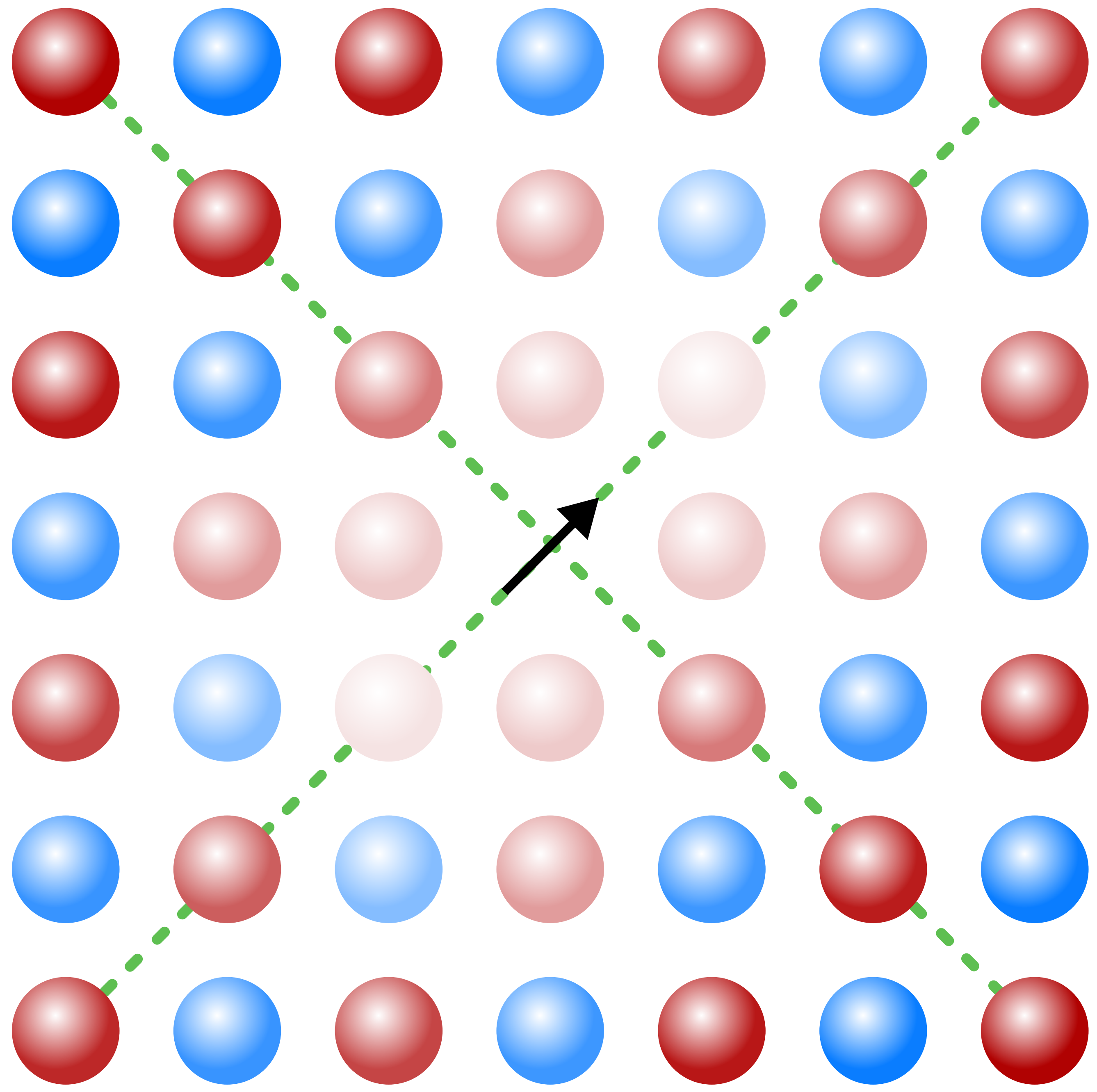
Magnetic polarons

Microscopic structure and dynamics



Georg M. Bruun, Center for Complex Quantum Systems, Aarhus University

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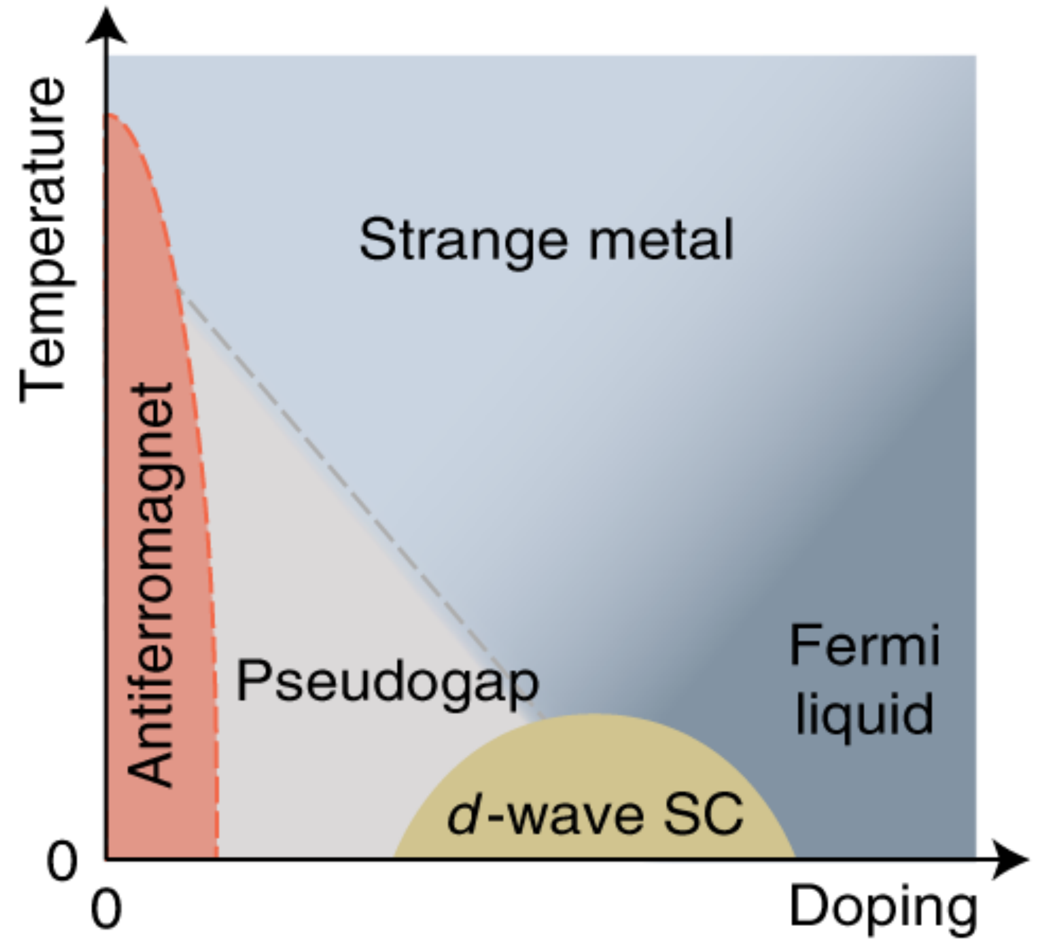
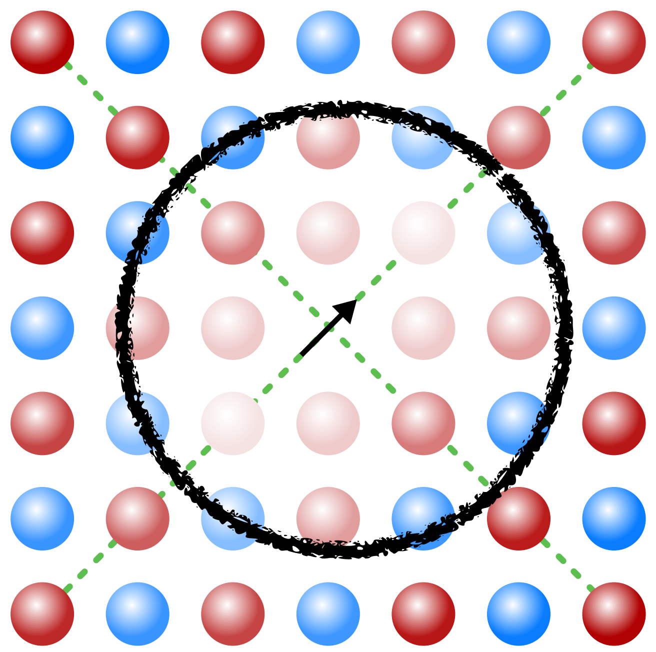
Overview

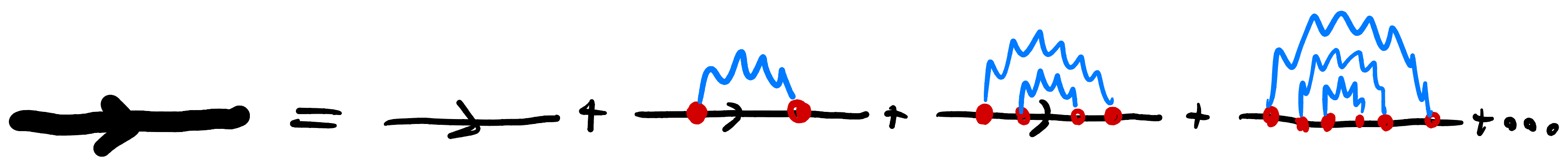
- Fermi-Hubbard model → t-J model close to half-filling. Holes in AF-background



- Motion of hole gives magnetic frustration ⇒ magnetic polaron

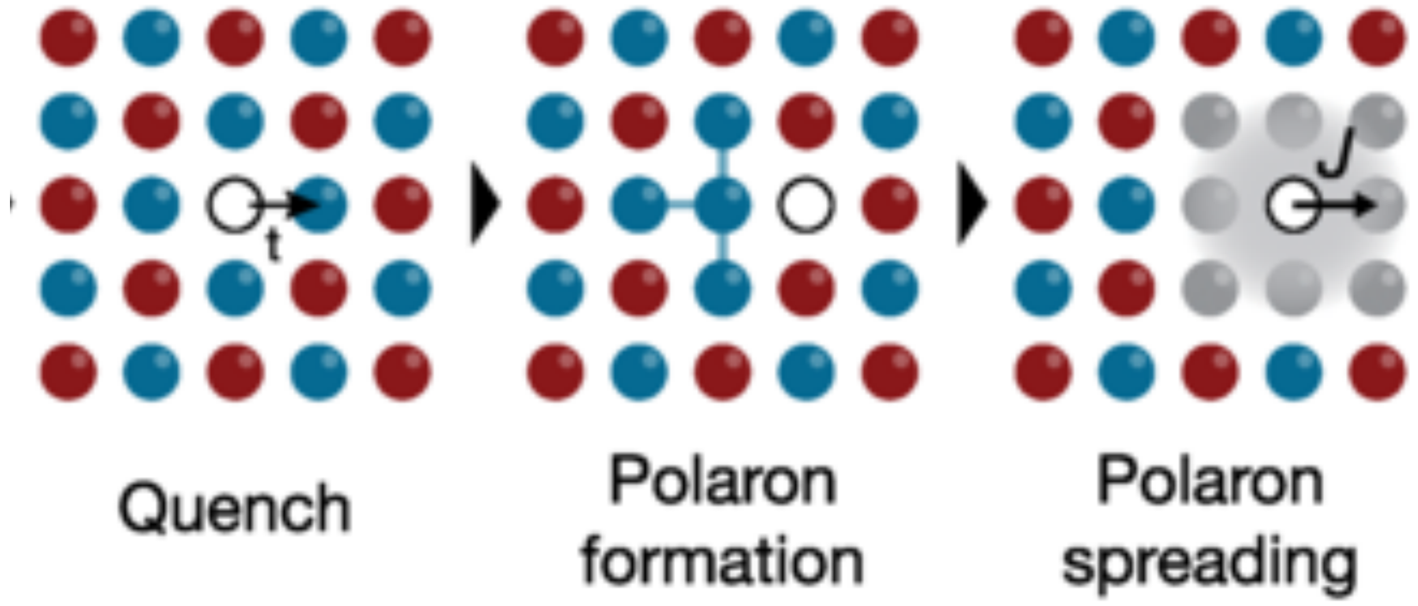


- Self-consistent Born approx. to describe polarons



- Dyson like eqn. for magnetization around hole for strong coupling

- Polaron dynamics for strong coupling



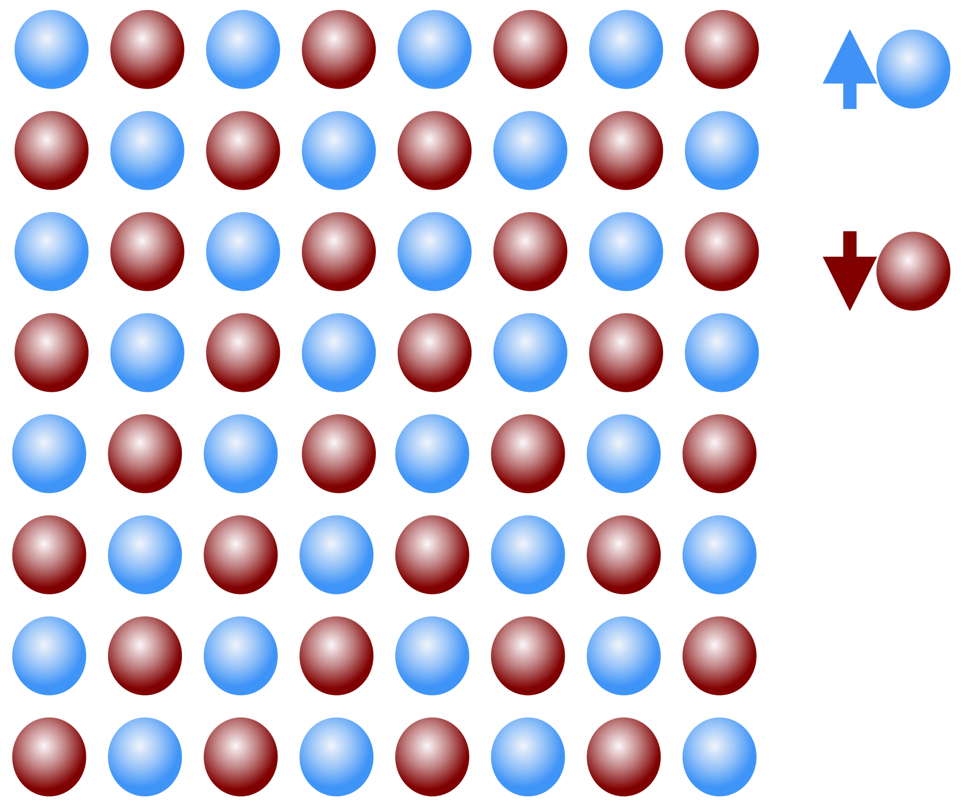
Doped anti-ferromagnets

Fermi-Hubbard model $$\hat{H}_{\mathrm{FH}} = -t \sum_{\langle \mathbf{i},\mathbf{j}\rangle,\sigma} \left[\hat{c}^{\dagger}_{\mathbf{i},\sigma}\hat{c}_{\mathbf{j},\sigma} + \mathrm{h.c.}\right] + U\sum_{\mathbf{i}} \hat{n}_{\mathbf{i},\uparrow}\hat{n}_{\mathbf{i},\downarrow}$$

Canonical model for quantum materials. But very hard to analyse in general

Anti-ferromagnet at half-filling for $U \gg t$:

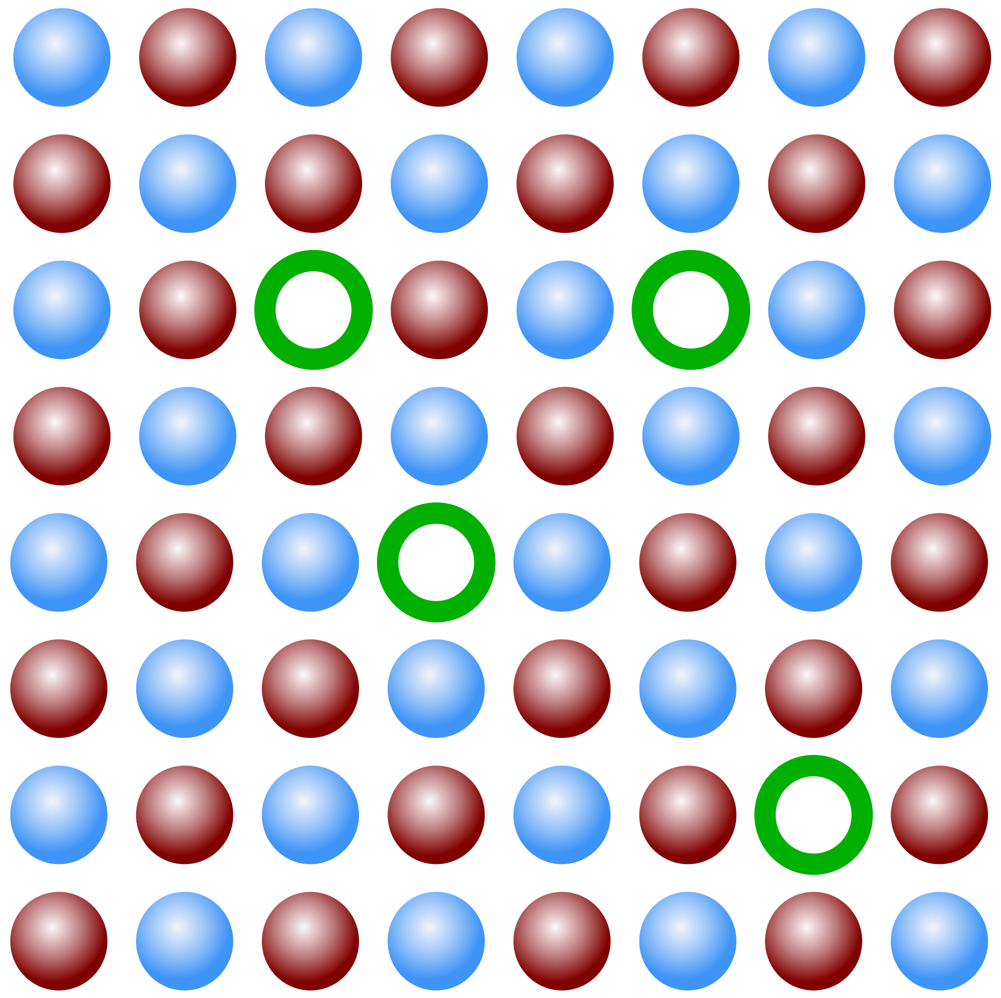
$$\hat{H} = J\sum_{\langle \mathbf{i},\mathbf{j}\rangle} \hat{\mathbf{S}}_{\mathbf{i}} \cdot \hat{\mathbf{S}}_{\mathbf{j}}$$

