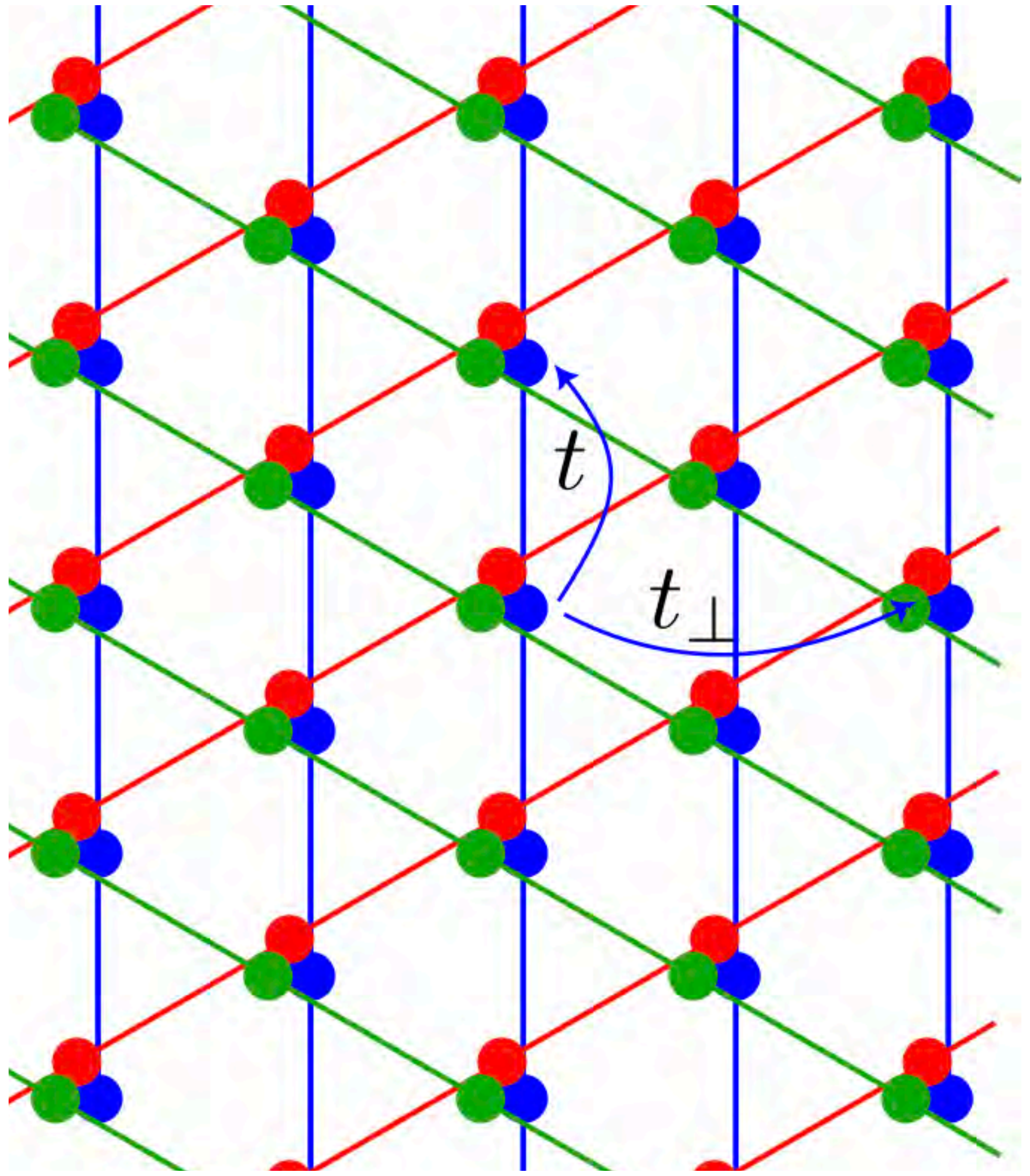
M-Point Moiré Materials II:
Electron Correlations and Sign-free Quantum Monte Carlo Techniques



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Theory Winter School, NHMFL, January 12-16, 2026

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UKRI
Engineering and Physical Sciences Research Council

Collaborators

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Oxford   Oxford/ENS   MPI-PKS Dresden

+discussions with **Haoyu Hu, Andrei Bernevig**

Division of Topics

Lecture 1: Basic Principles of Moiré Reconstruction applied to M-point Materials

[mostly adapted from Calugaru et al *Nature* **643**, 376 (2025) and its 100+ page supplementary material]

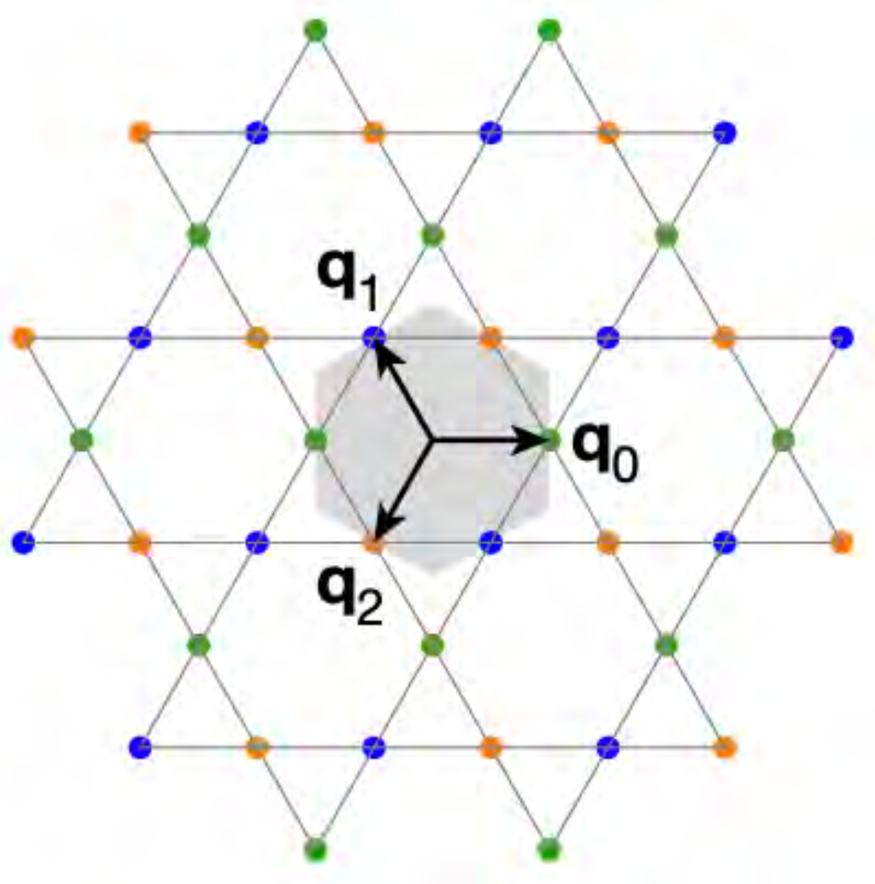
Lecture 2: Sign-Free Quantum Monte Carlo for (some) M-point Materials

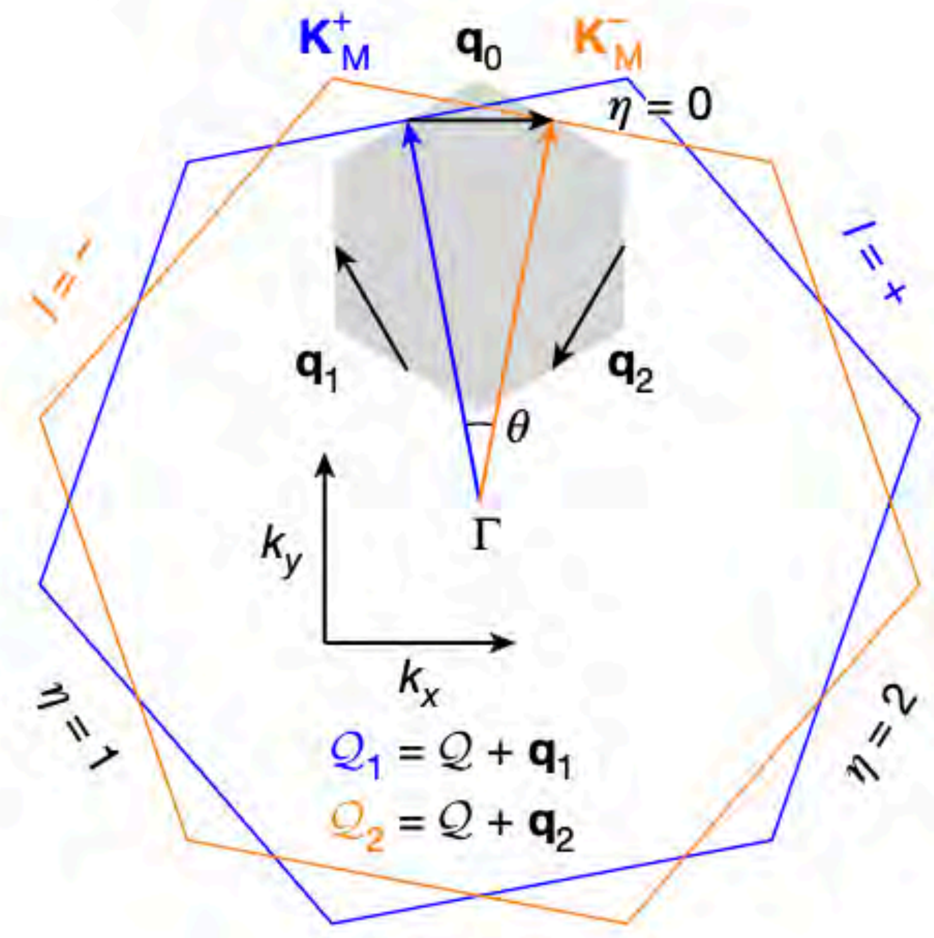
[mostly adapted from M.-R. Li, …, SAP,…, H. Hu 2508.10098 + work in progress]

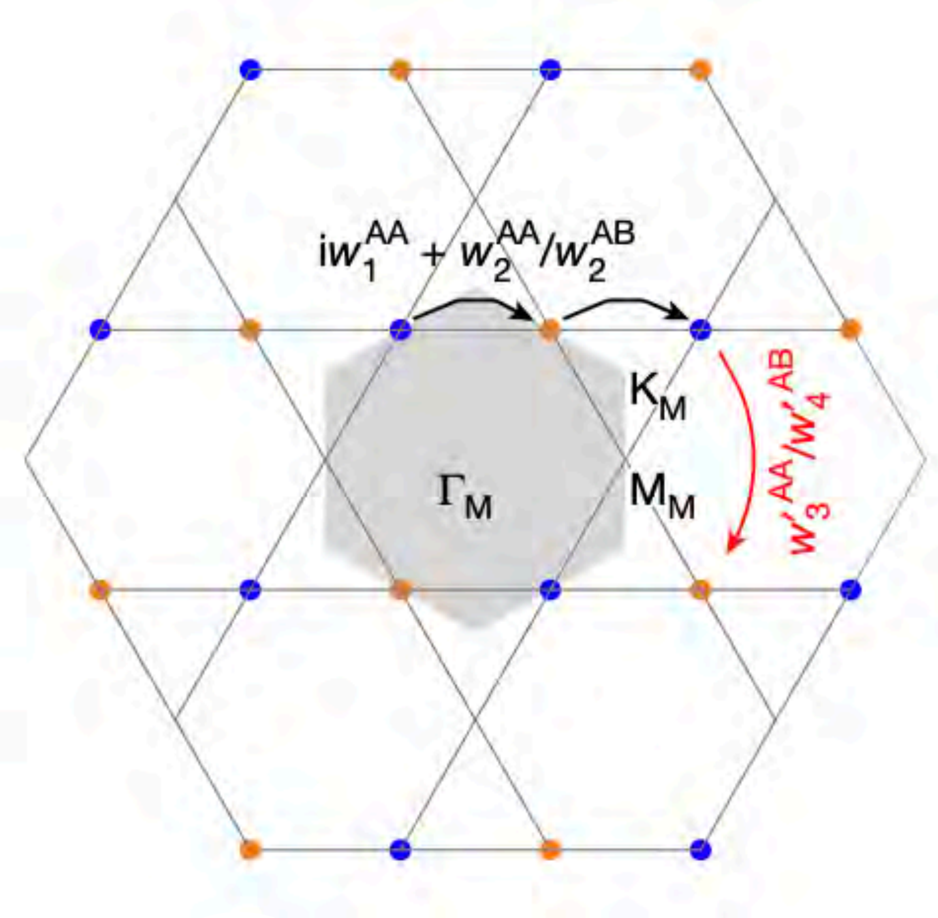
Recap of Lecture 1: *M*-Point Moiré Platforms

Moiré reconstruction ↔ "momentum space hopping problem" (cf. Bistritzer-MacDonald)

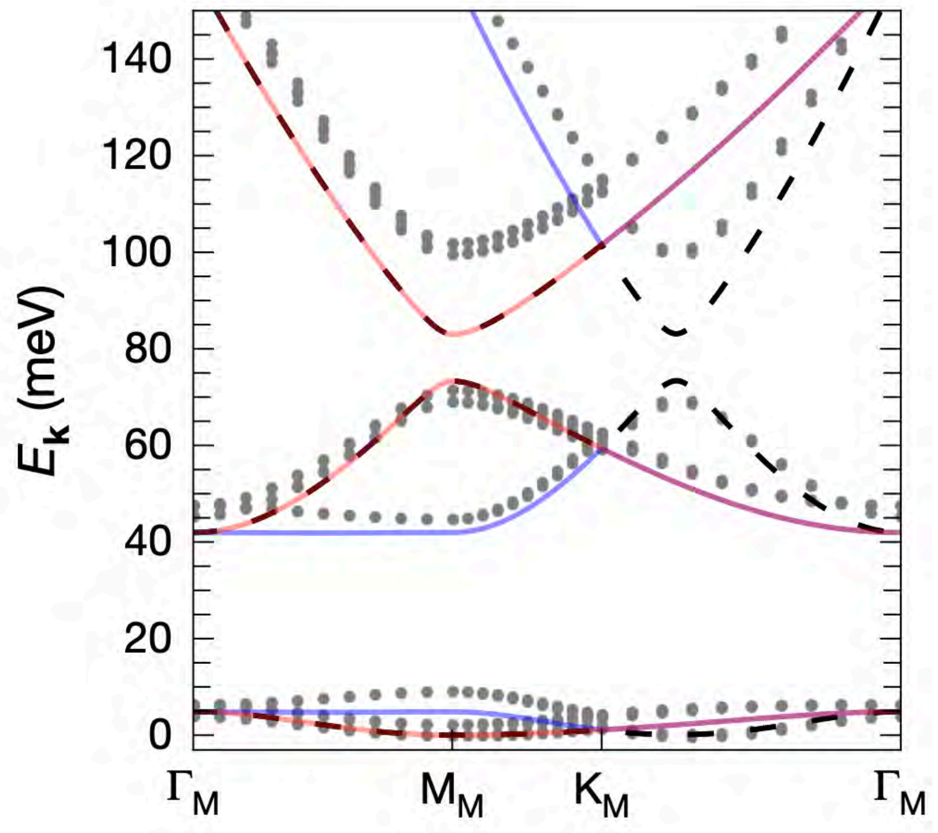
Homobilayers w/ low-energy electrons in each layer at M-point ⇒ momentum-space kagome lattice
(e.g. $SnSe_2$ ZrS_2)







Layers break inversion so AA/AB stacking differ



In each valley, *M*-point moiré potential only involves 2 of 3 k-space kagomé sublattices

Emergent k-space nonsymmorphic symmetry $\tilde{M}_z$ can enforce quasi-1D behavior
(eg. AA-stacked t-$SnSe_2$)

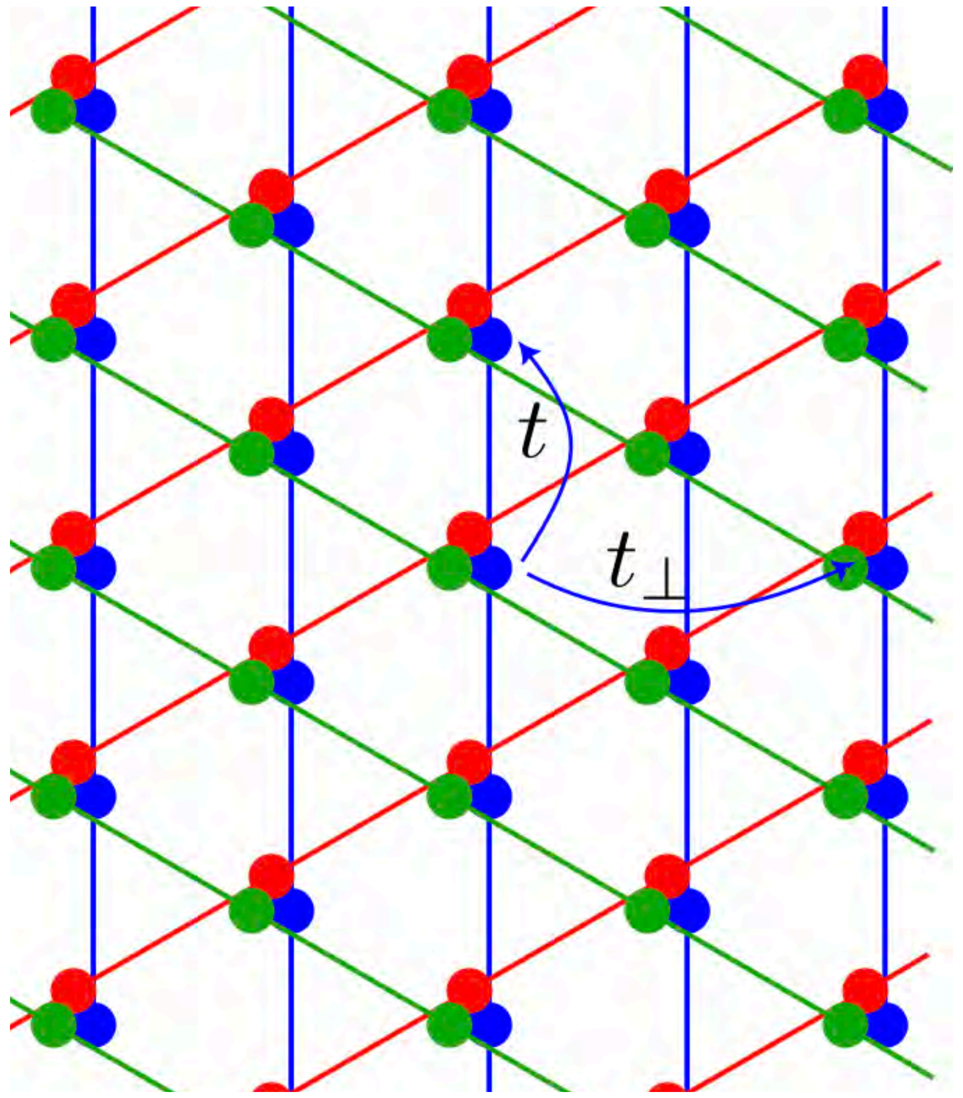
[Calugaru et al *Nature* **643**, 376 (2025) + **ask Dumitru!**]

Emergent Quasi-1D Physics in *M*-Point Moiré Systems

Focus on quasi-1D AA stacking e.g. *t*$SnSe_2$ at $\theta \approx 3.89°$

1 Wannier orbital/valley $\times$ 3 valleys $\times$ spin $\Rightarrow$ 6 states/site, triangular lattice

PHS maps $\nu \leftrightarrow 6 - \nu$



[M.-R. Li, …, SAP,…, H. Hu 2508.10098 + work in progress]

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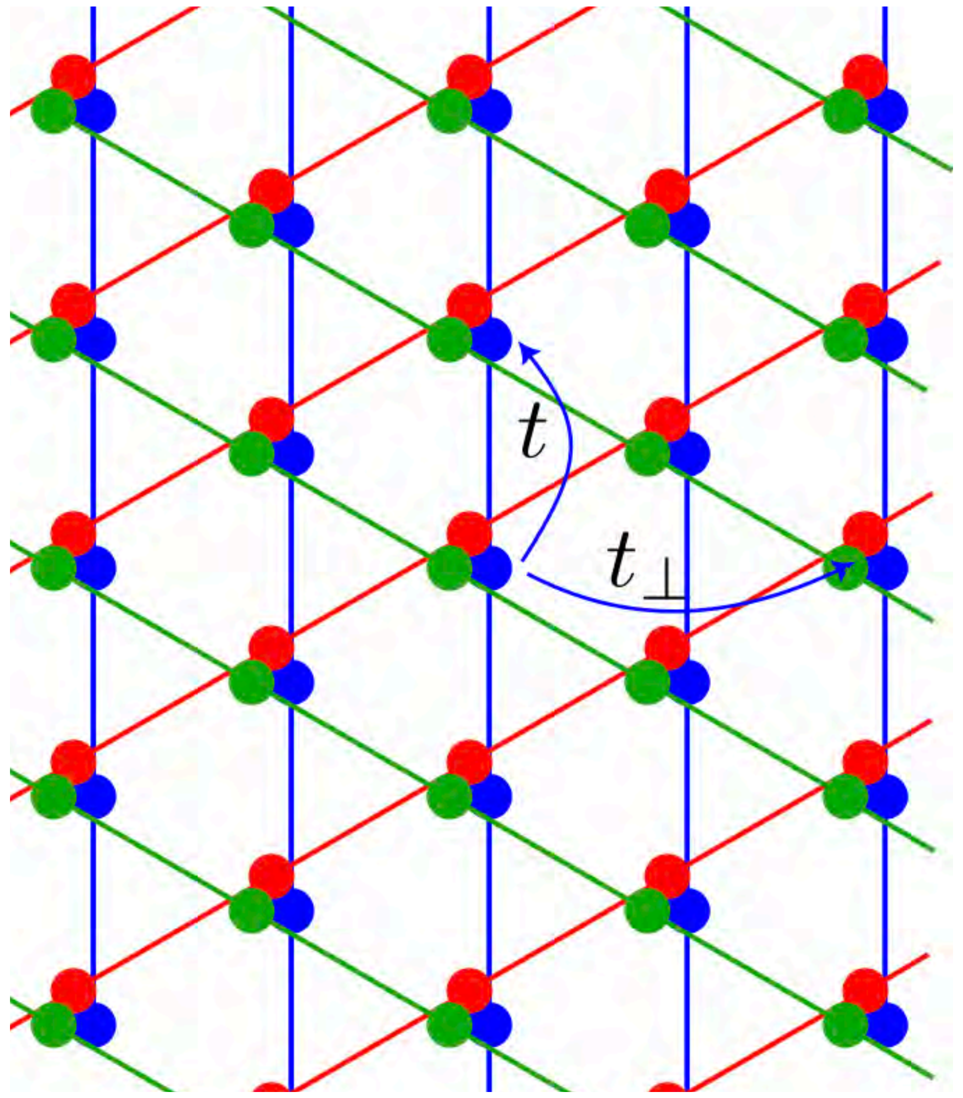

<u>Dispersion:</u> **orbitally-selective 1D hopping t**

Leading 2d kinetic term: **2nd-neighbor intravalley $t_\perp$**

(1st neighbor vanishes b/c approx. symmetry)

[M.-R. Li, …, SAP,…, H. Hu 2508.10098 + work in progress]

