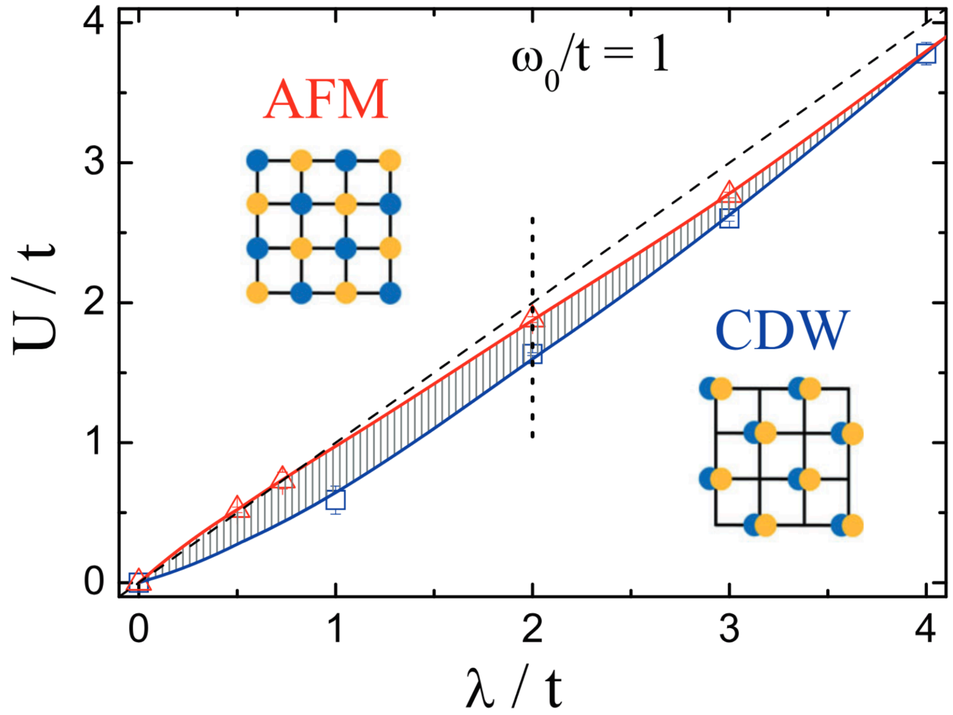
Electron-phonon models

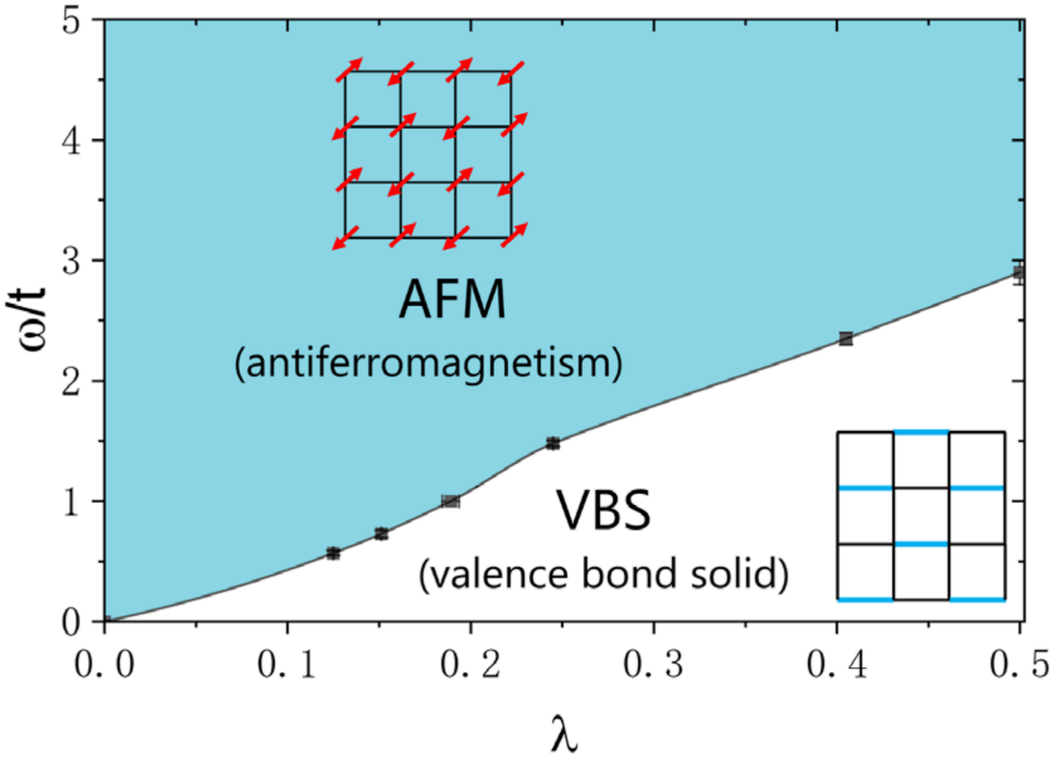
Hubbard-Holstein model



N.C. Costa et al. *Commun. Phys.* **3**, 80 (2020)