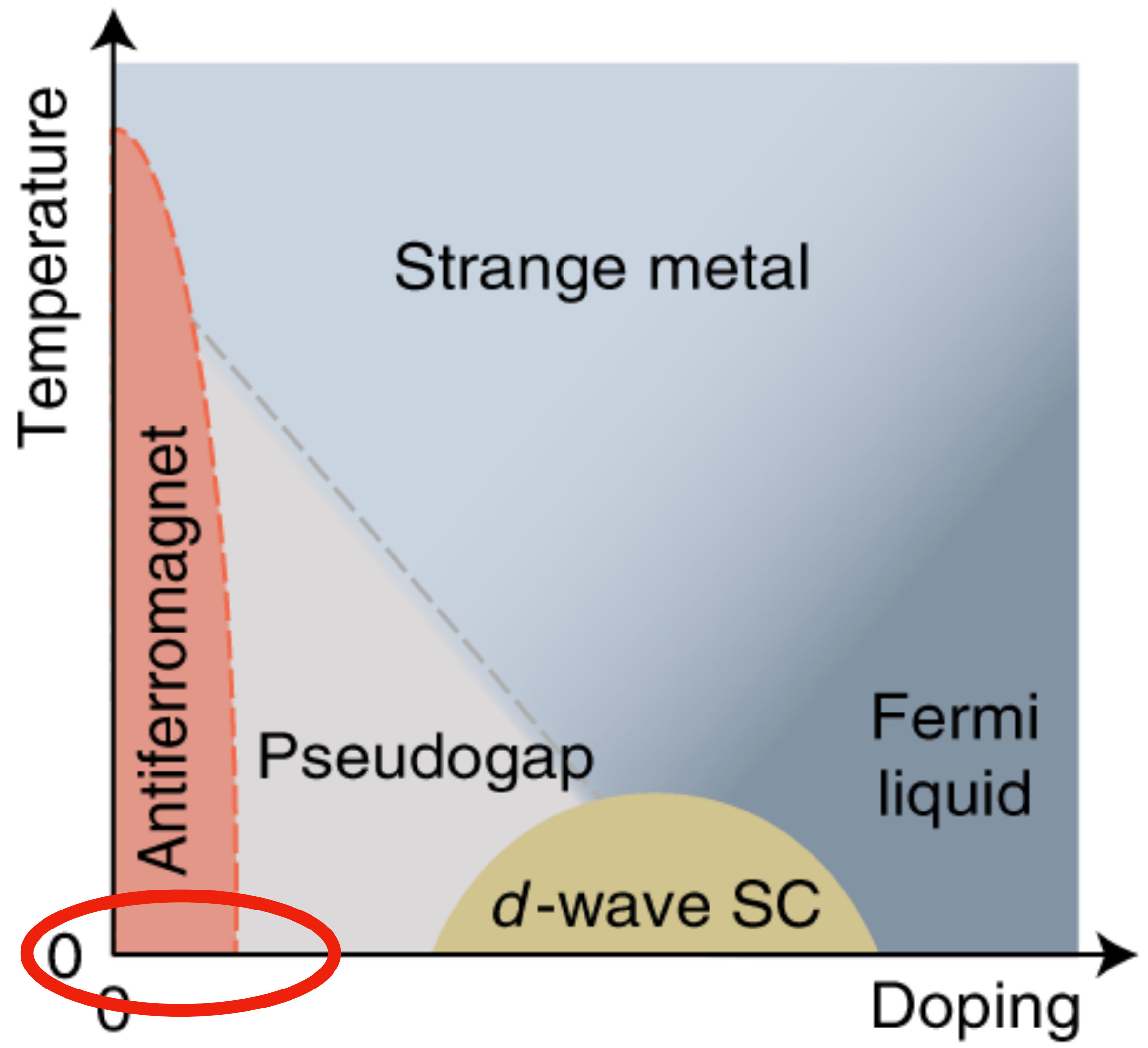


$$\mathbf{S}_{\mathbf{j}} = \frac{1}{2}\sum_{\sigma,\sigma'} \hat{c}^{\dagger}_{\mathbf{j},\sigma}\boldsymbol{\sigma}_{\sigma\sigma'}\hat{c}_{\mathbf{j},\sigma'}$$

$$J = 4t^2/U \ll t$$

What happens with hole doping?



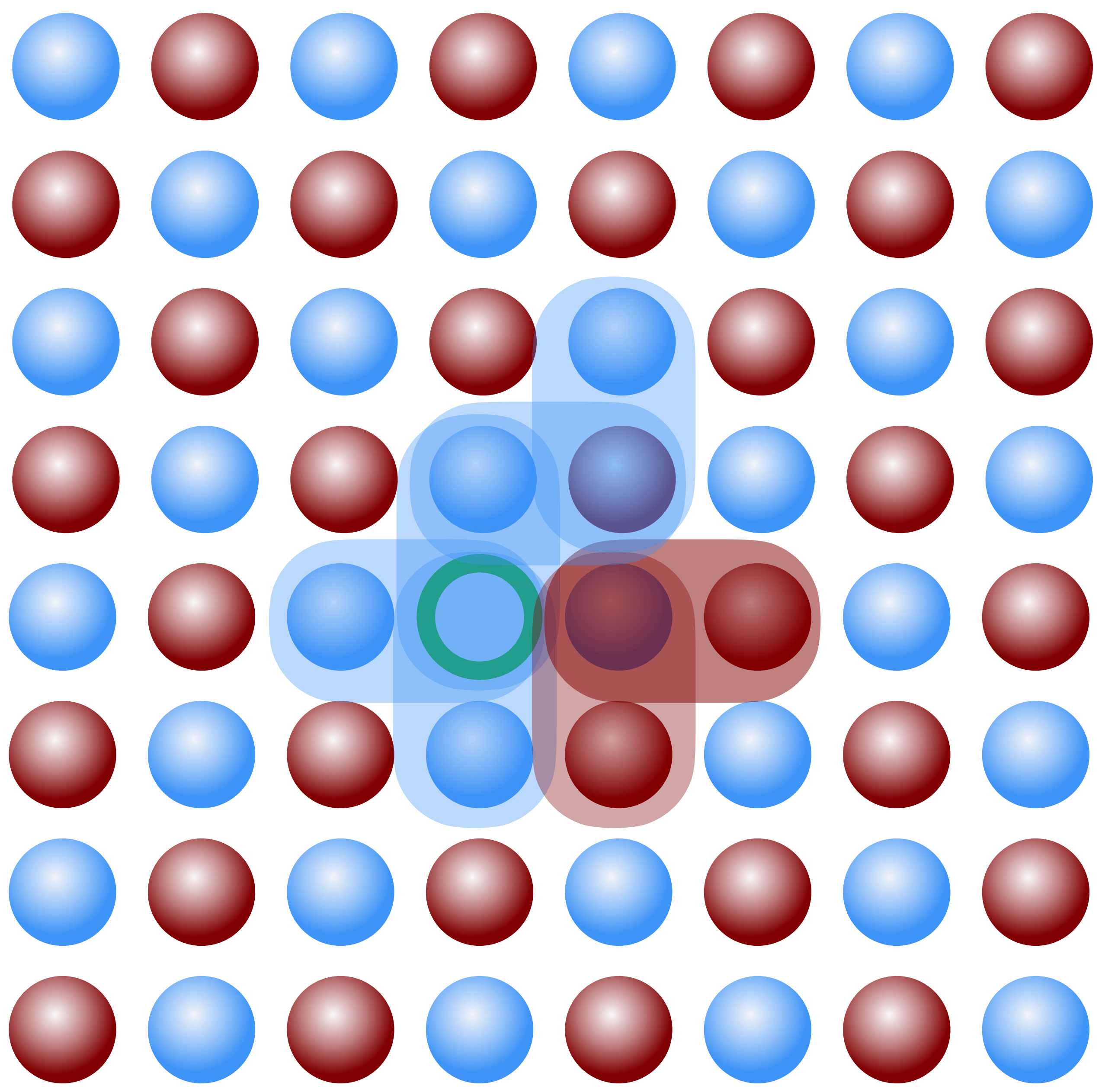


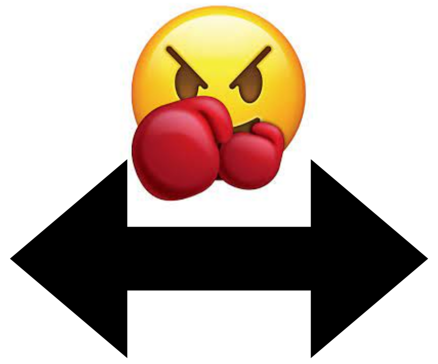
Patrick A. Lee, Naoto Nagaosa, and Xiao-Gang Wen, Rev. Mod. Phys. **78**, 17 (2006)

t-J model

Close to half-filling and $U \gg t$

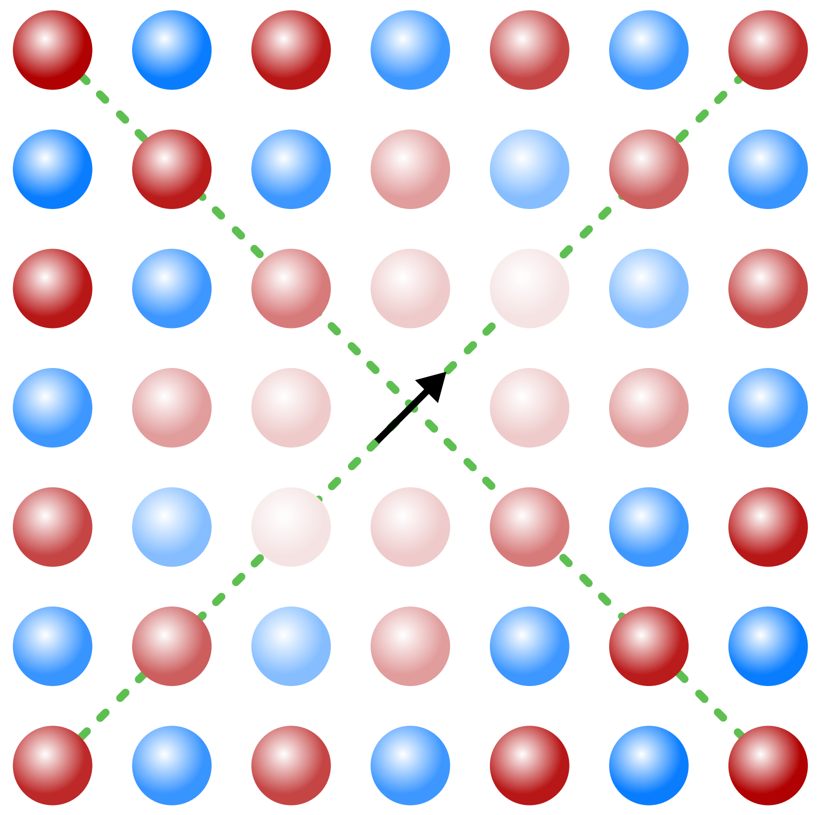
$$\hat{H} = -t \sum_{\langle \mathbf{i},\mathbf{j} \rangle, \sigma} \left[\tilde{c}^{\dagger}_{\mathbf{i},\sigma} \tilde{c}_{\mathbf{i},\sigma} + \mathrm{h.c.} \right] + J \sum_{\langle \mathbf{i},\mathbf{j} \rangle} \left[\hat{S}^z_{\mathbf{i}} \hat{S}^z_{\mathbf{j}} + \frac{\alpha}{2} \left(\hat{S}^+_{\mathbf{i}} \hat{S}^-_{\mathbf{j}} + \hat{S}^-_{\mathbf{i}} \hat{S}^+_{\mathbf{j}} \right) - \frac{\hat{n}_{\mathbf{i}} \hat{n}_{\mathbf{j}}}{4} \right]$$



Hole hopping  Magnetic order

Formation of

magnetic polaron



Huge high T_c literature

P. W. Anderson, Science **235**, 1196 (1987)

B. I. Shraiman and E. D. Siggia, PRL **61**, 467 (1988)

J. R. Schrieffer et al., PRL **60**, 944 (1988)

S. Schmitt-Rink et al., PRL **60**, 2793 (1988)

C. L. Kane et al., PRB **39**, 6880 (1989)

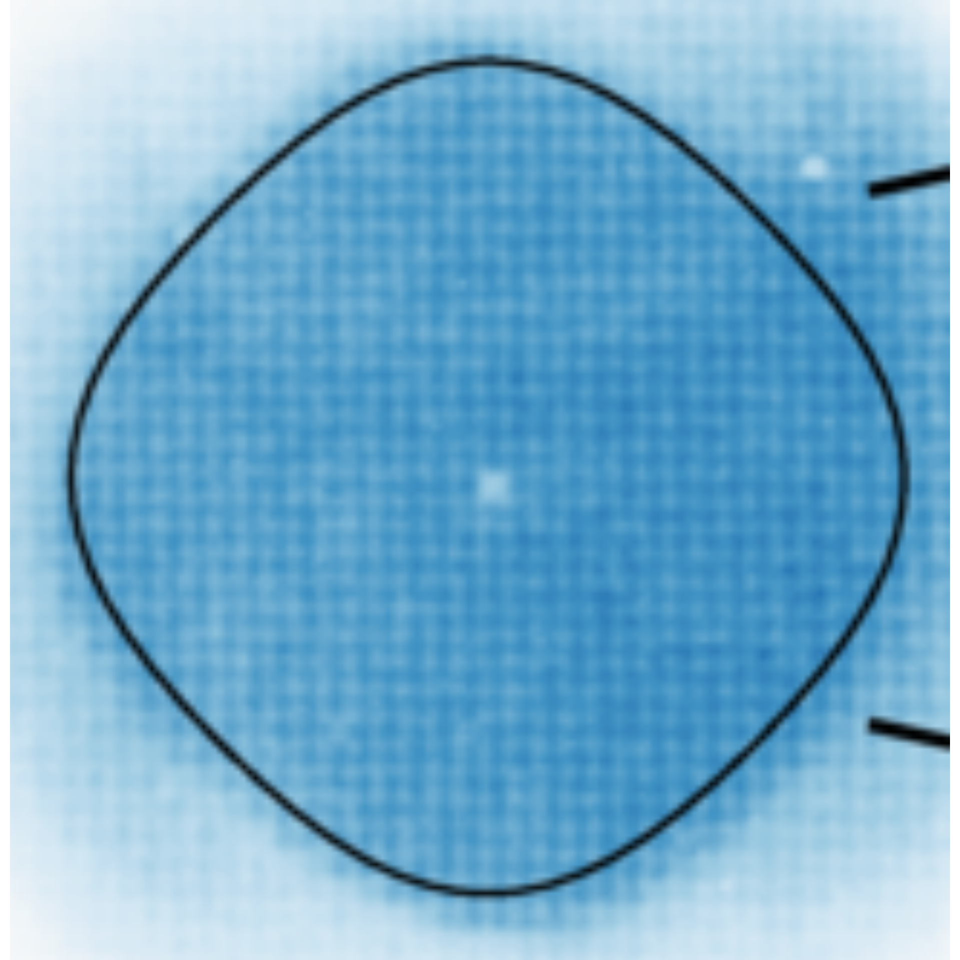
S. A. Trugman, PRB **41**, 892 (1990)

