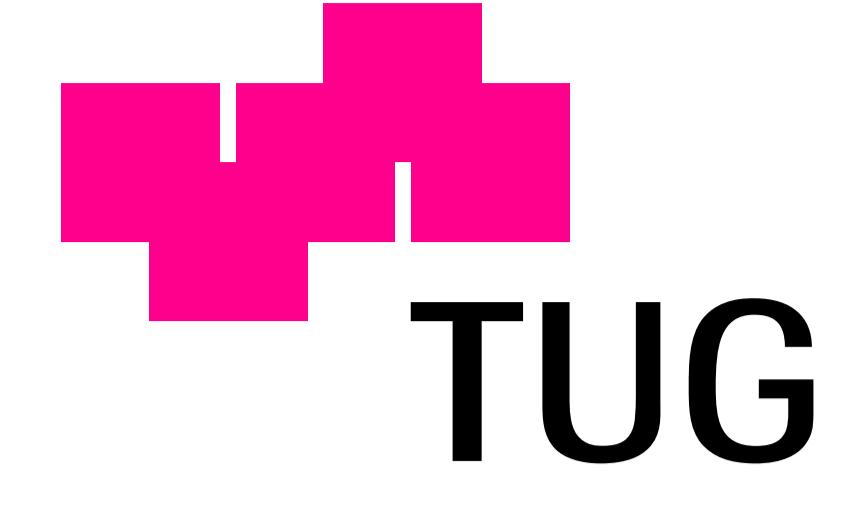


# Charge Ordering in Quarter-Filled Ladder Systems coupled to the Lattice

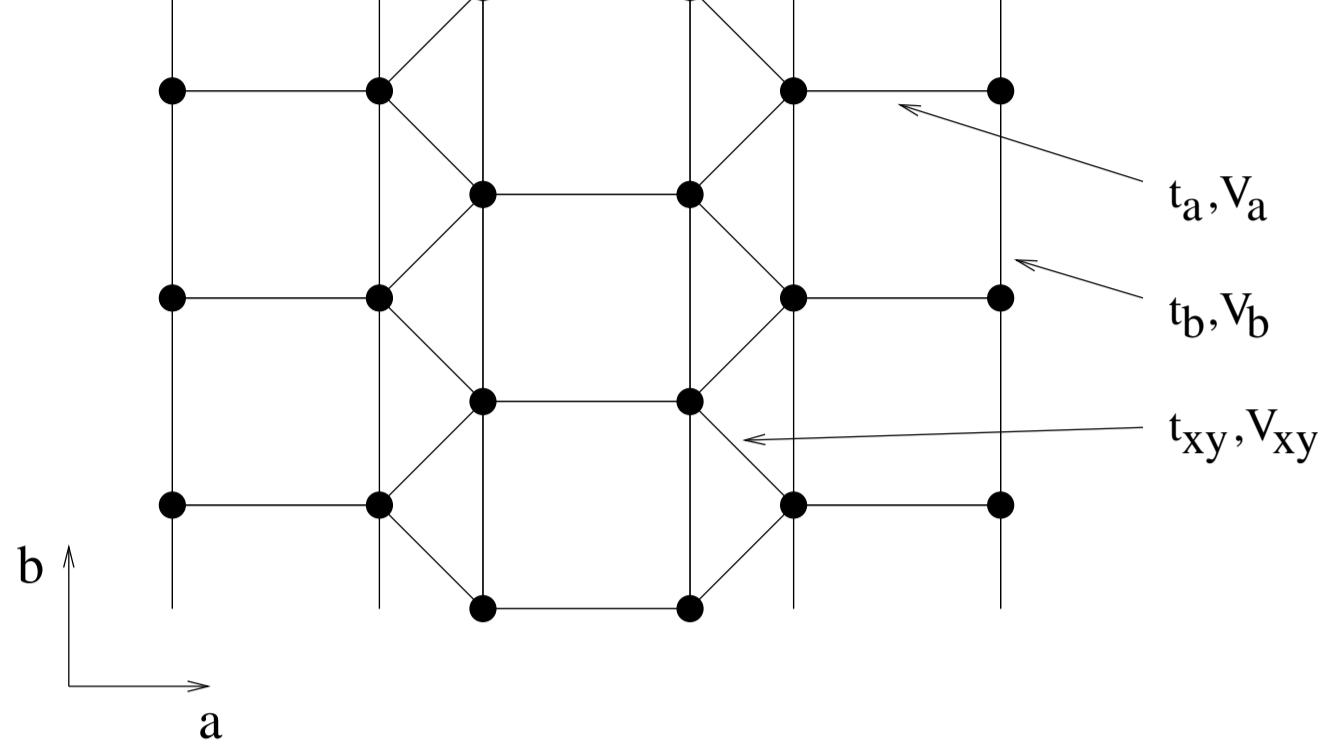
**itp**

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## Structure and Hamiltonian of NaV<sub>2</sub>O<sub>5</sub>