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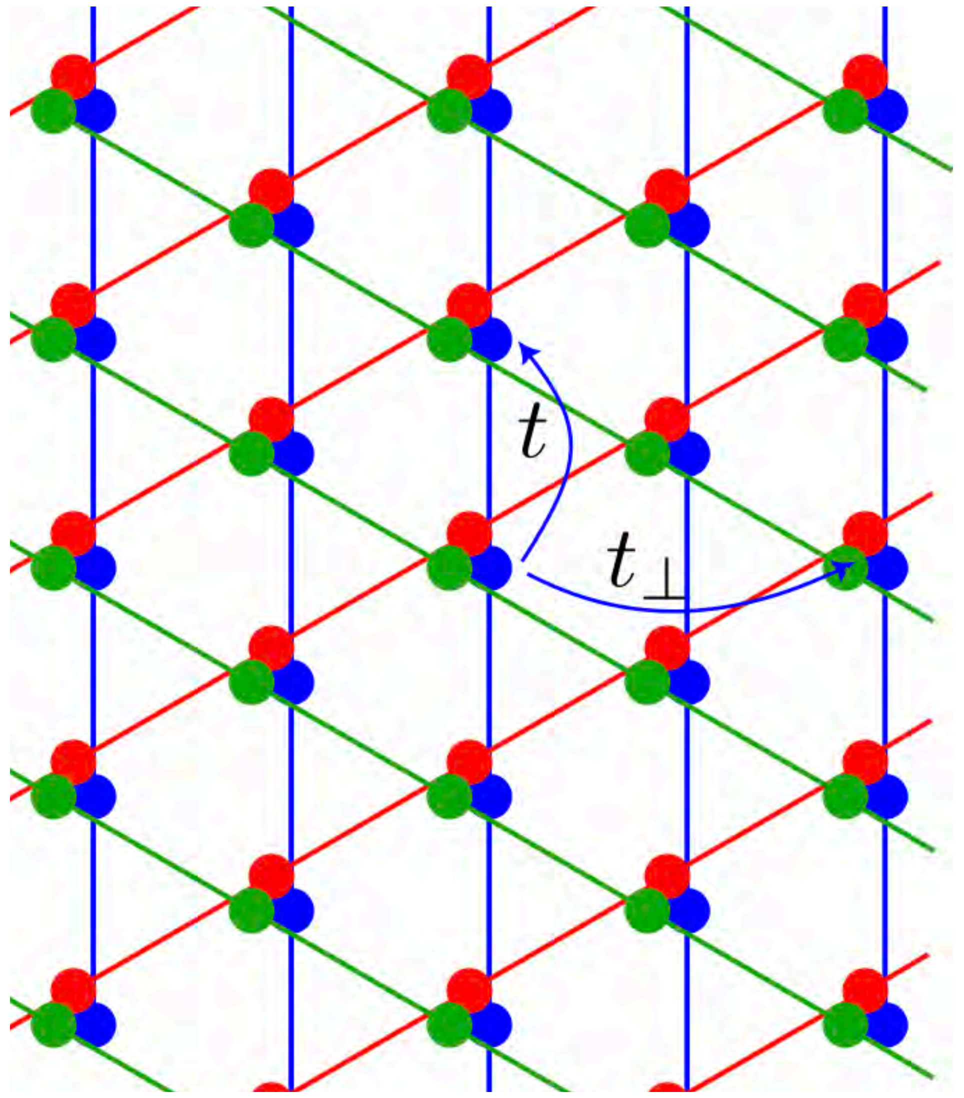

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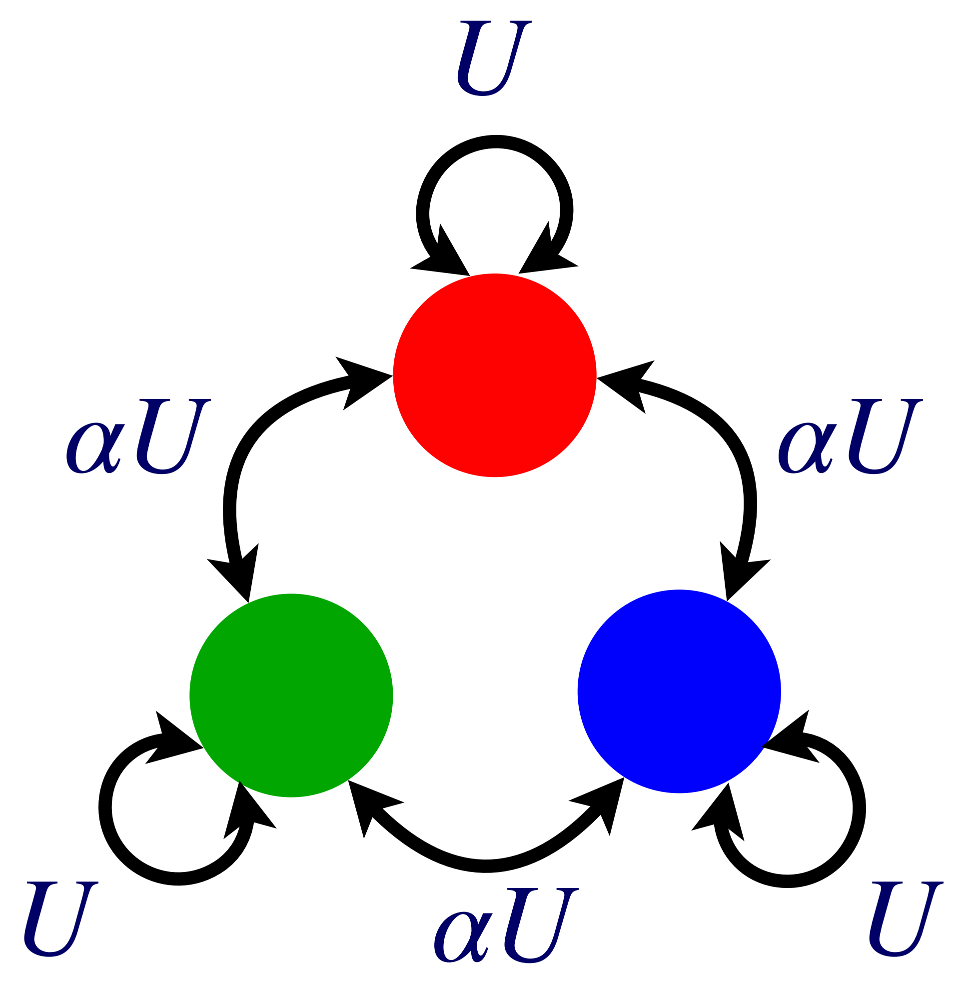

<u>Interactions:</u> On-site Hubbard U + nearest-neighbour V (fully 2D)

Orbital offsets ⇒ anisotropies in U, V (opp. sign for U, V)

- only retain U anisotropy

[M.-R. Li, …, SAP,…, H. Hu 2508.10098 + work in progress]

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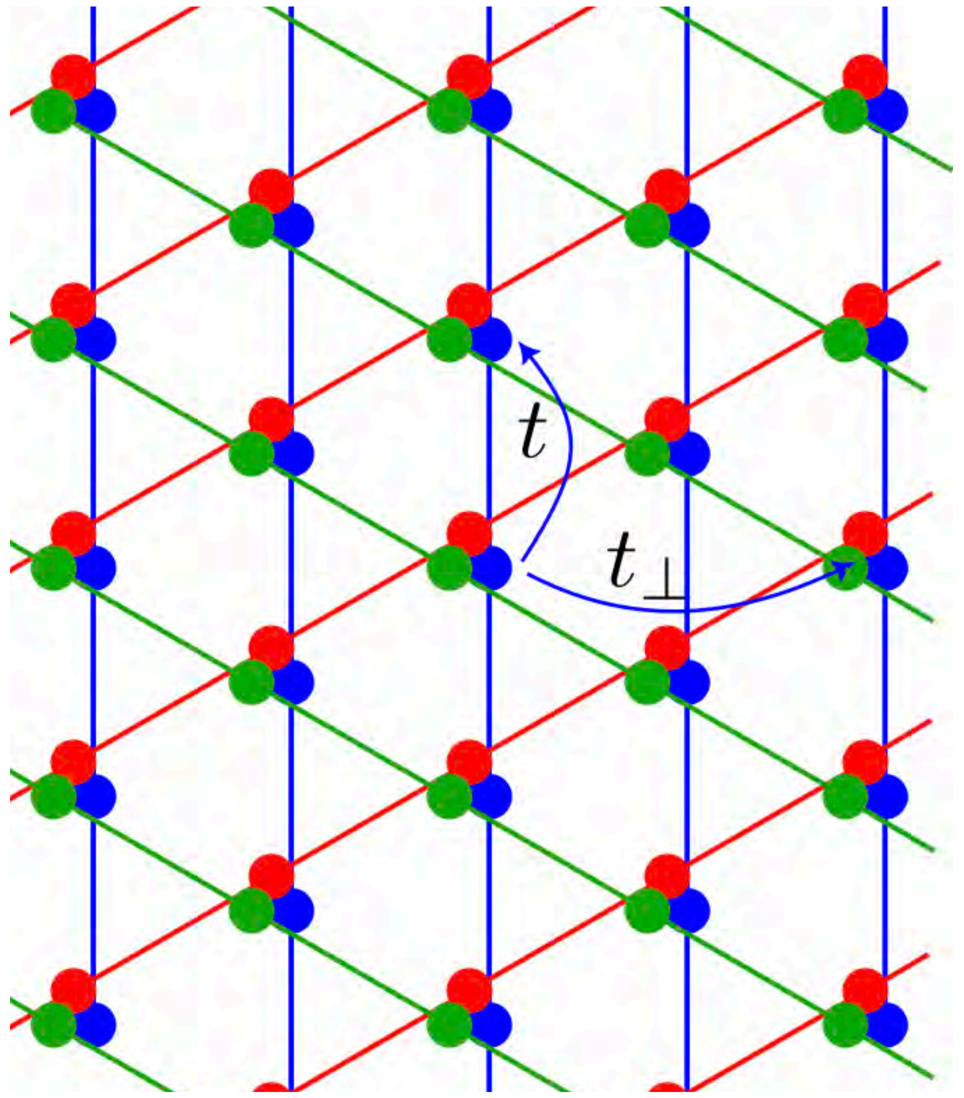

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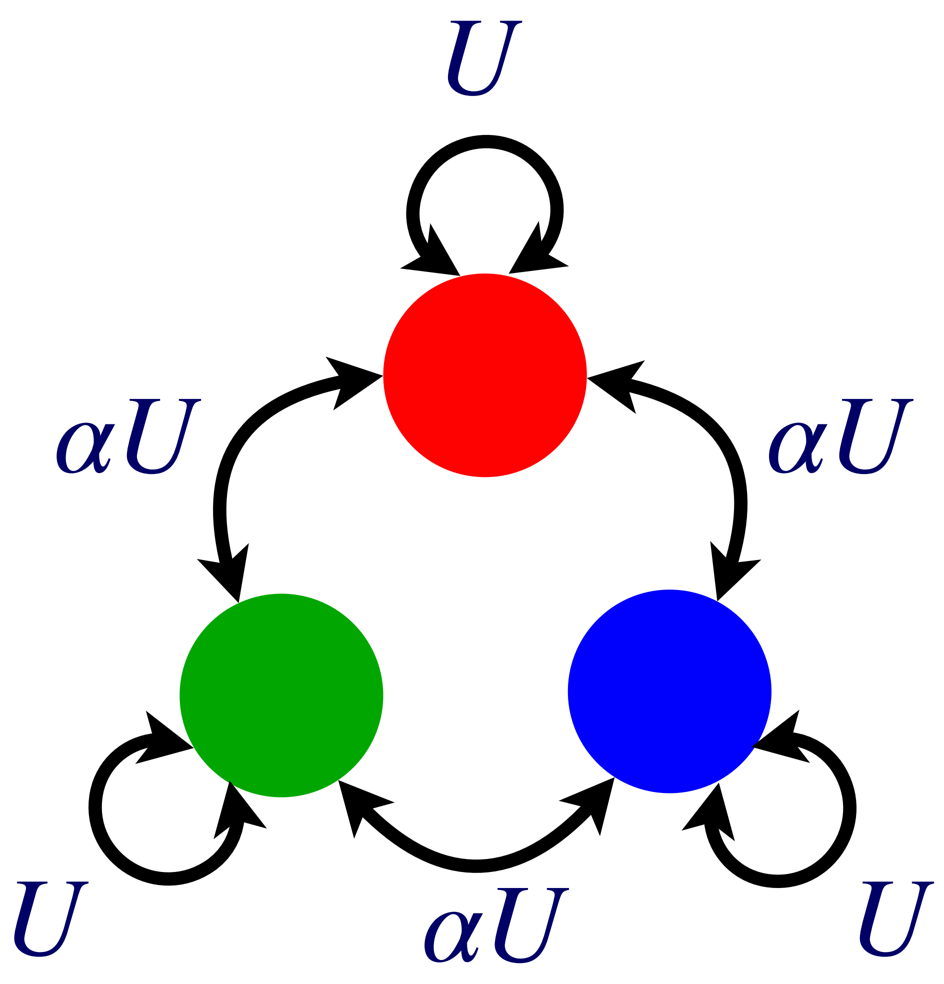
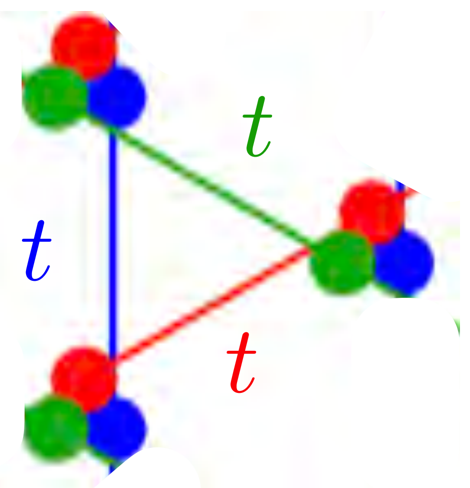
$\alpha = 1$: on-site terms $U(6)$-symmetric, only broken by hopping

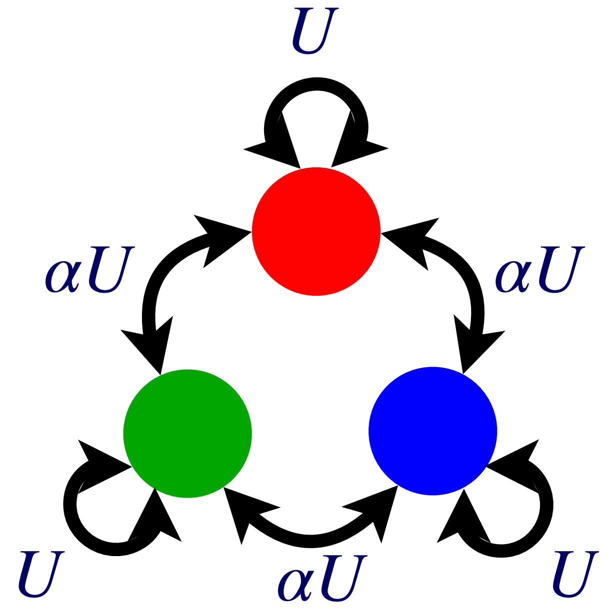


[M.-R. Li, …, SAP,…, H. Hu 2508.10098 + work in progress]

The Hamiltonian

$$H = -\sum_{\langle ij\rangle,\eta,\sigma} t_\eta c^\dagger_{i,\eta,\sigma} c_{j,\eta,\sigma} + U \sum_{i,\eta,\eta'} \{(1-\alpha)\delta_{\eta\eta'} + \alpha\} n_{i\eta} n_{i\eta'} + H_V + H_\perp$$





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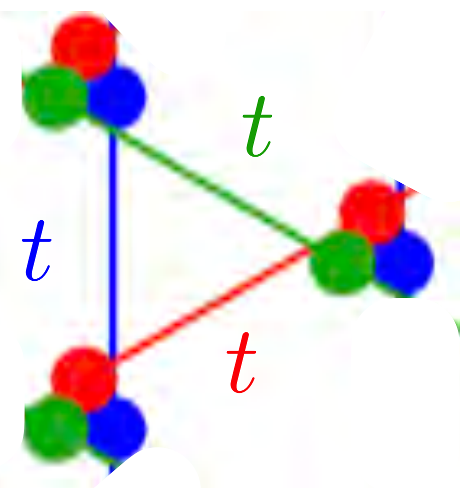
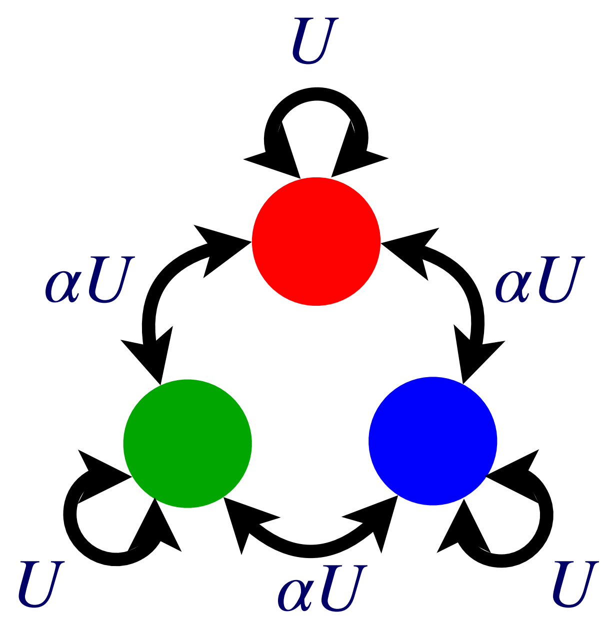
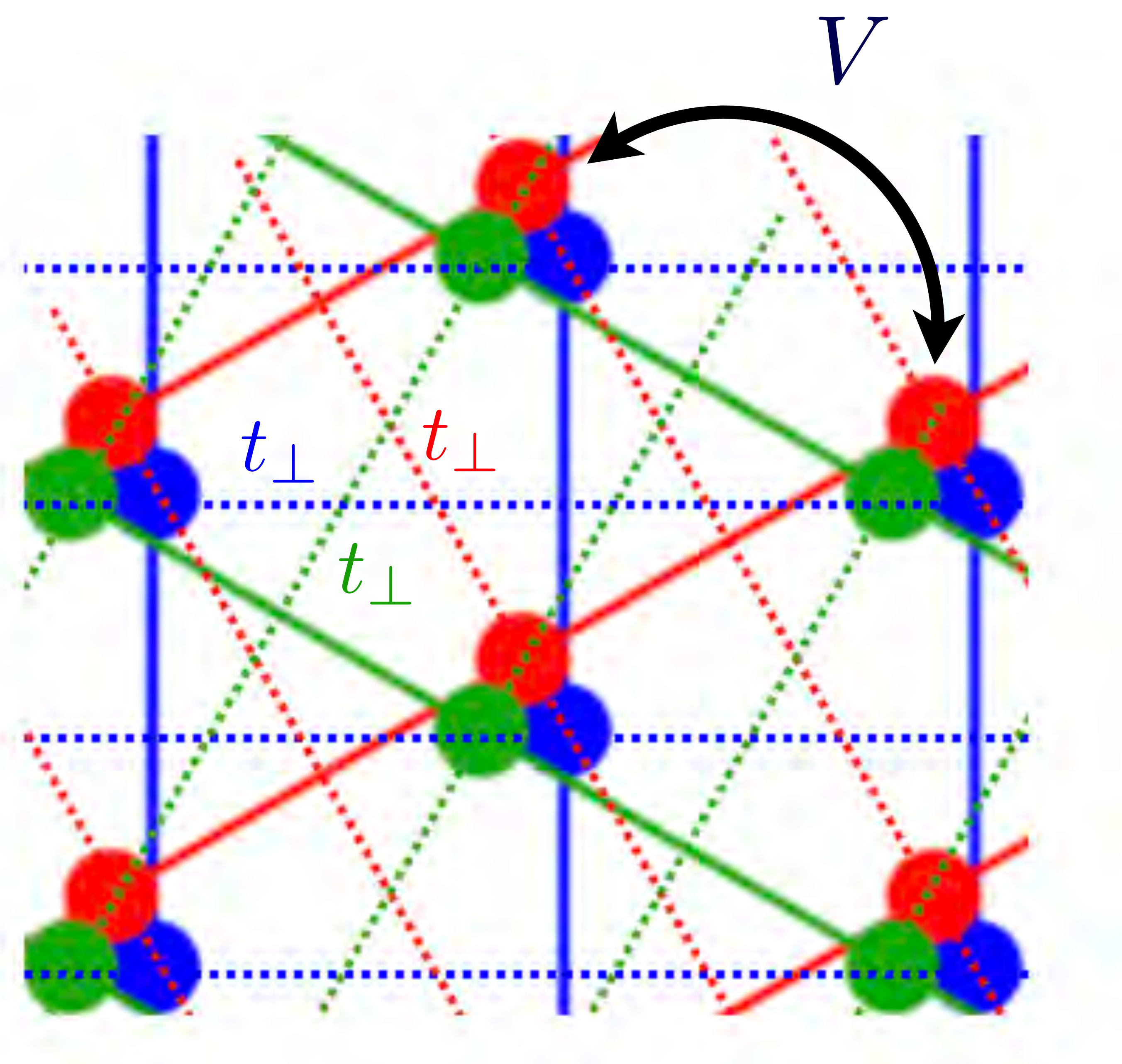




$$H_V = \sum_{\langle i,j\rangle,\eta,\sigma} V n_{i,\eta,\sigma} n_{j,\eta,\sigma}$$ (ignore anisotropies)

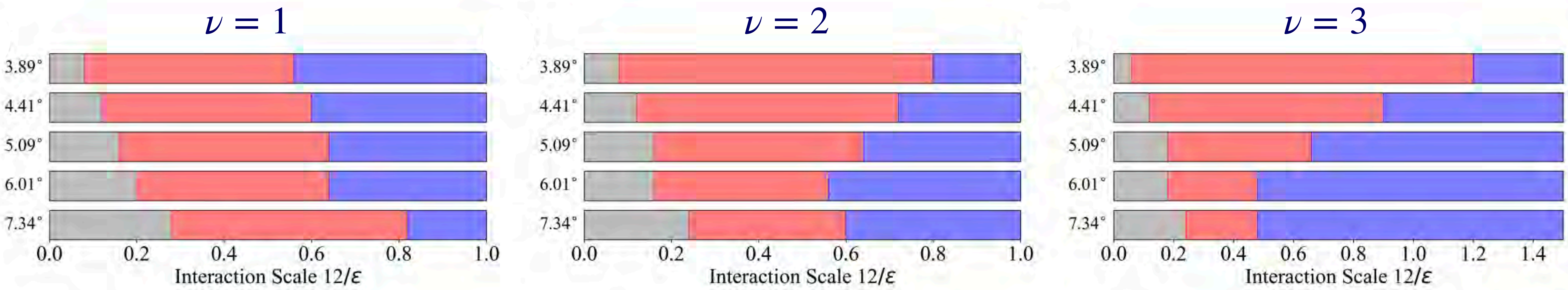
$$H_\perp = -\sum_{\langle\langle ij\rangle\rangle,\eta,\sigma} t_{\perp,\eta} c^\dagger_{i,\eta,\sigma} c_{j,\eta,\sigma}$$

"weak" 2nd nbr hopping: each valley → 2x2d rectangular lattices



First Pass: Hartree-Fock

Momentum- and **real- space** Hartree-Fock in continuum model + projected Coulomb interaction



(2×3 supercell) ($\sqrt{3} \times \sqrt{3}$ supercell) (2×2 supercell)

Qualitative Picture:

gapless metal → antiferromagnet (with and w/0 VP) → VP ferromagnet

"weak" "strong" "flat-band regime"

[M.-R. Li, …, SAP,…, H. Hu 2508.10098]

Strong-Coupling at Integer Fillings

AF super exchange at $O(t^2/U)$ breaks $U(6) \to SU(2) \times SU(2) \times SU(2)$

Exact results for $V = 0$ by mapping energetics to $\otimes$(spin chains of different lengths)

$\nu = 1$ case

[M.-R. Li, …, SAP,…, H. Hu 2508.10098]

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Step 1: Start with lattice model for all valleys

[M.-R. Li, …, SAP,…, H. Hu 2508.10098]

