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Static stripe correlations and pair-density-waves in the doped 2D Hubbard model

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Science

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Acknowledgments



Prof. Steve Johnston



Dr. Thomas Maier



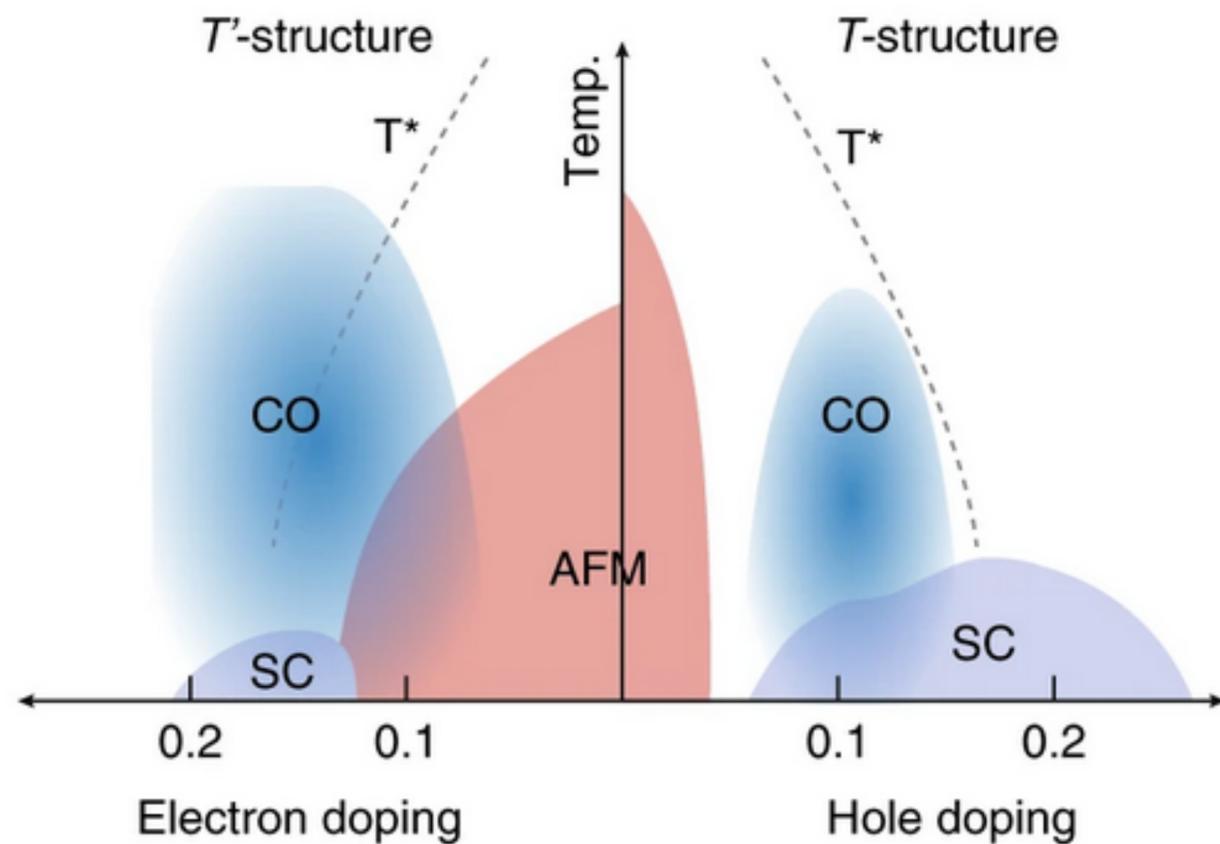
Special thanks



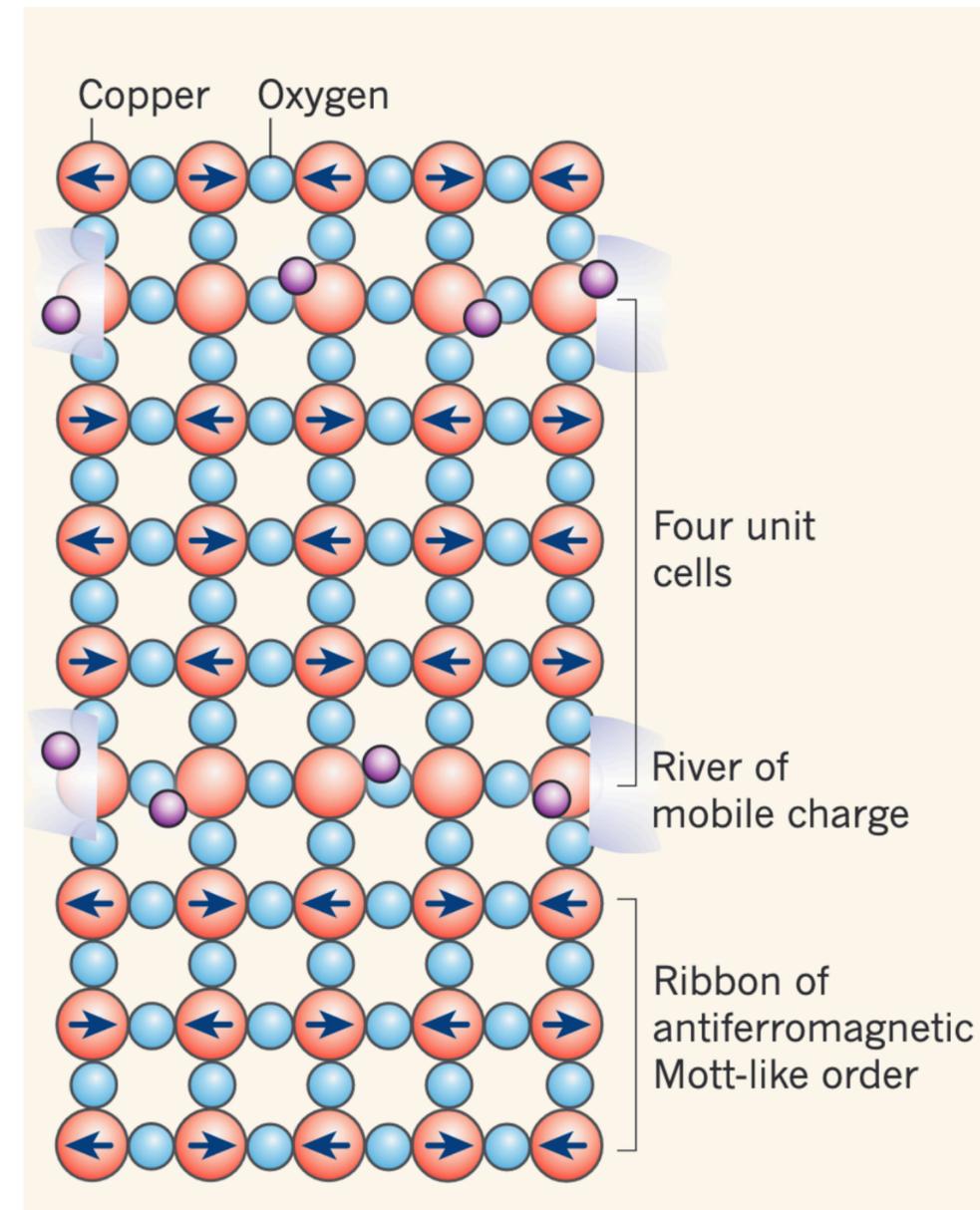
Dr. Seher Karakuzu



Stripes in the cuprates



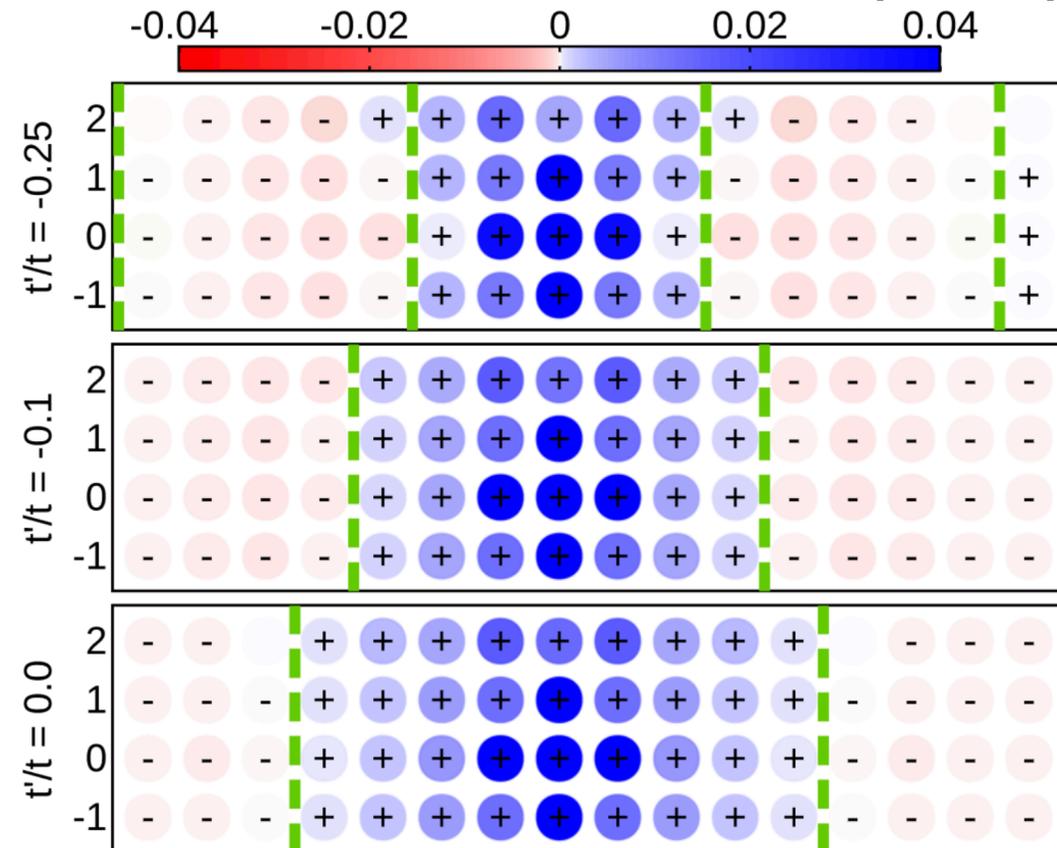
M. Kang et al. *Nat. Phys.* **15**, 335-340 (2019)



K.A. Moler. *Nature* **468**, 643-644 (2010)

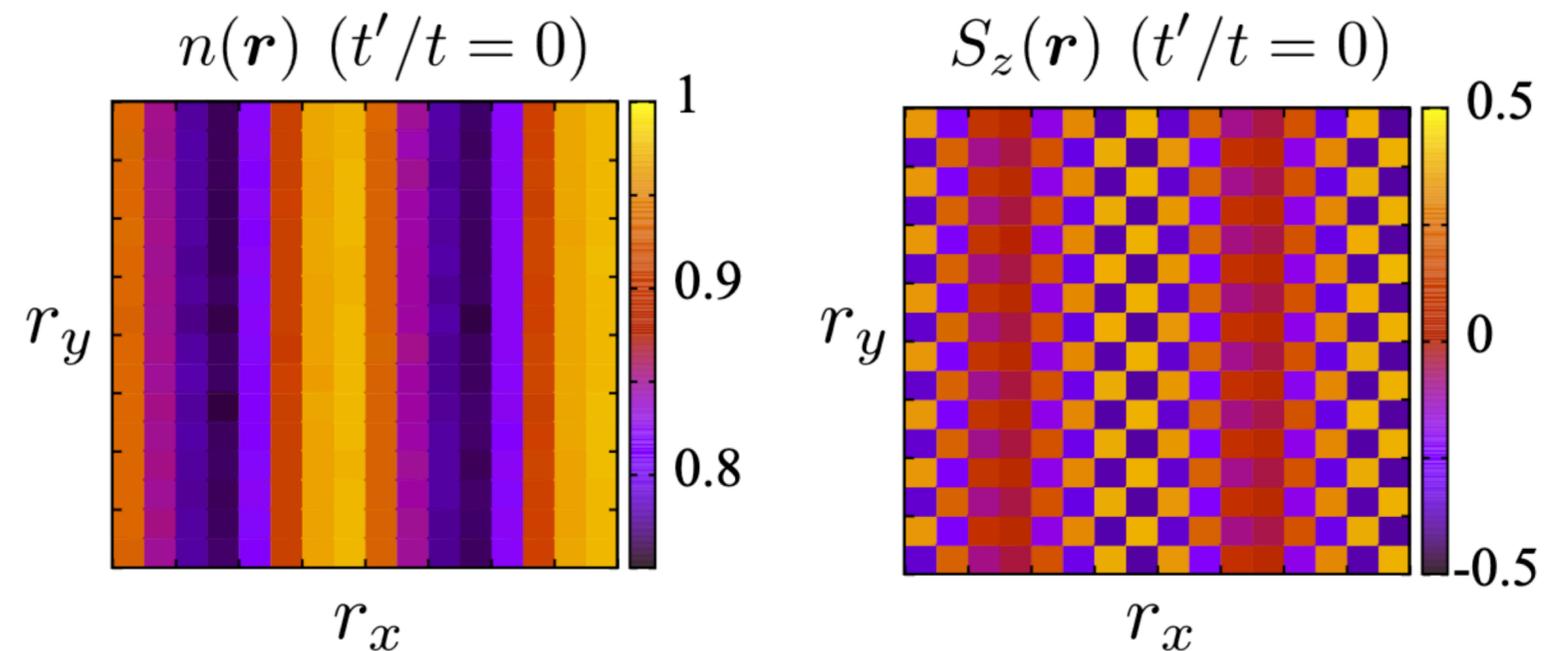
Stripes in the Hubbard model

Determinant Quantum Monte Carlo (DQMC)