Relevant electronic states: Vanadium 3d<sub>xy</sub> orbitals

Microscopic description: Extended Hubbard model (EHM):

$$H = - \sum_{\langle ij \rangle \sigma} t_{ij} (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow} + \sum_{\langle ij \rangle} V_{ij} n_i n_j \quad (1)$$

Parameters from first-principle calculations.<sup>1,2</sup> We use:

$$t_a = 0.38 \text{ eV} = 2t_b, \quad t_{xy} = 0.3t_a, \quad U = 8t_a.$$

Parameters  $V_a$ ,  $V_b$ , and  $V_{xy}$  undetermined  $\Rightarrow$  Free parameter  $V$

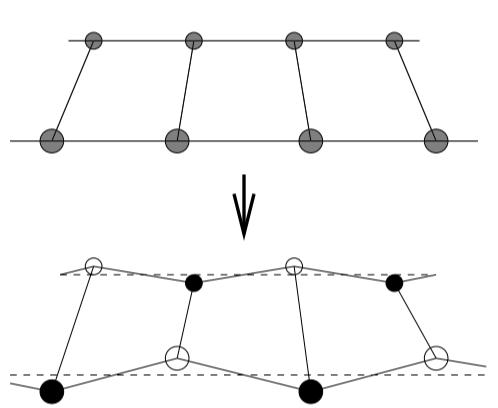
## Electron-Lattice Coupling

Phase transition at  $T_{CO} = 35 \text{ K}^3$

$T > T_{CO}$ : disordered

$T < T_{CO}$ : charge ordered,<sup>4</sup> lattice distortions<sup>5</sup>, spin gap<sup>3</sup>

Experiment: zig-zag distortions in  $z$  direction.



Lattice degrees of freedom important  $\Rightarrow$  Hamiltonian

$$H = H_{\text{EHM}} + \sum_i \left[ \frac{1}{2M} \dot{p}_i^2 + \frac{\kappa}{2} \dot{z}_i^2 - C \dot{z}_i n_i \right]. \quad (2)$$

First-principle calculations:<sup>2</sup>  $\kappa = 0.125$ ,  $C = 0.35$ ,  $[L] = 0.05 \text{ \AA}$

## Static distortions

Neglect phonon oscillations  $\Rightarrow \dot{p}_i^2 \equiv 0$ ,  $\dot{z}_i \rightarrow z_i$  (external parameters)

Classical MC over  $\{z_i\}$  (ED,  $6 \times 2$ )  $\Rightarrow$  find sharp zig-zag distortions

Now assume zig-zag order pattern  $z_j = z \cdot e^{iQr_j}$

DMRG calculations ( $64 \times 2$ ):

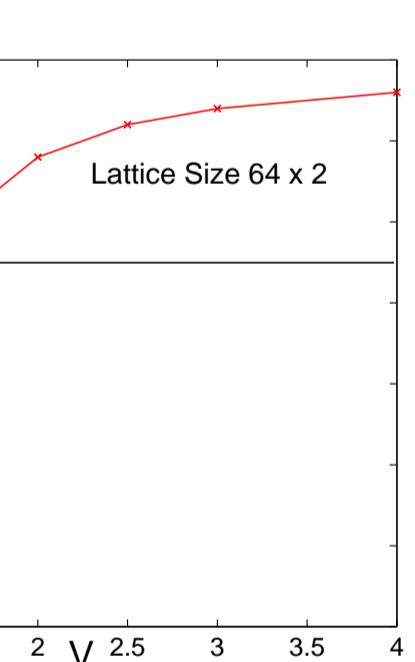
Optimal distortions:

Minimum in total energy  $\Leftrightarrow z_{\text{opt}}$

Finite for  $V \gtrsim 1$

Experiment:  $z_{\text{exp}} = 0.9$

$\Rightarrow$  eff. interaction  $V \simeq 1.4t_a$

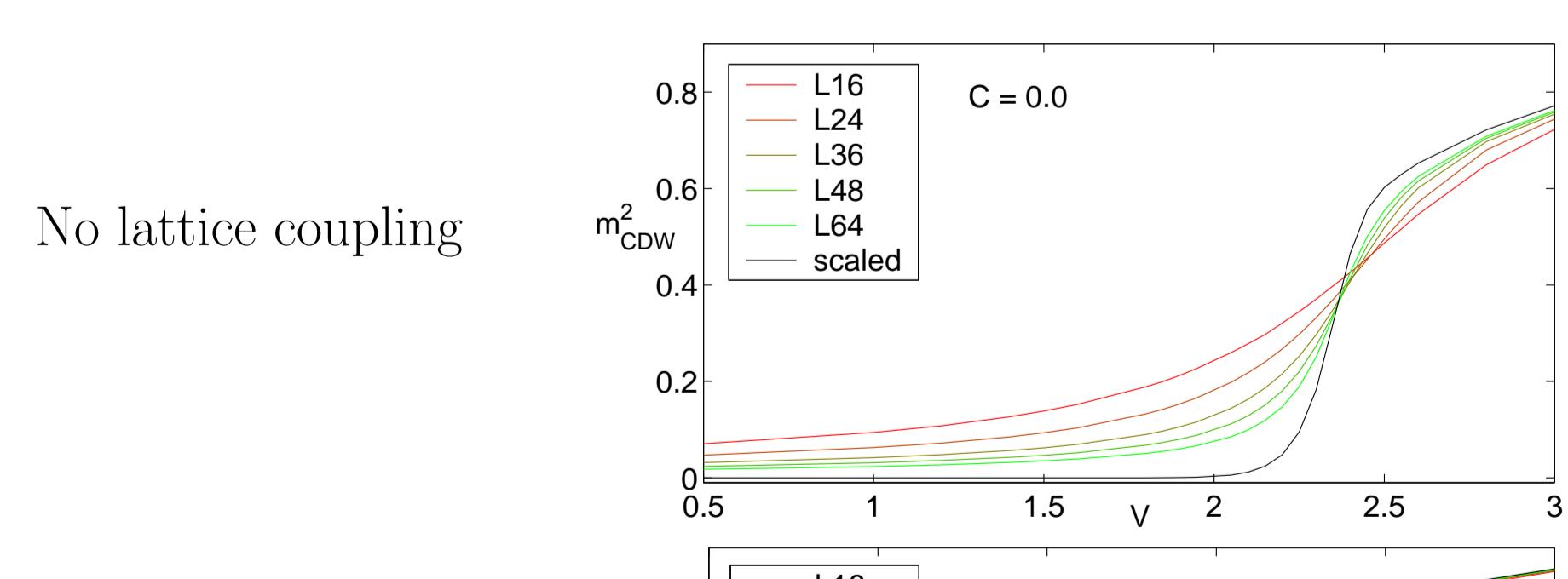


## Charge Order Parameter – Single Ladders

Order parameter calculated by DMRG:

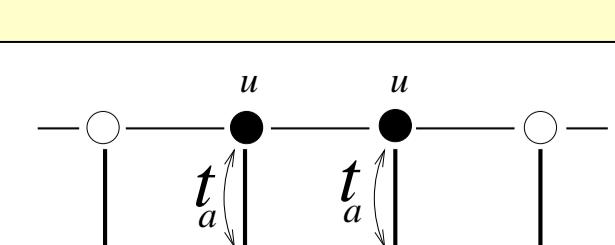
$$m_{CDW}^2 = \frac{1}{(2L)^2 \langle n \rangle} \sum_{ij} e^{iQ(r_i - r_j)} (\langle n_i n_j \rangle - \langle n \rangle^2) \quad (3)$$

No lattice coupling



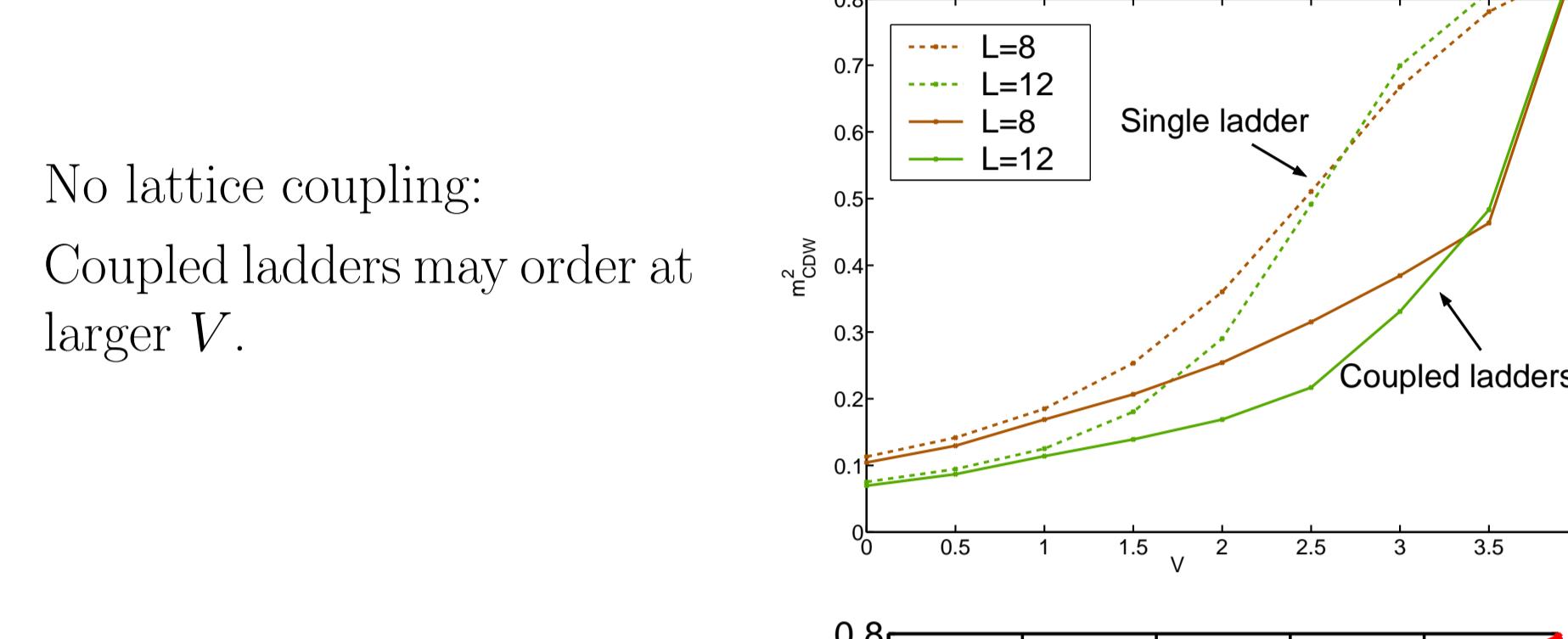
- 2nd-order phase transition at  $V_{\text{crit}} = 0.95$  and  $V_{\text{crit}} = 2.1$
- Change of critical exponent with lattice coupling
- No spin gap