G. Martinez and P. Horsch, PRB **44,** 317 (1991)

G. F. Reiter, PRB **49**, 1536 (1994)

A. Ramsak and P. Horsch, PRB **57**, 4308 (1998)

Probe microscopic structure with atoms in optical lattice



A. Mazurenko et al., Nature **545**, 462 (2017)

T. A. Hilker et al., Science **357**, 484 (2017)

F. Grusdt et al., SciPost Phys. **5**, 57 (2018)

F. Grusdt et al., PRX **8**, 011046 (2018)

J. Koepsell et al., Nature **572**, 358 (2019)

C. S. Chiu et al., Science **365**, 251 (2019)

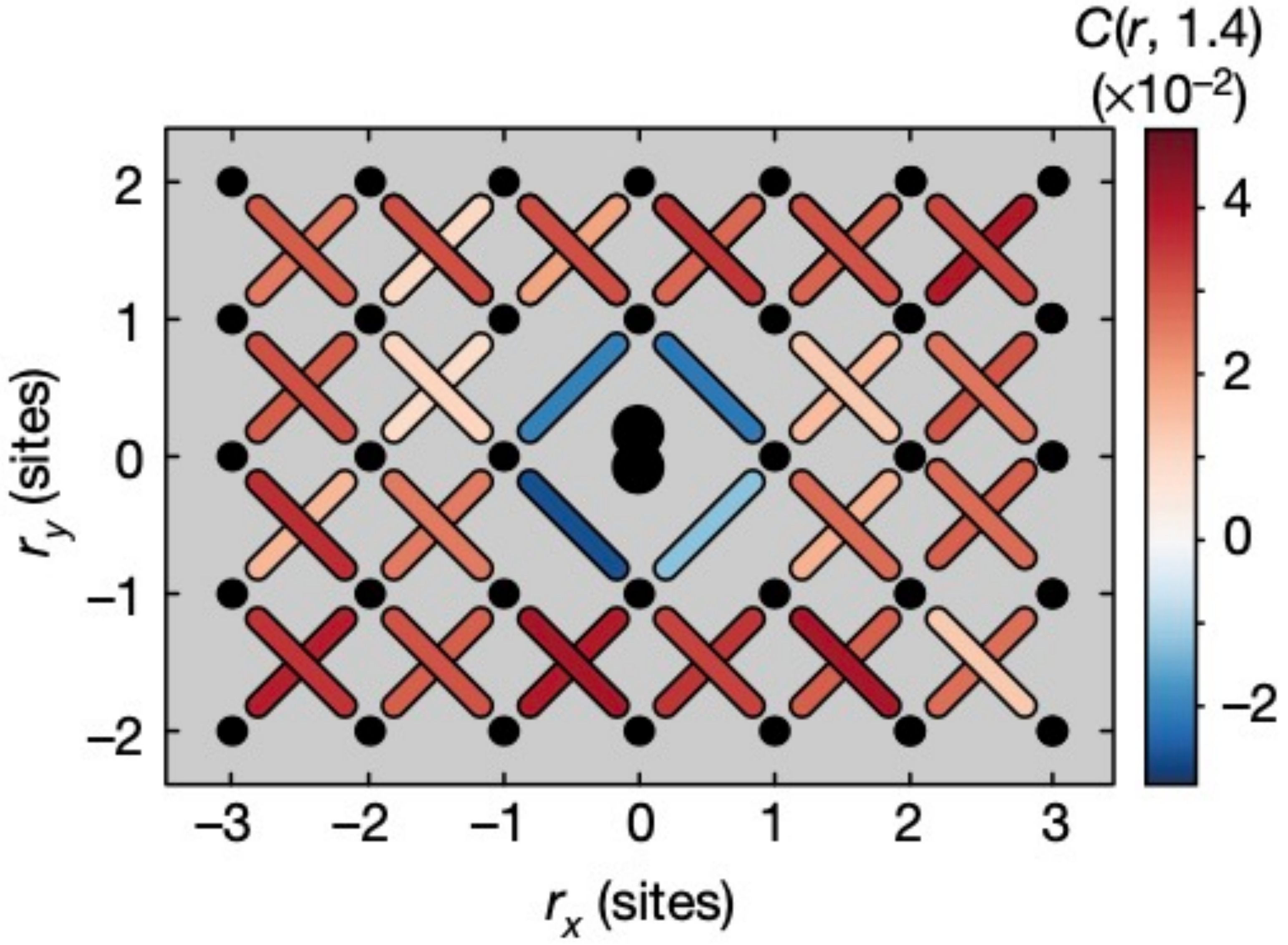
F. Grusdt et al., PRB **99**, 224422 (2019)

A. Bohrdt et al., Nature Physics **15**, 921 (2019)

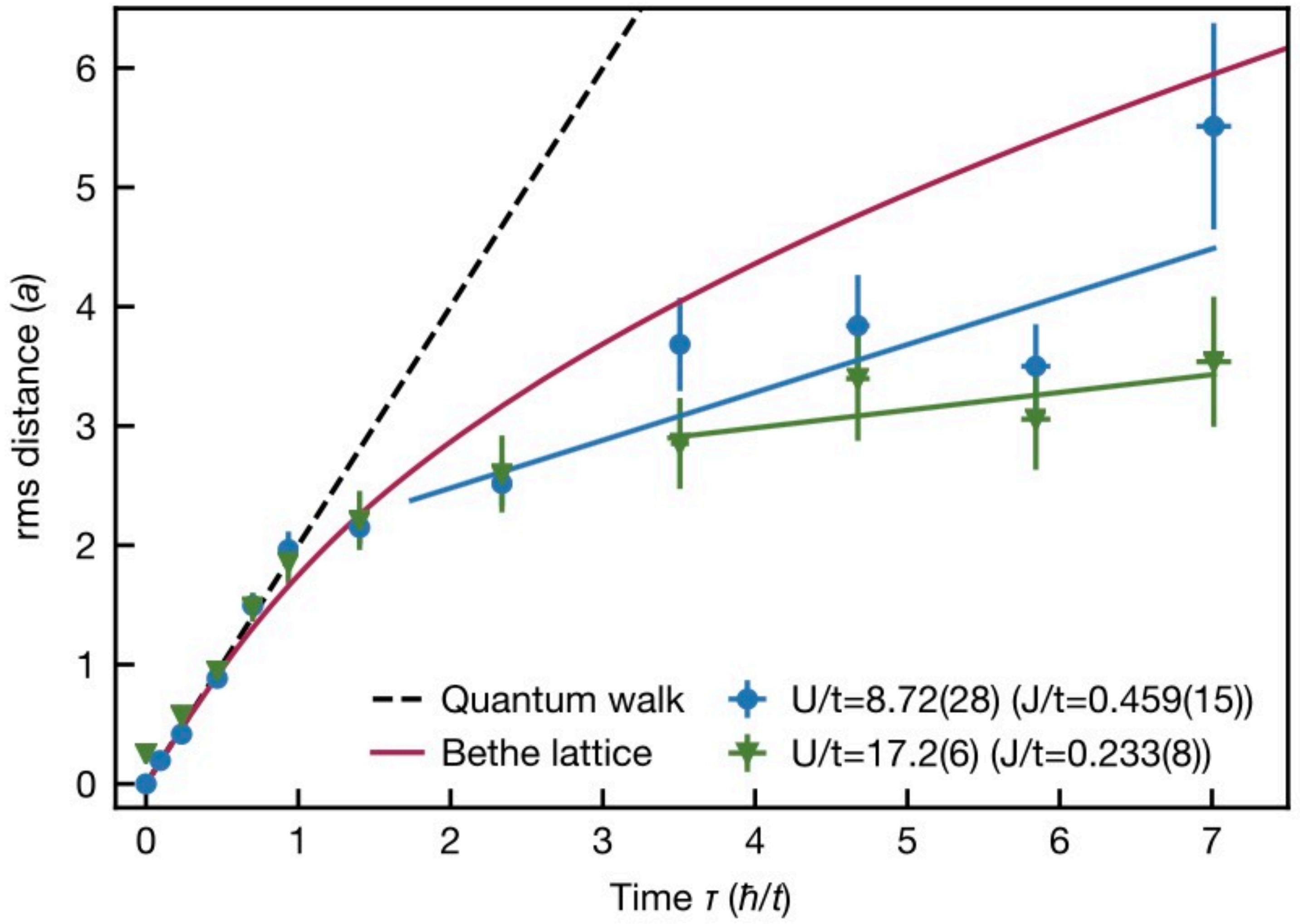
T. Hartke et al., PRL **125**, 113601 (2020)

G. Ji et al., PRX **11**, 021022 (2021)

Magnetic correlations around hole



Non-equilibrium dynamics



Self-consistent Born approximation

$$\hat{H} = -t \sum_{\langle \mathbf{i},\mathbf{j}\rangle,\sigma} \left[\tilde{c}^{\dagger}_{\mathbf{i},\sigma} \tilde{c}_{\mathbf{i},\sigma} + \text{h.c.} \right] + J \sum_{\langle \mathbf{i},\mathbf{j}\rangle} \left[\hat{S}^z_{\mathbf{i}} \hat{S}^z_{\mathbf{j}} + \frac{\alpha}{2} \left(\hat{S}^+_{\mathbf{i}} \hat{S}^-_{\mathbf{j}} + \hat{S}^-_{\mathbf{i}} \hat{S}^+_{\mathbf{j}} \right) - \frac{\hat{n}_{\mathbf{i}} \hat{n}_{\mathbf{j}}}{4} \right]$$

Holstein-Primakoff in presence of holes (Slave fermion)

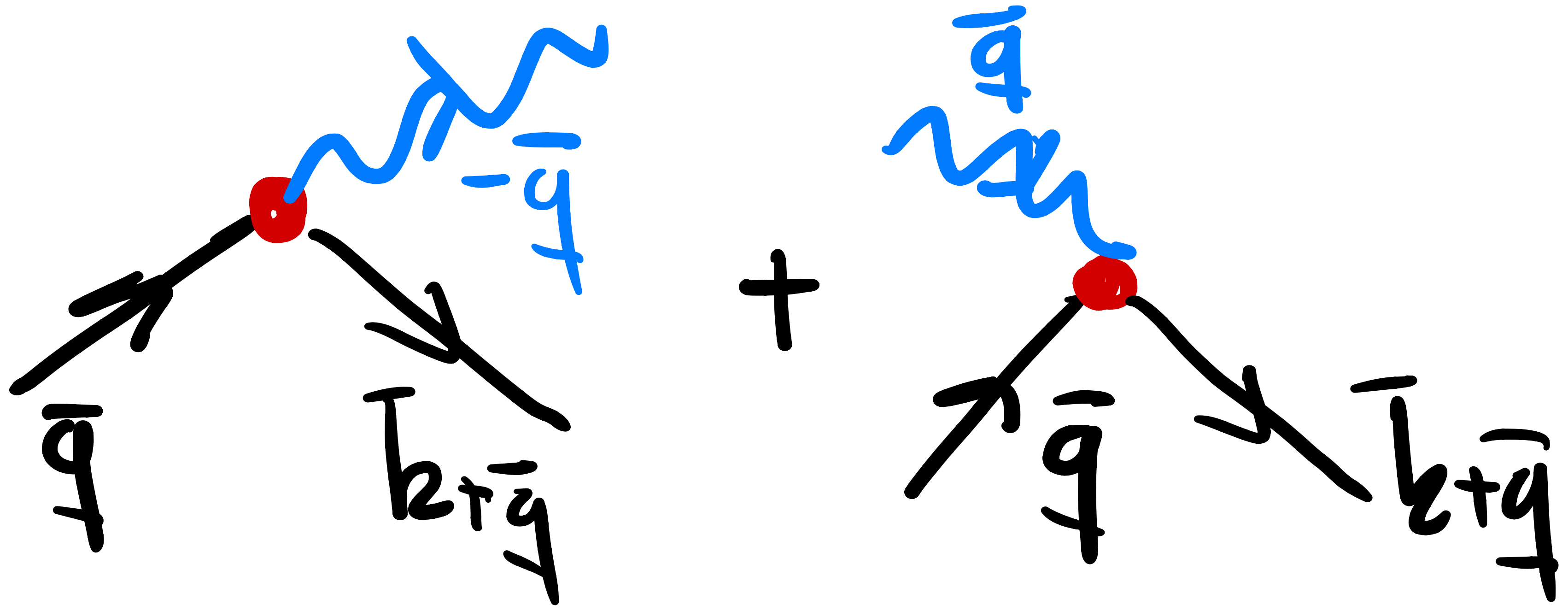
Hole hopping ⇒ emmission of spin waves

$$= \sum_{\mathbf{q},\mathbf{k}} \hat{h}^{\dagger}_{\mathbf{q}+\mathbf{k}} \hat{h}_{\mathbf{q}} \left[g(\mathbf{q},\mathbf{k}) \hat{b}^{\dagger}_{-\mathbf{k}} + g(\mathbf{q}+\mathbf{k},-\mathbf{k}) \hat{b}_{\mathbf{k}} \right] + \sum_{\mathbf{k}} \omega_{\mathbf{k}} \hat{b}^{\dagger}_{\mathbf{k}} \hat{b}_{\mathbf{k}}$$