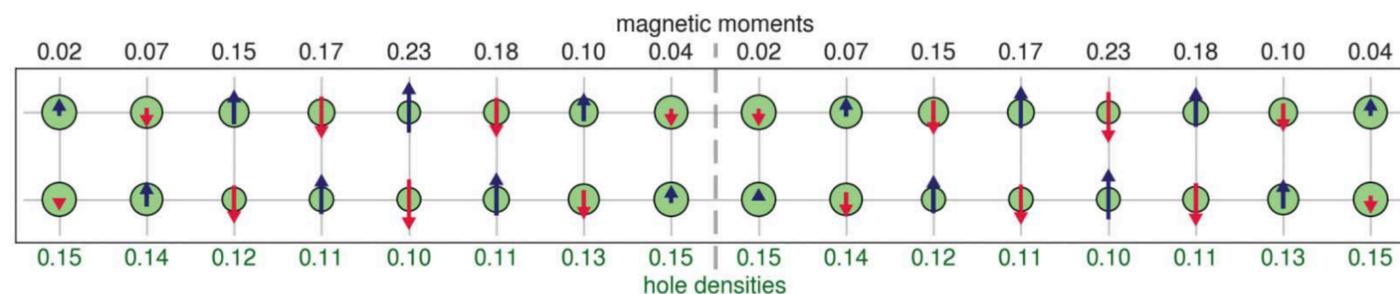
E.W. Huang et al. *npj Quant. Mat.* **3**, 22 (2018)

Variational Monte Carlo (VMC)

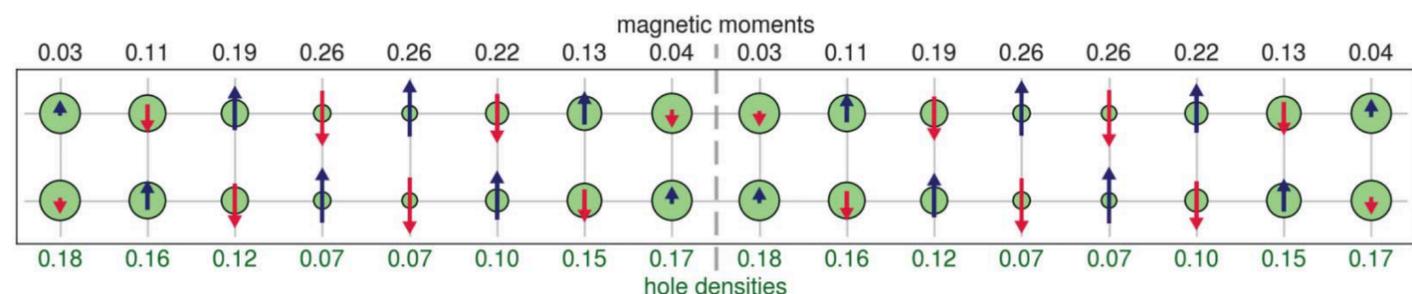


K.Ido et al. *Phys. Rev. B* **97**, 045138 (2018)

Auxiliary Field Quantum Monte Carlo (AFQMC)



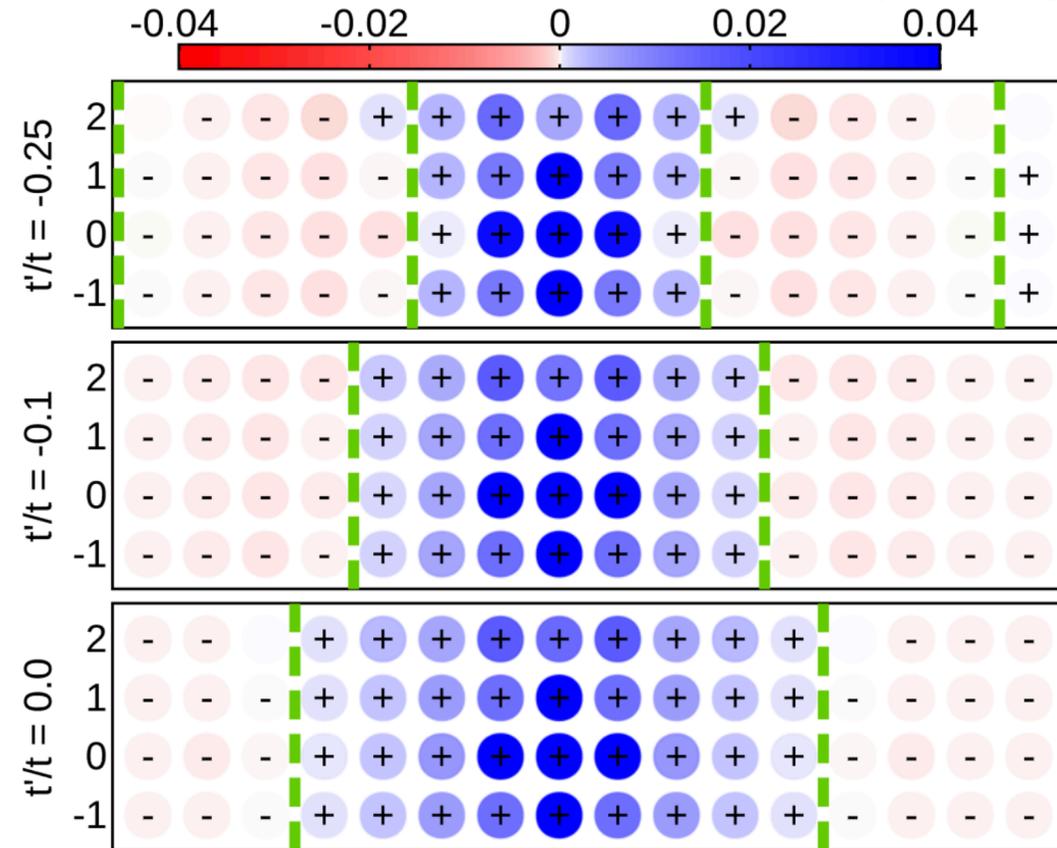
Density Matrix Renormalization Group (DMRG)



Zheng et al. *Science* **358**, 1155–1160 (2017)

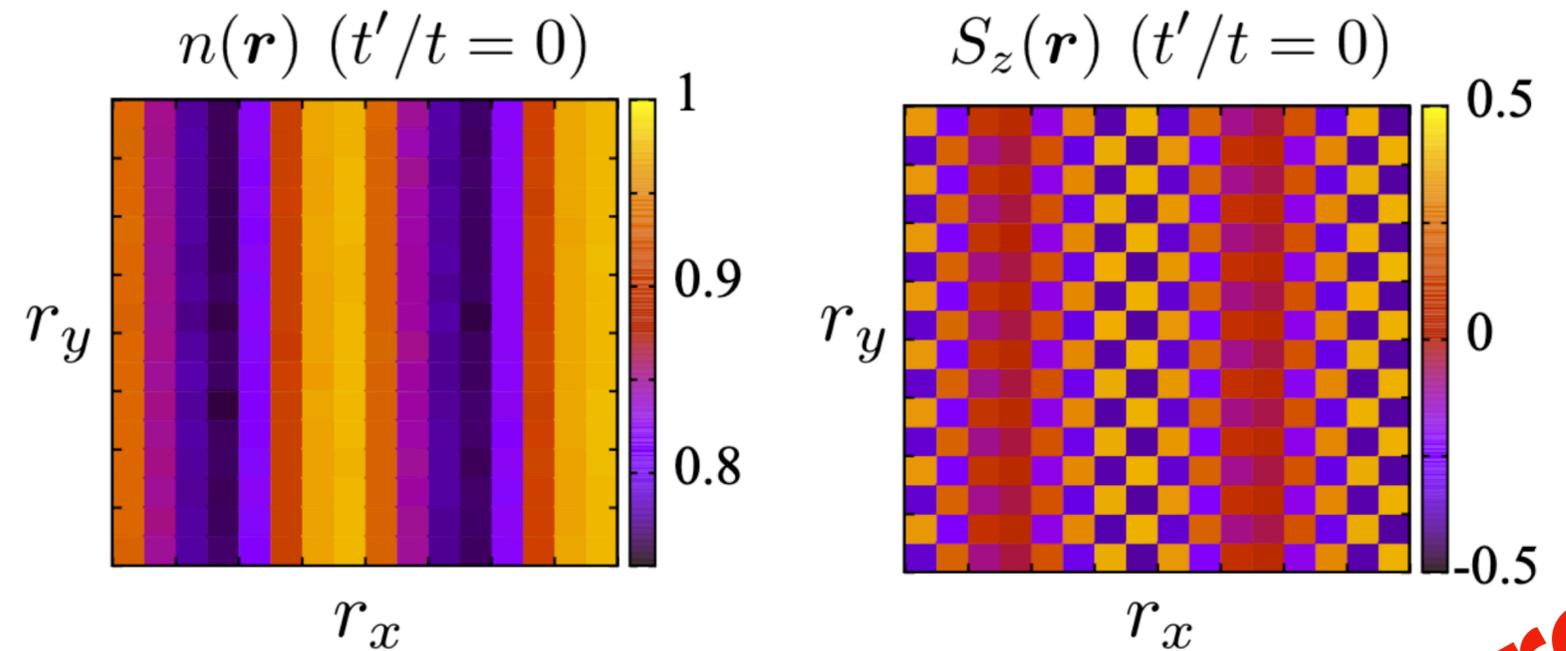
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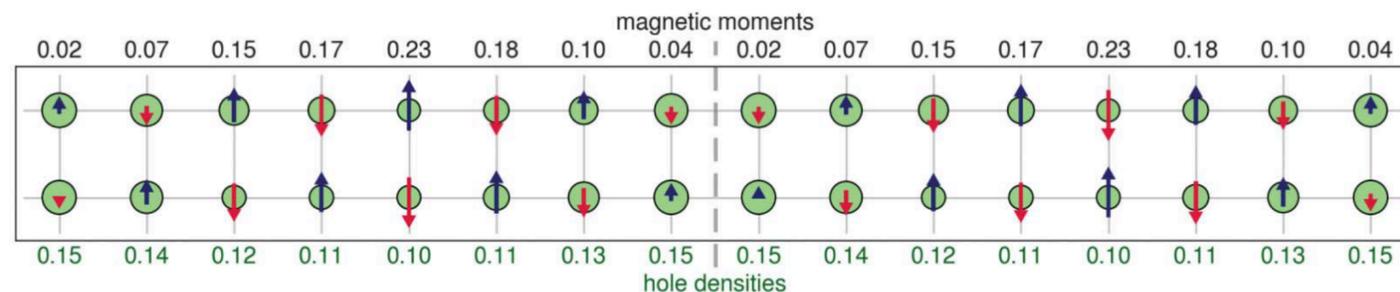
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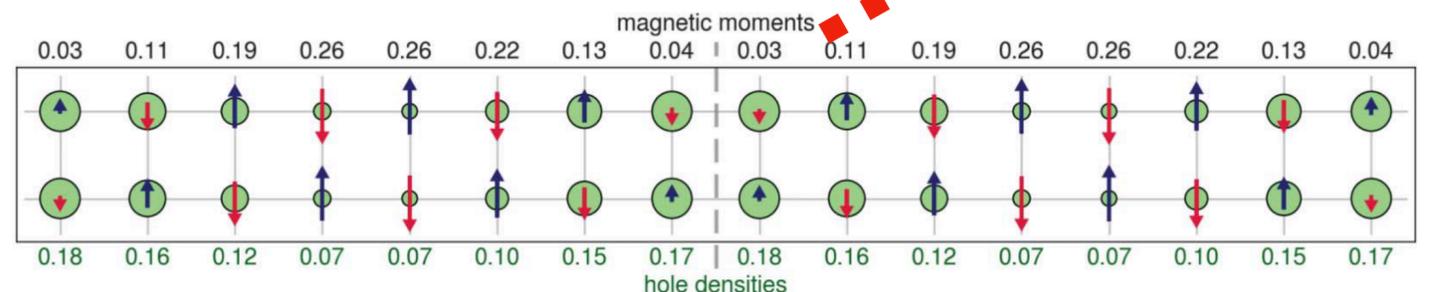
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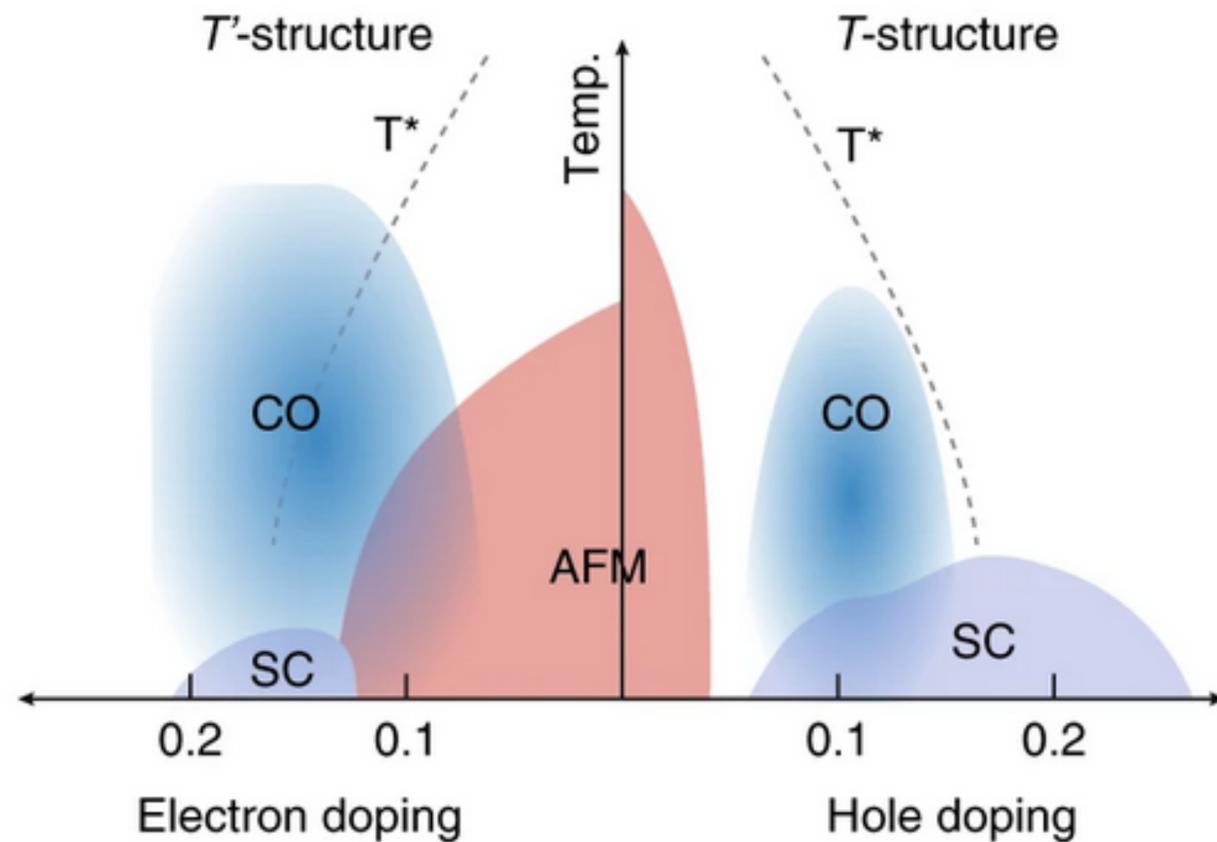
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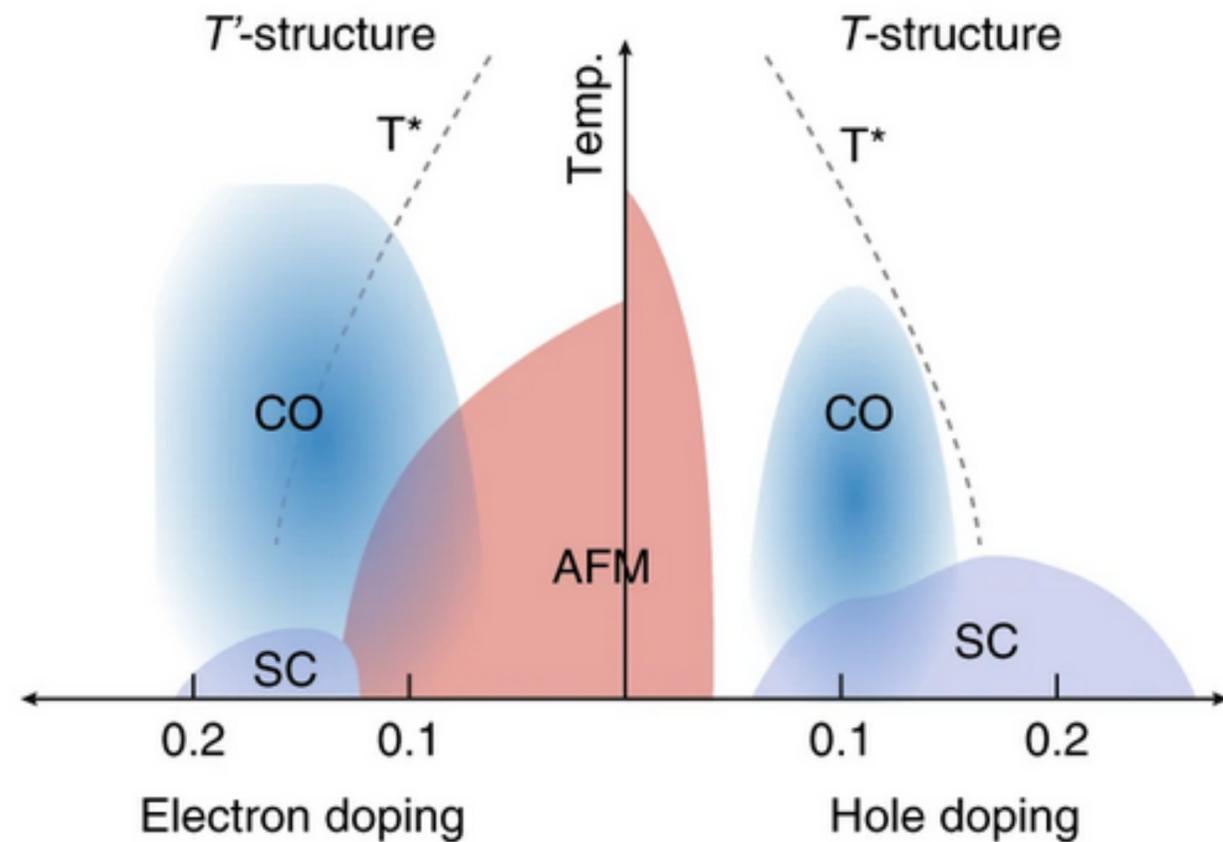
and more!

