Comparative Quantum Monte Carlo studies of the two-dimensional bond-Su-Schrieffer-Heeger and Holstein models

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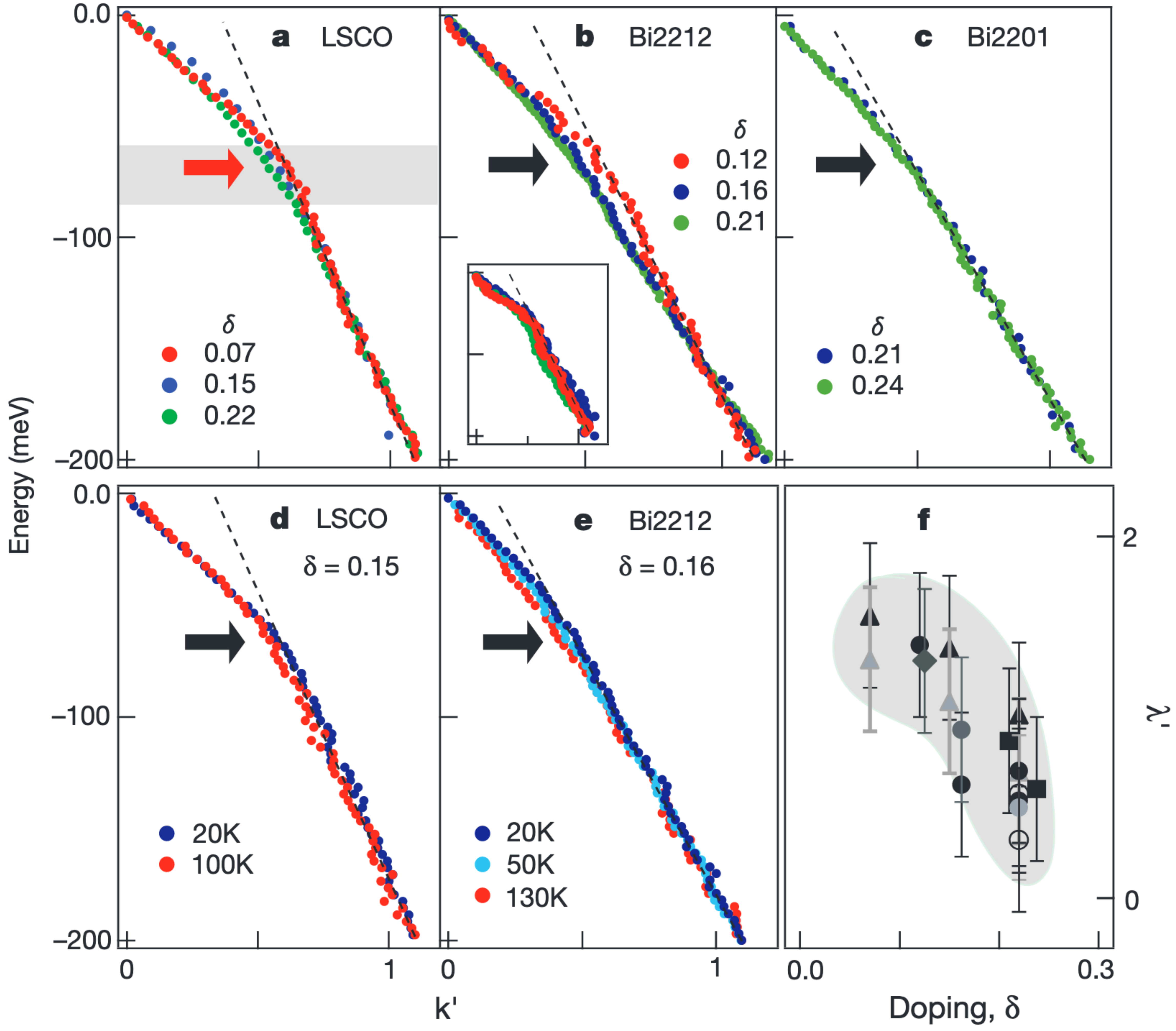
Electron-phonon (e-ph) interactions in materials



A. Lanzara et al. Nature **412**, 510 (2001)

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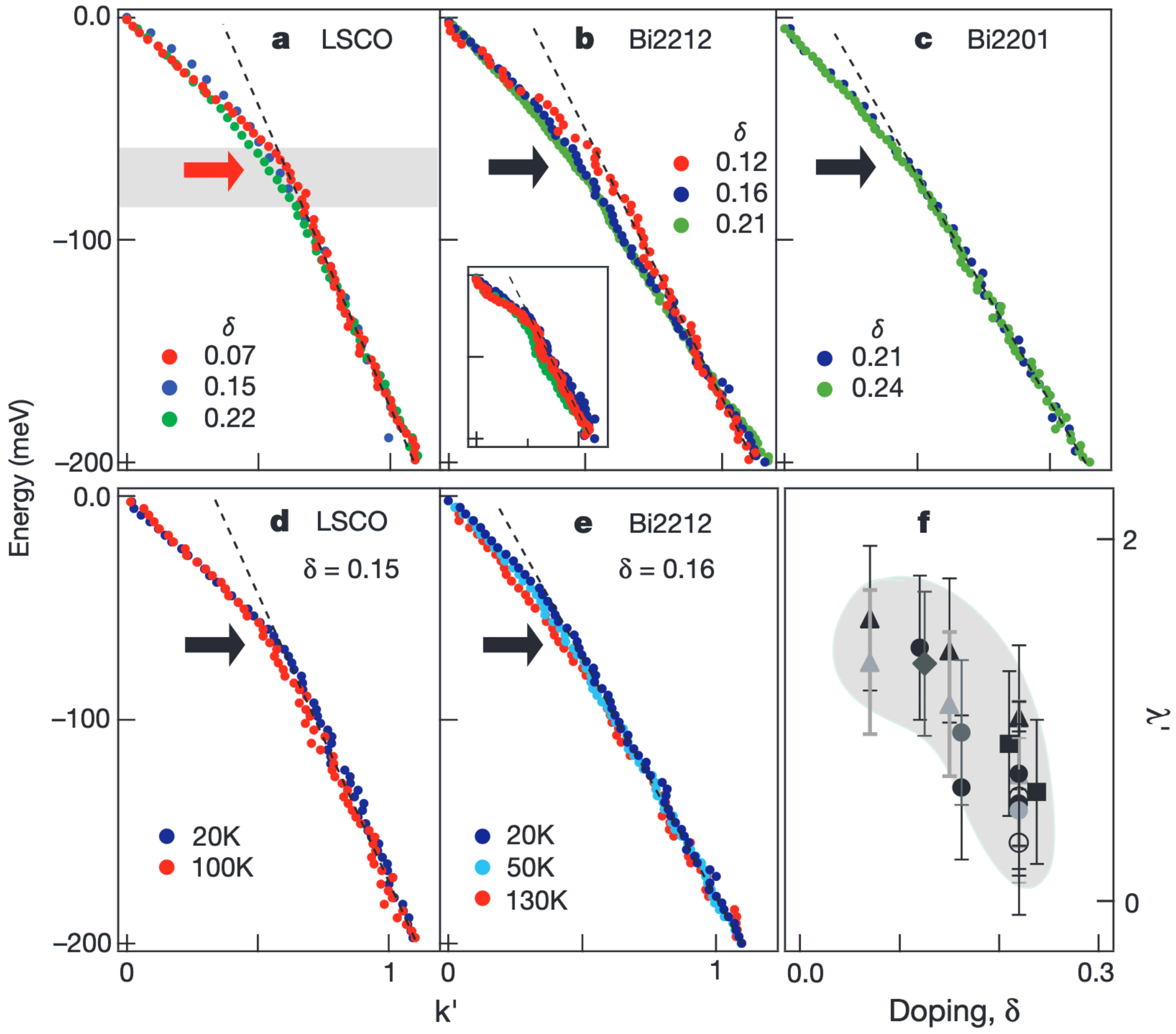