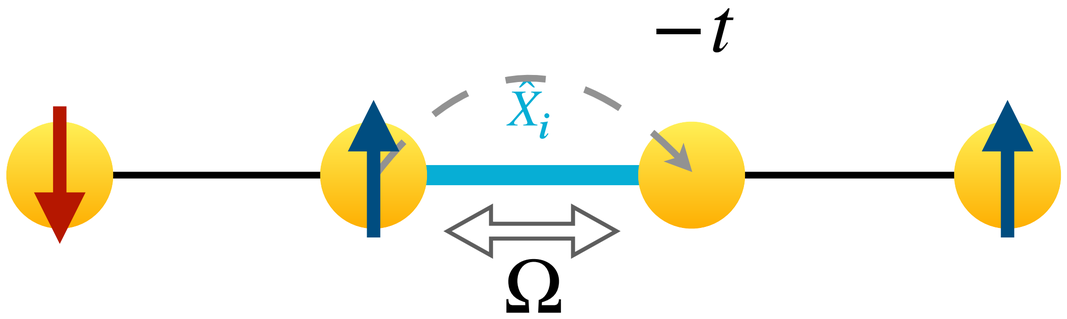
Electron-phonon models

Bond Su-Schrieffer-Heeger model



X.Cai et al. *Phys. Rev. Lett.* **127**, 247203 (2021)

$$\hat{H}_{e-\mathrm{ph}} = \alpha \sum_{\boldsymbol{i},\nu,\sigma} \hat{X}_{\boldsymbol{i},\nu} (\hat{c}^{\dagger}_{\boldsymbol{i}+\boldsymbol{a}_{\nu},\sigma} \hat{c}_{\boldsymbol{i},\sigma} + \mathrm{H.c.})$$



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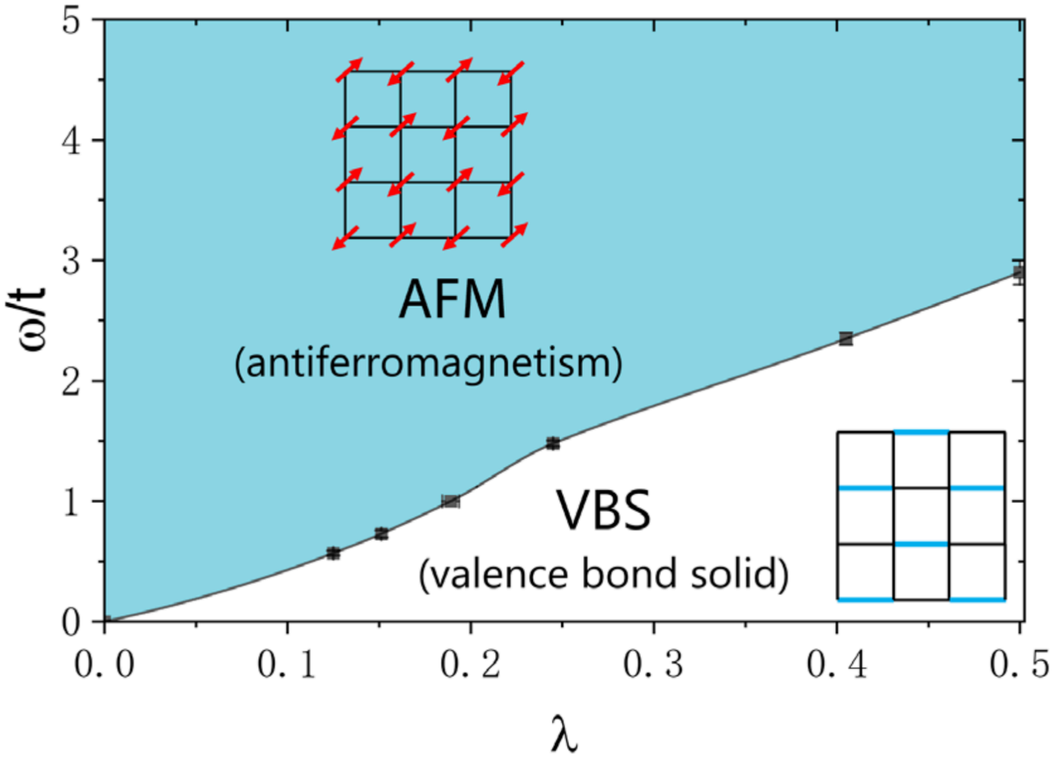

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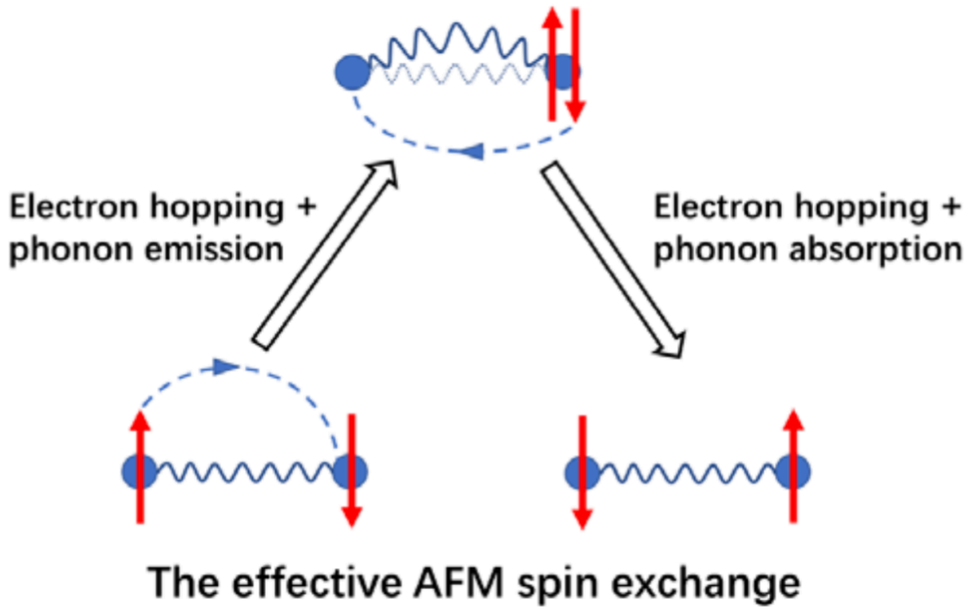

