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UNIVERSITÄT
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Fermion Monte Carlo: the auxiliary field determinantal approach

Fakher F. Assaad, Entanglement in Strongly Correlated Systems, Benasque, 04.03.2019

Lecture 1: A brief overview of the finite temperature auxiliary field algorithm.

Lecture 2: Selected applications

Review:

World-line and determinantal quantum monte carlo methods for spins, phonons and electrons
F.F.A and H.G. Evertz. Lecture Notes in Physics, vol. 739, Springer, Berlin Heidelberg, 2008, pp. 277–356

ALF: General Implementation:

Martin Bercx, Florian Goth, Johannes S. Hofmann, and Fakher F. Assaad
The ALF (Algorithms for Lattice Fermions) project release 1.0. Documentation for the auxiliary field quantum Monte Carlo code, SciPost Phys. 3 (2017), 013.

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Fermion Monte Carlo: the auxiliary field determinantal approach

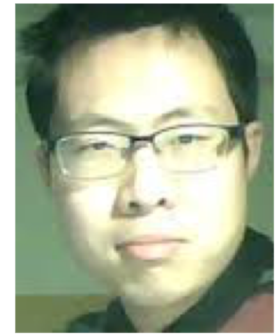
Many thanks to

M. Hohenadler

J. Hofmann

S. Beyl

M. Rackowski



Z. Wang

T. Sato

M. Ulybyshev

F. Parisen Toldin

J. Schwab

E. Huffman → Perimeter

Auxiliary field QMC. BSS: R. Blankenbecler, D. J. Scalapino, R. L. Sugar (1981)

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

Trotter

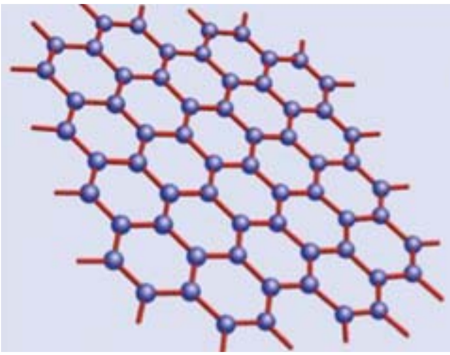
$\Phi(\mathbf{i},\tau)$: Hubbard-Stratonovich (or arbitrary field with predefined dynamics)

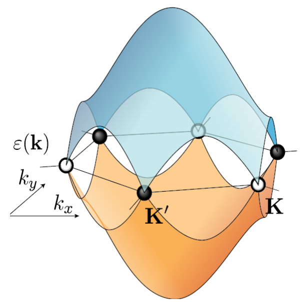
MC importance sampling

One body problem in external field

Auxiliary field QMC “Realistic models”

$$\hat{H} = -t \sum_{\langle i,j \rangle, \sigma=1}^{2} \left(\hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + \hat{c}^{\dagger}_{j,\sigma} \hat{c}_{i,\sigma} \right) + \sum_{i,j} \left(\hat{n}_i - 1 \right) V_{i,j} \left(\hat{n}_j - 1 \right)$$





Dirac fermions

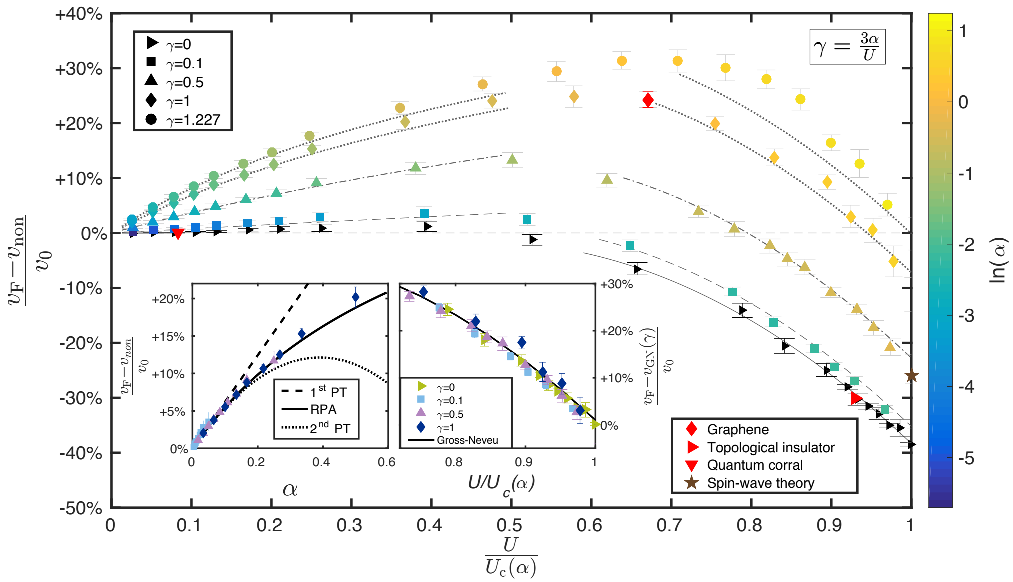
- Coulomb repulsion is not screened

→ Both short and long range part of the Coulomb repulsion has to be considered

- Velocity renormalization
- Mott transition

$$V_{i,j} = U \begin{cases} 1 & i = j \\ \frac{\gamma}{r_{i,j}} & i \neq j \end{cases}$$

$$\alpha = \gamma U$$



Ho-Kin Tang, J. N. Leaw, J. N. B. Rodrigues, I. F. Herbut, P. Sengupta, F. F. Assaad, and S. Adam, The role of electron-electron interactions in two dimensional Dirac fermions. Science 361, (2018), 570.

Auxiliary field QMC "Designer Hamiltonians"

Ising nematic quantum critical point in a metal: a Monte Carlo study

Yoni Schattner,[1,*] Samuel Lederer,[2,*] Steven A. Kivelson,[2] and Erez Berg[1]

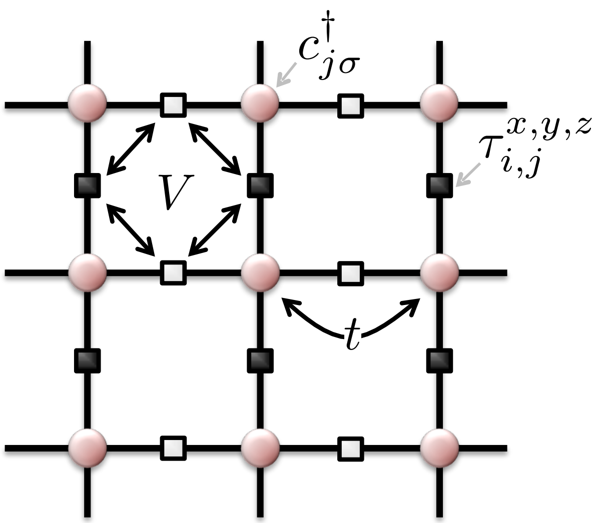
Phys. Rev. X 6, 031028 (2016)

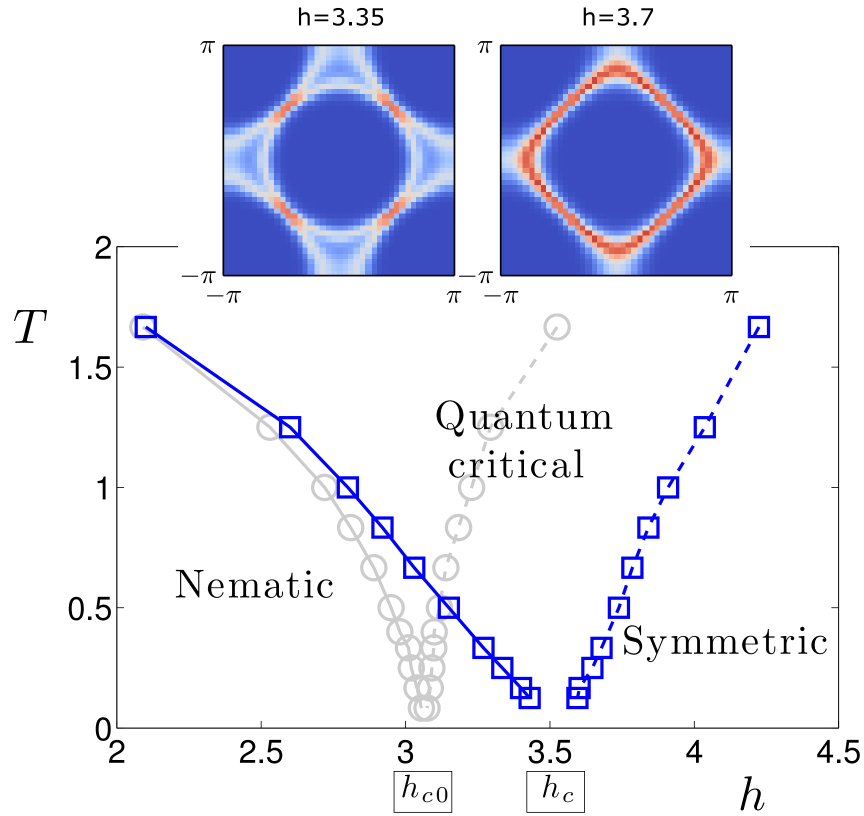
$$H = H_f + H_b + H_{\rm int},$$

$$H_f = -t \sum_{\langle i,j \rangle,\sigma} c^\dagger_{i\sigma} c_{j\sigma} - \mu \sum_{i,\sigma} c^\dagger_{i\sigma} c_{i\sigma},$$

$$H_b = V \sum_{\langle\langle i,j \rangle ; \langle k,l \rangle\rangle} \tau^z_{i,j} \tau^z_{k,l} - h \sum_{\langle i,j \rangle} \tau^x_{i,j},$$

$$H_{\rm int} = \alpha t \sum_{\langle i,j \rangle,\sigma} \tau^z_{i,j} c^\dagger_{i\sigma} c_{j\sigma}.$$





Designer Hamiltonians → Sign problem free Hamiltonians that capture the *correct* low energy physics

Science 1606 21 DECEMBER 2012 VOL 338 SCIENCE www.sciencemag.org

Sign-Problem–Free Quantum Monte Carlo of the Onset of Antiferromagnetism in Metals

Erez Berg, Max A. Metlitski and Subir Sachdev

PRL 119, 197203 (2017) PHYSICAL REVIEW LETTERS week ending 10 NOVEMBER 2017

Dirac Fermions with Competing Orders: Non-Landau Transition with Emergent Symmetry

Toshihiro Sato,[1] Martin Hohenadler,[1] and Fakher F. Assaad[1]

PHYSICAL REVIEW X 6, 041049 (2016)

Simple Fermionic Model of Deconfined Phases and Phase Transitions

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

nature physics ARTICLES
PUBLISHED ONLINE: 6 FEBRUARY 2017 | DOI: 10.1038/NPHYS4028

Emergent Dirac fermions and broken symmetries in confined and deconfined phases of Z_2 gauge theories

Snir Gazit[1]*, Mohit Randeria[2] and Ashvin Vishwanath[1,3]

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Fermion Monte Carlo: the auxiliary field determinantal approach

Auxiliary field QMC. BSS: R. Blankenbecler, D. J. Scalapino, R. L. Sugar (1981)

1) Trotter
2) Hubbard Stratonovitch
3) Integrating out the fermions
4) Measurements
5) Wicks theorem
6) Absence of sign problem
7) Organization of the code and fast updates.
8) Stabilization
9) ALF examples

Auxiliary field QMC.

$$\mathrm{Tr}\, e^{-\beta \hat{H}} \propto \int D\{\Phi(\mathbf{i},\tau)\}\, e^{-S(\{\Phi(\mathbf{i},\tau)\})}$$

Example For

$$\hat{H} = \hat{H}_0 + \overbrace{\frac{1}{4}\sum_{\mathbf{i},\mathbf{j}} V_{\mathbf{i},\mathbf{j}} (\hat{c}^\dagger_{\mathbf{i}}\hat{c}_{\mathbf{i}} - 1)(\hat{c}^\dagger_{\mathbf{j}}\hat{c}_{\mathbf{j}} - 1)}^{\hat{H}_V}, \quad \hat{c}^\dagger_{\mathbf{i}} = (\hat{c}^\dagger_{\mathbf{i},\uparrow}, \hat{c}^\dagger_{\mathbf{i},\downarrow})$$

$$e^{-S(\{\Phi(i,\tau)\})} = e^{-\sum_{\mathbf{i},\mathbf{j},\tau} \Delta\tau\, \Phi(\mathbf{i},\tau) V^{-1}_{\mathbf{i},\mathbf{j}} \Phi(\mathbf{j},\tau)} \mathrm{Tr}\left[\prod_{\tau=1}^{L_\tau} e^{-\Delta\tau \hat{H}_0} e^{-\Delta\tau \sum_{\mathbf{i}} i\Phi(\mathbf{i},\tau)\left[\hat{c}^\dagger_{\mathbf{i}}\hat{c}_{\mathbf{i}} - 1\right]}\right]$$

V has to be positive definite

R. Brower, C. Rebbi and D. Schaich PoS(Lattice 2011)056

M. V. Ulybyshev, P. V. Buividovich, M. I. Katsnelson, and M. I. Polikarpov. Phys. Rev. Lett., 111, 056801, (2013).

M. Hohenadler, F. Parisen Toldin, I. Herbut and F. F. Assaad, 90, 085146 (2014)

Ho-Kin Tang, E. Laksono, J. N. B. Rodrigues, P. Sengupta, F. F. Assaad, and S. Adam, Phys. Rev. Lett. 115 (2015), 186602.

M. Raczkowski and F. F. Assaad Phys. Rev. B 96 (2017), 115155.

Ho-Kin Tang, J. N. Leaw, J. N. B. Rodrigues, I. F. Herbut, P. Sengupta, F. F. Assaad, and S. Adam, Science 361 (2018), 570.

S. Karakuzu, K. Seki, S. Sorella, arXiv:1808.07759

Example $\hat{H} = \hat{H}_0 + \hat{H}_V, \qquad \hat{H}_V = \frac{1}{4}\sum_{\mathbf{i},\mathbf{j}} V_{\mathbf{i},\mathbf{j}} (\hat{c}^\dagger_{\mathbf{i}}\hat{c}_{\mathbf{i}} - 1)(\hat{c}^\dagger_{\mathbf{j}}\hat{c}_{\mathbf{j}} - 1), \qquad \hat{c}^\dagger_{\mathbf{i}} = (\hat{c}^\dagger_{\mathbf{i},\uparrow}, \hat{c}^\dagger_{\mathbf{i},\downarrow})$

$$e^{-S(\{\Phi(i,\tau)\})} = e^{-\sum_{\mathbf{i},\mathbf{j},\tau} \Delta\tau \Phi(\mathbf{i},\tau) V^{-1}_{\mathbf{i},\mathbf{j}} \Phi(\mathbf{j},\tau)} \mathrm{Tr}\left[\prod_{\tau=1}^{L_\tau} e^{-\Delta\tau \sum_{\mathbf{i}} i\Phi(\mathbf{i},\tau)\left[\hat{c}^\dagger_{\mathbf{i}}\hat{c}_{\mathbf{i}} - 1\right]} e^{-\Delta\tau \hat{H}_0}\right]$$

Trotter

R. M. Fye Phys. Rev. B **33, 6271 (1986)**

$$Z = \mathrm{Tr}\left[e^{-\beta\hat{H}}\right] = \mathrm{Tr}\left[\left(e^{-\Delta\tau\hat{H}_V} e^{-\Delta\tau\hat{H}_0}\right)^{L_\tau}\right] + O\left(\left(\Delta\tau V\right)^2\right), \qquad L_\tau \Delta\tau = \beta$$

Note 1 Resulting propagator is not Hermitian

$$e^{-\hat{H}_1} e^{-\hat{H}_2} = e^{-(\hat{H}_3 + i\hat{H}_4)} \qquad \hat{H}^\dagger_n = \hat{H}_n, \quad \hat{H}_3 = \hat{H}_1 + \hat{H}_2 + \cdots, \quad \hat{H}_4 = \tfrac{i}{2}\left[\hat{H}_1, \hat{H}_2\right] + \cdots$$

F. Casas and A. Murua, Journal of Mathematical Physics 50 (2009), no. 3, 033513.

If possible use a symmetric decomposition:

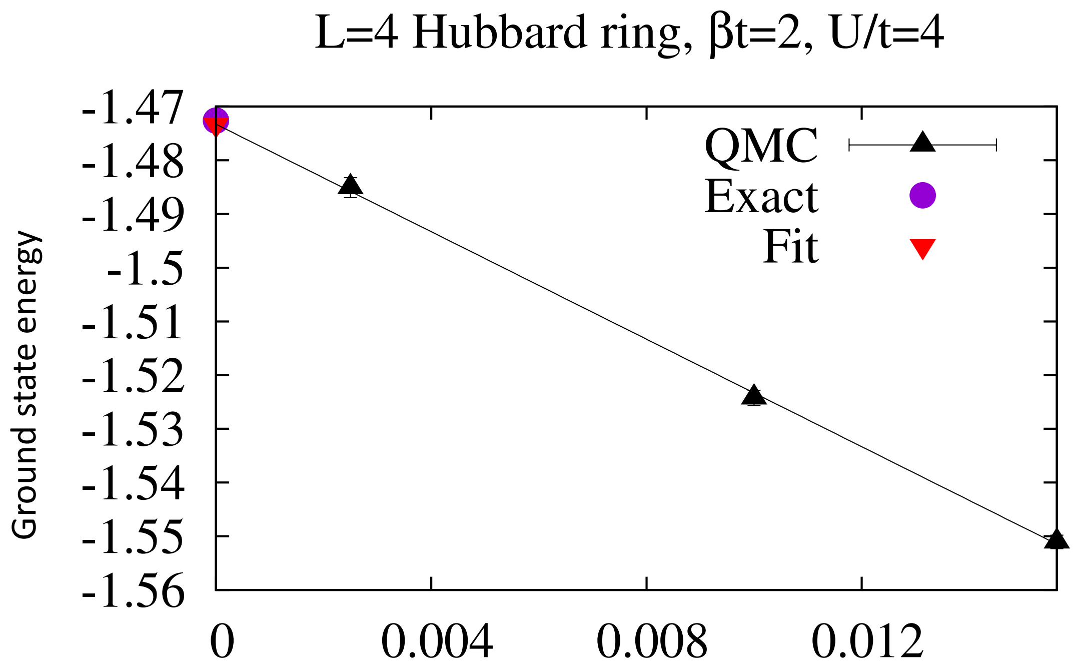
$$Z = \mathrm{Tr}\left[e^{-\beta\hat{H}}\right] = \mathrm{Tr}\left[\left(e^{-\Delta\tau\hat{H}_0/2} e^{-\Delta\tau\hat{H}_V} e^{-\Delta\tau\hat{H}_0/2}\right)^{L_\tau}\right] + O\left(\left(\Delta\tau V\right)^2\right)$$

Note 2

The Trotter systematic error can be avoided in certain cases: M. Iazzi and M. Troyer, Phys. Rev. B 91 (2015), 241118, L. Wang, Y. Liu, and M. Troyer, Phys. Rev. B 93 (2016), 155117. E. Huffman and S. Chandrasekharan, Phys. Rev. D 96 (2017), 114502.