Pair density waves in the cuprates

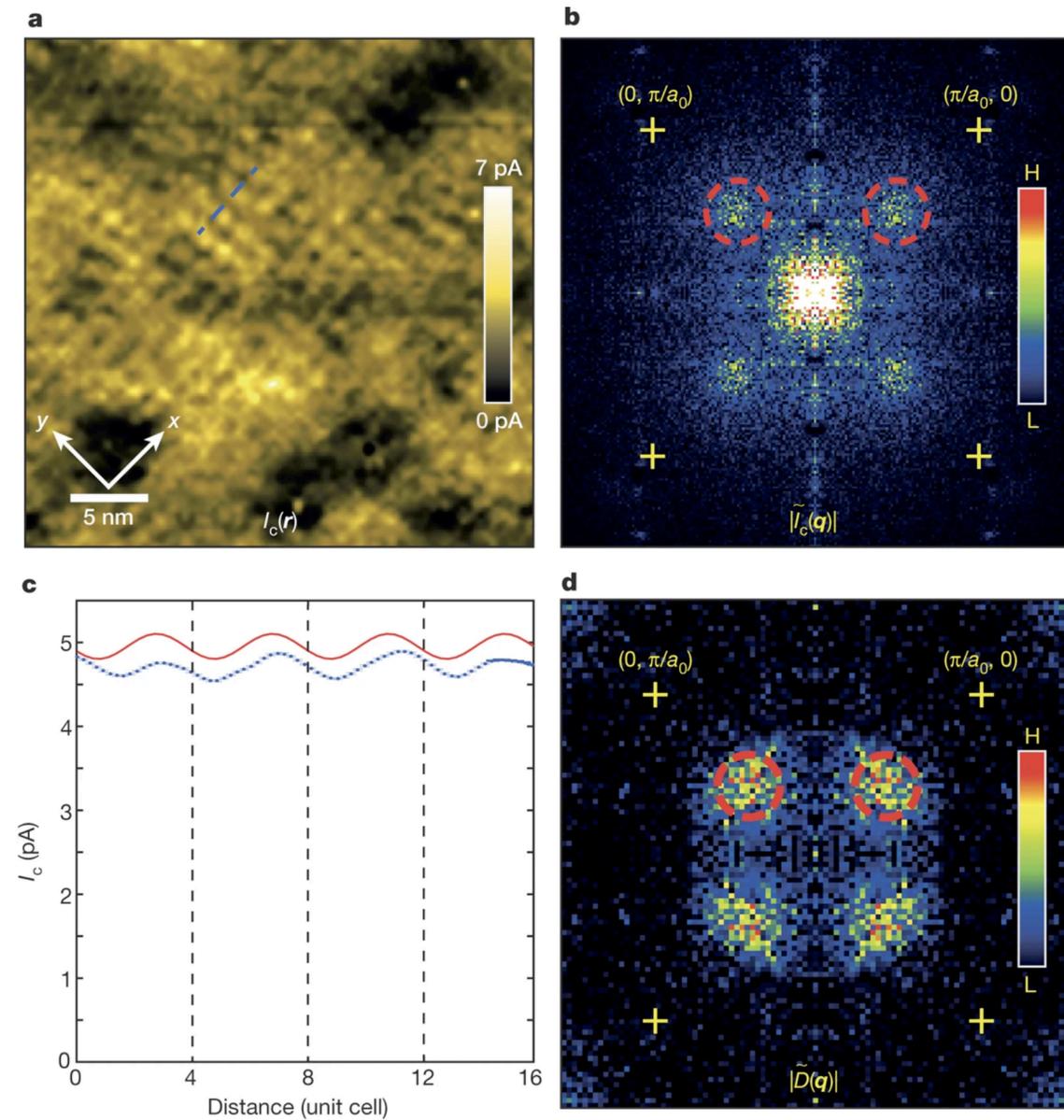


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Pair density waves in the cuprates



M. Kang et al. *Nat. Phys.* **15**, 335-340 (2019)



M. H. Hamidian et al. *Nature* **532**, 343–347 (2016)

Modeling pair density waves

Mean-field

$$\hat{H}_{\text{PDW}} = \sum_{i,\nu} \Delta_{i,\nu} \left(\mathcal{F}_i^\dagger \bar{\mathcal{F}}_{i+a_\nu} + \text{H.c.} \right)$$

$$\mathcal{F}_i = \left(\hat{c}_{i,\uparrow}, \hat{c}_{i,\downarrow} \right)^T$$
$$\bar{\mathcal{F}}_i = \left(\hat{c}_{i,\downarrow}^\dagger, -\hat{c}_{i,\uparrow}^\dagger \right)^T$$

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Fulde-Ferrell (FF)

$$\Delta_{i,\nu} = \tilde{\Delta}_\nu e^{iq \cdot r_i}$$

P. Fulde and R. A. Ferrell. *Phys. Rev.* **135**, A550 (1964)

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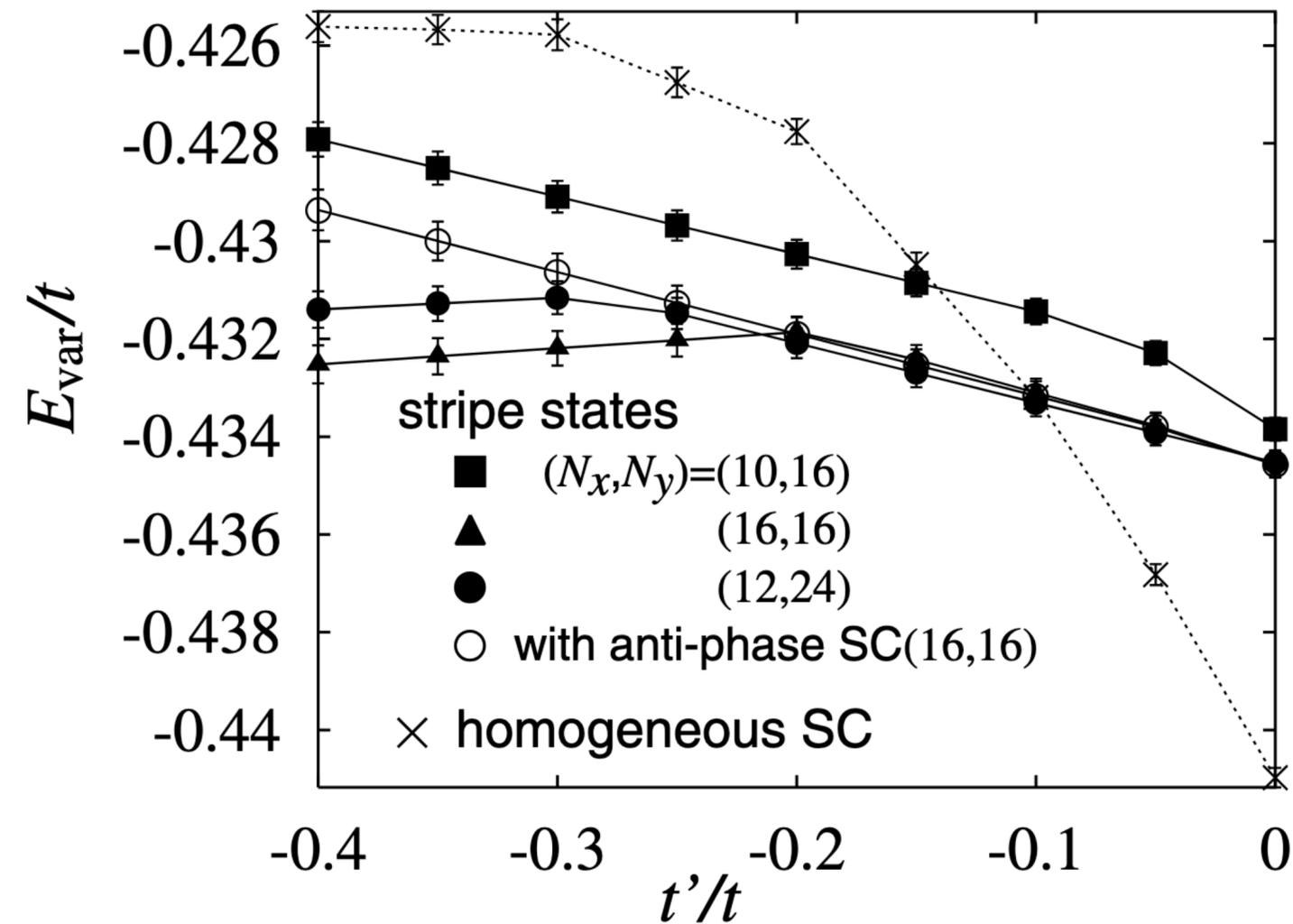
Larkin-Ovchinnikov (LO)

$$\Delta_{i,\nu} = \tilde{\Delta}_\nu \left(e^{iq \cdot r_i} + e^{-iq \cdot r_i} \right)$$