AF spin waves

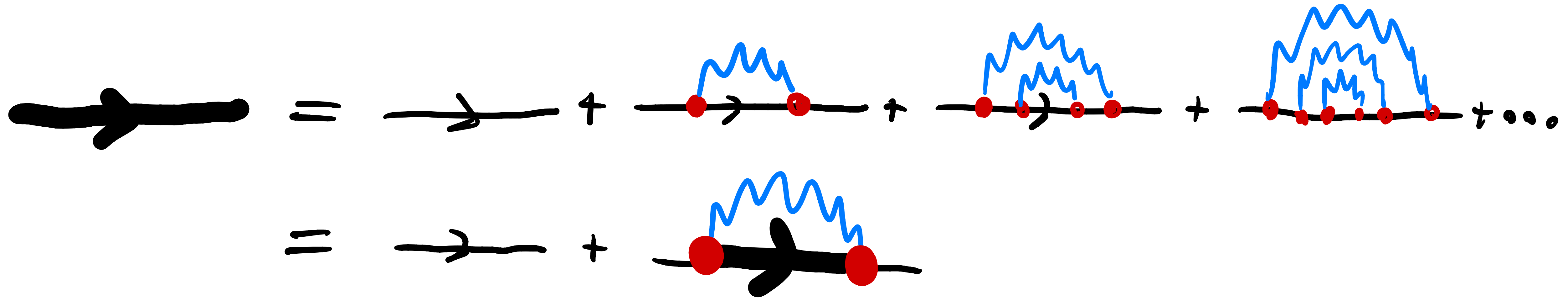
$\omega_{\mathbf{k}} \propto J$

$g(\mathbf{q},\mathbf{k}) \propto t$

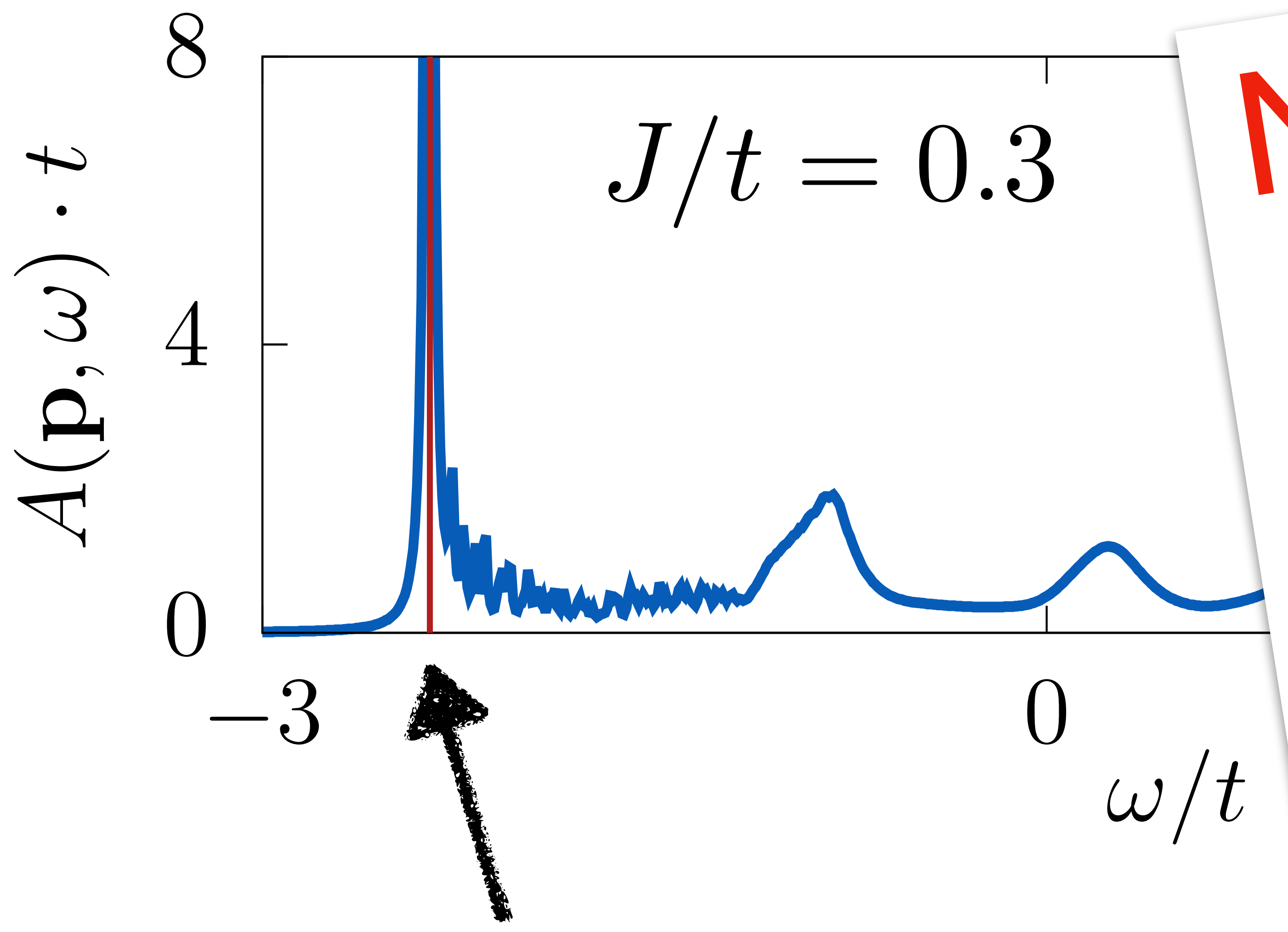


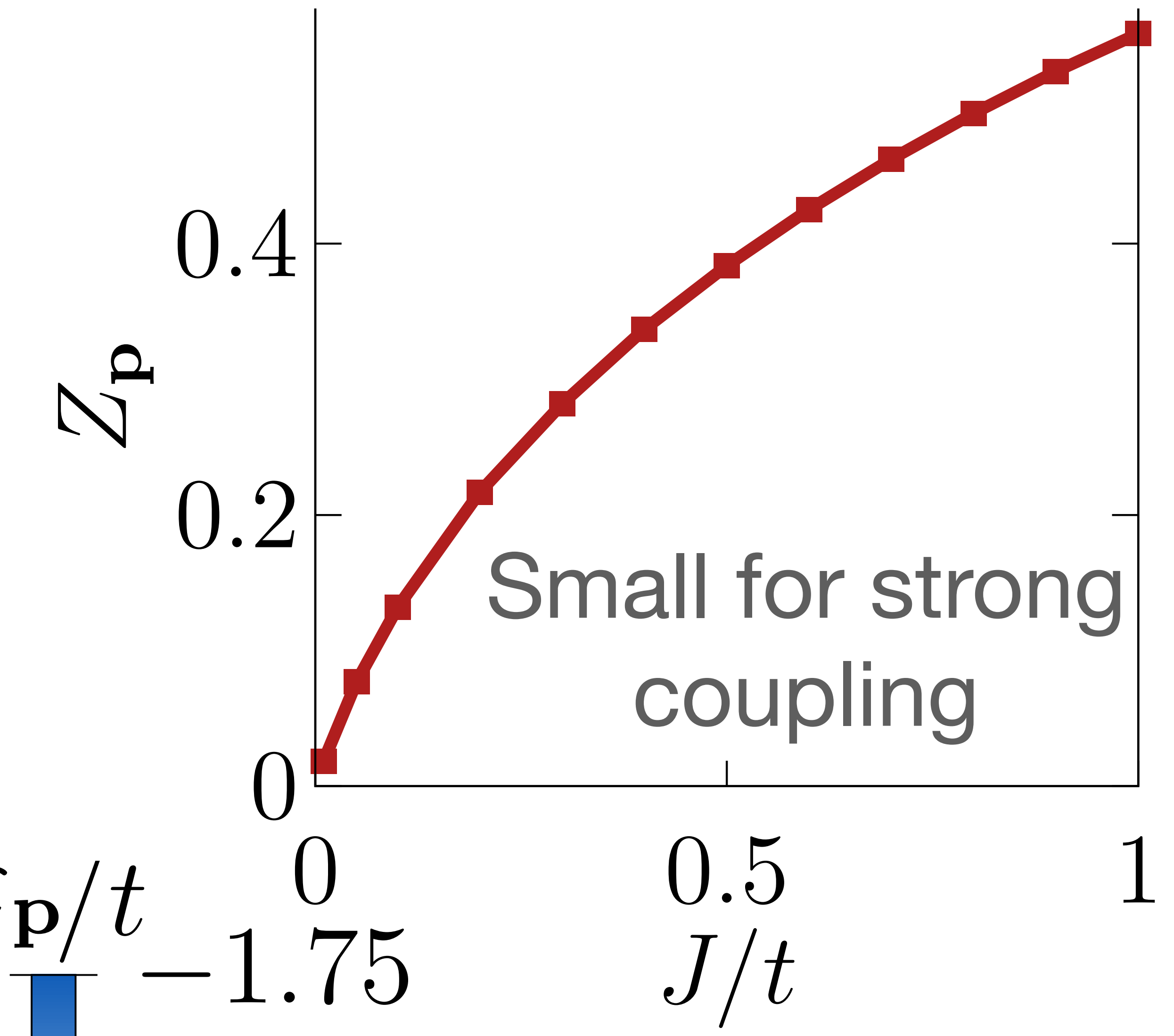
Strong coupling $J/t \ll 1$

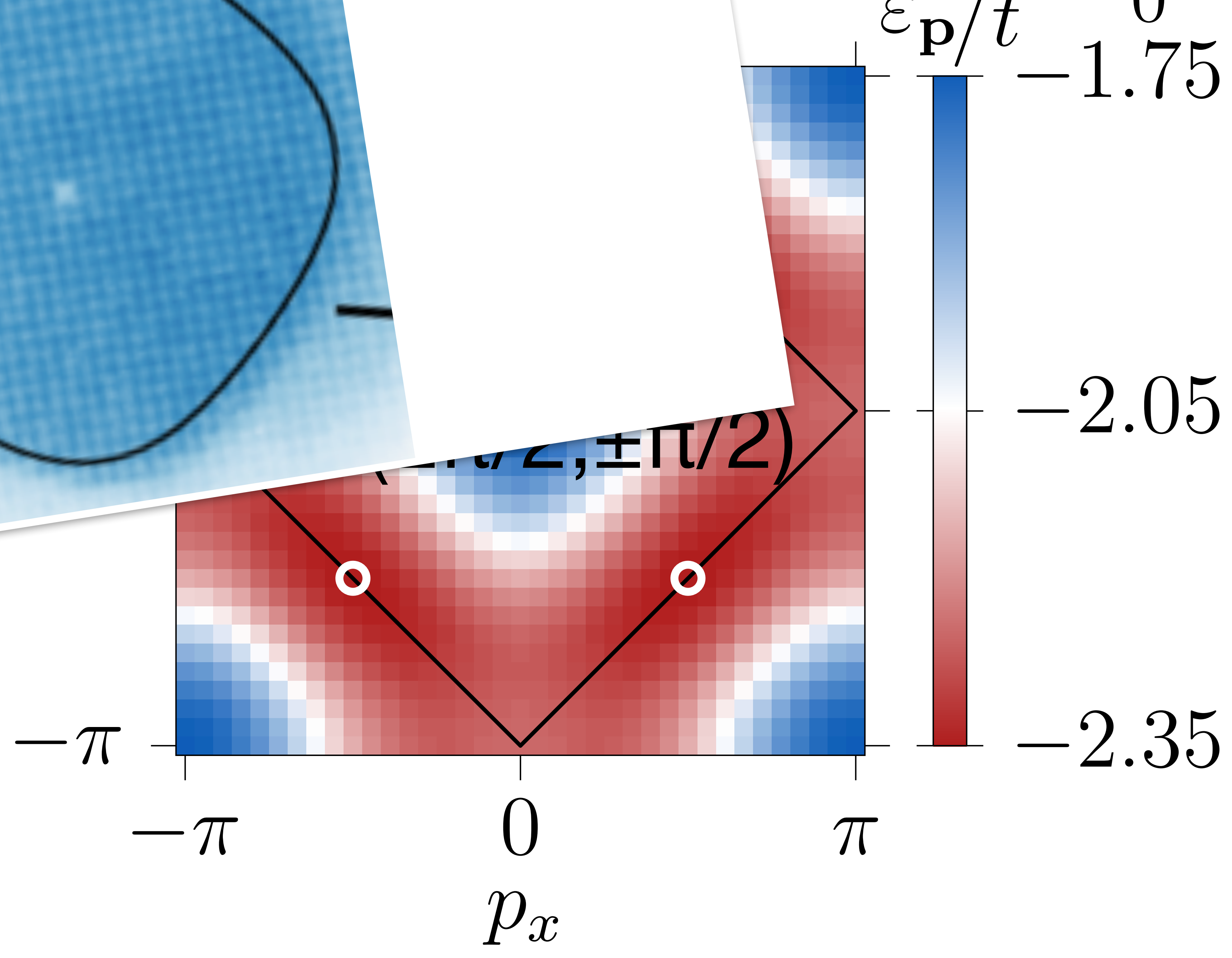
Self-consistent Born Approx. (SCBA) for hole Green's function :



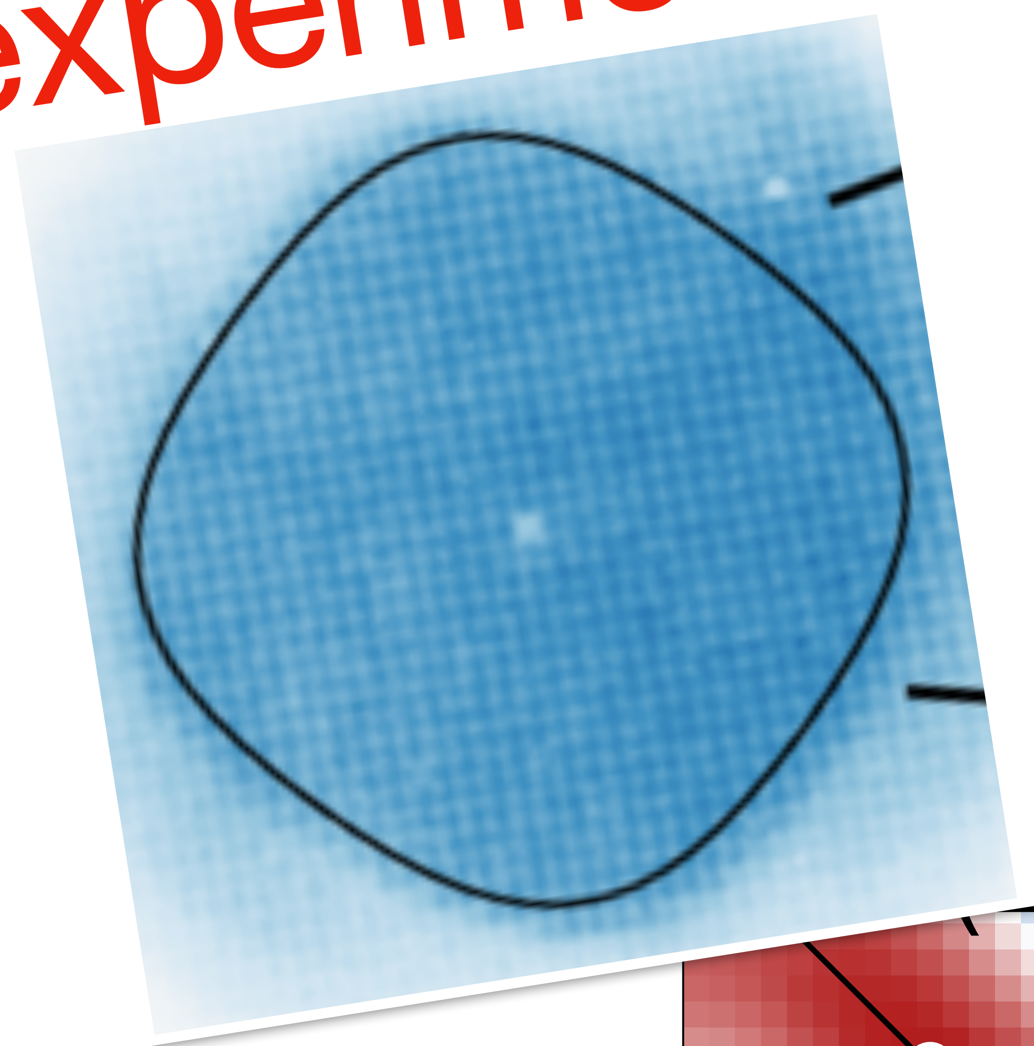
Spectral fn







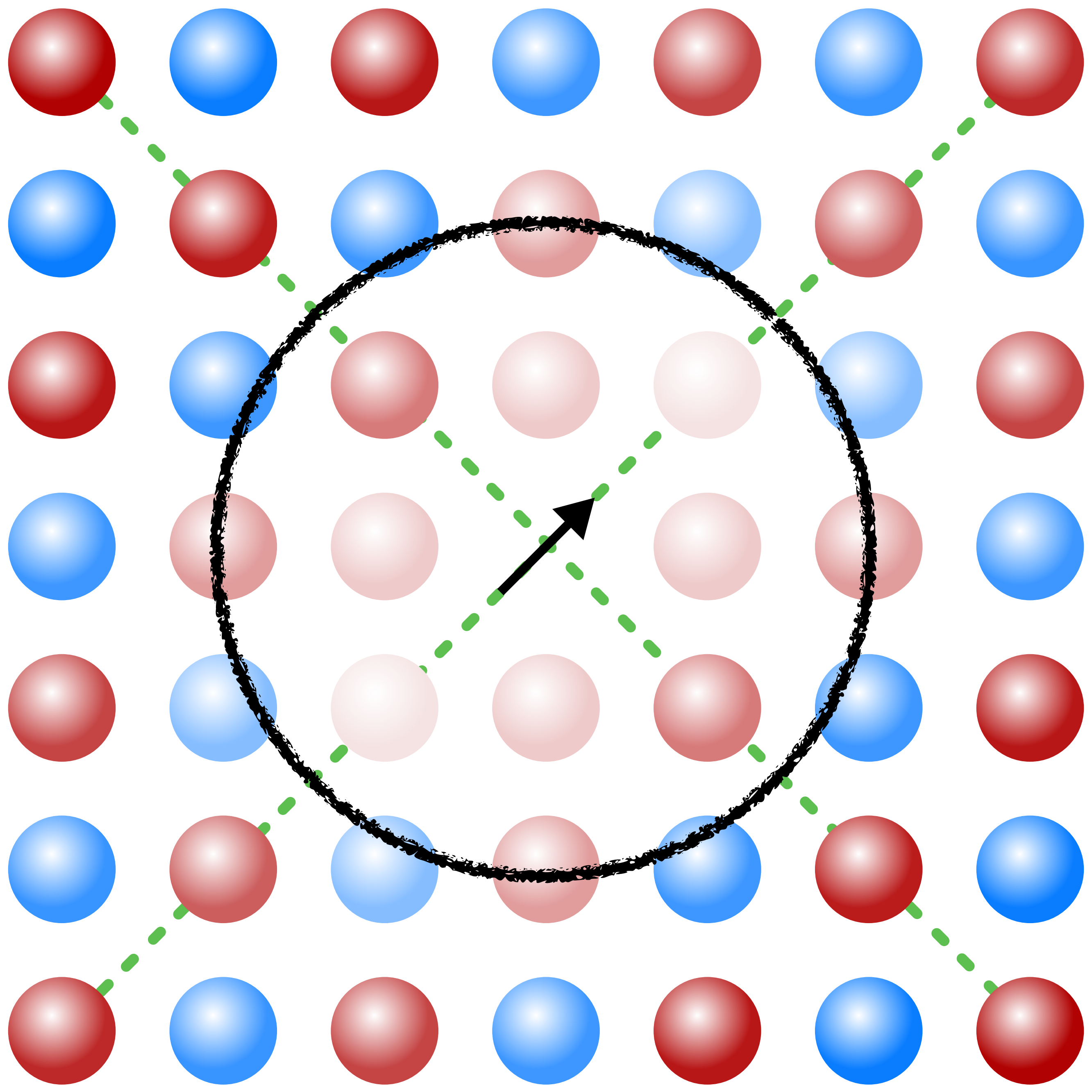
Not easily measurable in optical lattice experiments



S. Schmitt-Rink et al., PRL **60**, 2793 (1988)
C. L. Kane et al., PRB **39**, 6880 (1989)
G. Martinez and P. Horsch, PRB **44,** 317 (1991)

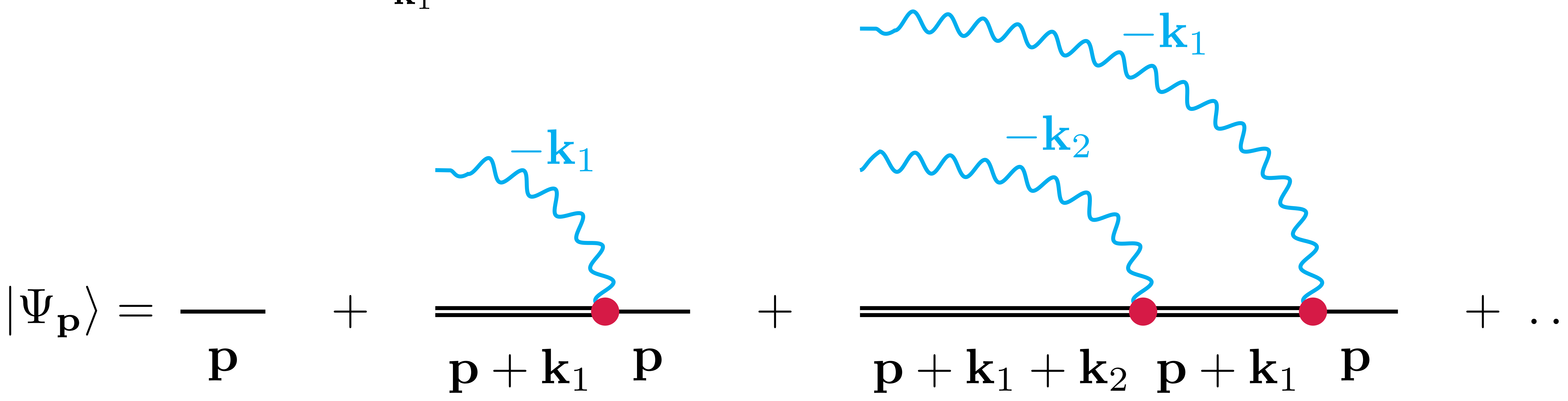
Microscopic structure of magnetic polaron

Magnetic dressing cloud



We need polaron wave function

$$|\Psi_{\mathbf{p}}\rangle = \sqrt{Z_{\mathbf{p}}}\left[\hat{h}^\dagger_{\mathbf{p}} + \sum_{\mathbf{k}_1} g(\mathbf{p},\mathbf{k}_1)G\left(\mathbf{p}+\mathbf{k}_1, \varepsilon_{\mathbf{p}} - \omega_{\mathbf{k}_1}\right)\hat{h}^\dagger_{\mathbf{p}+\mathbf{k}_1}\hat{b}^\dagger_{-\mathbf{k}_1} + \ldots\right]|\mathrm{AF}\rangle$$



