Emergent Majorana and Dirac fermions in spin and electronic systems

Fakher Assaad. Fractionalization and Emergent Gauge Fields in Quantum Matter (ICTP 4-8 – 14 December 2023)

Organization

- Fermion quantum Monte Carlo
- Numerical simulations of models of $RuCl_3$
- Deconfined quantum criticality in a two-dimensional Su-Schrieffer-Heeger model
- Conclusions

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Fakher Assaad. Fractionalization and Emergent Gauge Fields in Quantum Matter (ICTP 4-8 – 14 December 2023)

Many thanks to.....

T. Sato (IFW Dresden)

K. Modic (ISTA Vienna)

B. Ramshaw (Cornell University)

A. Götz (Würzburg)

M. Hohenadler (Münich)

Quantum Monte Carlo for fermions

$$Z = \mathrm{Tr} e^{-\beta \hat{H}} = \int D\left\{\Phi(i,\tau)\right\} e^{-S\{\Phi(i,\tau)\}}$$

$\Phi(\boldsymbol{x},\tau)$: Hubbard-Stratonovich (or arbitrary field with predefined dynamics)

Multidimensional integral → Monte Carlo

One body problem in external field → Polynomial complexity

R. Blankenbecler, D. J. Scalapino, and R. L. Sugar, Phys. Rev. D 24 (1981), 2278
J. E. Hirsch, Phys. Rev. B 31 (1985), 4403
White, D. Scalapino, R. Sugar, E. Loh, J. Gubernatis, and R. Scalettar, Phys. Rev. B 40 (1989), 506
....

Let $\hat{H} = \hat{H}_0 - \lambda \sum_n \left(\hat{\boldsymbol{c}}^\dagger O^{(n)} \hat{\boldsymbol{c}} \right)^2$ with $O^{(n)} = O^{(n),\dagger}$ and $\left\{ \hat{c}_x^\dagger, \hat{c}_y \right\} = \delta_{x,y}$

$$e^{-S(\Phi(n,\tau))} = e^{-\sum_{n,\tau} \Phi^2(n,\tau)/2} \, \mathrm{Tr} \prod_{\tau=1}^{L_\tau} \left(e^{-\Delta\tau \hat{H}_0} \prod_n e^{\sqrt{2\Delta\tau\lambda}\Phi(n,\tau) \hat{\boldsymbol{c}}^\dagger O^{(n)} \hat{\boldsymbol{c}}} \right) = e^{-\sum_{n,\tau} \Phi^2(n,\tau)/2 + \log \det M(\Phi)}$$

$L_\tau \Delta\tau = \beta$

Let $\hat{H} = \hat{H}_0 - \lambda \sum_n \left(\hat{\boldsymbol{c}}^\dagger O^{(n)} \hat{\boldsymbol{c}} \right)^2$ with $O^{(n)} = O^{(n),\dagger}$ and $\left\{ \hat{c}_x^\dagger, \hat{c}_y \right\} = \delta_{x,y}$

$$e^{-S(\Phi(n,\tau))} = e^{-\sum_{n,\tau} \Phi^2(n,\tau)/2} \, \mathrm{Tr} \prod_{\tau=1}^{L_\tau} \left(e^{-\Delta\tau \hat{H}_0} \prod_n e^{\sqrt{2\Delta\tau\lambda}\Phi(n,\tau) \hat{\boldsymbol{c}}^\dagger O^{(n)} \hat{\boldsymbol{c}}} \right) = e^{-\sum_{n,\tau} \Phi^2(n,\tau)/2 + \log\det M(\Phi)}$$

$L_\tau \Delta\tau = \beta$

- $S(\Phi)$ is complex → $\langle \mathrm{sign} \rangle = \dfrac{\int D\{\Phi\} e^{-S\{\Phi\}}}{\int D\{\Phi\} \left| e^{-S\{\Phi\}} \right|} \propto e^{-\alpha\beta V}$ Computational cost $e^{2\alpha\beta V}$ → Minimize α
- Long auto-correlations times
- .....

Algorithms for Lattice fermions @ http://alf.physik.uni-wuerzburg.de/

ALF 1.0: SciPost Phys. 3 (2017), 013 ALF 2.0 SciPost Phys. Codebases 1 (2022)

Kinetic

Potential (sum of perfect squares)

$$\hat{H} = \sum_{k=1}^{M_T}\sum_{\sigma=1}^{N_{\mathrm{col}}}\sum_{s=1}^{N_{\mathrm{fl}}}\sum_{x,y}^{N_{\mathrm{dim}}} \hat{c}^{\dagger}_{x\sigma s} T^{(ks)}_{xy} \hat{c}_{y\sigma s} + \sum_{k=1}^{M_V} U_k \left\{ \sum_{\sigma=1}^{N_{\mathrm{col}}}\sum_{s=1}^{N_{\mathrm{fl}}} \left[\left(\sum_{x,y}^{N_{\mathrm{dim}}} \hat{c}^{\dagger}_{x\sigma s} V^{(ks)}_{xy} \hat{c}_{y\sigma s} \right) + \alpha_{ks} \right] \right\}^2$$

Coupling of fermions to bosonic fields with predefined dynamics

$$+ \sum_{k=1}^{M_I} \hat{Z}_k \left(\sum_{\sigma=1}^{N_{\mathrm{col}}}\sum_{s=1}^{N_{\mathrm{fl}}}\sum_{x,y}^{N_{\mathrm{dim}}} \hat{c}^{\dagger}_{x\sigma s} I^{(ks)}_{xy} \hat{c}_{y\sigma s} \right) + \hat{H}_{\mathrm{Ising}}$$

- Block diagonal in flavors, N_{fl}
- SU(N_{col}) symmetric in colors N_{col}
- Arbitrary Bravais lattice for d=1,2
- Model can be specified at minimal programming cost
- Fortran 2003 standard
- MPI implementation
- Global and local moves, Parallel tempering, Langevin
- Projective and finite T approaches
- pyALF: easy access python interface
- Predefined models


F. Goth


M. Bercx


J. Hoffmann


J. S.E. Portela


J. Schwab


Z. Liu


E. Huffman


A. Götz


F. Parisen Toldin

DFG Wissenschaftliche Literaturversorgungs und Informationssysteme (LIS)

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A fermion approach generalized Kitaev models

PHYSICAL REVIEW B **104**, L081106 (2021)

Letter

Quantum Monte Carlo simulation of generalized Kitaev models

Toshihiro Sato[1] and Fakher F. Assaad[1,2]

[1] *Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany*

[2] *Würzburg-Dresden Cluster of Excellence ct.qmat, Am Hubland, 97074 Würzburg, Germany*

T. Sato

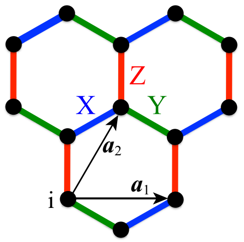
Scale-invariant magnetic anisotropy in α-$RuCl_3$: A quantum Monte Carlo study

Toshihiro Sato,[1,2] B. J. Ramshaw,[3,4] K. A. Modic,[5] and Fakher F. Assaad[1,6]

arXiv:2312.03080v1

K. Modic B. Ramshaw

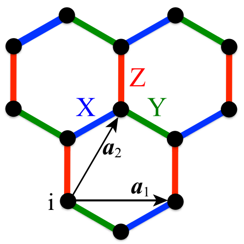
A fermion approach generalized Kitaev models



$$\hat{H} = 2K \sum_{i \in A, \delta} \hat{S}_i^\delta \hat{S}_{i+\delta}^\delta + J \sum_{i \in A, \boldsymbol{\delta}} \hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_{i+\delta}.$$

$$K = A \sin(\varphi), \; J = A \cos(\varphi), \; A = \sqrt{K^2 + J^2}$$

A fermion approach generalized Kitaev models



$$\hat{H} = 2K \sum_{i \in A, \delta} \hat{S}_i^{\delta} \hat{S}_{i+\delta}^{\delta} + J \sum_{i \in A, \boldsymbol{\delta}} \hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_{i+\delta}.$$

$$K = A \sin(\varphi), \ J = A \cos(\varphi), \ A = \sqrt{K^2 + J^2}$$

Simulating spins with fermions.

$$\hat{S}_i^{\delta} = \frac{1}{2} \sum_{s,s'} \hat{f}_{i,s}^{\dagger} \sigma_{s,s'}^{\delta} \hat{f}_{i,s'}$$

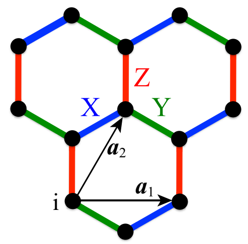
$$\sum_s \hat{f}_{i,s}^{\dagger} \hat{f}_{i,s} \equiv \hat{n}_i = 1$$

$$\hat{H}_{QMC} = |K| \sum_{i \in A, \delta} s_{\delta} \left(s_{\delta} \hat{S}_i^{\delta} + \frac{K}{|K|} \hat{S}_{i+\delta}^{\delta} \right)^2 - \frac{J}{8} \sum_{i \in A, \delta} \left(\left[\hat{D}_{i,\delta}^{\dagger} + \hat{D}_{i,\delta} \right]^2 + \left[i\hat{D}_{i,\delta} - i\hat{D}_{i,\delta}^{\dagger} \right]^2 \right) + U \sum_i (\hat{n}_i - 1)^2$$

$$\hat{D}_{i,\delta}^{\dagger} = \sum_s \hat{f}_{i,s}^{\dagger} \hat{f}_{i+\delta,s} \qquad s_{\delta} = \pm 1$$

Constraint commutes with Hamiltonian dynamics $\left[\hat{H}_{QMC}, \hat{n}_i \right] = 0$

A fermion approach generalized Kitaev models



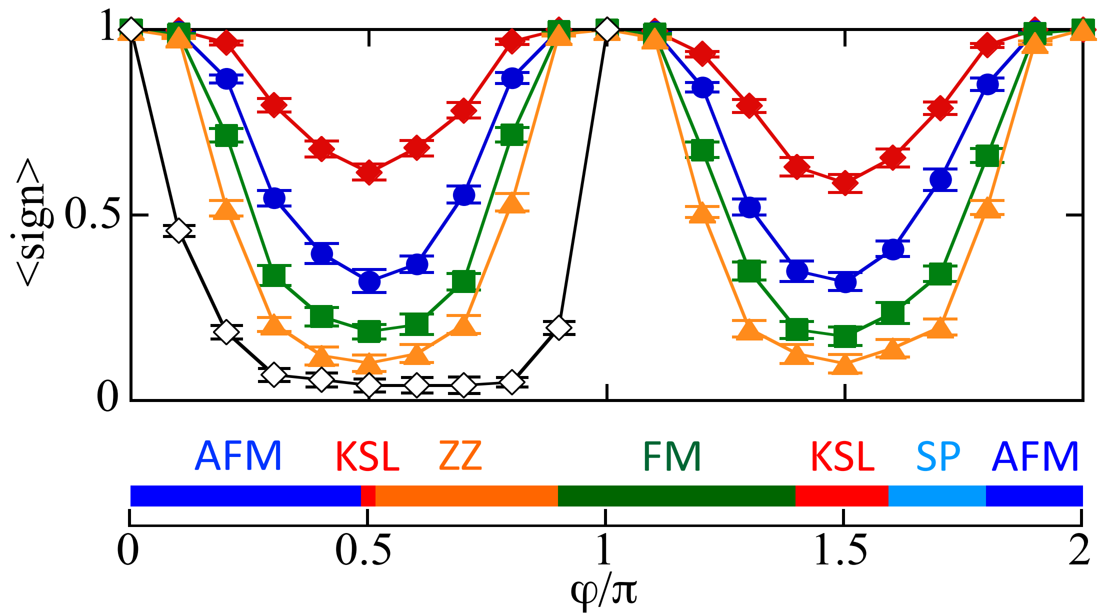
$$\hat{H} = 2K \sum_{i\in A,\delta} \hat{S}_i^\delta \hat{S}_{i+\delta}^\delta + J \sum_{i\in A,\boldsymbol{\delta}} \hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_{i+\delta}.$$

$$K = A\sin(\varphi),\ J = A\cos(\varphi),\ A = \sqrt{K^2+J^2}$$

$T/A = 1$

Filled symbols $s_x = 1, s_y = s_z = -1$

○ $s_x = s_y = s_z = 1$



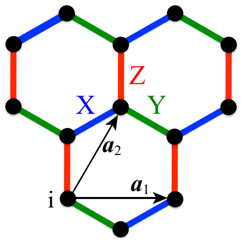
Possible to reach temperatures down to $\beta A \simeq 3$

$A \simeq 10meV \simeq 100K$

→ Experimentally relevant energy scales are accessible

J. Chaloupka, G. Jackeli, and G.Khaliullin Phys. Rev. Lett. 105 (2010), 027204.

A fermion approach generalized Kitaev models



$$\hat{H} = 2K \sum_{i \in A, \delta} \hat{S}_i^{\delta} \hat{S}_{i+\delta}^{\delta} + J \sum_{i \in A, \boldsymbol{\delta}} \hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_{i+\delta}.$$