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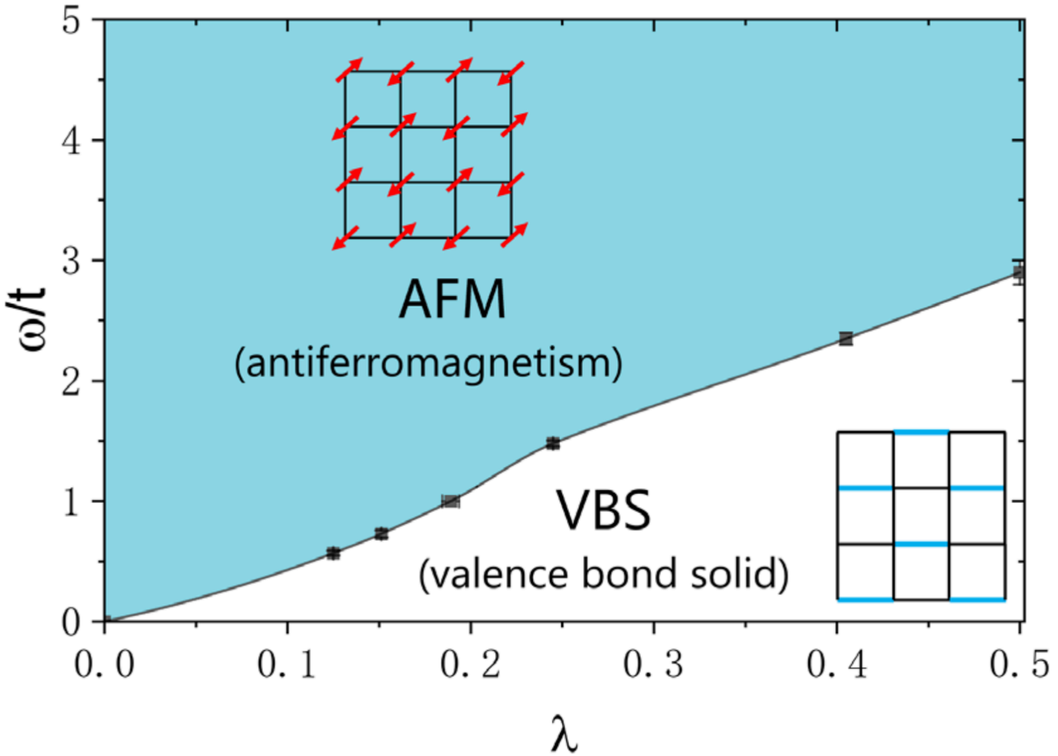
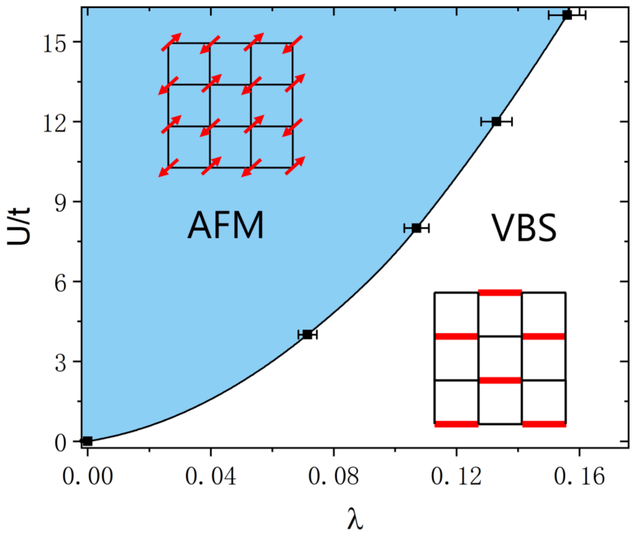
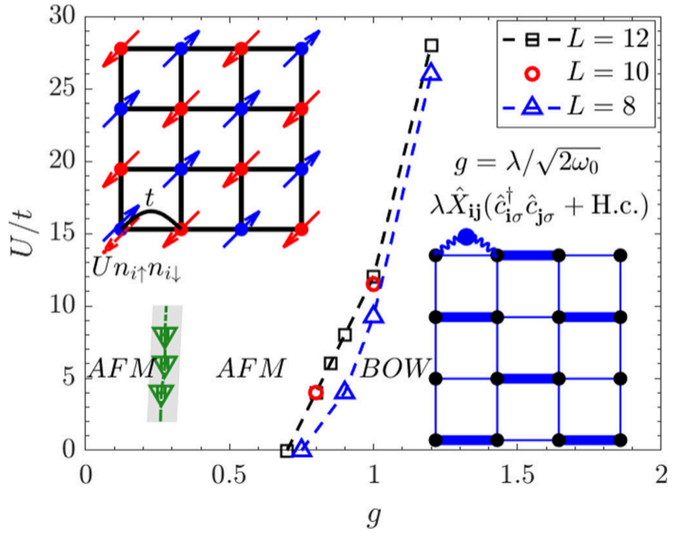


X.Cai et al. *Phys. Rev. Lett.* **127**, 247203 (2021)

+ Hubbard



X.Cai et al. *Phys. Rev. B* **106**, L081115 (2022)