Note 3 Trotter error can break symmetries and define a relevant perturbation at a critical point

Note 4 Tutorial https://git.physik.uni-wuerzburg.de/ALF



$(\Delta \tau t)^2$

QMC

-1.473 ± 0.002

Exact

-1.47261997

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Example $\hat{H} = \hat{H}_0 + \hat{H}_V, \qquad \hat{H}_V = \frac{1}{4}\sum_{\mathbf{i},\mathbf{j}} V_{\mathbf{i},\mathbf{j}} (\hat{c}^\dagger_{\mathbf{i}}\hat{c}_{\mathbf{i}} - 1)(\hat{c}^\dagger_{\mathbf{j}}\hat{c}_{\mathbf{j}} - 1), \qquad \hat{c}^\dagger_{\mathbf{i}} = (\hat{c}^\dagger_{\mathbf{i},\uparrow}, \hat{c}^\dagger_{\mathbf{i},\downarrow})$

$$e^{-S(\{\Phi(i,\tau)\})} = e^{-\sum_{\mathbf{i},\mathbf{j},\tau} \Delta\tau \Phi(\mathbf{i},\tau) V^{-1}_{\mathbf{i},\mathbf{j}} \Phi(\mathbf{j},\tau)} \mathrm{Tr}\left[\prod_{\tau=1}^{L_\tau} e^{-\Delta\tau \sum_{\mathbf{i}} i\Phi(\mathbf{i},\tau)\left[\hat{c}^\dagger_{\mathbf{i}}\hat{c}_{\mathbf{i}} - 1\right]} e^{-\Delta\tau \hat{H}_0} \right]$$

Hubbard Stratonovich

$$e^{\frac{-\Delta\tau}{4}\sum_{\mathbf{i},\mathbf{j}} V_{\mathbf{i},\mathbf{j}} (\hat{n}_{\mathbf{i}} - 1)(\hat{n}_{\mathbf{j}} - 1)} \propto \int \prod_{\mathbf{i}} d\Phi(\mathbf{i}) \; e^{-\sum_{\mathbf{i},\mathbf{j}} \Delta\tau \Phi(\mathbf{i}) V^{-1}_{\mathbf{i},\mathbf{j}} \Phi(\mathbf{j})} e^{-\Delta\tau \sum_{\mathbf{i}} i\Phi(\mathbf{i})\left[\hat{n}_{\mathbf{i}} - 1\right]}$$

Note: ALF implementation

$$e^{\Delta\tau \hat{A}^2} = \sum_{l=\pm1,\pm2} \gamma(l) e^{\sqrt{\Delta\tau}\,\eta(l)\,\hat{A}} + O(\Delta\tau^4)$$

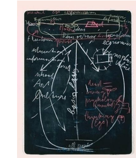
$\gamma(\pm1) = 1 + \sqrt{6}/3, \quad \gamma(\pm2) = 1 - \sqrt{6}/3$

$\eta(\pm1) = \pm\sqrt{2(3-\sqrt{6})}, \quad \eta(\pm2) = \pm\sqrt{2(3+\sqrt{6})}$

$-\frac{1}{2}\left(n_{i,\uparrow} - n_{i,\downarrow}\right)^2 = \left(n_{i,\uparrow} - \frac{1}{2}\right)\left(n_{i,\downarrow} - \frac{1}{2}\right) - \frac{1}{4}$ → Hubbard Mz

$\frac{1}{2}\left(n_{i,\uparrow} + n_{i,\downarrow} - 1\right)^2 = \left(n_{i,\uparrow} - \frac{1}{2}\right)\left(n_{i,\downarrow} - \frac{1}{2}\right) + \frac{1}{4}$ → Hubbard SU(2)

$-\left(c^\dagger_i c_j + c^\dagger_j c_i\right)^2 = 2\left(c^\dagger_i c_i - \frac{1}{2}\right)\left(c^\dagger_j c_j - \frac{1}{2}\right) - \frac{1}{2}$ → t-V



Perfect squares

$$H = H_{\text{Spin}} + H_{\text{Fermion}} + H_{\text{Kondo}}$$

$$H_{\text{Spin}} = \sum_{i,j} \left(J^z_{ij} S^z_i S^z_j + J^{\perp}_{ij} \left(S^+_i S^-_j + h.c. \right) \right) \quad (1)$$

$$H_{\text{Fermion}} = \sum_{x,y,\sigma} c^{\dagger}_{x\sigma} T_{x,y} c_{y\sigma} + U \sum_{x} (n_{x,\downarrow} - \frac{1}{2})(n_{x,\uparrow} - \frac{1}{2})$$

$$H_{\text{Kondo}} = \sum_{i,x} J^{\text{K}}_{i,x} \mathbf{c}^{\dagger}_x \left[\frac{\sigma^z}{2} \cdot S^z_i - \frac{(-1)^x}{2} \left(\sigma^+ S^-_i + \sigma^- S^+_i \right) \right] \mathbf{c}_x .$$

No sign problem if graph x is bipartite and $J^{\perp}_{i,j} < 0$

PHYSICAL REVIEW LETTERS **120,** 107201 (2018)

Quantum Monte Carlo Simulation of Frustrated Kondo Lattice Models

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

Perfect squares

$$H = H_{\text{Spin}} + H_{\text{Fermion}} + H_{\text{Kondo}}$$

$$H_{\text{Spin}} = \sum_{i,j} \left(J^z_{ij} S^z_i S^z_j + J^{\perp}_{ij} \left(S^+_i S^-_j + h.c. \right) \right) \quad (1)$$

$$H_{\text{Fermion}} = \sum_{x,y,\sigma} c^{\dagger}_{x\sigma} T_{x,y} c_{y\sigma} + U \sum_{x} (n_{x,\downarrow} - \frac{1}{2})(n_{x,\uparrow} - \frac{1}{2})$$

$$H_{\text{Kondo}} = \sum_{i,x} J^{\text{K}}_{i,x} \mathbf{c}^{\dagger}_x \left[\frac{\sigma^z}{2} \cdot S^z_i - \frac{(-1)^x}{2} \left(\sigma^+ S^-_i + \sigma^- S^+_i \right) \right] \mathbf{c}_x .$$

$$\tilde{\boldsymbol{f}}^{\dagger}_i = \left(\tilde{f}^{\dagger}_{i,\uparrow}, \tilde{f}^{\dagger}_{i,\downarrow} \right) = \left(f^{\dagger}_{i,\uparrow}, f_{i,\downarrow} \right)$$

$$\tilde{\mathbf{c}}^{\dagger}_x = \left(\tilde{c}^{\dagger}_{x,\uparrow}, \tilde{c}^{\dagger}_{x,\downarrow} \right) = \left(c^{\dagger}_{x,\uparrow}, (-1)^x c_{x,\downarrow} \right)$$

No sign problem if graph x is bipartite and $J^{\perp}_{i,j} < 0$

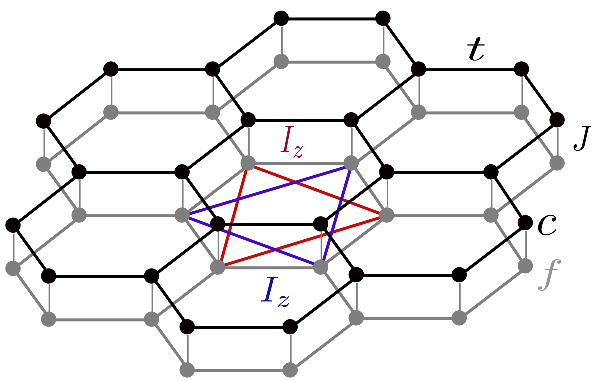
$$H_{\text{QMC}} = -\sum_{i,j} \left| J^{\perp}_{i,j} \right| \left[\frac{1}{2} \left(\widetilde{\mathbf{f}}^{\dagger}_i \widetilde{\mathbf{f}}_j + \widetilde{\mathbf{f}}^{\dagger}_j \widetilde{\mathbf{f}}_i \right)^2 + \frac{1}{4} \left(\left(\widetilde{\mathbf{f}}^{\dagger}_i \widetilde{\mathbf{f}}_i - 1 \right) + \left(\widetilde{\mathbf{f}}^{\dagger}_j \widetilde{\mathbf{f}}_j - 1 \right) \right)^2 \right]$$
$$- \frac{1}{8} \sum_{i,j} |J^z_{i,j}| \left(\left(\widetilde{\mathbf{f}}^{\dagger}_i \widetilde{\mathbf{f}}_i - 1 \right) - \frac{J^z_{i,j}}{|J^z_{i,j}|} \left(\widetilde{\mathbf{f}}^{\dagger}_j \widetilde{\mathbf{f}}_j - 1 \right) \right)^2 - U_f \sum_i \left(\widetilde{\mathbf{f}}^{\dagger}_i \widetilde{\mathbf{f}}_i - 1 \right)^2$$
$$+ \sum_{x,y} \widetilde{\mathbf{c}}^{\dagger}_x T_{x,y} \widetilde{\mathbf{c}}_y - \frac{U}{2} \sum_x \left(\widetilde{\mathbf{c}}^{\dagger}_x \widetilde{\mathbf{c}}_x - 1 \right)^2 - \frac{1}{4} \sum_{i,x} J^{\text{K}}_{i,x} \left(\widetilde{\mathbf{f}}^{\dagger}_i \widetilde{\mathbf{c}}_x + \widetilde{\mathbf{c}}^{\dagger}_x \widetilde{\mathbf{f}}_i \right)^2$$

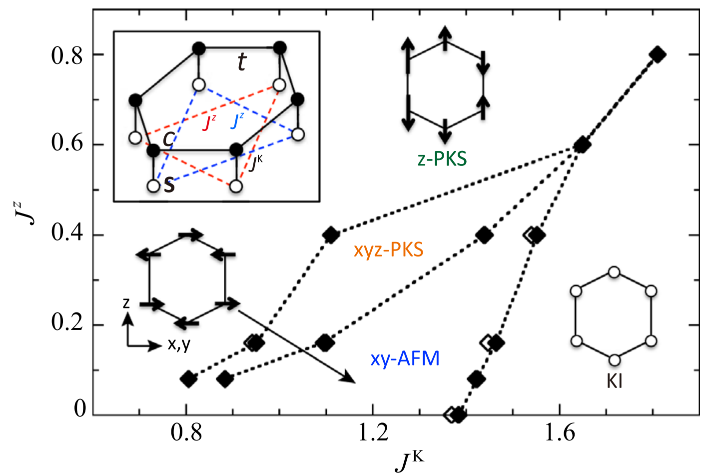
Half-filled Kondo Lattice with classical frustration

PHYSICAL REVIEW LETTERS **120**, 107201 (2018)

Quantum Monte Carlo Simulation of Frustrated Kondo Lattice Models

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



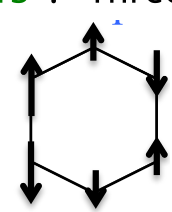


$$\hat{H} = -t \sum_{<i,j>,\sigma} \hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + J^K \sum_i \hat{\mathbf{S}}^c_i \bullet \hat{\mathbf{S}}^f_j + J^Z \sum_{<<i,j>>} \hat{S}^{z,f}_i \hat{S}^{z,f}_j$$

1) Kondo — U(1) spin

2) xy-AF: Ordering in xy-spin direction — Broken U(1) spin

3) z-TS : Three sub-lattice ordering — U(1) spin, Broken translation, "Partial Kondo Screening"



See also S. Capponi and F. F. Assaad Phys. Rev. B 63 (2001), 155114

Example $\hat{H} = \hat{H}_0 + \hat{H}_V$, $\hat{H}_V = \frac{1}{4}\sum_{\mathbf{i},\mathbf{j}} V_{\mathbf{i},\mathbf{j}} (\hat{c}^\dagger_{\mathbf{i}}\hat{c}_{\mathbf{i}} - 1)(\hat{c}^\dagger_{\mathbf{j}}\hat{c}_{\mathbf{j}} - 1)$, $\hat{c}^\dagger_{\mathbf{i}} = (\hat{c}^\dagger_{\mathbf{i},\uparrow}, \hat{c}^\dagger_{\mathbf{i},\downarrow})$

$$e^{-S(\{\Phi(i,\tau)\})} = e^{-\sum_{\mathbf{i},\mathbf{j},\tau} \Delta\tau \Phi(\mathbf{i},\tau) V^{-1}_{\mathbf{i},\mathbf{j}} \Phi(\mathbf{j},\tau)} \mathrm{Tr}\left[\prod_{\tau=1}^{L_\tau} e^{-\Delta\tau \sum_{\mathbf{i}} i\Phi(\mathbf{i},\tau)\left[\hat{c}^\dagger_{\mathbf{i}}\hat{c}_{\mathbf{i}} - 1\right]} e^{-\Delta\tau \hat{H}_0}\right]$$

Notation

$$e^{-S(\{\Phi(i,\tau)\})} = e^{-S_0(\{\Phi(i,\tau)\})} \mathrm{Tr}\left[\prod_{\tau=1}^{L_\tau} e^{-\Delta\tau \hat{\mathbf{c}}^\dagger V(\Phi_\tau)\hat{\mathbf{c}}} e^{-\Delta\tau \hat{\mathbf{c}}^\dagger T \hat{\mathbf{c}}}\right]$$

Def: $$\mathbf{B}(\Phi_\tau) = e^{-\Delta\tau V(\Phi_\tau)} e^{-\Delta\tau T}$$

Auxiliary field QMC. BSS: R. Blankenbecler, D. J. Scalapino, R. L. Sugar (1981)

✓ 1) Trotter

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Integrating out the fermions → coherent state path integral. (Negele-Orland)

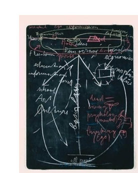
Let: $\hat{c}_x|\xi\rangle = \xi_x|\xi\rangle, \quad \{\xi_x^{\#},\xi_y^{\#'}\} = \{\hat{c}_x^{\#},\xi_y^{\#'}\} = 0, \quad \xi_y$ are Grassmann numbers, $x=(i,\sigma), \quad \# = \ ,\dagger$

States	$|\xi\rangle = \prod_x \left(1-\xi_x\hat{c}_x^\dagger\right)|0\rangle$
Overlaps	$\langle\xi|\xi'\rangle = \exp\left(\sum_x \xi_x^\dagger\xi_x'\right)$
Integration	$\int d\xi = 0, \quad \int d\xi\ \xi = 1$
Resolution of unity	$\hat{1} = \int \prod_x d\xi_x^\dagger d\xi_x\ \mathrm{e}^{-\sum_x \xi_x^\dagger\xi_x} |\xi\rangle\langle\xi|$
Trace	$\mathrm{Tr}\left[\hat{\mathbf{A}}\right] = \int \prod_x d\xi_x^\dagger d\xi_x\ \mathrm{e}^{-\sum_x \xi_x^\dagger\xi_x} \langle -\xi|\hat{\mathbf{A}}|\xi\rangle$

$$\mathrm{Tr}\, e^{-\beta\hat{H}} = \int \prod_{x,\tau=1}^{L_\tau} d\xi_{x,\tau}^\dagger d\xi_{x,\tau} \exp\left(\sum_{x,\tau=1}^{L_\tau} -\xi_{x,\tau+1}^\dagger\left(\xi_{x,\tau+1}-\xi_{x,\tau}\right) - \Delta\tau\, H(\xi_{x,\tau+1}^\dagger,\xi_{x,\tau})\right), \qquad \xi_{x,L_\tau+1}^\dagger = -\xi_{x,1}^\dagger$$

$$\prod_{\tau=1}^{L_\tau} e^{-\Delta\tau\hat{\mathbf{c}}^\dagger V(\Phi_\tau)\hat{\mathbf{c}}} e^{-\Delta\tau\,\hat{\mathbf{c}}^\dagger T\hat{\mathbf{c}}}$$

$$\xi_{\tau+1}^\dagger T\xi_\tau + \xi_{\tau+1}^\dagger V(\Phi_{\tau+1})\xi_\tau$$



Integrating out the fermions → coherent state path integral. (Negele-Orland)

$$\mathrm{Tr}\prod_{\tau=1}^{L_\tau} e^{-\Delta\tau \hat{\mathbf{c}}^\dagger V(\Phi_\tau)\hat{\mathbf{c}}} e^{-\Delta\tau \hat{\mathbf{c}}^\dagger T \hat{\mathbf{c}}} = \int \prod_{x,\tau=1}^{L_\tau} d\xi^\dagger_{x,\tau} d\xi_{x,\tau} \exp\left(\sum_{x,\tau=1}^{L_\tau} -\xi^\dagger_{x,\tau+1}\left(\xi_{x,\tau+1}-\xi_{x,\tau}\right) - \Delta\tau \xi^\dagger_{\tau+1}(T+V(\Phi_\tau))\xi_\tau \right)$$

$$\equiv \int \prod_\alpha d\xi^\dagger_\alpha d\xi_\alpha \exp\left(\sum -\xi^\dagger_\alpha M_{\alpha,\beta}\xi_\beta \right) =$$

$$= \det \underbrace{\begin{pmatrix} 1 & 0 & \cdot & \cdot & \cdot & 1-\Delta\tau(T+V(\Phi_{L_\tau})) \\ -1+\Delta\tau(T+V(\Phi_1)) & 1 & 0 & \cdot & \cdot & 0 \\ 0 & -1+\Delta\tau(T+V(\Phi_2)) & 1 & 0 & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & \cdot & \cdot & 0 & -1+\Delta\tau(T+V(\Phi_{L_\tau-1})) & 1 \end{pmatrix}}_{\equiv M \;:\; NL_\tau \times NL_\tau \text{ Matrix}}$$

Here we have used:

$$\int \prod_\alpha d\xi^\dagger_\alpha d\xi_\alpha \exp\left(\sum -\xi^\dagger_\alpha M_{\alpha,\beta}\xi_\beta \right) = \det(M)$$

With $-1+\Delta\tau(T+V(\Phi_n)) = -e^{-\Delta\tau V(\Phi_n)}e^{-\Delta\tau T} + O(\Delta\tau^2) \equiv -B(\Phi_n) + O(\Delta\tau^2)$

we obtain the final result:

Integrating out the fermions → coherent state path integral. (Negele-Orland)

$$\mathrm{Tr}\prod_{\tau=1}^{L_\tau} e^{-\Delta\tau \hat{\mathbf{c}}^\dagger V(\Phi_\tau)\hat{\mathbf{c}}} e^{-\Delta\tau\, \hat{\mathbf{c}}^\dagger T \hat{\mathbf{c}}} = \det\begin{pmatrix} 1 & 0 & \cdot & \cdot & \cdot & B(\Phi_{L_\tau}) \\ -B(\Phi_1) & 1 & 0 & \cdot & \cdot & 0 \\ 0 & -B(\Phi_2) & 1 & 0 & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & \cdot & \cdot & 0 & -B(\Phi_{L_\tau-1}) & 1 \end{pmatrix} =$$

Schur's determinant identity

$$\det\begin{pmatrix} A & B \\ C & D \end{pmatrix} = \det(D)\det(A - BD^{-1}C)$$

$$= \det\begin{pmatrix} 1 & 0 & \cdot & \cdot & \cdot & B(\Phi_{L_\tau})B(\Phi_{L_\tau-1}) \\ -B(\Phi_1) & 1 & 0 & \cdot & \cdot & 0 \\ 0 & -B(\Phi_2) & 1 & 0 & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & \cdot & \cdot & 0 & -B(\Phi_{L_\tau-2}) & 1 \end{pmatrix} =$$

$$= \cdots = \det\left(1 + B(\Phi_{L_\tau})\cdots B(\Phi_3)B(\Phi_2)\, B(\Phi_1)\right)$$

Integrating out the fermions → coherent state path integral. (Negele-Orland)

$$Z = \int D\{\Phi(\mathbf{i},\tau)\}\, e^{-S_0(\{\Phi(\mathbf{i},\tau)\})} \det \overbrace{\left[1 + B(\Phi_{L_\tau}) \cdots B(\Phi_1)\right]}^{N\times N \text{ Matrix}}$$

Numerical stabilization required !
$V^3 L_\tau$ scaling → 2592 particles
Sorella et al PRX 2016

$$= \int D\{\Phi(\mathbf{i},\tau)\}\, e^{-S_0(\{\Phi(\mathbf{i},\tau)\})} \det \underbrace{\begin{pmatrix} 1 & 0 & \cdot & \cdot & \cdot & B(\Phi_{L_\tau}) \\ -B(\Phi_1) & 1 & 0 & \cdot & \cdot & 0 \\ 0 & -B(\Phi_2) & 1 & 0 & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & \cdot & \cdot & 0 & -B(\Phi_{L_\tau -1}) & 1 \end{pmatrix}}_{\equiv M:\quad NL_\tau \times NL_\tau \quad \text{Matrix}}$$

No numerical stabilization required !
$N^3 L_\tau^3$ scaling (Hirsch-Fye)

Sub-cubic scaling? Stochastic sampling of det.

$$\left|\det(M)\right| = (2\pi)^{n/2} \int d^n\varphi\, e^{-\varphi^T \left(M^T M\right)^{-1} \varphi/2}$$

Note: Matrix is sparse.
Checkerboard decomposition of hopping → $O(NL_\tau)$ non-zero elements!