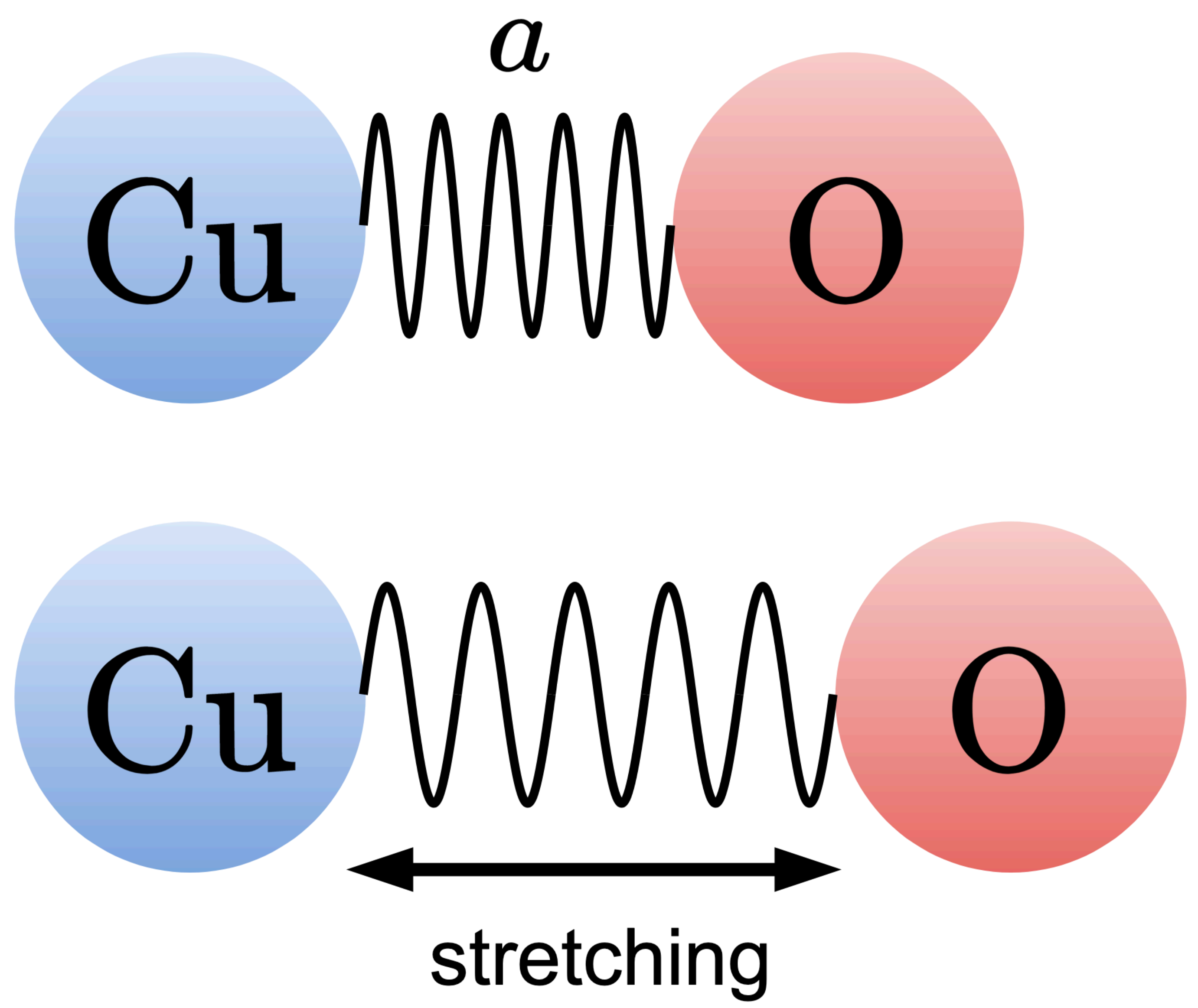

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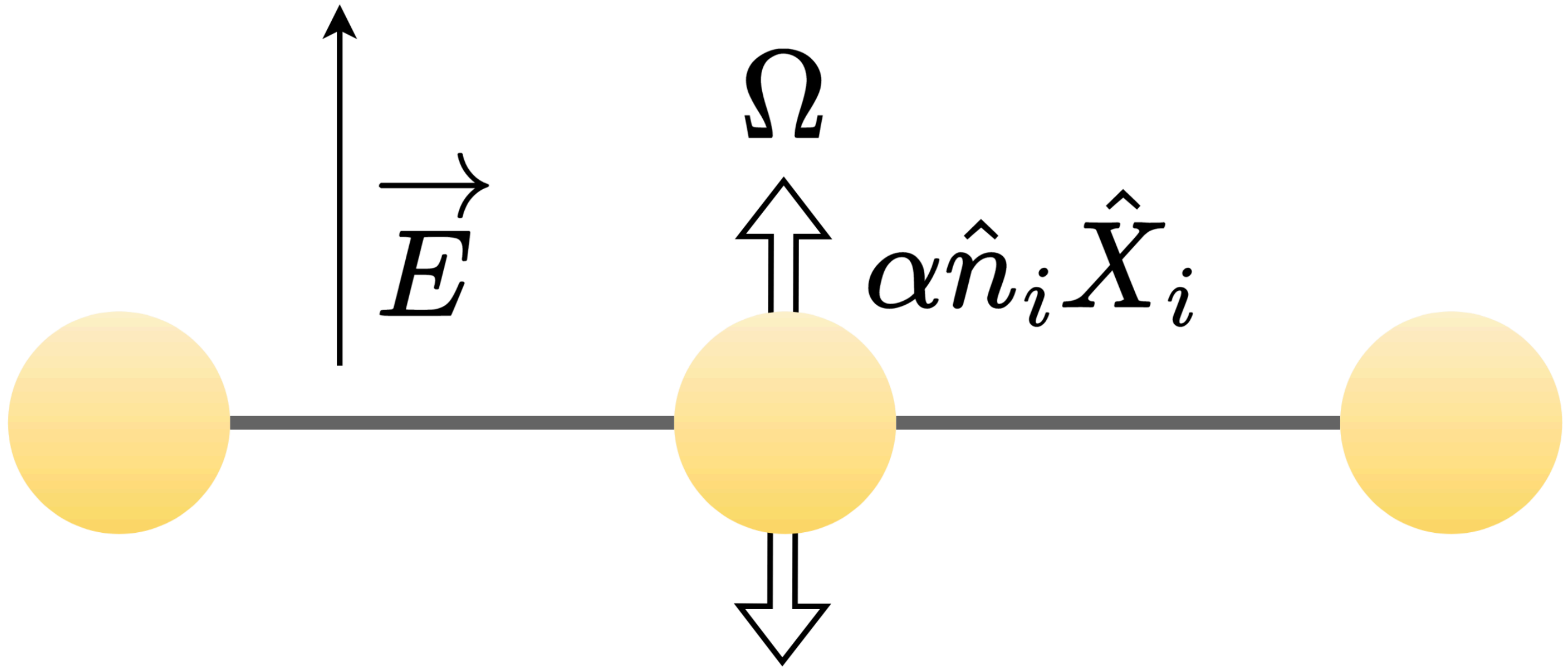
Models of e-ph interactions

“Buckling” modes



Holstein model

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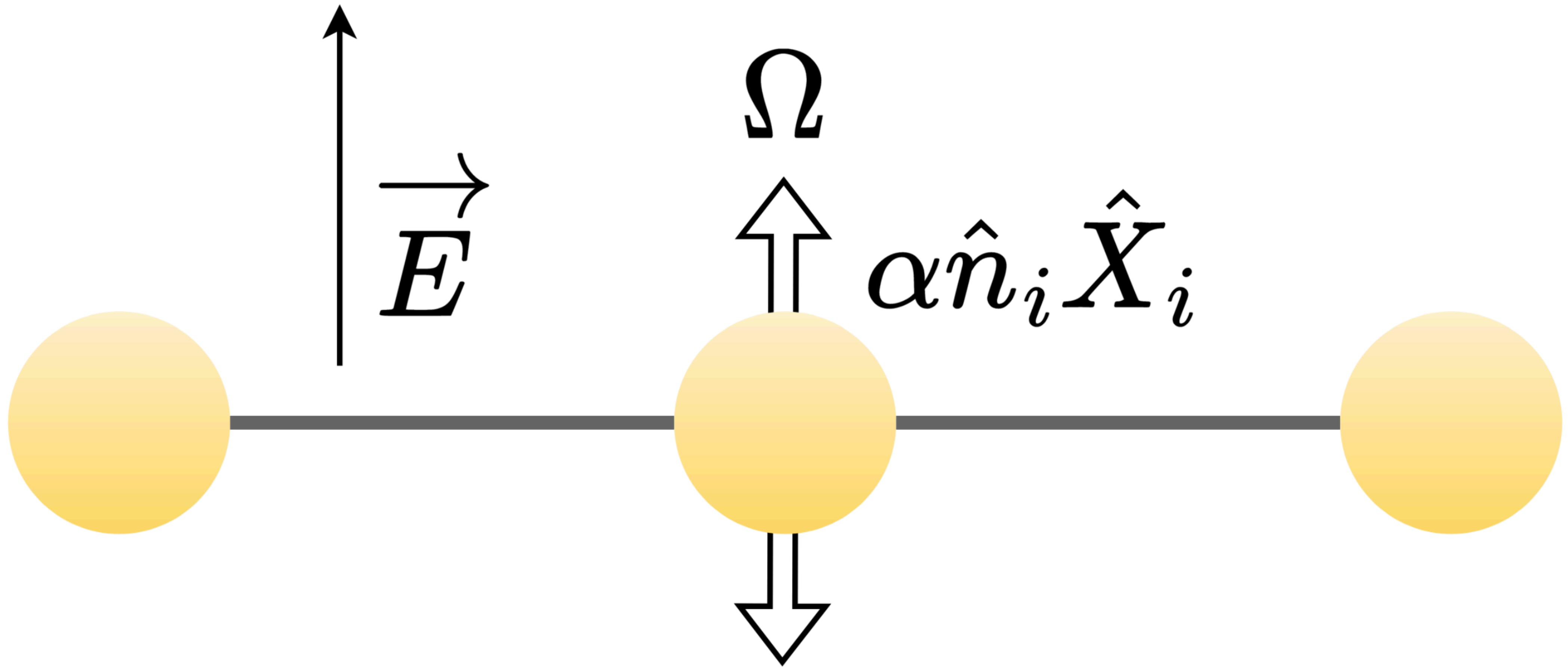