A.I. Larkin and Y. N. Ovchinnikov. *Zh. Eksperim. i Teor. Fiz.*, **47** (1964)

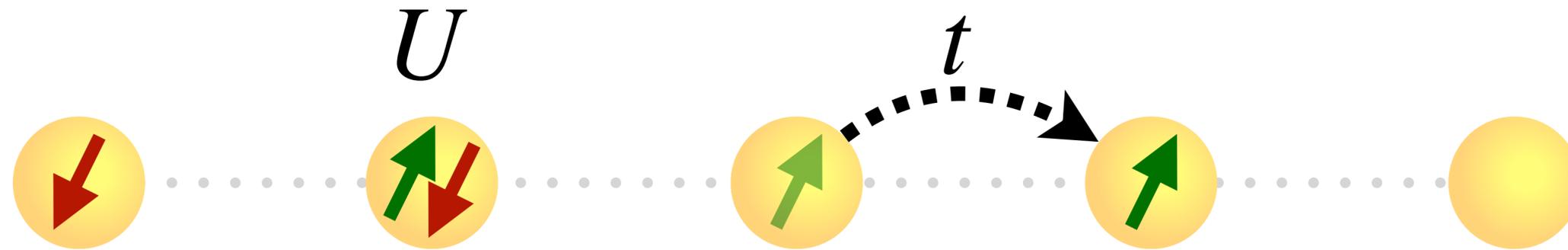
Pair density waves and stripes

$$\hat{H}_{t,t',J} = -t \sum_{\langle ij \rangle, \sigma} (\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \text{H.c.}) - t' \sum_{\langle\langle ij \rangle\rangle, \sigma} (\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \text{H.c.}) + J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$



Methods

Hubbard model



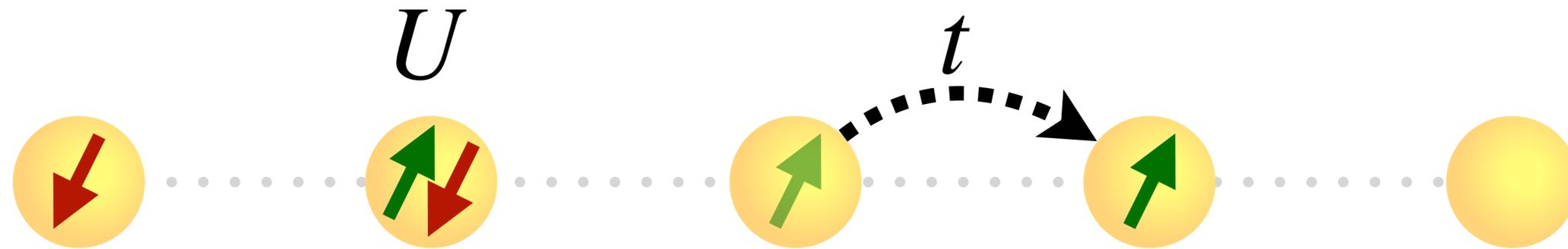
Variational Monte Carlo (VMC)

- Zero temperature
- Markov chain Monte Carlo
- Rectangular clusters: $L_x, L_y = (16, 4)$
- **VariationalMC** package (in development)

VariationalMC
<https://github.com/atanjaro/VariationalMC.jl>

Methods

Hubbard model



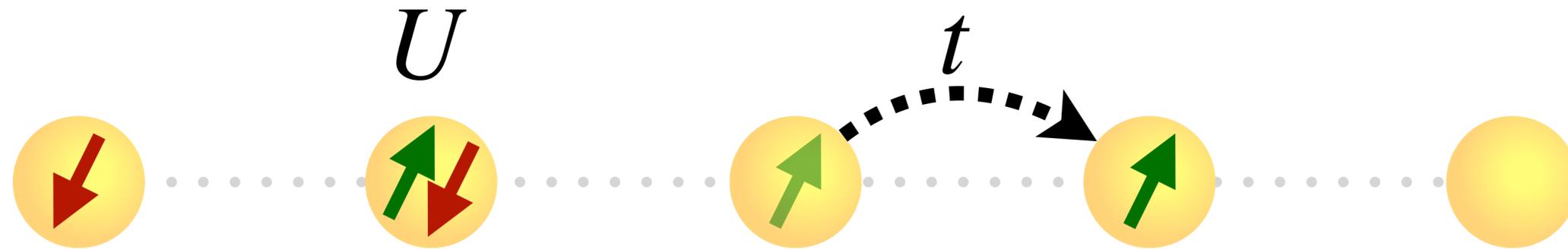
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Hubbard model



Variational Monte Carlo (VMC)

- Jastrow-Slater wavefunctions: $|\Psi_T\rangle = J_d^{e-e} J_s^{e-e} P(N_e) |\Phi_\alpha\rangle$

1. $\hat{H}_\alpha = \hat{H}_e + \hat{H}_{\text{stripe}}^s + \hat{H}_{\text{stripe}}^c$

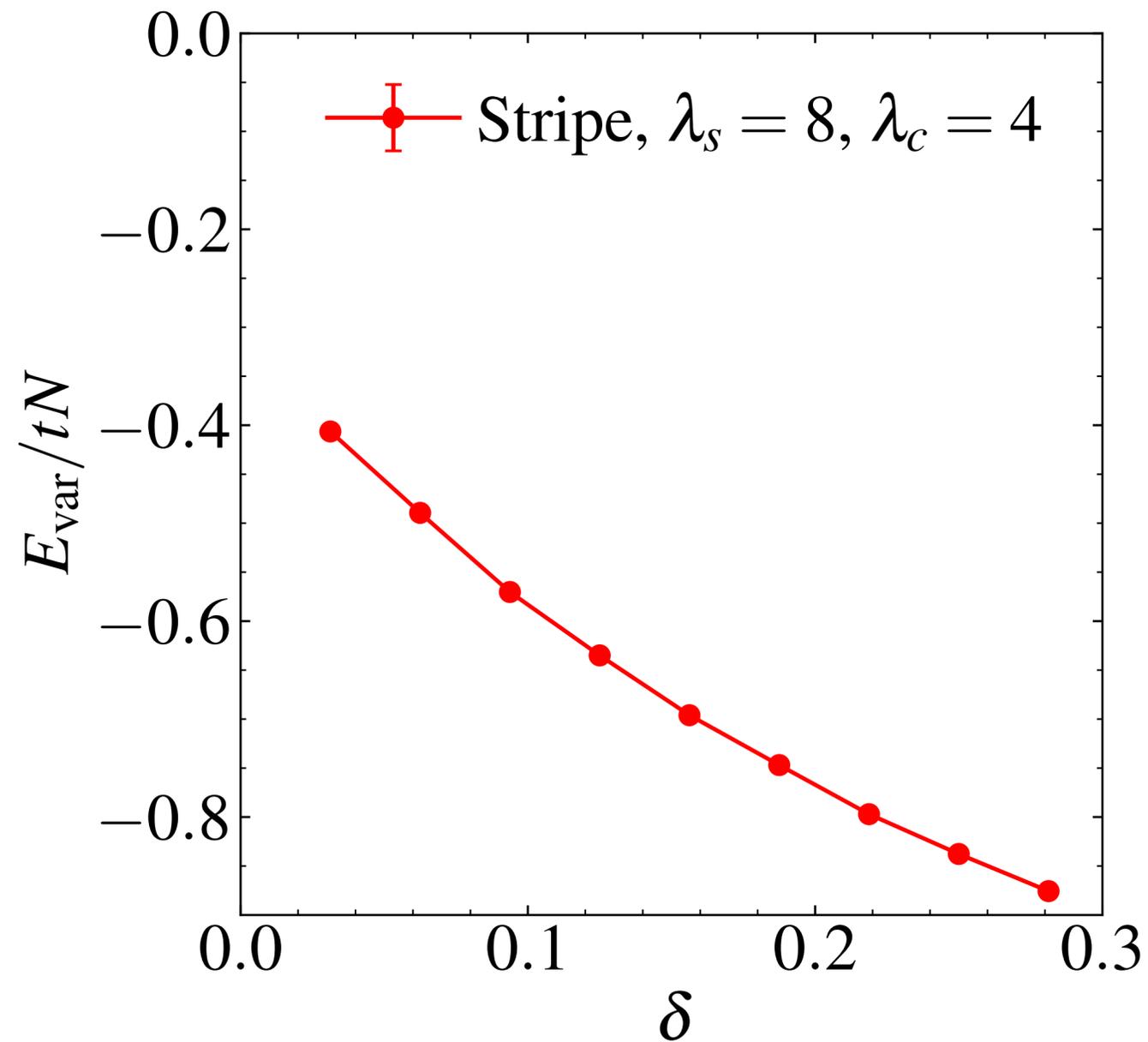
2. $\hat{H}_\alpha = \hat{H}_e + \hat{H}_{\text{FF}} + \hat{H}_{\text{LO}}$

VariationalMC

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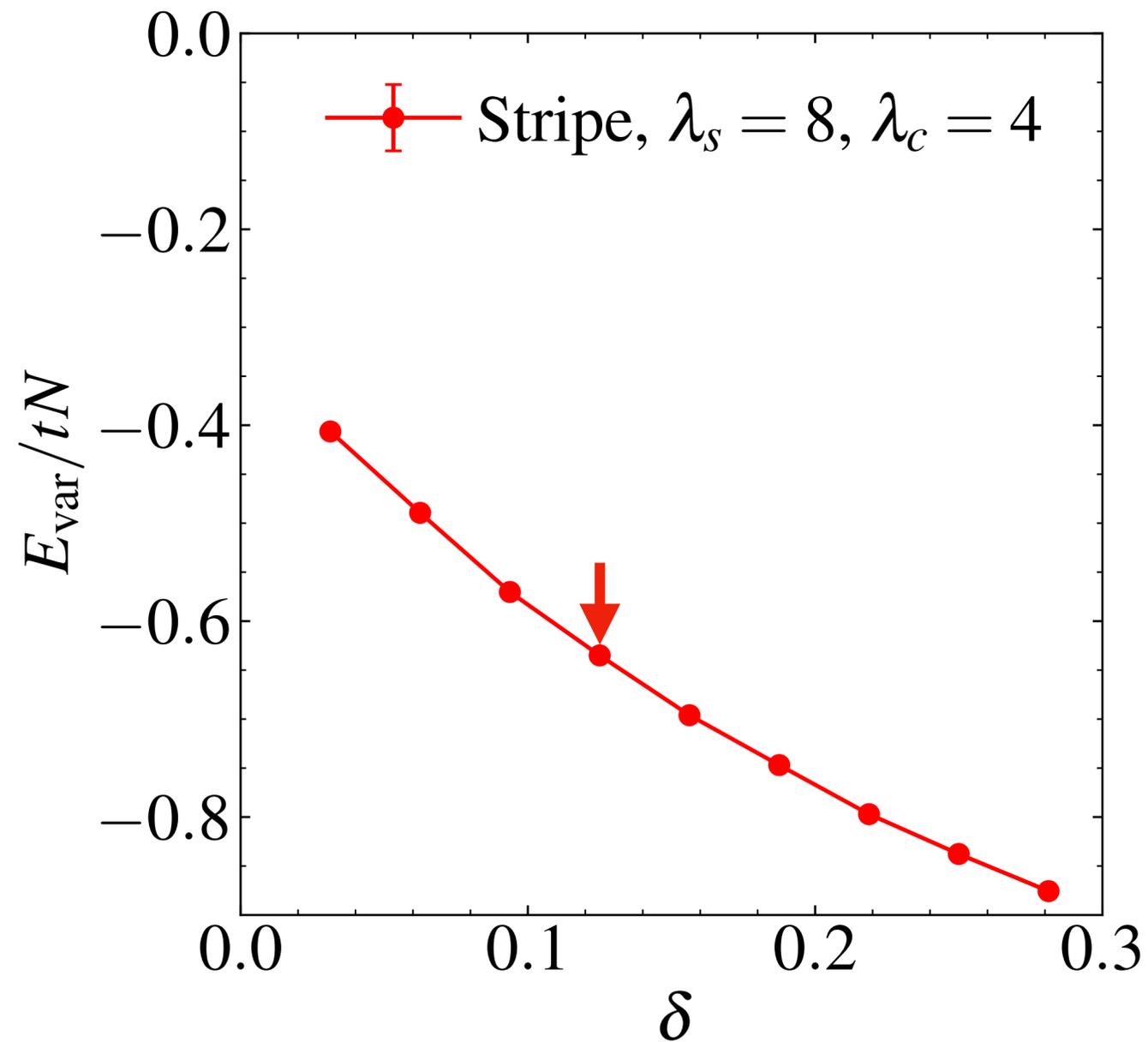
Stripe energies and correlations