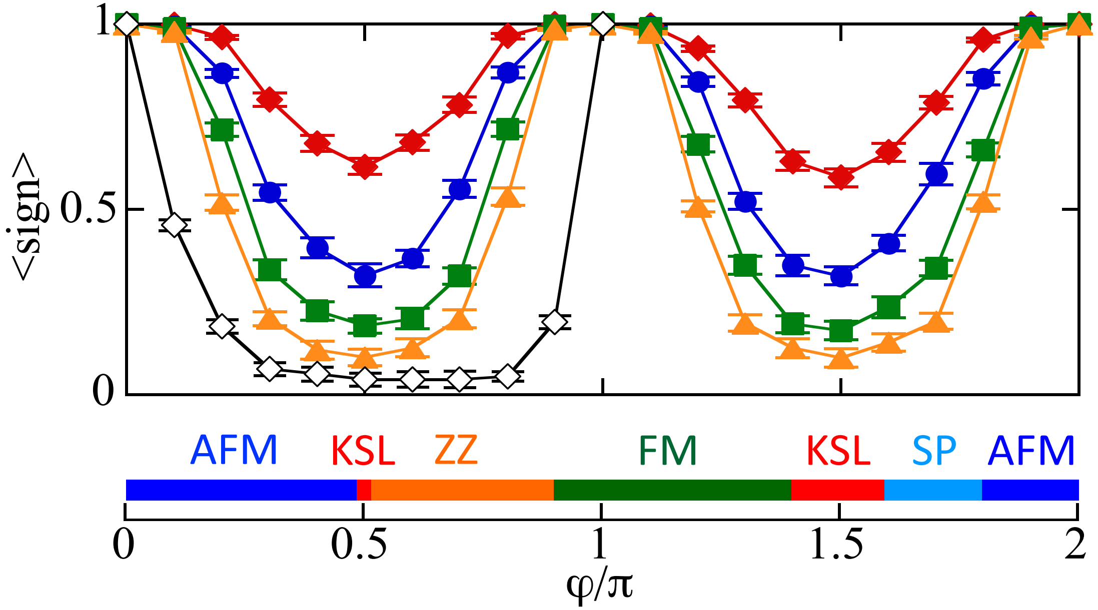
$$K = A \sin(\varphi), \; J = A \cos(\varphi), \; A = \sqrt{K^2 + J^2}$$

$T/A = 1$

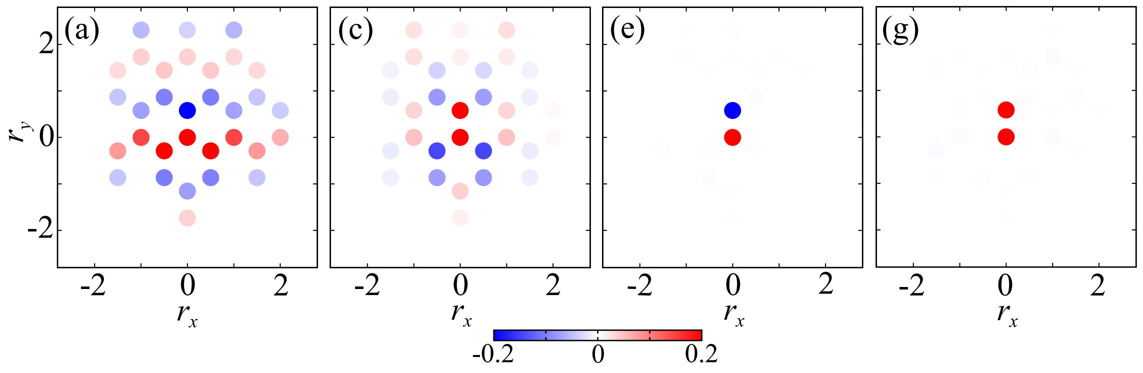
◆ V=18 ▲ V=72 Filled symbols $s_x = 1, s_y = s_z = -1$

● V=32 ○ V=18 ○ $s_x = s_y = s_z = 1$

■ V=50



$\varphi/\pi = 0.8$ $\varphi/\pi = 1.7$ $\varphi/\pi = 0.5$ $\varphi/\pi = 1.5$

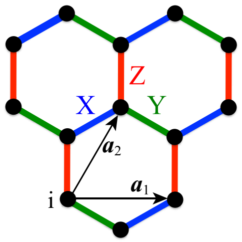


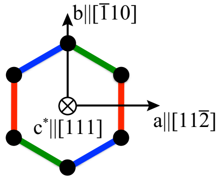
$\langle \hat{S}_{\boldsymbol{r}}^1 \hat{S}_{\boldsymbol{0}}^1 \rangle$

J. Chaloupka, G. Jackeli, and G.Khaliullin Phys. Rev. Lett. 105 (2010), 027204.

A fermion approach generalized Kitaev models

$RuCl_3$



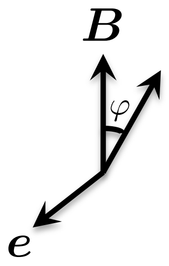


$$\hat{H}(\varphi) = \sum_{\langle i,j \rangle} \left[K \hat{S}_i^\gamma \hat{S}_j^\gamma + \Gamma \hat{S}_i^\alpha \hat{S}_j^\beta + J_1 \hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_j \right] + J_3 \sum_{\langle\langle i,j \rangle\rangle} \hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_j - \mu_B \sum_i \boldsymbol{B}(\varphi) \cdot \boldsymbol{g} \hat{\boldsymbol{S}}_i$$

$$(J_1, J_3, K, \Gamma) = (-0.5, 0.5, -5.0, 2.5) \ [\mathrm{meV}] \qquad \boldsymbol{g} = \mathrm{diag}\left[2.3, 2.3, 1.3\right]$$

Winter et al. Nat. Comm. 8 (2017), PRL. 120 (2018)

Magnetotropic susceptibility



$$e^{i\varphi \boldsymbol{K}\cdot \boldsymbol{e}} \boldsymbol{B} \equiv \boldsymbol{B}(\varphi)$$

PHYSICAL REVIEW B **108**, 035111 (2023)

Magnetotropic susceptibility

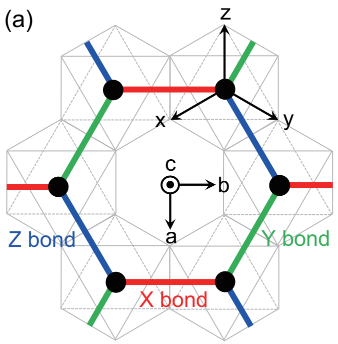
A. Shekhter,[1,*] R. D. McDonald,[1] B. J. Ramshaw,[2] and K. A. Modic[3]

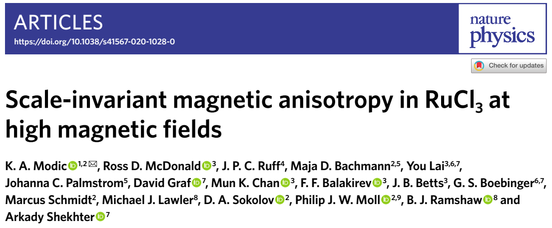
$$\frac{\partial F}{\partial \varphi} = \mu_B \sum_{\boldsymbol{i}} \hat{t}_{\boldsymbol{i}} \quad \text{with} \quad \hat{t}_{\boldsymbol{i}} = (\boldsymbol{e} \times \boldsymbol{B}) \cdot \boldsymbol{g} \hat{\boldsymbol{S}}_{\boldsymbol{i}}$$

$$k \equiv \frac{1}{V} \frac{\partial^2}{\partial \varphi^2} F(\varphi) \Big|_{\varphi=0} = \frac{1}{V} \left[\mu_B \boldsymbol{e} \times (\boldsymbol{e} \times \boldsymbol{B}) \cdot \boldsymbol{g} \langle \hat{\boldsymbol{S}}_{tot} \rangle - \mu_B^2 \sum_{\boldsymbol{i},\boldsymbol{j}} \int_0^\beta d\tau \ \left[\langle \hat{t}_{\boldsymbol{i}}(\tau) \hat{t}_{\boldsymbol{j}} \rangle - \langle \hat{t}_{\boldsymbol{i}} \rangle \langle \hat{t}_{\boldsymbol{j}} \rangle \right] \right.$$

Independent local moments: $\beta k = f(\beta B)$

A fermion approach generalized Kitaev models




ARTICLES

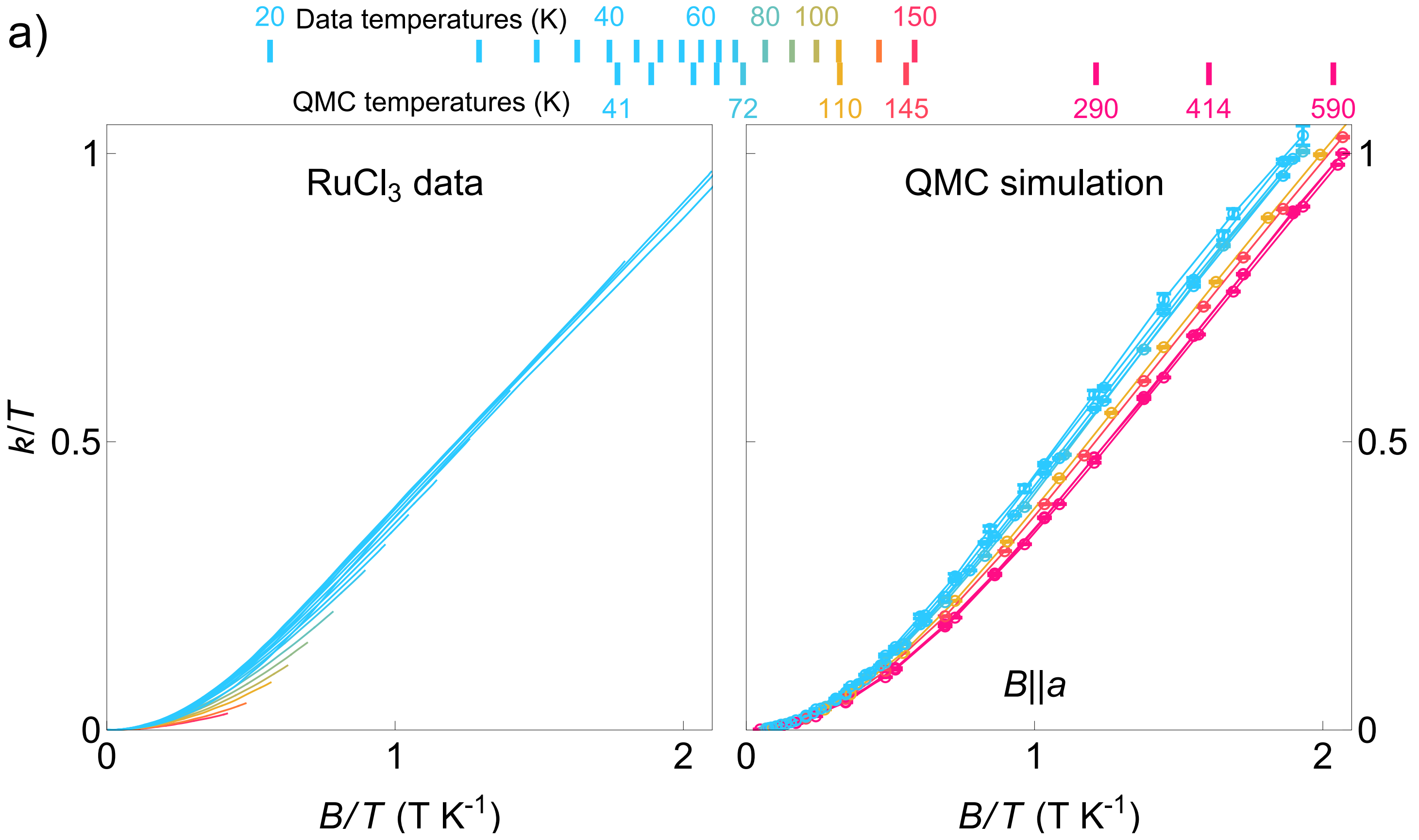
https://doi.org/10.1038/s41567-020-1028-0

nature physics

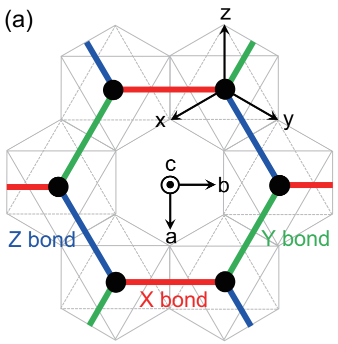
Check for updates

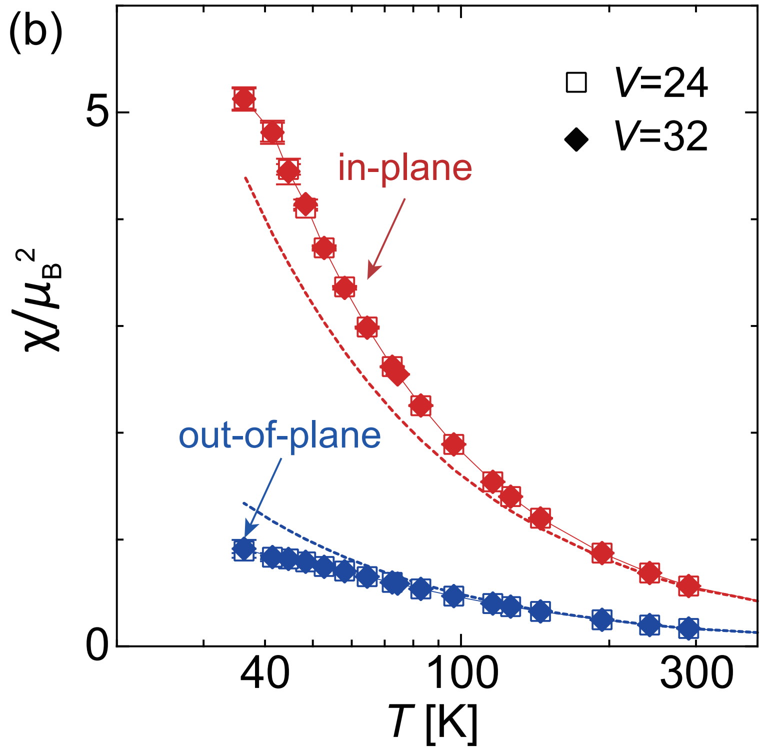
Scale-invariant magnetic anisotropy in $RuCl_3$ at high magnetic fields