$N^x L_\tau^y$ scaling (Hybrid Molecular Dynamics)

Stefan Beyl, Florian Goth, and FFA, PRB 97 (2018).

Fermion Monte Carlo: the auxiliary field determinantal approach

Auxiliary field QMC. BSS: R. Blankenbecler, D. J. Scalapino, R. L. Sugar (1981)

✓ 1) Trotter

✓ 2) Hubbard Stratonovitch

✓ 3) Integrating out the fermions

4) Measurements

5) Wicks theorem

6) Absence of sign problem

7) Organization of the code and fast updates.

8) Stabilization

9) ALF examples

Measuring observables:

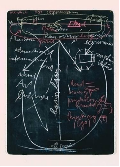
$$\frac{\mathrm{Tr}\left[e^{-\beta\hat{H}}\hat{O}\right]}{\mathrm{Tr}\, e^{-\beta\hat{H}}} = \frac{\int D\Phi\, e^{-S_0(\Phi)}\mathrm{Tr}\left[\prod_{\tau=1}^{L_\tau} e^{-\Delta\tau\hat{\mathbf{c}}^\dagger T\hat{\mathbf{c}}} e^{-\Delta\tau\hat{\mathbf{c}}^\dagger V(\Phi_\tau)\hat{\mathbf{c}}}\hat{O}\right]}{\int D\Phi\, e^{-S_0(\Phi)}\mathrm{Tr}\left[\prod_{\tau=1}^{L_\tau} e^{-\Delta\tau\hat{\mathbf{c}}^\dagger T\hat{\mathbf{c}}} e^{-\Delta\tau\hat{\mathbf{c}}^\dagger V(\Phi_\tau)\hat{\mathbf{c}}}\right]}$$

$$= \frac{\int D\Phi\, e^{-S_0(\Phi)}\mathrm{Tr}\left[\prod_{\tau=1}^{L_\tau} e^{-\Delta\tau\hat{\mathbf{c}}^\dagger T\hat{\mathbf{c}}} e^{-\Delta\tau\hat{\mathbf{c}}^\dagger V(\Phi_\tau)\hat{\mathbf{c}}}\right] \dfrac{\mathrm{Tr}\left[\prod_{\tau=1}^{L_\tau} e^{-\Delta\tau\hat{\mathbf{c}}^\dagger T\hat{\mathbf{c}}} e^{-\Delta\tau\hat{\mathbf{c}}^\dagger V(\Phi_\tau)\hat{\mathbf{c}}}\hat{O}\right]}{\mathrm{Tr}\left[\prod_{\tau=1}^{L_\tau} e^{-\Delta\tau\hat{\mathbf{c}}^\dagger T\hat{\mathbf{c}}} e^{-\Delta\tau\hat{\mathbf{c}}^\dagger V(\Phi_\tau)\hat{\mathbf{c}}}\right]}}{\int D\Phi\, e^{-S_0(\Phi)}\mathrm{Tr}\left[\prod_{\tau=1}^{L_\tau} e^{-\Delta\tau\hat{\mathbf{c}}^\dagger T\hat{\mathbf{c}}} e^{-\Delta\tau\hat{\mathbf{c}}^\dagger V(\Phi_\tau)\hat{\mathbf{c}}}\right]}$$

Implicit assumption: $\mathrm{Tr}\left[\prod_{\tau=1}^{L_\tau} e^{-\Delta\tau\hat{\mathbf{c}}^\dagger T\hat{\mathbf{c}}} e^{-\Delta\tau\hat{\mathbf{c}}^\dagger V(\Phi_\tau)\hat{\mathbf{c}}}\right]$ does not vanish!

If this is not the case, then wrong results can be obtained and/or variance may not be finite.

Hao Shi and Shiwei Zhang, Phys. Rev. E 93 (2016), 033303.



Measuring observables:

$$\frac{\mathrm{Tr}\left[e^{-\beta\hat{H}}\hat{O}\right]}{\mathrm{Tr}\, e^{-\beta\hat{H}}} = \frac{\int D\Phi\, e^{-S_0(\Phi)}\mathrm{Tr}\left[\prod_{\tau=1}^{L_\tau} e^{-\Delta\tau\hat{\mathbf{c}}^\dagger T\hat{\mathbf{c}}} e^{-\Delta\tau\hat{\mathbf{c}}^\dagger V(\Phi_\tau)\hat{\mathbf{c}}}\hat{O}\right]}{\int D\Phi\, e^{-S_0(\Phi)}\mathrm{Tr}\left[\prod_{\tau=1}^{L_\tau} e^{-\Delta\tau\hat{\mathbf{c}}^\dagger T\hat{\mathbf{c}}} e^{-\Delta\tau\hat{\mathbf{c}}^\dagger V(\Phi_\tau)\hat{\mathbf{c}}}\right]}$$

$$= \frac{\int D\Phi\, e^{-S_0(\Phi)}\mathrm{Tr}\left[\prod_{\tau=1}^{L_\tau} e^{-\Delta\tau\hat{\mathbf{c}}^\dagger T\hat{\mathbf{c}}} e^{-\Delta\tau\hat{\mathbf{c}}^\dagger V(\Phi_\tau)\hat{\mathbf{c}}}\right] \dfrac{\mathrm{Tr}\left[\prod_{\tau=1}^{L_\tau} e^{-\Delta\tau\hat{\mathbf{c}}^\dagger T\hat{\mathbf{c}}} e^{-\Delta\tau\hat{\mathbf{c}}^\dagger V(\Phi_\tau)\hat{\mathbf{c}}}\hat{O}\right]}{\mathrm{Tr}\left[\prod_{\tau=1}^{L_\tau} e^{-\Delta\tau\hat{\mathbf{c}}^\dagger T\hat{\mathbf{c}}} e^{-\Delta\tau\hat{\mathbf{c}}^\dagger V(\Phi_\tau)\hat{\mathbf{c}}}\right]}}{\int D\Phi\, e^{-S_0(\Phi)}\mathrm{Tr}\left[\prod_{\tau=1}^{L_\tau} e^{-\Delta\tau\hat{\mathbf{c}}^\dagger T\hat{\mathbf{c}}} e^{-\Delta\tau\hat{\mathbf{c}}^\dagger V(\Phi_\tau)\hat{\mathbf{c}}}\right]}$$

$$= \int D\Phi\; P(\Phi) \ll \hat{O} \gg_{(\Phi)}$$

Auxiliary field QMC. BSS: R. Blankenbecler, D. J. Scalapino, R. L. Sugar (1981)

✓ 1) Trotter

✓ 2) Hubbard Stratonovitch

✓ 3) Integrating out the fermions

✓ 4) Measurements

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Measuring observables: Calculating $O(\Phi)$ → Wick's theorem (Negele Orland)

Let $\prod_{\tau=\tau_1+1}^{\tau_2} e^{-\Delta\tau \hat{\mathbf{c}}^\dagger V(\Phi_\tau)\hat{\mathbf{c}}} e^{-\Delta\tau \hat{\mathbf{c}}^\dagger T \hat{\mathbf{c}}} = \hat{U}_\Phi(\tau_2,\tau_1)$ if $\tau_2 > \tau_1$ and $\hat{U}_\Phi(\tau_2,\tau_1) = \hat{U}_\Phi^{-1}(\tau_1,\tau_2)$ if $\tau_1 > \tau_2$

Let $\hat{O} = T_\tau \, \hat{c}^\dagger_{x_1}(\tau_1)\hat{c}_{x'_1}(\tau'_1)\hat{c}^\dagger_{x_2}(\tau_2)\hat{c}_{x'_2}(\tau'_2)\cdots\hat{c}^\dagger_{x_n}(\tau_n)\hat{c}_{x'_n}(\tau'_n)$ $\qquad T_\tau$: Time ordering

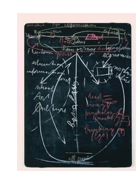
with $\hat{c}^\dagger_x(\tau) = \hat{U}_\Phi(0,\tau)\,\hat{c}^\dagger_x\,\hat{U}_\Phi(\tau,0)$

$$\frac{\mathrm{Tr}\left[\prod_{\tau=1}^{L_\tau} e^{-\Delta\tau \hat{\mathbf{c}}^\dagger V(\Phi_\tau)\hat{\mathbf{c}}} e^{-\Delta\tau \hat{\mathbf{c}}^\dagger T \hat{\mathbf{c}}}\hat{O}\right]}{\mathrm{Tr}\left[\prod_{\tau=1}^{L_\tau} e^{-\Delta\tau \hat{\mathbf{c}}^\dagger V(\Phi_\tau)\hat{\mathbf{c}}} e^{-\Delta\tau \hat{\mathbf{c}}^\dagger T \hat{\mathbf{c}}}\right]} = \frac{\int \prod_\alpha d\xi^\dagger_\alpha d\xi_\alpha \exp\left(\sum_{\alpha,\beta} -\xi^\dagger_\alpha M_{\alpha,\beta}\,\xi_\beta\right)\xi^\dagger_{x_1,\tau_1}\xi_{x'_1,\tau'_1}\cdots\xi^\dagger_{x_n,\tau_n}\xi_{x'_n,\tau'_n}}{\int \prod_\alpha d\xi^\dagger_\alpha d\xi_\alpha \exp\left(\sum_{\alpha,\beta} -\xi^\dagger_\alpha M_{\alpha,\beta}\,\xi_\beta\right)} =$$

$$= \det\begin{pmatrix} -M^{-1}_{(x_1\tau_1),(x'_1\tau'_1)} & \cdots & -M^{-1}_{(x_1\tau_1),(x'_n\tau'_n)} \\ \vdots & \ddots & \vdots \\ -M^{-1}_{(x_n\tau_n),(x'_1\tau'_1)} & \cdots & -M^{-1}_{(x_n\tau_n),(x'_n\tau'_n)} \end{pmatrix}$$

→ $M^{-1}_{(x_1\tau_1),(x'_1\tau'_1)} = -\ll T_\tau \hat{c}_{x_1}(\tau_1)\hat{c}^\dagger_{x'_1}(\tau'_1)\gg$

Green function



Measuring observables:

Since we know the matrix M explicitly we can find a form for M^{-1}. For instance the equal time Green function reeds:

$$M^{-1}_{(x_1\tau),(x'_1\tau)} = - \ll T_\tau \hat{c}_{x_1}(\tau) \hat{c}^\dagger_{x'_1}(\tau) \gg = -\Big(1 + B(\Phi_\tau)\cdots B(\Phi_1) B(\Phi_{L_\tau})\cdots B(\Phi_{\tau+1})\Big)^{-1}_{x_1,x'_1}$$

$$\text{Def:} \quad G_\Phi(\tau) = \Big(1 + B(\Phi_\tau)\cdots B(\Phi_1) B(\Phi_{L_\tau})\cdots B(\Phi_{\tau+1})\Big)^{-1}$$

The equal time Green function is the central quantity in the algorithm.

Measuring observable:

$$\frac{\mathrm{Tr}\left[e^{-\beta\hat{H}}\hat{c}_x\hat{c}_y^\dagger\right]}{\mathrm{Tr}\,e^{-\beta\hat{H}}} = \int D\Phi\; P(\Phi)\; G_{x,y}\left(\Phi\right)$$

$$P(\Phi) = \frac{e^{-S(\Phi)}}{\int D\Phi\; e^{-S(\Phi)}}\;, \qquad G(\Phi) \;=\; (1 + B_{L_\tau}\cdots B_1)^{-1}$$

Wicks theorem holds for a given field configuration →

Any equal time observable can be computed from G

A different way of writing Wick's theorem. T. Grover Phys. Rev. Lett., 111, 130402, (2013).

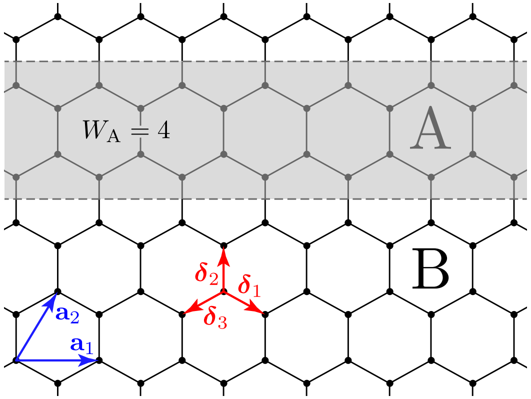
$$\hat{\rho} \equiv \frac{e^{-\beta\hat{H}}}{Z} = \int d\Phi\, P(\Phi)\hat{\rho}(\Phi), \qquad \hat{\rho}(\Phi) = \det\left[G(\Phi)\right] e^{-\hat{c}^\dagger \ln\left[\frac{1}{1-G(\Phi)}-1\right]\hat{c}}$$

$$\rightarrow \int d\Phi\, P(\Phi)\mathrm{Tr}\left[\hat{\rho}(\Phi)\hat{O}\right] = \left\langle \hat{O}\right\rangle$$

For all equal time observables.

Renyi entanglement entropies

T. Grover Phys. Rev. Lett., 111, 130402, (2013).



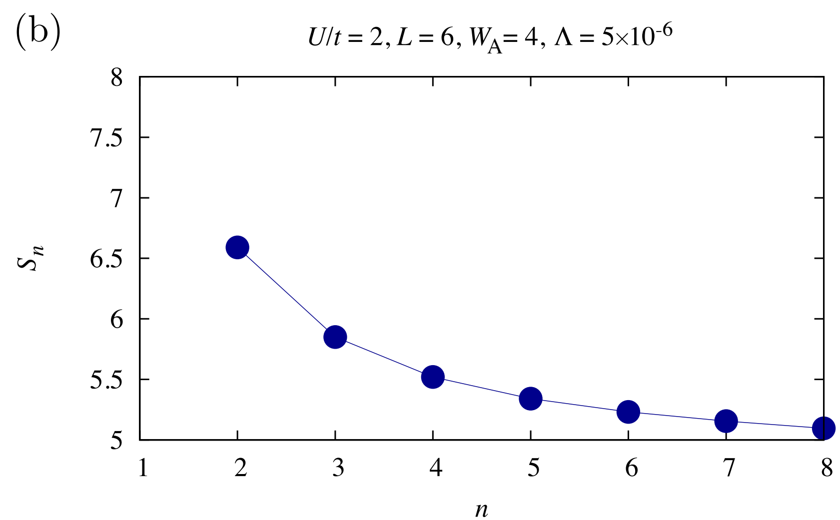
$$\hat{\rho}_A = \mathrm{Tr}_B \hat{\rho} \equiv \int d\Phi\, P(\Phi) \hat{\rho}_A(\Phi)$$

n-replicas

$$\mathrm{Tr} \hat{\rho}_A{}^n = \int \overbrace{d\Phi^1 \cdots d\Phi^n P(\Phi^1) \cdots P(\Phi^n)}^{\text{n-replicas}} \mathrm{Tr}\left[\hat{\rho}_A(\Phi^1) \cdots \hat{\rho}_A(\Phi^n) \right]$$

$$S_n = -\frac{1}{n-1} \ln \mathrm{Tr} \hat{\rho}_A{}^n$$

F. F. Assaad, T. C. Lang, and F. Parisen Toldin
Phys. Rev. B, 89, 125121, (2014)



Mutual information in heavy fermions systems

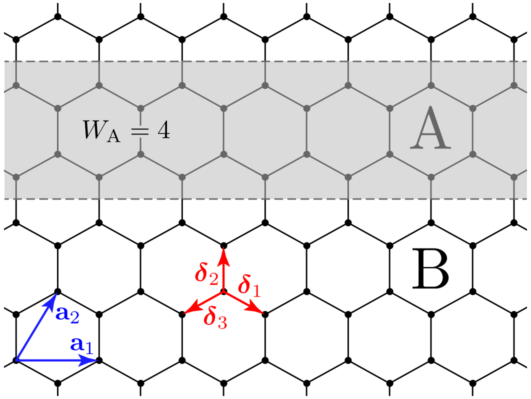
Francesco Parisen Toldin,[1,*] Toshihiro Sato,[1,†] and Fakher F. Assaad[1,‡]

arXiv:1811.11194v2

$$I_n(\Gamma_c, \Gamma_S) \equiv S_n(\Gamma_c) + S_n(\Gamma_S) - S_n(\Gamma_c \cup \Gamma_S)$$

Entanglement Hamiltonian

T. Grover Phys. Rev. Lett., 111, 130402, (2013).



$$\hat{\rho}_A = e^{-\hat{H}_E} = \mathrm{Tr}_B \hat{\rho} \equiv \int d\Phi\, P(\Phi) \hat{\rho}_A(\Phi),$$

with $$\hat{\rho}_A(\Phi) = \overbrace{\det\left[1 - G_A(\Phi)\right]}^{\equiv e^{-\alpha(\Phi)}} e^{-\hat{c}^\dagger \overbrace{\ln\left[G_A^{-1}(\Phi) - 1\right]}^{\equiv h(\Phi)} \hat{c}}$$

Cumulant expansion: $$\hat{H}_E = \sum_{x,y} t_{x,y} \hat{c}_x^\dagger \hat{c}_y + \sum_{x,y,w,z} U_{x,y,w,z} \hat{c}_x^\dagger \hat{c}_y \hat{c}_w^\dagger \hat{c}_z + \cdots$$

$$t_{x,y} = \left\langle h(\Phi)_{x,y} \right\rangle - \left[\left\langle \alpha(\Phi) h(\Phi)_{x,y} \right\rangle - \left\langle \alpha(\Phi) \right\rangle \left\langle h(\Phi)_{x,y} \right\rangle \right]$$

$$\left\langle h(\Phi)_{x,y} \right\rangle = \int d\Phi P(\Phi) h(\Phi)_{x,y}$$

$$U_{x,y,w,z} = -\left[\left\langle h(\Phi)_{x,y} h(\Phi)_{w,z} \right\rangle - \left\langle h(\Phi)_{x,y} \right\rangle \left\langle h(\Phi)_{w,z} \right\rangle \right]$$

PHYSICAL REVIEW LETTERS **121,** 200602 (2018)

Entanglement Hamiltonian of Interacting Fermionic Models

Francesco Parisen Toldin[*] and Fakher F. Assaad[†]
Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

Fermion Monte Carlo: the auxiliary field determinantal approach

Auxiliary field QMC. BSS: R. Blankenbecler, D. J. Scalapino, R. L. Sugar (1981)

✔ 1) Trotter

✔ 2) Hubbard Stratonovitch

✔ 3) Integrating out the fermions

✔ 4) Measurements

✔ 5) Wicks theorem

6) Absence of sign problem

7) Organization of the code and fast updates.