$$N = 16 \times 4, t = 1, U/t = 8$$



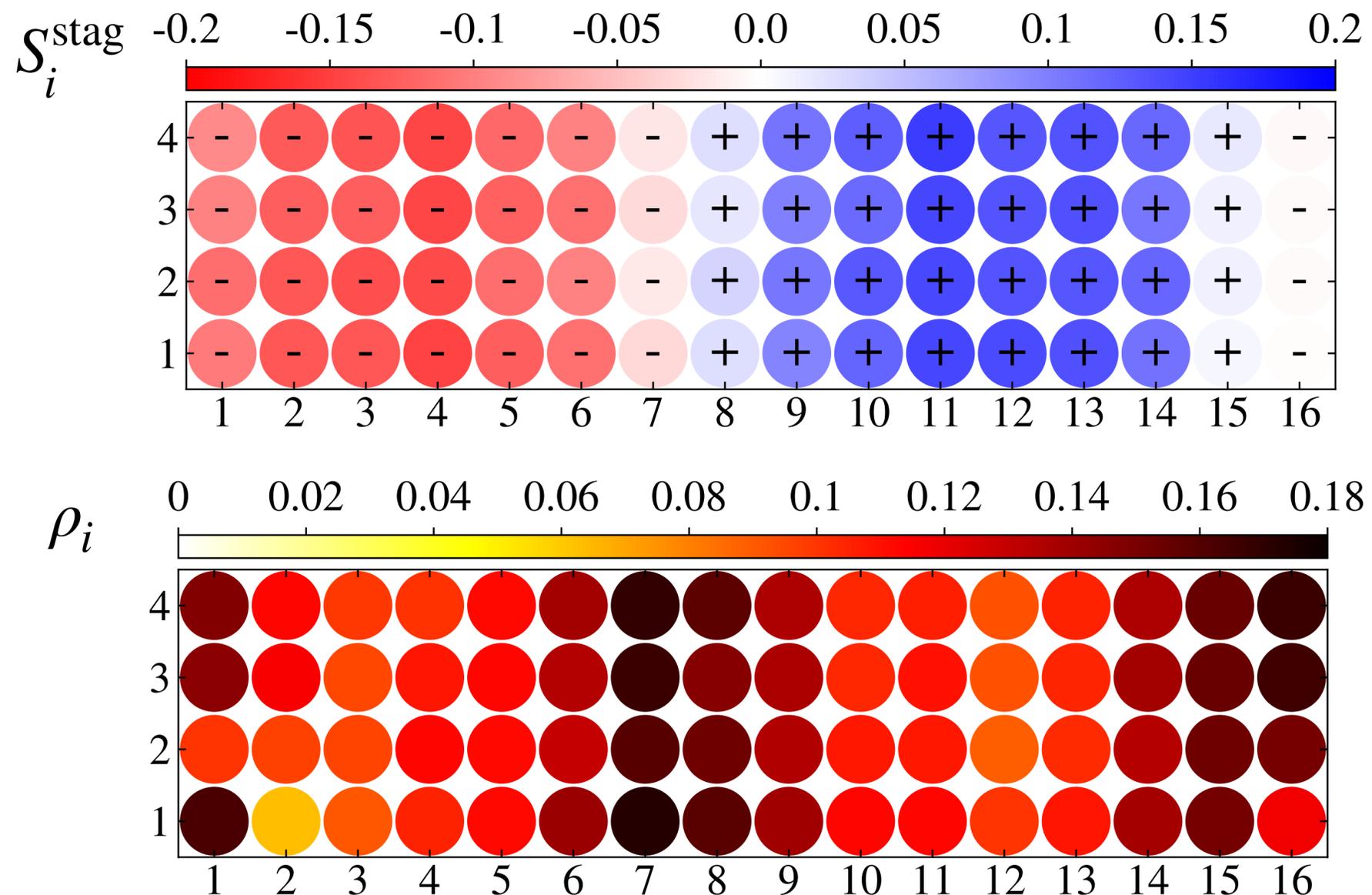
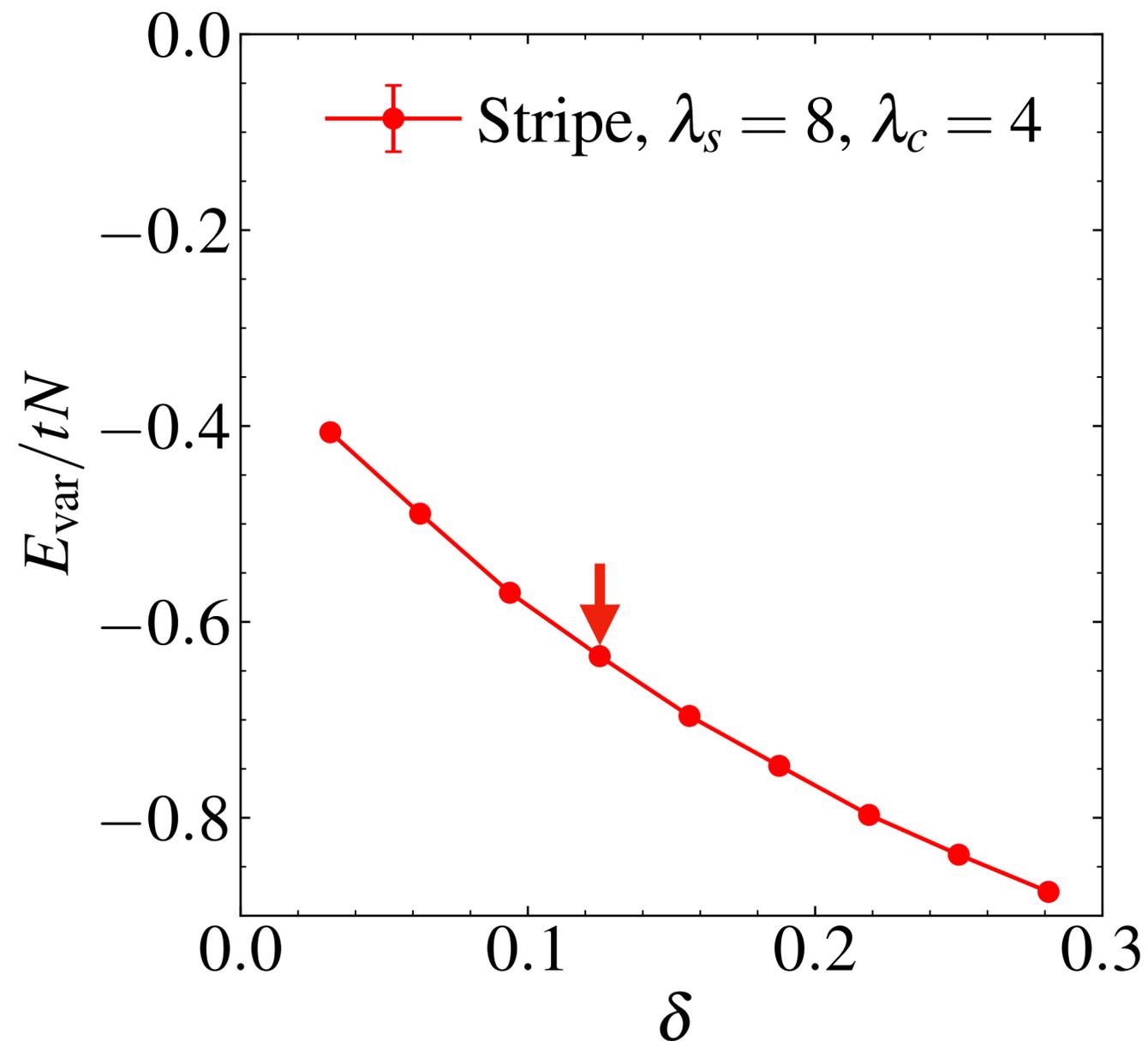
Stripe energies and correlations

$N = 16 \times 4$, $t = 1$, $U/t = 8$, $\langle \hat{n} \rangle = 0.875$ ($\delta = 0.125$)