C. Feng et al. *Phys. Rev. B* **106**, L081114 (2022)

Optical Su-Schrieffer-Heeger-Hubbard model

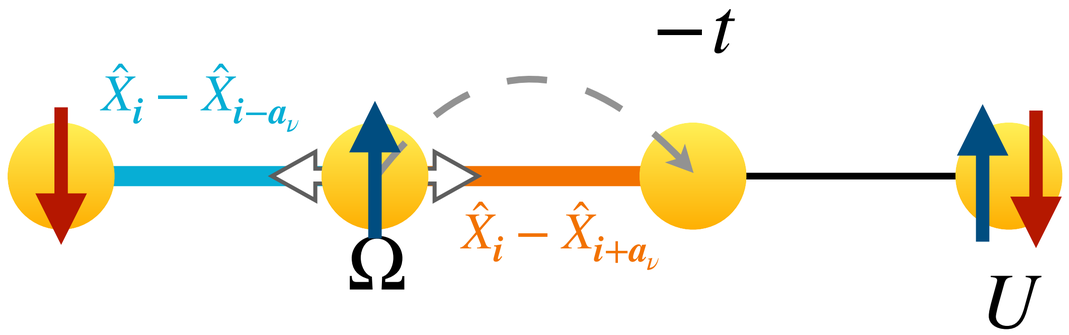
Hubbard model

$$\hat{H}_e = -t \sum_{i,\nu,\sigma} (\hat{c}^{\dagger}_{i+a_\nu,\sigma} \hat{c}_{i,\sigma} + \mathrm{H.c.}) + U \sum_i \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow}$$

Optical SSH model

$$\hat{H}_{e-\mathrm{ph}} = \alpha \sum_{i,\nu,\sigma} (\hat{X}_{i+a_\nu,\nu} - \hat{X}_{i,\nu})(\hat{c}^{\dagger}_{i+a_\nu,\sigma} \hat{c}_{i,\sigma} + \mathrm{H.c.})$$

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



M. Capone, W. Stephen, M Grilli. *Phys. Rev. B.* **56**, 4484 (1997)

Comparative studies: **ATL** et al. *Phys. Rev. B* **108**, 184501 (2023)
S. Malkaruge Costa et al. *Phys. Rev. B* **108**, 165138 (2023)

Methods

Dimensionless coupling constant

$$\lambda = \frac{2}{WN^2} \sum_{\boldsymbol{k},\boldsymbol{q},\nu} \frac{|g_\nu(\boldsymbol{k},\boldsymbol{q})|^2}{\Omega(\boldsymbol{q})} = \boxed{\frac{8\alpha^2}{M\Omega^2 W}}$$

See **ATL** et al. *Phys. Rev. B* **108**, 184501 (2023) and S. Malkaruge Costa et al. *Phys. Rev. B* **108**, 165138 (2023)

Determinant quantum Monte Carlo

- with hybrid Monte Carlo updates
- Finite temperature
- Square clusters ($L = 8 - 14$)
- Phonon energy: $\Omega/t = 0.5$
- Half-filling: $\langle n \rangle = 1$
- **SmoQyDQMC** package

SmoQy Suite: https://github.com/SmoQySuite

B. Cohen-Stead et al. *SciPost Physics Codebases.* **24** (2024)

Correlation Ratios

$$U/t = 3$$
$$\Omega/t = 0.5$$

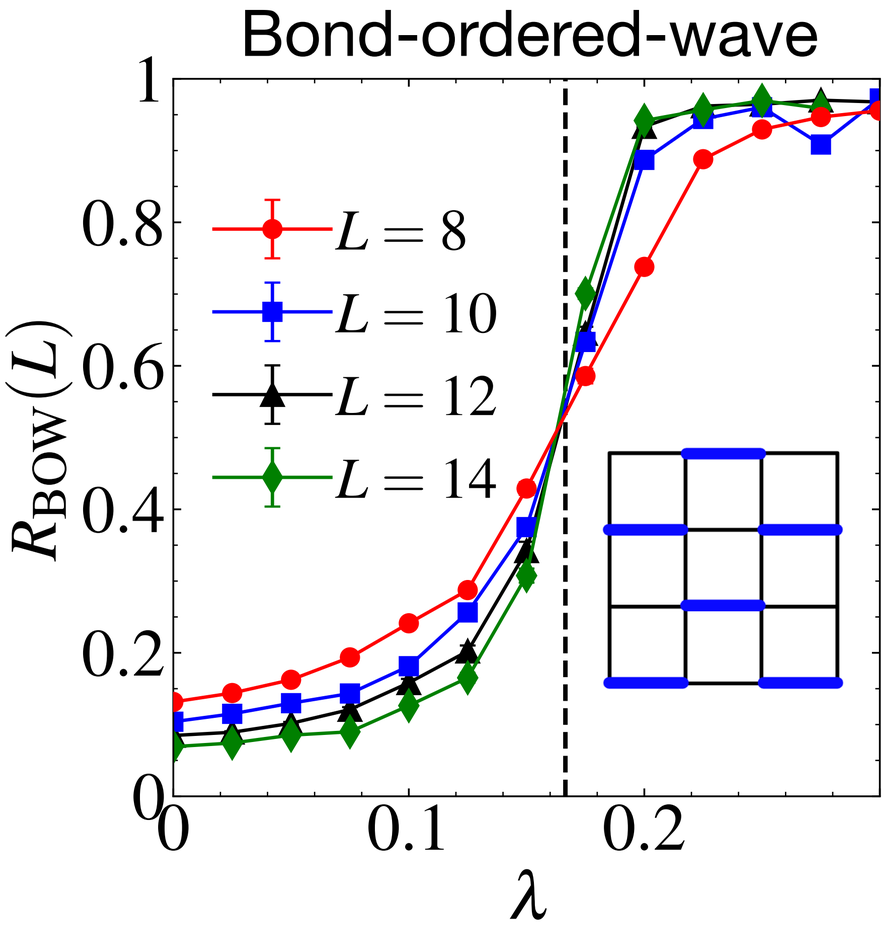
$$R_\gamma(L) = 1 - \frac{S_\gamma(\boldsymbol{Q} - \delta\boldsymbol{q}_L, 0)}{S_\gamma(\boldsymbol{Q}, 0)}$$

$$|\,\delta\boldsymbol{q}_L\,| = \frac{2\pi}{La}$$

$$\boldsymbol{Q} = (\pi/a, \pi/a)$$

Finite size scaling

$$\beta t = L$$



ATL, B. Cohen-Stead, S. Johnston. arXiv:2502.14196 (2025)