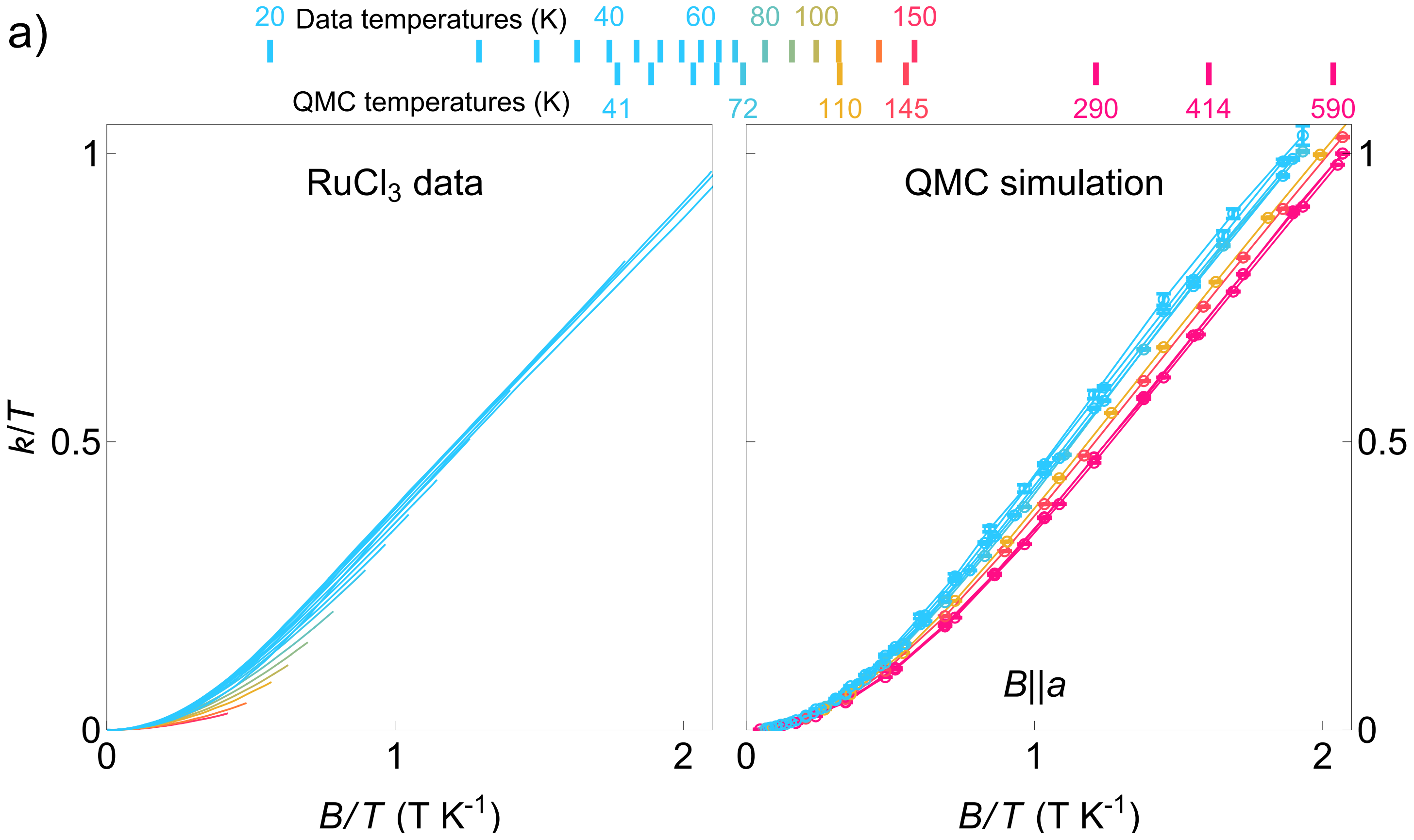
K. A. Modic, Ross D. McDonald, J. P. C. Ruff, Maja D. Bachmann, You Lai, Johanna C. Palmstrom, David Graf, Mun K. Chan, F. F. Balakirev, J. B. Betts, G. S. Boebinger, Marcus Schmidt, Michael J. Lawler, D. A. Sokolov, Philip J. W. Moll, B. J. Ramshaw and Arkady Shekhter



A fermion approach generalized Kitaev models

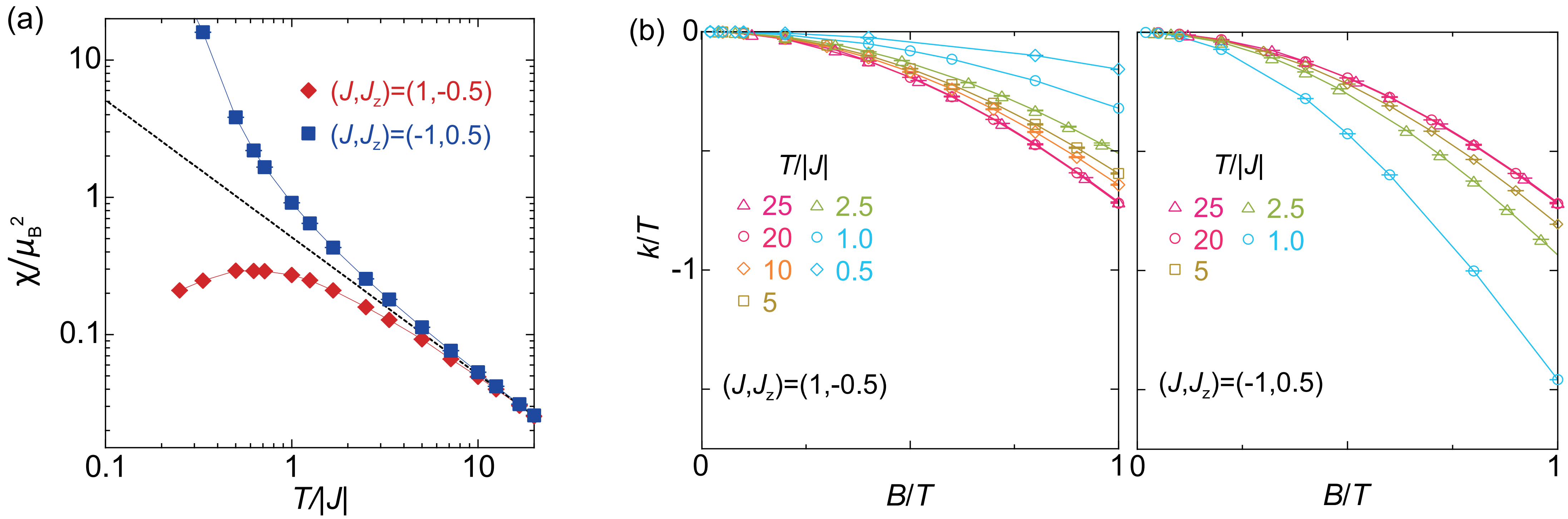






A fermion approach generalized Kitaev models

$$\hat{H}_{XXZ} = \sum_{\langle \boldsymbol{i},\boldsymbol{j} \rangle} J \left[\hat{S}^x_{\boldsymbol{i}} \cdot \hat{S}^x_{\boldsymbol{j}} + \hat{S}^y_{\boldsymbol{i}} \cdot \hat{S}^y_{\boldsymbol{j}} \right] + [J + J_z] \, \hat{S}^z_{\boldsymbol{i}} \hat{S}^z_{\boldsymbol{j}}$$

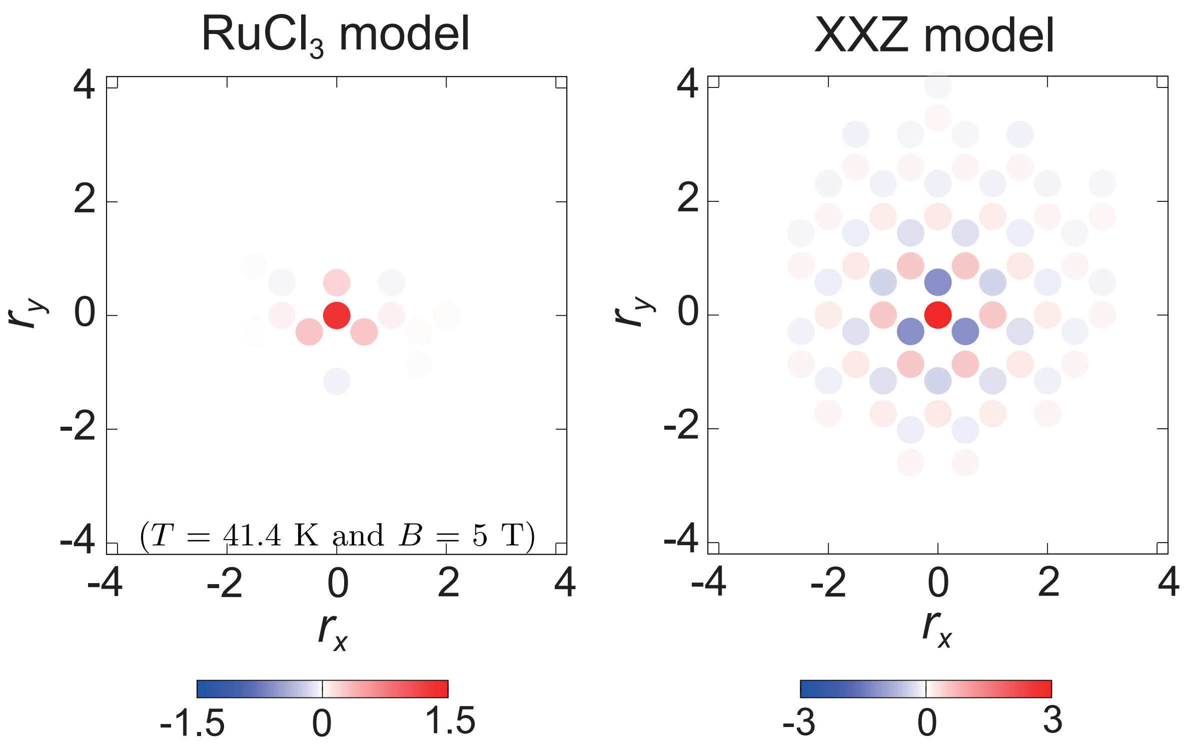


A fermion approach generalized Kitaev models

Torque fluctuations

$$\frac{\partial F}{\partial \varphi} = \mu_B \sum_{\boldsymbol{i}} \hat{t}_{\boldsymbol{i}} \quad \text{with} \quad \hat{t}_{\boldsymbol{i}} = (\boldsymbol{e} \times \boldsymbol{B}) \cdot \boldsymbol{g}\hat{\boldsymbol{S}}_{\boldsymbol{i}}$$

$$\langle \hat{t}_{\boldsymbol{r}} \hat{t}_{\boldsymbol{0}} \rangle - \langle \hat{t}_{\boldsymbol{r}} \rangle \langle \hat{t}_{\boldsymbol{0}} \rangle$$



Low temperature magnetic anisotropy is that of a renormalized local magnetic moment

Emergent low-lying particles have small contribution to magnetic anisotropy

A fermion approach generalized Kitaev models

Next steps? Debye temperature ~ 200K Magnetic energy scale ~ 100K

$$\hat{H} = \sum_{b=[i\in A,\delta]} \frac{\hat{P}_b^2}{2m} + \frac{k}{2}\hat{Q}_b + 2K(1+\hat{Q}_b)\hat{S}_i^\delta \hat{S}_{i+\delta}^\delta + J(1+\hat{Q}_b)\boldsymbol{S}_i\cdot\boldsymbol{S}_{i+\delta}$$

$$\omega_0 = \sqrt{\frac{k}{m}}, \quad \lambda = \frac{1}{2k}$$

32 sites lattice.

$$\omega_0 = 0.5, \lambda = 0.0, J = 0, K = 1, \beta K = 1$$

<sign> = 0.33(1)

$$\omega_0 = 0.5, \lambda = 0.1, J = 0, K = 1, \beta K = 1$$

<sign> = 0.30(1)

Coupling to phonons does not lead to more severe sign problem!