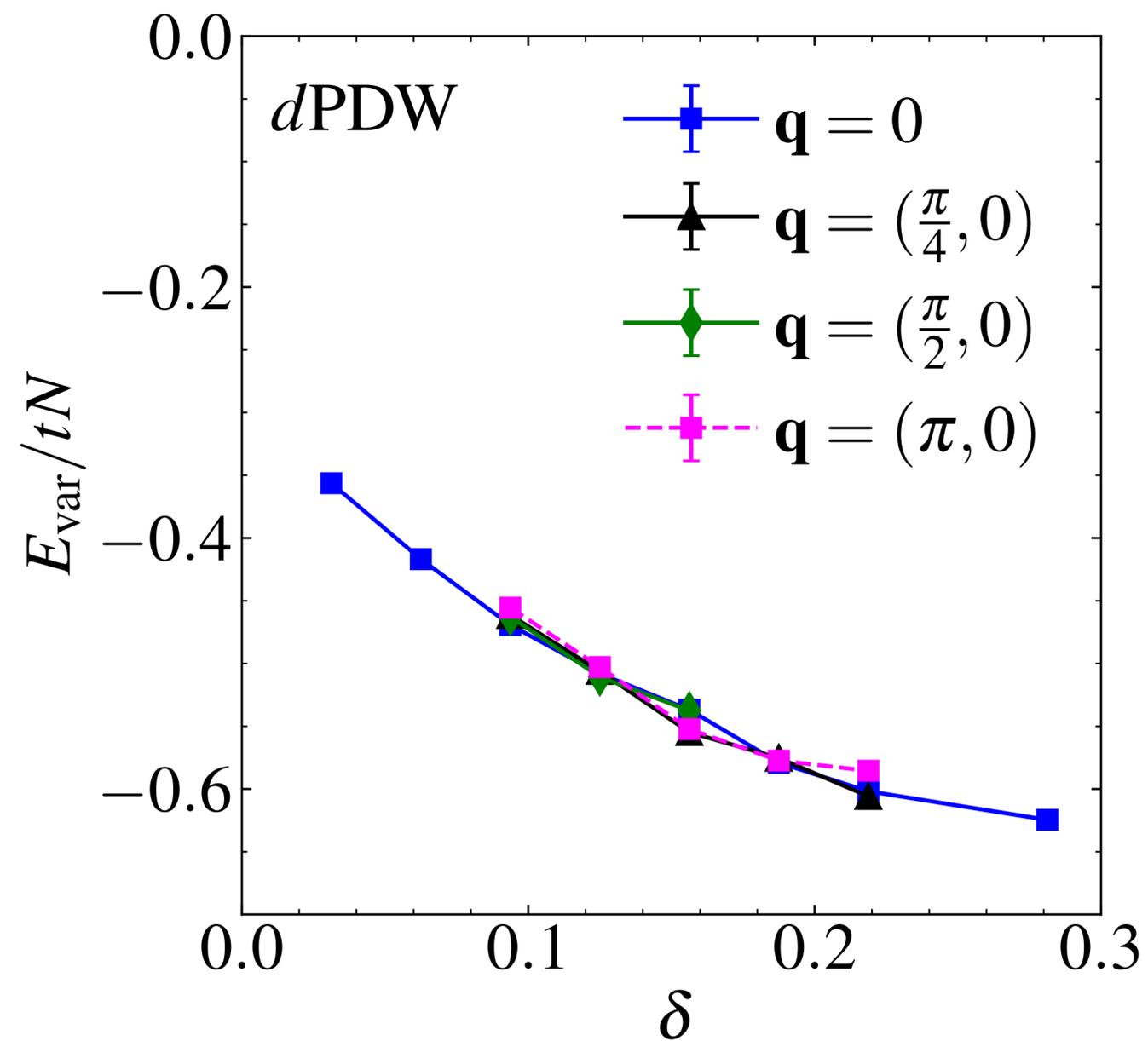
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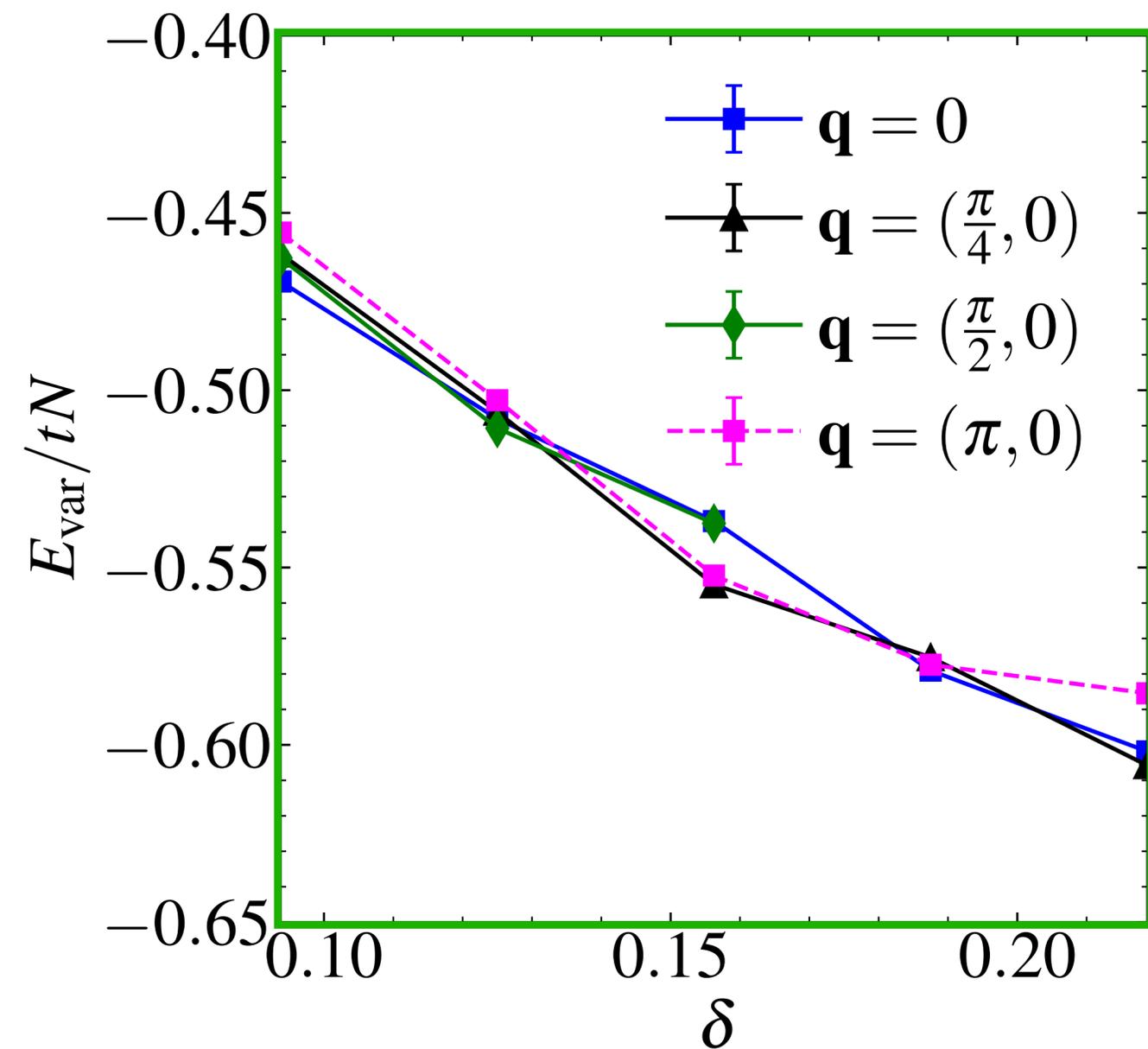
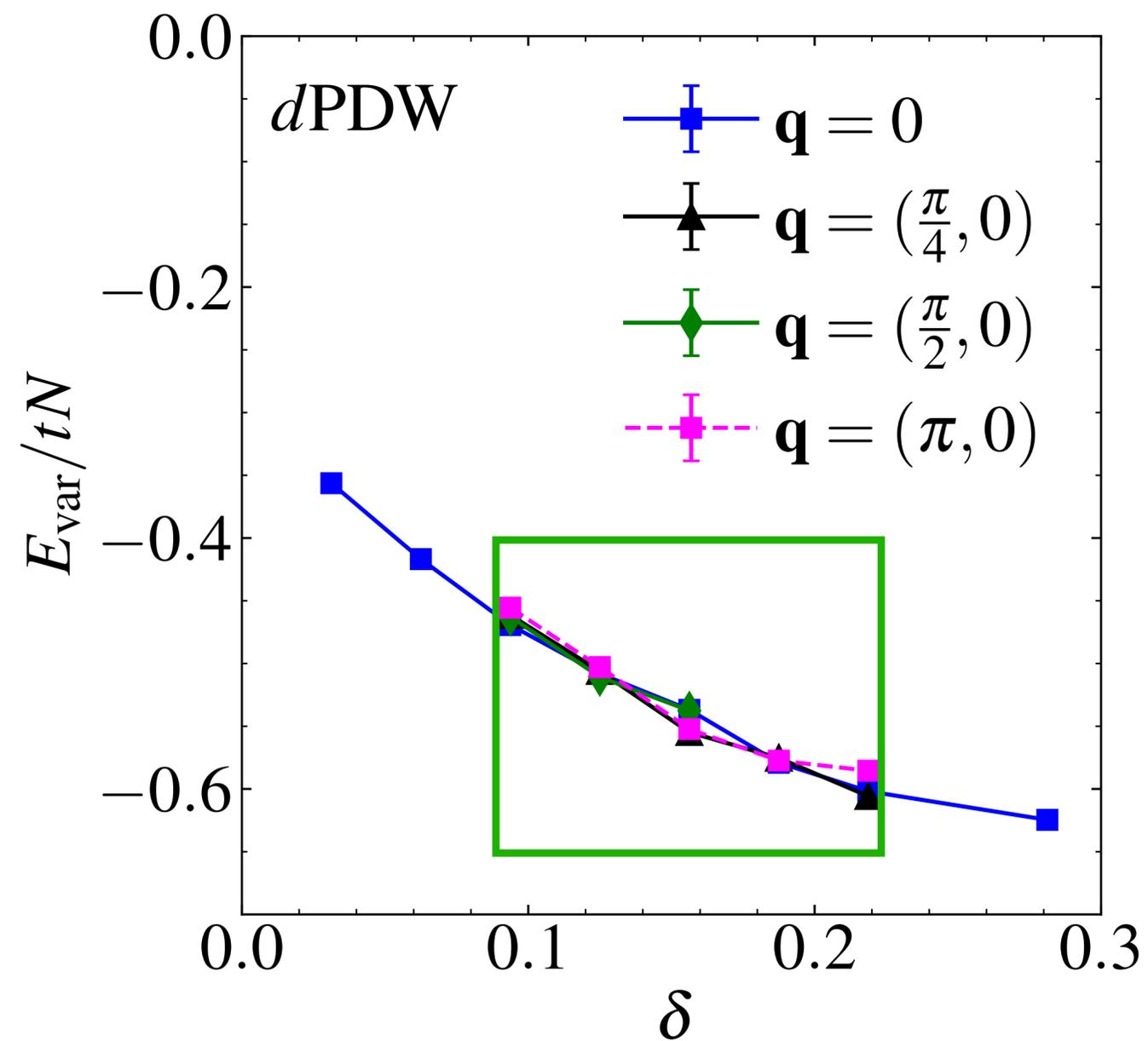
Superconducting energies