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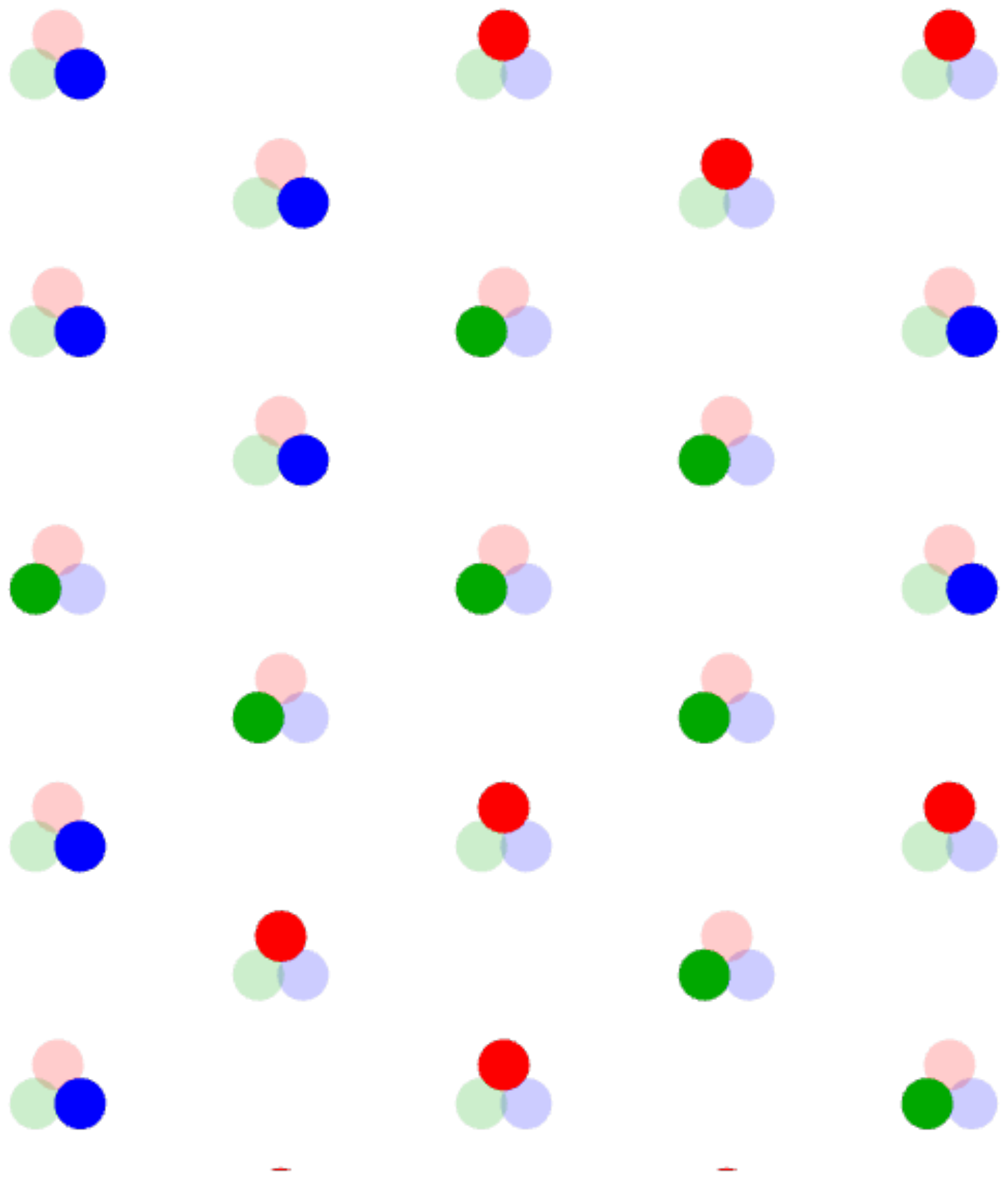

Step 2: place 1 electron per site in fixed valley

[M.-R. Li, …, SAP,…, H. Hu 2508.10098]

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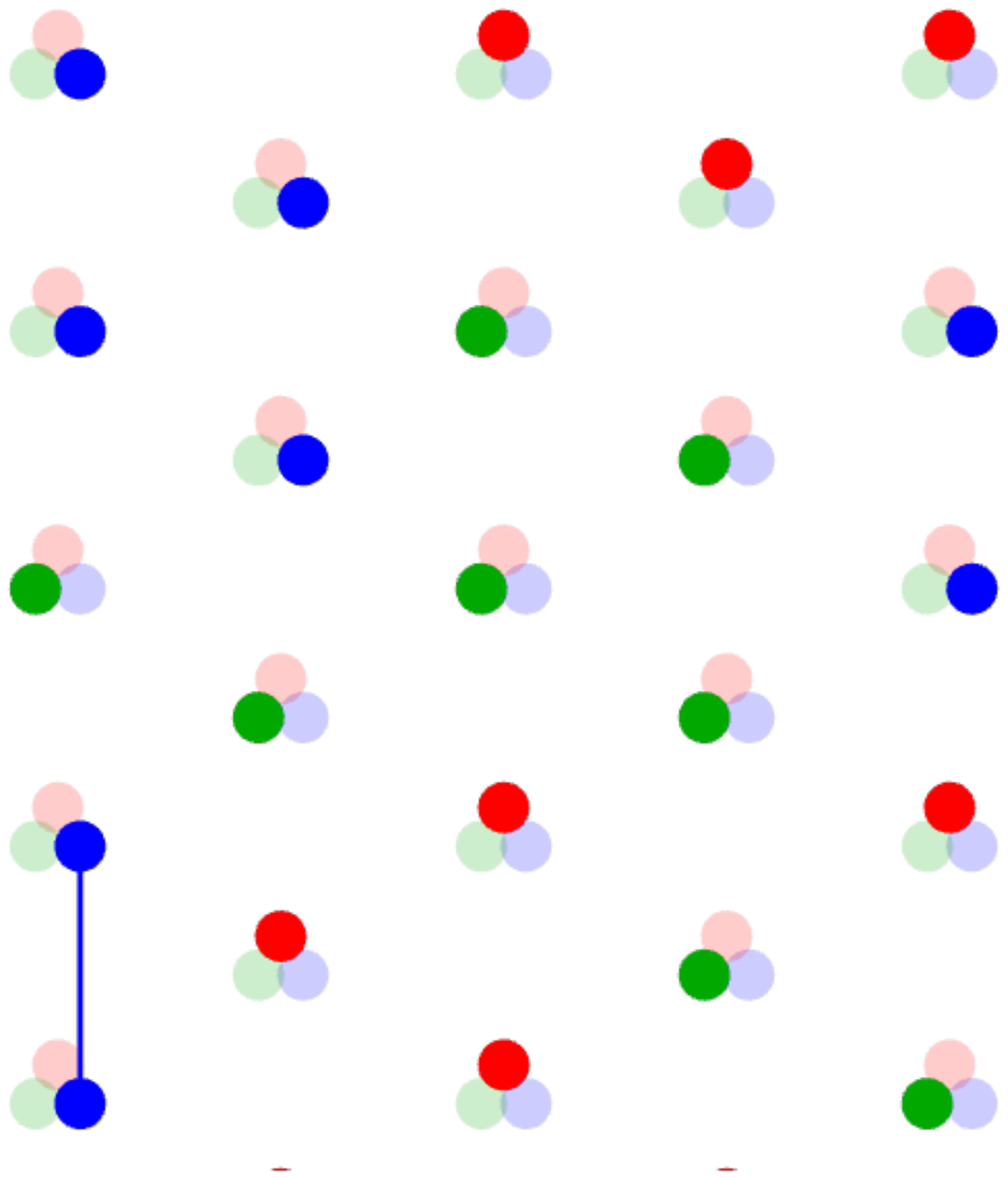

Step 3: consider strong-coupling effective Hamiltonian

(usual Hubbard→Heisenberg AF, but valley-selective — cf. $\eta_{\langle ij \rangle}$)

$$H_{\rm eff} = -\frac{4t^2}{U} \sum_{\langle ij \rangle} \mathcal{P}_{\nu=1} \left[\mathbf{S}_{i,\eta_{\langle ij \rangle}} \cdot \mathbf{S}_{j,\eta_{\langle ij \rangle}} + \frac{1}{4} n_{i\eta_{\langle ij \rangle}} n_{j,\eta_{\langle ij \rangle}} \right] \mathcal{P}_{\nu=1}$$

$\Rightarrow$ 1d AF valley-selective coupling that tracks valley anisotropy

[M.-R. Li, …, SAP, …, H. Hu 2508.10098]

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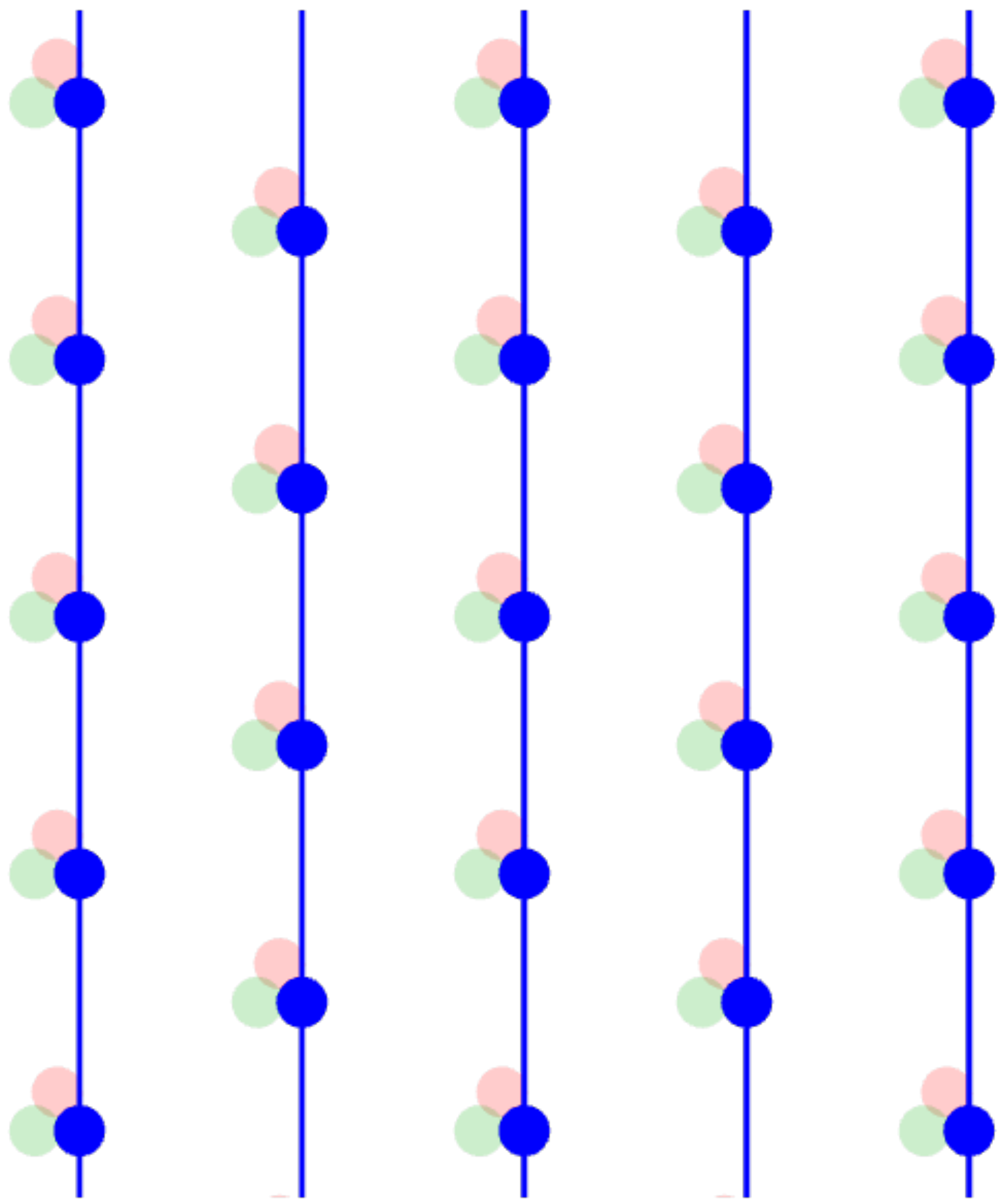

Step 4: determine optimum valley configuration

Since H_{eff} is valley-selective, if we change valley, spin chains "end"

$\Rightarrow$ calculate energy by linking "connected" sites

[M.-R. Li, …, SAP, …, H. Hu 2508.10098]

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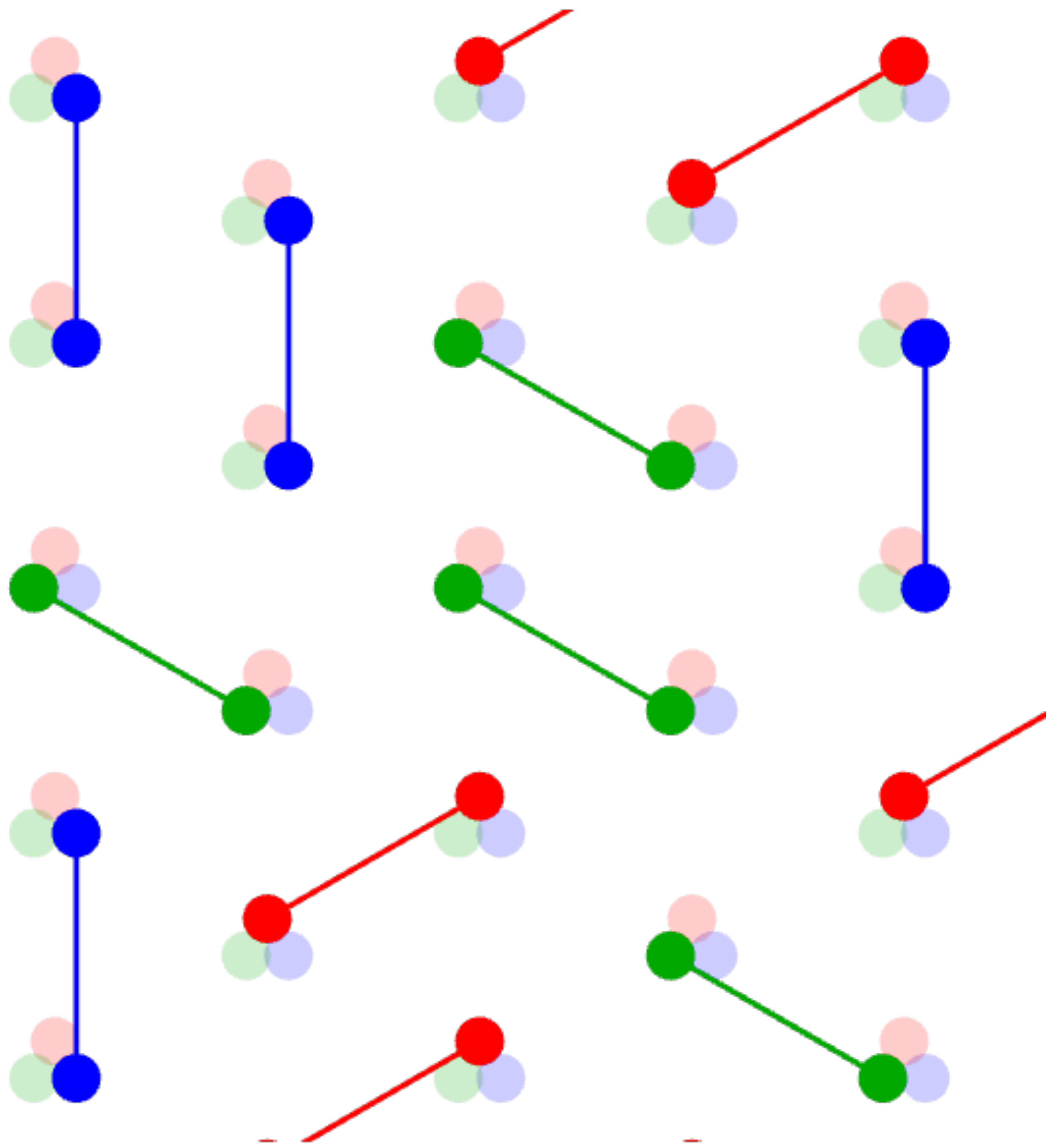

Result: "dimerize" since $\min_L \frac{E(L)}{L}$ is at $L = 2$ for Heisenberg AF

"classical dimer solid" with no-turn rule

extensive degeneracy ($S_{T=0} \approx 0.307 N k_B$)

(needs some work to compute!)

[M.-R. Li, …, SAP, …, H. Hu 2508.10098]

Strong-Coupling at Integer Fillings

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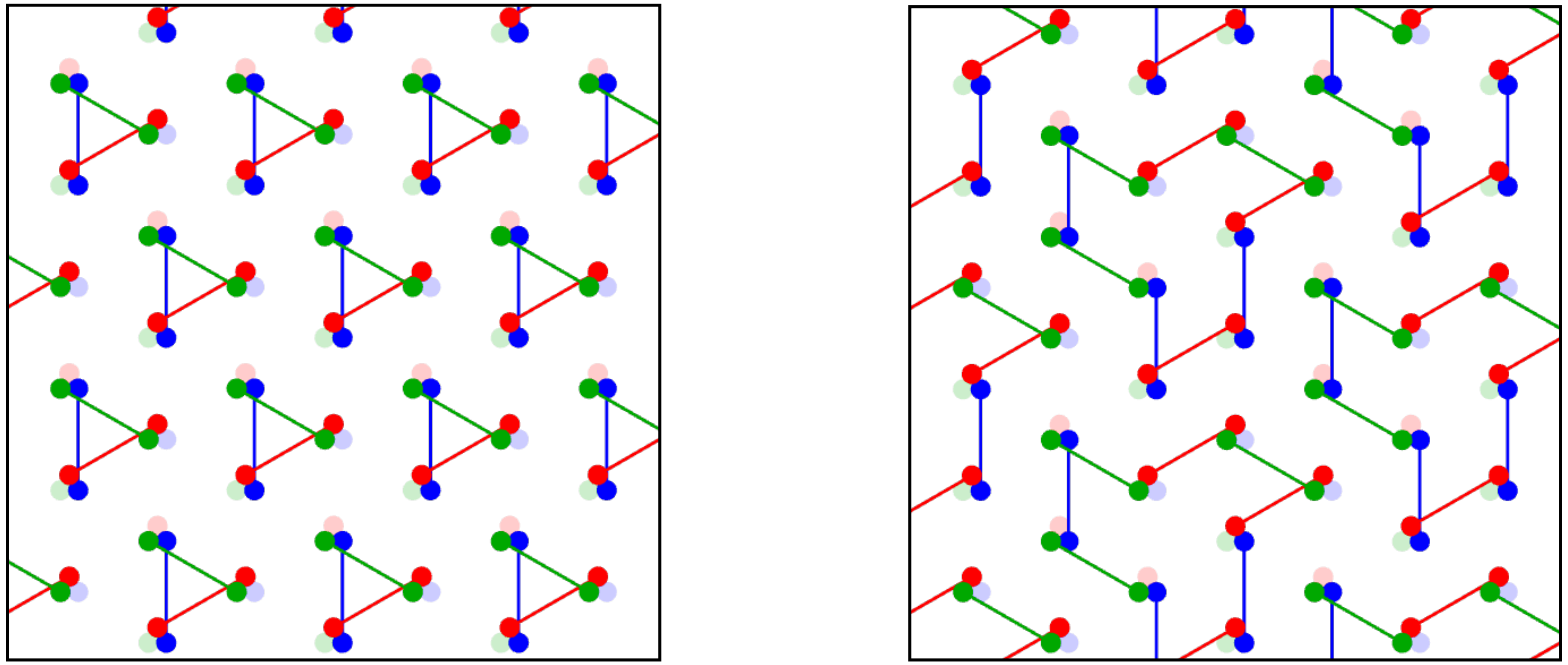
Exact results for $V = 0$ by mapping energetics to $\otimes$(spin chains of different lengths)

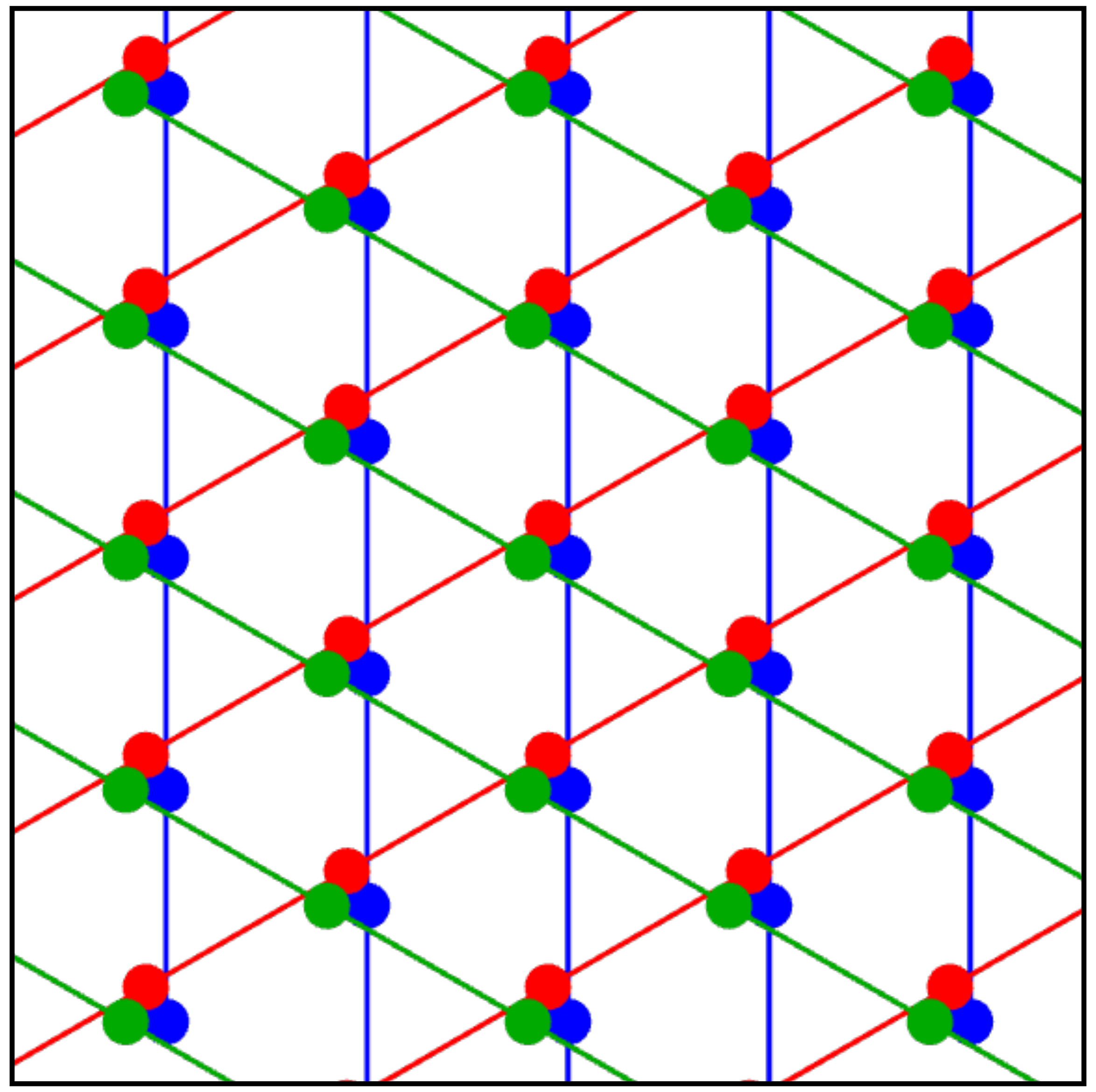
$\nu = 2$ case

similar logic to $\nu = 1$ but now get 2 distinct VBS states



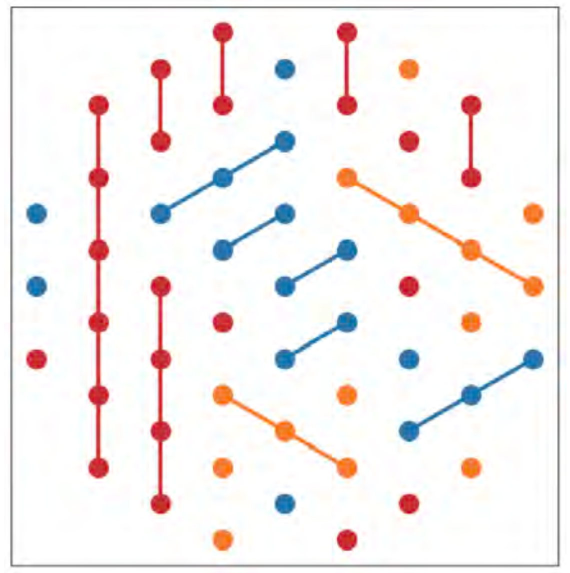
$\nu = 3$ case

just get 3 sets of Heisenberg chains



[M.-R. Li, …, SAP, …, H. Hu 2508.10098]