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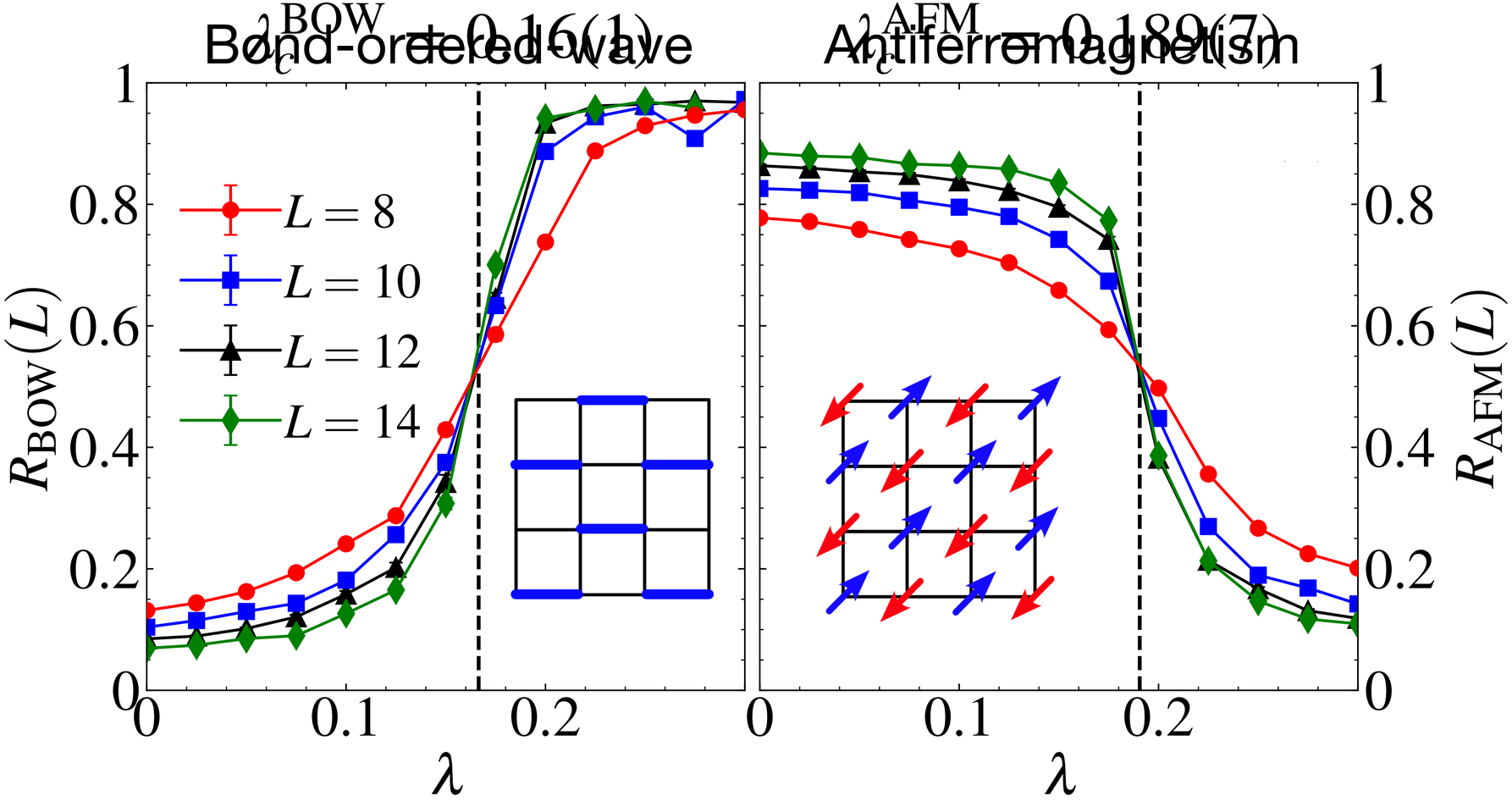
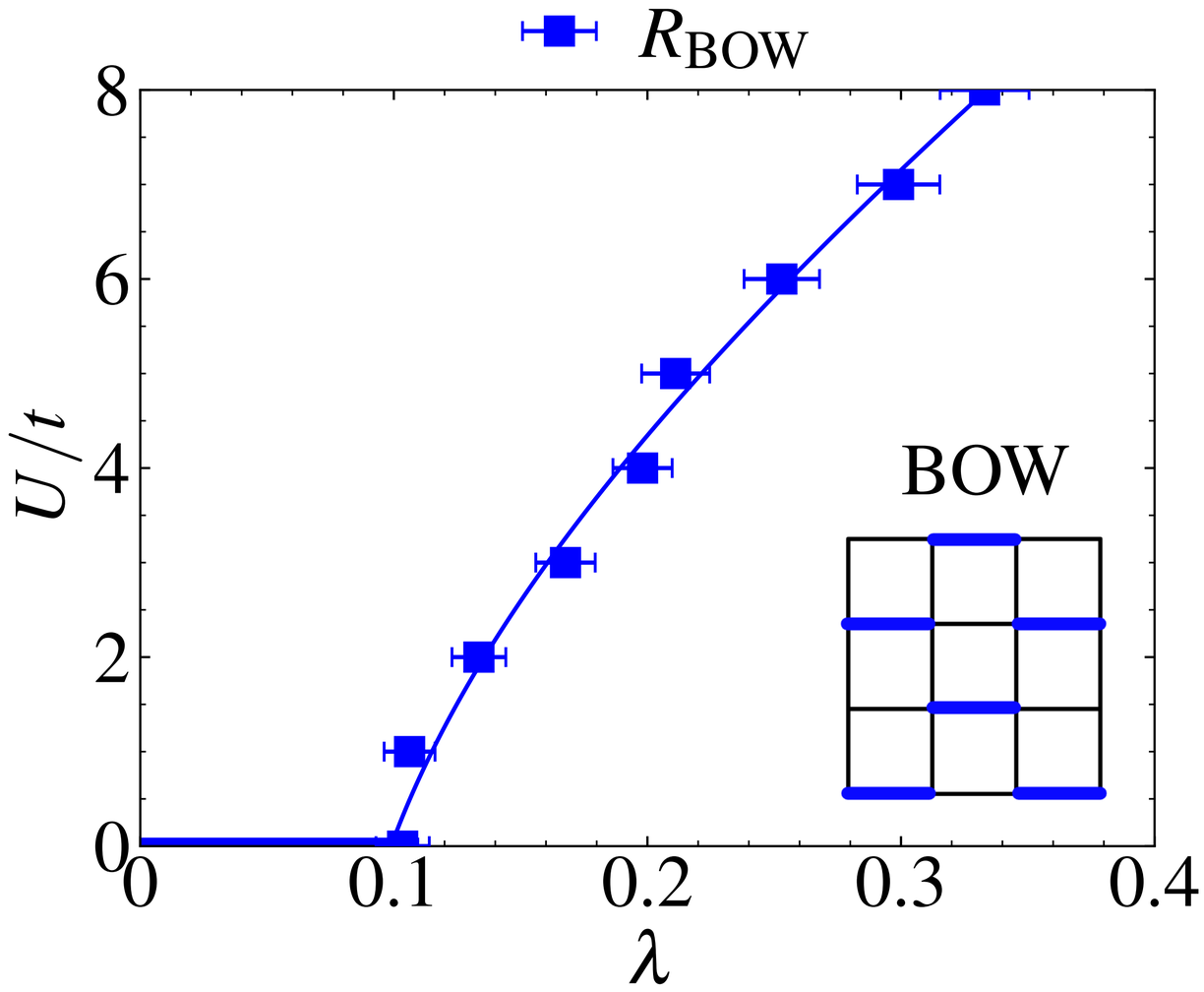