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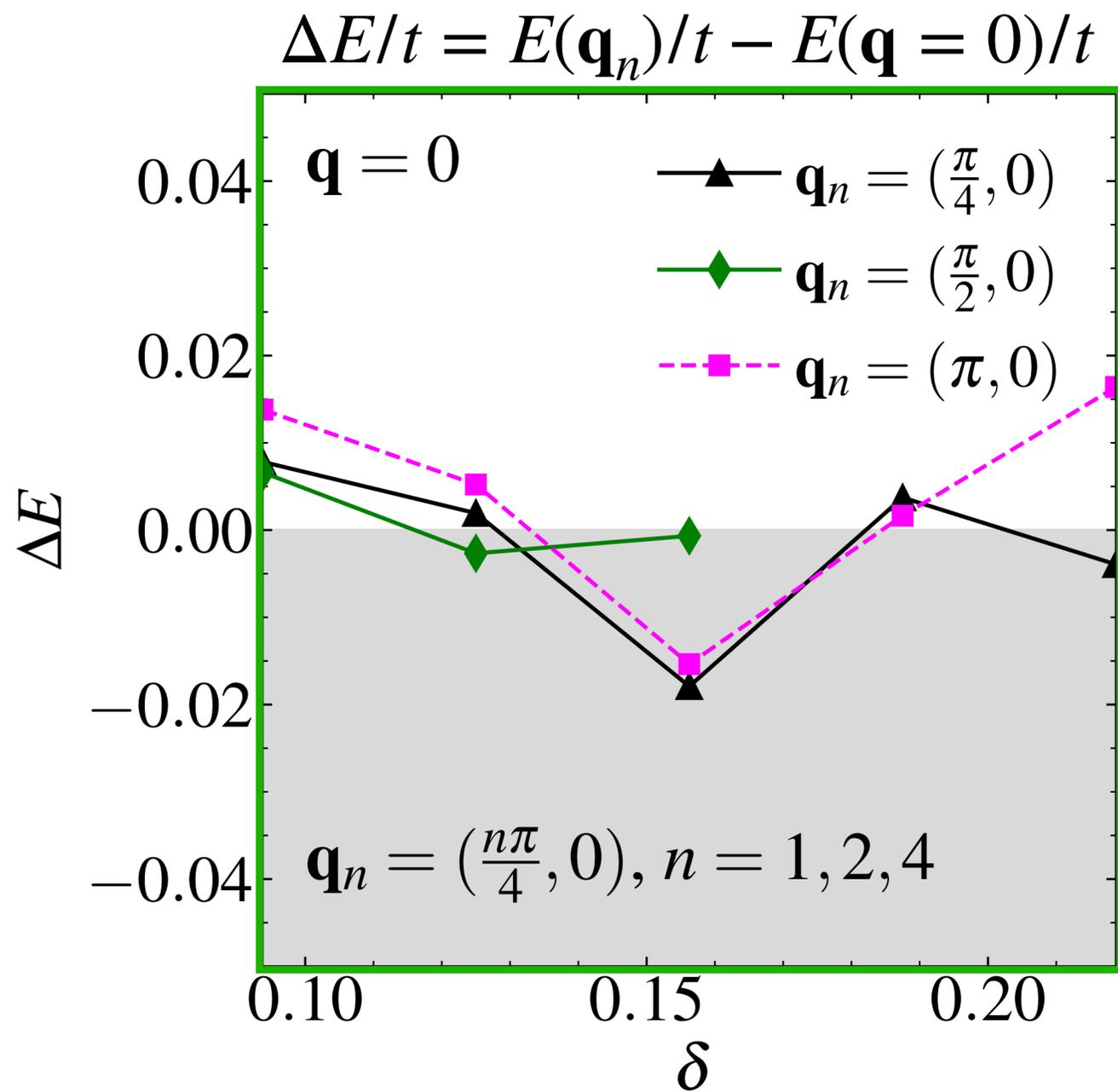
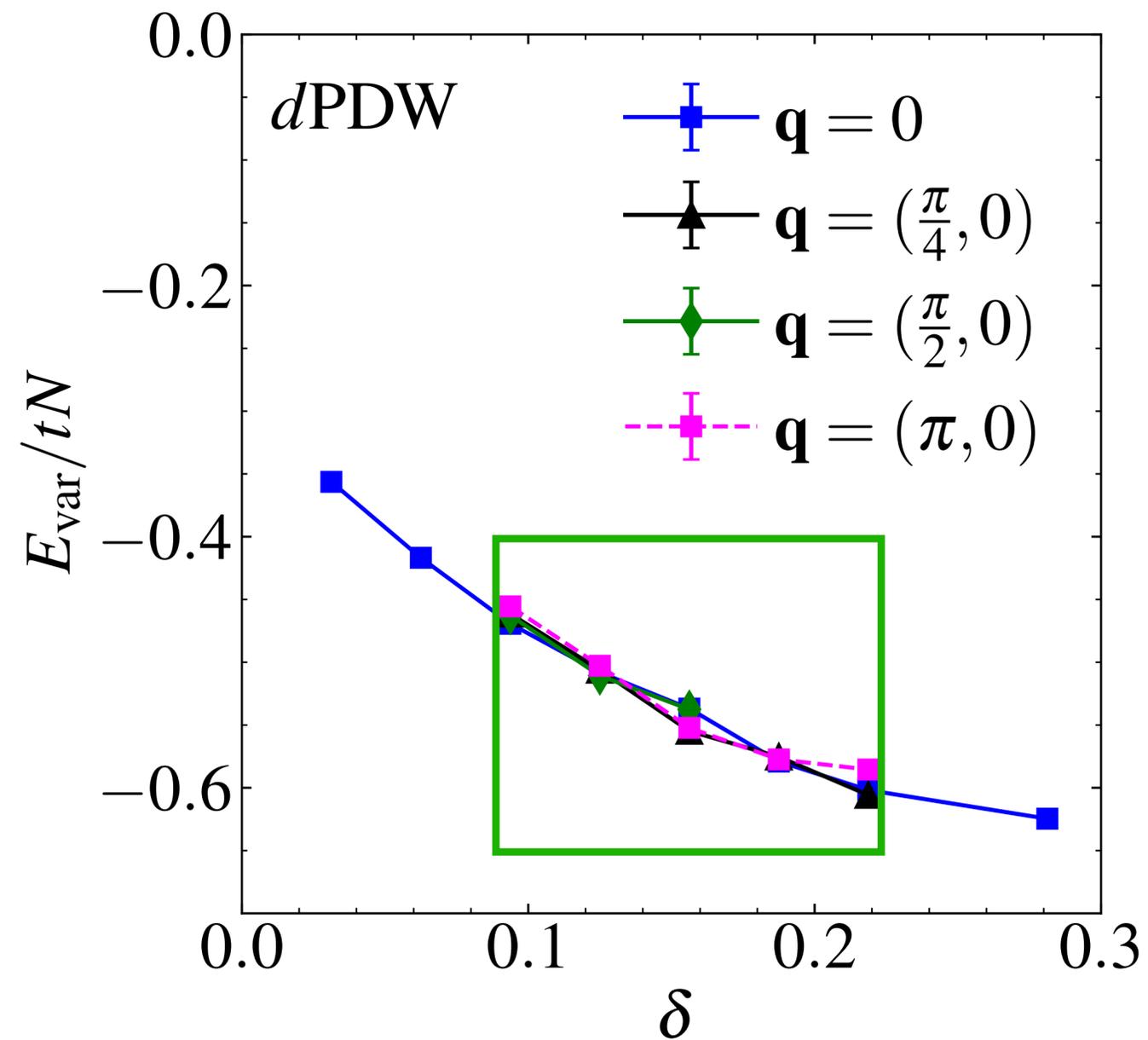
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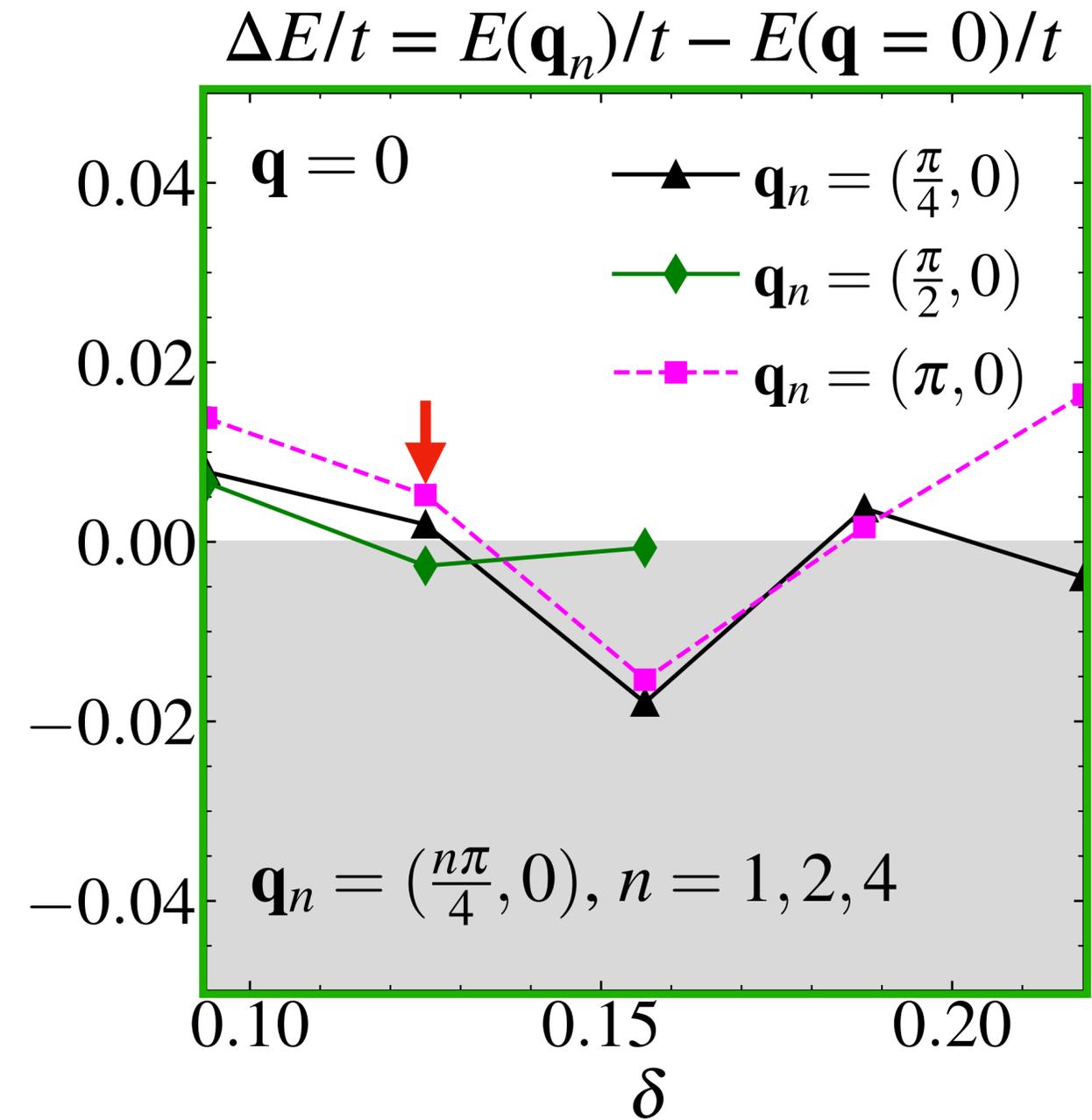
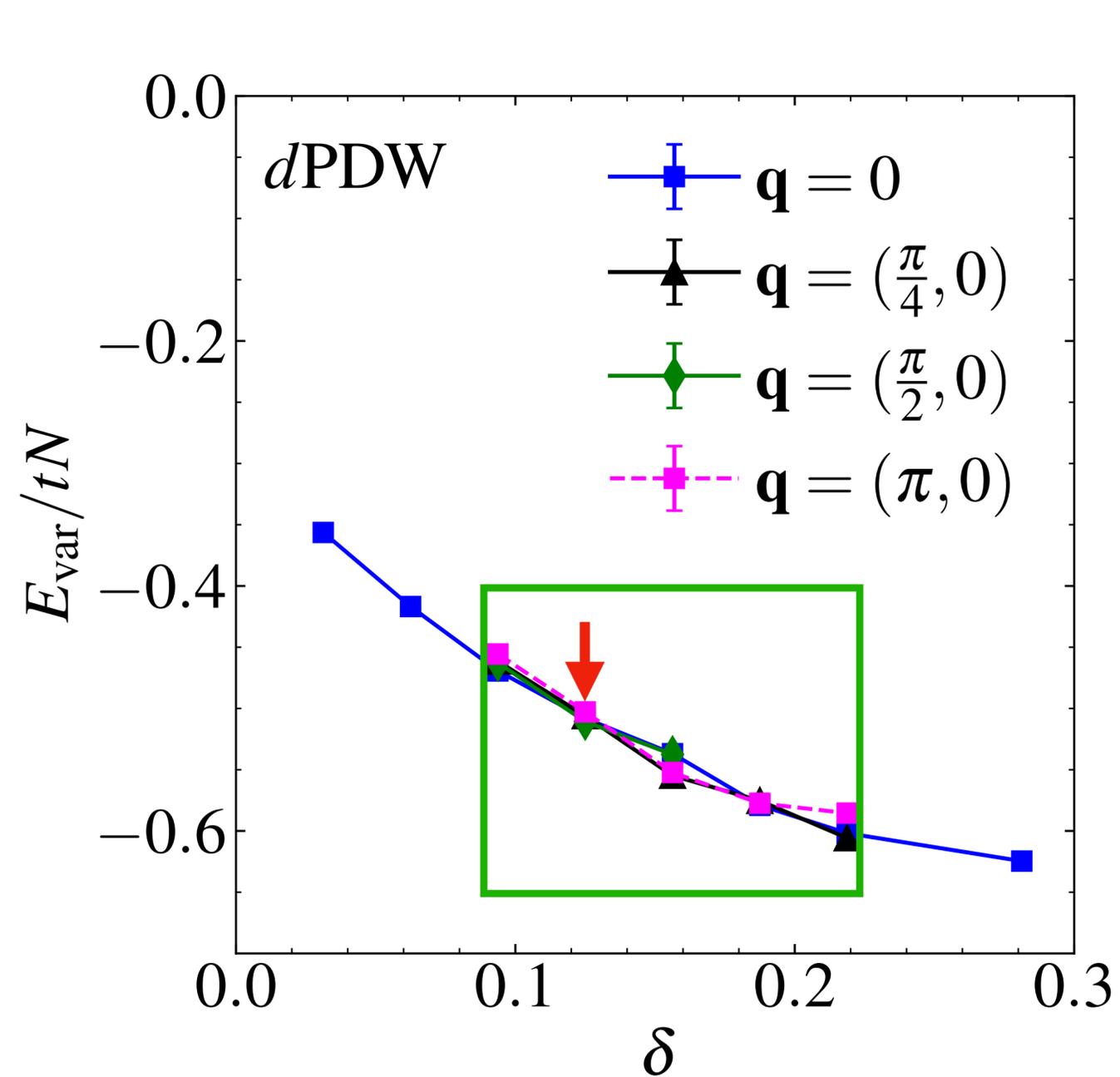
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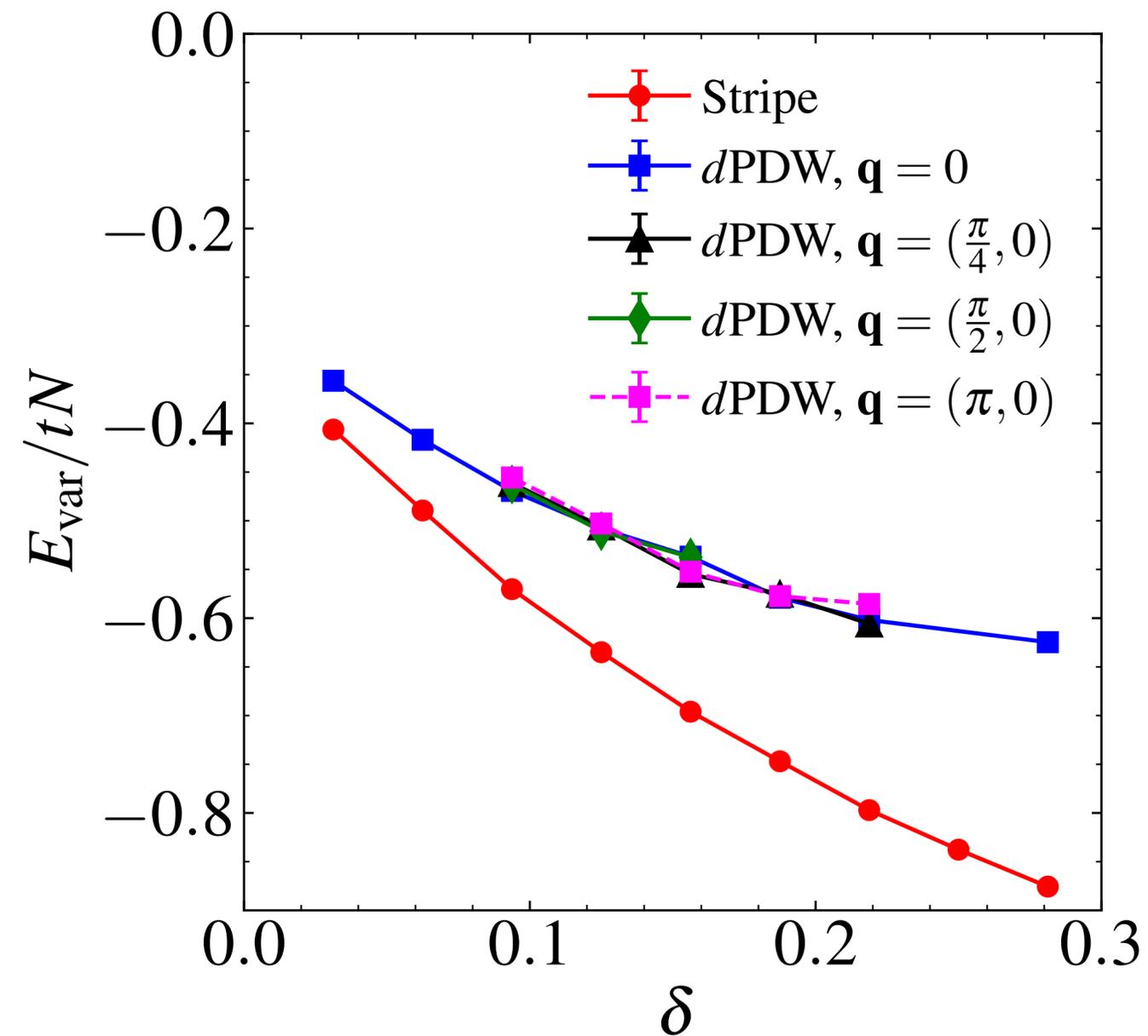
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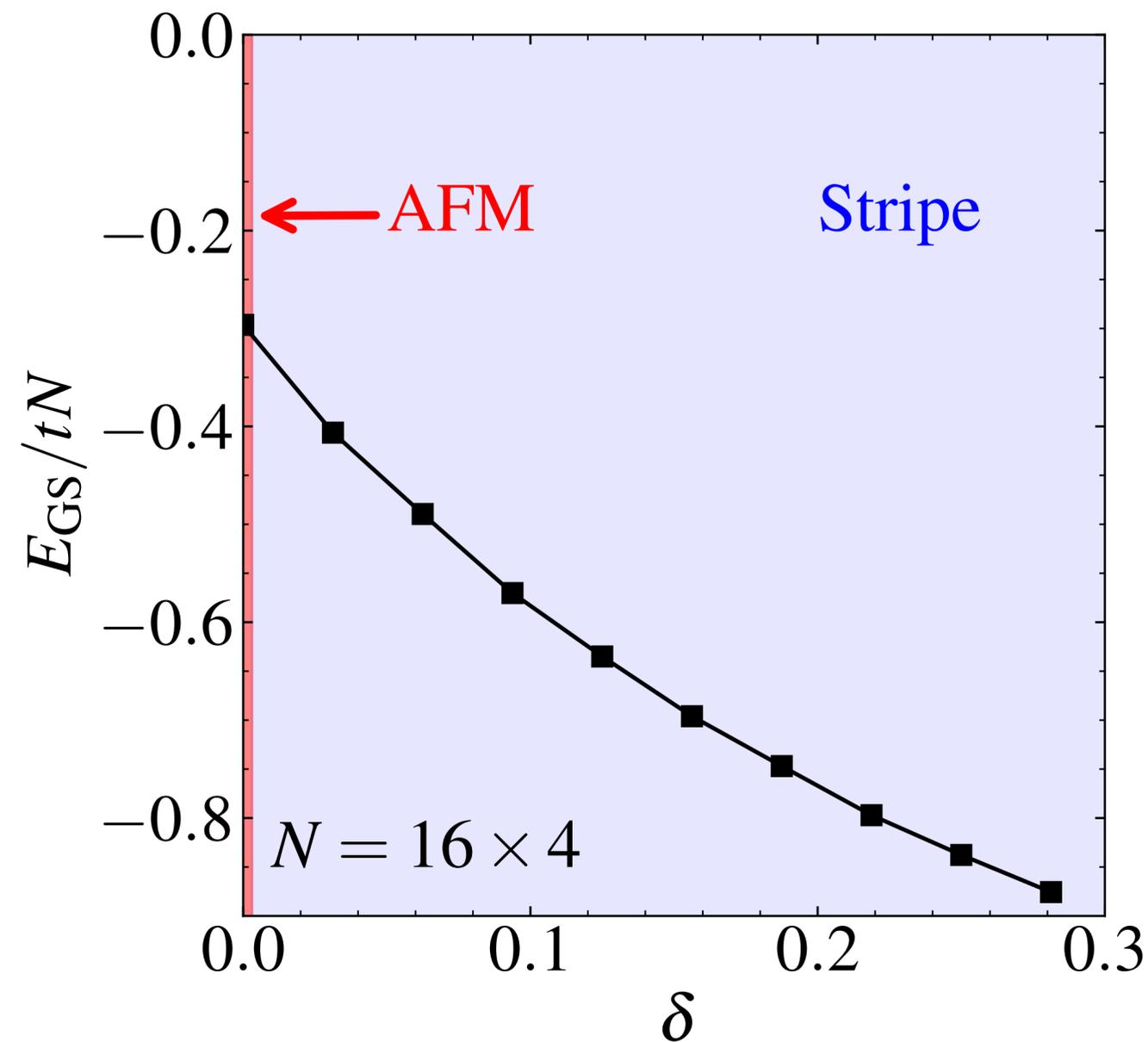
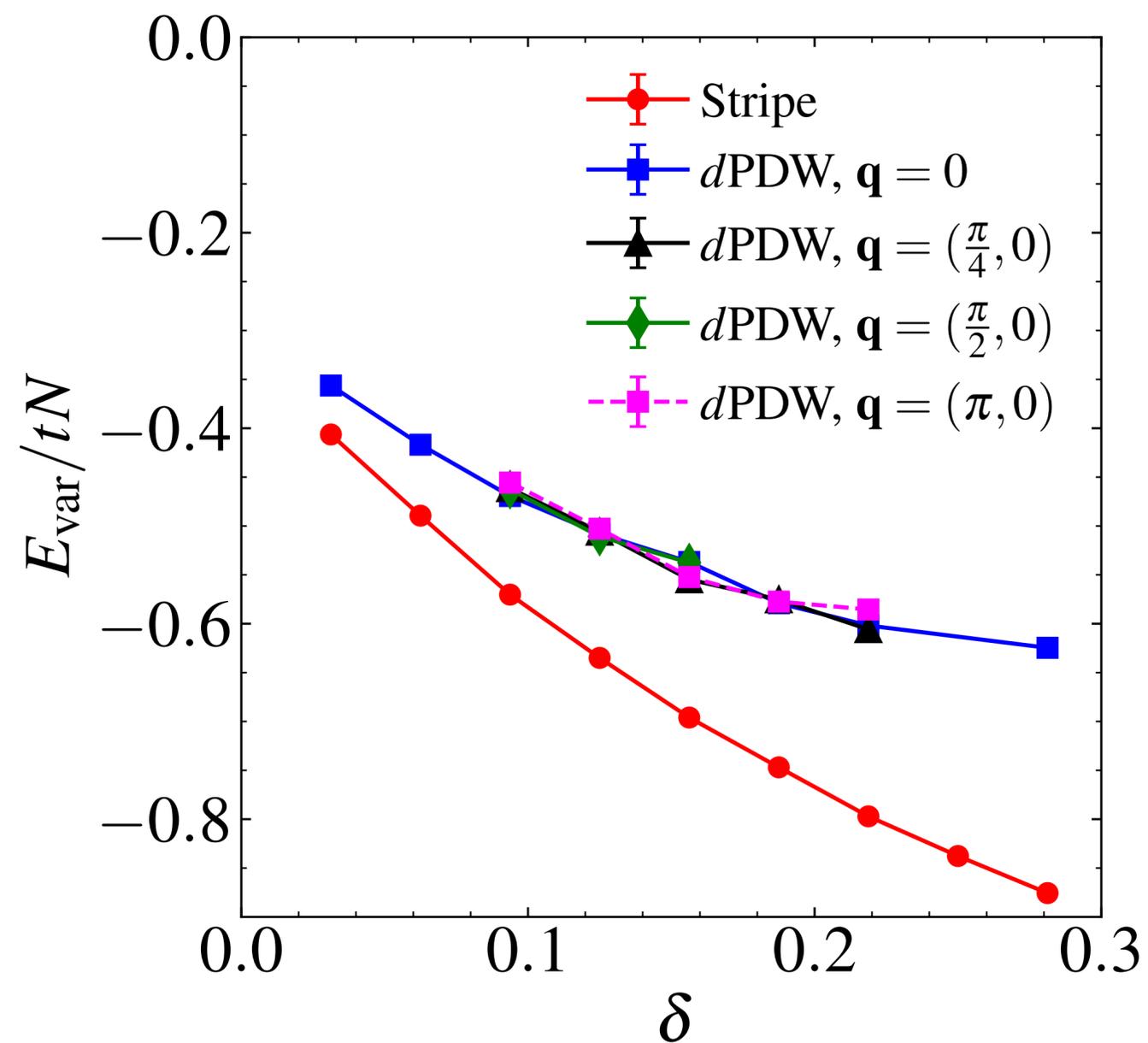
Ground state energies