Strong-Coupling Model at Integer Fillings: Summary



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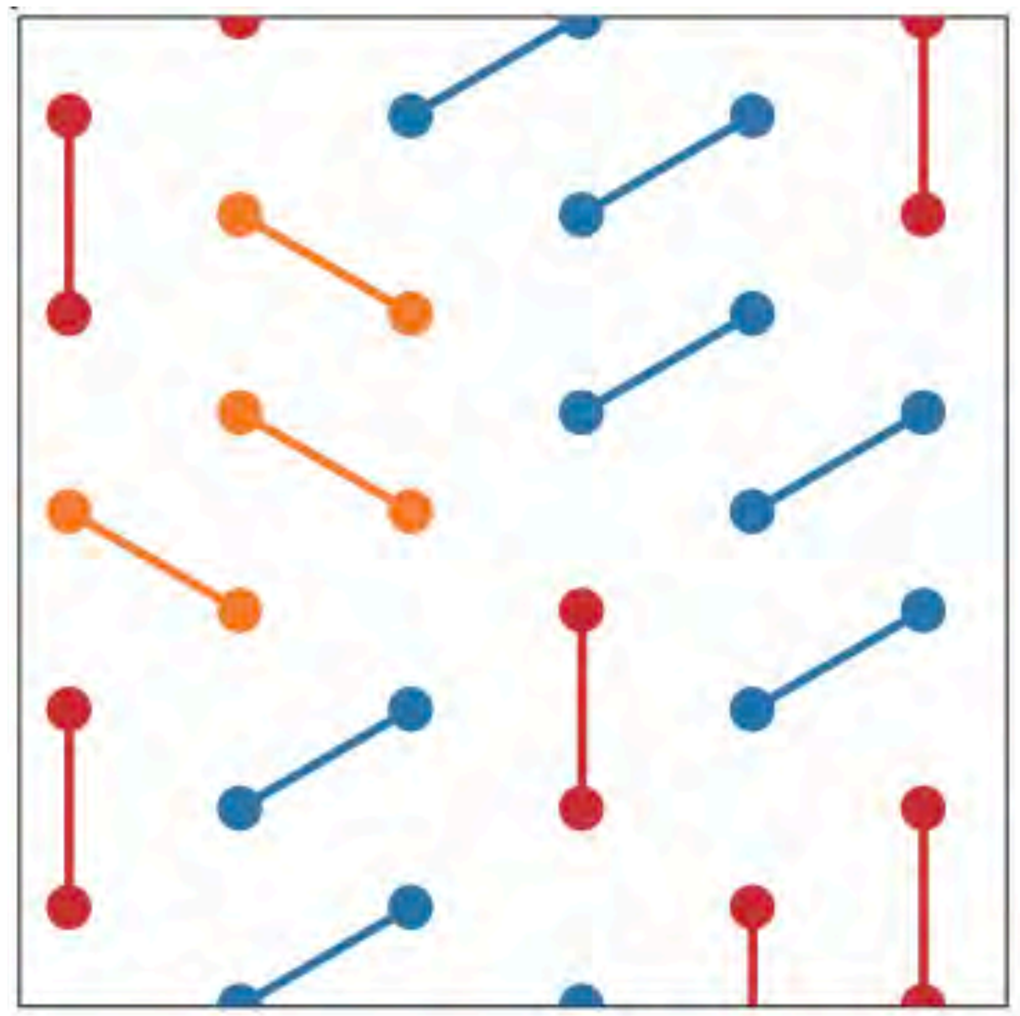
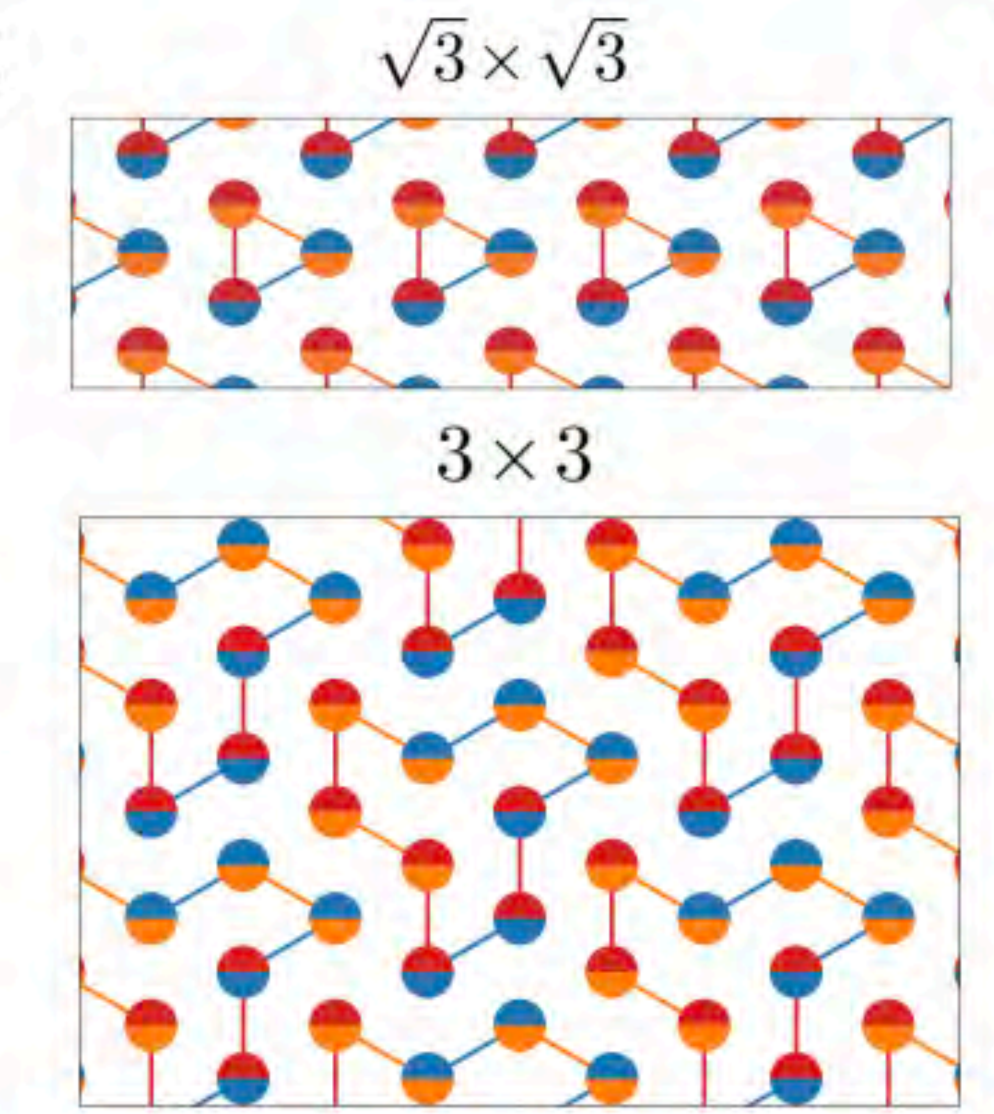
$\nu = 1$



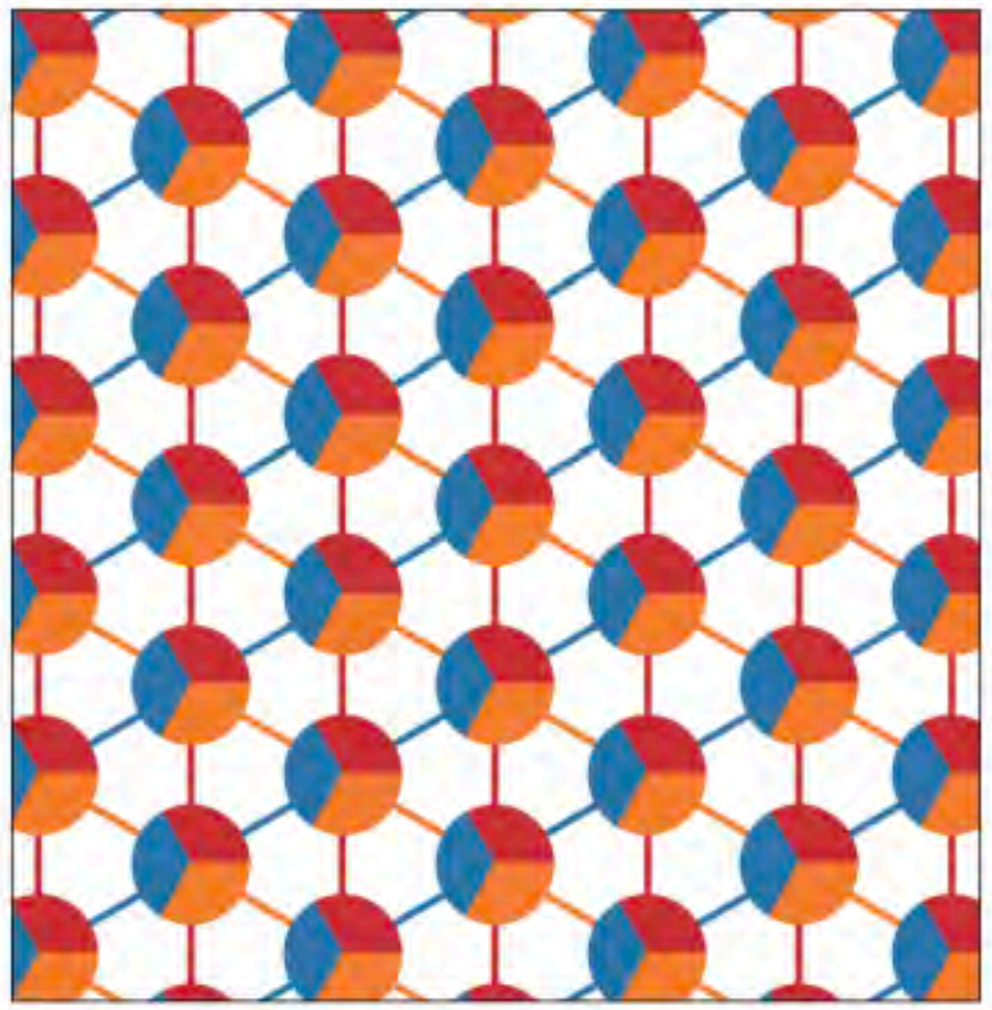
disordered classical dimer solid
w/ "forced turn" rule

$\nu = 2$



two types of
degnerate VBS

$\nu = 3$



stacked-chain-state
(quantum-disordered spins)

[M.-R. Li, …, SAP, …, H. Hu 2508.10098]

As is often the case, intermediate coupling is likely to be interesting

Can we do *controlled* calculations away from strong/weak coupling?
(rest of this talk)

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(rest of this talk)

Possibly useful pictures to keep in mind:

"crossed sliding Luttinger liquids"

[R. Mukhopadhyay, C.L. Kane, and T. Lubensky, *PRB* **63**, 081103 (2001); *PRB* **64**, 045120 (2001)]

multi-orbital Hubbard with anisotropic hopping (à la Kugel-Khomskii)

mixed-dimensional Hubbard model

[see e.g., A. Bohrdt et al, Nature Physics **18**, 651 (2022)]

Aside: How strong is "strong coupling"?

Extended Hubbard with $U, V \approx$ on-site Hubbard with $U^* \approx U + \frac{1}{2}\sum_{\substack{i\neq j\\ \sigma,\sigma'}} V_{ij}\frac{\partial_{U^*}\langle n_{i\sigma}n_{j\sigma'}\rangle^*}{\sum_l \partial_{U^*}\langle n_{l\uparrow}n_{l\downarrow}\rangle^*} \approx U - V$

[M. Schüler et al *PRL* **111**, 036601 (2013)]

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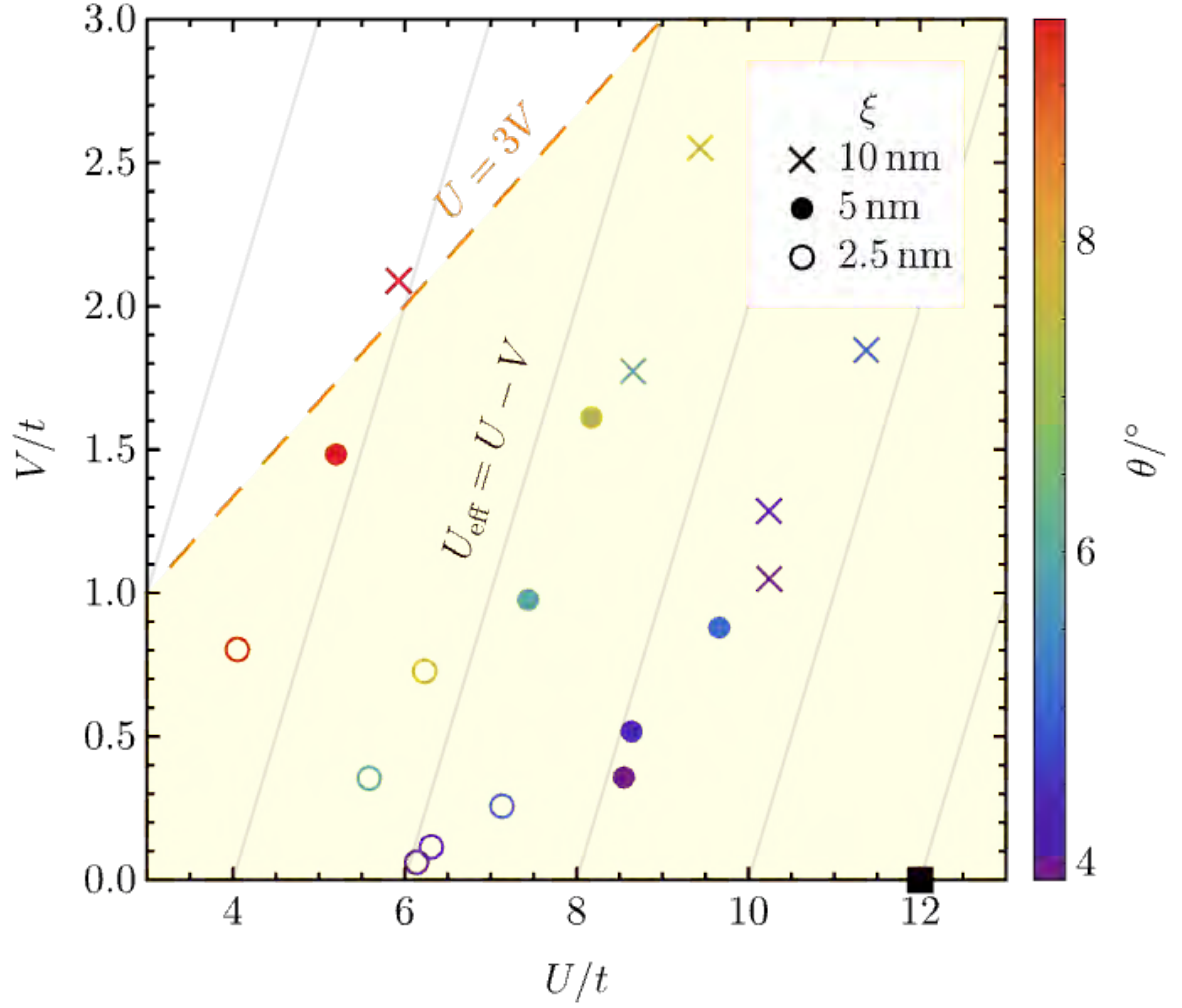