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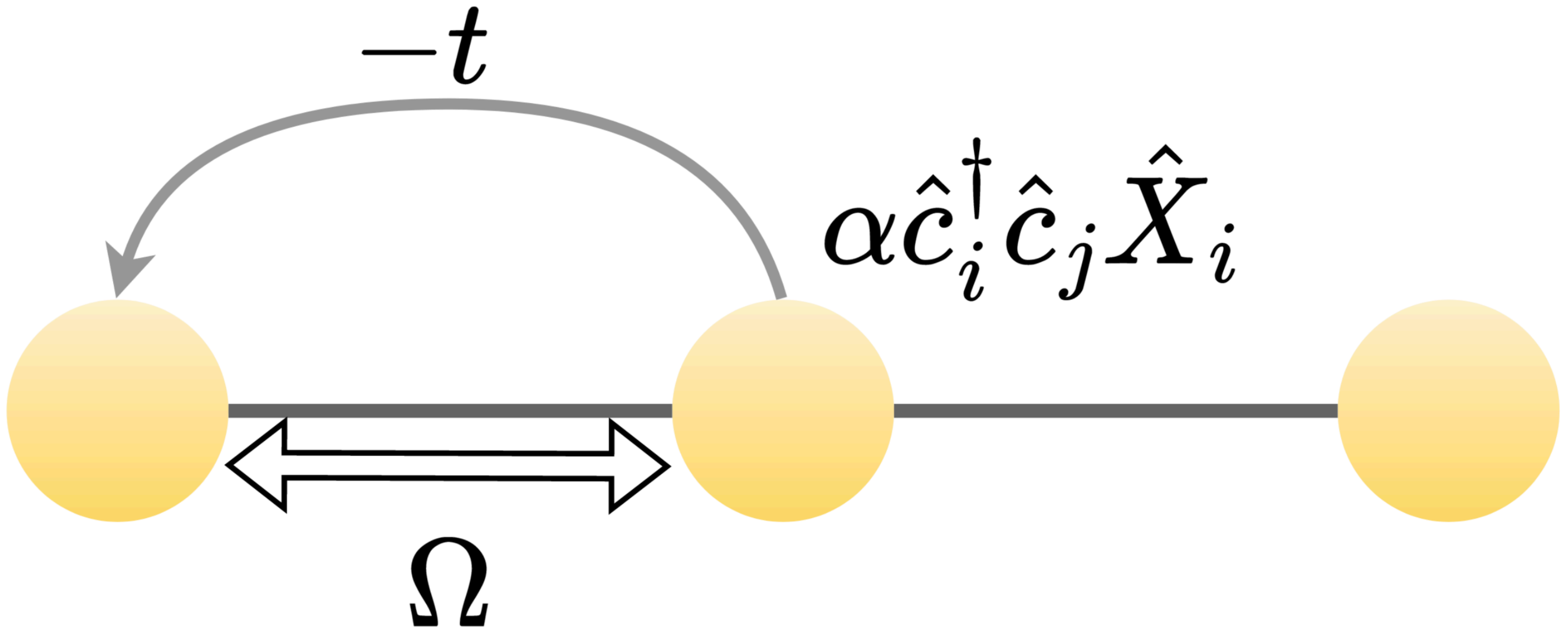

bond-Su-Schrieffer-Heeger (bSSH) model

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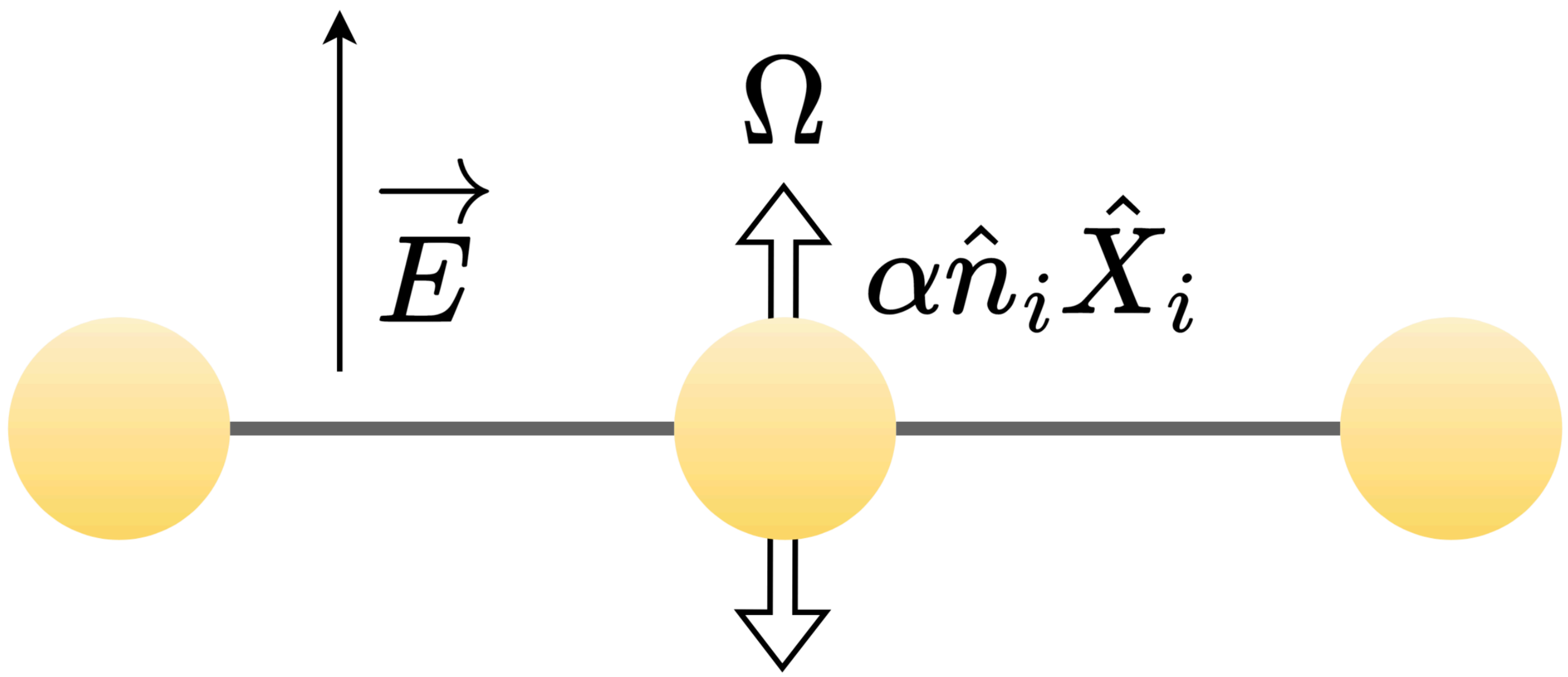

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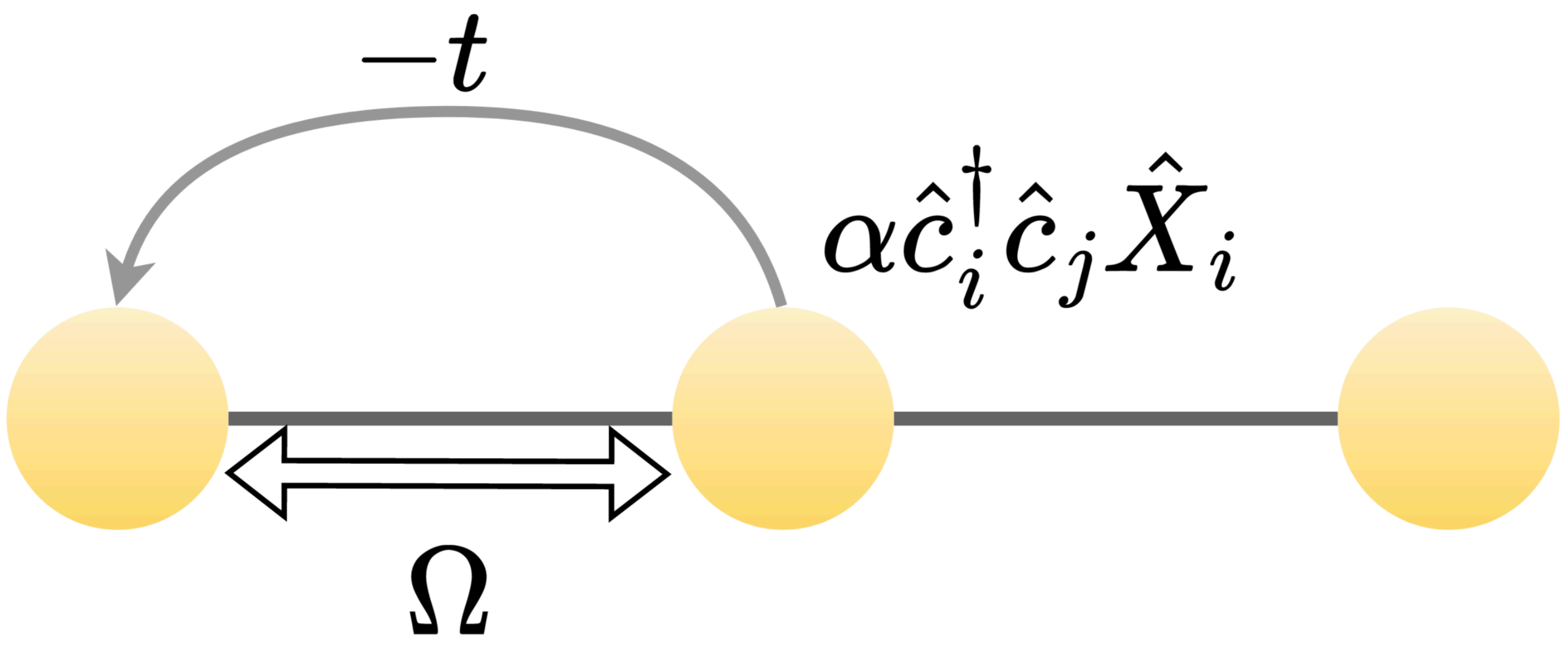

bond-Su-Schrieffer-Heeger (bSSH) model

Proposal by C. Zhang et al., Phys. Rev. X 13, 011010 (2023)

Methods

Tight-binding model and phonon modes

$$\hat{H}_{\text{el}} = -t \sum_{\langle i,j \rangle,\sigma} \left(\hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + \text{h.c.} \right) - \mu \sum_{i\sigma} \hat{n}_{i\sigma}$$

$$\hat{H}_{\text{lat}} = \sum_{i} \left(\frac{1}{2} M \Omega^2 \hat{X}_i^2 + \frac{1}{2M} \hat{P}_i^2 \right)$$

e-ph coupling

$$\hat{H}_{\text{H}} = \alpha \sum_{i\sigma} \hat{n}_{i\sigma} \hat{X}_i$$

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Determinant Quantum Monte Carlo[1,2] (DQMC) and Hybrid Monte Carlo[3] (HMC)