ATL, B. Cohen-Stead, S. Johnston. arXiv:2502.14196 (2025)

Phase diagram $\Omega/t = 0.5$



ATL, B. Cohen-Stead, S. Johnston. arXiv:2502.14196 (2025)

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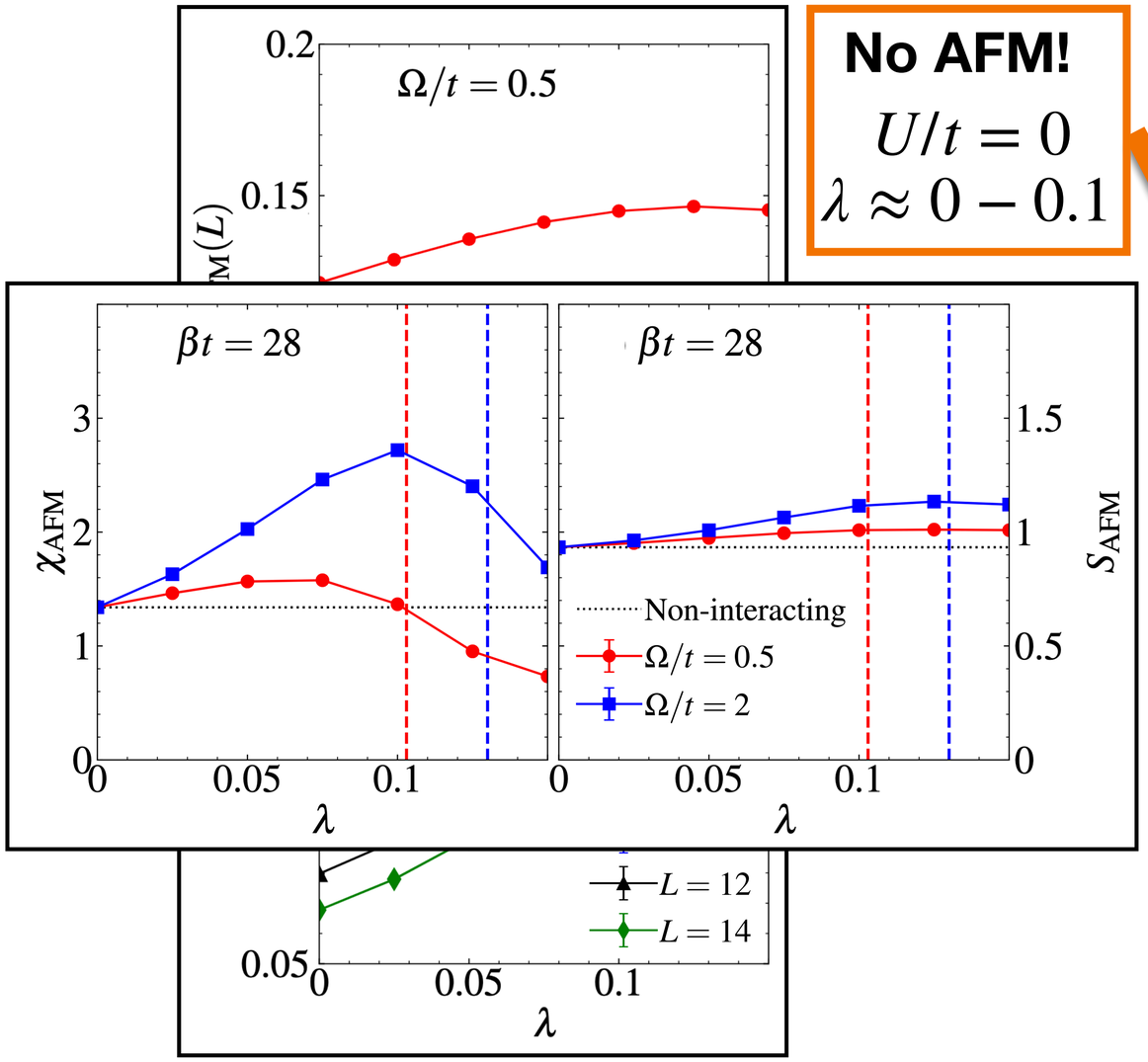
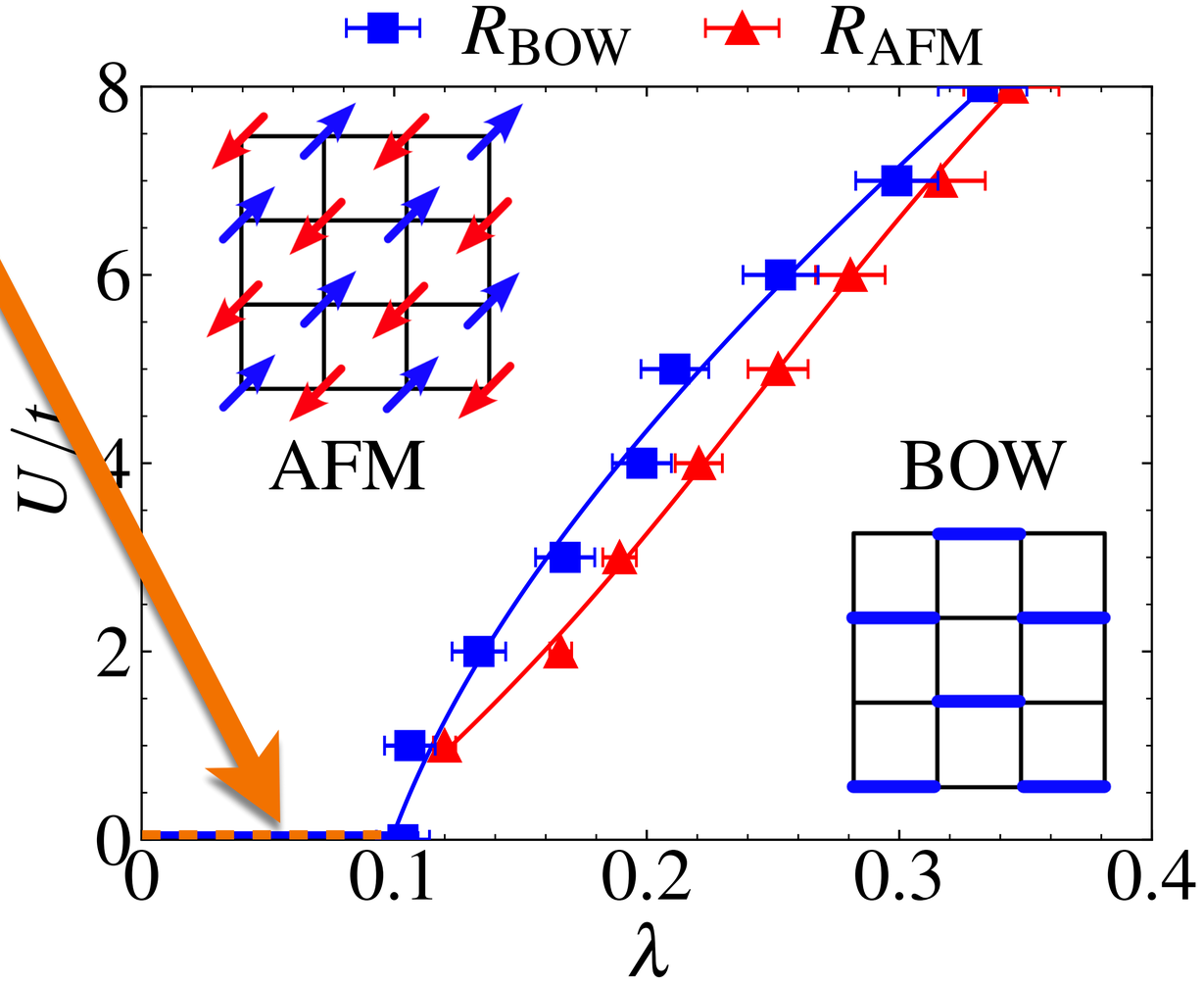


No AFM!

$U/t = 0$

$\lambda \approx 0 - 0.1$



ATL, B. Cohen-Stead, S. Johnston. arXiv:2502.14196 (2025)