Elementary excitations: Kinks

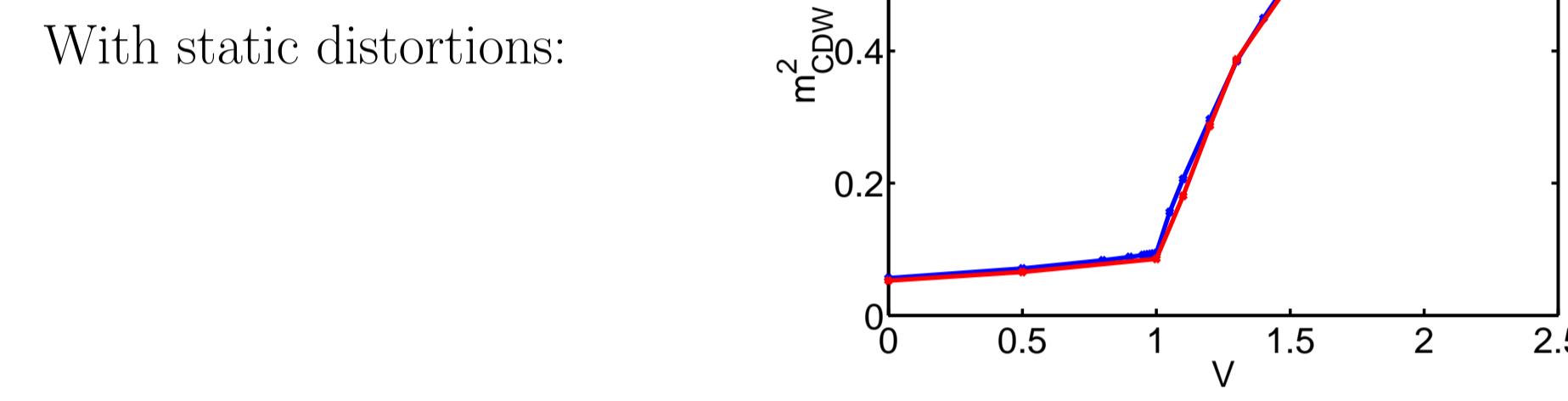


## Charge Order Parameter – Coupled Ladders

We find: Both ladders order simultaneously!



No lattice coupling:  
Coupled ladders may order at larger  $V$ .