- Auxiliary field Monte Carlo
- DQMC: $\Omega \geq t$, HMC: $\Omega \leq t$
- Finite temperature
- 8 x 8 square clusters

[1] S. Johnston, E. A. Nowadnick, Y. F. Kung, B. Moritz, R. T. Scalettar, and T. P. Devereaux, Phys. Rev. B **87**, 235133 (2013)

[2] C. Feng, B. Xing, D. Poletti, R. Scalettar, and G. Batrouni, Phys. Rev. B **106**, L081114 (2022)

[3] B. Cohen-Stead, O. Bradley, C. Miles, G. Batrouni, R. Scalettar, and K. Barros, Phys. Rev. E, **105** 065302 (2022)

Electron-phonon coupling constant

- Dimensionless coupling: $\lambda = N_F \left\langle \left\langle \frac{\alpha^2_{\mathbf{k}-\mathbf{k}'}}{\Omega^2_{\mathbf{k}-\mathbf{k}'}} \right\rangle \right\rangle_{FS}$

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- Bond-SSH: **Momentum independent:**

$$\lambda_{bSSH} \approx \frac{4\alpha^2}{\Omega^2 W}$$

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Momentum averaged:

$$\lambda_{bSSH} \approx \frac{4\alpha^2}{\Omega^2 W} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \partial k \partial q \cos^2[(k + q/2)/2]$$

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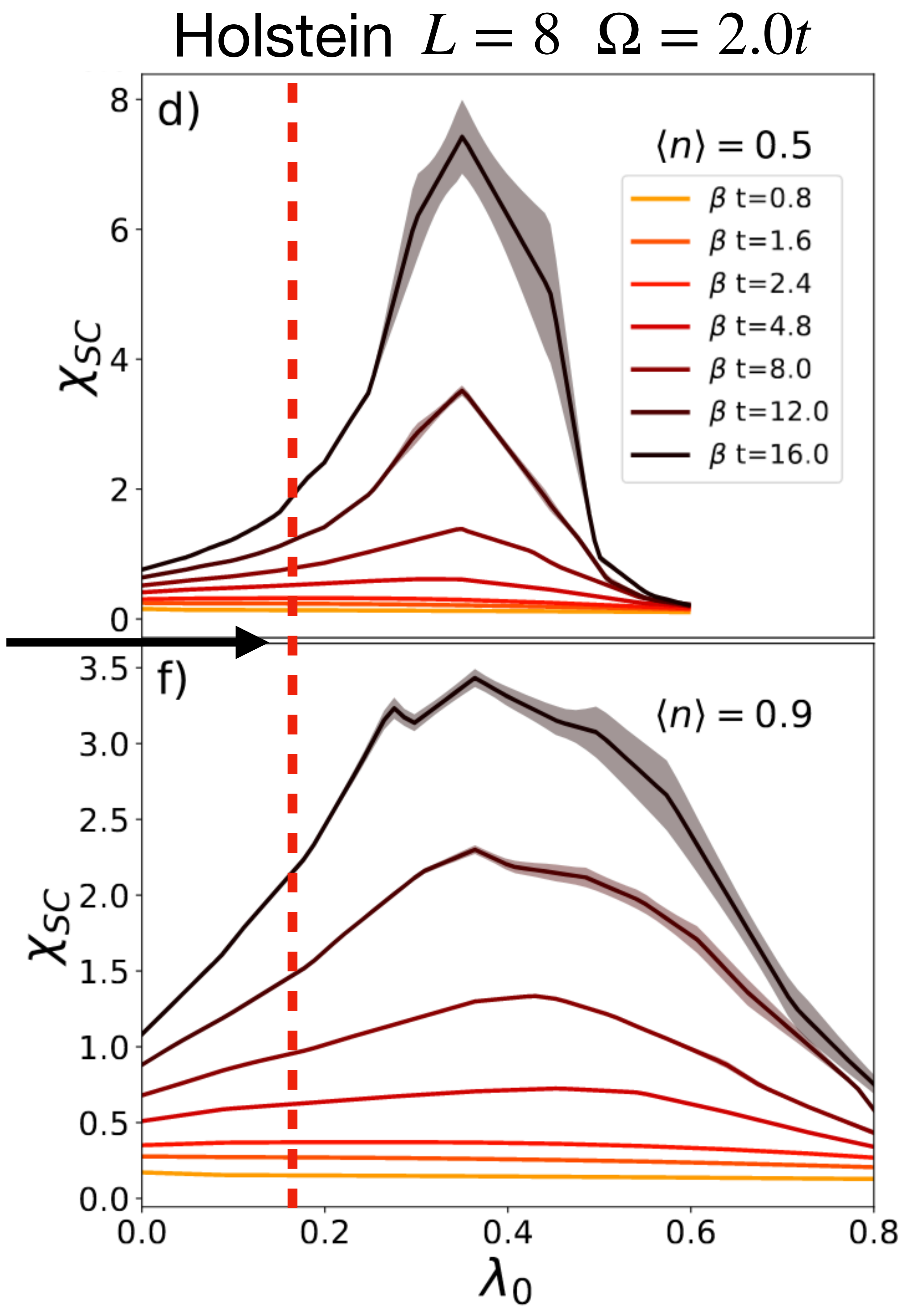
$\lambda = 0.15$



B. Nosarzewski et al. Phys. Rev. B **103**, 235156 (2021)

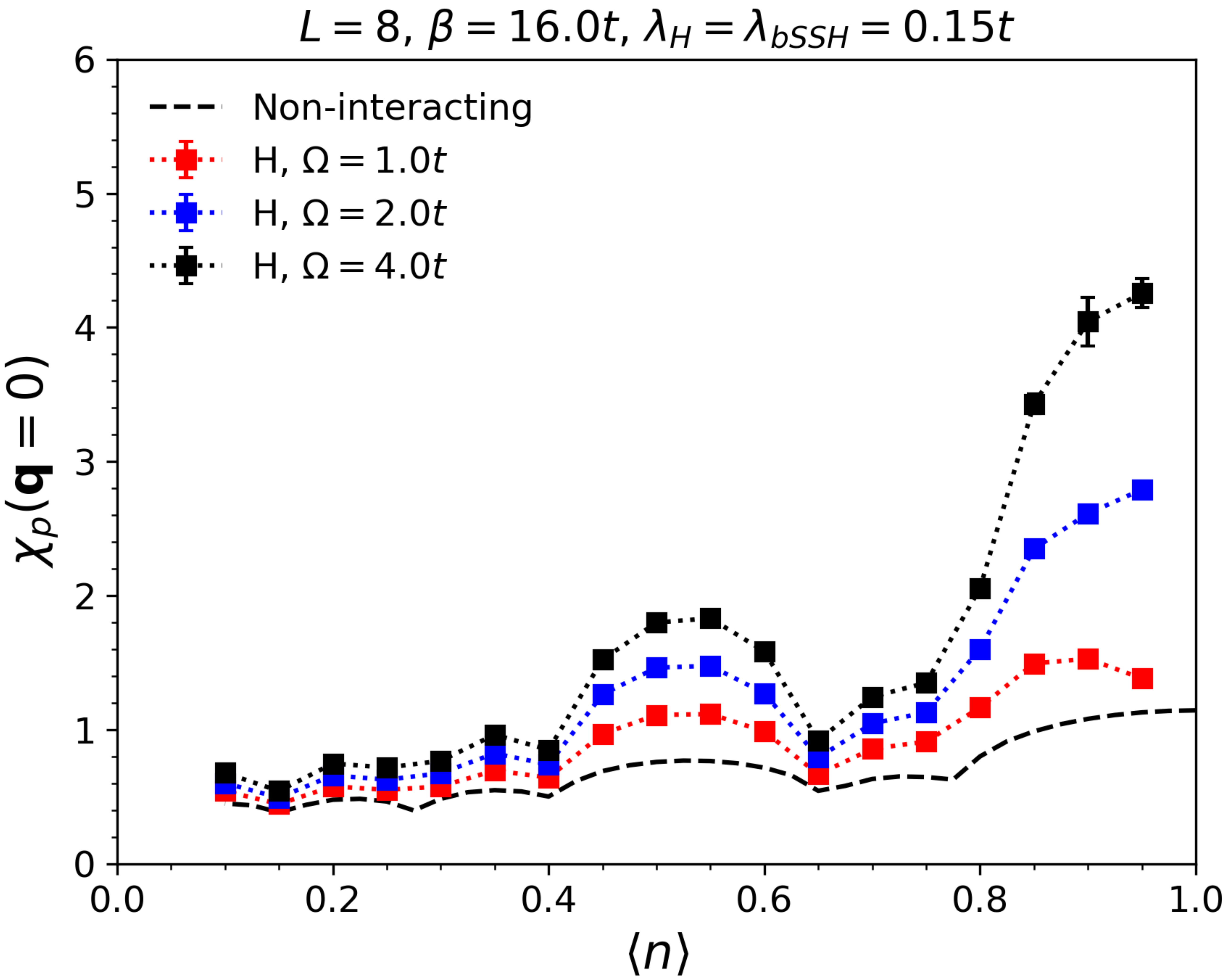
Density dependent pairing correlations

Pair-field operator

$$\hat{\Delta}(\tau) = \sum_i \hat{c}_{i\uparrow}(\tau)\hat{c}_{i\downarrow}(\tau)$$