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Fakher Assaad. Fractionalization and Emergent Gauge Fields in Quantum Matter (ICTP 4-8 – 14 December 2023)

Phases and Exotic Phase Transitions of a Two-Dimensional Su-Schrieffer-Heeger Model

Anika Götz,[1] Martin Hohenadler,[1] and Fakher F. Assaad[1,2]

arXiv:2307.07613v1

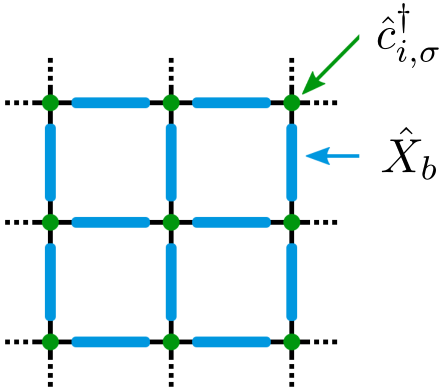
A. Götz

M. Hohenadler

The two-dimensional SSH model

$$\hat{H} = \sum_{\langle i,j \rangle} \left(-t + g\hat{X}_{\langle i,j \rangle} \right) \sum_{\sigma=1}^{N} \left(\hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + \text{h.c.} \right) + \sum_{\langle i,j \rangle} \left[\frac{\hat{P}^2_{\langle i,j \rangle}}{2m} + \frac{k}{2} \hat{X}^2_{\langle i,j \rangle} \right]$$

$$\omega_0 = \sqrt{\frac{k}{m}} \qquad \left[\hat{X}_b, \hat{P}_{b'} \right] = i\hbar\, \delta_{b,b'}$$

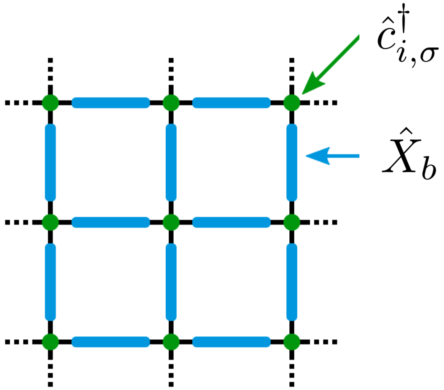


The two-dimensional SSH model

$$\hat{H} = \sum_{\langle i,j \rangle} \left(-t + g\hat{X}_{\langle i,j \rangle}\right) \sum_{\sigma=1}^{N} \left(\hat{c}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma} + \text{h.c.}\right) + \sum_{\langle i,j \rangle} \left[\frac{\hat{P}^2_{\langle i,j \rangle}}{2m} + \frac{k}{2}\hat{X}^2_{\langle i,j \rangle}\right]$$

$$\omega_0 = \sqrt{\frac{k}{m}} \qquad \left[\hat{X}_b, \hat{P}_{b'}\right] = i\hbar\, \delta_{b,b'}$$

$$\hat{c}^{\dagger}_{i,\sigma} = \frac{1}{2}\left(\hat{\gamma}_{i,\sigma,1} - i\hat{\gamma}_{i,\sigma,2}\right) \ \text{for } i \in A \qquad \hat{c}^{\dagger}_{i,\sigma} = \frac{i}{2}\left(\hat{\gamma}_{i,\sigma,1} - i\hat{\gamma}_{i,\sigma,2}\right) \ \text{for } i \in B$$

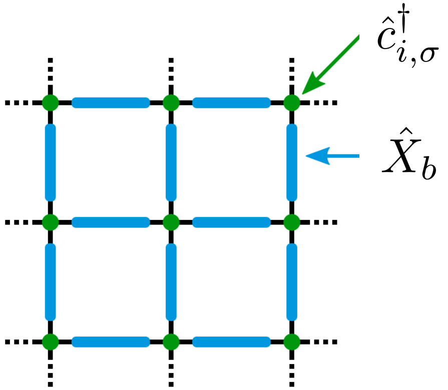


The two-dimensional SSH model

$$\hat{H} = \sum_{\langle i,j\rangle} \left(-t + g\hat{X}_{\langle i,j\rangle}\right) \sum_{\sigma=1}^{N}\sum_{n=1}^{2} \frac{i}{2}\, \hat{\gamma}_{i,\sigma,n}\hat{\gamma}_{j,\sigma,n} + \sum_{\langle i,j\rangle}\left[\frac{\hat{P}^2_{\langle i,j\rangle}}{2m} + \frac{k}{2}\hat{X}^2_{\langle i,j\rangle}\right]$$

$\omega_0 = \sqrt{\frac{k}{m}}$ $\left[\hat{X}_b, \hat{P}_{b'}\right] = i\hbar\, \delta_{b,b'}$

$\hat{c}^\dagger_{i,\sigma} = \frac{1}{2}\left(\hat{\gamma}_{i,\sigma,1} - i\hat{\gamma}_{i,\sigma,2}\right)$ for $i \in A$ $\hat{c}^\dagger_{i,\sigma} = \frac{i}{2}\left(\hat{\gamma}_{i,\sigma,1} - i\hat{\gamma}_{i,\sigma,2}\right)$ for $i \in B$



$O(2N)$ Symmetry $\hat{\boldsymbol{\gamma}}_{\boldsymbol{i}} \rightarrow O\hat{\boldsymbol{\gamma}}_{\boldsymbol{i}}$

For N=2 $O(4) = SU(2) \times SU(2) \times \mathbb{Z}_2$

$\hat{\boldsymbol{S}} = \frac{1}{2}\sum_i \boldsymbol{c}^\dagger_i \boldsymbol{\sigma} \boldsymbol{c}_i$

AFM

$\hat{\boldsymbol{\eta}} = \hat{P}^{-1}\hat{\boldsymbol{S}}\hat{P}$

CDW/SC

$\hat{P}^{-1}\hat{c}_{i,\sigma}\hat{P} = (-1)^i \hat{c}^\dagger_{i,\sigma}\delta_{\sigma,\uparrow} + \hat{c}_{i,\sigma}\delta_{i,\downarrow}$

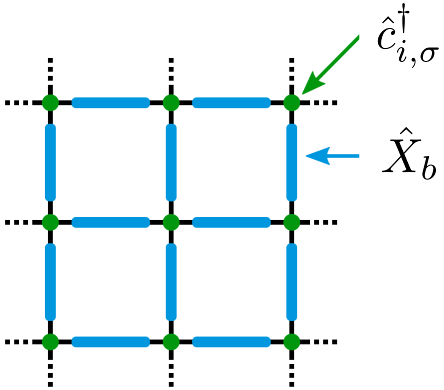
Parity

$(-1)^{\hat{n}^c_i} = \hat{\gamma}_{i,1}\hat{\gamma}_{i,2}\hat{\gamma}_{i,3}\hat{\gamma}_{i,4} \rightarrow \det(O)\, \hat{\gamma}_{i,1}\hat{\gamma}_{i,2}\hat{\gamma}_{i,3}\hat{\gamma}_{i,4}$

$$\hat{H} = \frac{g}{\sqrt{2m\omega_0}} \sum_{\langle i,j \rangle} \left(\hat{a}^\dagger_{\langle i,j \rangle} + \hat{a}_{\langle i,j \rangle} \right) \sum_{\sigma=1}^{N} \left(\hat{c}^\dagger_{i,\sigma} \hat{c}_{j,\sigma} + \text{h.c.} \right) + \sum_{\langle i,j \rangle} \omega_0 \left(\hat{a}^\dagger_{\langle i,j \rangle} \hat{a}_{\langle i,j \rangle} + \frac{1}{2} \right)$$

$$\hat{a}^\dagger_{\langle i,j \rangle} = \frac{\omega_0 m \hat{X}_{\langle i,j \rangle} - i \hat{P}_{\langle i,j \rangle}}{\sqrt{2\omega_0 m}}$$

$$\omega_0 = \sqrt{\frac{k}{m}} \qquad \left[\hat{X}_b, \hat{P}_{b'} \right] = i\hbar \, \delta_{b,b'}$$



Local $\mathbb{Z}_2$ symmetry

Let $\hat{Q}_i = (-1)^{\hat{n}^a_{\langle i,i+a_x \rangle} + \hat{n}^a_{\langle i,i-a_x \rangle} + \hat{n}^a_{\langle i,i+a_y \rangle} + \hat{n}^a_{\langle i,i-a_y \rangle}} (-1)^{\hat{n}^c_i}$ with

$$\hat{n}^a_{\langle i,j \rangle} = \hat{a}^\dagger_{\langle i,j \rangle} \hat{a}_{\langle i,j \rangle} \qquad \hat{n}^c_i = \sum_\sigma \hat{c}^\dagger_{i,\sigma} \hat{c}_{i,\sigma}$$

$\left[\hat{Q}_i, \hat{H} \right] = 0 \qquad \hat{Q}_i^2 = 1$ → Unconstrained $\mathbb{Z}_2$ lattice gauge theory

Gauge invariant invariant quantities: Spin: $\hat{\boldsymbol{S}}_{\boldsymbol{i}} = \frac{1}{2} \hat{\boldsymbol{c}}^\dagger_i \boldsymbol{\sigma} \hat{\boldsymbol{c}}_i$ Dimer: $\Delta_{b=(\boldsymbol{i},\boldsymbol{j})} = \hat{\boldsymbol{S}}_{\boldsymbol{i}} \cdot \hat{\boldsymbol{S}}_{\boldsymbol{j}}$ Flux: $\prod_{b \in \partial \square} \hat{X}_b$

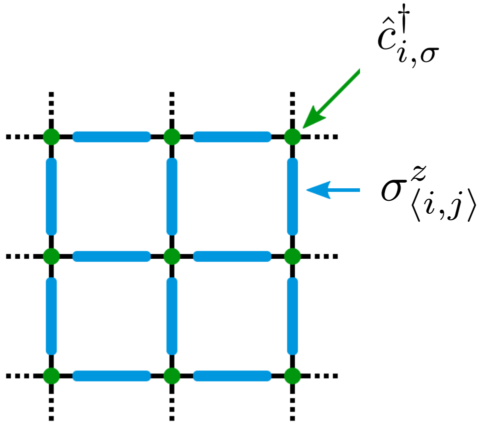
The two-dimensional SSH model

PHYSICAL REVIEW X **6,** 041049 (2016)

Simple Fermionic Model of Deconfined Phases and Phase Transitions

F. F. Assaad[1] and Tarun Grover[2,3]

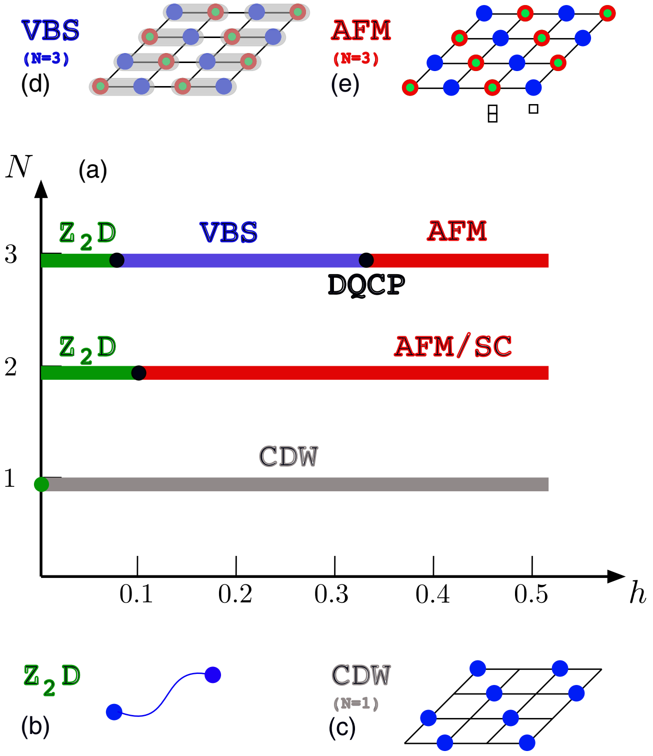
$$\hat{H} = \sum_{\langle i,j\rangle} \sigma^z_{\langle i,j\rangle} \sum_{\sigma=1}^{N} \left(\hat{c}^\dagger_{i,\sigma} \hat{c}_{j,\sigma} + \text{h.c.} \right) - h \sum_{\langle i,j\rangle} \sigma^x_{\langle i,j\rangle}$$



Global $O(2N)$ symmetry

Local $\mathbb{Z}_2$ symmetry

$$\hat{Q}_i = \sigma^x_{i,i+a_x}\sigma^x_{i,i-a_x}\sigma^x_{i,i-a_y}\sigma^x_{i,i+a_y}(-1)^{\hat{n}^c_i}$$



S. Gazit, A Vishwanath, M. Randeria, S. Sachdev, C. Wang Nat Phys 13 (2017), PNAS 2018

Quantum Monte Carlo simulations

$$\hat{H} = \sum_{\langle i,j \rangle} \left(-t + g \hat{X}_{\langle i,j \rangle} \right) \sum_{\sigma=1}^{N} \left(\hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + \text{h.c.} \right) + \sum_{\langle i,j \rangle} \left[\frac{\hat{P}^2_{\langle i,j \rangle}}{2m} + \frac{k}{2} \hat{X}^2_{\langle i,j \rangle} \right]$$

Formulation: Integrate out the phonons

PHYSICAL REVIEW B **98**, 201108(R) (2018)

Rapid Communications Editors' Suggestion

Solution of the sign problem for the half-filled Hubbard-Holstein model

Seher Karakuzu,[1] Kazuhiro Seki,[1,2,3] and Sandro Sorella[1,2]
[1] *International School for Advanced Studies (SISSA), Via Bonomea 265, 34136 Trieste, Italy*
[2] *Computational Materials Science Research Team, RIKEN Center for Computational Science (R-CCS), Hyogo 650-0047, Japan*
[3] *Computational Condensed Matter Physics Laboratory, RIKEN Cluster for Pioneering Research (CPR), Saitama 351-0198, Japan*