8) Stabilization

9) ALF examples

Auxiliary field QMC. Positivity of weight?

$$e^{-S\left(\left\{\Phi(i,\tau)\right\}\right)} = e^{-\sum_{\mathbf{i},\mathbf{j},\tau}\Delta\tau\,\Phi(\mathbf{i},\tau)V^{-1}_{\mathbf{i},\mathbf{j}}\Phi(\mathbf{j},\tau)}\,\mathrm{Tr}\underbrace{\left[\prod_{\tau=1}^{L_\tau} e^{-\Delta\tau\sum_{\mathbf{i}} i\Phi(\mathbf{i},\tau)\left[\hat{c}^\dagger_{\mathbf{i}}\hat{c}_{\mathbf{i}}-1\right]} e^{-\Delta\tau\hat{H}_0}\right]}_{\equiv\hat{\mathbf{U}}}$$

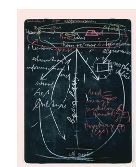
Is the action real ? Let $\hat{T}$ be an anti-unitary operator, $\hat{T}=\hat{K}\hat{U}$, $\hat{U}^\dagger\hat{U}=1$, $\hat{K}$: complex conjugation with

$\hat{T}^2=-1$ and $\left[\hat{T},\hat{\mathbf{U}}\right]=0$ then $e^{-S\left(\left\{\Phi(i,\tau)\right\}\right)}\geq 0$

C. Wu and S.-C. Zhang. Phys. Rev. B, 71, 155115, (2005).

Let $\hat{\mathbf{U}}\left|v\right\rangle=\lambda\left|v\right\rangle \Rightarrow \hat{\mathbf{U}}\hat{T}\left|v\right\rangle=\bar{\lambda}\hat{T}\left|v\right\rangle$ From $\hat{T}^2=-1$, $\left\langle v\right|\hat{T}\left|v\right\rangle=0$

→ Eigenvalues of $\hat{\mathbf{U}}$ occur in complex conjugate pairs. Implicit assumption: U(1) symmetry



Auxiliary field QMC. Positivity of weight?

$$e^{-S(\{\Phi(i,\tau)\})} = e^{-\sum_{\mathbf{i},\mathbf{j},\tau} \Delta\tau \Phi(\mathbf{i},\tau) V^{-1}_{\mathbf{i},\mathbf{j}} \Phi(\mathbf{j},\tau)} \mathrm{Tr} \underbrace{\left[\prod_{\tau=1}^{L_\tau} e^{-\Delta\tau \sum_{\mathbf{i}} i\Phi(\mathbf{i},\tau)\left[\hat{c}^\dagger_{\mathbf{i}} \hat{c}_{\mathbf{i}} - 1\right]} e^{-\Delta\tau \hat{H}_0} \right]}_{\equiv \hat{\mathbf{U}}}$$

Is the action real ? Let $\hat{T}$ be an anti-unitary operator, $\hat{T} = \hat{K}\hat{U}$, $\hat{U}^\dagger \hat{U} = 1$, $\hat{K}$: complex conjugation with

$\hat{T}^2 = -1$ and $\left[\hat{T}, \hat{\mathbf{U}}\right] = 0$ then $e^{-S(\{\Phi(i,\tau)\})} \geq 0$

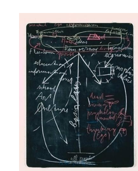
C. Wu and S.-C. Zhang. Phys. Rev. B, 71, 155115, (2005).

Let $\hat{\mathbf{U}} |v\rangle = \lambda |v\rangle \Rightarrow \hat{\mathbf{U}} \hat{T} |v\rangle = \overline{\lambda} \hat{T} |v\rangle$ From $\hat{T}^2 = -1$, $\langle v | \hat{T} | v \rangle = 0$

→ Eigenvalues of $\hat{\mathbf{U}}$ occur in complex conjugate pairs. Implicit assumption: U(1) symmetry

Time reversal symmetry

$$\hat{T} \begin{pmatrix} \hat{c}^\dagger_{\mathbf{i},\uparrow} \\ \hat{c}^\dagger_{\mathbf{i},\downarrow} \end{pmatrix} \hat{T}^{-1} = \begin{pmatrix} -\hat{c}^\dagger_{\mathbf{i},\downarrow} \\ \hat{c}^\dagger_{\mathbf{i},\uparrow} \end{pmatrix}$$



Auxiliary field QMC. Positivity of weight?

$$e^{-S(\{\Phi(i,\tau)\})} = e^{-\sum_{\mathbf{i},\mathbf{j},\tau}\Delta\tau\,\Phi(\mathbf{i},\tau)V^{-1}_{\mathbf{i},\mathbf{j}}\Phi(\mathbf{j},\tau)}\,\mathrm{Tr}\underbrace{\left[\prod_{\tau=1}^{L_\tau} e^{-\Delta\tau\sum_{\mathbf{i}} i\Phi(\mathbf{i},\tau)\left[\hat{c}^\dagger_{\mathbf{i}}\hat{c}_{\mathbf{i}}-1\right]} e^{-\Delta\tau\hat{H}_0}\right]}_{\equiv\hat{\mathbf{U}}}$$

Is the action real ?

Ever growing class of *interesting* negative sign free models.

C. Wu and S.-C. Zhang. Phys. Rev. B, 71, 155115, (2005)

E. Huffman and S. Chandrasekharan, Phys. Rev. B 89, 111101, (2014)

Zi-Xiang Li, Yi-Fan Jiang, and H. Yao Phys. Rev. Lett. 117, 267002, (2016)

Z. C. Wei, C. Wu, Yi Li, Shiwei Zhang, and T. Xiang. Phys. Rev. Lett. 116, 250601 (2016)
.
Z. C. Wei, arXiv:1712.09412

Conditions on $A_1 \cdots A_n,\;\; A_i^T = -A_i \;\mid\; \mathrm{Tr}\left(e^{\gamma^T A_1 \gamma}\cdots e^{\gamma^T A_n \gamma}\right) \geq 0$?

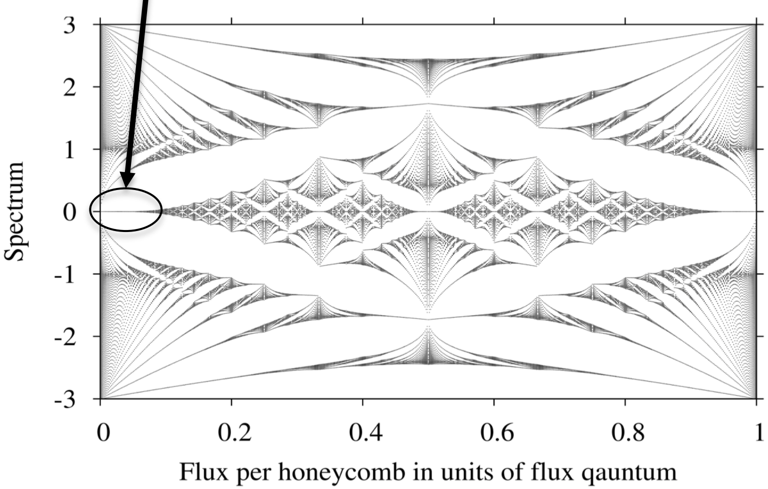
PHYSICAL REVIEW B **98**, 235108 (2018)

Half-filled Landau levels: A continuum and sign-free regularization for three-dimensional quantum critical points

Matteo Ippoliti,[1] Roger S. K. Mong,[2] Fakher F. Assaad,[3] and Michael P. Zaletel[1,4]

$$\hat{H} = \hat{P} \int d^2\boldsymbol{x} \left[U_M \left(\hat{\psi}^\dagger(\boldsymbol{x}) \tau_z \boldsymbol{\sigma} \hat{\psi}(\boldsymbol{x}) \right)^2 + U_K \left(\hat{\psi}^\dagger(\boldsymbol{x}) \tau_x \hat{\psi}(\boldsymbol{x}) \right)^2 + U_K \left(\hat{\psi}^\dagger(\boldsymbol{x}) \tau_y \hat{\psi}(\boldsymbol{x}) \right)^2 \right] \hat{P}$$

4 component spinor.
Single particle Hilbert space has dimension $4N_\phi$



PRL **114**, 226801 (2015) PHYSICAL REVIEW LETTERS

Wess-Zumino-Witten Terms in Graphene Landau Levels

Junhyun Lee[1] and Subir Sachdev[1,2]

$U_K = U_M$

$$S = \int d^2\boldsymbol{x} d\tau \frac{1}{G} \left(\partial_\mu \hat{\boldsymbol{\varphi}}(\boldsymbol{x}, \tau) \right)^2 + 2\pi i \Gamma \left[\hat{\boldsymbol{\varphi}} \right]$$

$$\Gamma \left[\hat{\boldsymbol{\varphi}} \right] = \frac{\epsilon_{abcde}}{\mathrm{Area}(S^4)} \int_0^1 du \int d^2\boldsymbol{x} d\tau \hat{\varphi}_a \partial_x \hat{\varphi}_b \partial_y \hat{\varphi}_c \partial_\tau \hat{\varphi}_d \partial_u \hat{\varphi}_e$$

Candidate theory for critical point of DQCP.

Auxiliary field QMC. Sign problem

Generically the action will be complex

$$\langle O\rangle_P = \frac{\int d\{\Phi\} e^{-S(\{\Phi\})} O(\{\Phi\})}{\int d\{\Phi\} e^{-S(\{\Phi\})}} = \frac{\dfrac{\int d\{\Phi\} \left| e^{-S(\{\Phi\})}\right| e^{i\varphi(\{\Phi\})} O(\{\Phi\})}{\int d\{\Phi\} \left| e^{-S(\{\Phi\})}\right|}}{\dfrac{\int d\{\Phi\} \left| e^{-S(\{\Phi\})}\right| e^{i\varphi(\{\Phi\})}}{\int d\{\Phi\} \left| e^{-S(\{\Phi\})}\right|}} \equiv \frac{\left\langle e^{i\varphi(\{\Phi\})} O \right\rangle_{\bar{P}}}{\left\langle e^{i\varphi(\{\Phi\})} \right\rangle_{\bar{P}}}$$

Auxiliary field QMC. Sign problem

Generically the action will be complex

$$\langle O \rangle_P = \frac{\int d\{\Phi\} e^{-S(\{\Phi\})} O(\{\Phi\})}{\int d\{\Phi\} e^{-S(\{\Phi\})}} = \frac{\dfrac{\int d\{\Phi\} \left| e^{-S(\{\Phi\})} \right| e^{i\varphi(\{\Phi\})} O(\{\Phi\})}{\int d\{\Phi\} \left| e^{-S(\{\Phi\})} \right|}}{\dfrac{\int d\{\Phi\} \left| e^{-S(\{\Phi\})} \right| e^{i\varphi(\{\Phi\})}}{\int d\{\Phi\} \left| e^{-S(\{\Phi\})} \right|}} \equiv \frac{\left\langle e^{i\varphi(\{\Phi\})} O \right\rangle_{\bar{P}}}{\left\langle e^{i\varphi(\{\Phi\})} \right\rangle_{\bar{P}}}$$

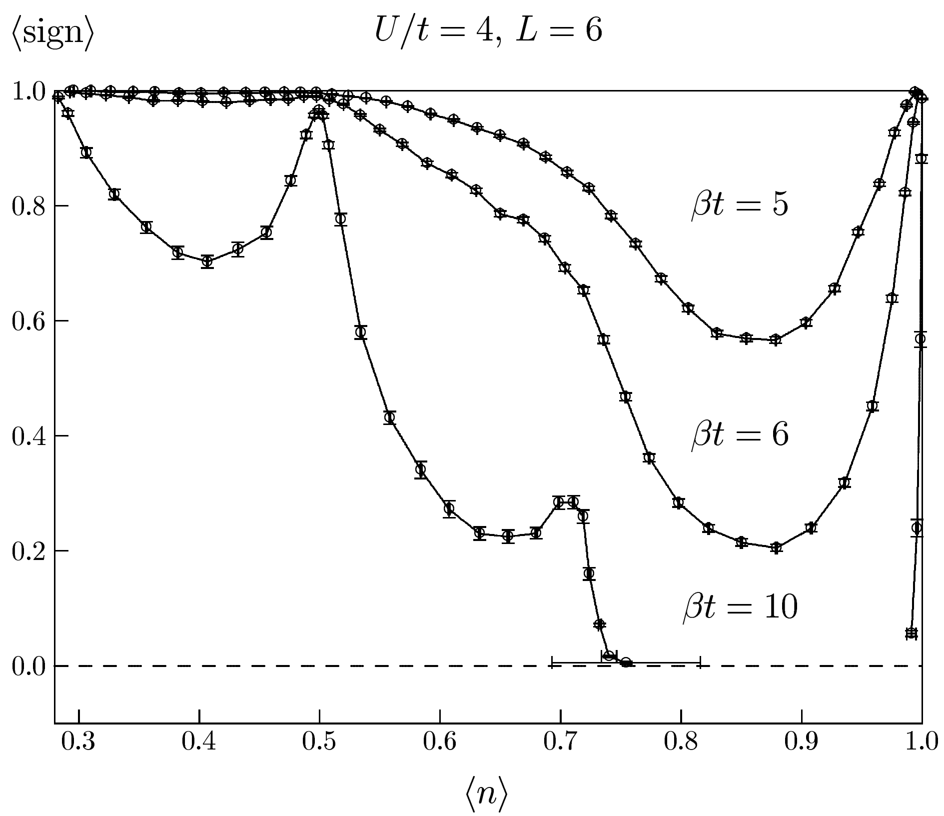
But in the low temperature limit: $\left\langle e^{i\varphi(\{\Phi\})} \right\rangle_{\bar{P}} = Z / \bar{Z} \propto e^{-\beta N (e_0 - \bar{e}_0)} = e^{-\beta N \delta}$

$$\Delta(Z/\bar{Z}) \Big/ Z/\bar{Z} << 1 \quad \text{but} \quad \Delta(Z/\bar{Z}) \approx 1 \Big/ \sqrt{\text{CPU}} \quad \text{so that CPU} >> \quad \mathrm{e}^{2\beta V \delta}$$

Note:

- δ is method dependent.

Hubbard model on square lattice away from half-filling



$$-\frac{U}{2}\left(\hat{n}_{i,\uparrow}-\hat{n}_{i,\downarrow}\right)^2 \quad = U\left(\hat{n}_{i,\uparrow}-\frac{1}{2}\right)\left(\hat{n}_{i,\downarrow}-\frac{1}{2}\right)-\frac{1}{4}$$

$$e^{\Delta\tau U\left(\hat{n}_{i,\uparrow}-\hat{n}_{i,\downarrow}\right)^2/2} = \sum_{l=\pm1,\pm2}\gamma(l)e^{\sqrt{\Delta\tau U/2}\,\eta(l)\left(\hat{n}_{i,\uparrow}-\hat{n}_{i,\downarrow}\right)} + O(\Delta\tau^4)$$

Fermion Monte Carlo: the auxiliary field determinantal approach

Auxiliary field QMC. BSS: R. Blankenbecler, D. J. Scalapino, R. L. Sugar (1981)

✓ 1) Trotter

✓ 2) Hubbard Stratonovitch

✓ 3) Integrating out the fermions

✓ 4) Measurements

✓ 5) Wicks theorem

✓ 6) Absence of sign problem

7) Organization of the code and fast updates.

8) Stabilization

9) ALF examples

All in all we have:

$$< \hat{O} > = \frac{\int D\{\Phi(\mathbf{i},\tau)\}\, e^{-S_0(\{\Phi(\mathbf{i},\tau)\})} \det\left[1 + B(\Phi_{L_\tau}) \cdots B(\Phi_1)\right] \ll \hat{O} \gg}{\int D\{\Phi(\mathbf{i},\tau)\}\, e^{-S_0(\{\Phi(\mathbf{i},\tau)\})} \det\left[1 + B(\Phi_{L_\tau}) \cdots B(\Phi_1)\right]}$$

Sum over HS fields → Metropolis importance sampling. Adopt a sequential single spin-flip upgrading scheme.