Pair-field susceptibility

$$\chi_p = \frac{1}{N}\int_0^\beta d\tau \langle \hat{\Delta}(\tau)\hat{\Delta}(0)\rangle$$



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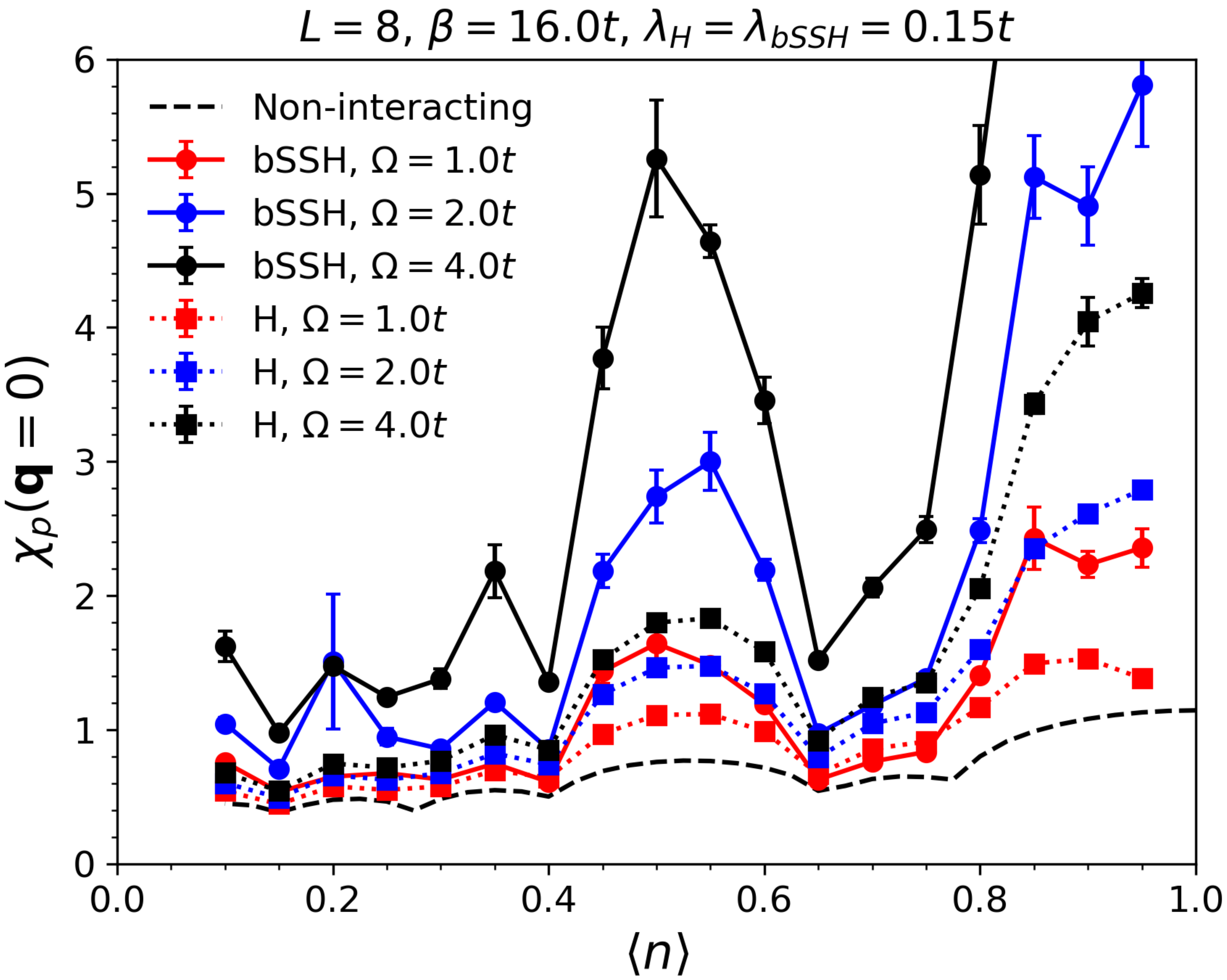
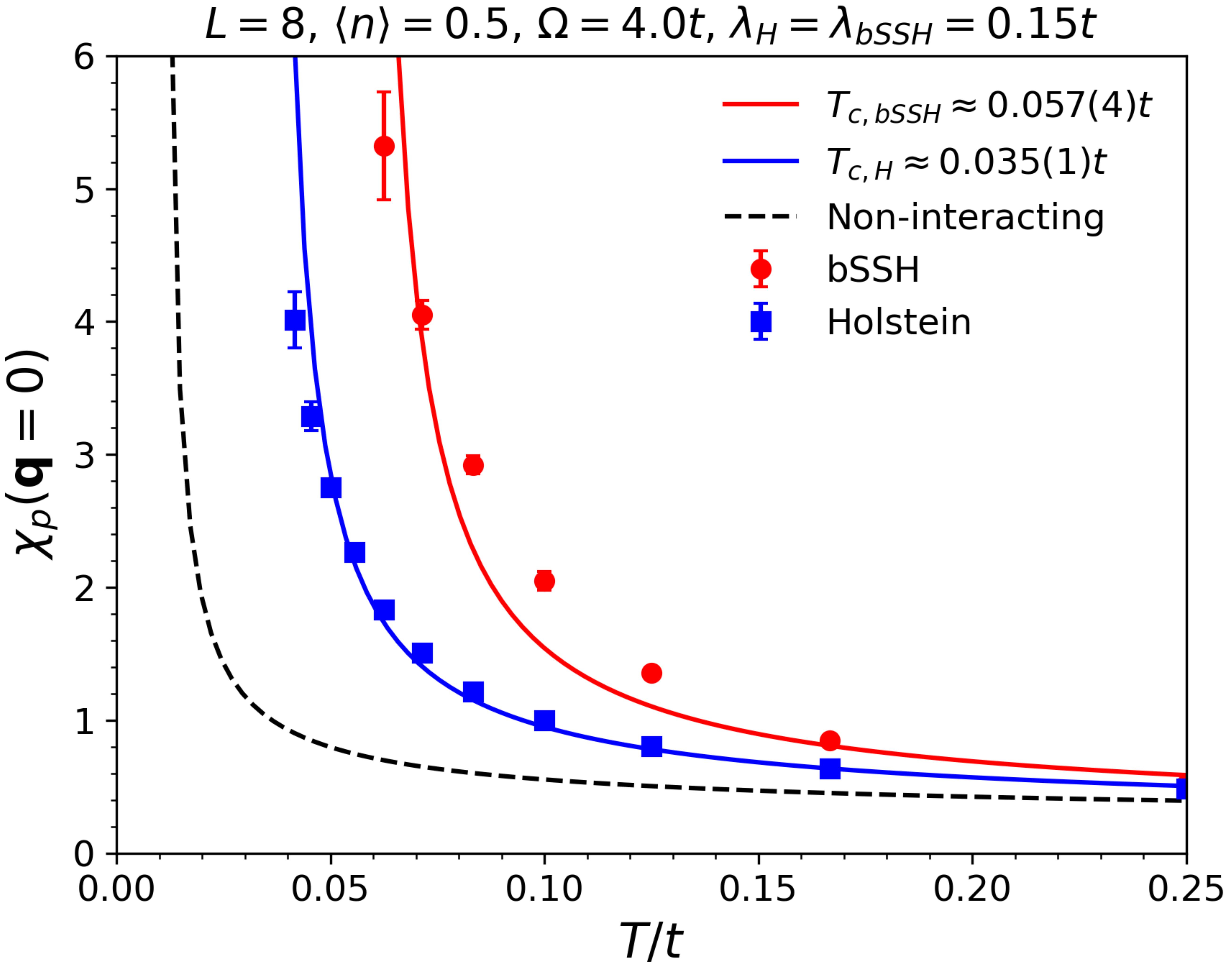