Quantum Monte Carlo simulations

$$\hat{H} = \sum_{\langle i,j \rangle} \left(-t + g\hat{X}_{\langle i,j \rangle} \right) \sum_{\sigma=1}^{N} \left(\hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + \text{h.c.} \right) + \sum_{\langle i,j \rangle} \left[\frac{\hat{P}^2_{\langle i,j \rangle}}{2m} + \frac{k}{2} \hat{X}^2_{\langle i,j \rangle} \right] - \lambda \sum_{\langle i,j \rangle} \left(\sum_{\sigma=1}^{N} \hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + \text{h.c.} \right)^2$$

Formulation: Integrate out the phonons

PHYSICAL REVIEW B **98**, 201108(R) (2018)

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$$\hat{H} = \sum_{\langle i,j\rangle} \left(-t + g\hat{X}_{\langle i,j\rangle}\right) \sum_{\sigma=1}^{N} \left(\hat{c}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma} + \text{h.c.}\right) + \sum_{\langle i,j\rangle} \left[\frac{\hat{P}^2_{\langle i,j\rangle}}{2m} + \frac{k}{2}\hat{X}^2_{\langle i,j\rangle}\right] - \lambda \sum_{\langle i,j\rangle} \Bigg(\underbrace{\sum_{\sigma=1}^{N} \hat{c}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma} + \text{h.c.}}_{\hat{K}_{b=\langle i,j\rangle}}\Bigg)^2$$

Formulation: Integrating out the phonons

$$\hat{H} = -t\sum_b \hat{K}_b - \lambda \sum_b \left(\hat{K}_b - \frac{g}{2\lambda}\hat{X}_b\right)^2 + \sum_b \frac{1}{2m}\hat{P}_b^2 + \left(\frac{k}{2} + \frac{g^2}{4\lambda}\right)\hat{X}_b^2$$

For the perfect square use (Gauss-Hermite quadrature)

$$e^{\lambda\Delta\tau\left(\hat{K}_b - \frac{g}{2\lambda}\hat{X}_b\right)^2} = \frac{1}{4}\sum_{l=\pm1,\pm2} \gamma(l) e^{\sqrt{\Delta\tau\lambda}\,\eta(l)\left(\hat{K}_b - \frac{g}{2\lambda}\hat{X}_b\right)} + \mathcal{O}((\Delta\tau\lambda)^4)$$

$$\gamma(\pm1) = 1 + \sqrt{6}/3\,, \qquad \eta(\pm1) = \pm\sqrt{2\left(3-\sqrt{6}\right)}$$

$$\gamma(\pm2) = 1 - \sqrt{6}/3\,, \qquad \eta(\pm2) = \pm\sqrt{2\left(3+\sqrt{6}\right)}$$

Choose a real space basis $\hat{X}_b|x_b\rangle = x_b|x_b\rangle$

Quantum Monte Carlo simulations

$$\hat{H} = -t\sum_{b}\hat{K}_b - \lambda\sum_{b}\left(\hat{K}_b - \frac{g}{2\lambda}\hat{X}_b\right)^2 + \sum_{b}\frac{1}{2m}\hat{P}_b^2 + \left(\frac{k}{2}+\frac{g^2}{4\lambda}\right)\hat{X}_b^2$$

Formulation: Integrating out the phonons

$$Z = \sum_{l_{b,\tau}}\prod_{b,\tau}\gamma(l_{b,\tau})\int D\left\{x_{b,\tau}\right\} e^{-\boldsymbol{x}^T\boldsymbol{A}\,\boldsymbol{x}-\boldsymbol{J}^T(\{l_{b,\tau}\})\,\boldsymbol{x}}\ \mathrm{Tr}_{\mathrm{F}}\prod_{\tau=1}^{L_\tau} e^{-\Delta\tau\sum_b\hat{K}_b} e^{-\sqrt{\Delta\tau\lambda}\sum_b\eta(l_{b,\tau})\hat{K}_b}$$

$$= \frac{(\pi)^{L^2L_\tau}}{\sqrt{det(A)}}\sum_{l_{b,\tau}}\prod_{b,\tau}\gamma(l_{b,\tau}) e^{\frac{1}{4}\boldsymbol{J}^T(\{l_{b,\tau}\})\boldsymbol{A}^{-1}\boldsymbol{J}(\{l_{b,\tau}\})}\mathrm{Tr}_{\mathrm{F}}\prod_{\tau=1}^{L_\tau} e^{-\Delta\tau\sum_b\hat{K}_b} e^{-\sqrt{\Delta\tau\lambda}\sum_b\eta(l_{b,\tau})\hat{K}_b}$$

Since A is positive definite, one can explicitly integrate out the phonons, and sample the discrete fields $l_{b,\tau}$

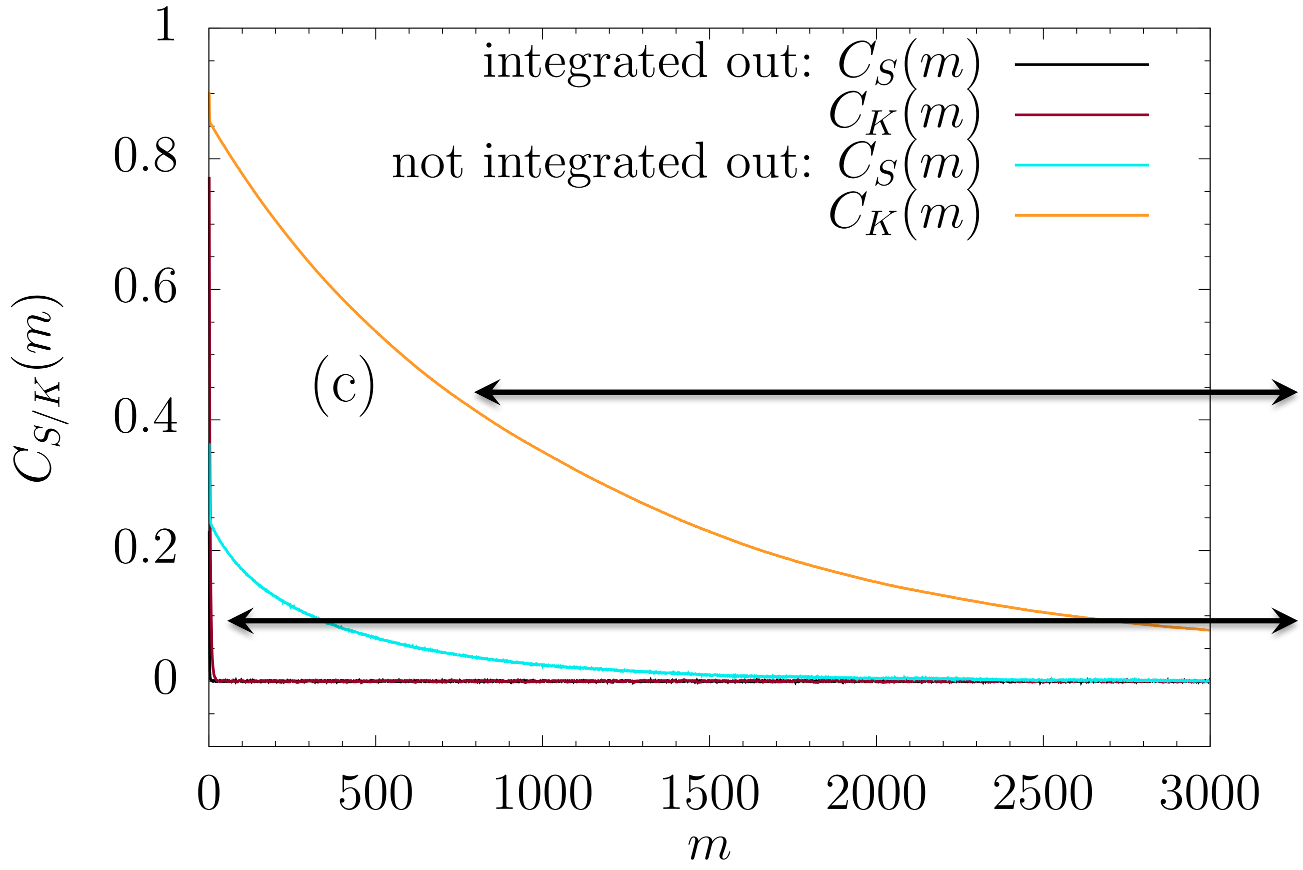
Quantum Monte Carlo simulations

$$L = 4, \beta = 1, t = 1, k = 2, \omega_0 = 3, \lambda = 0.5$$

Auto-correlation time

as a function of

Monte Carlo time, m



Single spin flips of phonon and HS fields (Dimer correlations)

Phonons are integrated out. HS fields acquire time dependence. (Dimer correlations)

A. Götz, M. Hohenadler, and FFA to appear

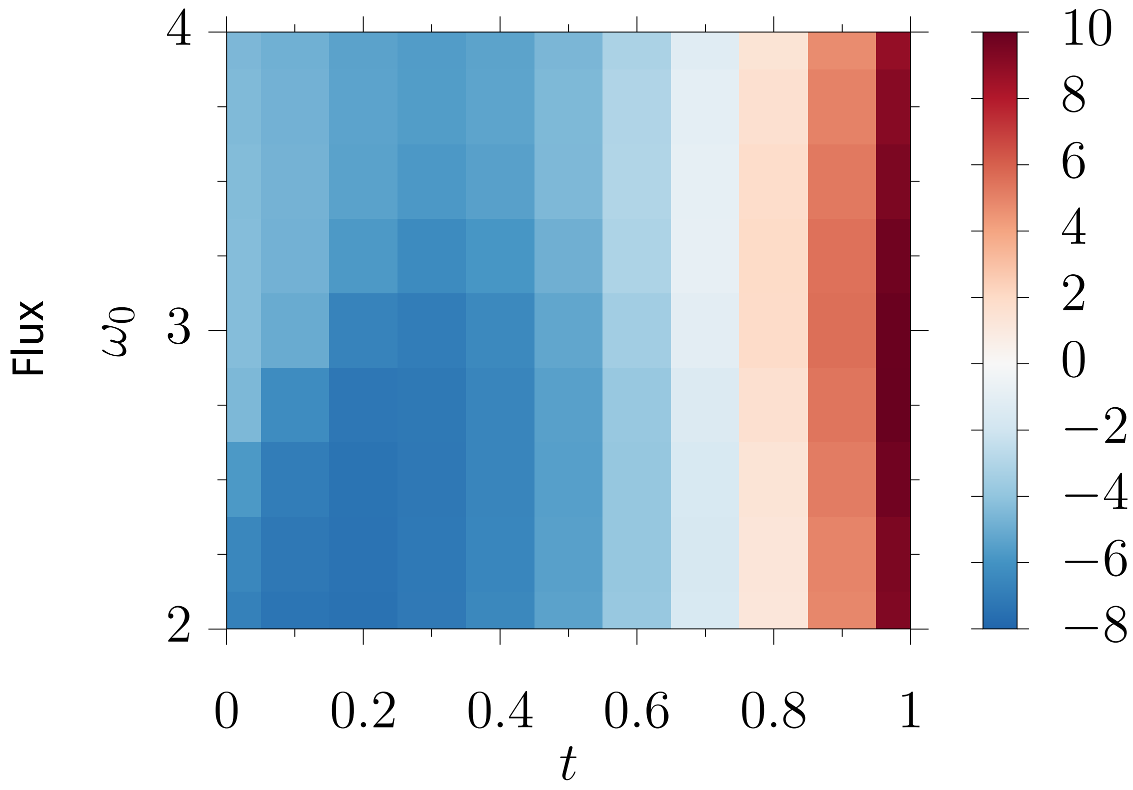
Numerical results

$k = 2, g = 2, \lambda = 0.5 \qquad \beta = L$

$$\hat{H} = \sum_{\langle i,j \rangle} \left(-t + g\hat{X}_{\langle i,j \rangle} \right) \sum_{\sigma=1}^{N} \left(\hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + \text{h.c.} \right) + \sum_{\langle i,j \rangle} \left[\frac{\hat{P}^2_{\langle i,j \rangle}}{2m} + \frac{k}{2} \hat{X}^2_{\langle i,j \rangle} \right] - \lambda \sum_{\langle i,j \rangle} \left(\sum_{\sigma=1}^{N} \hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + \text{h.c.} \right)^2$$

$$\left\langle \prod_{\langle i,j \rangle \in \partial \square} -t + g\hat{X}_{\langle i,j \rangle} \right\rangle$$