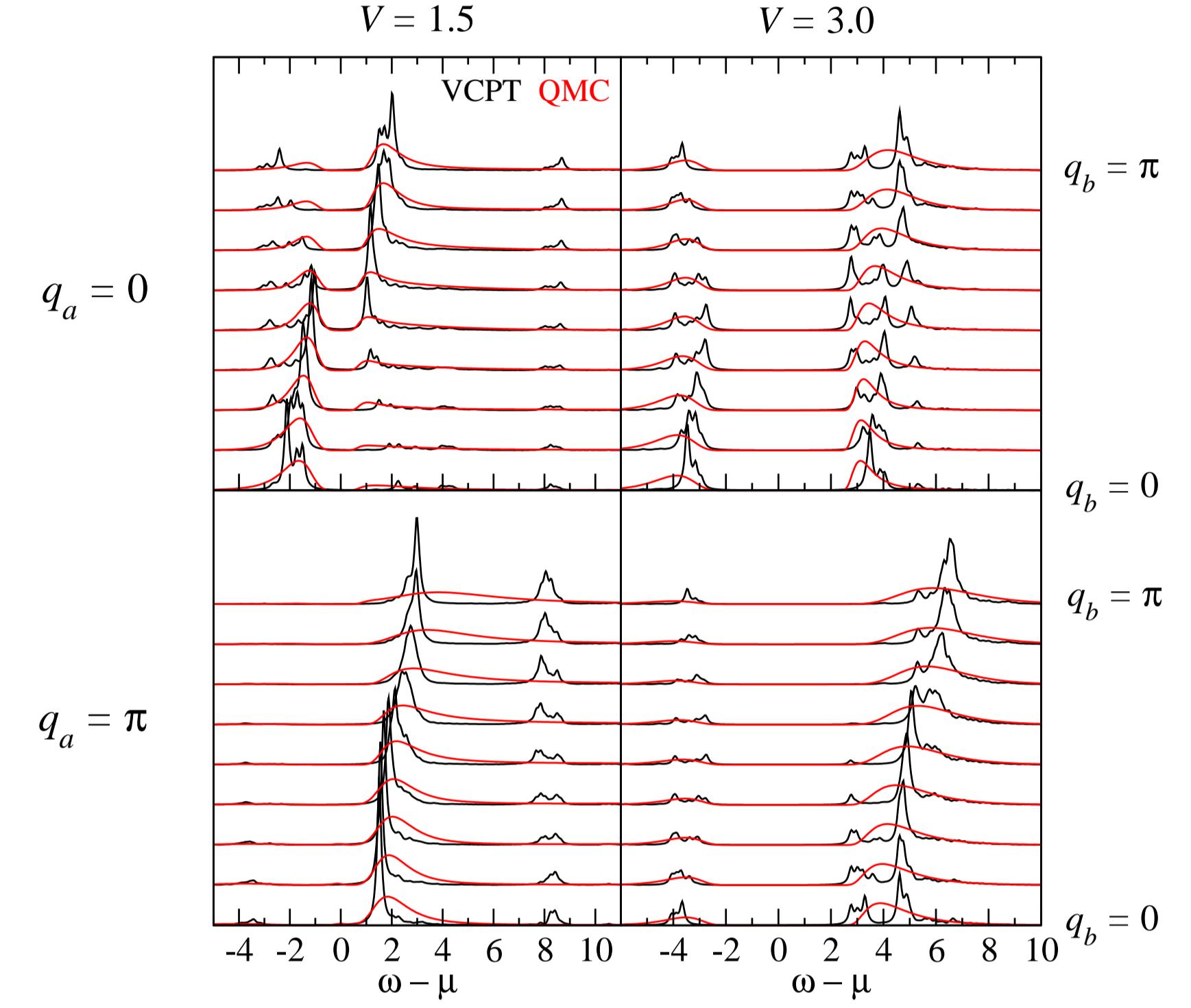


With static distortions:

No spin gap, no preference for 2a unit cell

## Single-Particle Spectral Function

Spectral function calculated by variational cluster perturbation theory (VCPT,  $T = 0$ ) and QMC (at  $\beta = 6t_a$ ).



Good agreement between VCPT and QMC:

- For  $q_a = 0$ : Similar to the half-filled 1D Hubbard model
- Gap determined by  $V$  (not  $U$ ), bandwidth set by  $t_b$

Difference between  $q_a = 0$  and  $q_a = \pi$ :

For  $q_a = 0$ : Occupied states (bonding orbital)

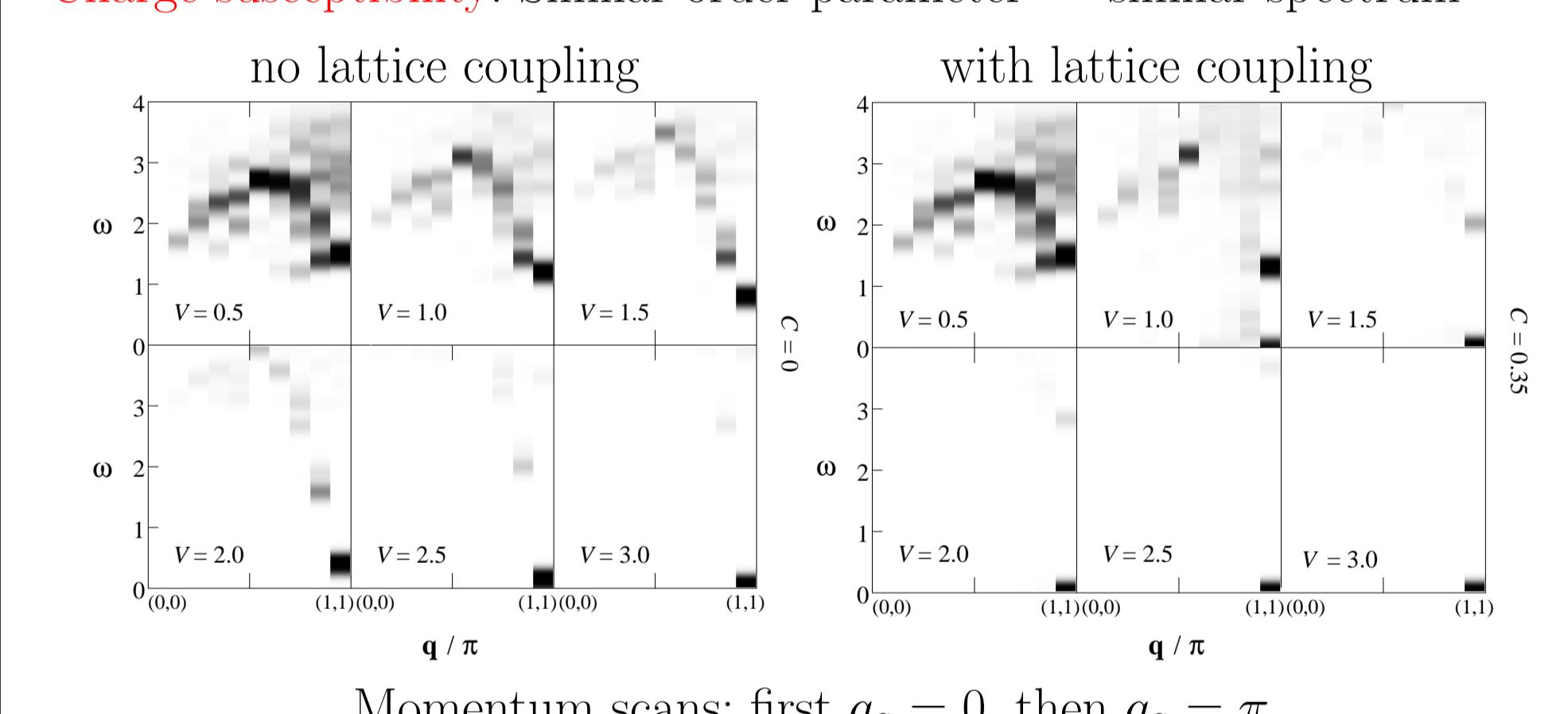
For  $q_a = \pi$ : not occupied in the ground state (antibonding)!