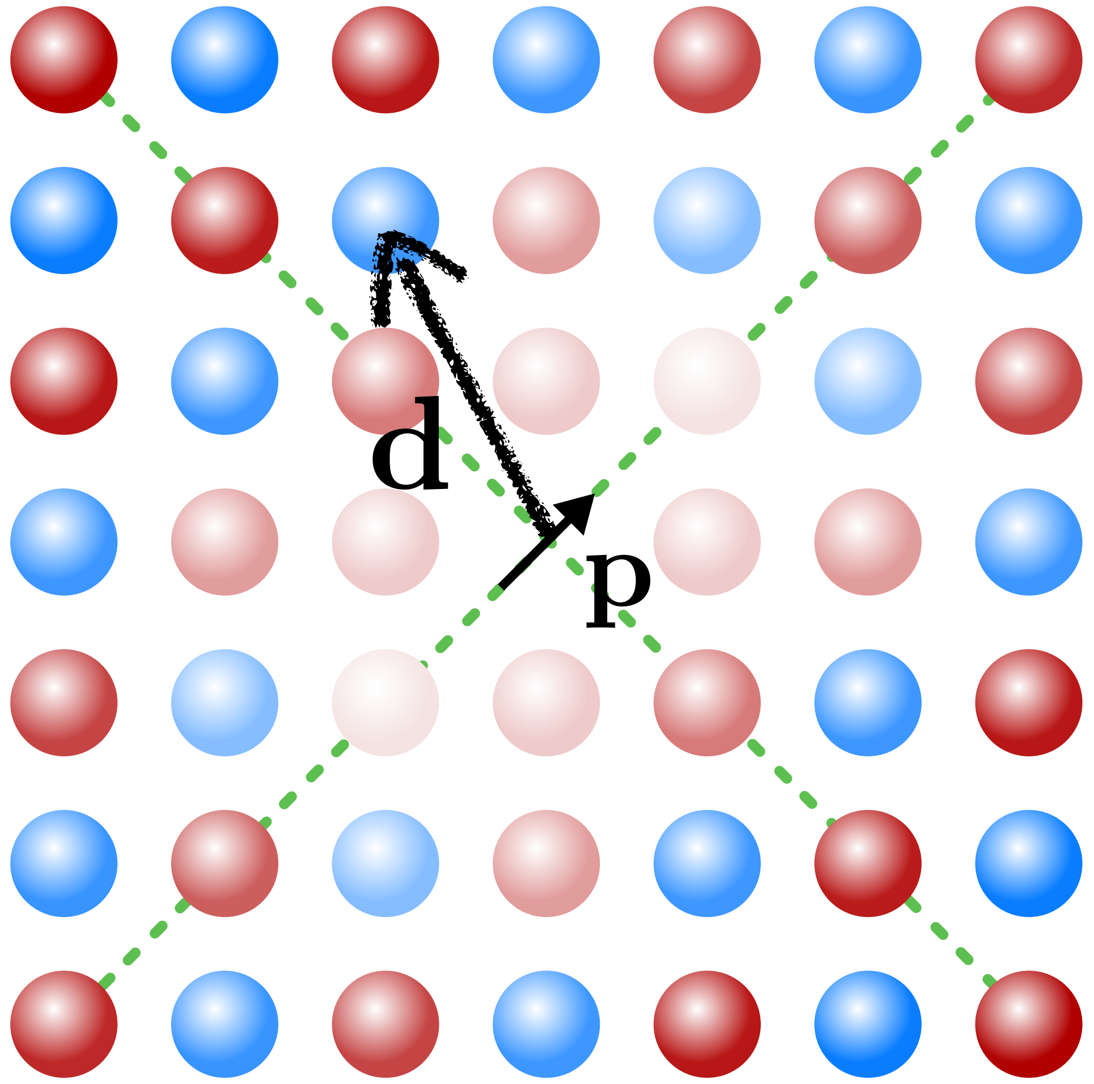
“Diagrammatic” rules for wave f^n construction

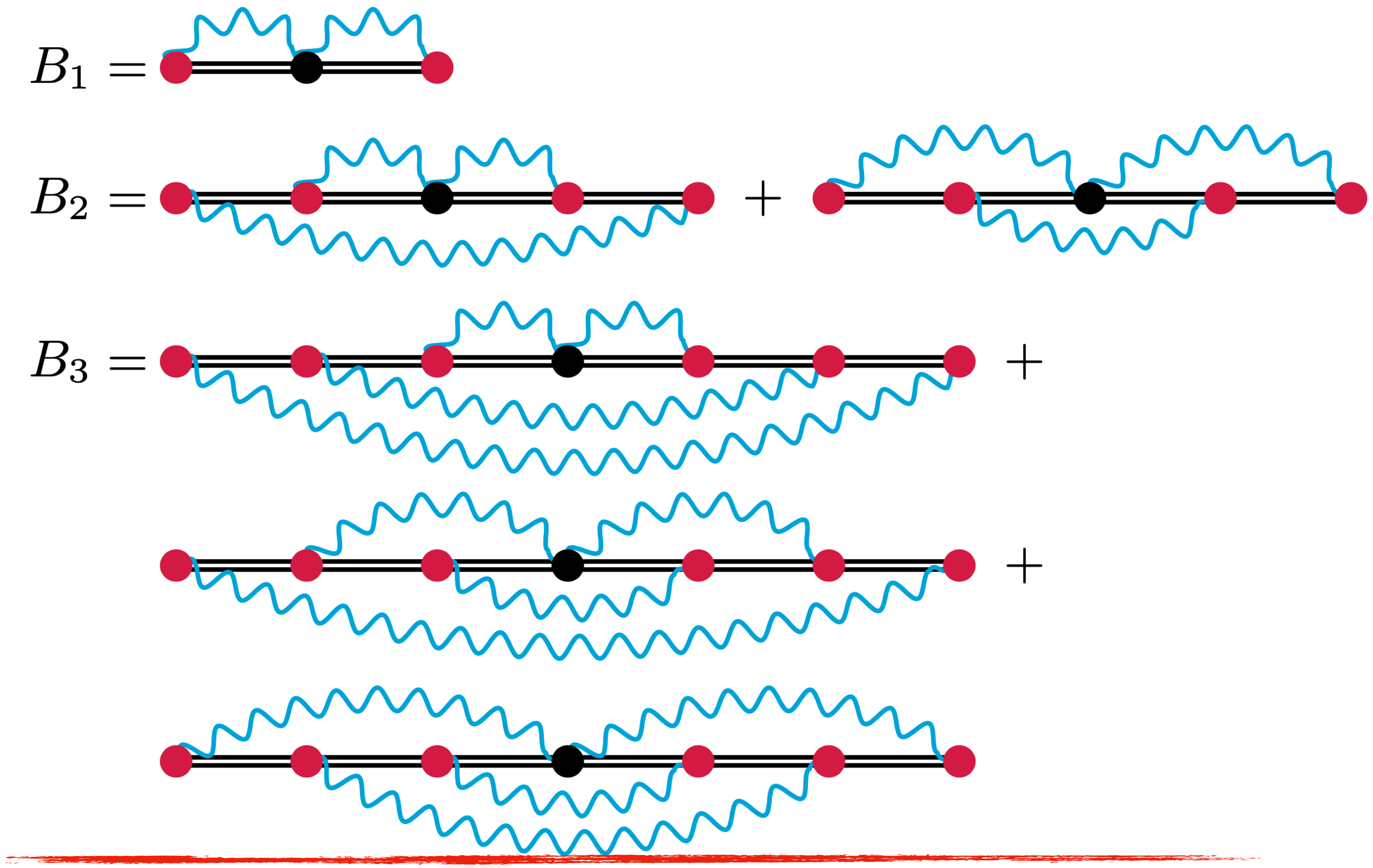
G. F. Reiter, PRB **49**, 1536 (1994)

Magnetisation around hole

$\sim \langle \Psi_{\mathbf{p}} | \hat{h}^\dagger \hat{h} \hat{b}^\dagger \hat{b} | \Psi_{\mathbf{p}} \rangle$ gives structure

$$M_{\mathbf{p}}(\mathbf{d}) = \frac{\langle \hat{h}_{\mathbf{r}}^\dagger \hat{h}_{\mathbf{r}} \, \hat{S}_{\mathbf{r}+\mathbf{d}}^{(z)} \rangle_{\mathbf{p}}}{\langle \hat{h}_{\mathbf{r}}^\dagger \hat{h}_{\mathbf{r}} \rangle_{\mathbf{p}} \, \langle \hat{S}_{\mathbf{r}+\mathbf{d}}^{(z)} \rangle_{\mathbf{p}}}$$