Temperature dependent pairing correlations



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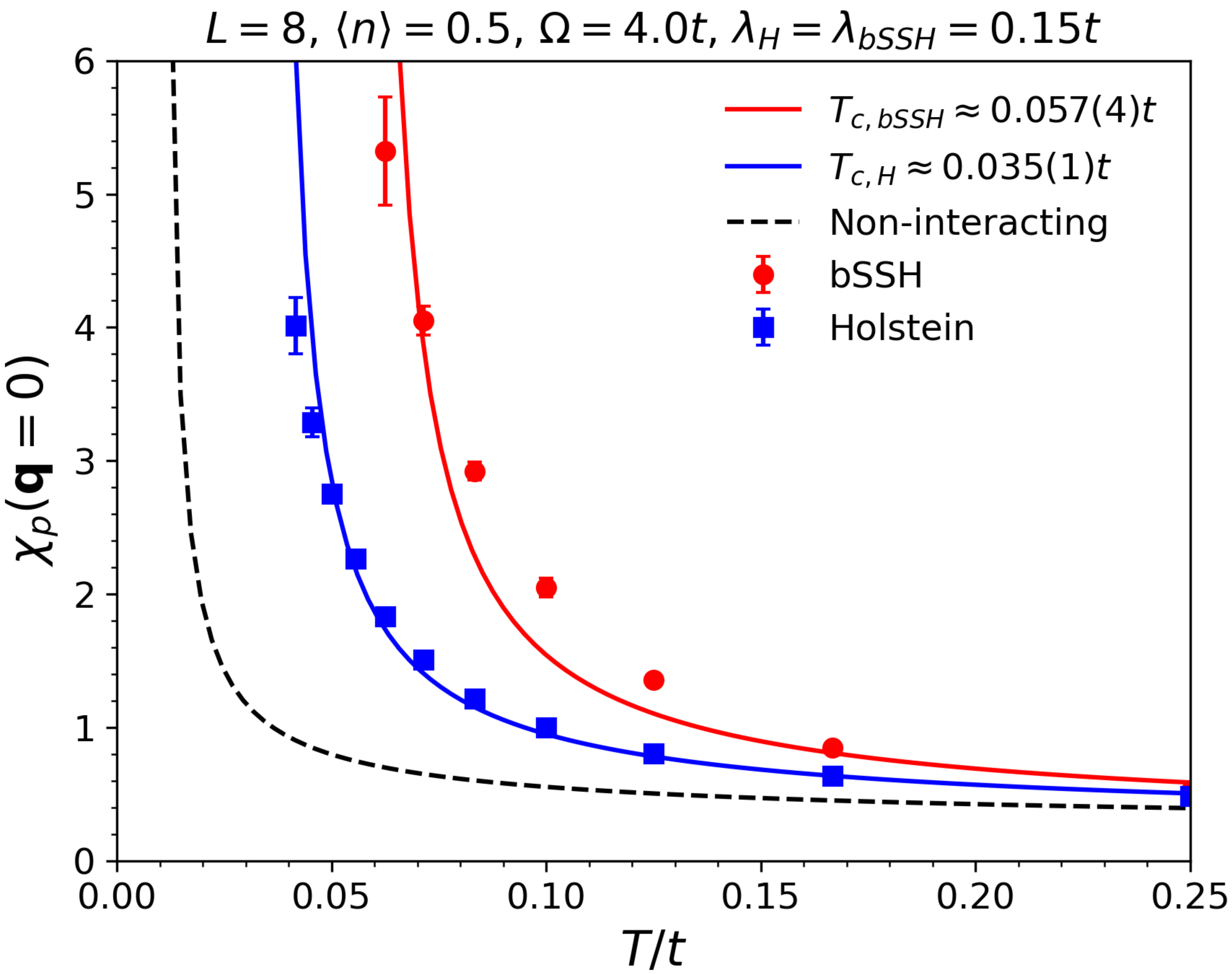
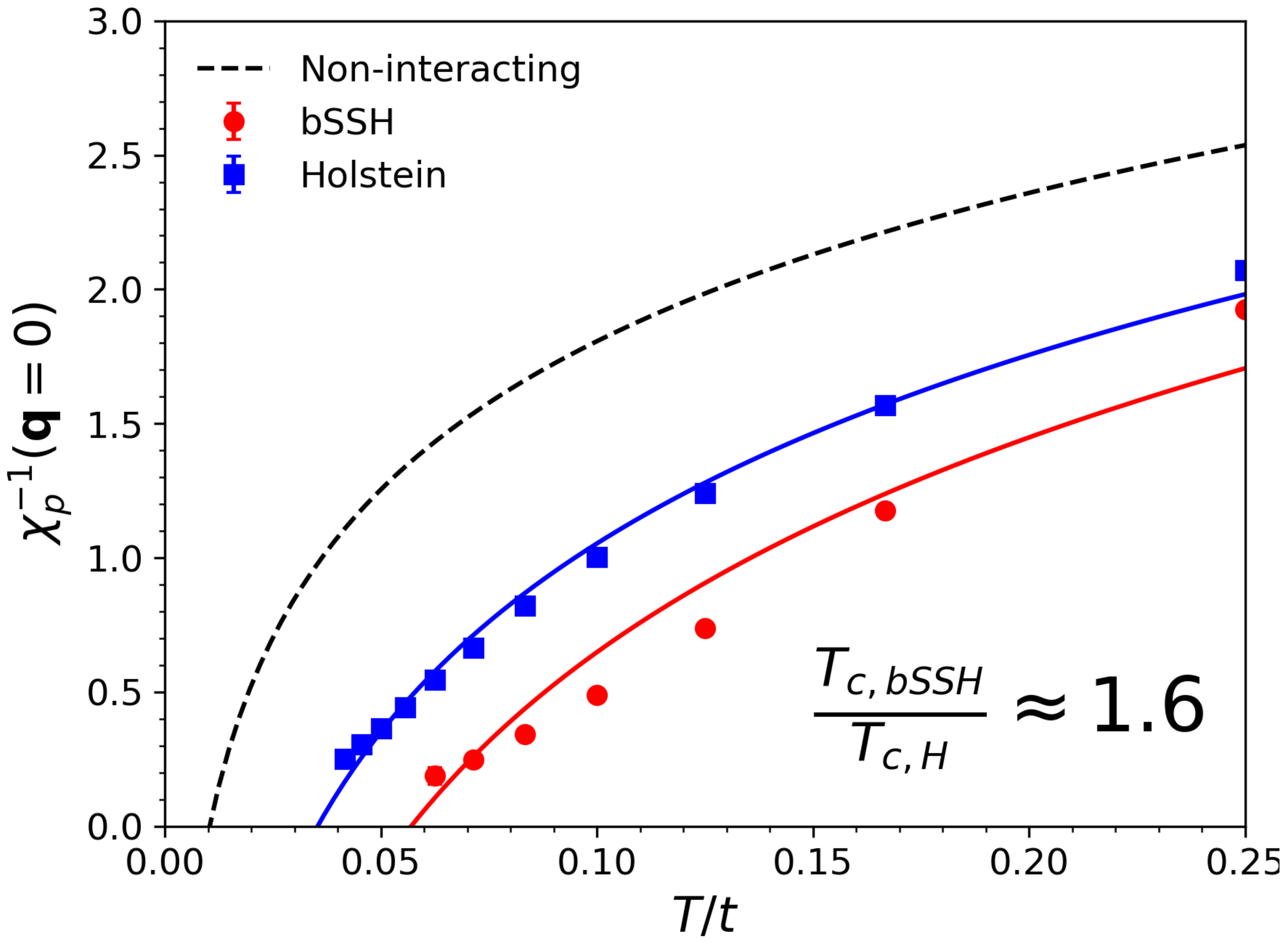
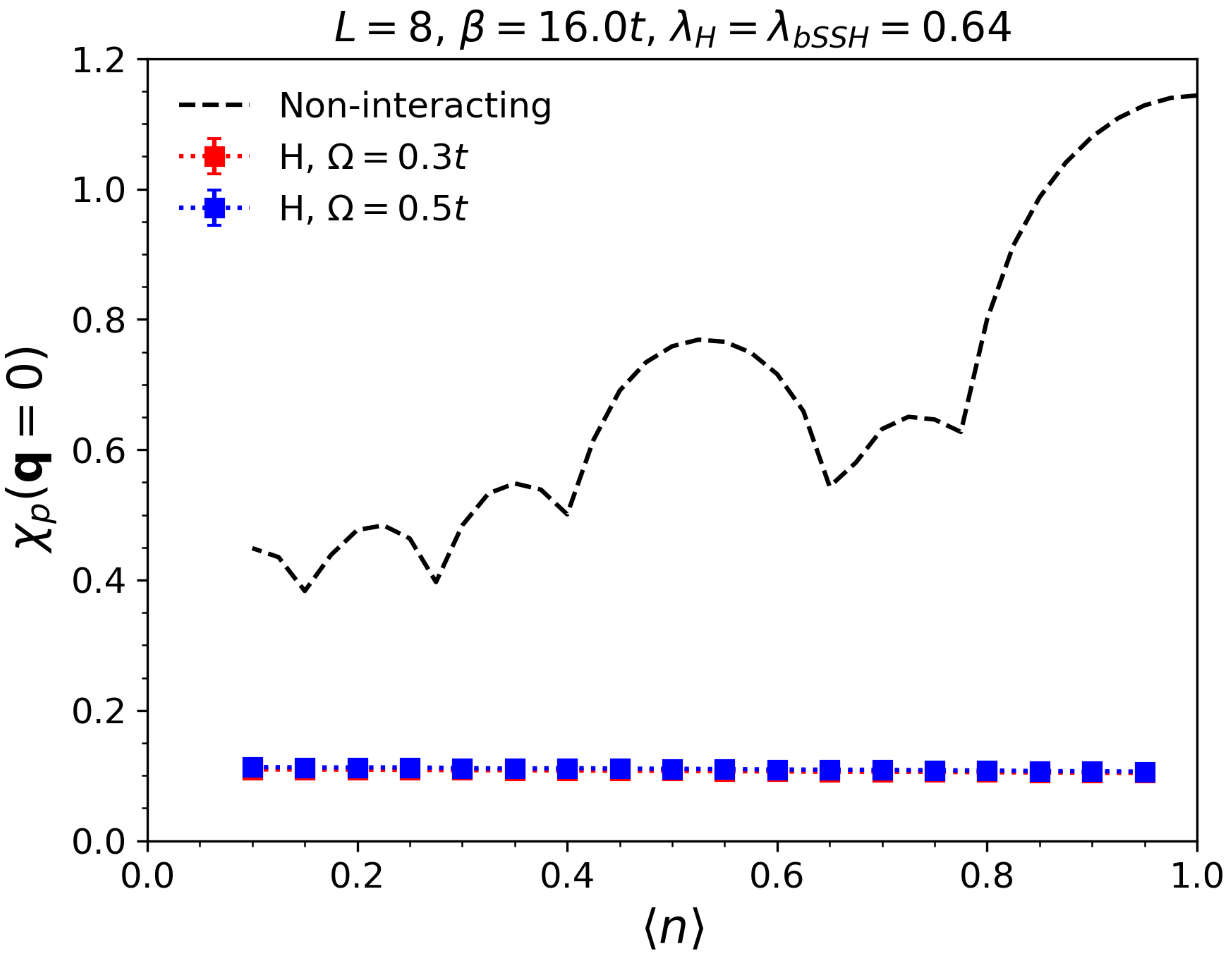