$\Rightarrow$  no spectral weight below  $\mu$

## Dynamical Susceptibilities at $T = 0$

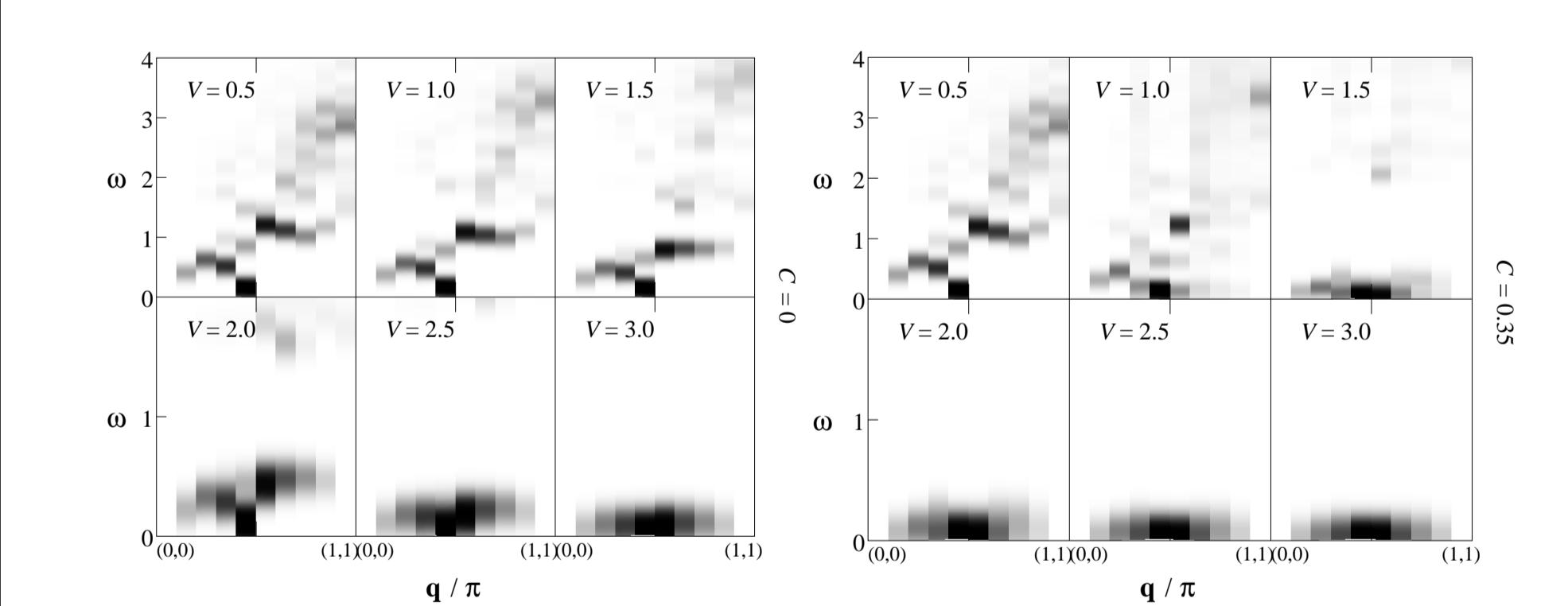
ED calculations on an  $8 \times 2$  ladder

Charge susceptibility: Similar order parameter  $\leftrightarrow$  similar spectrum