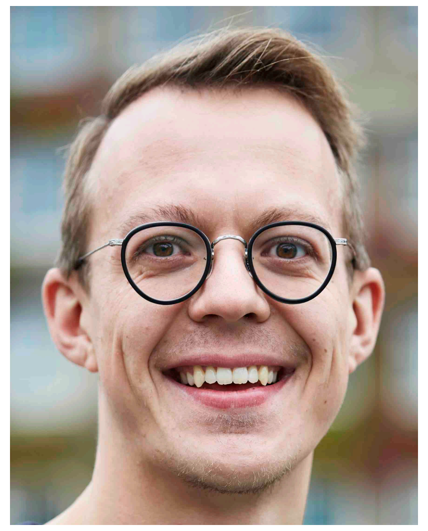


$B_4 = \cdots$

A. Ramsak and P. Horsch, PRB **57**, 4308 (1998)

Describe strong coupling regime

- Hubbard → t-J model assumes t≫J=4t²/U
- SCBA most accurate for t≫J

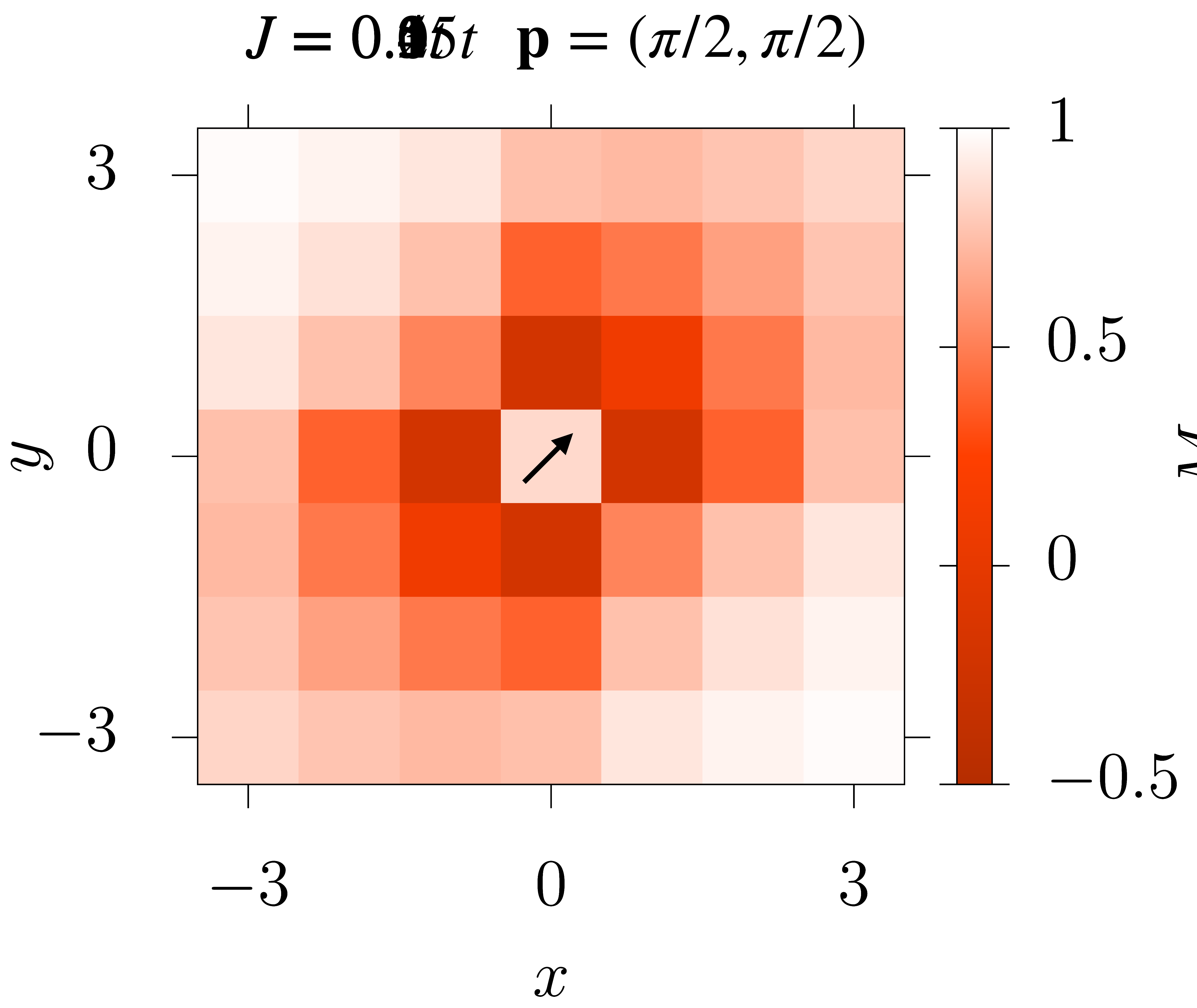


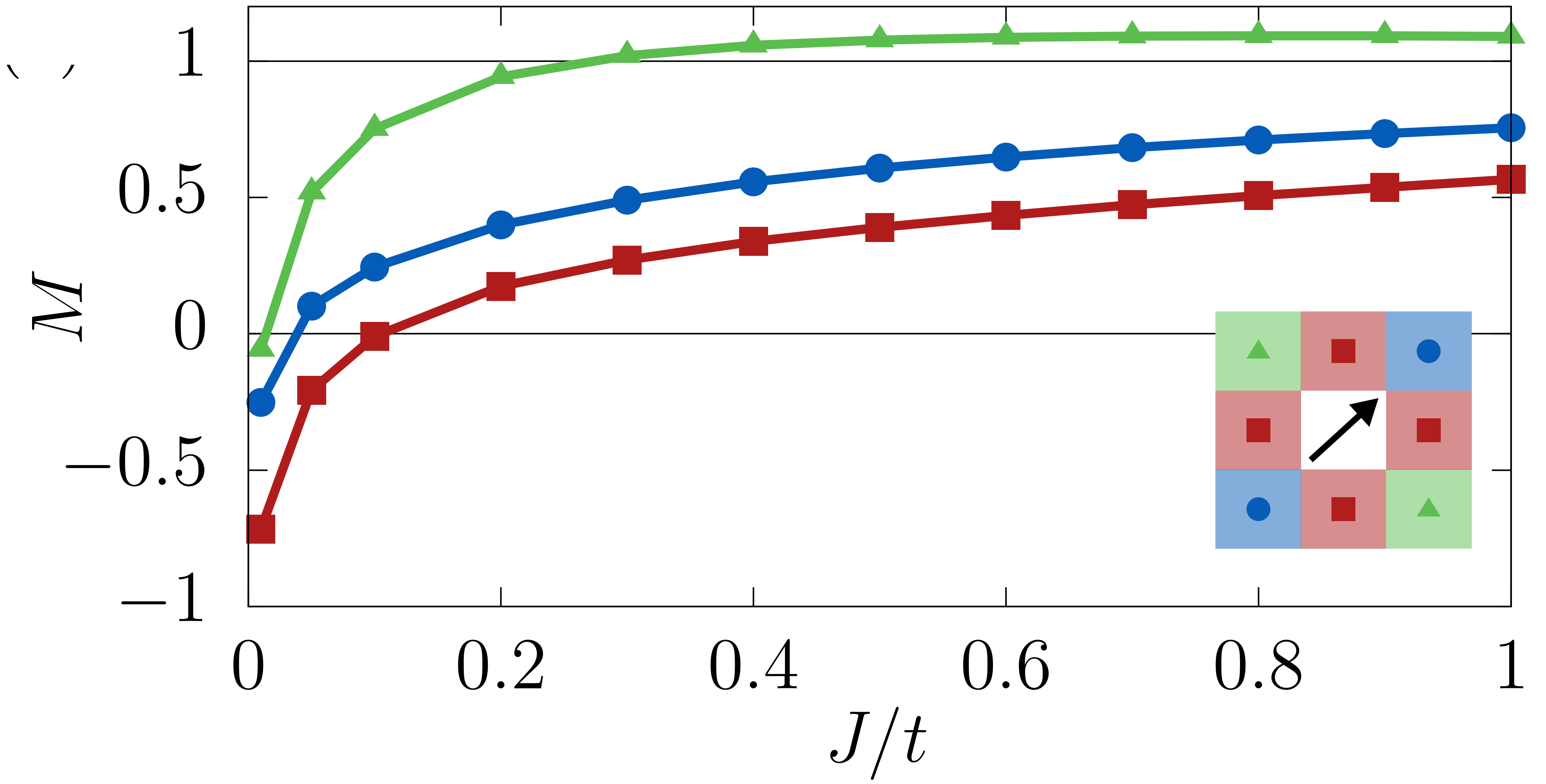
Infinite order

K. Knakkergaard arXiv:2106.14510

Numerical results

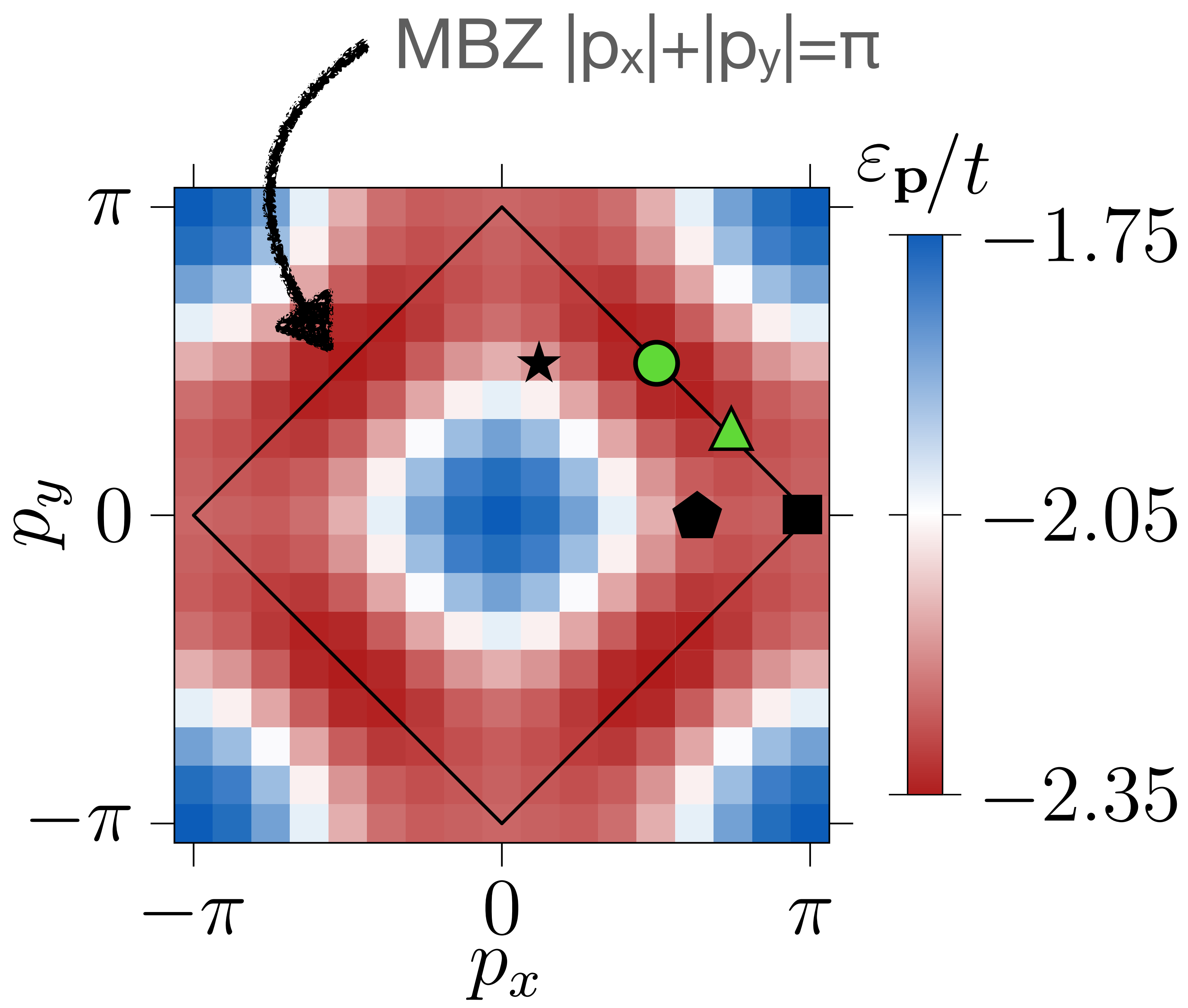
$$M_{\mathbf{p}}(\mathbf{d}) = \frac{\langle \hat{h}^\dagger_{\mathbf{r}} \hat{h}_{\mathbf{r}}\, \hat{S}^{(z)}_{\mathbf{r}+\mathbf{d}} \rangle_{\mathbf{p}}}{\langle \hat{h}^\dagger_{\mathbf{r}} \hat{h}_{\mathbf{r}} \rangle_{\mathbf{p}}\, \langle \hat{S}^{(z)}_{\mathbf{r}+\mathbf{d}} \rangle_{\mathbf{p}}}$$



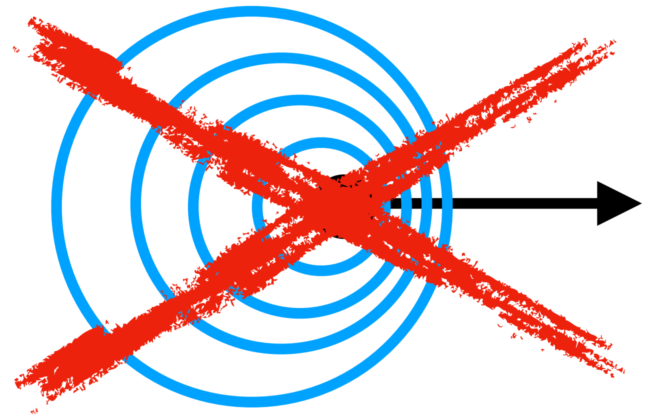


- Magnetic dressing cloud grows in magnitude and extend with t/J
- Magnetisation flipped for strong coupling
- Elongated shape

Look closer at shape of dressing cloud:



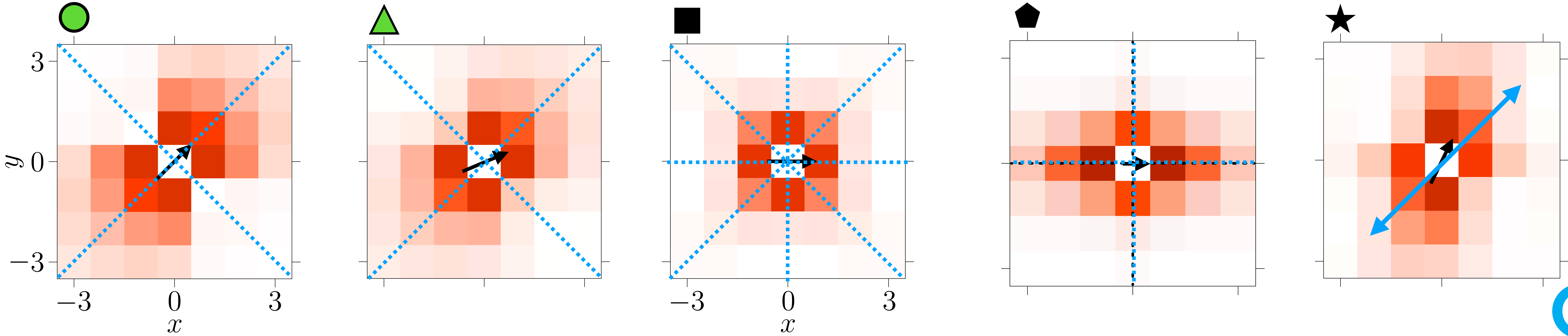
- Time-reversal symmetry ⇒ inversion symmetry



- AF translational symmetry ⇒ mirror symmetries along diagonals for $|p_x|+|p_y|=\pi$

Full C_{4v} symmetry of AF lattice!

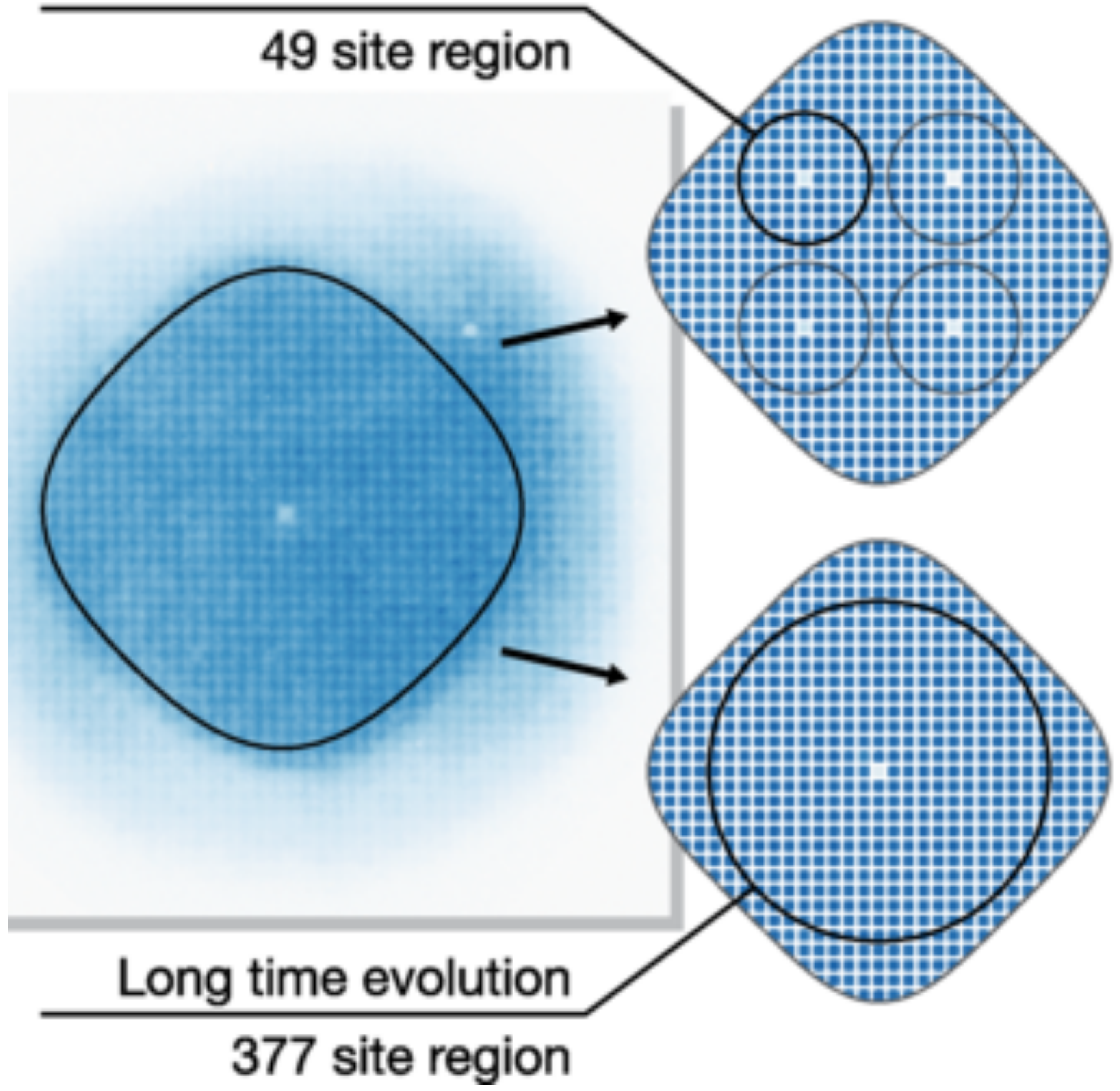
$J/t = 0.3$



Non-equilibrium dynamics of holes

Formation of the magnetic polaron

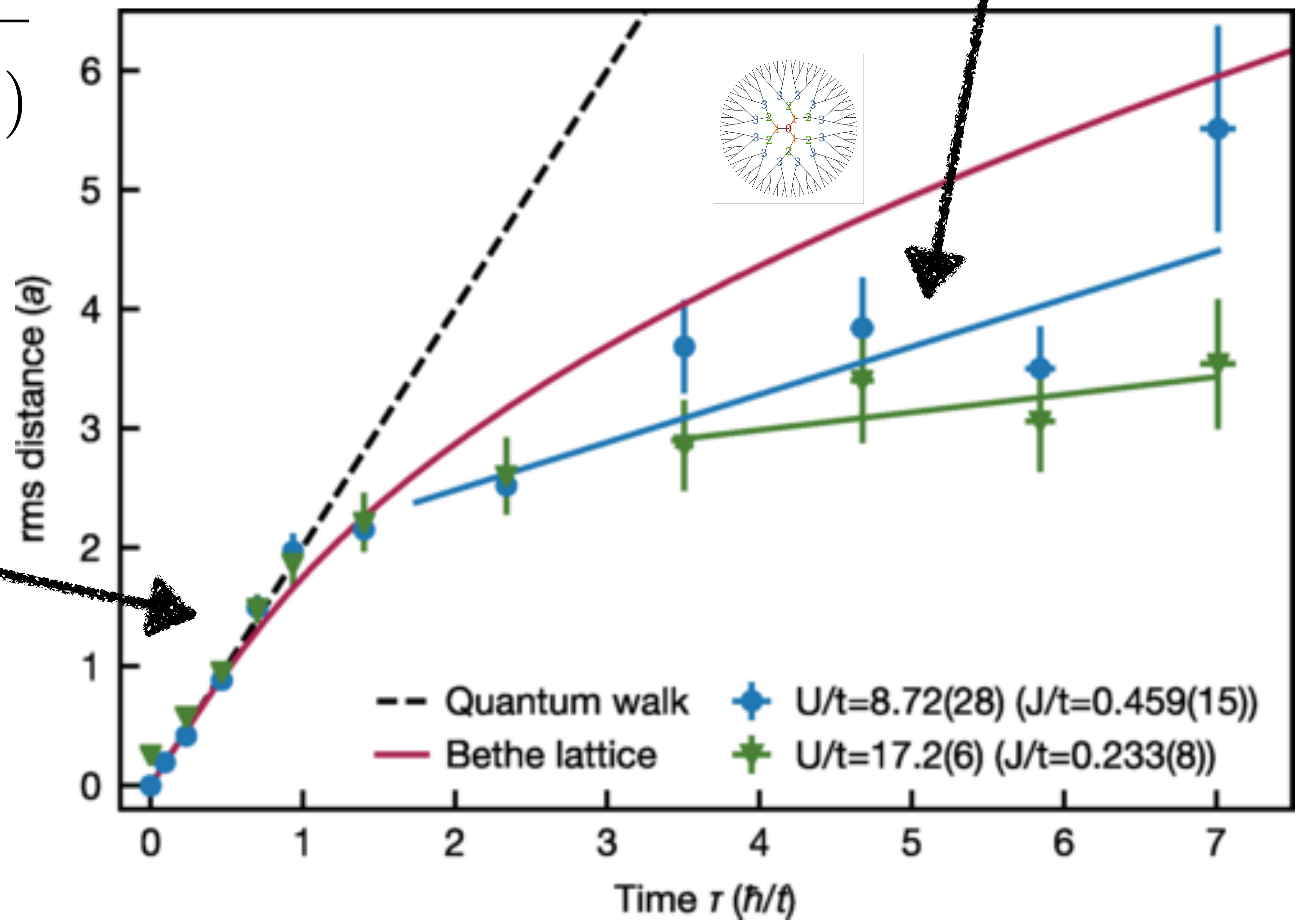
Experiments release hole and observes how it evolves:



$$d = \sqrt{\sum_{\mathbf{r}} r^2 \cdot n_h(\mathbf{r})}$$

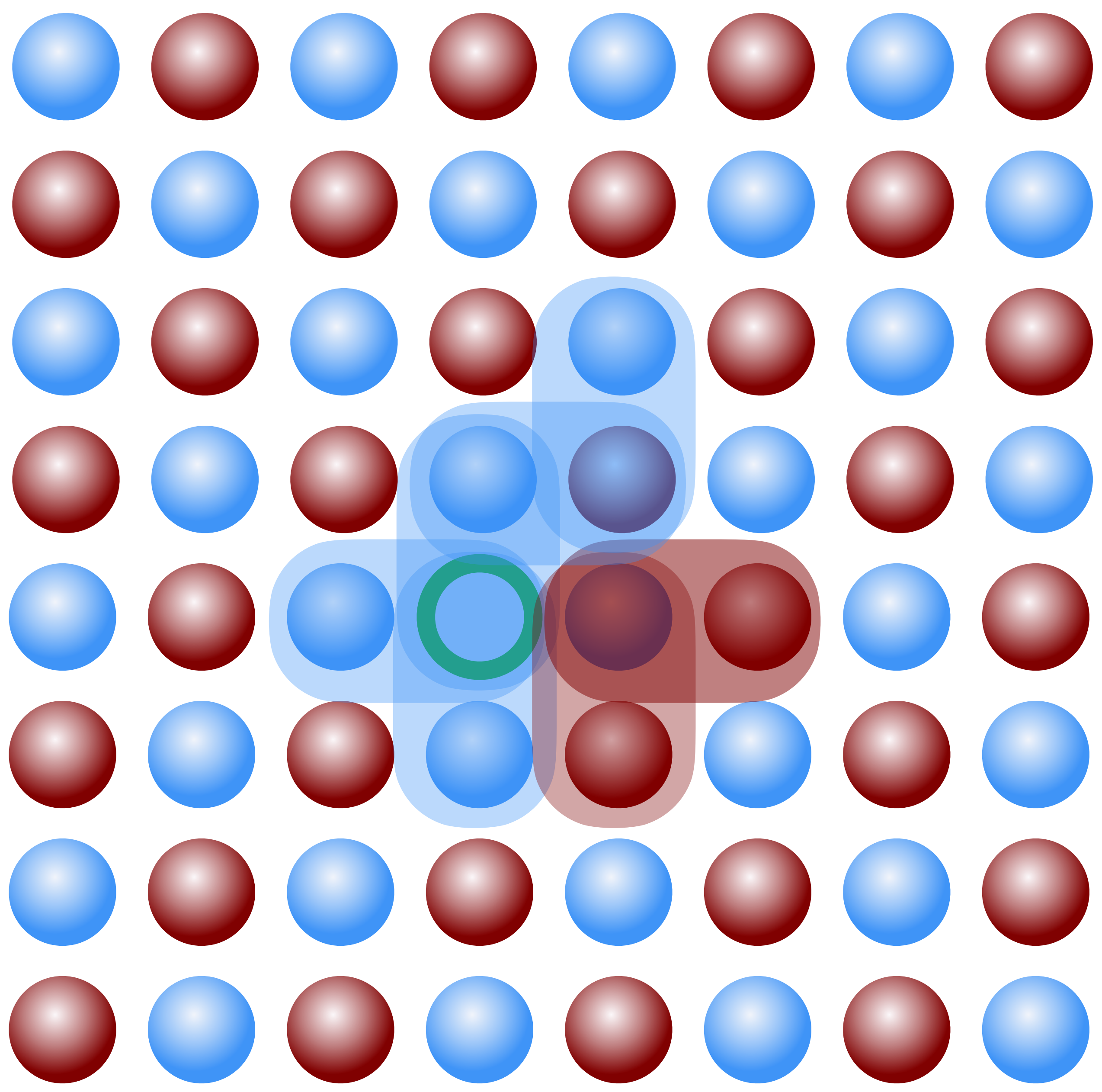
Initial fast quantum walk

Slower long time dynamics



Ji *et al.*, PRX **11**, 021022 (2021)