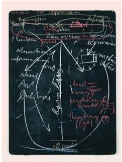
$$\Phi_{i,\tau} \rightarrow \Phi'_{i,\tau}$$

$$B(\Phi_\tau) \rightarrow B(\Phi'_\tau) = (1+\Delta) B(\Phi_\tau)$$

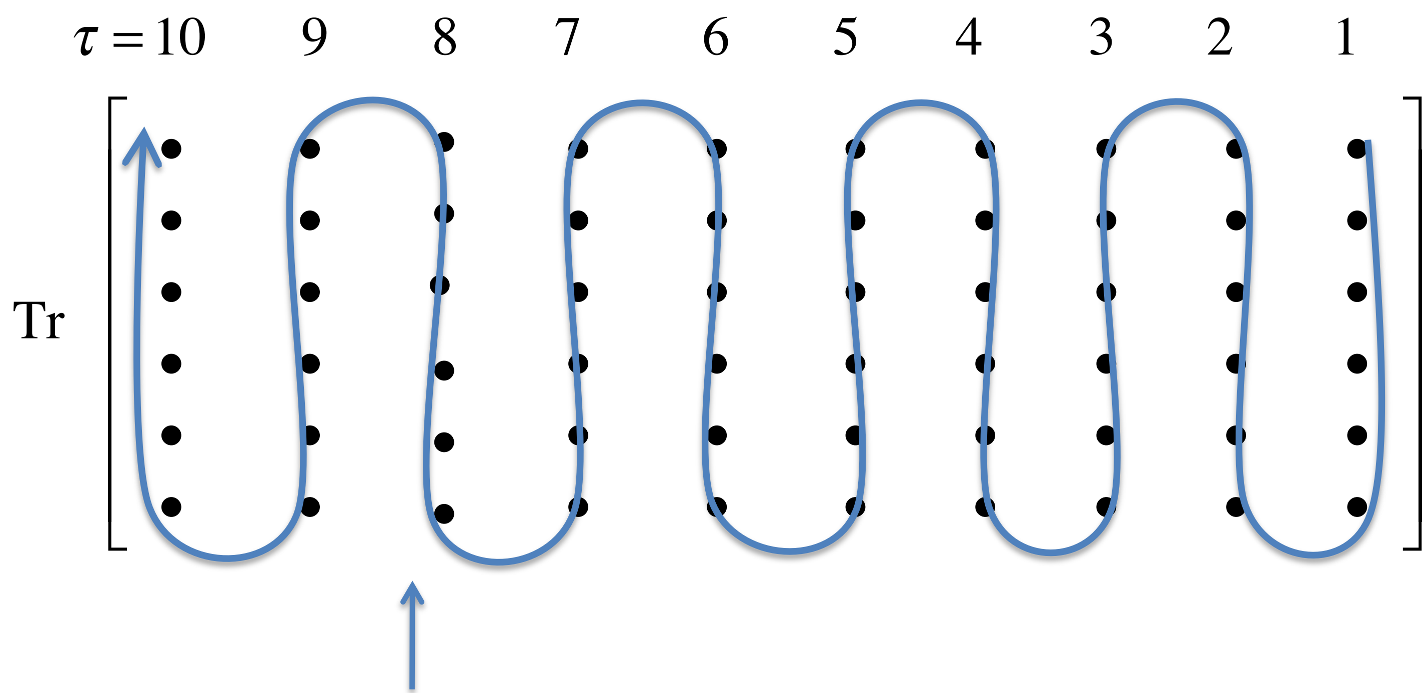
$$\frac{e^{-S_0(\{\Phi'(\mathbf{i},\tau)\})} \det\left[1 + B(\Phi_{L_\tau}) \cdots (1+\Delta) B(\Phi_\tau) \cdots B(\Phi_1)\right]}{e^{-S_0(\{\Phi(\mathbf{i},\tau)\})} \det\left[1 + B(\Phi_{L_\tau}) \cdots B(\Phi_1)\right]} = \frac{e^{-S_0(\{\Phi'(\mathbf{i},\tau)\})}}{e^{-S_0(\{\Phi(\mathbf{i},\tau)\})}} \det\left[1 + \Delta\left(1 - G_\Phi(\tau)\right)\right]$$

The equal time Green function matrix is the central quantity of the algorithm. It determines

i) The Monte Carlo dynamics
ii) All equal time observables (Wick's theorem)



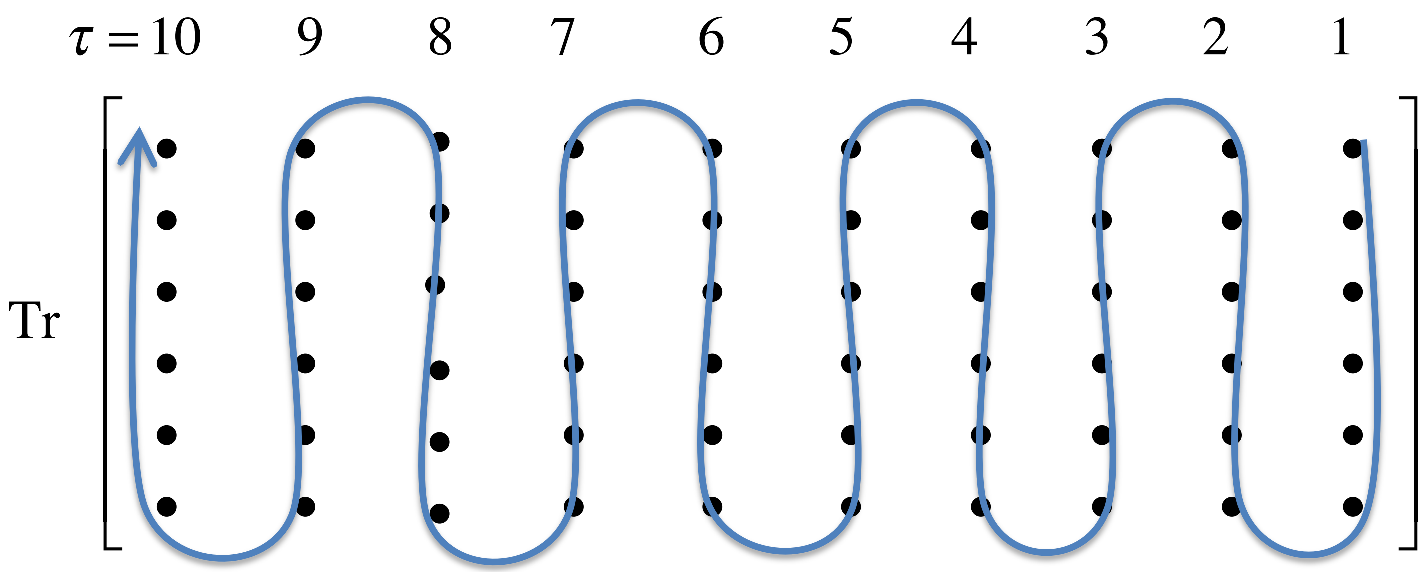
Organization of the code.



Real space lattice, with replica at each imaginary time slice.

Independent Hubbard Stratonovitch field at each imaginary time and lattice site. $\Phi_{i,\tau}$

Organization of the code.



Start on time slice $\tau = 1$ with $G_{\Phi}(\tau = 1)$

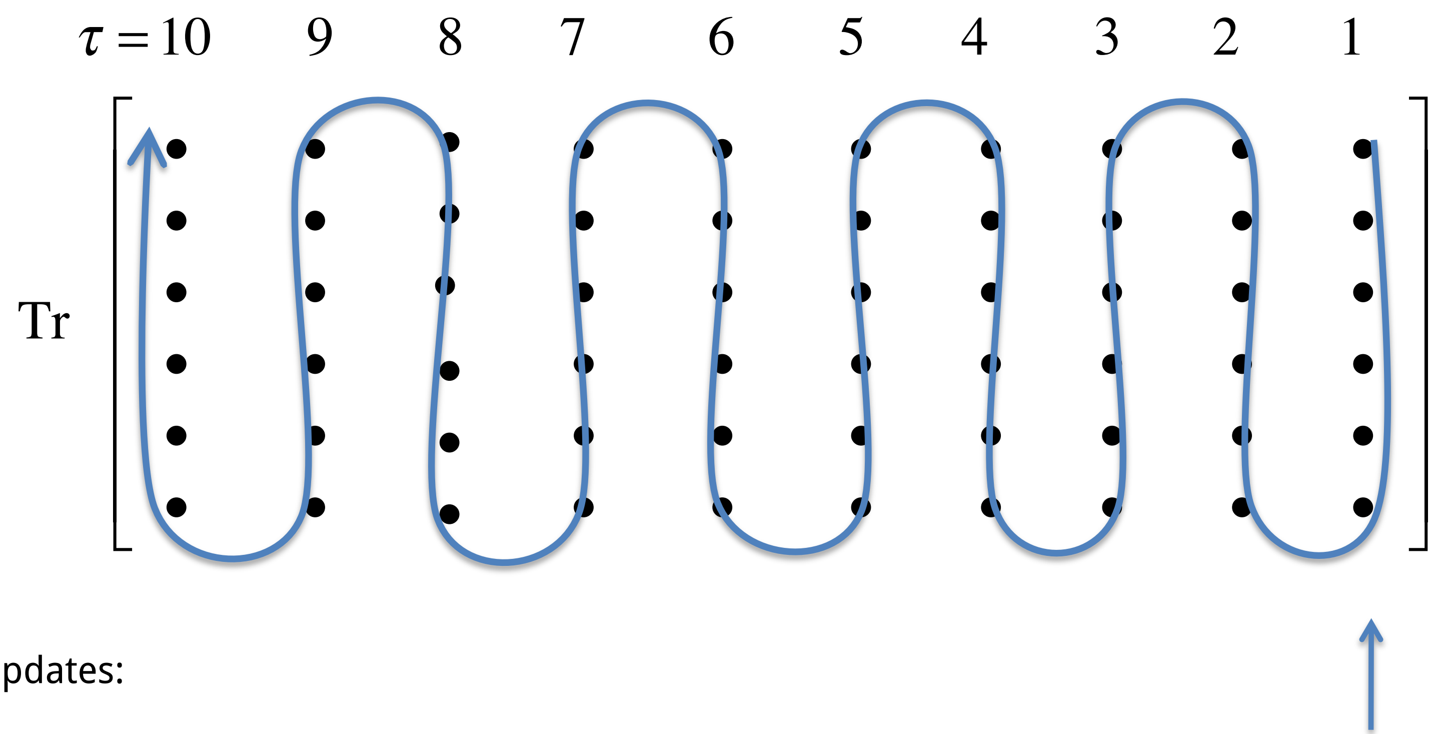
Scan through the real space lattice and flip spin sequentially
Accept move with probability:

$$\frac{e^{-S_0(\{\Phi'(\mathbf{i},\tau)\})}}{e^{-S_0(\{\Phi(\mathbf{i},\tau)\})}} \det\left[1+\Delta\left(1-G_{\Phi}(\tau)\right)\right]$$

If the move is accepted, upgrade the Green function.

$$G_{\Phi}(\tau = 1) \rightarrow G_{\Phi'}(\tau = 1)$$

Organization of the code.

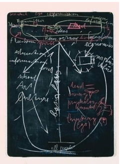


Fast updates:

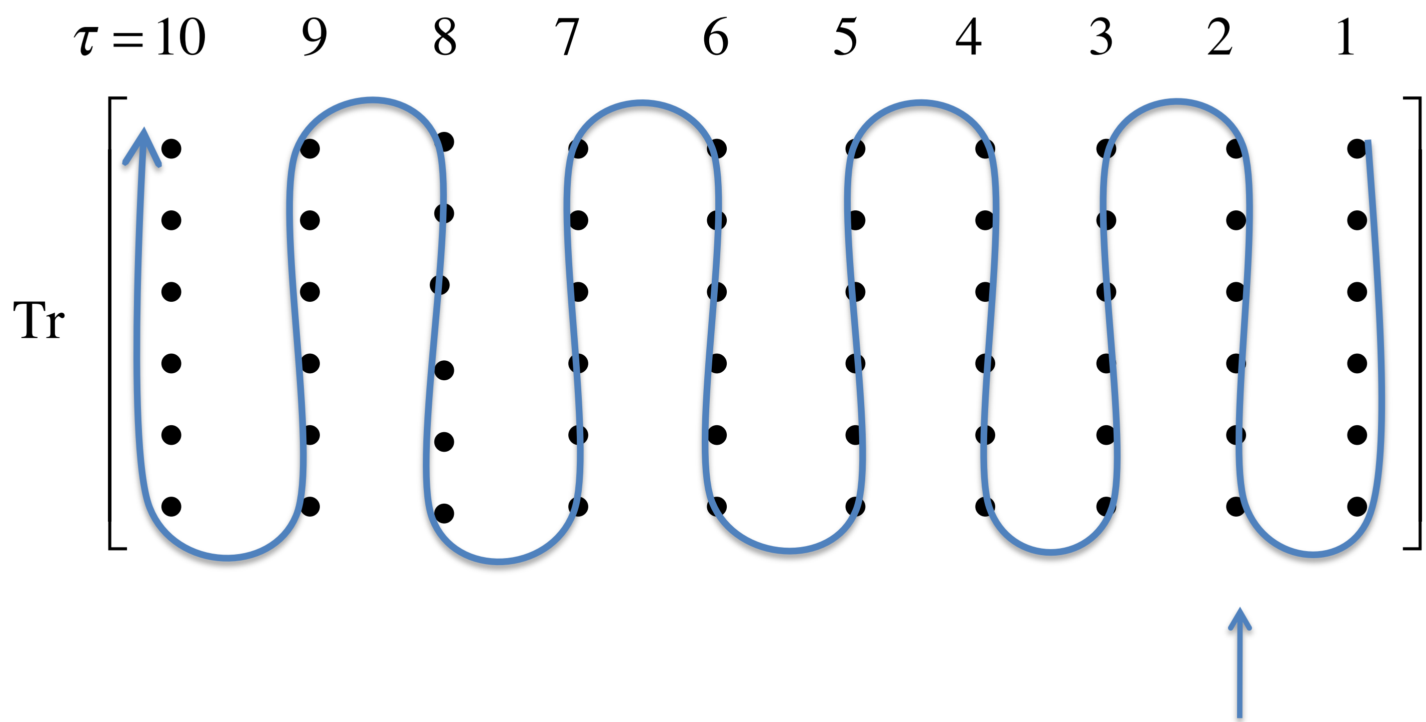
$$G_{\Phi'}(\tau) = \left(1 + (1+\Delta) B(\Phi_\tau) \cdots B(\Phi_1) B(\Phi_{L_\tau}) \cdots B(\Phi_{\tau+1})\right)^{-1}, \quad \Delta_{x,y} = \delta_{x,z}\delta_{y,z}\eta$$

$$G_{\Phi'}(\tau)_{x,y} = G_{\Phi}(\tau)_{x,y} - \frac{G_{\Phi}(\tau)_{x,z}\,\eta\left[1 - G_{\Phi}(\tau)\right]_{z,y}}{1 + \left[1 - G_{\Phi}(\tau)\right]_{z,z}\eta}$$

Use: $$\left(A + \vec{u} \otimes \vec{v}\right)^{-1} = A^{-1} - \frac{A^{-1}\vec{u} \otimes \vec{v} A^{-1}}{1 + \vec{v} \bullet A^{-1}\vec{u}}$$



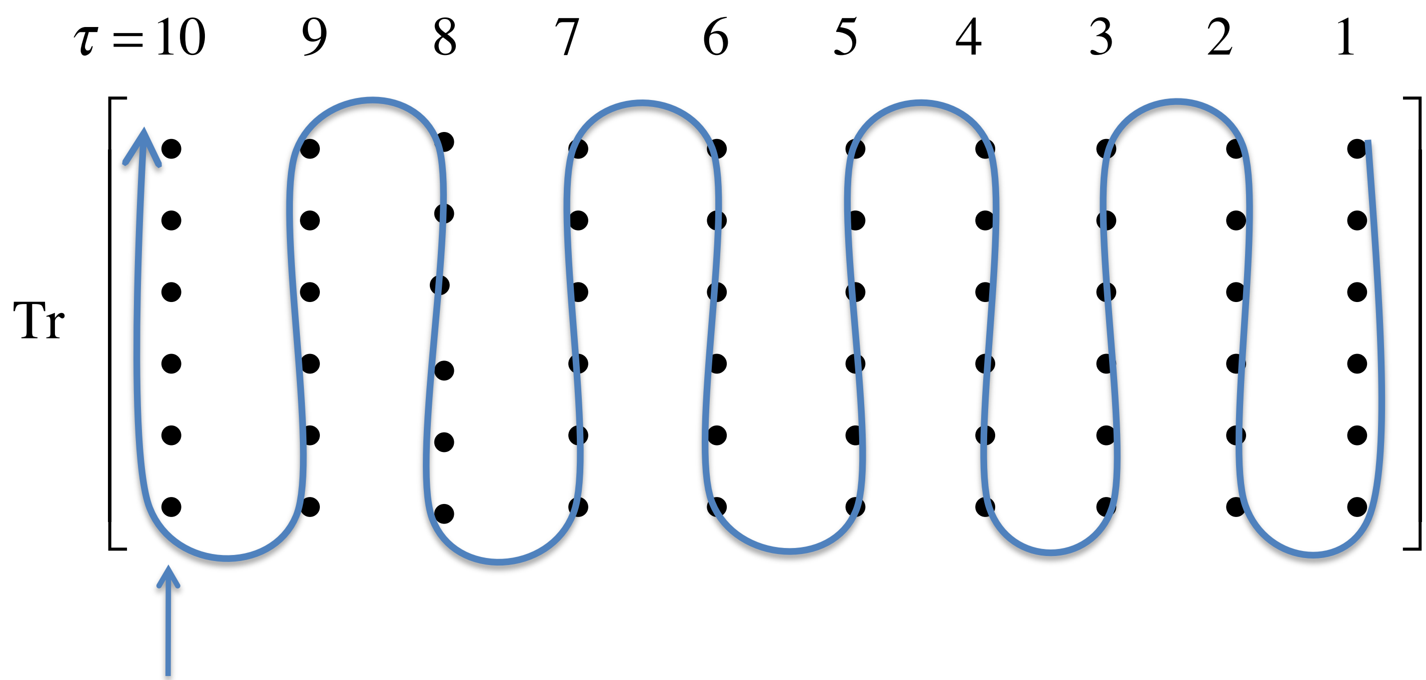
Organization of the code.



Propagate the Green function
from $\tau = 1$ to $\tau = 2$

$$G_\Phi(\tau+1) = \left(1 + B(\Phi_{\tau+1})\cdots B(\Phi_1) B(\Phi_{L_\tau})\cdots B(\Phi_{\tau+2})\right)^{-1} = B(\Phi_{\tau+1}) G_\Phi(\tau) B^{-1}(\Phi_{\tau+1})$$

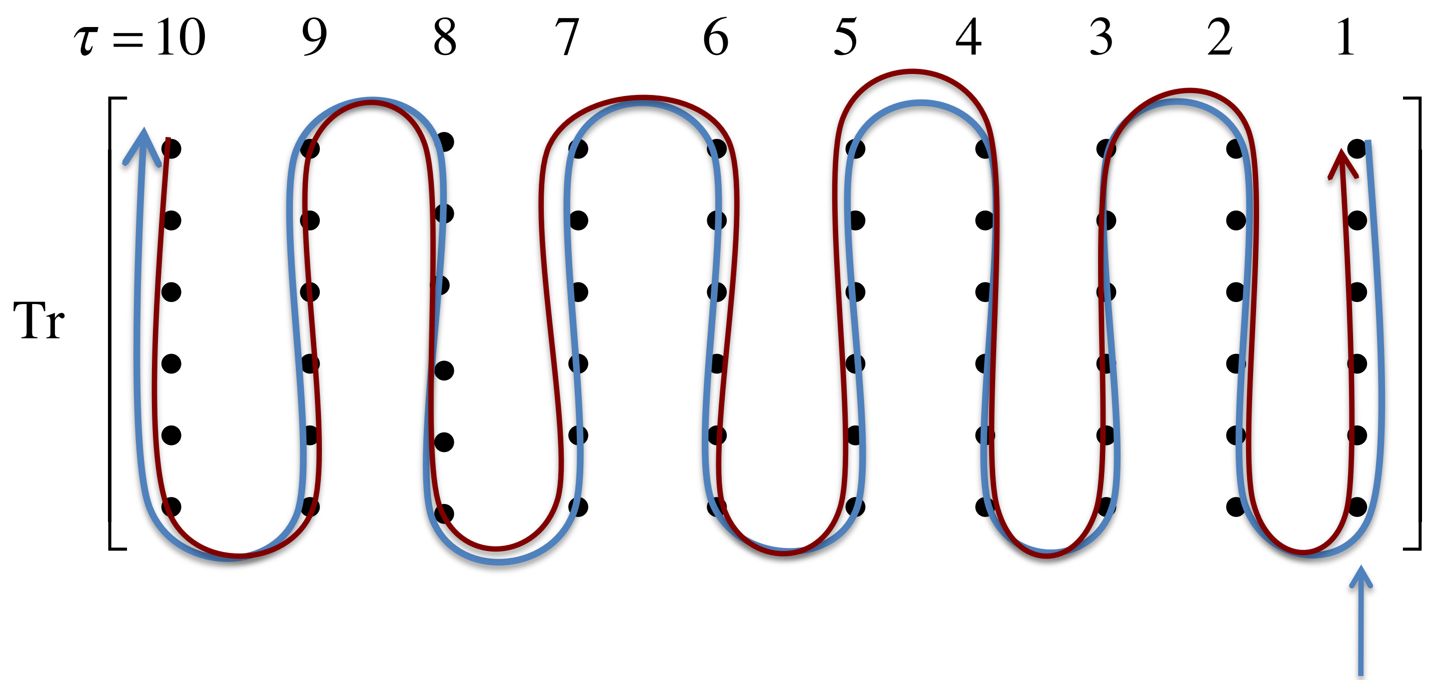
Organization of the code.