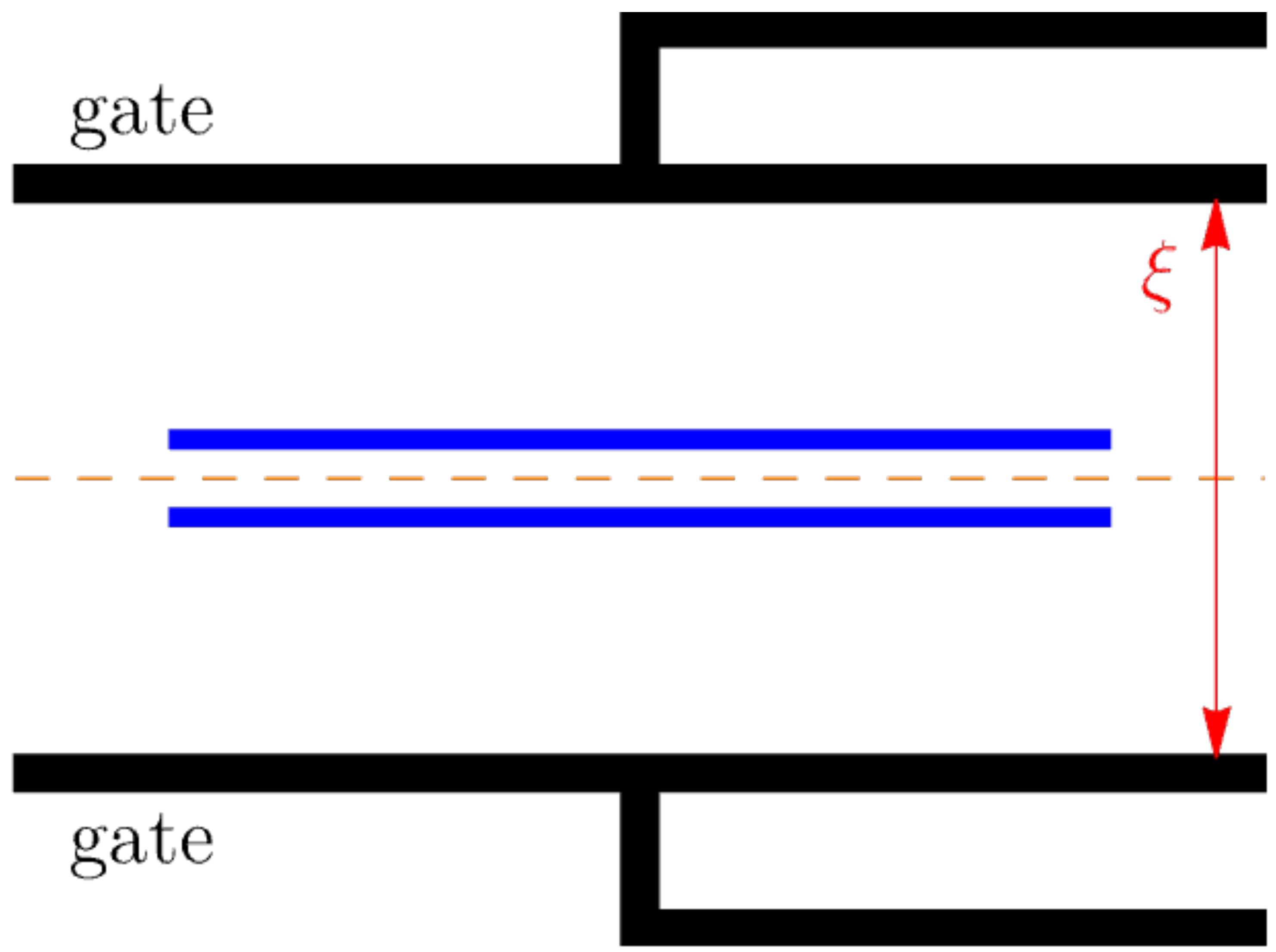

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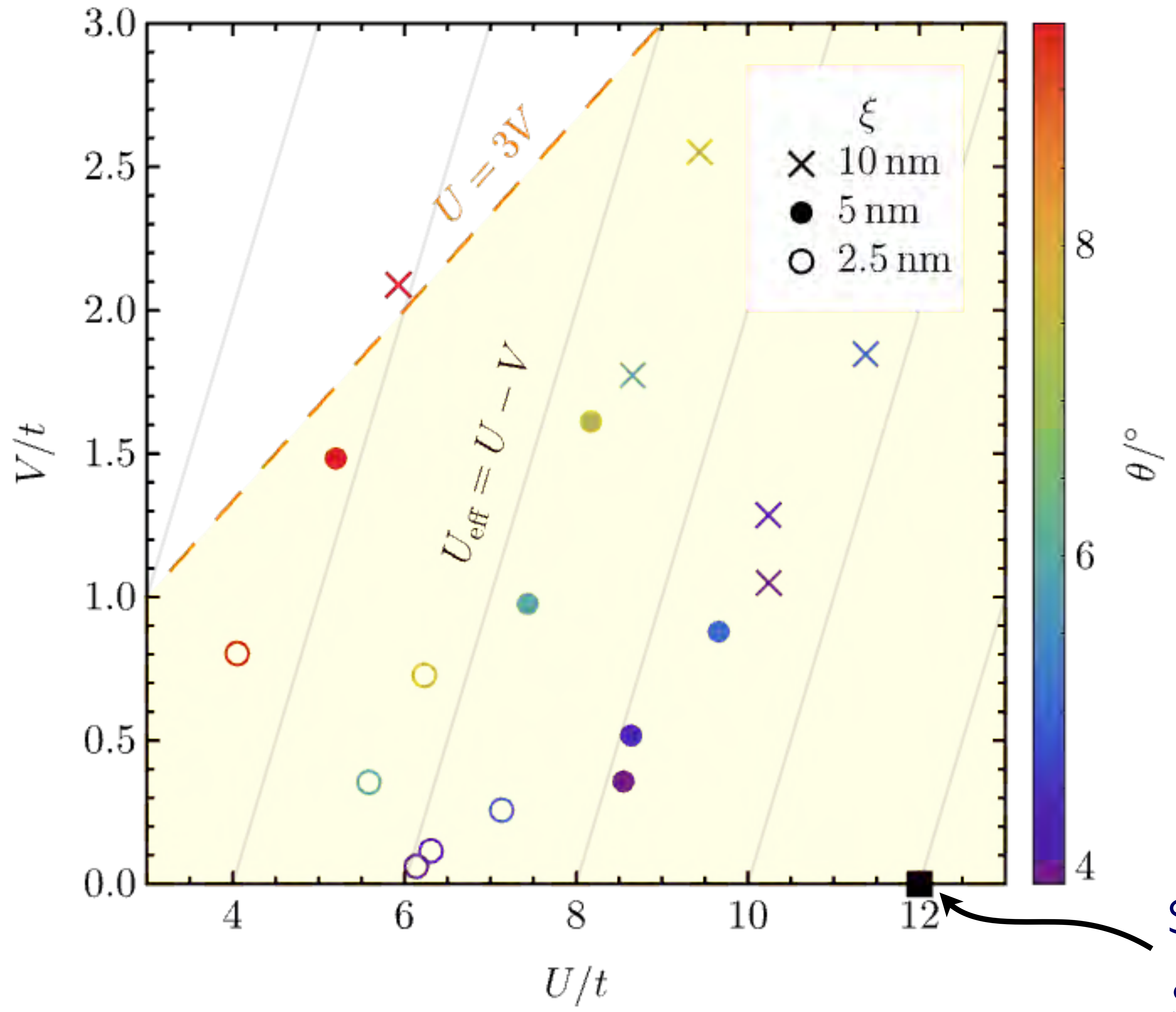
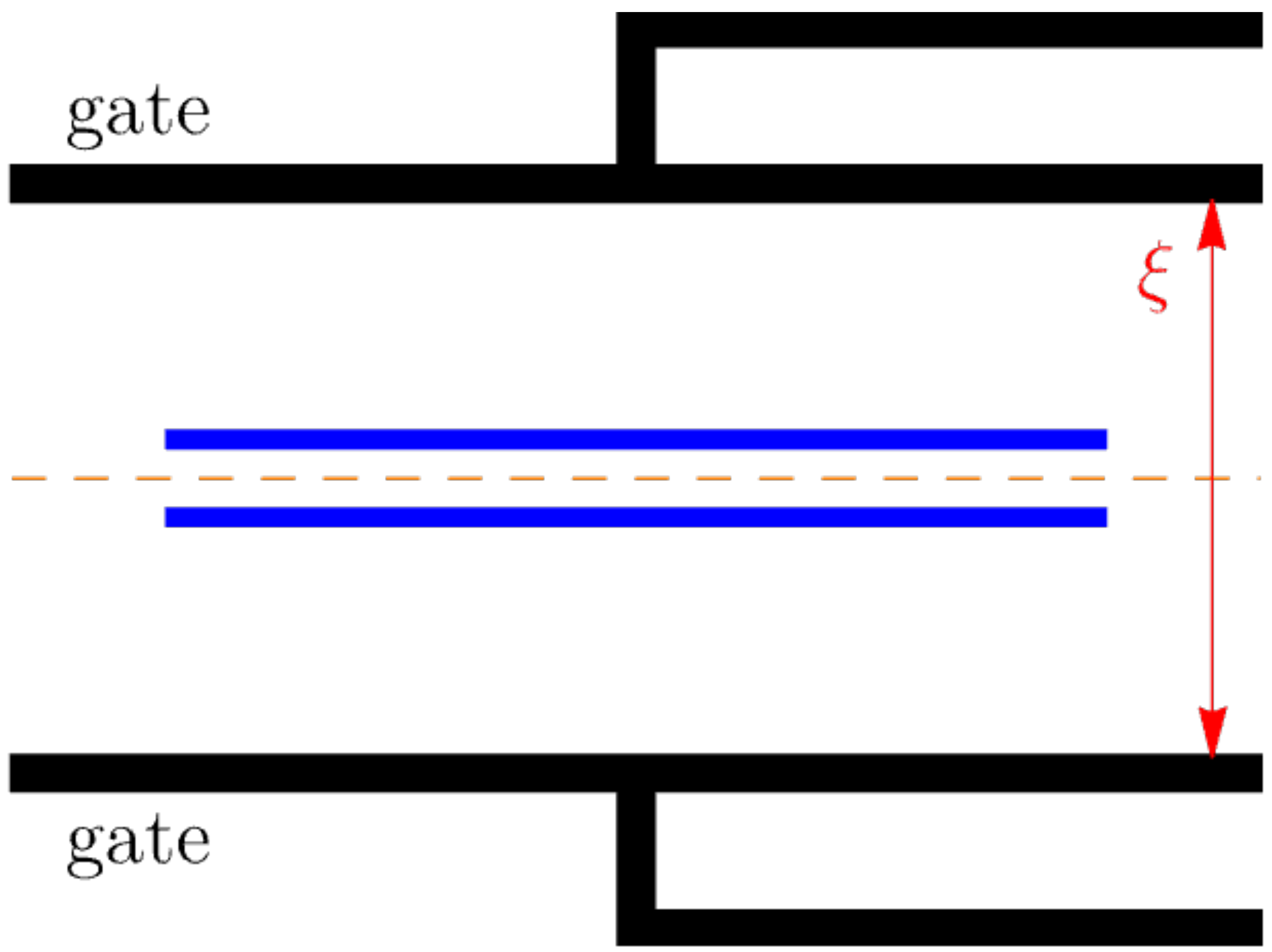
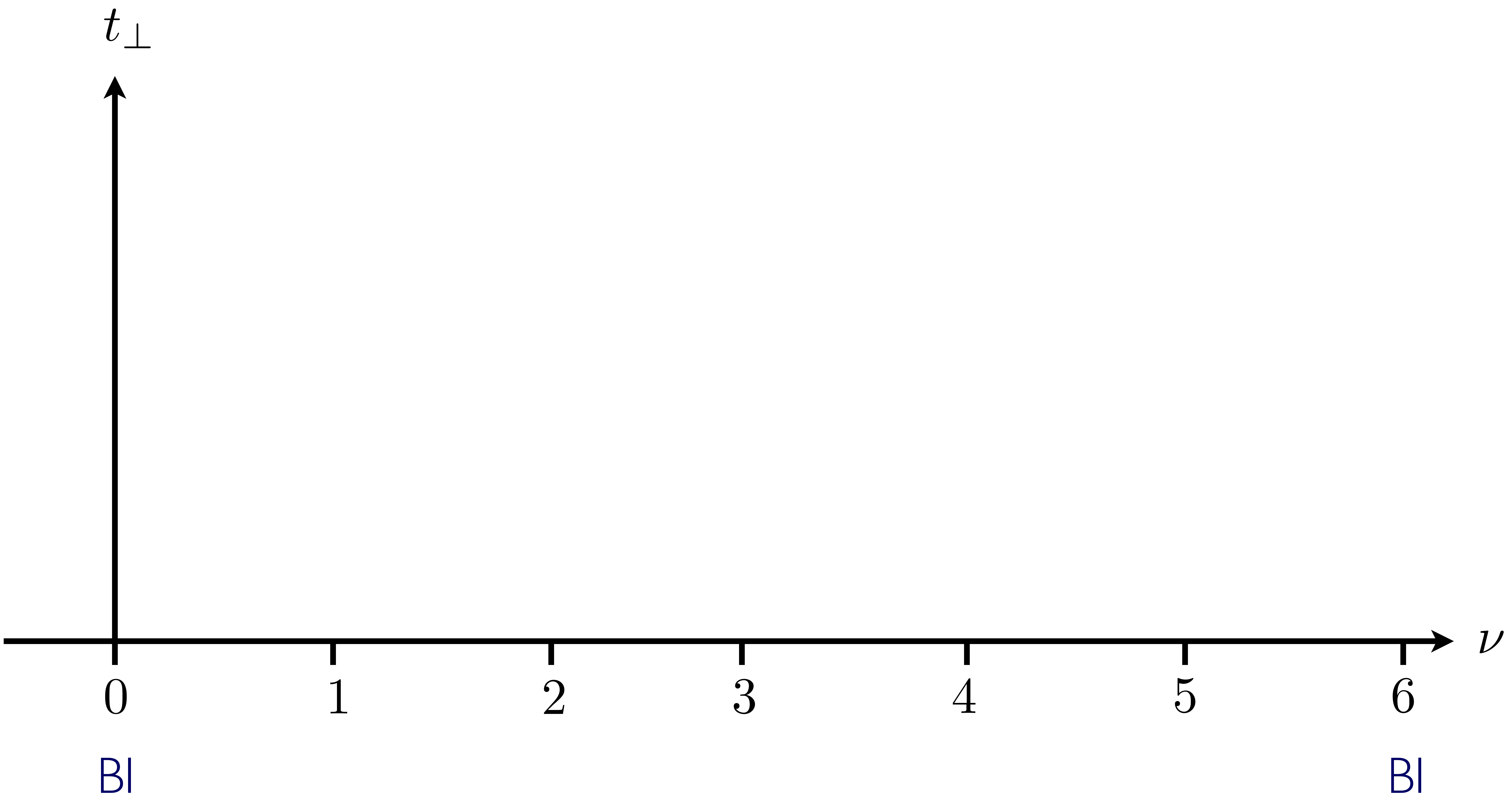


strong coupling seems to work



Controlled Calculations at Intermediate Coupling?



*some minor constraints on U, V, α

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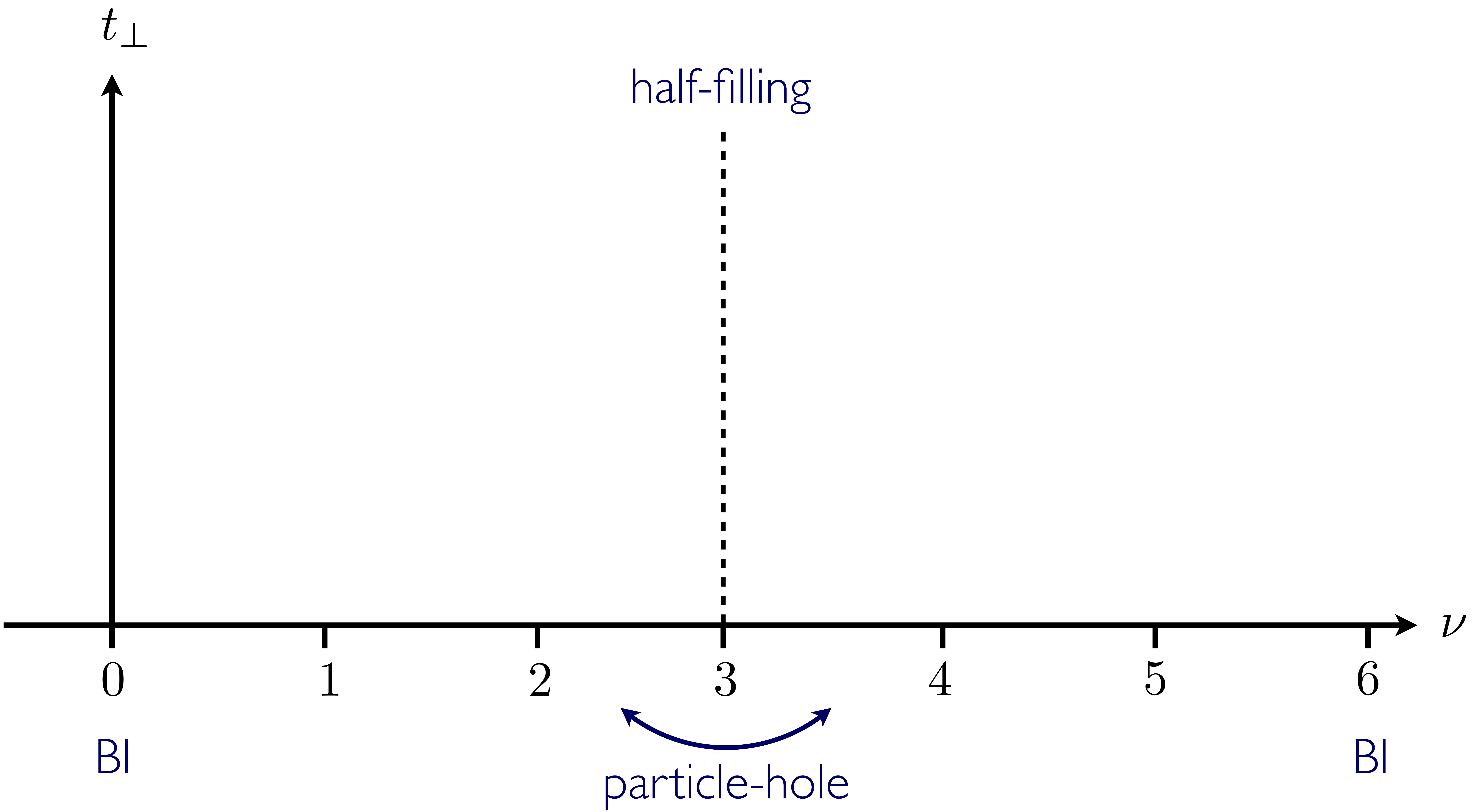

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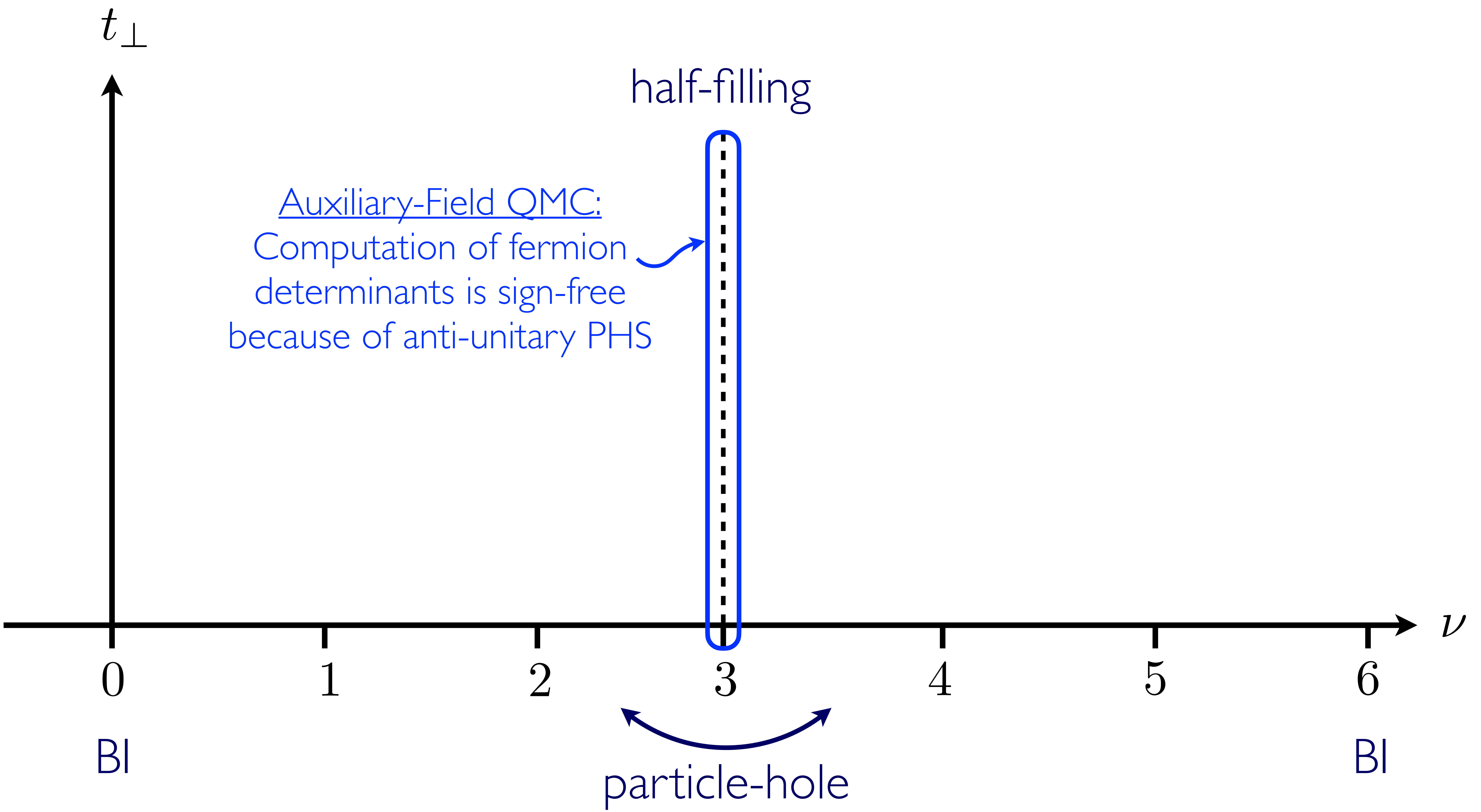

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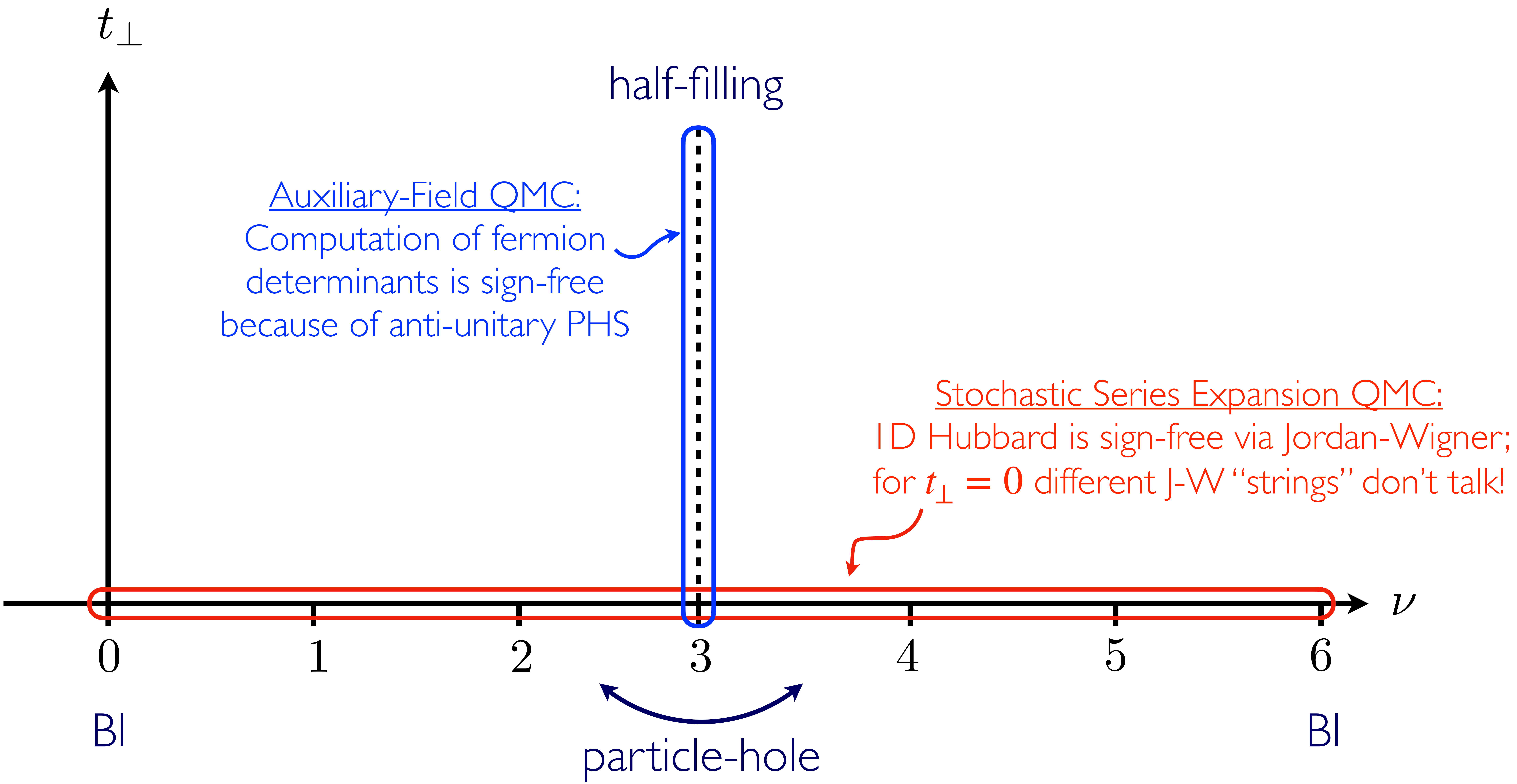

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Controlled Calculations at Intermediate Coupling?

Today:

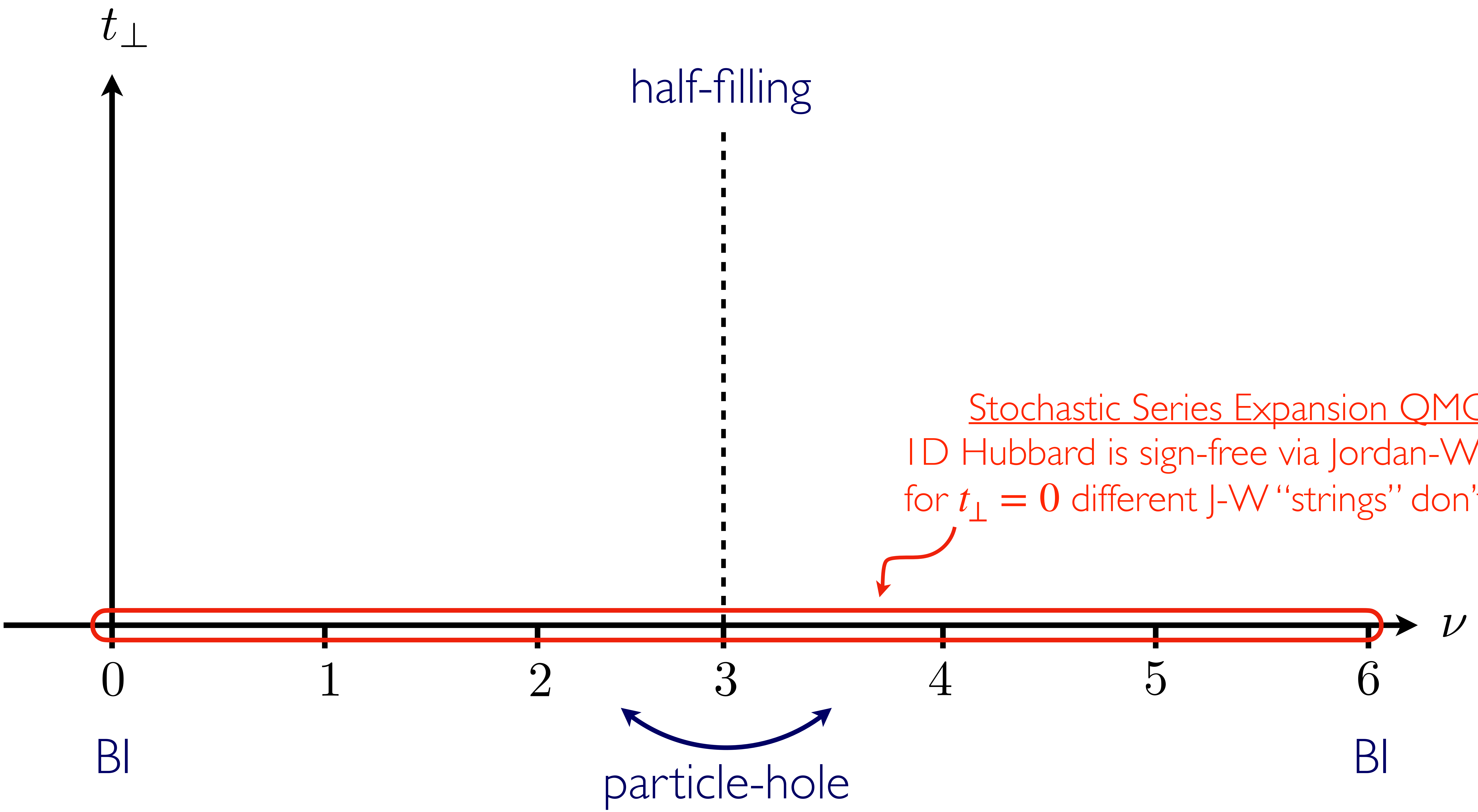
First results* from Monte Carlo studies along these two axes

I. Doping the "Sliding Point"

II. "Going 2D" at Half-Filling

*Disclaimer: this is work in progress, so final story might be more refined

I. Doping the "Sliding Point"



Stochastic Series Expansion QMC:
1D Hubbard is sign-free via Jordan-Wigner;
for $t_\perp = 0$ different J-W "strings" don't talk!