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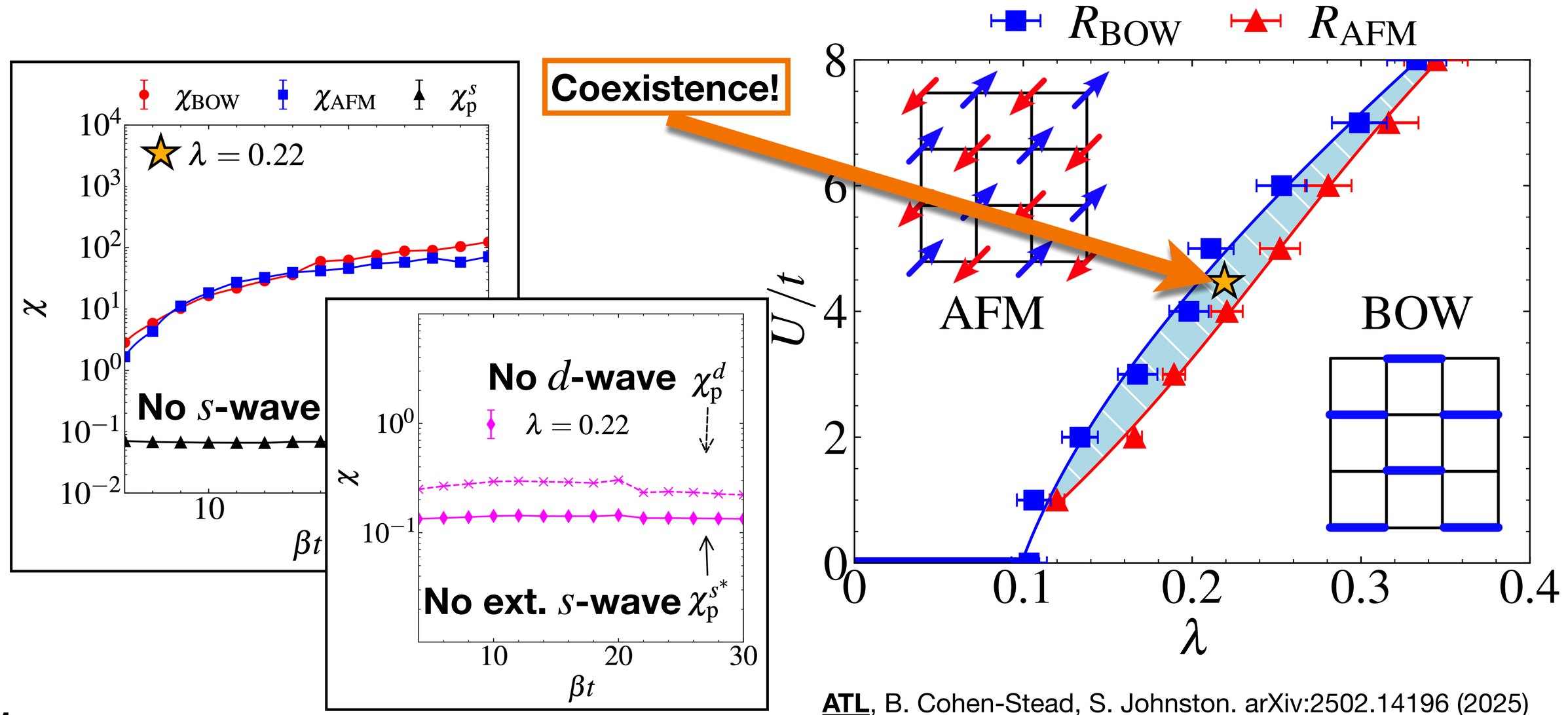
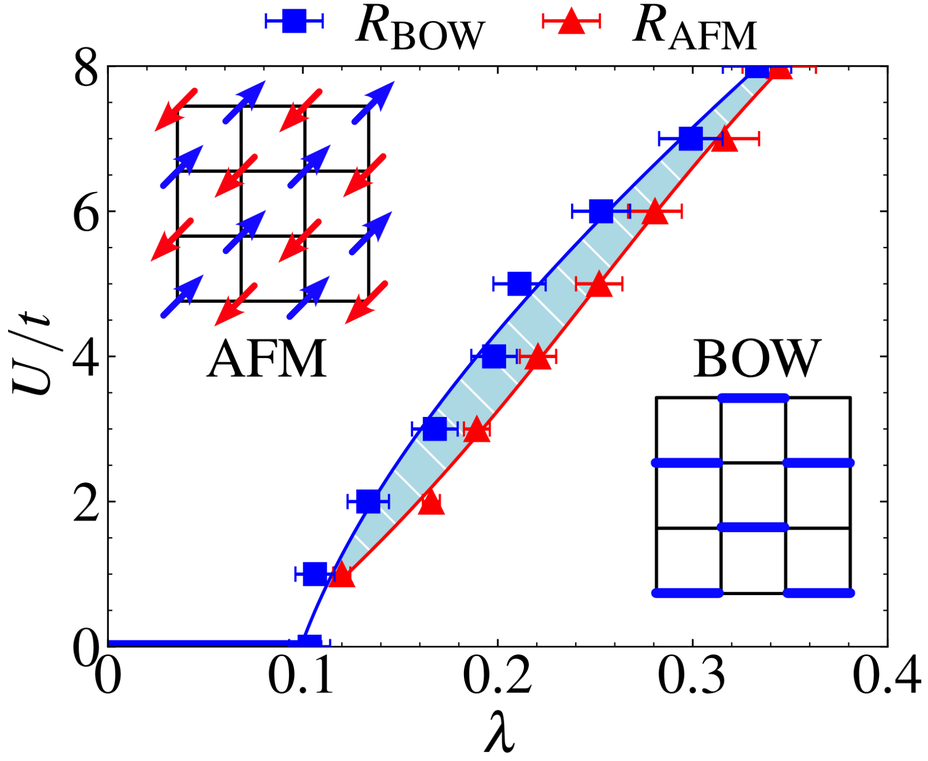


ATL, B. Cohen-Stead, S. Johnston. arXiv:2502.14196 (2025)

Summary

- Ground state phase diagram of the optical SSH-Hubbard model.
- No (long-range) antiferromagnetism in the small coupling ($\lambda = 0 - 0.1$) limit at $U/t = 0$.
- Narrow region of coexistence between antiferromagnetic and bond-ordered-wave phases.
- Overall, the pure ($U/t = 0$) optical SSH model behaves quite differently from the pure bond SSH model.
- Preprint available at: **arXiv:2502.14196 (2025)**



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