Repeat till $\tau = 10$ and do not forget to measure observables.

$$G_{\Phi}(\tau+1) = \left(1 + B(\Phi_{\tau+1})\cdots B(\Phi_{1}) B(\Phi_{L_\tau})\cdots B(\Phi_{\tau+2})\right)^{-1} = B(\Phi_{\tau+1}) G_{\Phi}(\tau) B^{-1}(\Phi_{\tau+1})$$

Organization of the code.



Retrace your steps back to $\tau = 1$

$$G_{\Phi}(\tau-1) = \left(1 + B(\Phi_{\tau-1})\cdots B(\Phi_{1})B(\Phi_{L_\tau})\cdots B(\Phi_{\tau})\right)^{-1} = B^{-1}(\Phi_{\tau})G_{\Phi}(\tau)B(\Phi_{\tau})$$

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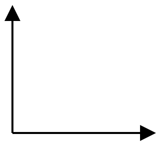
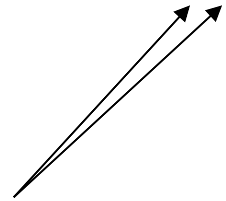
9) ALF examples

Numerical stabilization: Problem. $e^{-\beta H}$

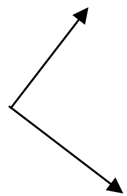
$1:$ 

$$U(l) = B(\Phi_l)\cdots B(\Phi_1)1$$



When β gets big, then vectors become linearly dependent and the Green function is ill defined.

QR (Gram Schmidt)

$U(l) = \mathbf{U}_1 D_1 V_1$ $\quad \mathbf{U}_1 :$  $\mathbf{U}_1^{\dagger}\mathbf{U}_1 = 1,\ V_1 :$ Unit triangular $\quad D_1 :$ Real Diagonal

Do not mix scales during propagation.

$$U(2l) = \underbrace{\left(B(\Phi_{2l})\cdots B(\Phi_{l+1})\mathbf{U}_1 \right) D_1}_{\mathbf{U}_2 D_2 V} V_1 = \mathbf{U}_2 D_2 \underbrace{V V_1}_{V_2}$$

Handle scales only when computing the Green function. Internal check: difference between wrapped and freshly computed Green functions

ALF: $l = \mathrm{NWRAP}$ Variable: *Precision Green Mean, Max* in info file

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ALF @ http://alf.physik.uni-wuerzburg.de

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 Ising field 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
- Parallel tempering, projective and finite T approaches
- Long range Coulomb


F. Goth


M. Bercx


J. Hoffmann


M. Ulybyshev

KONWIHR

DFG Wissenschaftliche Literaturversorgungs und Informationssysteme (LIS)

M. Bercx, F. Goth, J. S. Hofmann and F. F. Assaad, SciPost Phys. 3 (2017), 013

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SU(N) Hubbard model on the square lattice.

Da Wang, Yi Li, Zi Cai, Zhichao Zhou, Yu Wang, and Congjun Wu, Phys. Rev. Lett. 112 (2014), 156403.

$$\hat{H} = \sum_{i,j,\sigma=1}^{N} \hat{c}^{\dagger}_{i,\sigma} T_{i,j} \hat{c}_{j,\sigma} + \frac{U}{N} \sum_{k} \left(\sum_{\sigma=1}^{N} (\hat{c}^{\dagger}_{k,\sigma} \hat{c}_{k,\sigma} - \tfrac{1}{2}) \right)^2$$

Here i,j,k denote Wannier orbitals

- Lattice vectors $\vec{a}_1 = (1,0),\ \vec{a}_2 = (0,1)$ → Lattice class will make the lattice (tilted lattices are possible)
- $N_{\rm dim}$ = # of lattice sites
- $N_{\rm fl}$ = 1
- $N_{\rm col}$ = N
- M_T = 1 (Possible to include checkerboard decomposition $M_T = 2*N_{\rm dim}$)
- T = Hopping matrix (bipartite)
- U_k = U/N
- M_V = # of lattice sites
- $\left(V^{(k)}\right)_{i,j} = \delta_{i,k}\delta_{k,j}$
- α_{ks} = - ½

No sign problem for even values of N

Conclusions Lecture 1

Recent progress allows to simulate an ever growing class of models without encountering the negative sign problem

Challenges

Sign problem. Can one find new sign free formulations for an even bigger class of models?

Global updates. Single spin flip formulations will suffer from critical slowing down.
Ergodicity issues for some problems.

Order Nβ methods. Present fermion QMC algorithms scale as $N^3\beta$. → Pseudofermions?

.....

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der Bayerischen Akademie der Wissenschaften
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Gauss Centre for Supercomputing

Lecture 2. Selected applications

- Superconductivity from condensation of skyrmions in a quantum spin Hall insulator

  Y. Liu, Z. Wang, T. Sato, M. Hohenadler, C. Wang, W. Guo and FFA arXiv:1811.02583

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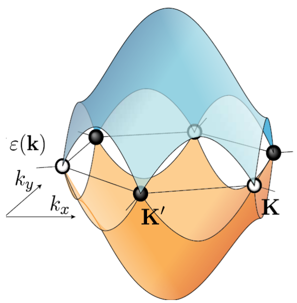
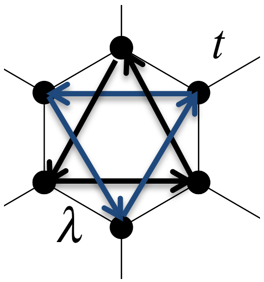
Why would it be interesting to dynamically generate a QSH state?

$$\hat{H} = -t \sum_{\langle \boldsymbol{i},\boldsymbol{j}\rangle} (\hat{\boldsymbol{c}}_{\boldsymbol{i}}^{\dagger}\hat{\boldsymbol{c}}_{\boldsymbol{j}} + \mathrm{H.c.}) + \lambda \sum_{\hexagon=\boldsymbol{x}} \boldsymbol{N}(\boldsymbol{x}) \cdot \sum_{\langle\langle \boldsymbol{i},\boldsymbol{j}\rangle\rangle \in \hexagon} \left(\mathrm{i}\nu_{\boldsymbol{ij}} \hat{\boldsymbol{c}}_{\boldsymbol{i}}^{\dagger} \boldsymbol{\sigma} \hat{\boldsymbol{c}}_{\boldsymbol{j}} + \mathrm{H.c.} \right)$$



$$L_0 = \sum_{\sigma} \bar{\psi}_{\sigma}(\mathbf{x},\tau)\partial_{\mu}\gamma_{\mu}\psi_{\sigma}(\mathbf{x},\tau)$$

$$\{\gamma_{\mu},\gamma_{\nu}\} = 2\delta_{\mu,\nu}, \quad \bar{\psi}_{\sigma} = \psi_{\sigma}^{\dagger}\gamma_0$$



$$\boldsymbol{N}(\boldsymbol{x}) \in S^2$$

$$\hat{c}_i^{\dagger} = \left(\hat{c}_{i,\uparrow}^{\dagger}, \hat{c}_{i,\downarrow}^{\dagger}\right)$$

$$j = i + \delta_1 + \delta_2 \rightarrow \nu_{i,j} = \mathrm{sign}\left[e_z \cdot (\delta_1 \times \delta_2)\right]$$

Superconductivity from condensation of topological defects in QSH insulator

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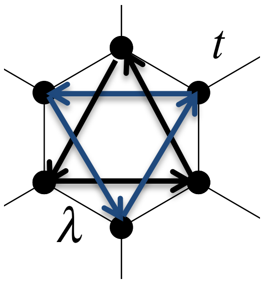
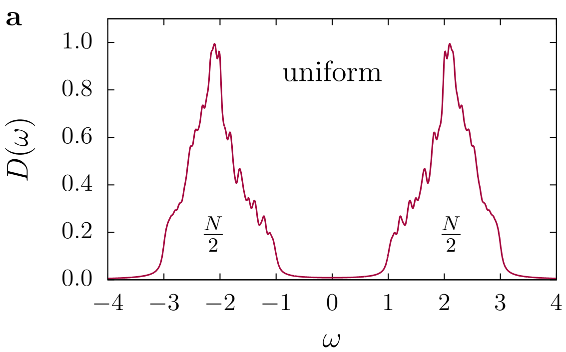
Uniform



$$\boldsymbol{N}(\boldsymbol{x}) = \boldsymbol{e}_z$$

Quantum spin Hall insulator



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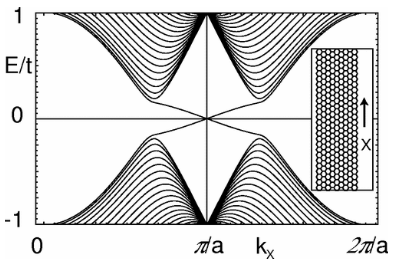

C. L. Kane and E. J. Mele, PRL, 2005

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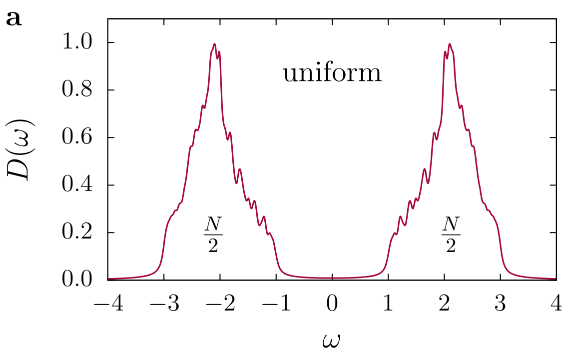
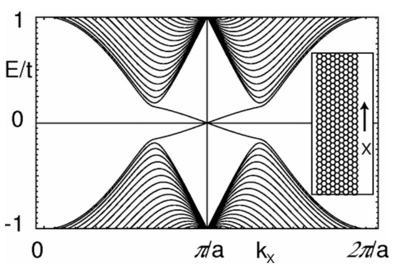
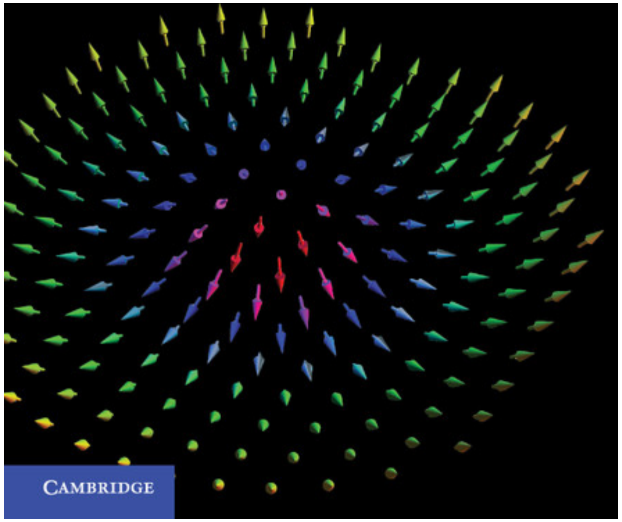




C. L. Kane and E. J. Mele, PRL, 2005

One Skyrmion

$$Q = \frac{1}{4\pi} \int dxdy \boldsymbol{N}(\boldsymbol{x}) \cdot (\partial_x \boldsymbol{N}(\boldsymbol{x}) \times \partial_y \boldsymbol{N}(\boldsymbol{x})) = 1$$



Field theories of condensed matter physics. E. Fradkin

Superconductivity from condensation of topological defects in QSH insulator

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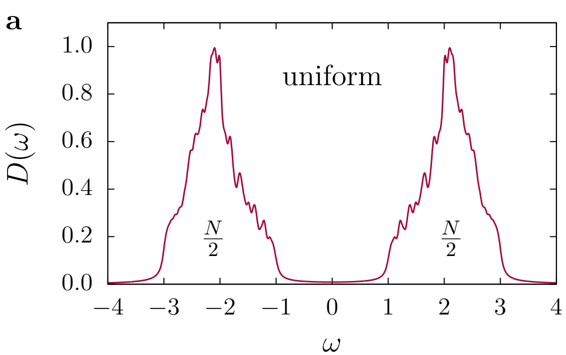
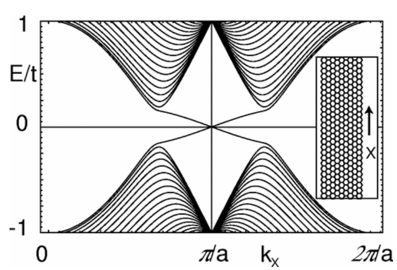
Quantum spin Hall insulator





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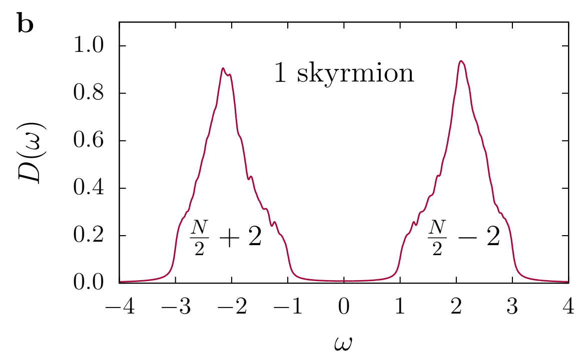

Skyrmion carries charge 2e → proliferation of skyrmions destroys QSH and could lead to SC.

T. Grover and T. Senthil, PRL. 2008.

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$$\hat{H} = -t\sum_{\langle \boldsymbol{i},\boldsymbol{j}\rangle}(\hat{\boldsymbol{c}}^{\dagger}_{\boldsymbol{i}}\hat{\boldsymbol{c}}_{\boldsymbol{j}} + \mathrm{H.c.}) + \lambda\sum_{\hexagon=\boldsymbol{x}}\boldsymbol{N}(\boldsymbol{x})\cdot\sum_{\langle\langle \boldsymbol{i},\boldsymbol{j}\rangle\rangle\in\hexagon}\left(\mathrm{i}\nu_{\boldsymbol{ij}}\hat{\boldsymbol{c}}^{\dagger}_{\boldsymbol{i}}\boldsymbol{\sigma}\hat{\boldsymbol{c}}_{\boldsymbol{j}} + \mathrm{H.c.}\right)$$

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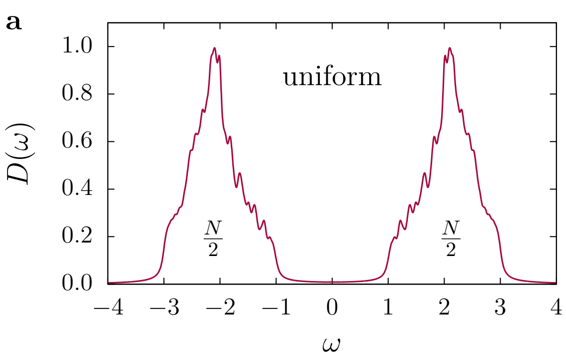
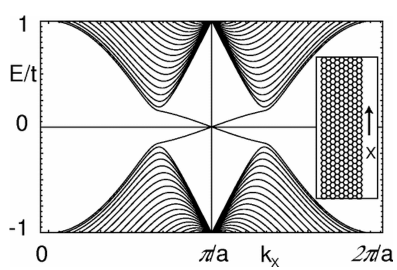
Quantum spin Hall insulator



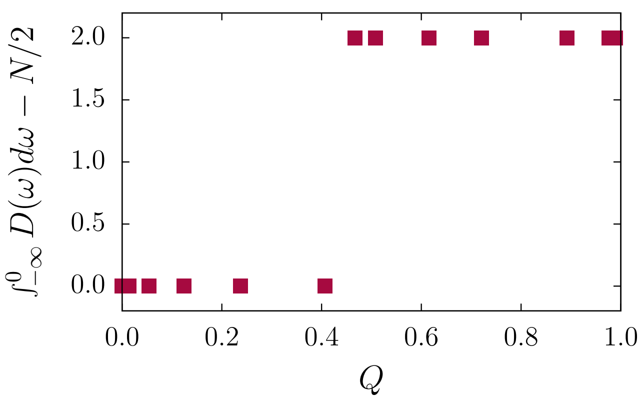


C. L. Kane and E. J. Mele, PRL, 2005

One Skyrmion

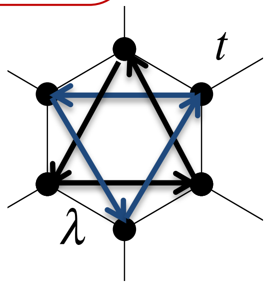
$$Q = \frac{1}{4\pi}\int dxdy\boldsymbol{N}(\boldsymbol{x})\cdot(\partial_x\boldsymbol{N}(\boldsymbol{x})\times\partial_y\boldsymbol{N}(\boldsymbol{x}))$$

Open boundary conditions. Q is not quantized



T. Grover and T. Senthil, PRL. 2008.

$$\hat{H} = -t\sum_{\langle ij\rangle}(\hat{c}_i^\dagger\hat{c}_j + \hat{c}_j^\dagger\hat{c}_i) - \lambda\sum_{\hexagon}\left(\sum_{\langle\langle i,j\rangle\rangle\in\hexagon}\nu_{i,j}i\left(\hat{c}_i^\dagger\boldsymbol{\sigma}\hat{c}_j - \hat{c}_j^\dagger\boldsymbol{\sigma}\hat{c}_i\right)\right)^2$$



$$\hat{c}_i^\dagger = \left(\hat{c}_{i,\uparrow}^\dagger, \hat{c}_{i,\downarrow}^\dagger\right)$$

$$j = i + \delta_1 + \delta_2 \rightarrow \nu_{i,j} = \text{sign}\left[e_z \cdot (\delta_1 \times \delta_2)\right]$$

Order parameters

$$\vec{J}_{\hexagon} = \sum_{\langle\langle i,j\rangle\rangle\in\hexagon}\nu_{i,j}\left(i\hat{c}_i^\dagger\boldsymbol{\sigma}\hat{c}_j - i\hat{c}_j^\dagger\boldsymbol{\sigma}\hat{c}_i\right)$$

Quantum spin Hall [SO(3)]

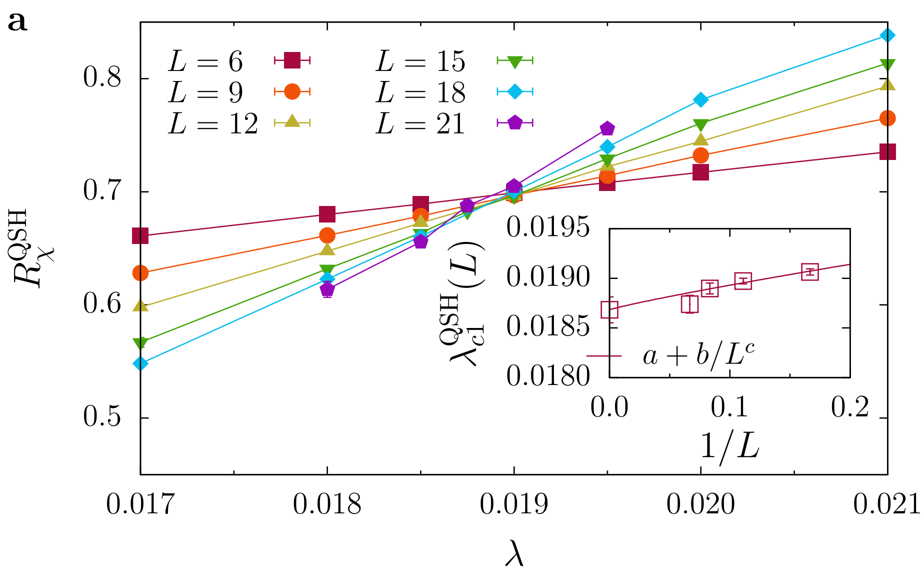
$$\hat{\Delta}_i^\dagger = \hat{c}_{i,\uparrow}^\dagger\hat{c}_{i,\downarrow}^\dagger$$

s-wave superconductor [U(1)]

$$\chi_{QSH}(q) = \frac{1}{N}\int_0^{\beta} d\tau \sum_{i,j} \langle \vec{J}_{\hexagon_i}(\tau)\vec{J}_{\hexagon_j}\rangle e^{iq(i-j)}$$

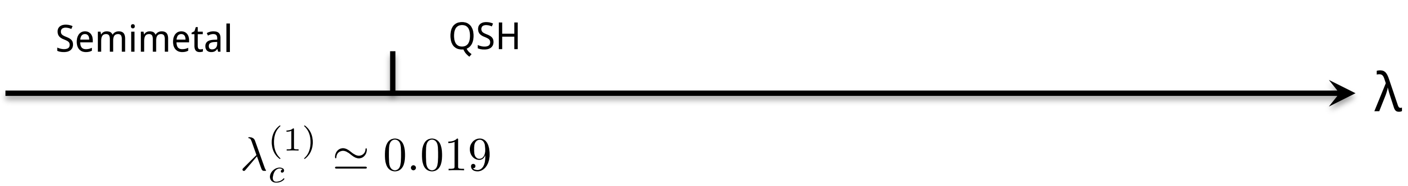
$$R_{QSH} = 1 - \frac{\chi_{QSH}(q_0+\delta q)}{\chi_{QSH}(q_0)}$$

$$R_{\mathrm{QSH}}(L,\lambda) = F(L^z/\beta, (\lambda-\lambda_c)L^{1/\nu}, L^{-\omega})$$



Assumption z=1

Critical exponents ?