*some minor constraints on U, V, α

Method: Stochastic Series Expansion w/ Directed-Loop Updates

P. Sengupta, A.W. Sandvik, D.K. Campbell, Phys. Rev. B **65**, 155113 (2002)

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$$Z = \mathrm{Tr}[e^{-\beta H}] = \sum_{\alpha} \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \langle \alpha | (-H)^n | \alpha \rangle$$

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Sequence of operators ("strings")
(together w/ initial state)

$$S_L = [a_0, b_0], [a_1, b_1], \ldots, [a_{L-1}, b_{L-1}]$$

P. Sengupta, A.W. Sandvik, D.K. Campbell, Phys. Rev. B **65**, 155113 (2002)

Method: Stochastic Series Expansion w/ Directed-Loop Updates

"simple enough" states
(e.g. Fock basis)

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Sequence of operators ("strings")
(together w/ initial state)

$$S_L = [a_0, b_0], [a_1, b_1], \ldots, [a_{L-1}, b_{L-1}]$$

P. Sengupta, A.W. Sandvik, D.K. Campbell, Phys. Rev. B **65**, 155113 (2002)

Method: Stochastic Series Expansion w/ Directed-Loop Updates

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e.g. 1D Hubbard:

$$H_{0,b} = -\mathbf{1} \qquad H_{1,b} = -\frac{U}{2}(N_b^2 + N_{b+1}^2) + VN_b N_{b+1}$$

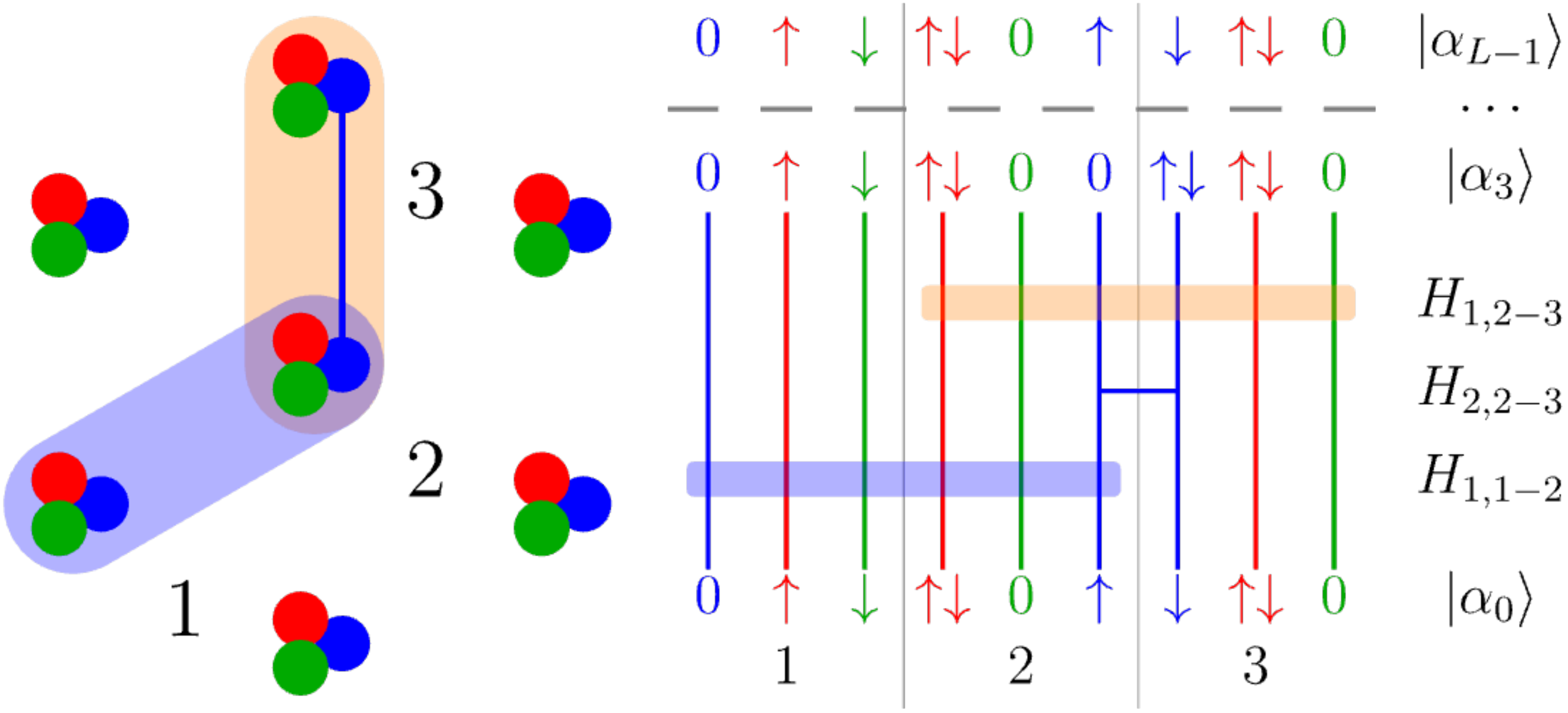
$$H_{2,b} = -t(c^\dagger_{b+1,\uparrow} c_{b,\uparrow} + \mathrm{h.c.}) \qquad H_{3,b} = -t(c^\dagger_{b+1,\downarrow} c_{b,\downarrow} + \mathrm{h.c.})$$

P. Sengupta, A.W. Sandvik, D.K. Campbell, Phys. Rev. B **65**, 155113 (2002)

SSE for *M*-Point Moiré

When $t_\perp = 0$, fermion worldlines on different chains never cross + each chain is sign-free for SSE

Can do large-scale SSE for up to 12×12 systems (needs good basis choice* + clever updates, $O(\beta L^2)$ scaling)



*previous SSE at $U = \infty$ in different basis [S. Xu, Y. Li, C. Wu *PRX* **5**, 021032 (2015)] doesn't generalize; need valley-flip updates

Observables in SSE

Inverse compressibility: $\tilde{\chi}_c^{-1} = \frac{1}{t}\frac{d\mu}{d\nu}$

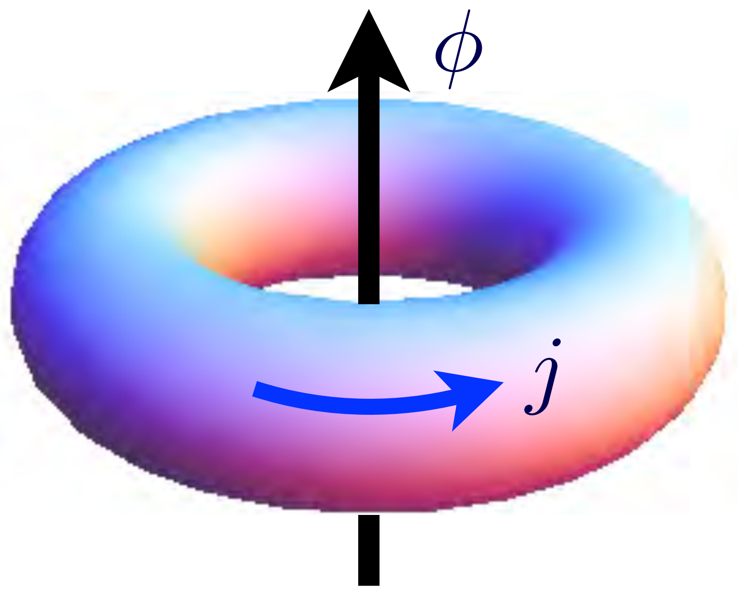
Measures energy cost for adding/removing charges

Peaks at insulating states, small in metallic states

SSE Estimator: $\tilde{\chi}_c = \frac{\beta t}{L^2}\left(\langle \hat{N}^2\rangle - \langle \hat{N}\rangle^2\right)$

Charge stiffness: $\tilde{\rho}_c = \frac{\partial^2 E(\phi)}{\partial \phi^2}$

[W. Kohn, Phys. Rev. **133**, A171 (1964)]



Intuitively, measures "flux response" of torus: $\boldsymbol{\phi}$ tries to drive current

Large in metal, vanishes in Mott insulator

SSE Estimator: use "winding number" of loops

— relate to ⟨difference⟩ of "right"/"left" KE terms **+ sum over wires**

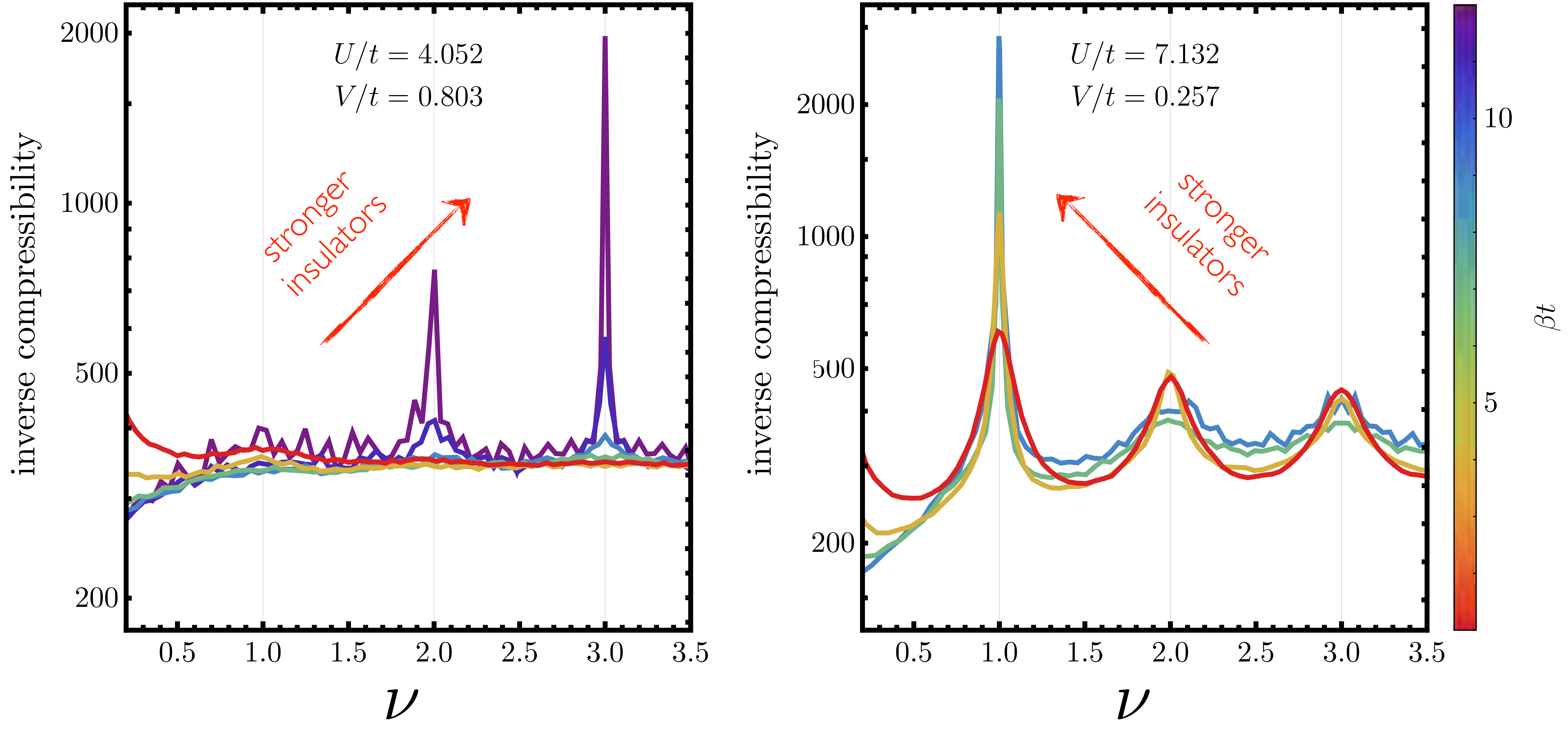
$$\rho_c = \frac{1}{\beta L^2}\sum_{\substack{\eta_1,\eta_2\\ s_1,s_2}} \left(C_{3z}^{\eta_1}\delta\mathbf{R}\cdot\hat{\mathbf{x}}\right)\left(C_{3z}^{\eta_2}\delta\mathbf{R}\cdot\hat{\mathbf{x}}\right)\langle\left(N^+_{\eta_1,s_1} - N^-_{\eta_1,s_1}\right)\left(N^+_{\eta_2,s_2} - N^-_{\eta_2,s_2}\right)\rangle$$

P. Sengupta, A.W. Sandvik, D.K. Campbell, Phys. Rev. B **65**, 155113 (2002)

*in "real" 2D, distinction between charge/superfluid stiffness is subtle, but we are in quasi-1d limit

"Hierarchy Reversal"

Trend in strength of $\nu = 1,2,3$ correlated insulators is reversed between weak and strong coupling*



* SSE data shown here is for 6×6 systems; 12×12 also shows this but weak-coupling states shift to lower T

Bosonization & Weak-Coupling Hierarchy

Standard bosonization with charge and spin modes per species, per wire:

$$\psi^j_{\eta,\sigma,R/L}(x_\eta) \sim \frac{\kappa_{\eta\sigma}}{\sqrt{2\pi a}} e^{\pm i k_{F,\eta} x_\eta} e^{i(\theta^j_{\mu,\sigma}(x_\eta) \pm \phi^j_{\mu,\sigma}(x_\eta))} \qquad \phi^j_{\eta,c} = \frac{\phi^j_{\eta,\uparrow} + \phi^j_{\eta,\downarrow}}{\sqrt{2}} \qquad \phi^j_{\eta,s} = \frac{\phi^j_{\eta,\uparrow} - \phi^j_{\eta,\downarrow}}{\sqrt{2}}$$

2D coarse-graining ($j \to$ continuous): $H \sim \sum_{\eta,a=c,s} \frac{v_{\eta,a}}{2\pi} \int d^2\mathbf{r} \left[K_\eta (\nabla_\eta \theta_{\eta,a})^2 + \frac{1}{K_\eta} (\nabla_\eta \phi_{\eta,a})^2 \right] + \begin{pmatrix} \text{umklapp} \\ \text{cosines} \end{pmatrix}$

1d gradients along $\mathbf{e}_\eta$

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Focus on 2 specific umklapps from rewriting $\sum_i n_i^2$:

Intra-chain $2k_F$: $\mathcal{O}_\eta \sim \cos(2\phi_{\eta,c})$ — more relevant, commensurate when $2k_F\nu \in 6\mathbb{Z}$

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(survives 2D sum b/c $\Delta\mathbf{Q}_{2D} = 0$)

Roughly: $\nu = 3$ ~ strong "intrachain Mott state" via $\mathcal{O}_\eta$, whereas $\nu = 1,2$ ~ weaker "inter-chain Mott" via $\mathcal{O}_\triangle$

Strong-Coupling Hierarchy & Pomeranchuk Physics

Trend tracks the number of "fluctuation directions" that destabilize insulator: $\binom{6}{3} > \binom{6}{2} > \binom{6}{1}$

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[S. Florens, A. Georges, Phys. Rev. B **70**, 035114 (2004)]

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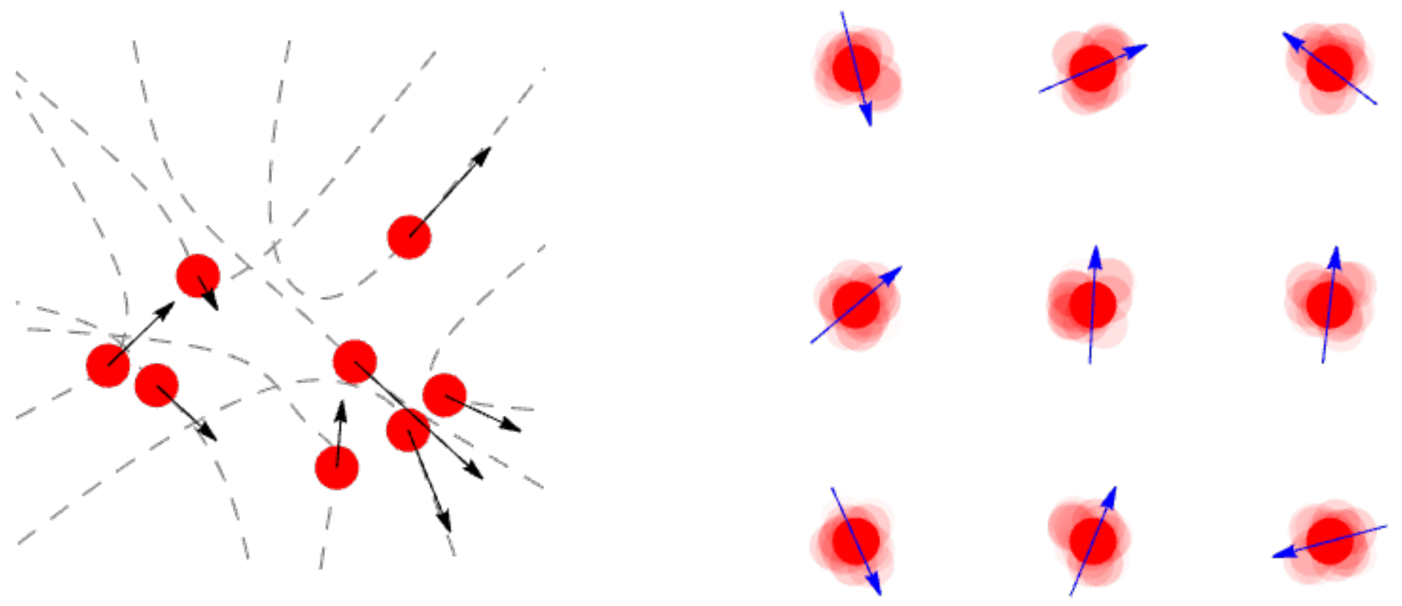
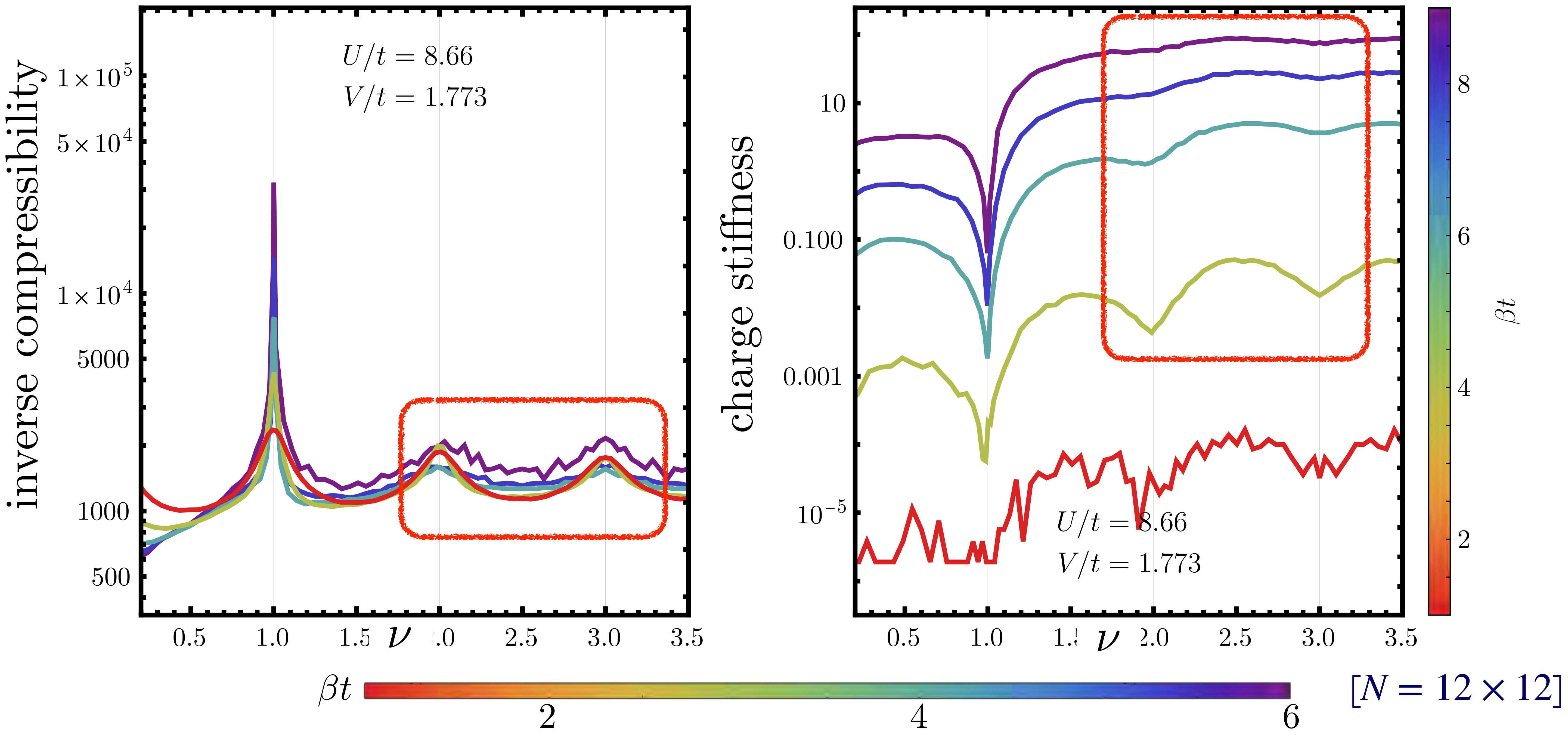
Also gives rise to "Pomeranchuk effect": For $U_{\text{Mott}}(1) < U < U_{\text{Mott}}(2)$, $\nu = 2{,}3$ are **not** insulators as $T \to 0$

Increasing T *stabilizes* Mott insulators at these fillings b/c of high entropy!

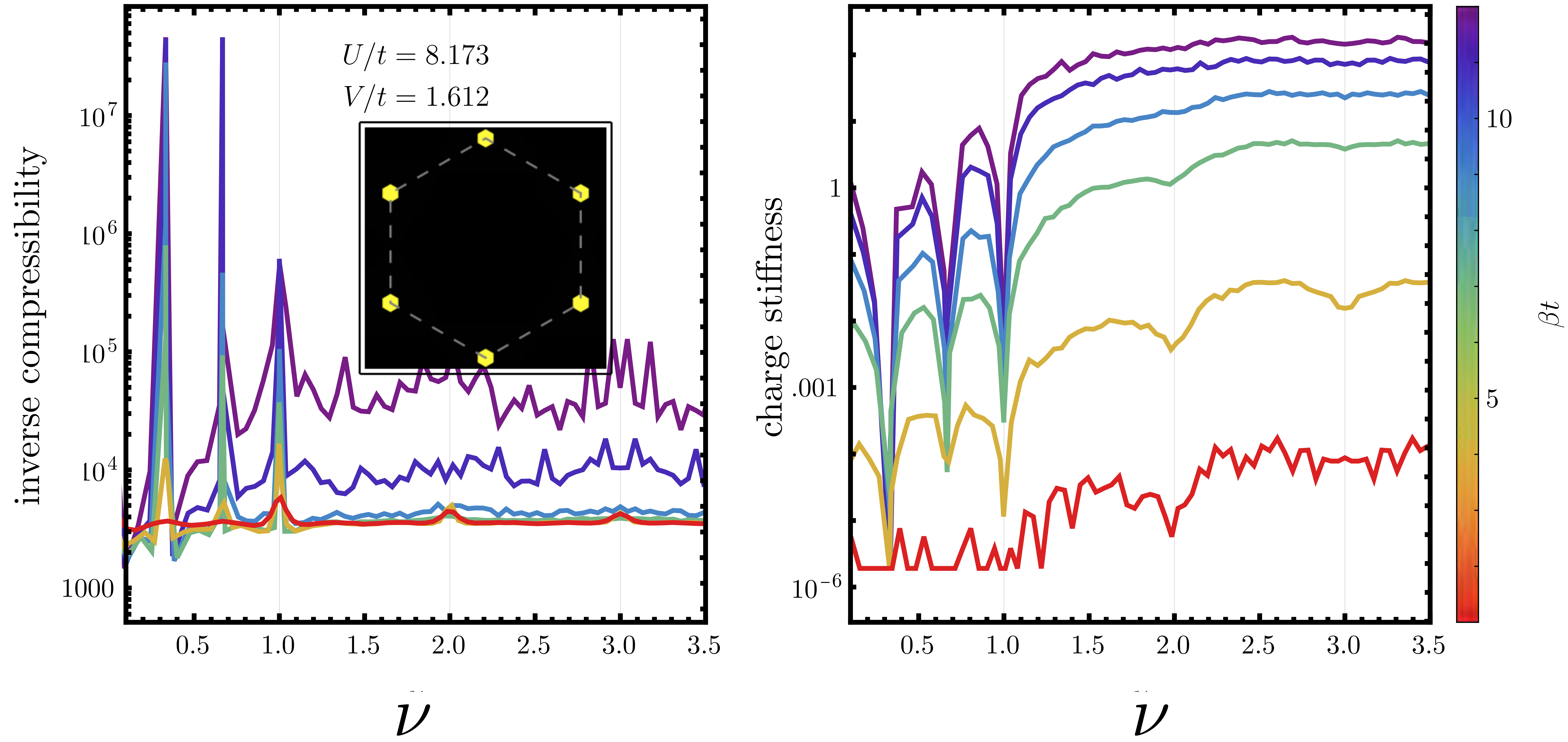


[cf. TBG: A. Rozen, et al., *Nature* **592**, 214 (2021); Y. Saito, et al., *Nature* **592**, 220 (2021)]