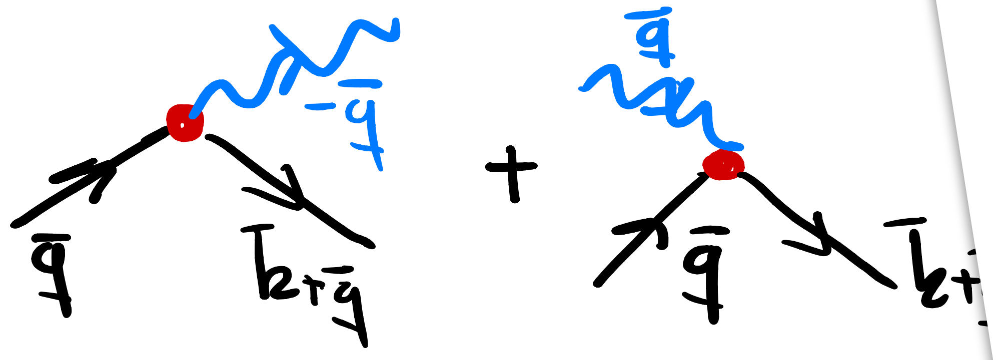
Time-dependent version of SCBA



Initial wave fn $|\Psi_{\mathbf{p}}(\tau=0)\rangle = \hat{h}^\dagger_{\mathbf{p}}|\mathrm{AF}\rangle$

Subsequent motion creates spin waves

$$\hat{H} = \sum_{\mathbf{q},\mathbf{k}} \hat{h}^\dagger_{\mathbf{q}+\mathbf{k}}\hat{h}_{\mathbf{q}}\Big[g(\mathbf{q},\mathbf{k})\hat{b}^\dagger_{-\mathbf{k}} + g(\mathbf{q}+$$



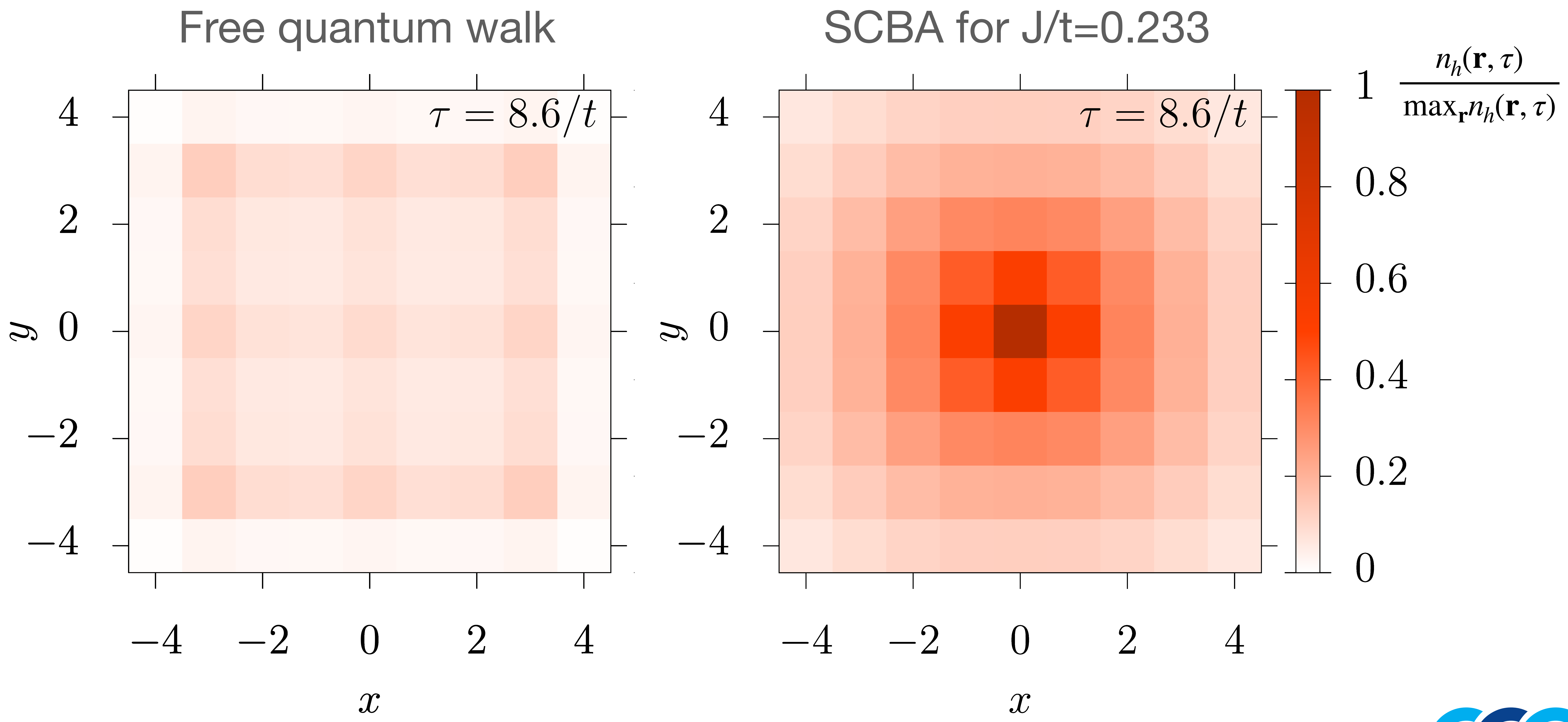
Solve to infinite order within SCBA

Time-dependent wave fn

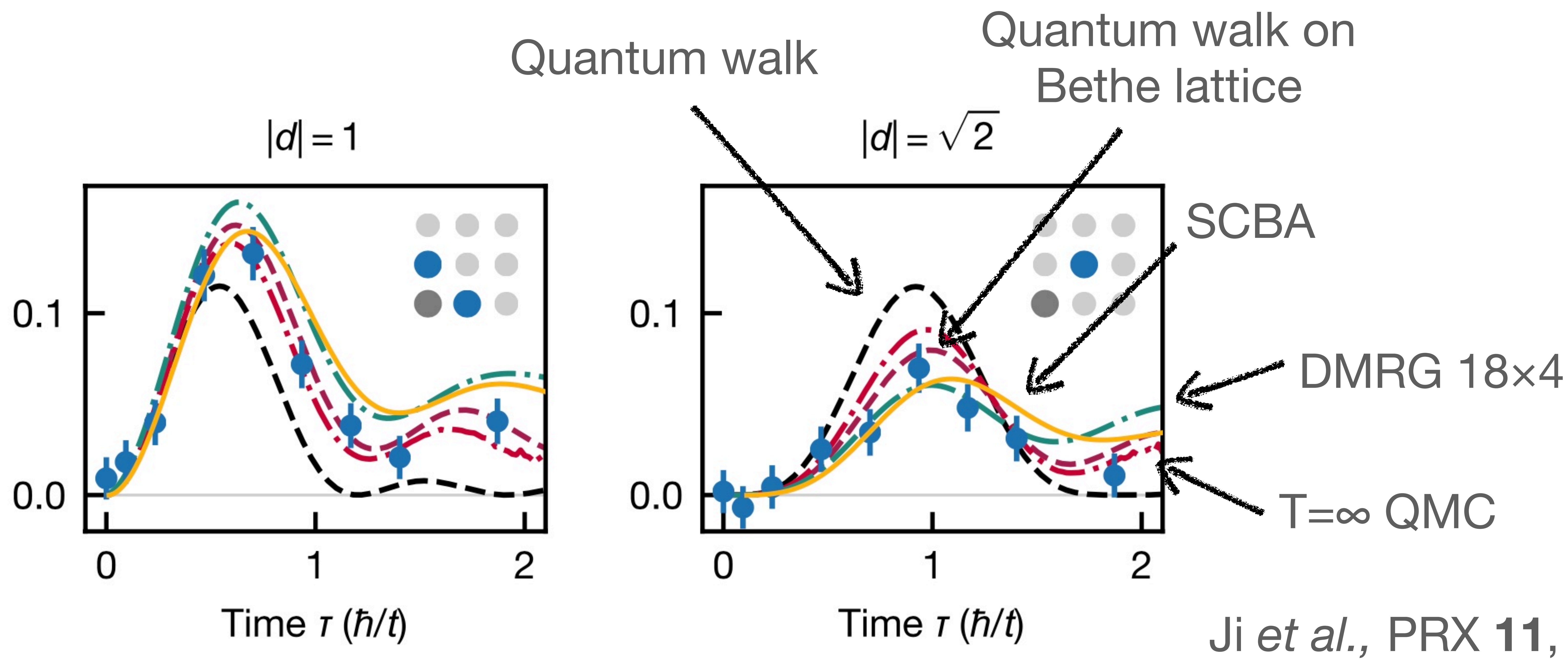
$$|\Psi_{\mathbf{p}}(\tau)\rangle = [c_0(\mathbf{p};\tau)\hat{h}^\dagger_{\mathbf{p}} + \sum_{\mathbf{k}_1} c_1(\mathbf{p},\mathbf{k}_1;\tau)\hat{h}^\dagger_{\mathbf{p}+\mathbf{k}_1}\hat{b}^\dagger_{-\mathbf{k}_1} + \sum_{\mathbf{k}_1,\mathbf{k}_2} c_2(\mathbf{p},\mathbf{k}_1,\mathbf{k}_1;\tau)\hat{h}^\dagger_{\mathbf{p}+\mathbf{k}_1+\mathbf{k}_2}\hat{b}^\dagger_{-\mathbf{k}_2}\hat{b}^\dagger_{-\mathbf{k}_1} + \ldots]|\mathrm{AF}\rangle$$

Create hole at **r=0** and see what happens:

$$\langle \Psi(\tau) | \hat{h}^\dagger_{\mathbf{r}} \hat{h}_{\mathbf{r}} | \Psi(\tau) \rangle$$



Catches short time behaviour



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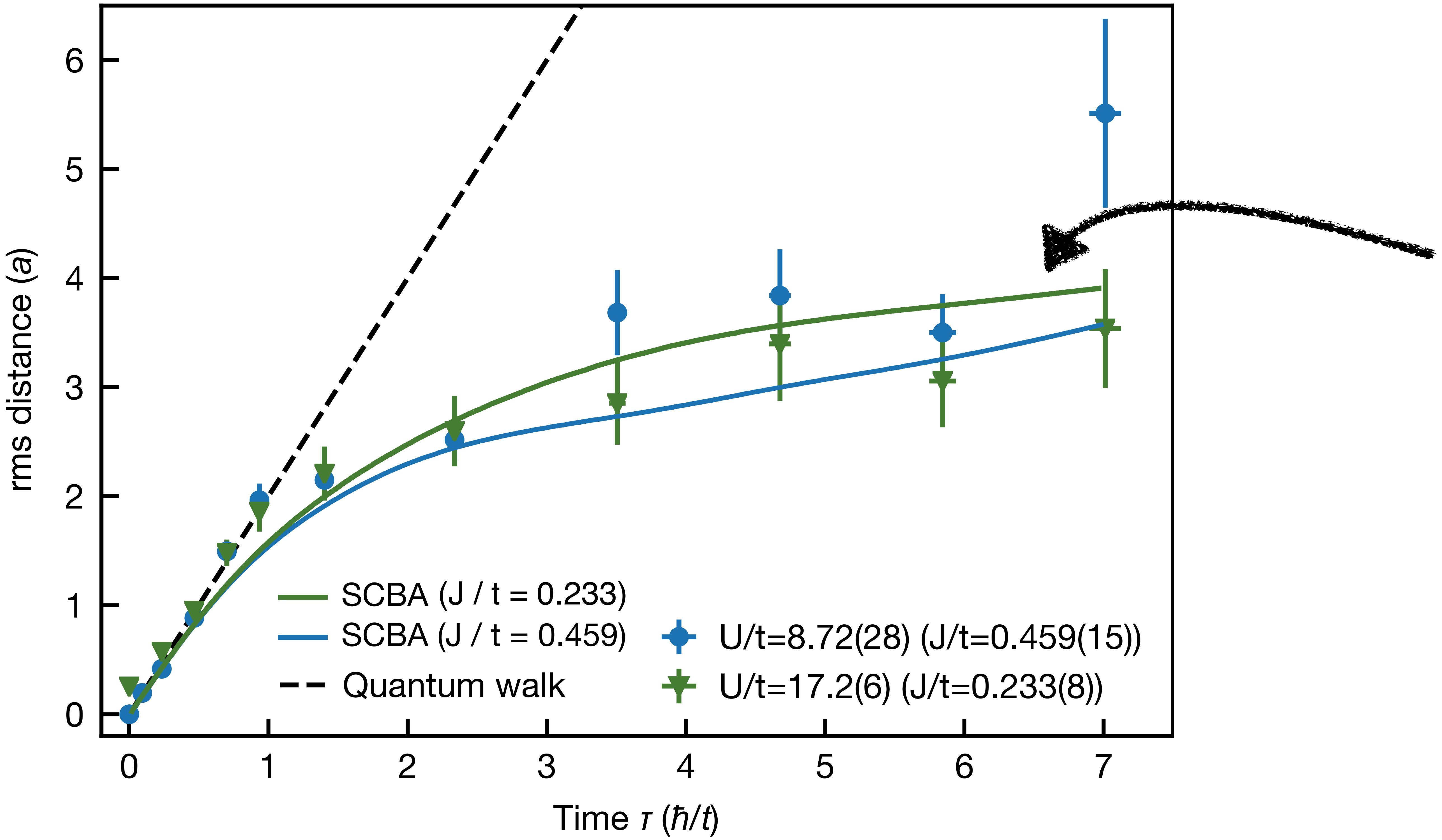
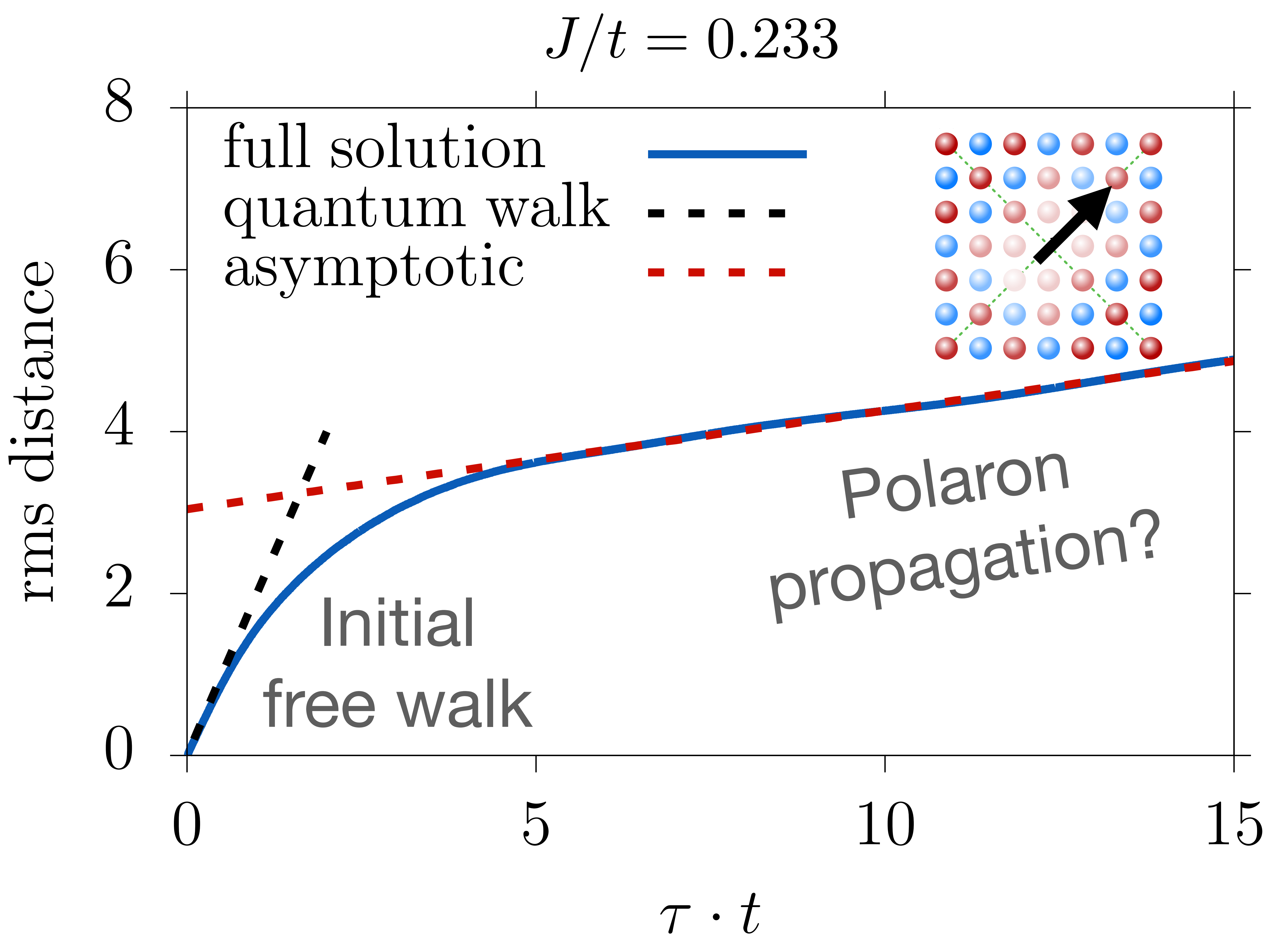
As well as long time dynamics