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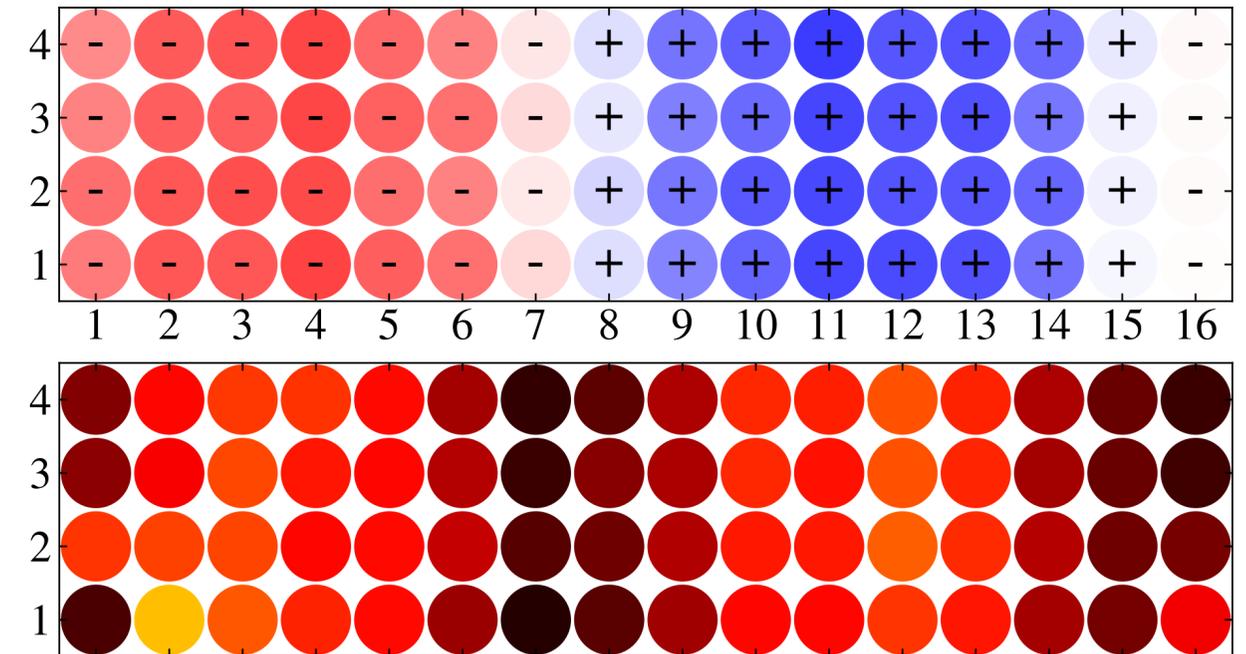
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Summary and outlook

- Results suggest that charge and spin stripes win out against uniform d-wave and dPDW.
- Further work will push to larger lattice sizes, better statistics.
- Results for stripe + SC wavefunctions
- Additional observables and correlation measurements.



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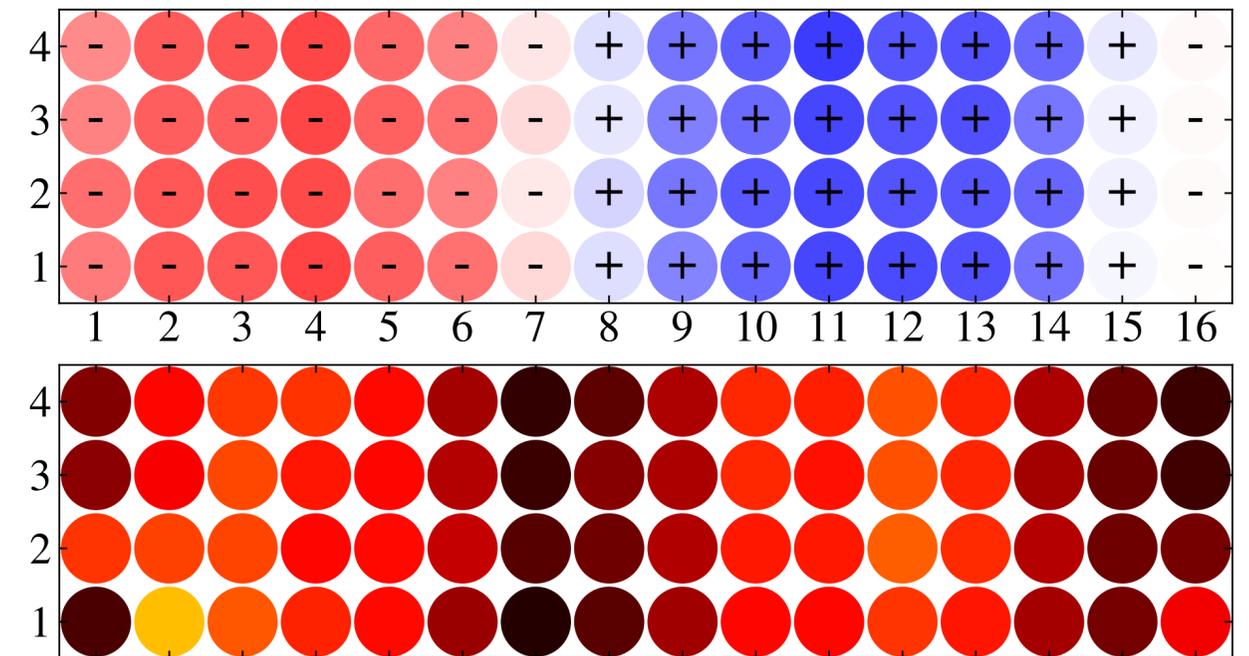
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