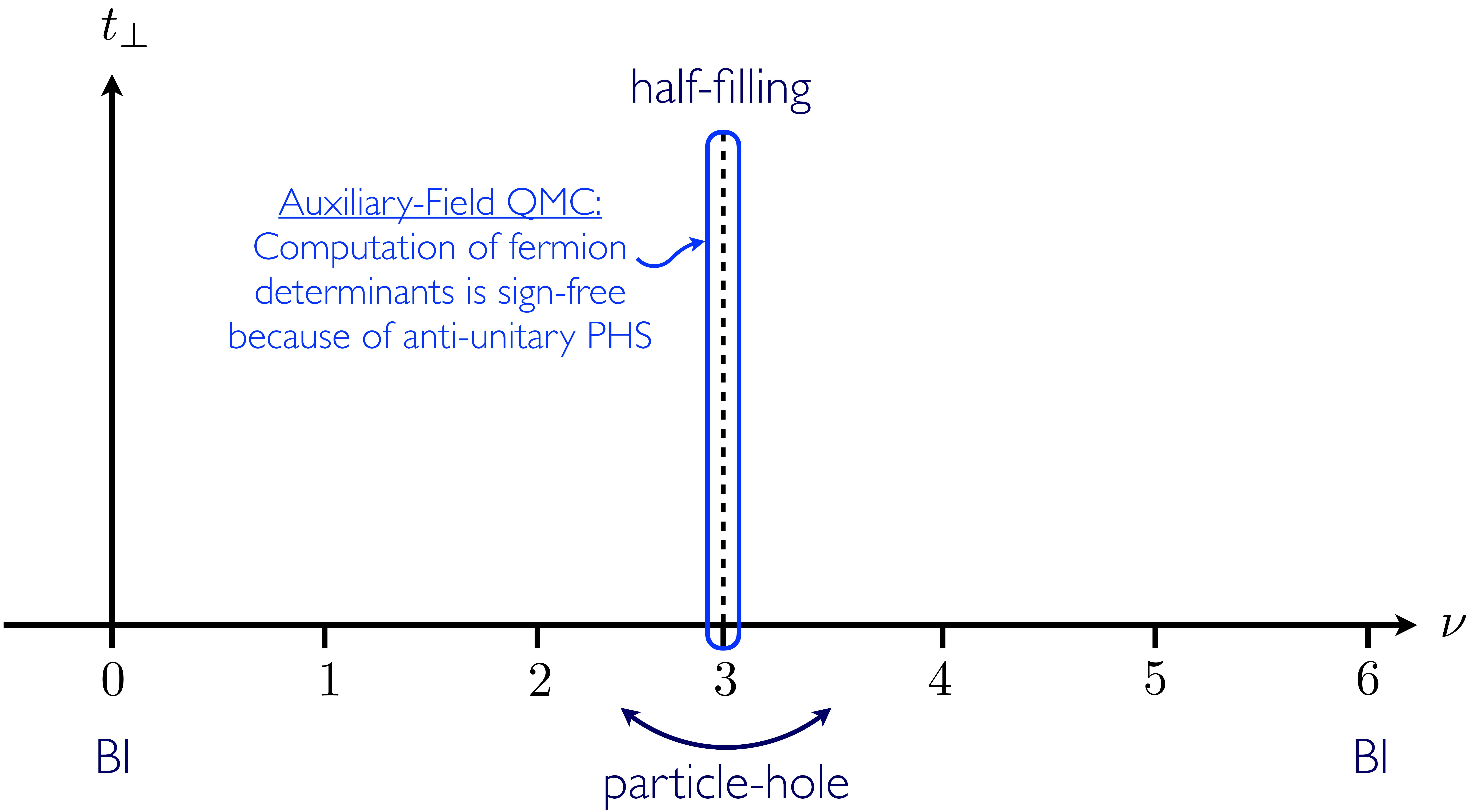
Teaser: Wigner-Mott Phases

w/ moderate V: inverse compressibility peaks at **fractional** filling $\nu \in (0,1)$ with vanishing "charge stiffness"



*SSE for 12×12 systems

II. "Going 2D" at Half-Filling



*some minor constraints on U, V, α

Method: Auxiliary-Field QMC

Basic idea: Hubbard-Stratonovich: interacting fermions → free fermion problem $\mathscr{H}_{\mathscr{C}}$ + auxiliary field $\mathscr{C}$

importance-sample auxiliary field configurations: $Z = \mathrm{Tr}[e^{-\beta H}] = \sum_{\mathscr{C}} e^{-S_0(\mathscr{C})} \times \det \mathscr{H}_{\mathscr{C}}$

if antiunitary PHS present *and* acts trivially on $\mathscr{C}$: "sign free" ($\det \mathscr{H}_{\mathscr{C}} \sim \prod_{\lambda} \lambda\lambda^* > 0$)

imaginary-time fermion Green's functions: Wick's theorem + sampling (complexity $O(\beta L^6)$)

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$$\frac{U}{2}\sum_{\bullet} \hat{n}_i^2 + V \sum_{\bullet\!-\!\bullet} \hat{n}_i \hat{n}_j = \frac{U-3V}{2} \sum_{\bullet} \hat{n}_i^2 + \frac{V}{4} \sum_{\triangle} (\hat{n}_i + \hat{n}_j + \hat{n}_k)^2$$

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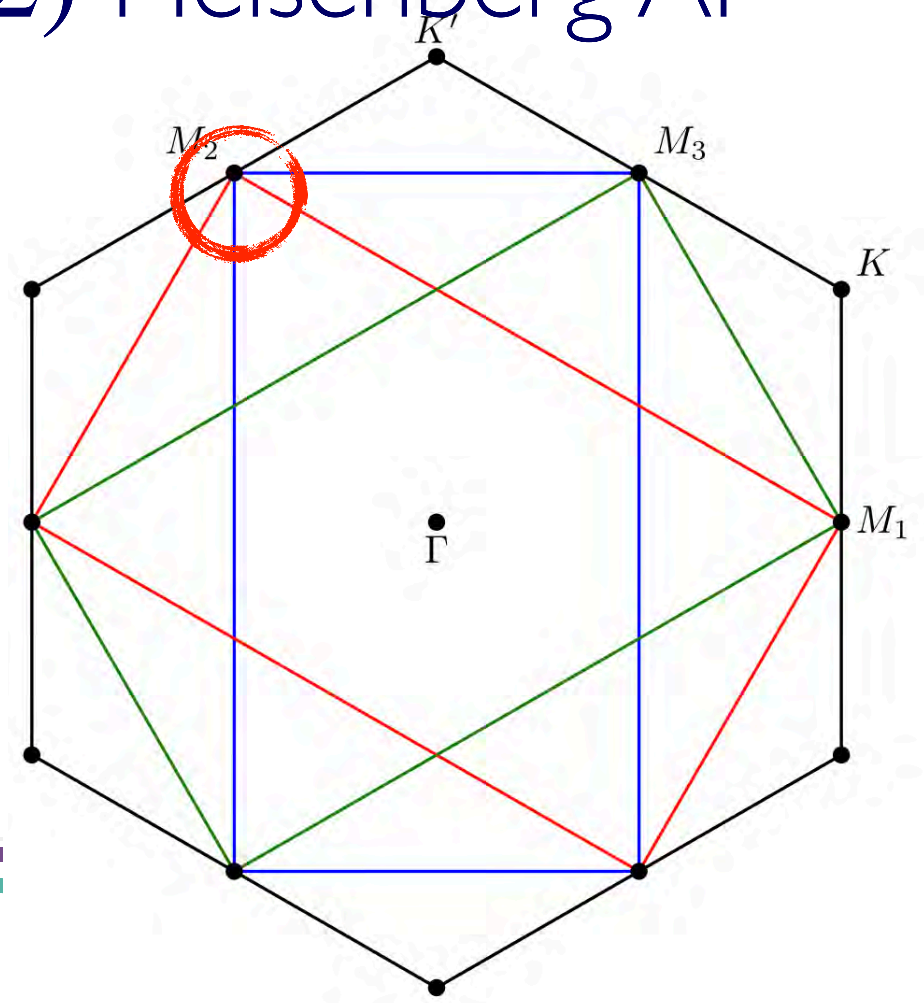
Check PHS condition: sign free at half-filling for $\alpha \in [0,1]$ if $\dfrac{V}{U} \leq \dfrac{2\alpha+1}{9}$

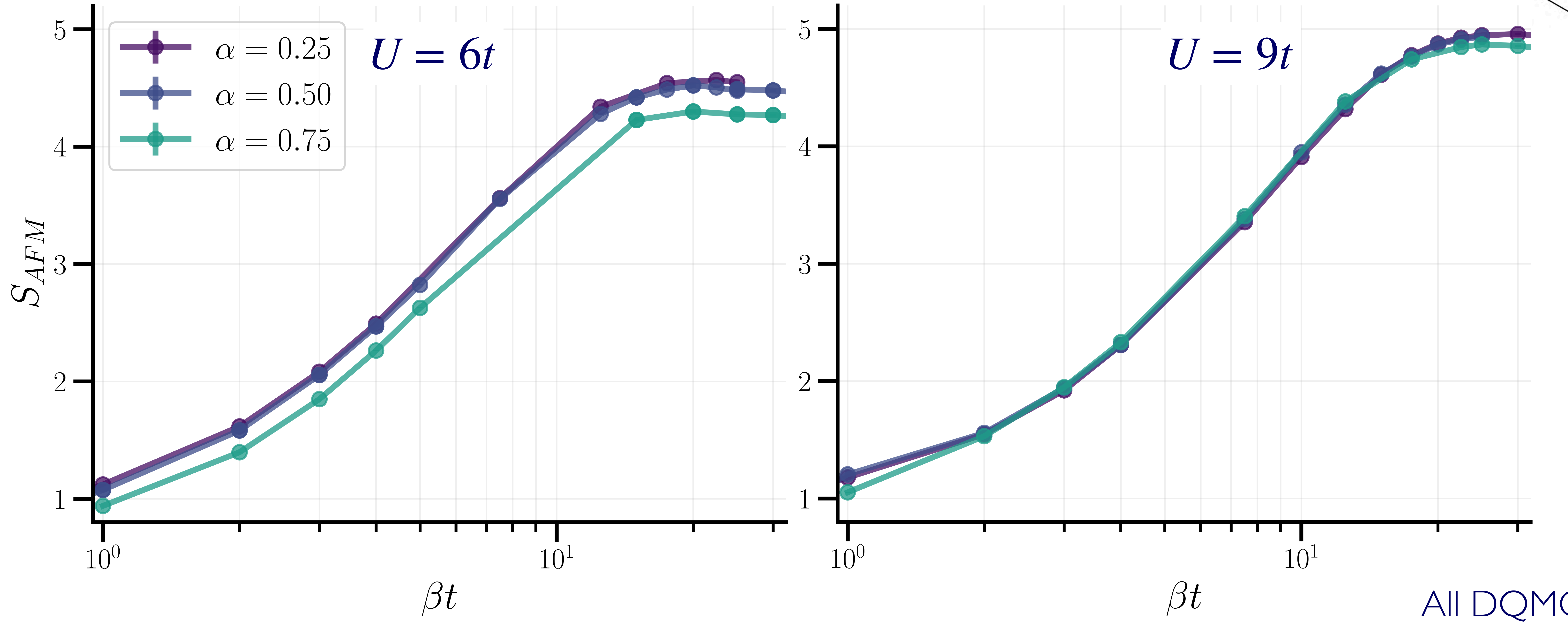
"Standard" Antiferromagnetism for Anisotropic Case ($\alpha \neq 1$)

$t_\perp \neq 0$: two decoupled rectangular lattices in each valley leading to 6 copies of usual $SU(2)$ Heisenberg AF



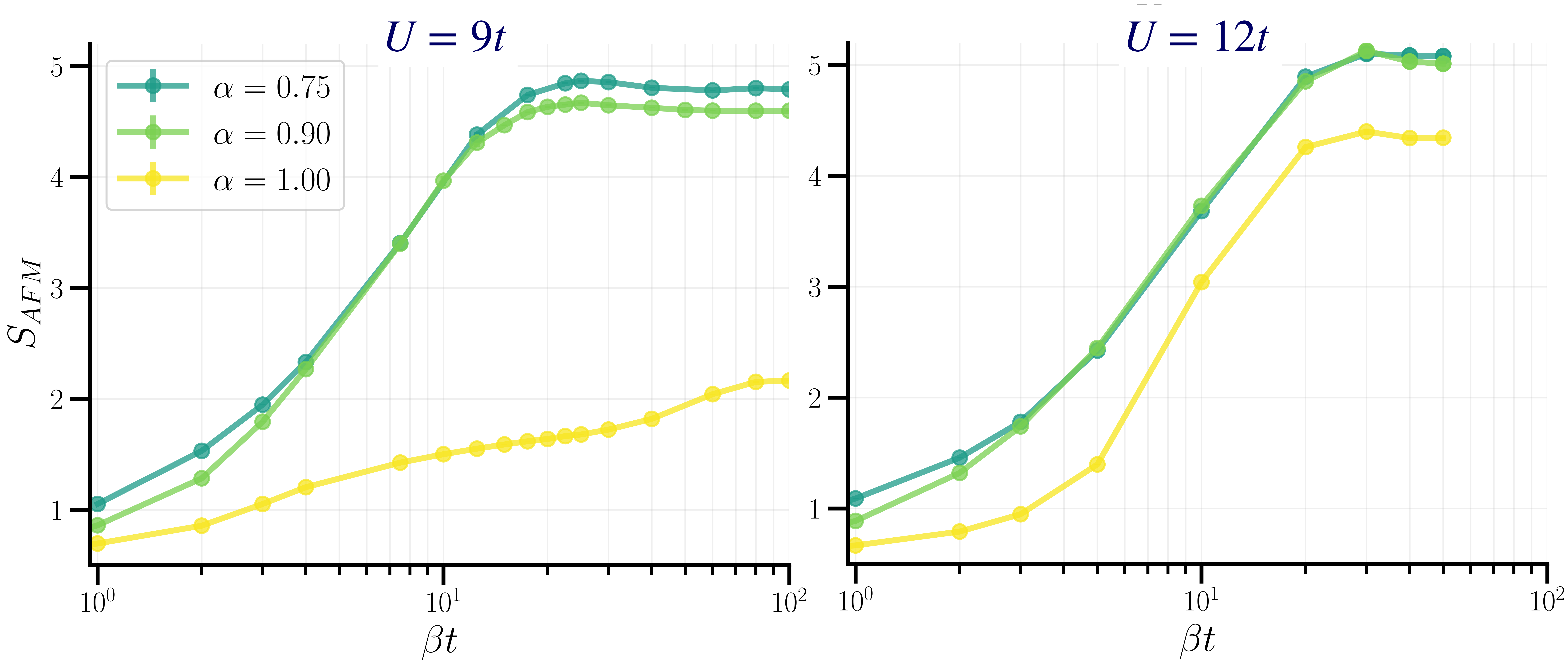
Néel order in each valley $\eta \Rightarrow$ AF peak at *rectangular* BZ corners = triangular *M*-points

Clear saturation of $S_{AFM} = \frac{1}{3} \sum_\eta \langle \hat{\mathbf{S}}^{(\eta)}_{\mathbf{Q}_\eta} \cdot \hat{\mathbf{S}}^{(\eta)}_{-\mathbf{Q}_\eta} \rangle$ as $T \to 0$



All DQMC data for $N = 12 \times 12$

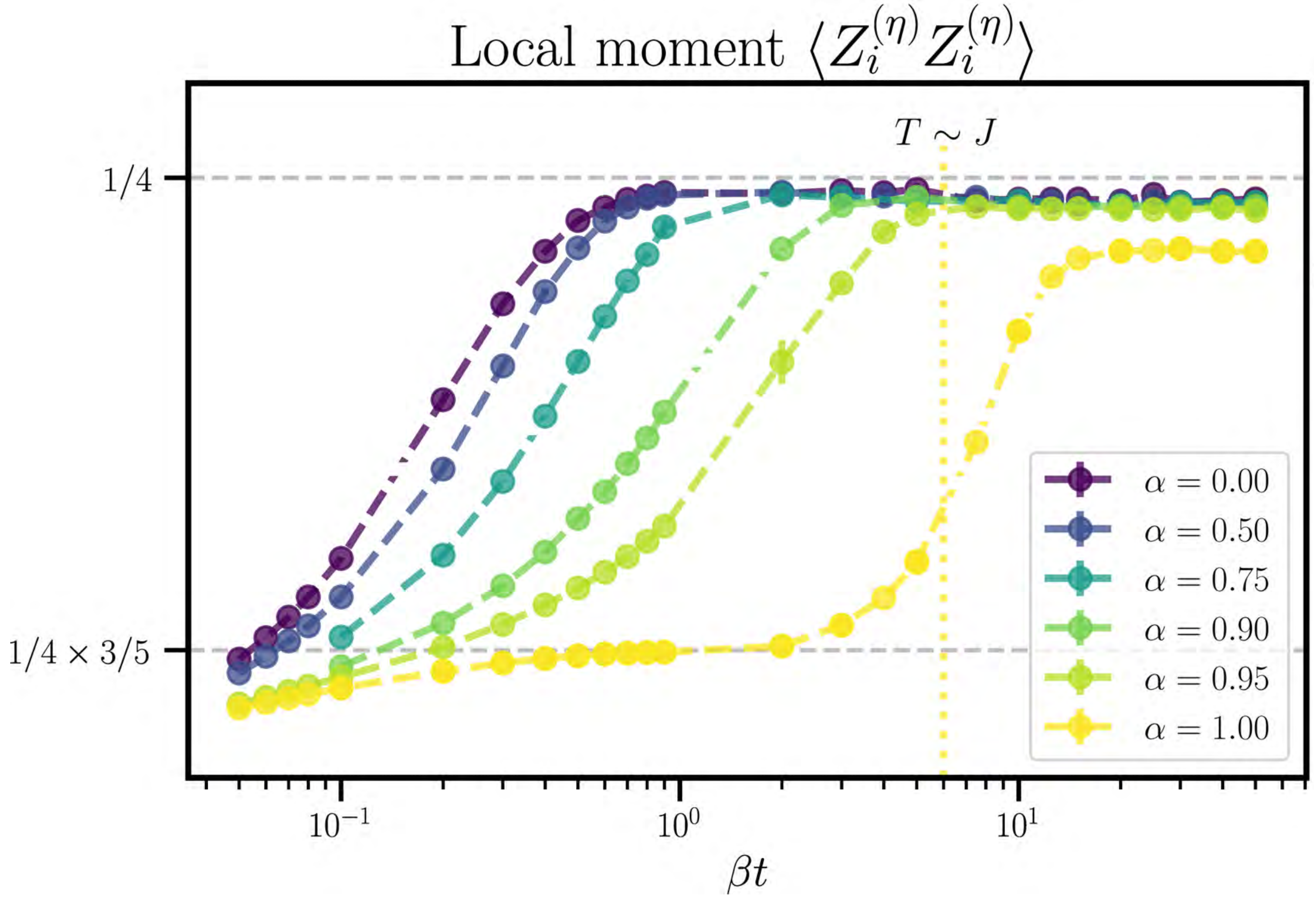
$\alpha \to 1$: Suppression of AF Order

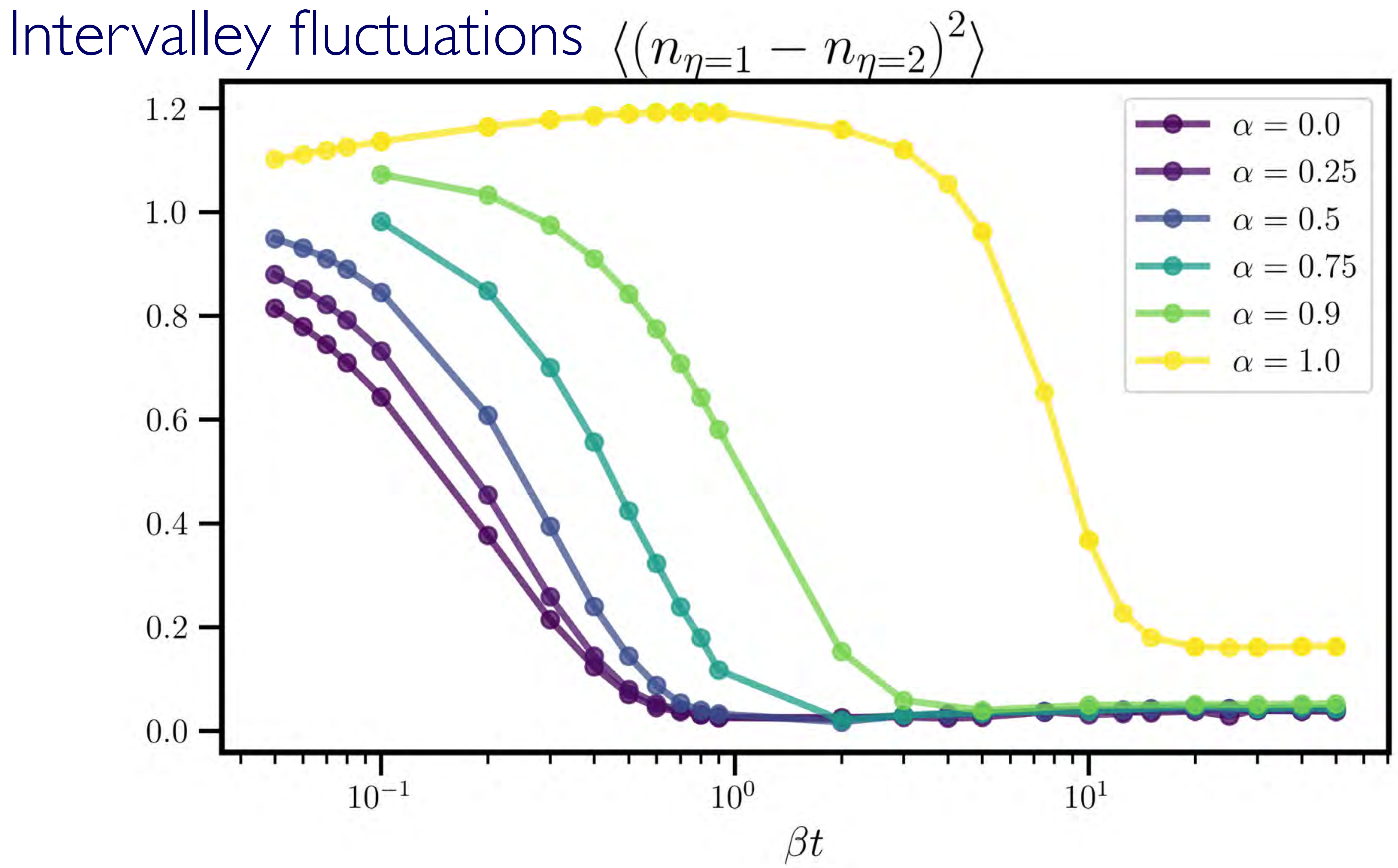


As $\alpha \to 1$, AF order only saturates at much larger U/t — likely consequence of $U(6)$ on-site degeneracy

Apparent finite-size effects for $\alpha \to 1$ even for $\beta t \gg 1$ ~ metal survives to very low T even at strong coupling?