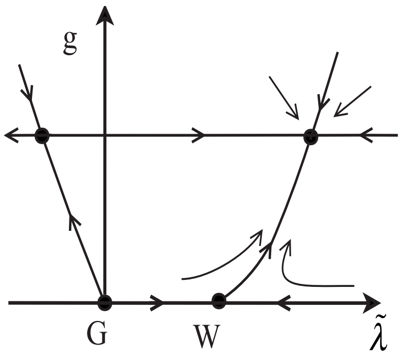


One expects the the SM-QSH quantum phase transition to belong to the same universality class as of the SM-AFM transition.

Gross Neveu Yukawa

$$L_0 = \sum_{\sigma,\sigma'} \bar{\psi}_\sigma(\mathbf{x},\tau)\left[\partial_\mu \gamma_\mu \delta_{\sigma,\sigma'} + g\vec{m}_{AFM}(\mathbf{x},\tau)\cdot\vec{\sigma}_{\sigma,\sigma'}\right]\psi_{\sigma'}(\mathbf{x},\tau)$$

$$L_b = \left(\partial_\mu \vec{m}_{AFM}(\mathbf{x},\tau)\right)^2 + \tilde{\lambda}\left(\vec{m}_{AFM}(\mathbf{x},\tau)\bullet\vec{m}_{AFM}(\mathbf{x},\tau)\right)^2$$



I. Herbut, V. Juričić, O. Vafek PRB 80, 075432, (2009)

$M = \gamma_0 \vec{\boldsymbol{\sigma}}$ is a mass term such that when $\vec{m}_{AFM}$ acquires a non-zero vacuum expectation value a mass gap opens.

Mass term: $$H(k) = \overbrace{\sum_{i=1}^{2} ik_i \gamma_0 \gamma_i}^{H_0(k)} + m\, M$$

M is a mass term if $\{M, H_0(k)\} = 0$ and $M^2 = 1 \rightarrow E(k) = \pm\sqrt{k^2 + m^2}$

One expects the the SM-QSH quantum phase transition to belong to the same universality class as of the SM-AFM transition.

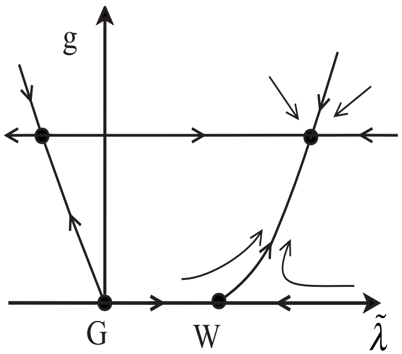
Gross Neveu Yukawa

$$L_0 = \sum_{\sigma,\sigma'} \bar{\psi}_\sigma(\mathbf{x},\tau)\left[\partial_\mu \gamma_\mu \delta_{\sigma,\sigma'} + g\vec{m}_{AFM}(\mathbf{x},\tau)\cdot\vec{\sigma}_{\sigma,\sigma'}\right]\psi_{\sigma'}(\mathbf{x},\tau)$$

$$L_b = \left(\partial_\mu \vec{m}_{AFM}(\mathbf{x},\tau)\right)^2 + \tilde{\lambda}\left(\vec{m}_{AFM}(\mathbf{x},\tau)\bullet\vec{m}_{AFM}(\mathbf{x},\tau)\right)^2$$

$$L_0 = \sum_{\sigma,\sigma'} \bar{\psi}_\sigma(\mathbf{x},\tau)\left[\partial_\mu \gamma_\mu \delta_{\sigma,\sigma'} + g\vec{m}_{QSH}(\mathbf{x},\tau)\cdot\vec{\sigma}_{\sigma,\sigma'} i\gamma_3\gamma_5\right]\psi_{\sigma'}(\mathbf{x},\tau)$$

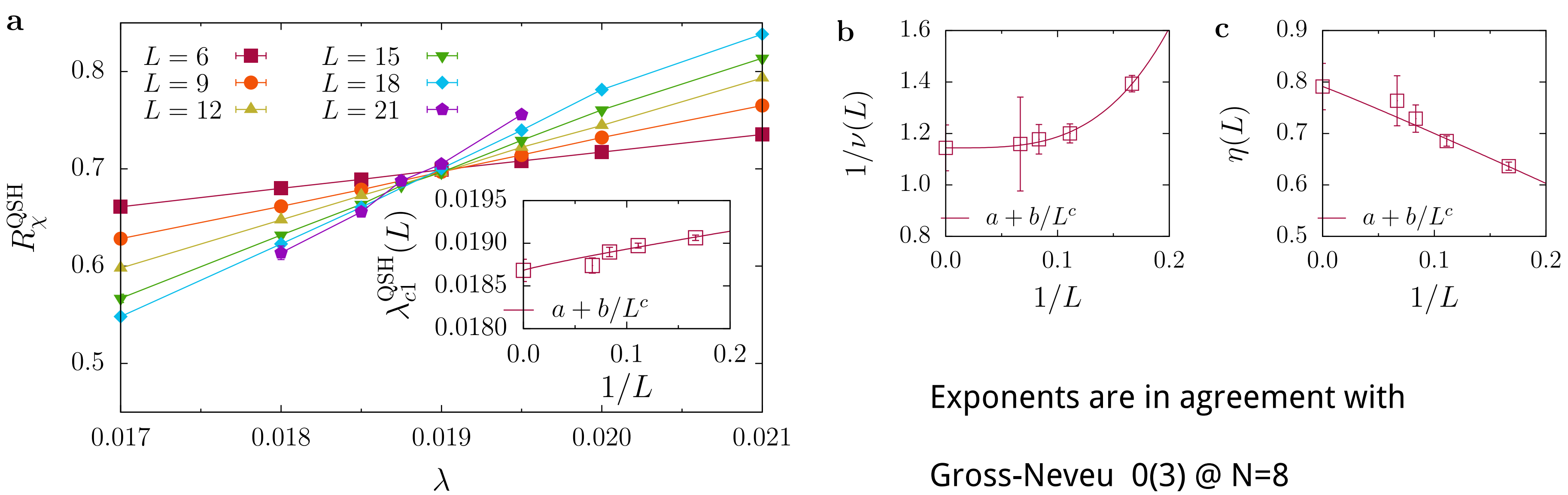
$$L_b = \left(\partial_\mu \vec{m}_{QSH}(\mathbf{x},\tau)\right)^2 + \tilde{\lambda}\left(\vec{m}_{QSH}(\mathbf{x},\tau)\bullet\vec{m}_{QSH}(\mathbf{x},\tau)\right)^2$$



I. Herbut, V. Juričić, O. Vafek
PRB 80, 075432, (2009)

The only difference between the γ_0 and $i\gamma_0\gamma_3\gamma_5$ is a sign difference between the two valleys. Since the transition is a $Q = 0$ transition, we do not expect this sign difference to have any effect.

$$\chi_{QSH}(q) = \frac{1}{N}\int_0^\beta d\tau \sum_{i,j} \langle \vec{J}_{\hexagon_i}(\tau)\vec{J}_{\hexagon_j}\rangle e^{iq(i-j)}$$



Exponents are in agreement with

Gross-Neveu 0(3) @ N=8

$\nu = 0.84(4)$
$\eta = 0.70(15)$
$z=1$

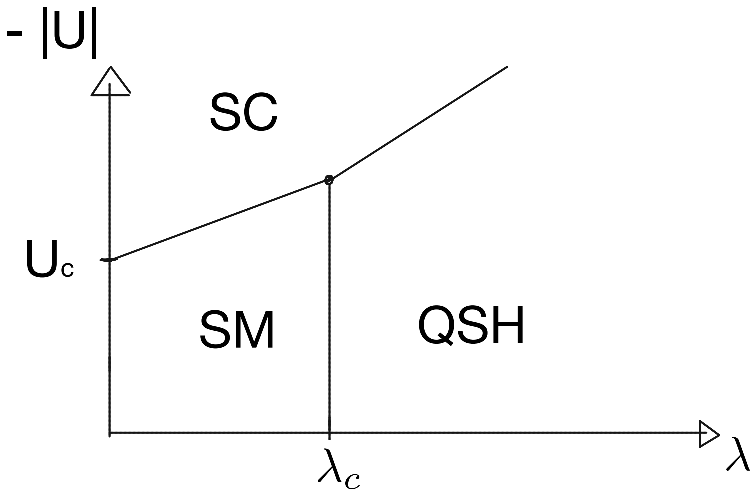
F. Parisen Toldin, M. Hohenadler, F. F. Assaad, and I. Herbut, Phys. Rev. B 91 (2015), 165108.

$$\lambda_c^{(1)} \simeq 0.019$$

How should we trigger the proliferation of skyrmions in the QSH insulator?

Add an attractive Hubbard U-term

(Is technically possible and does not trigger
a negative sign problem)



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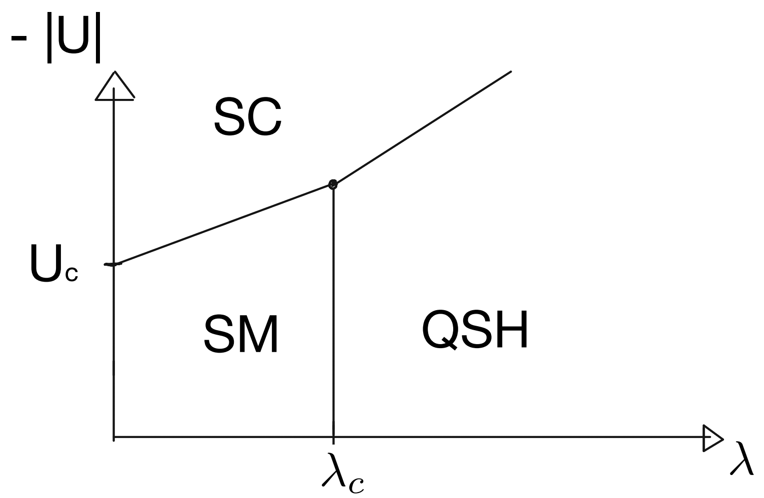
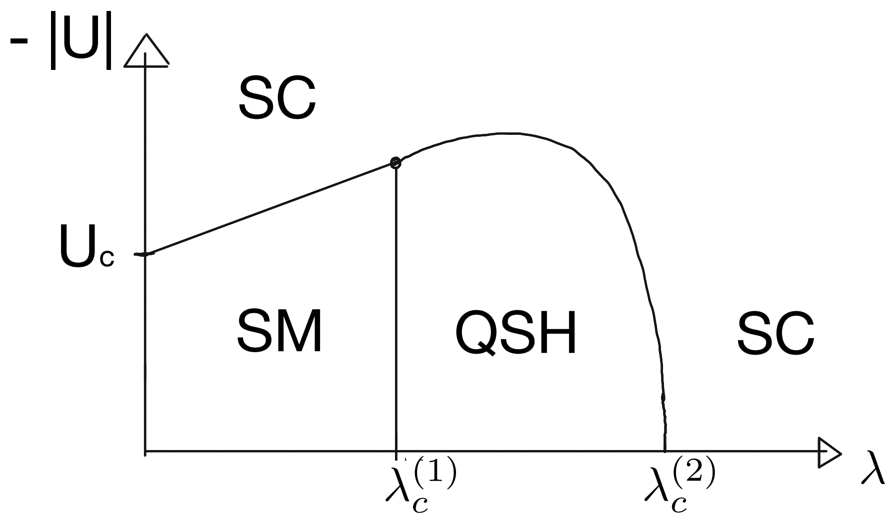
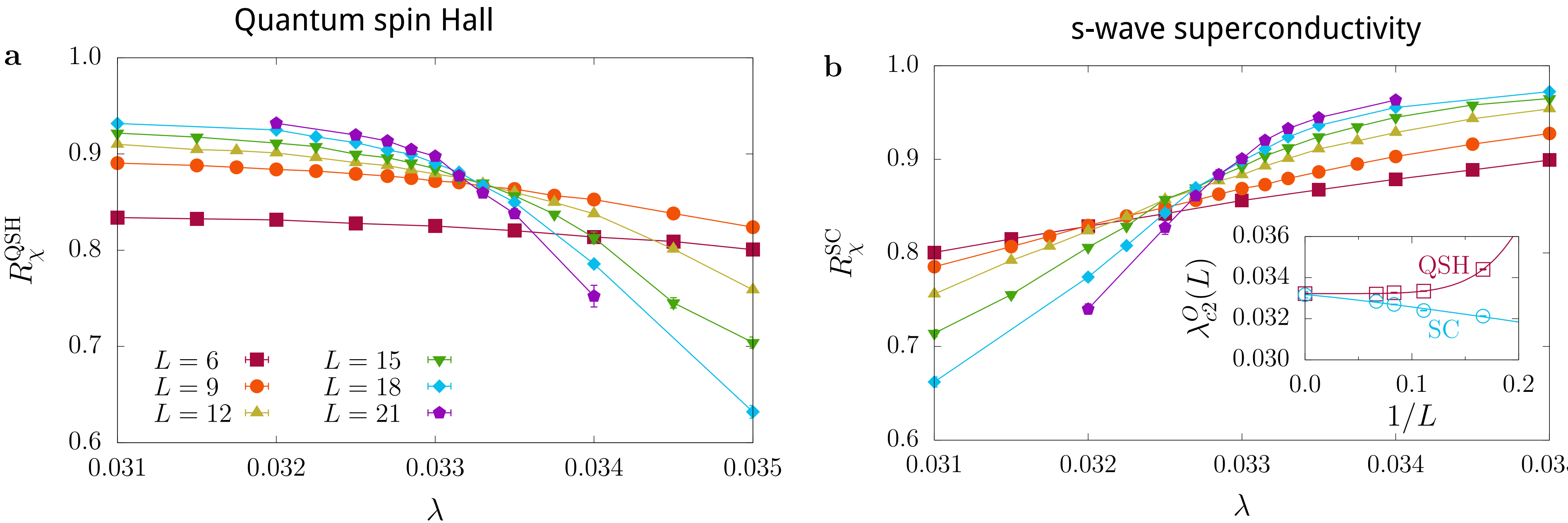
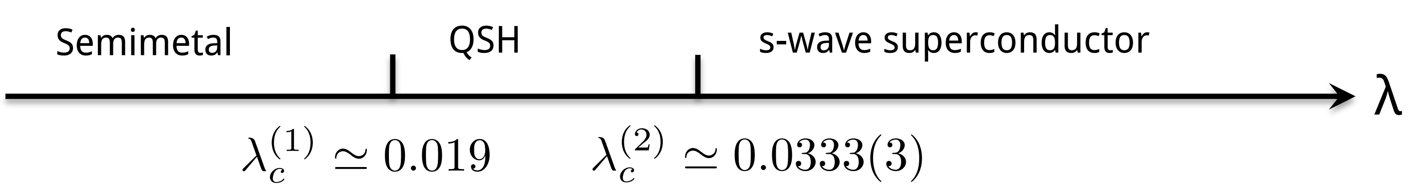


Adding a Hubbard U-term is not necessary!