Emergent Dirac fermions



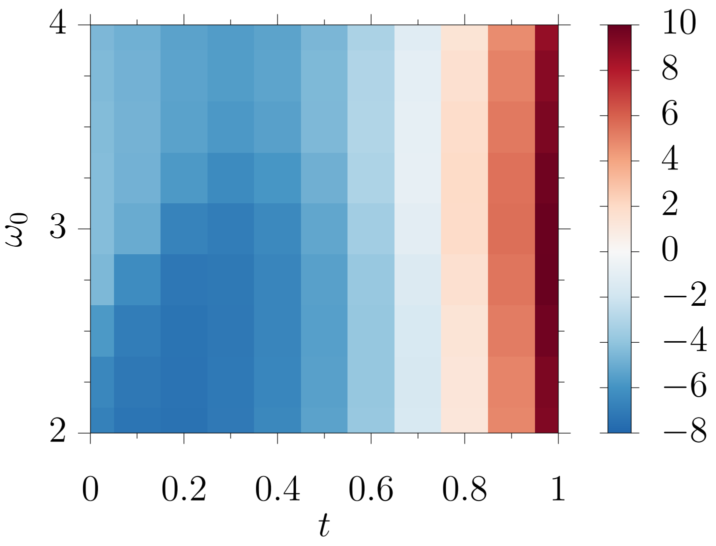
Numerical results

$k = 2, g = 2, \lambda = 0.5 \qquad \beta = L$

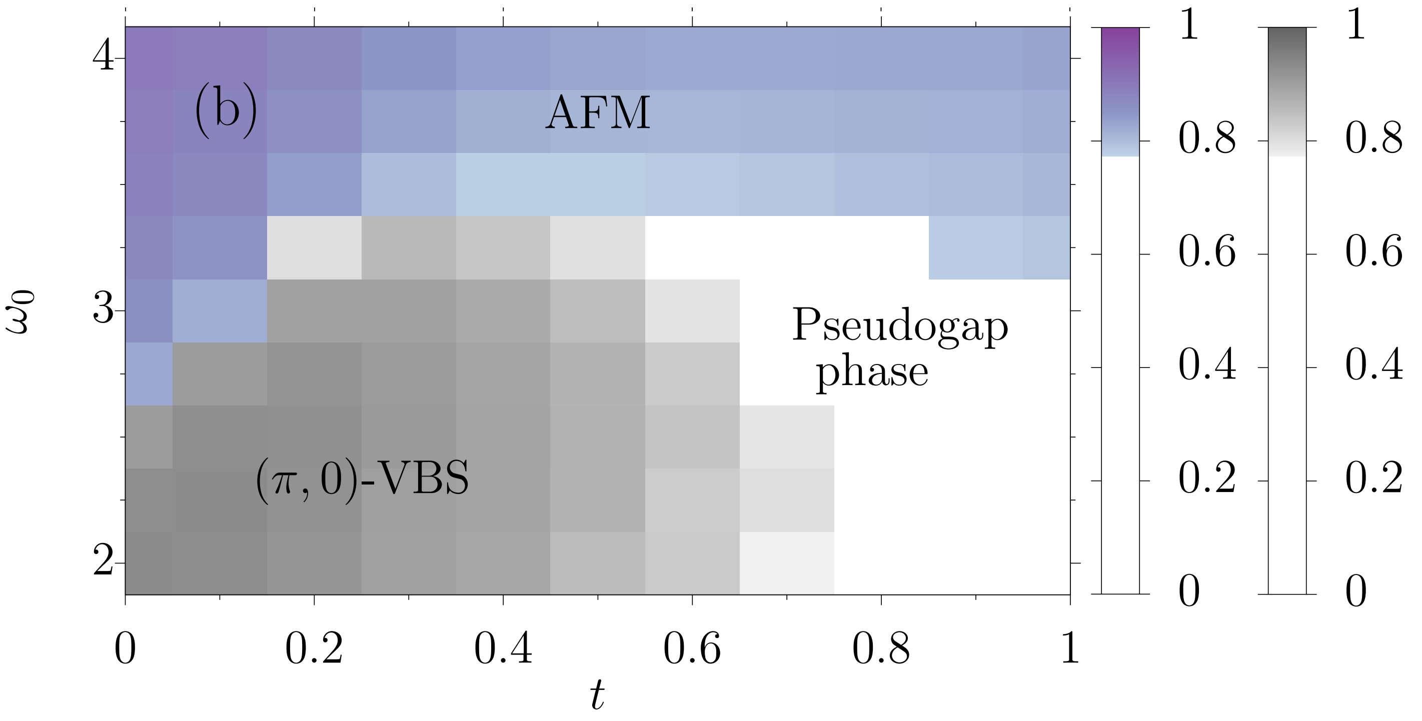
$$\hat{H} = \sum_{\langle i,j \rangle} \left(-t + g\hat{X}_{\langle i,j \rangle} \right) \sum_{\sigma=1}^{N} \left(\hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + \text{h.c.} \right) + \sum_{\langle i,j \rangle} \left[\frac{\hat{P}^2_{\langle i,j \rangle}}{2m} + \frac{k}{2} \hat{X}^2_{\langle i,j \rangle} \right] - \lambda \sum_{\langle i,j \rangle} \left(\sum_{\sigma=1}^{N} \hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + \text{h.c.} \right)^2$$

$$\left\langle \prod_{\langle i,j \rangle \in \partial \square} -t + g\hat{X}_{\langle i,j \rangle} \right\rangle$$

Flux



Spin and Dimer correlation ratios on 8x8 lattice



Numerical results

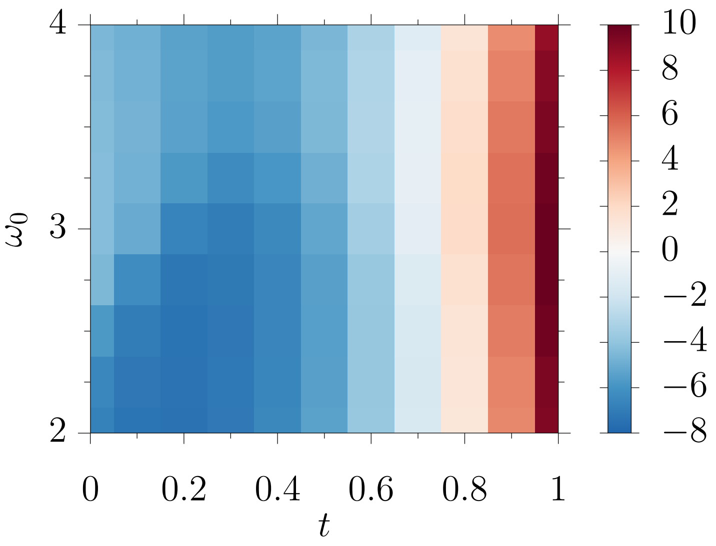
$k = 2, g = 2, \lambda = 0.5 \qquad \beta = L$

$$\hat{H} = \sum_{\langle i,j \rangle} \left(-t + g\hat{X}_{\langle i,j \rangle} \right) \sum_{\sigma=1}^{N} \left(\hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + \text{h.c.} \right) + \sum_{\langle i,j \rangle} \left[\frac{\hat{P}^2_{\langle i,j \rangle}}{2m} + \frac{k}{2} \hat{X}^2_{\langle i,j \rangle} \right] - \lambda \sum_{\langle i,j \rangle} \left(\sum_{\sigma=1}^{N} \hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + \text{h.c.} \right)^2$$

Instance of deconfined quantum *pseudo* criticality ?

Flux

$$\left\langle \prod_{\langle i,j \rangle \in \partial \square} -t + g\hat{X}_{\langle i,j \rangle} \right\rangle$$



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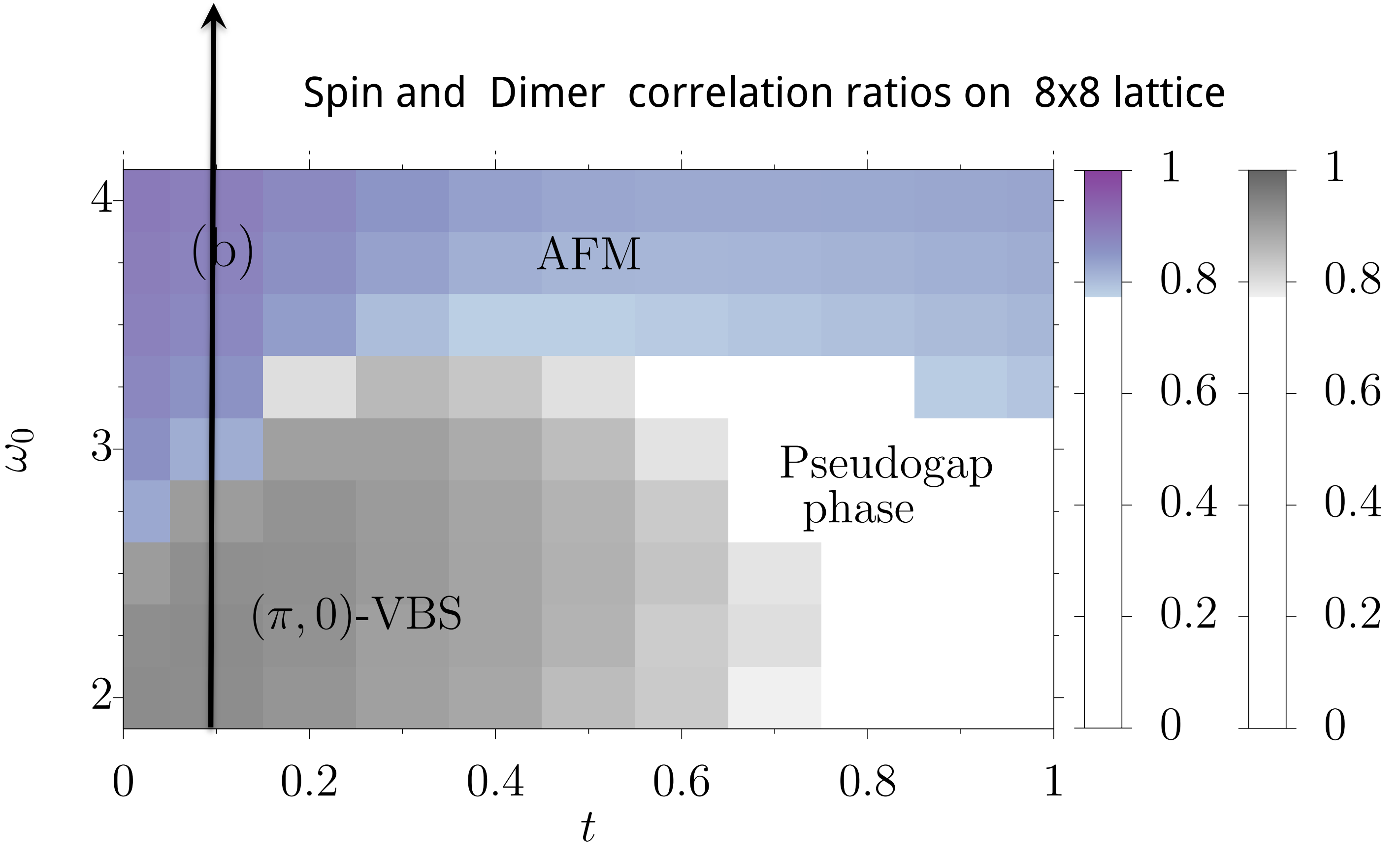
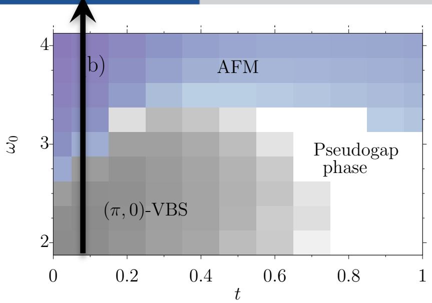