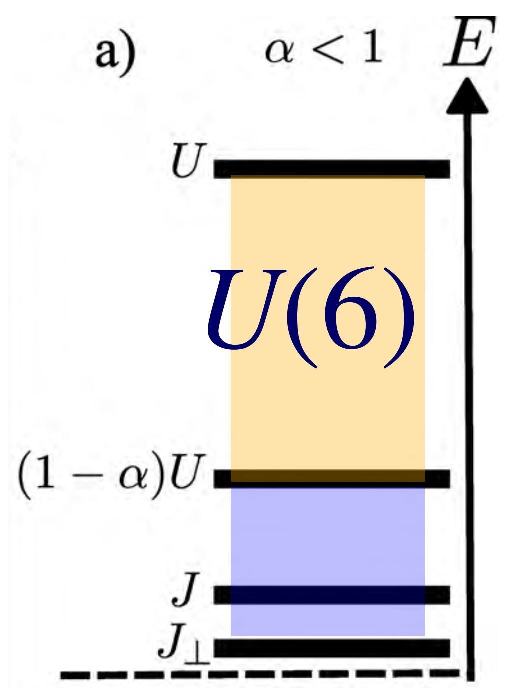
"Local Moment formation" and $U(6)$



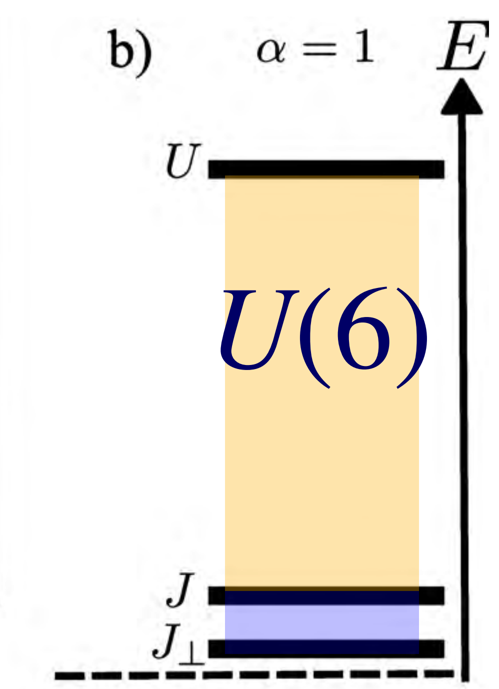


Can rationalize based on difference in the scale of SU(6) breaking

Anisotropic case:
$U(6)$broken at scale U

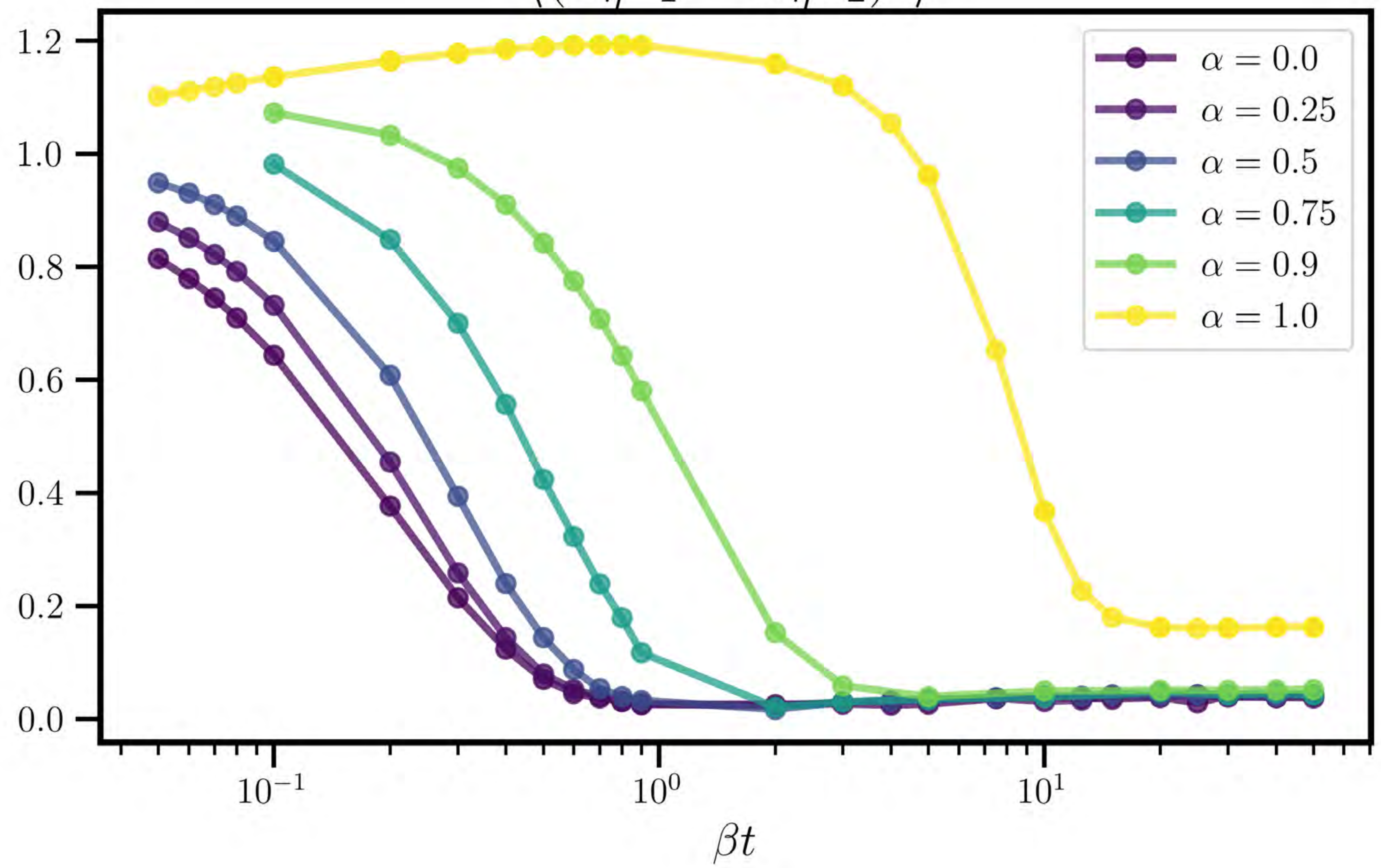


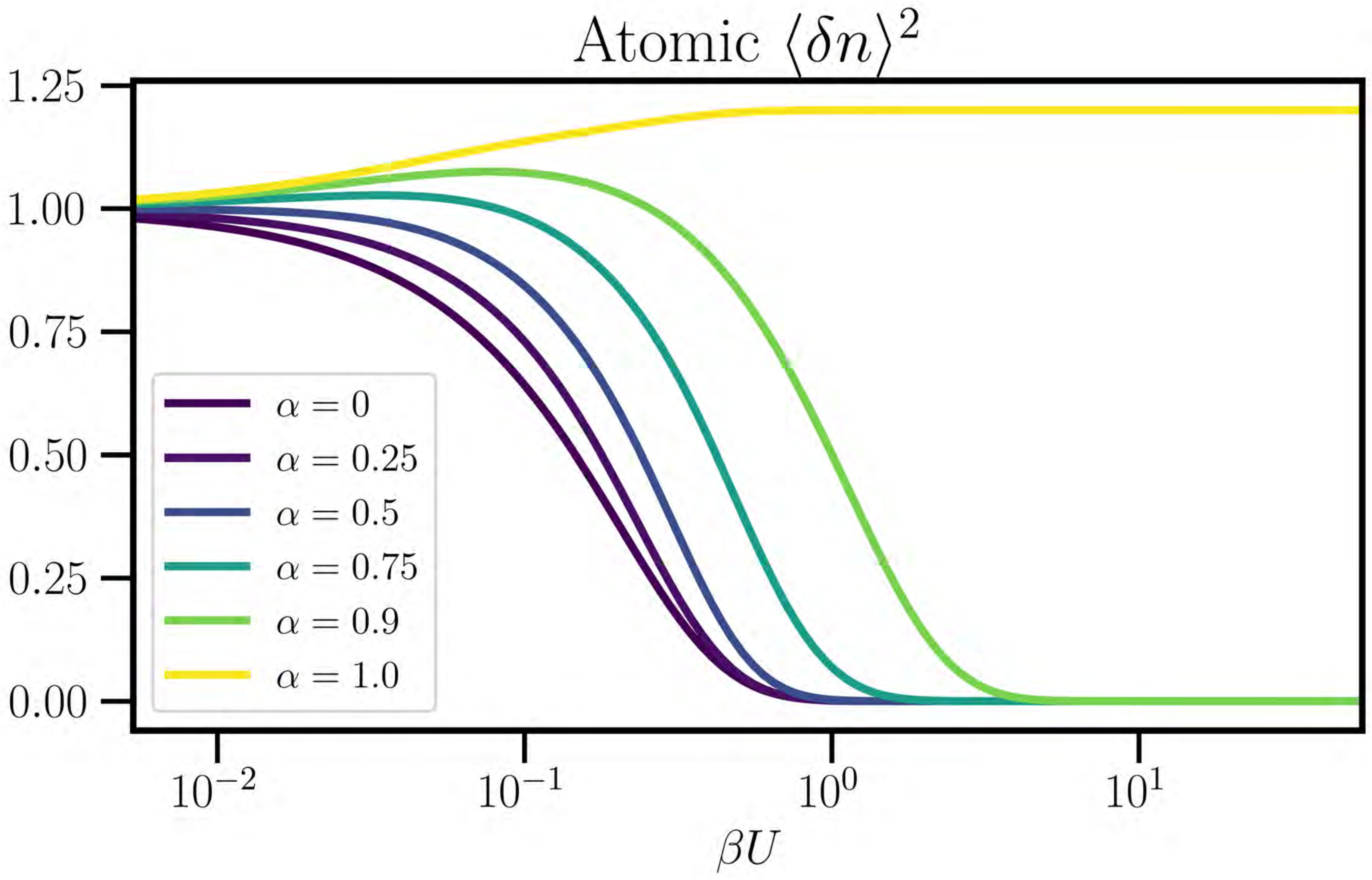
Isotropic case:
SU(6) broken only at $J \sim t^2/U$



Local Moment formation vs. Atomic Limit

Intervalley fluctuations $\langle (n_{\eta=1} - n_{\eta=2})^2 \rangle$



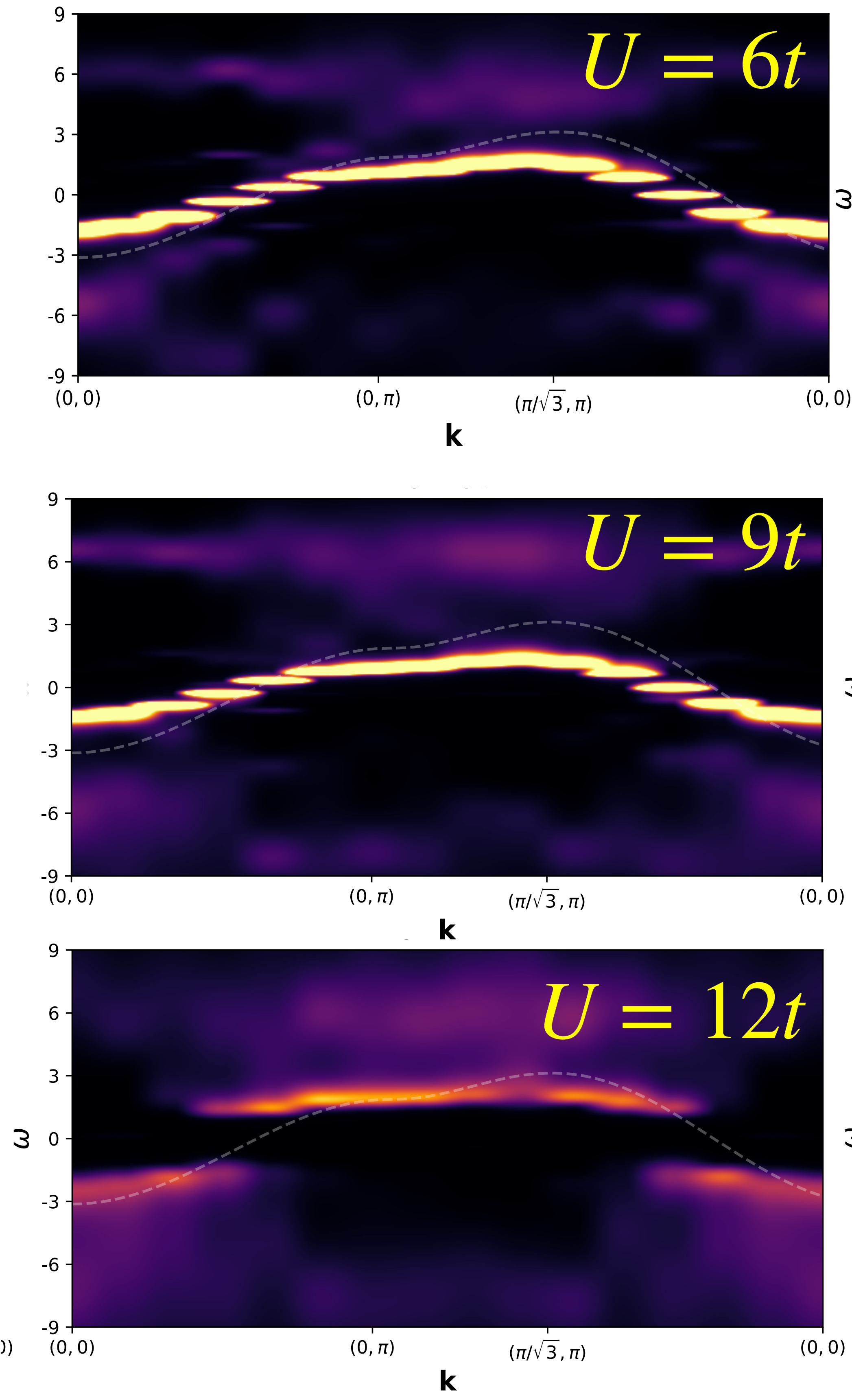


For wide range of $T, \alpha = 0$ curves for full model tracks atomic limit
$\Rightarrow$ "SU(6)" symmetric local moment over wide temperature scale

Spectral Functions

Can analytically continue to real-time & extract $A(\boldsymbol{k}, \omega)$

Stronger Interactions



Anisotropic system: emergence of clear Mott gap for $U \gg t$

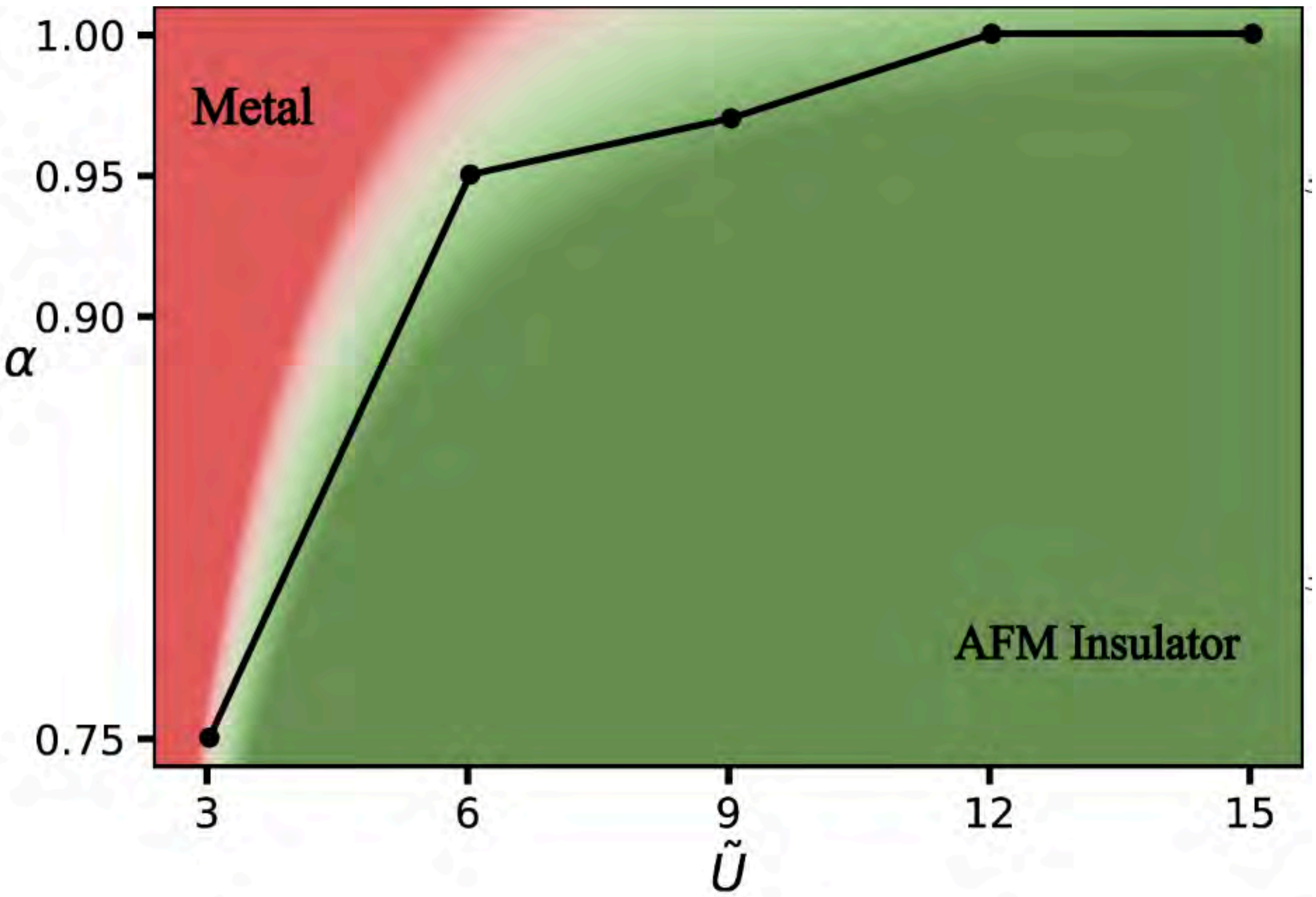
Isotropic point ~ very broad features down to low T

More isotropic

$\alpha = 0$ $\alpha = 0.5$ $\alpha = 0.75$ $\alpha = 0.9$ $\alpha = 1$

Low-T Crossover Diagram

$T = 0.01t$

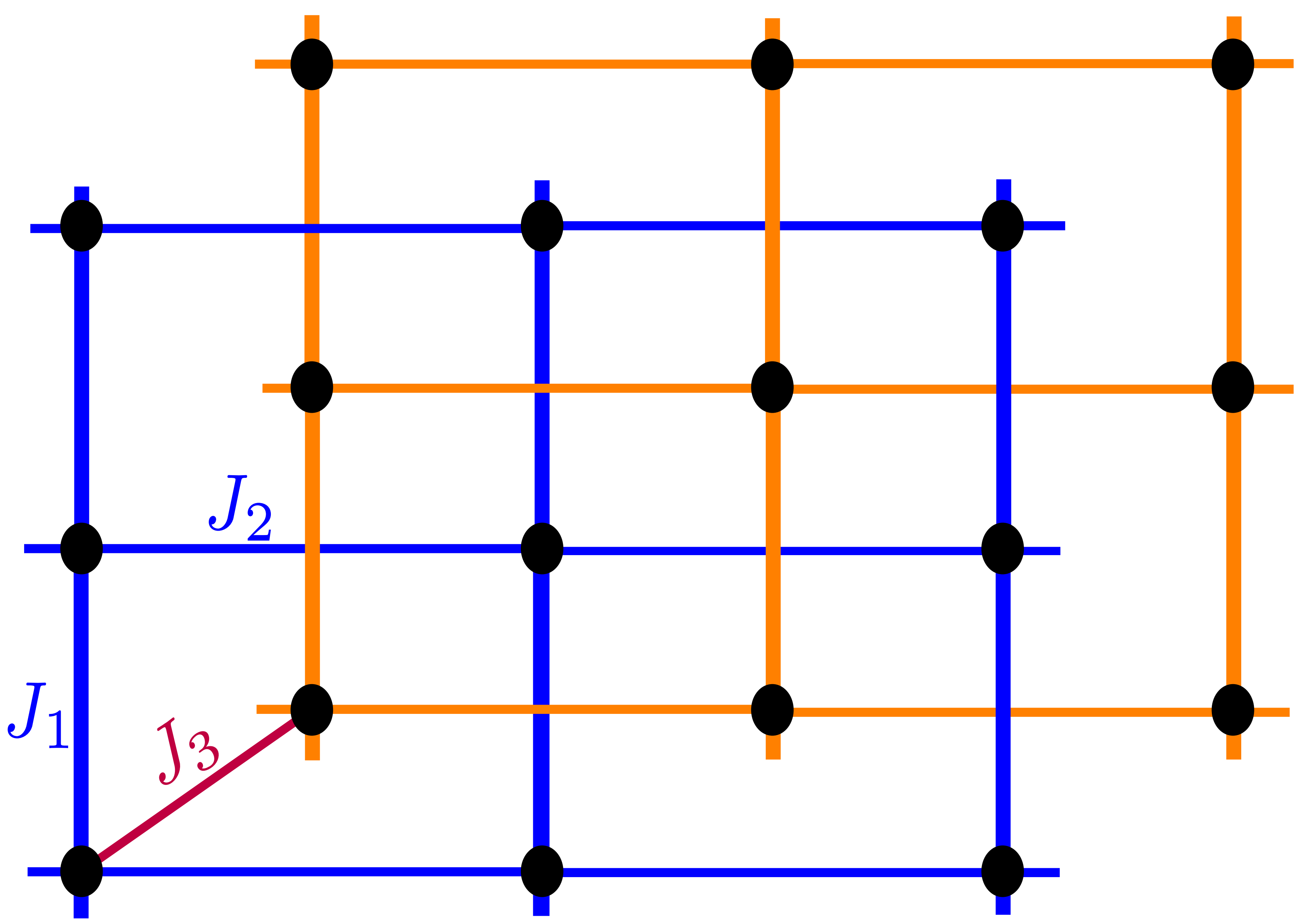


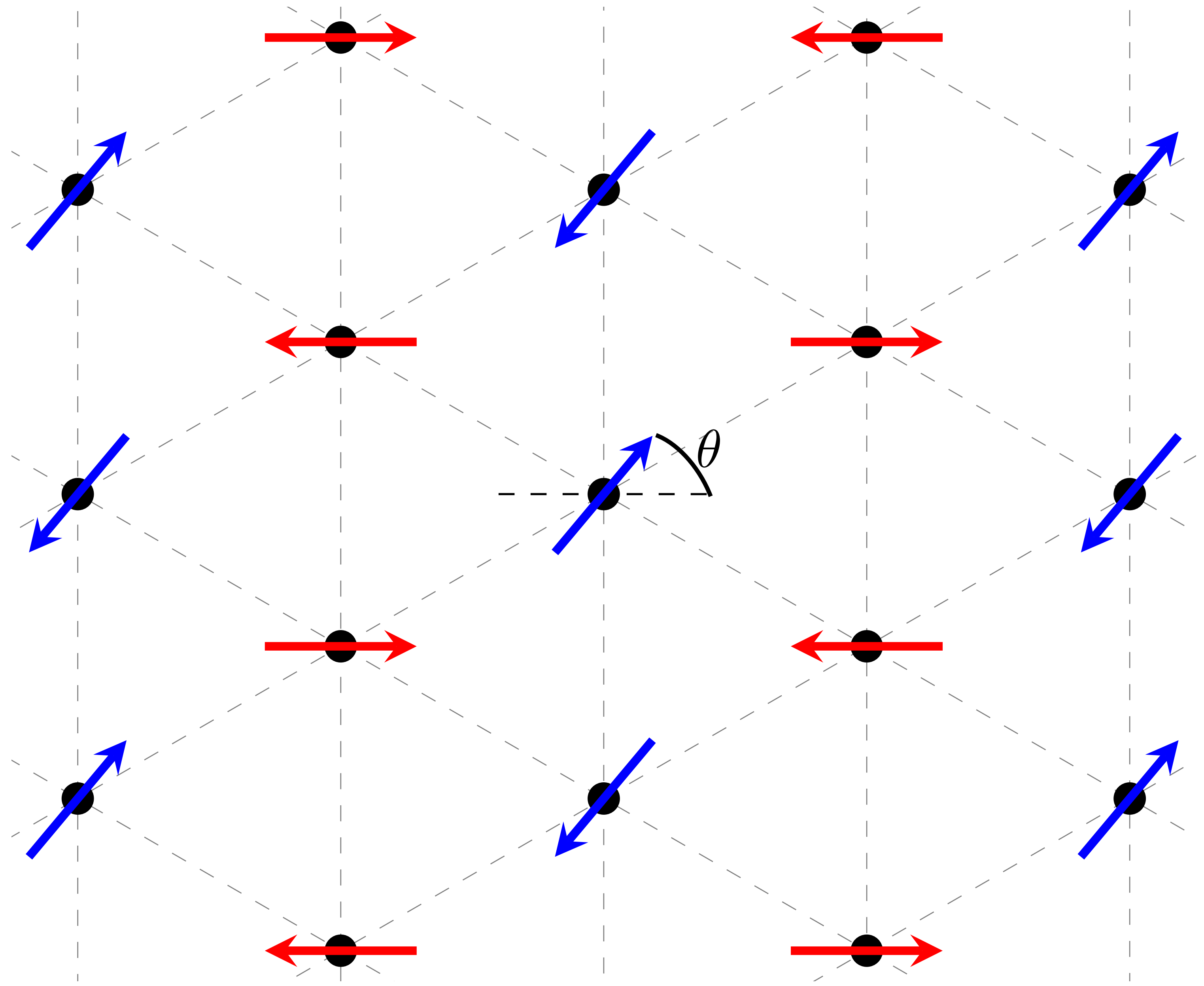
Aside: More on the AF Insulator for $\alpha \neq 1$

Even in a *single* valley: since second neighbor $t_\perp \gg$ first-neighbor $t_\perp$, splits into two rectangular sub lattices (effective $J_1 - J_2 - J_3$ model — so not as frustrated as usual triangular lattice)

Each sublattice Néel-ordered but *relative* orientation θ of Néel vectors is "free" at leading order in J_3 — "order-by disorder"* selects collinear states w/ $\theta = 0, \pi$ (cf. classic work on $J_1 - J_2$ square lattice)

[C. Henley, PRL **62**, 2056 (1989)]





*competing scale for OBD via inter-valley tunneling as well…

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Remarkably, **two limiting cases of phase diagram can be accessed with sign-free QMC!**

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Rich physics: "hierarchy reversal", Pomeranchuk, Wigner-Mott physics

Future: Green's functions, superconductivity, possible CDWs

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For $t_\perp = 0$, rare example of unbiased numerical access (SSE) to doped Mott insulator w/o local approx.

Rich physics: "hierarchy reversal", Pomeranchuk, Wigner-Mott physics

Future: Green's functions, superconductivity, possible CDWs

For half-filling and $t_\perp \neq 0$, can use DQMC to access AF ordering

AF order suppressed $U(6)$; possible strongly renormalized metal accessed via spectral function

Future: more extensive study of metal and the AF phases

Thanks for listening!