BCS instability:

$$\chi_p^{-1} = A \log\left(\frac{T}{T_c}\right)$$



Strong coupling



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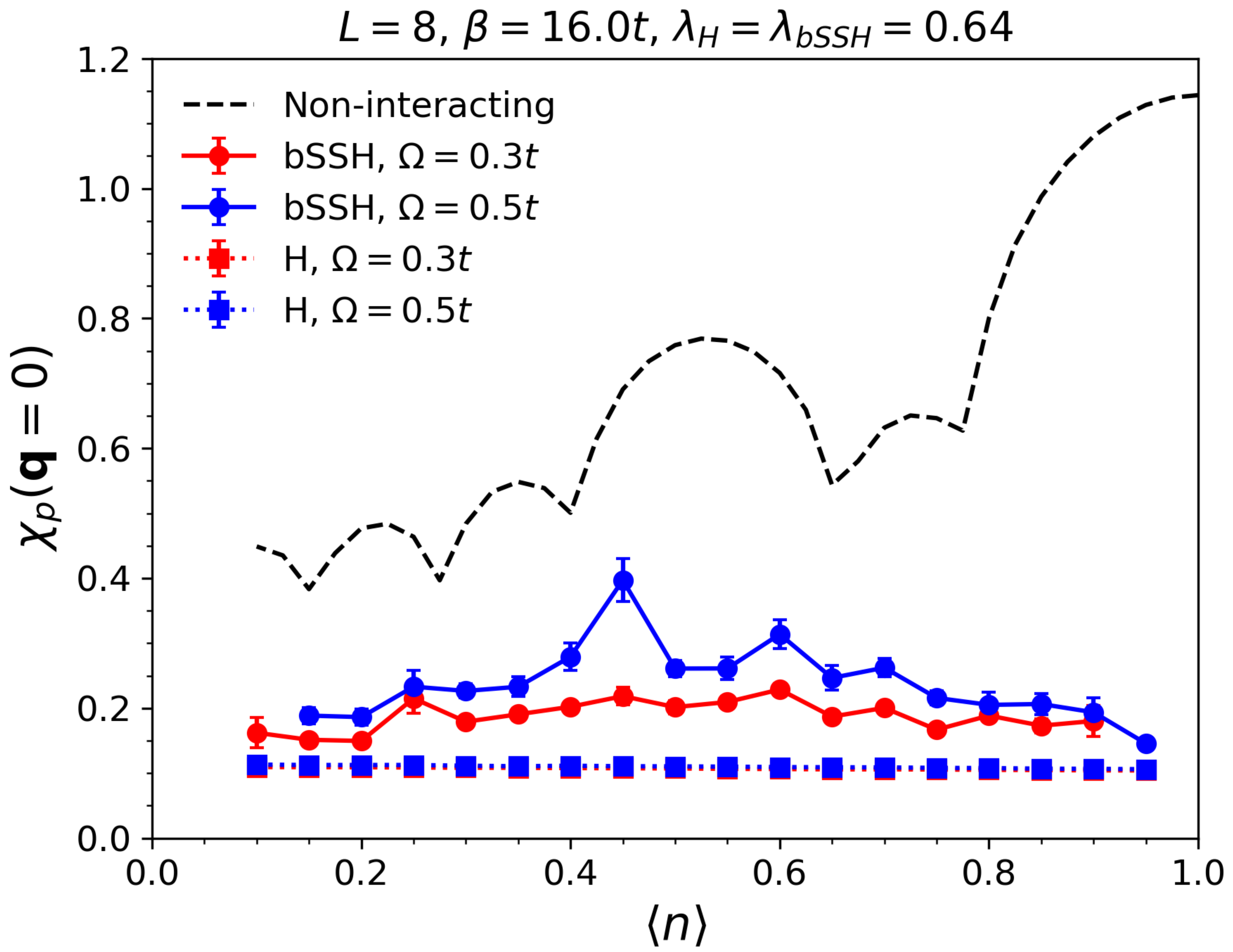

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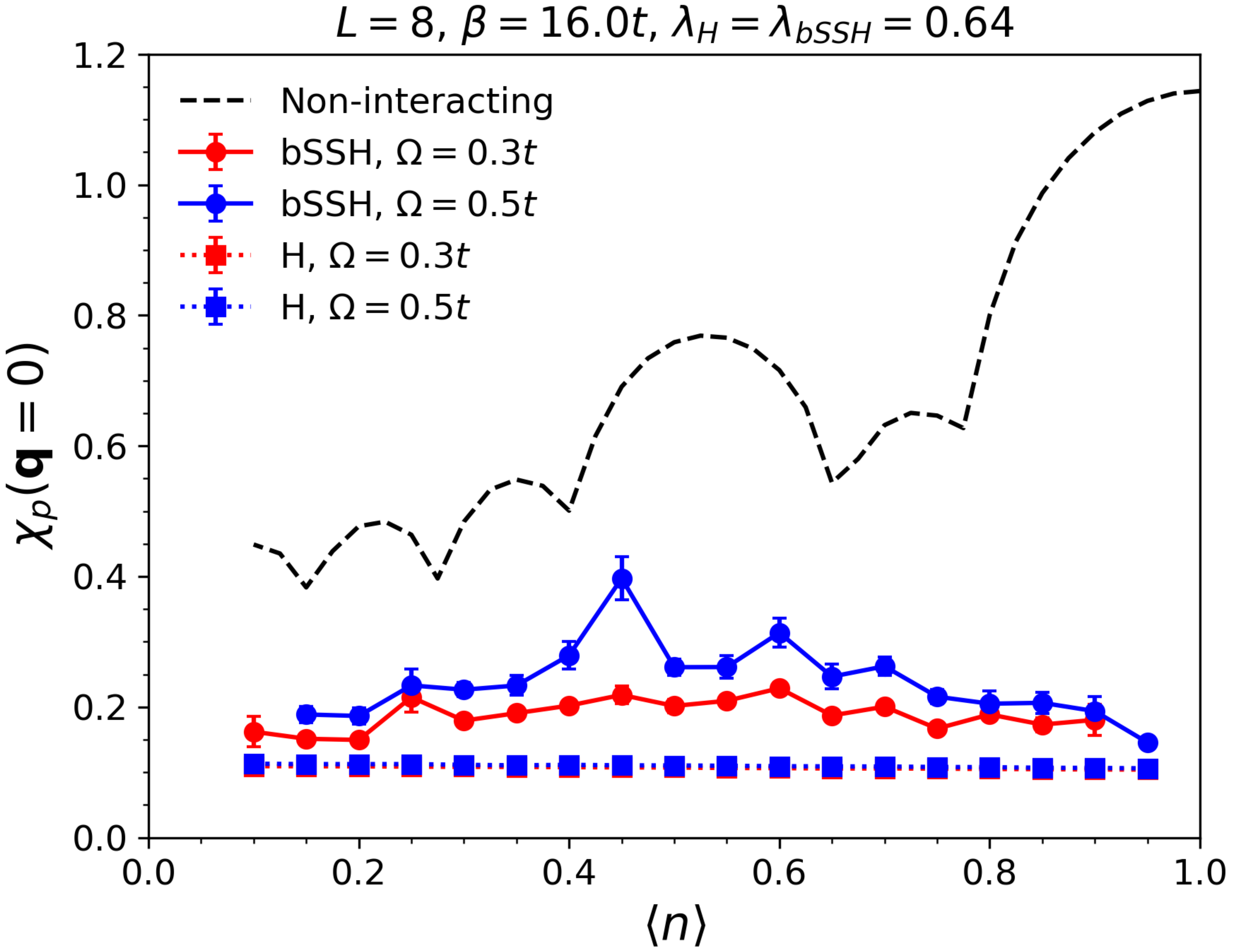