Numerical results

$k = 2, g = 2, \lambda = 0.5 \qquad \beta = L$



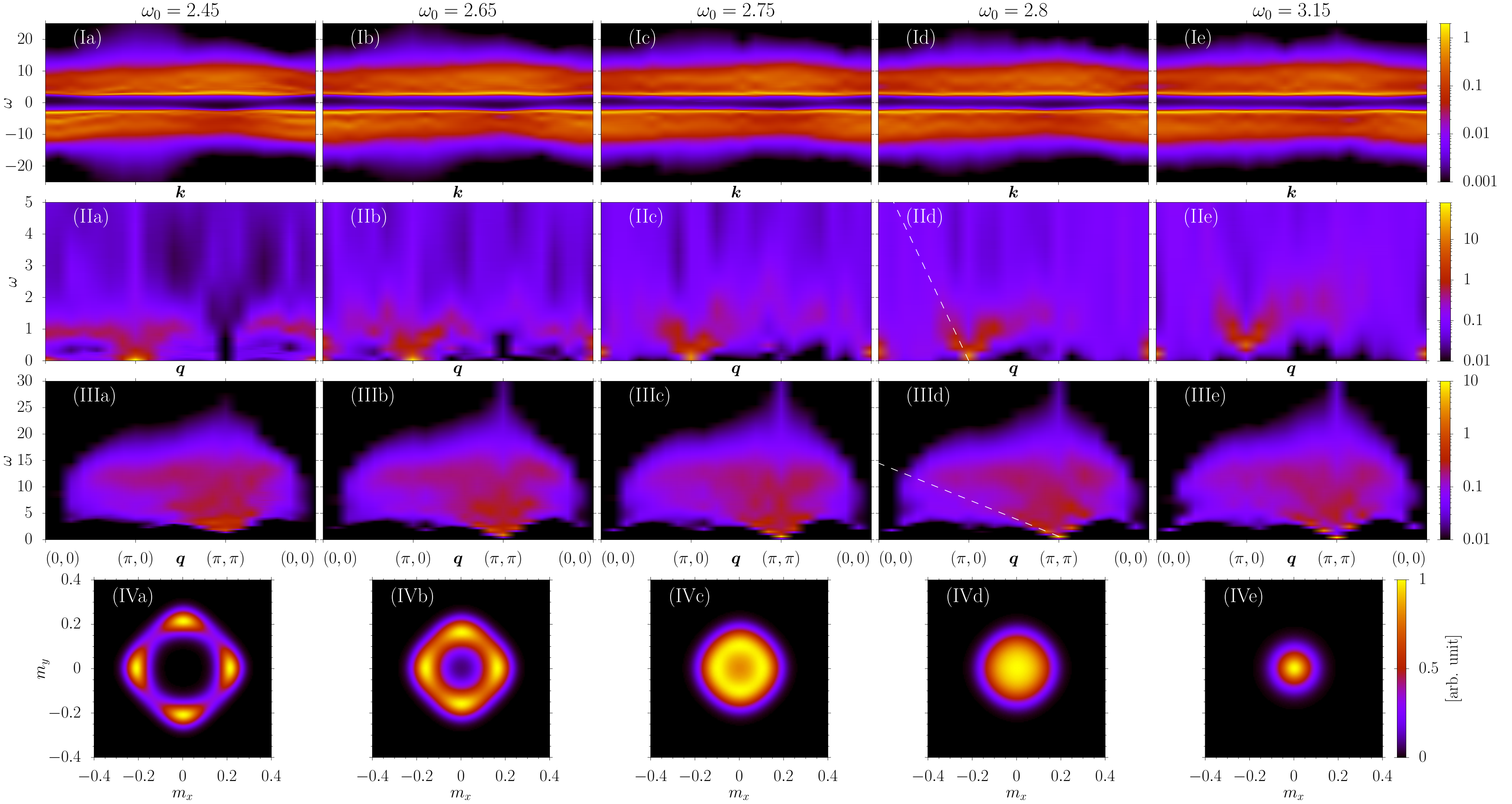
ω_0^c

Green

VBS

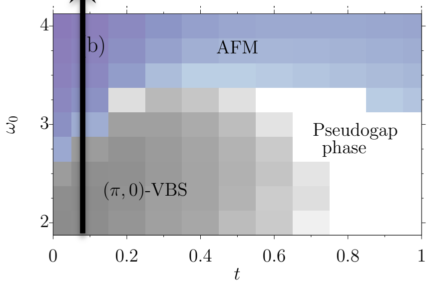
Spin

VBS Histograms



Numerical results

$k = 2, g = 2, \lambda = 0.5 \qquad \beta = L$

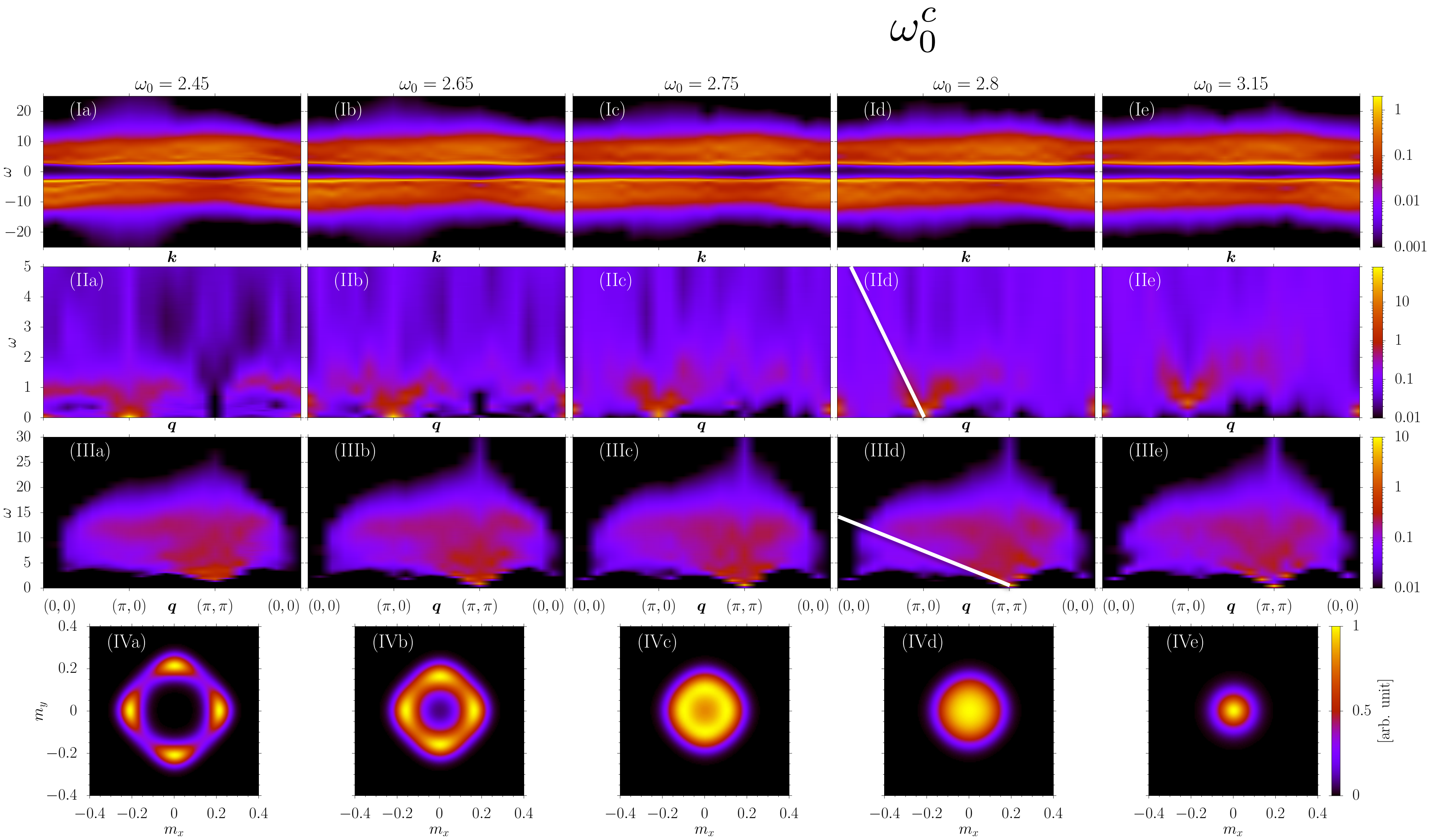


Green

VBS

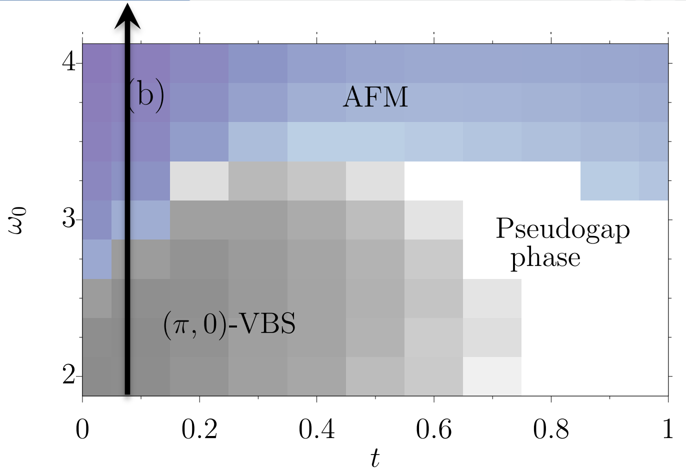
Spin

VBS Histograms



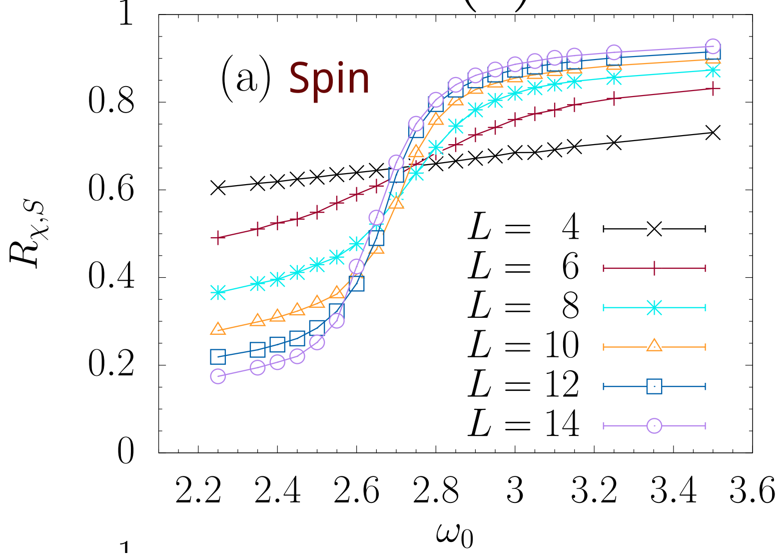
Numerical results

$k = 2, g = 2, \lambda = 0.5 \qquad \beta = L$

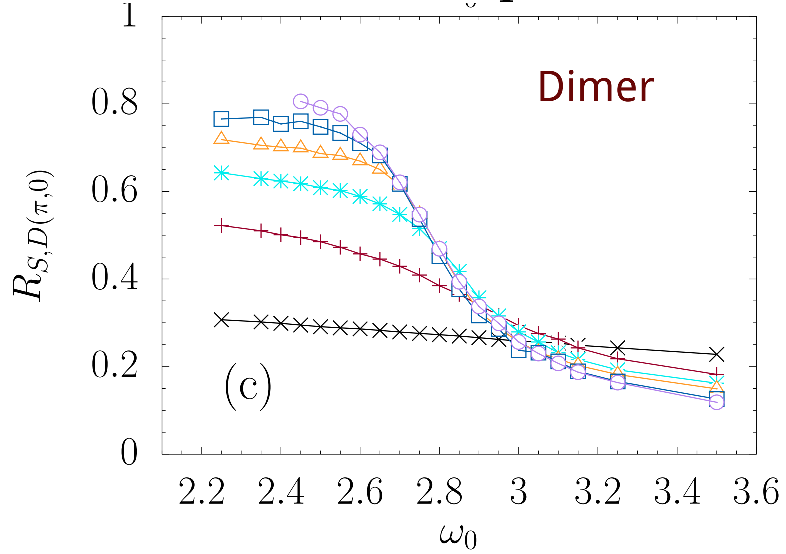


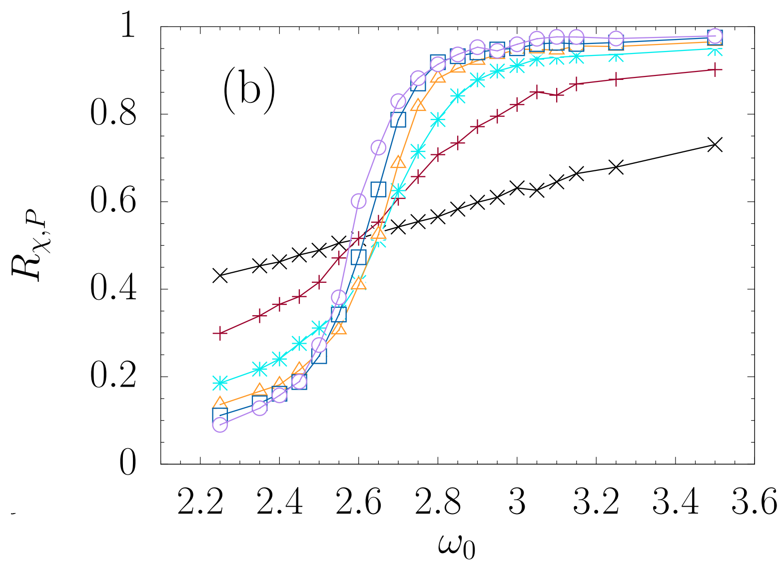
Correlation ratio

$SU(2)$



$\mathbb{Z}_4$





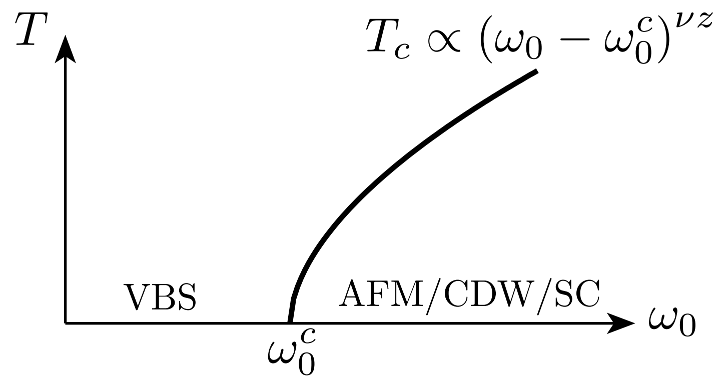
<u>Parity</u> Order parameter is

$$\hat{\gamma}_{i,1}\hat{\gamma}_{i,2}\hat{\gamma}_{i,3}\hat{\gamma}_{i,4} \rightarrow$$

$$\det O \, \hat{\gamma}_{i,1}\hat{\gamma}_{i,2}\hat{\gamma}_{i,3}\hat{\gamma}_{i,4}$$

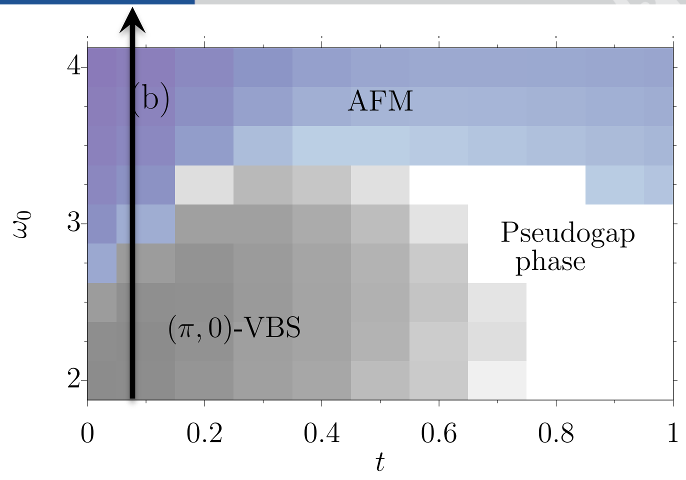
$$\hat{\boldsymbol{\gamma}}_{\boldsymbol{i}} \rightarrow O\hat{\boldsymbol{\gamma}}_{\boldsymbol{i}}$$

$$\hat{\gamma}_{i,1}\hat{\gamma}_{i,2}\hat{\gamma}_{i,3}\hat{\gamma}_{i,4} = (-1)^{\hat{n}_i^c}$$