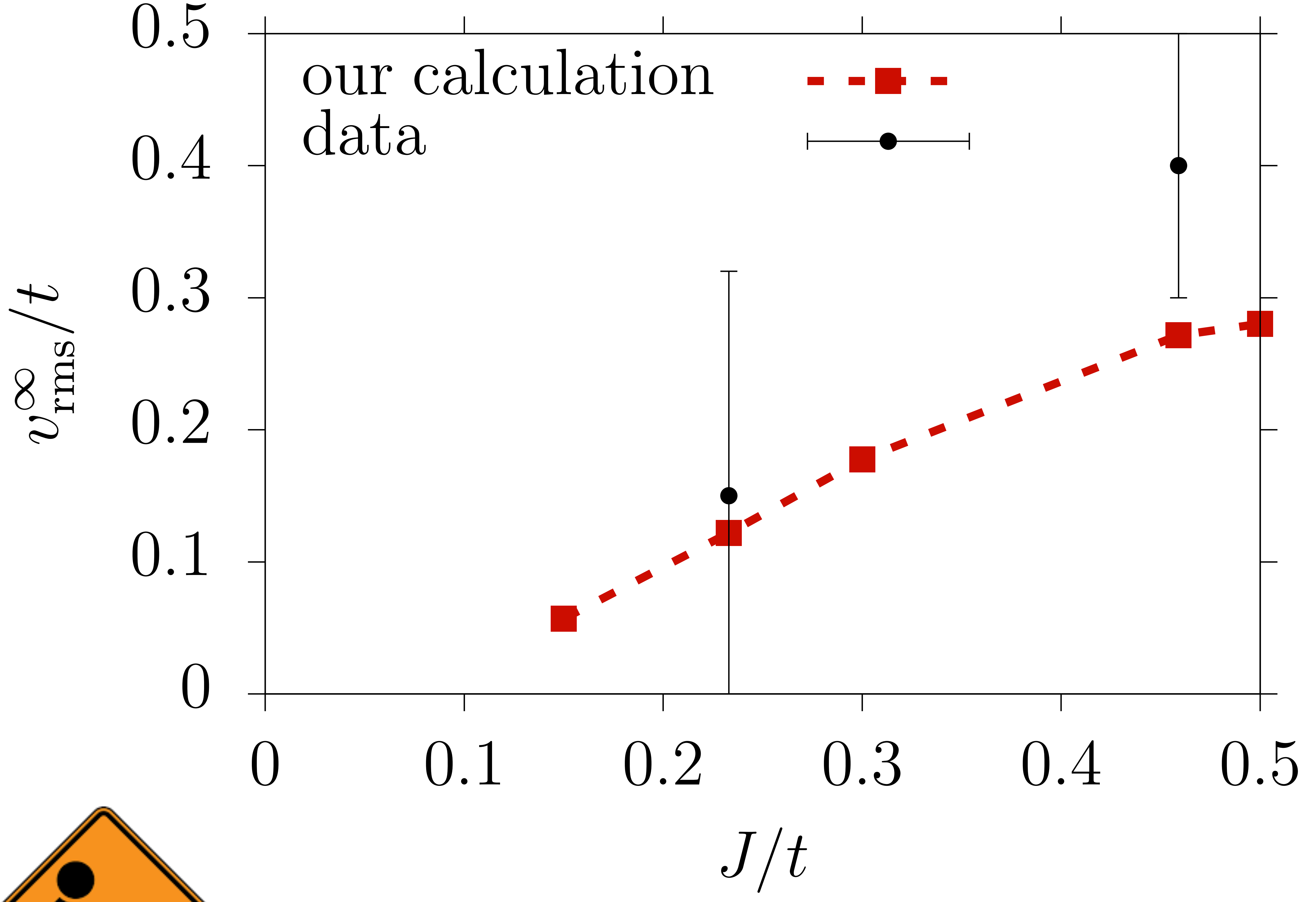
$$d = \sqrt{\sum_{\mathbf{r}} r^2 \cdot n_h(\mathbf{r})}$$



Works better for stronger coupling

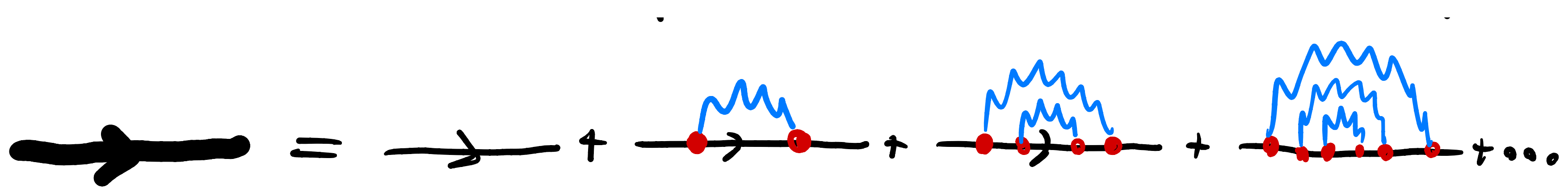
Formation of magnetic polaron



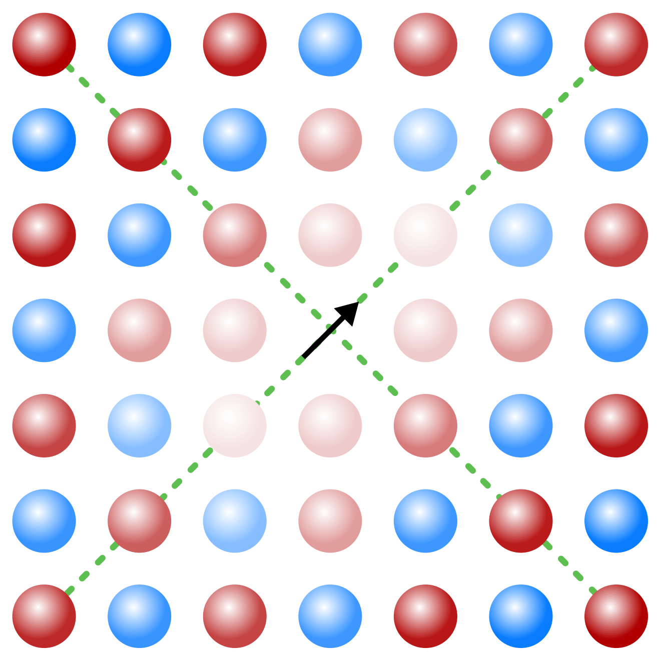


Conclusions

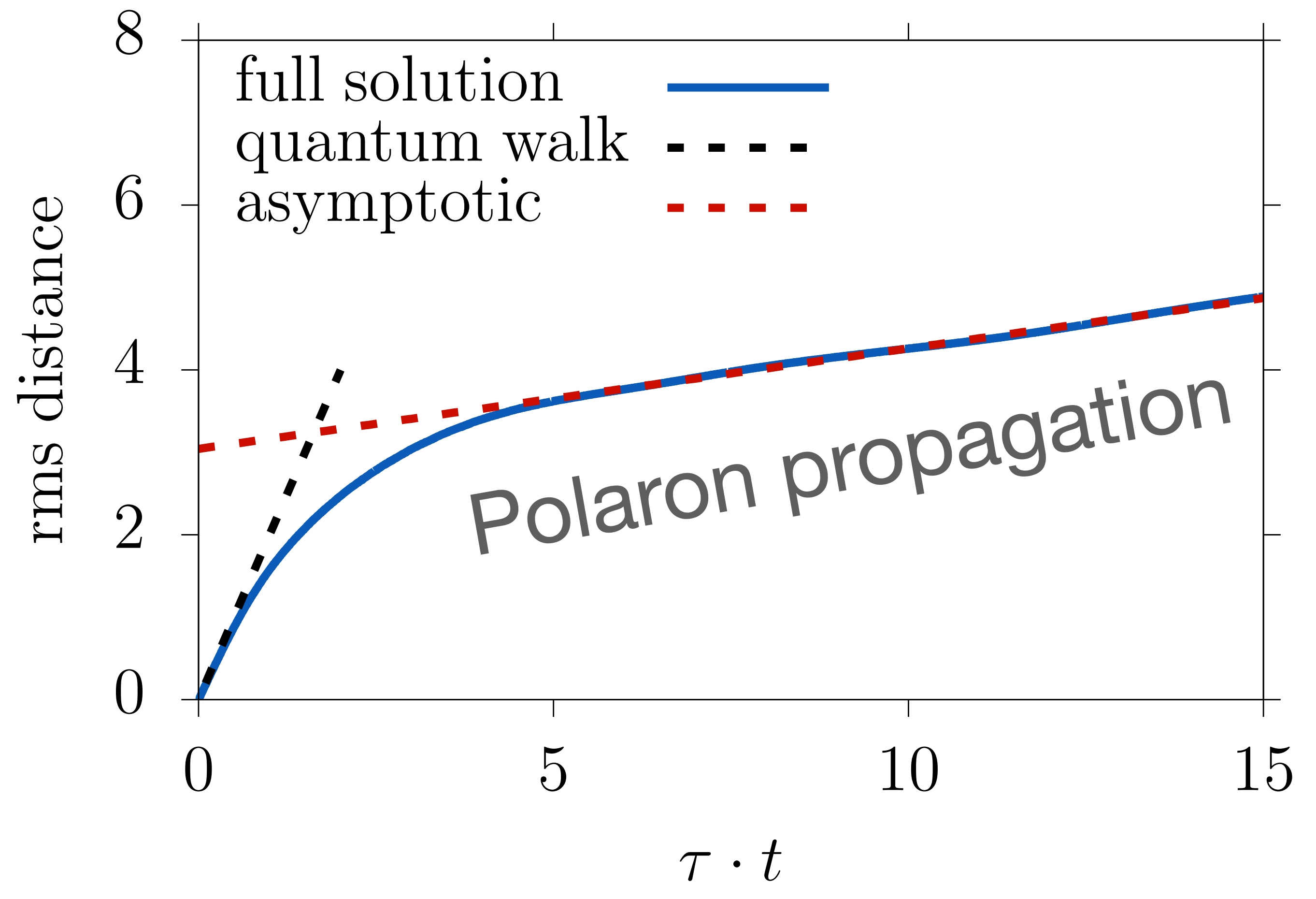
- SCBA to describe polarons



- Include spin waves to infinite order to calculate magnetic dressing cloud



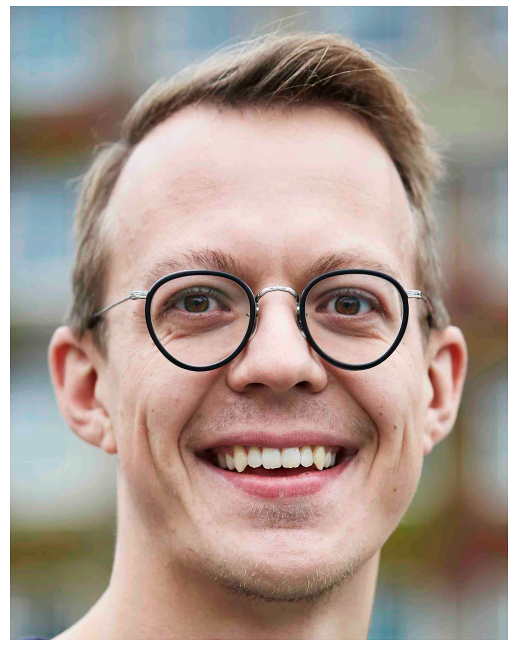
- Extend SCBA to non-equil. dynamics



arXiv:2106.14510

T. Pohl

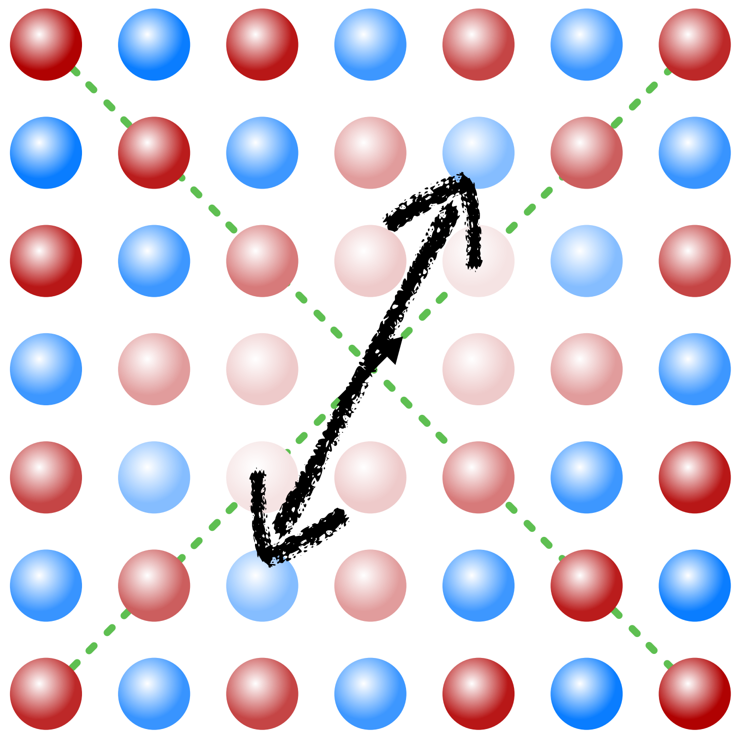
M. Bastarrachea-Magnani

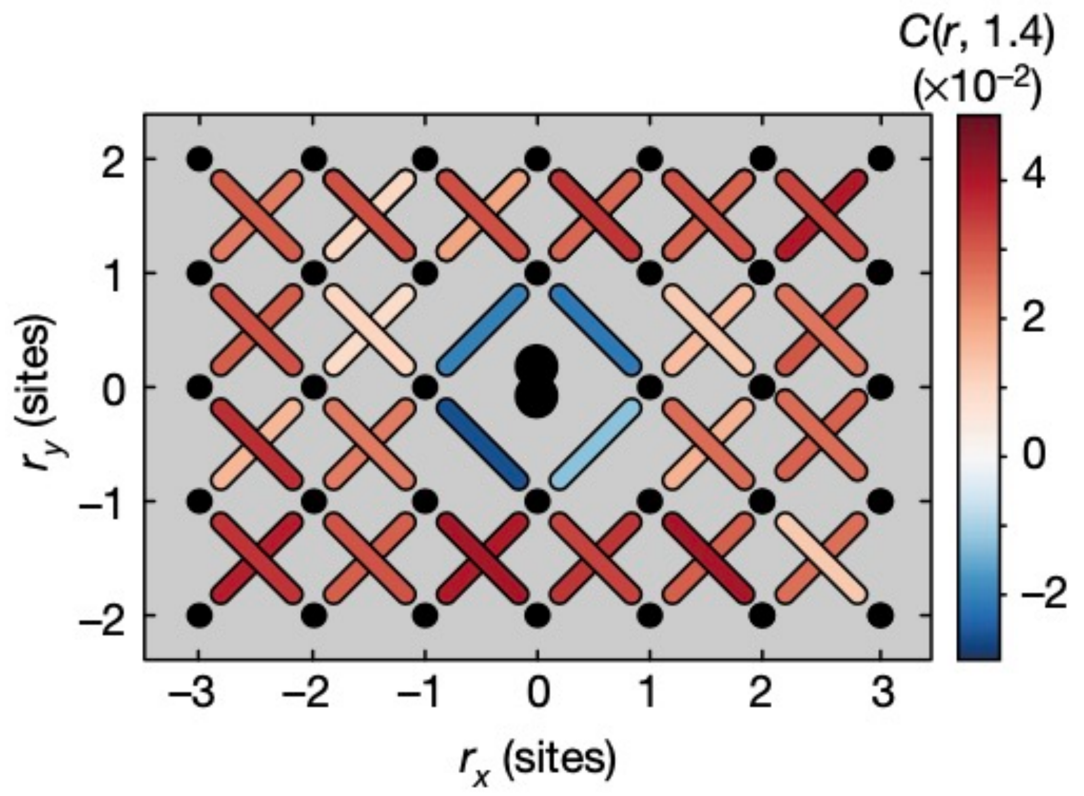


K. Knakkergaard

Outlook

- Non-zero temperature effects (T≈0.5J)
- Higher order correlation functions





J. Koepsell *et al*., Nature **572**, 358 (2019)

- Hole-hole correlations and pairing?