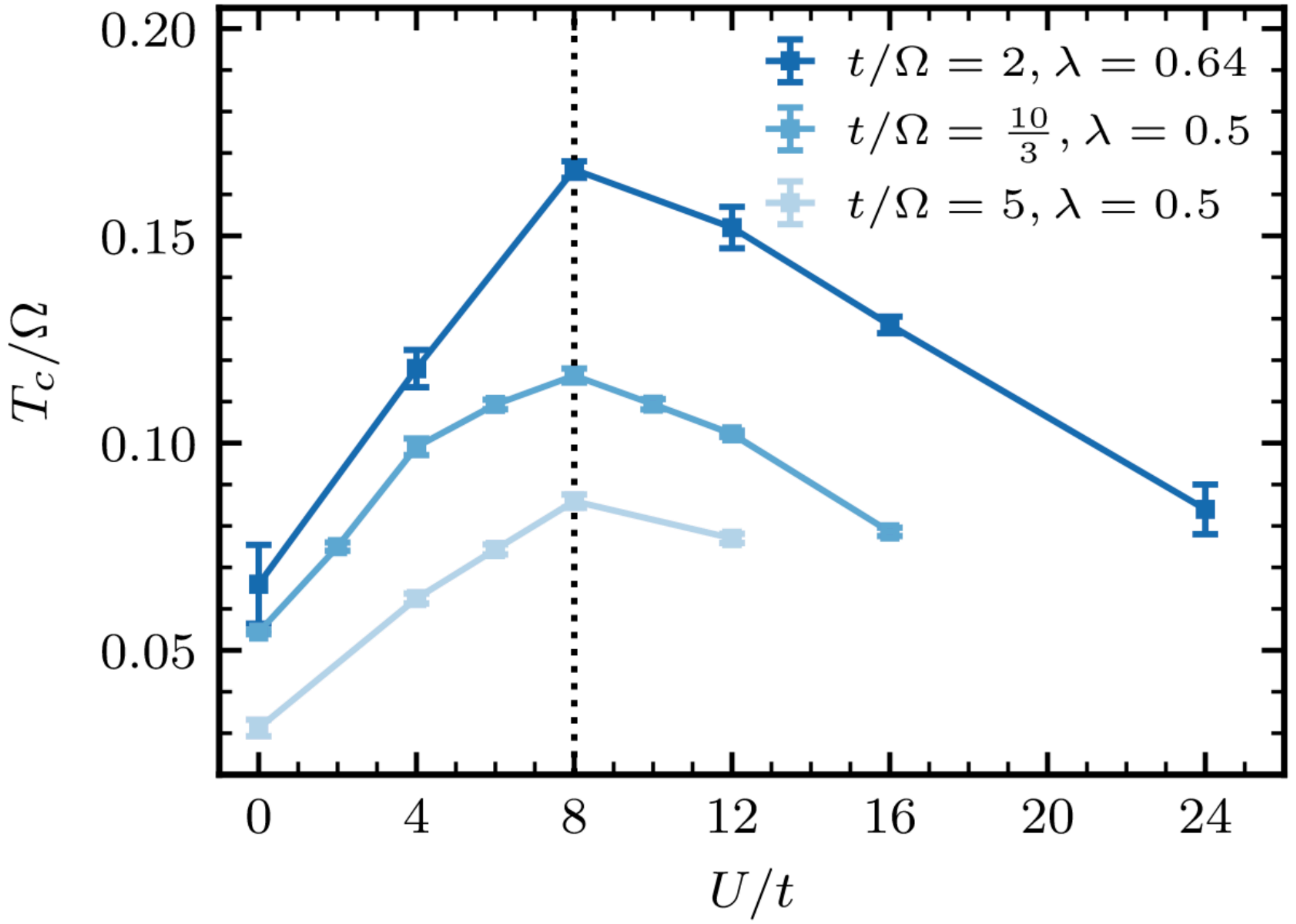

C. Zhang et al., Phys. Rev. X 13, 011010 (2023)

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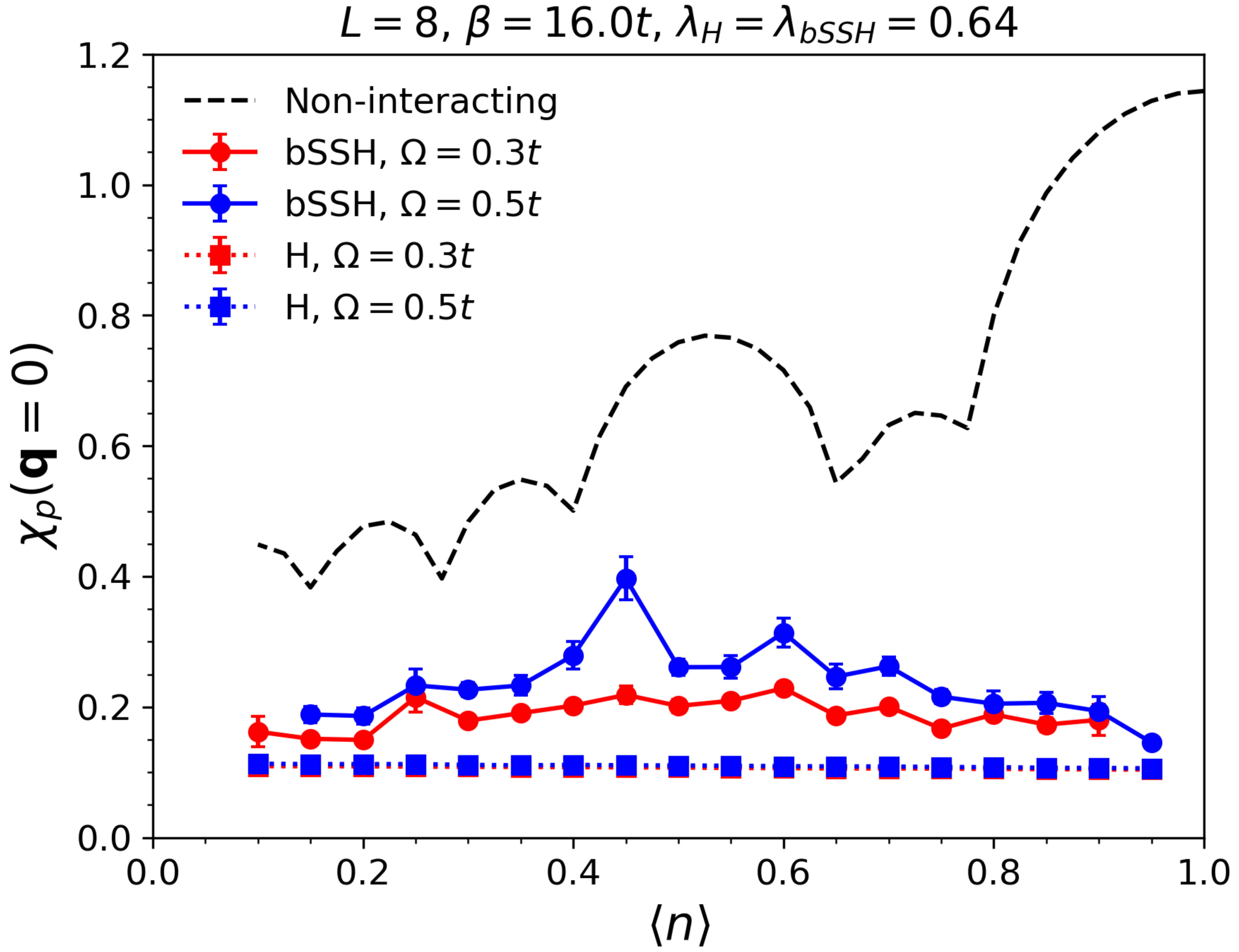

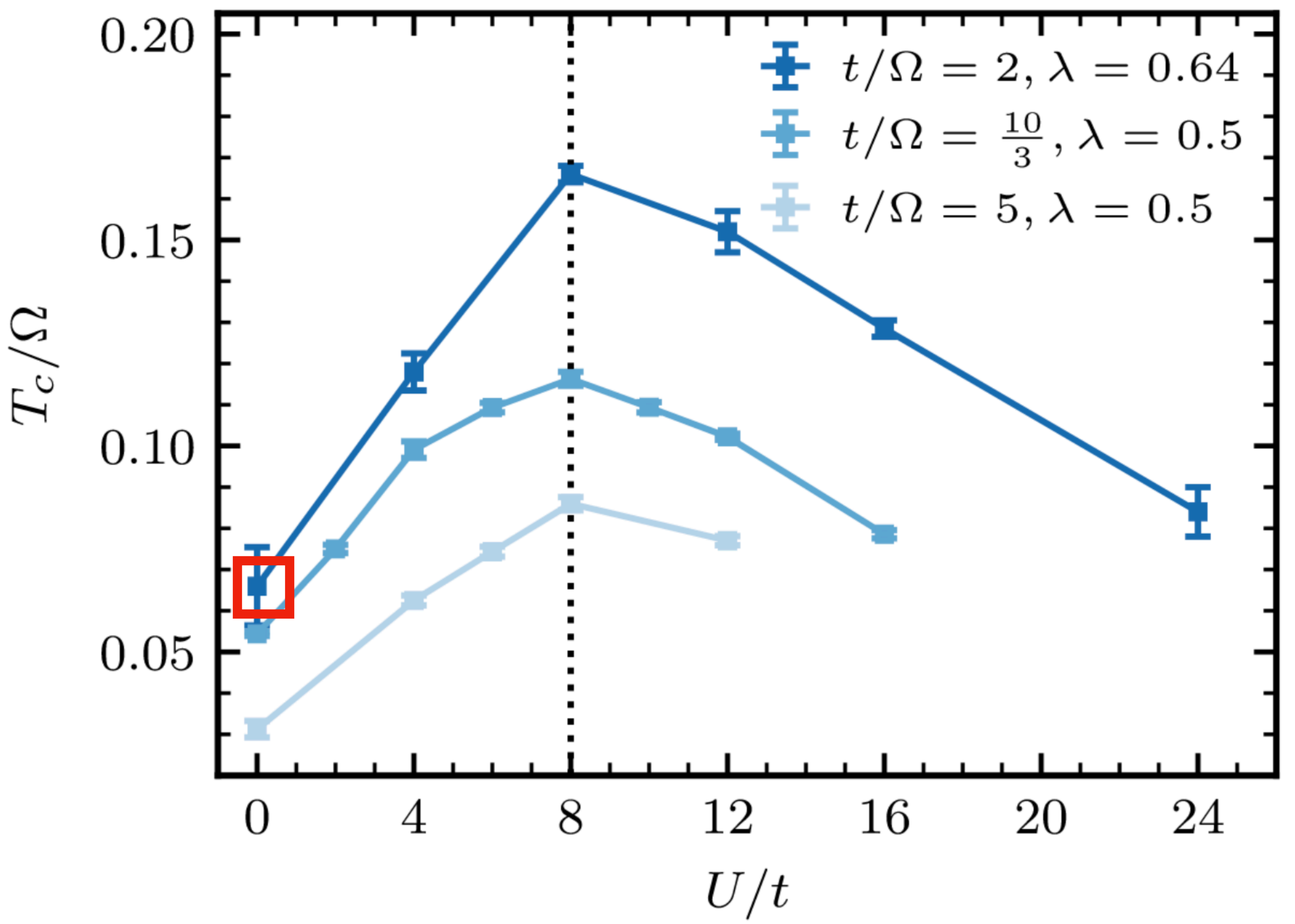

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$$\beta^{-1} = 0.0625t < T_c$$

Summary

- Holstein (density coupled) versus bond-SSH models (bond modulated)
- Significant enhancements to *s*-wave pairing in bSSH model the anti-adiabatic limit
- Could potentially be applicable to explain “flat band” systems
- Little pairing enhancement for smaller frequencies, strong coupling