Numerical results

$k = 2, g = 2, \lambda = 0.5$ $\beta = L$

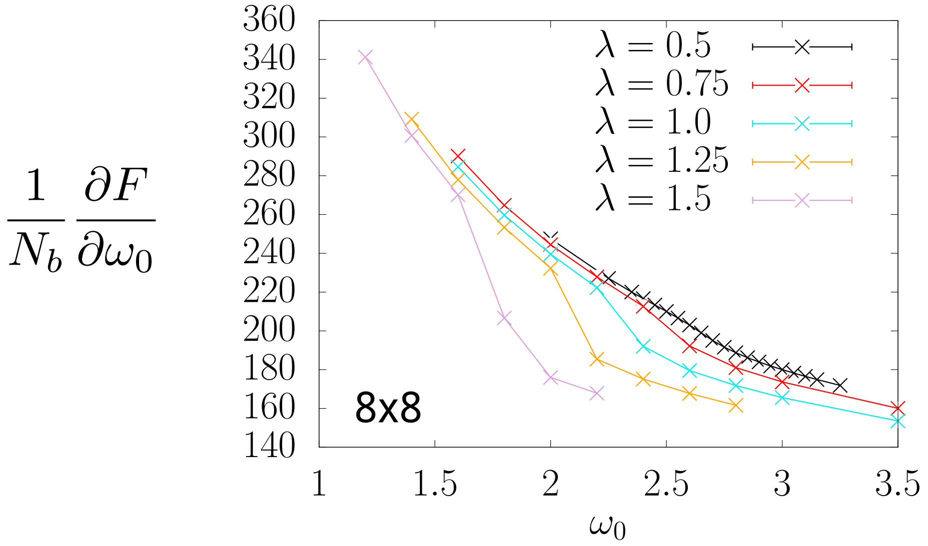


Spin-Peierls instability of the U(1) Dirac spin liquid

arXiv:2307.12295v3

Urban F. P. Seifert,[1,*] Josef Willsher,[2,3,*] Markus Drescher,[2,3] Frank Pollmann,[2,3] and Johannes Knolle[2,3,4]

Decreasing the value of ω_0^c by increasing λ or adding a Hubbard U-term should drive the DQCP to a strong first order transition.



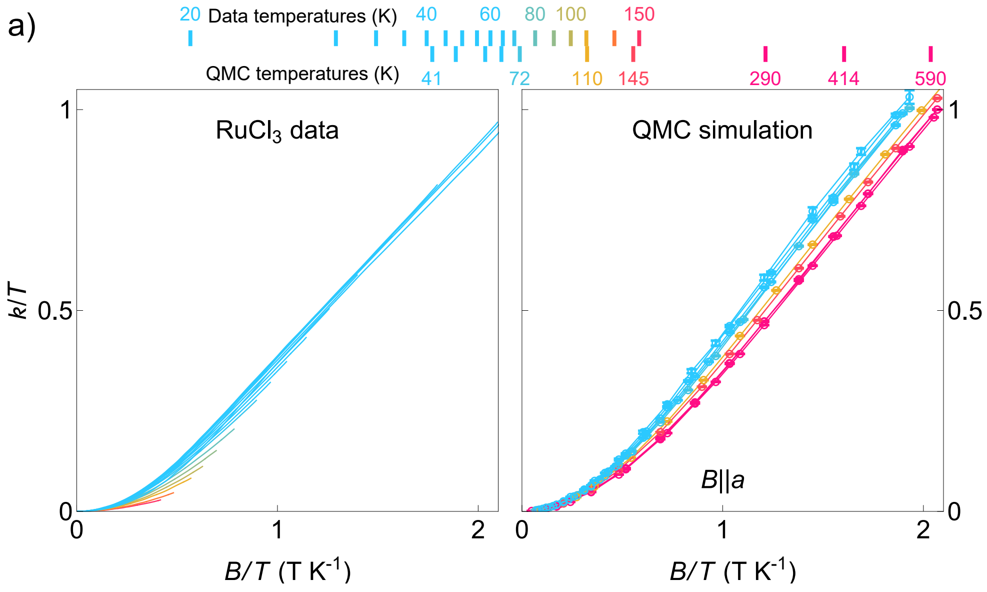
Conclusions

$$\hat{H}(\varphi) = \sum_{\langle i,j\rangle}\left[K\hat{S}_i^{\gamma}\hat{S}_j^{\gamma} + \Gamma\hat{S}_i^{\alpha}\hat{S}_j^{\beta} + J_1\hat{\boldsymbol{S}}_i\cdot\hat{\boldsymbol{S}}_j\right] + J_3\sum_{\langle\langle i,j\rangle\rangle}\hat{\boldsymbol{S}}_i\cdot\hat{\boldsymbol{S}}_j - \mu_B\sum_i \boldsymbol{B}(\varphi)\cdot\boldsymbol{g}\hat{\boldsymbol{S}}_i$$

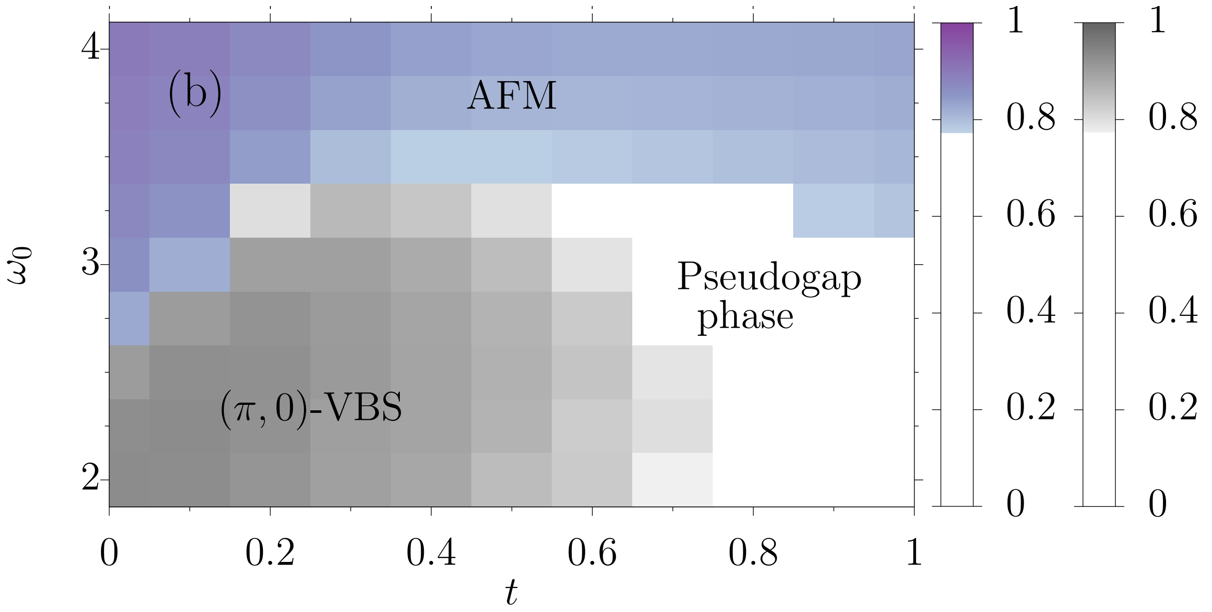
$$(J_1, J_3, K, \Gamma) = (-0.5, 0.5, -5.0, 2.5)\ [\text{meV}] \qquad \boldsymbol{g} = \text{diag}\,[2.3, 2.3, 1.3]$$

$$\hat{H} = \sum_{\langle i,j\rangle}\left(-t + g\hat{X}_{\langle i,j\rangle}\right)\sum_{\sigma=1}^{N}\left(\hat{c}_{i,\sigma}^{\dagger}\hat{c}_{j,\sigma} + \text{h.c.}\right) + \sum_{\langle i,j\rangle}\left[\frac{\hat{P}_{\langle i,j\rangle}^2}{2m} + \frac{k}{2}\hat{X}_{\langle i,j\rangle}^2\right] - \lambda\sum_{\langle i,j\rangle}\left(\sum_{\sigma=1}^{N}\hat{c}_{i,\sigma}^{\dagger}\hat{c}_{j,\sigma} + \text{h.c.}\right)^2$$

$$k = 2, g = 2, \lambda = 0.5 \qquad \beta = L$$



Coupling to phonons



DQCP. Fate of DQCP as a function of λ?

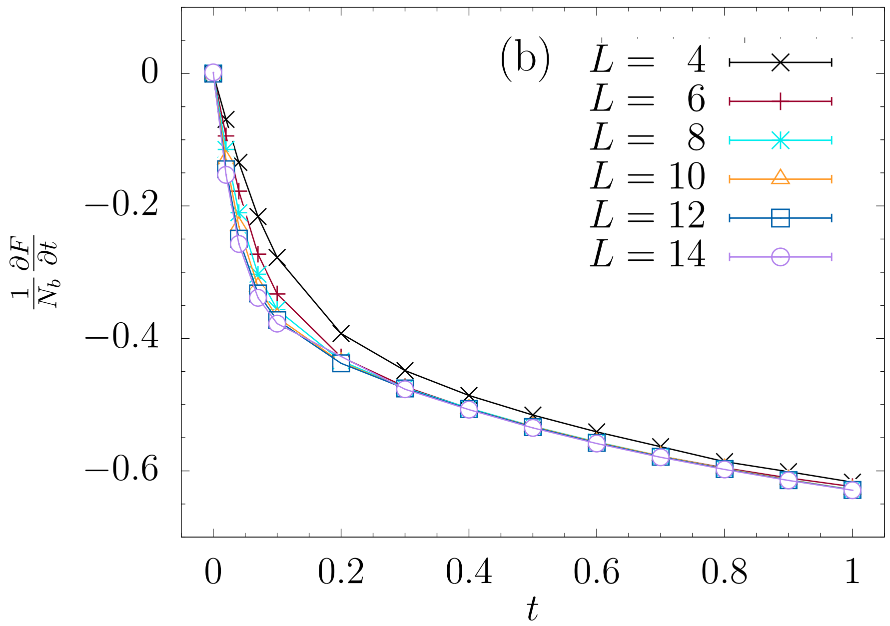
Numerical results

$k = 2, g = 2, \lambda = 0.5 \qquad \beta = L$

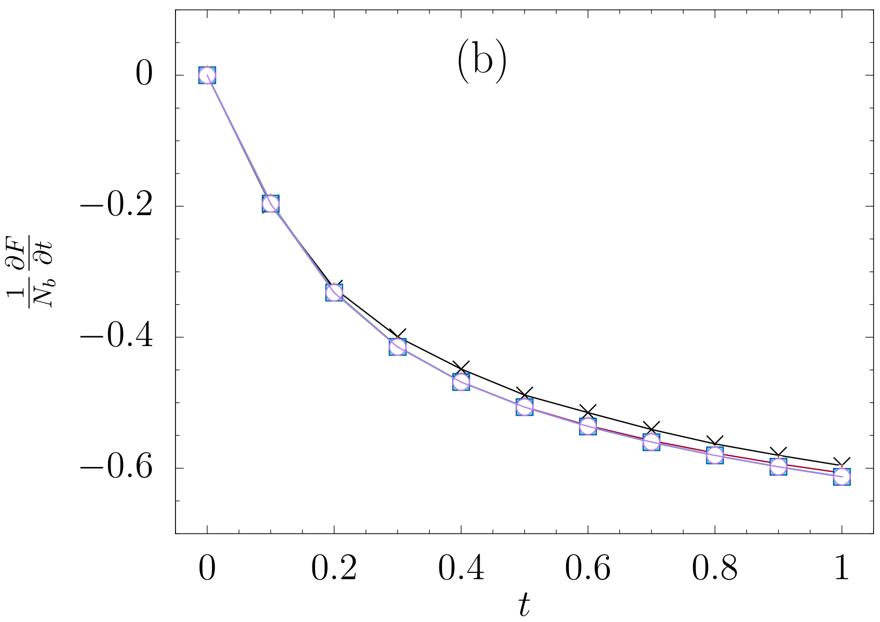
$$\hat{H} = \sum_{\langle i,j \rangle} \left(-t + g\hat{X}_{\langle i,j \rangle} \right) \sum_{\sigma=1}^{N} \left(\hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + \text{h.c.} \right) + \sum_{\langle i,j \rangle} \left[\frac{\hat{P}^2_{\langle i,j \rangle}}{2m} + \frac{k}{2} \hat{X}^2_{\langle i,j \rangle} \right] - \lambda \sum_{\langle i,j \rangle} \Bigg(\underbrace{\sum_{\sigma=1}^{N} \hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + \text{h.c.}}_{\hat{K}_{b=\langle i,j \rangle}} \Bigg)^2$$

Is the t=0 limit singular ?

$\omega_0 = 2.0$



$\omega_0 = 4$



$$F = F_0 - t^2 \int_0^{\beta} d\tau \sum_b \langle \hat{K}_b(\tau) \hat{K}_b(0) \rangle_0 + \cdots$$