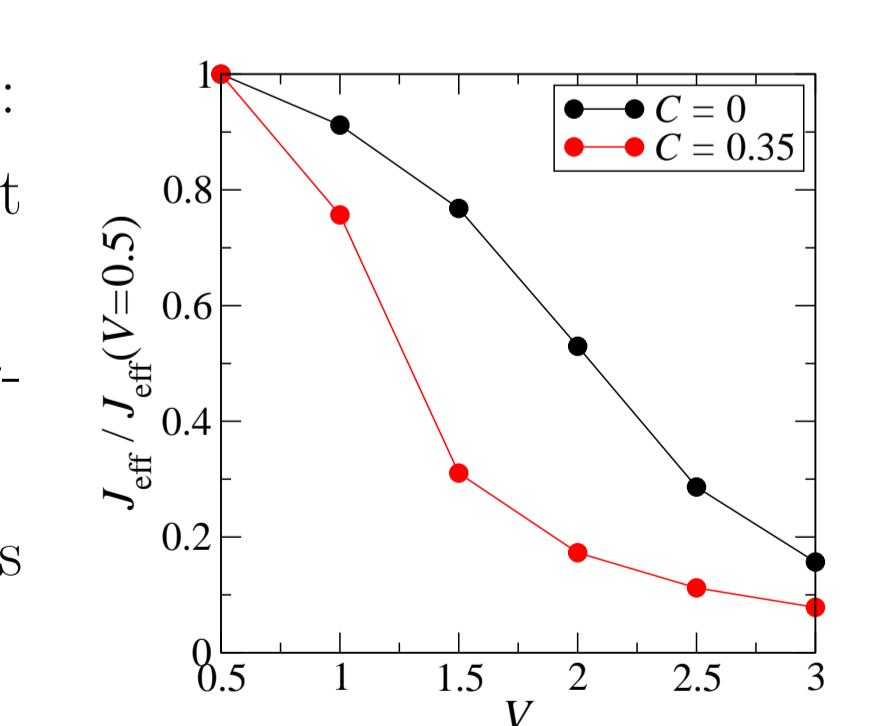
Momentum scans: first  $q_a = 0$ , then  $q_a = \pi$

Spin susceptibility:

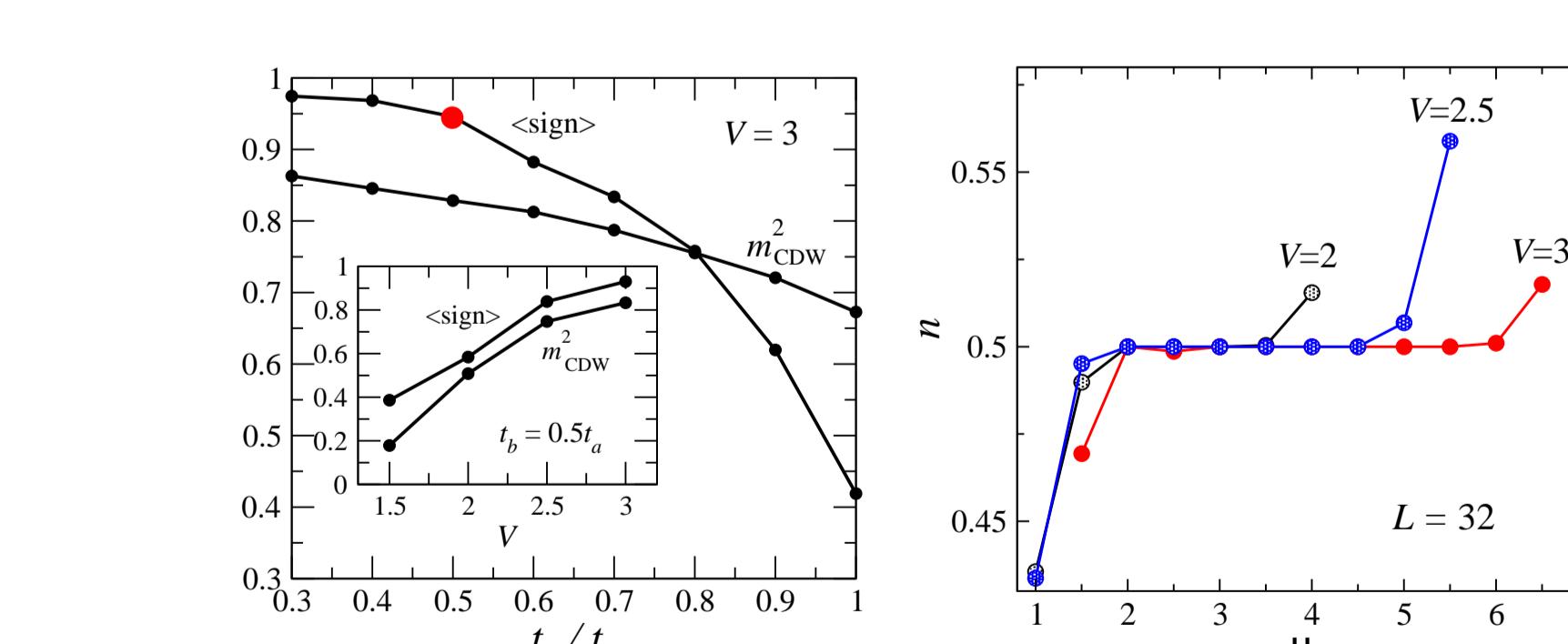


$q_a = 0$ : Quasi-1D-Heisenberg behavior:

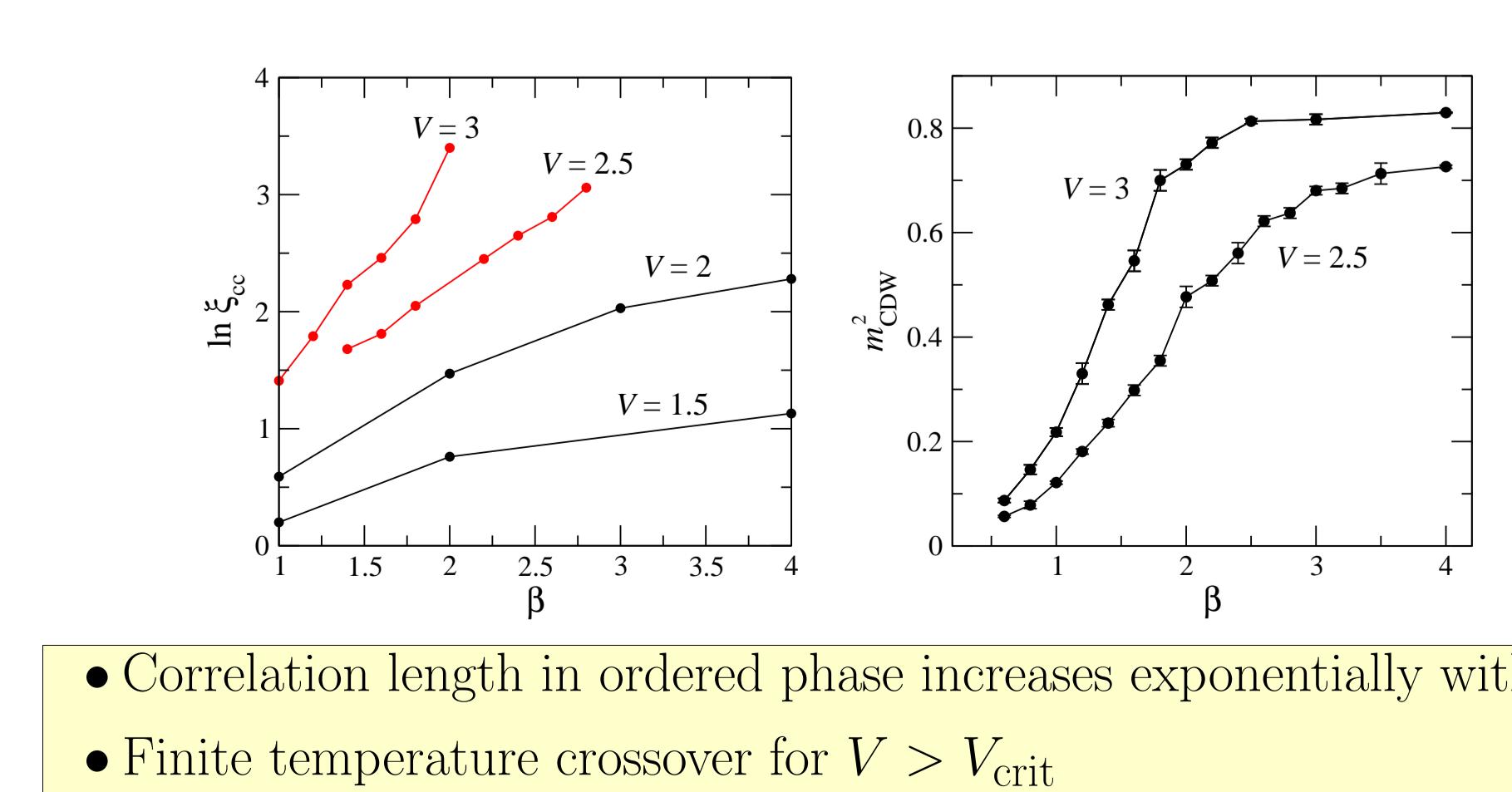
- Effective interaction  $J_{\text{eff}}$  consistent with perturbation theory
- Reduction of  $J_{\text{eff}}$  with increasing order
- At  $V = 1.4t_a$ :  $J_{\text{eff}} \approx 67 \text{ meV}$  matches experiment.<sup>6</sup>



## Finite-Temperature Investigations – QMC



- Sign problem is moderate at quarter filling and  $t_b/t_a = 0.5$  in the ordered phase ( $\beta = 6$ ,  $L = 16$ ).
- Finite single-particle gap in the ordered phase



- Correlation length in ordered phase increases exponentially with  $\beta$
- Finite temperature crossover for  $V > V_{\text{crit}}$   
– shifts to larger  $\beta$  for larger  $L$ , similar to 1D Ising

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