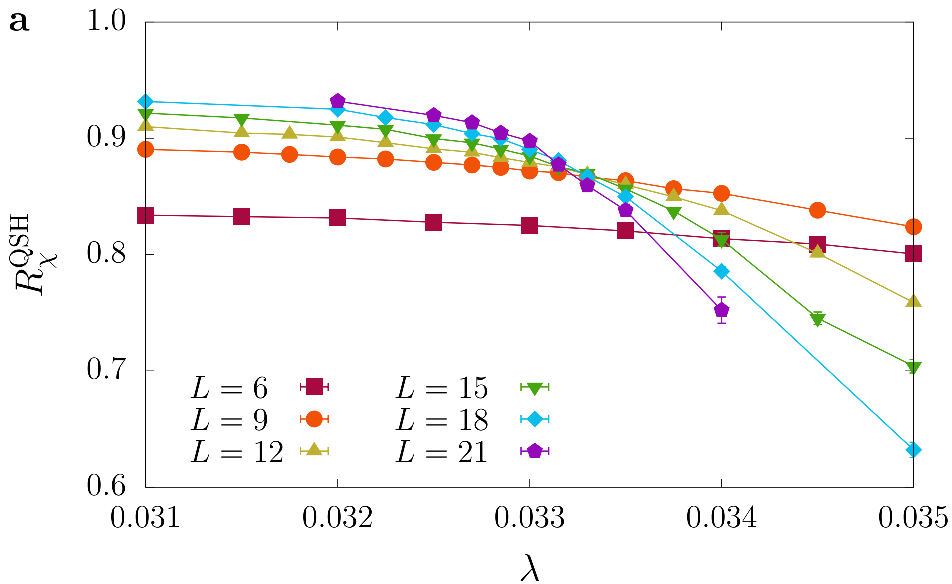
Superconductivity from condensation of topological defects in QSH insulator



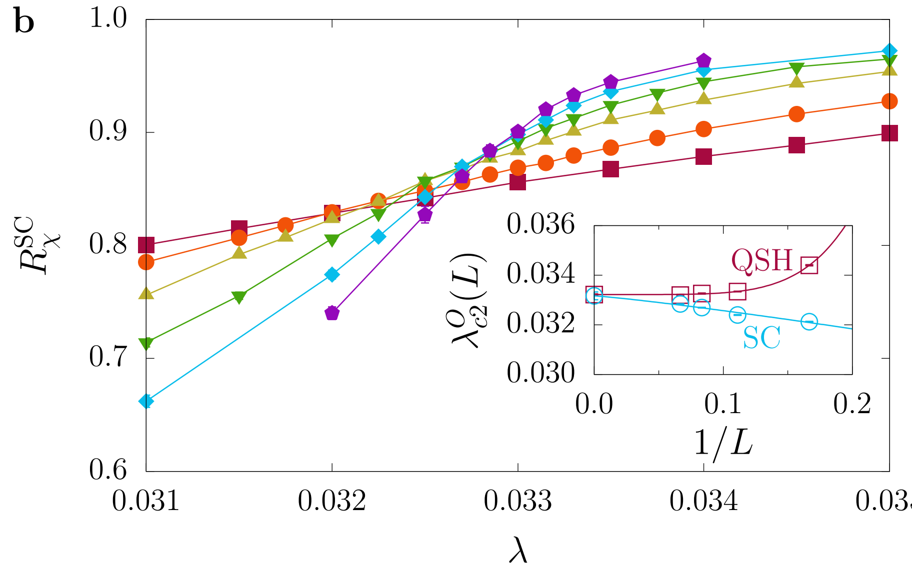


Superconductivity from condensation of topological defects in QSH insulator

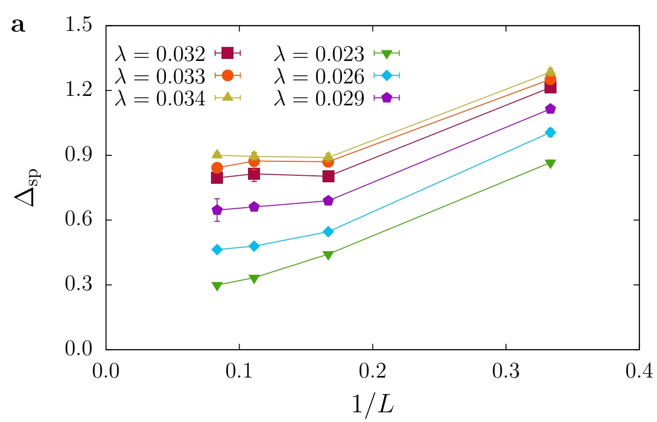
Quantum spin Hall

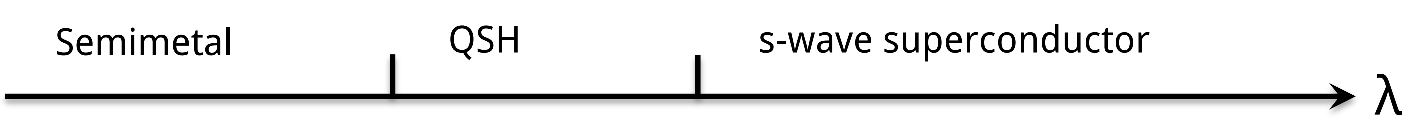


s-wave superconductivity



Single particle gap remains open over the transition

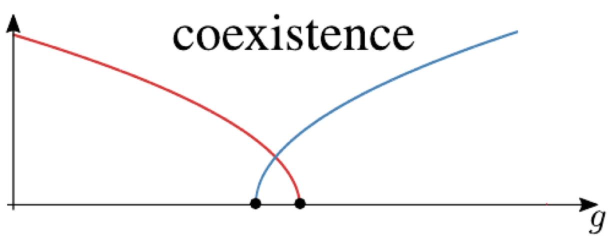


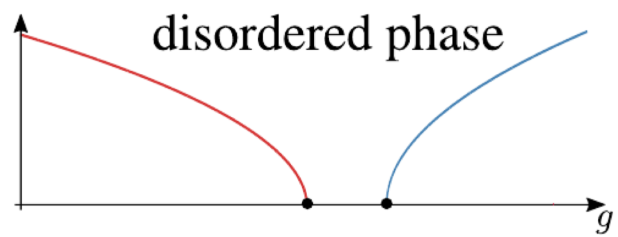


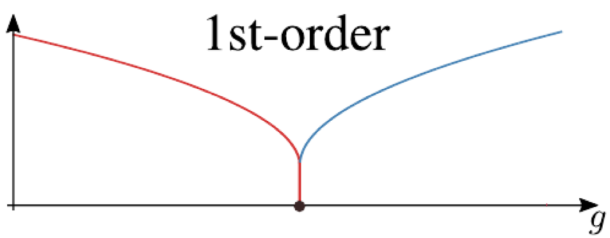
$\lambda_c^{(1)} \simeq 0.019$ $\lambda_c^{(2)} \simeq 0.0333(3)$

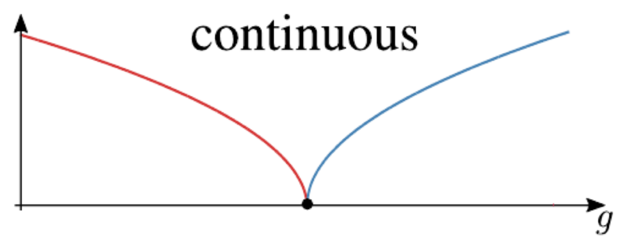
Direct and continuous transition between two broken symmetry phases.

Can we understand this in the realm of Ginzburg-Landau order parameter theory?







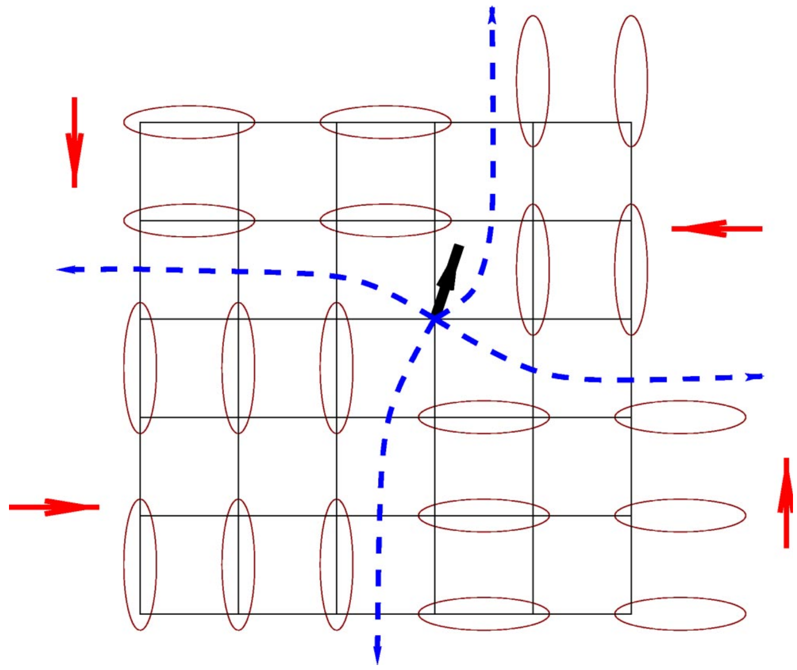


Fine tuning → not generic

Deconfined quantum criticality

F. D. M. Haldane Phys. Rev. Lett. 61 (1988), 1029–1032.
T. Senthil, A. Vishwanath, L. Balents, S. Sachdev, and M. P. A. Fisher, Science 303 (2004), 1490–1494.

Topological defects of one phase carry the charge of the other. When they condense they simultaneously destroy one phase and create the other.



C_4 VBS vortex carries a spinon. Proliferation of vortices destroys the VBS and generates SDW order. M. Levin and T. Senthil, Phys. Rev. B 70 220403 (2004).

Why is the quantum spin Hall state intertwined with s-wave superconductivity?

The three quantum spin Hall mass terms are part of the quintuplet of mutually **anti-commuting** QSH and s-wave superconductivity mass terms.

$$\boldsymbol{M} = \{ \overbrace{\tau_z\sigma_x i\gamma_0\gamma_3\gamma_5, \;\; \tau_0\sigma_y i\gamma_0\gamma_3\gamma_5, \;\; \tau_z\sigma_z i\gamma_0\gamma_3\gamma_5}^{\boldsymbol{M}_{\rm QSH}}, \;\; \underbrace{\tau_y\sigma_y i\gamma_0\gamma_2\gamma_3, \;\; \tau_x\sigma_y i\gamma_0\gamma_2\gamma_3}_{\boldsymbol{M}_{\rm SC}} \}$$

Bogoliubov index

s-wave superconductivity

A. Tanaka and X. Hu, PRL, 2005
T. Senthil and M. Fisher, PRB, 2006
T. Grover and T. Senthil, PRL. 2008

$$\mathcal{L}_0 = \mathcal{L}_{\text{Dirac}} + g\Psi^\dagger(\boldsymbol{x},\tau)\overbrace{\begin{bmatrix}\boldsymbol{\Phi}(\boldsymbol{x},\tau)\\ \boldsymbol{\chi}(\boldsymbol{x},\tau)\end{bmatrix}}^{\equiv \boldsymbol{\varphi}(\boldsymbol{x},\tau)} \cdot \begin{bmatrix}\boldsymbol{M}_{QSH}\\ \boldsymbol{M}_{SC}\end{bmatrix}\Psi(\boldsymbol{x},\tau)$$

This Lagrangian has an SO(5) symmetry

$$\mathcal{L}_{\text{Dirac}} + g\Psi^\dagger(\boldsymbol{x},\tau)\left(R^{SO(5)}\begin{bmatrix}\boldsymbol{\Phi}(\boldsymbol{x},\tau)\\ \boldsymbol{\chi}(\boldsymbol{x},\tau)\end{bmatrix}\right) \cdot \begin{bmatrix}\boldsymbol{M}_{QSH}\\ \boldsymbol{M}_{SC}\end{bmatrix}\Psi(\boldsymbol{x},\tau) = \mathcal{L}'_{\text{Dirac}} + g\Psi'^\dagger(\boldsymbol{x},\tau)\begin{bmatrix}\boldsymbol{\Phi}(\boldsymbol{x},\tau)\\ \boldsymbol{\chi}(\boldsymbol{x},\tau)\end{bmatrix} \cdot \begin{bmatrix}\boldsymbol{M}_{QSH}\\ \boldsymbol{M}_{SC}\end{bmatrix}\Psi'(\boldsymbol{x},\tau)$$

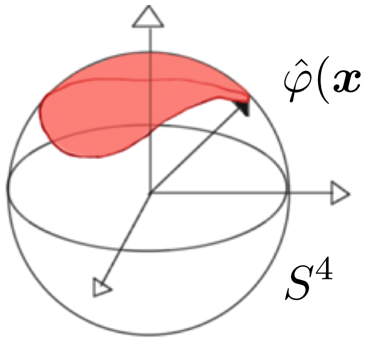
Thereby the single particle gap is given by: $\Delta_{sp} = g|\varphi|$

Assume that the single particle gap remains finite across the transition, then one can omit amplitude fluctuations of the field $\varphi(\boldsymbol{x},\tau)$ and retain only phase fluctuations $\hat{\varphi}(\boldsymbol{x},\tau)$, $|\hat{\varphi}(\boldsymbol{x},\tau)| = 1$

Integrating out the fermions gives and effective field theory for the field $\hat{\varphi}(\boldsymbol{x},\tau)$

$$S = \int d^2\boldsymbol{x} d\tau \frac{1}{G}\left(\partial_\mu \hat{\boldsymbol{\varphi}}(\boldsymbol{x},\tau)\right)^2 + 2\pi i \Gamma\left[\hat{\boldsymbol{\varphi}}\right] + S_{SO(3)\times U(1)}$$

$$\Gamma\left[\hat{\boldsymbol{\varphi}}\right] = \frac{\epsilon_{abcde}}{\text{Area}(S^4)} \int_0^1 du \int d^2\boldsymbol{x} d\tau \hat{\varphi}_a \partial_x \hat{\varphi}_b \partial_y \hat{\varphi}_c \partial_\tau \hat{\varphi}_d \partial_u \hat{\varphi}_e$$



$$\hat{\boldsymbol{\varphi}}(\boldsymbol{x},\tau,u=0) = \boldsymbol{e}_z$$
$$\hat{\boldsymbol{\varphi}}(\boldsymbol{x},\tau,u=1) = \hat{\boldsymbol{\varphi}}(\boldsymbol{x},\tau)$$

$$S_{SO(3)\times U(1)} = \int d^2\boldsymbol{x} d\tau \; \alpha_{SO(3)\times U(1)} \left(\hat{\varphi}_1^2 + \hat{\varphi}_2{}^2 + \hat{\varphi}_3{}^2 - \hat{\varphi}_4{}^2 - \hat{\varphi}_5{}^2\right)$$

Why is anti-ferromagnetism intertwined with the valence bond solid ?

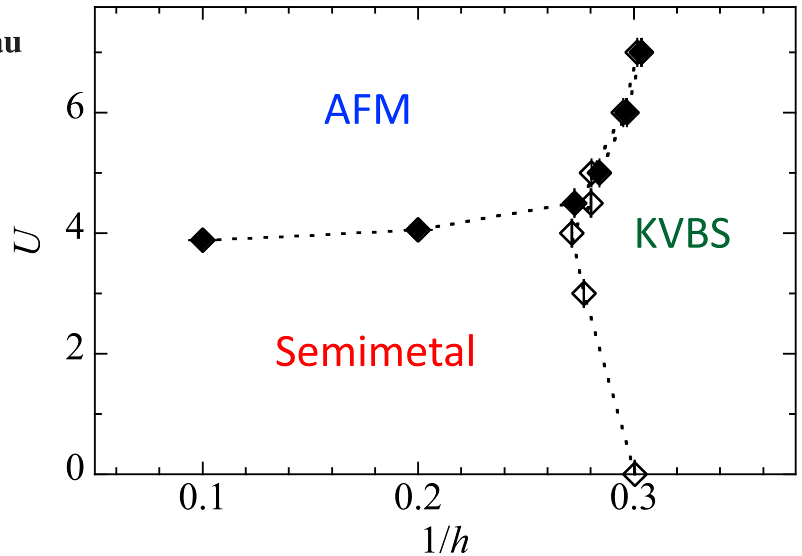
The three AFM mass terms are part of mutually **anti-commuting** quintuplet of AFM and VBS masses

$$\boldsymbol{M} = \{ \overbrace{\sigma_x\gamma_0, \quad \sigma_y\gamma_0, \quad \sigma_z\gamma_0}^{\boldsymbol{M}_{\mathrm{AFM}}}, \quad \underbrace{i\gamma_0\gamma_3, \quad i\gamma_0\gamma_5}_{\boldsymbol{M}_{\mathrm{VBS}}} \}$$

PRL **119**, 197203 (2017) PHYSICAL REVIEW LETTERS week ending 10 NOVEMBER 2017

Dirac Fermions with Competing Orders: Non-Landau Transition with Emergent Symmetry

Toshihiro Sato,[1] Martin Hohenadler,[1] and Fakher F. Assaad[1]



$$\mathcal{L}_0 = \mathcal{L}_{\text{Dirac}} + g\Psi^\dagger(\boldsymbol{x},\tau)\overbrace{\begin{bmatrix}\boldsymbol{\Phi}(\boldsymbol{x},\tau)\\ \boldsymbol{\chi}(\boldsymbol{x},\tau)\end{bmatrix}}^{\equiv\boldsymbol{\varphi}(\boldsymbol{x},\tau)}\cdot\begin{bmatrix}\boldsymbol{M}_{AFM}\\ \boldsymbol{M}_{VBS}\end{bmatrix}\Psi(\boldsymbol{x},\tau)$$

This Lagrangian has an SO(5) symmetry

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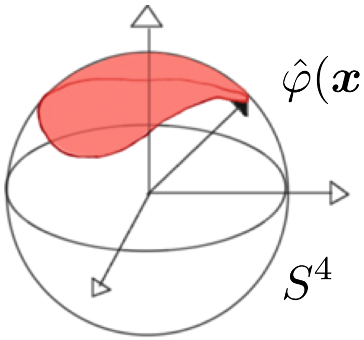


$$\hat{\boldsymbol{\varphi}}(\boldsymbol{x},\tau,u=0)=\boldsymbol{e}_z$$
$$\hat{\boldsymbol{\varphi}}(\boldsymbol{x},\tau,u=1)=\hat{\boldsymbol{\varphi}}(\boldsymbol{x},\tau)$$

$$S_{SO(3)\times U(1)}=\int d^2\boldsymbol{x}d\tau\;\alpha_{SO(3)\times U(1)}\left(\hat{\varphi}_1^2+\hat{\varphi}_2{}^2+\hat{\varphi}_3{}^2-\hat{\varphi}_4{}^2-\hat{\varphi}_5{}^2\right)$$

PHYSICAL REVIEW B **80**, 205319 (2009)

Masses in graphenelike two-dimensional electronic systems: Topological defects in order parameters and their fractional exchange statistics

Shinsei Ryu,[1] Christopher Mudry,[2] Chang-Yu Hou,[3] and Claudio Chamon[3]

TABLE III. Enumeration of the 56 distinct five-tuplets of maximally pairwise anticommuting PHS $X_{\mu_1\mu_2\mu_3\mu_4}$. The 56 five-tuplets are broken into 28 pairs related by the operation of C conjugation (9.12).

Five tuplet	Partner five-tuplet by C conjugation
{Re VBS, Im VBS, Re SSC, Im SSC, CDW}	{Re VBS, Im VBS, Néel$_x$, Néel$_y$, Néel$_z$}
{Im VBS, CDW, Re VBS$_x$, Re VBS$_y$, Re VBS$_z$}	{Im VBS, Néel$_z$, Im TSC$_{32z}$, Re TSC$_{32z}$, Re VBS$_z$}
{Re VBS, CDW, Im VBS$_x$, Im VBS$_y$, Im VBS$_z$}	{Re VBS, Néel$_z$, Re TSC$_{02z}$, Im TSC$_{02z}$, Im VBS$_z$}
{Re SSC, Im SSC, QSHE$_x$, QSHE$_y$, QSHE$_z$}	{Néel$_x$, Néel$_y$, Im TSC$_z$, Re TSC$_z$, QSHE$_z$}
{Re VBS, Re SSC, Re TSC$_{02x}$, Im TSC$_{02y}$, Re TSC$_{02z}$}	{Re VBS, Néel$_x$, Re TSC$_{02x}$, Im TSC$_{02x}$, Im VBS$_x$}
{Re VBS, Im SSC, Im TSC$_{02x}$, Re TSC$_{02y}$, Im TSC$_{02z}$}	{Re VBS, Néel$_y$, Im TSC$_{02y}$, Re TSC$_{02y}$, Im VBS$_y$}
{Im VBS, Im SSC, Re TSC$_{32x}$, Im TSC$_{32y}$, Re TSC$_{32z}$}	{Im VBS, Néel$_y$, Re TSC$_{32y}$, Im TSC$_{32y}$, Re VBS$_y$}
{Im VBS, Re SSC, Im TSC$_{32x}$, Re TSC$_{32y}$, Im TSC$_{32z}$}	{Im VBS, Néel$_x$, Im TSC$_{32x}$, Re TSC$_{32x}$, Re VBS$_x$}
{CDW, Im SSC, Im TSC$_x$, Re TSC$_y$, Im TSC$_z$}	{Néel$_z$, Néel$_y$, Im TSC$_x$, Re TSC$_x$, QSHE$_x$}
{CDW, Re SSC, Re TSC$_x$, Im TSC$_y$, Re TSC$_z$}	{Néel$_z$, Néel$_x$, Re TSC$_y$, Im TSC$_y$, QSHE$_y$}
{Im VBS$_x$, QSHE$_y$, Im VBS$_z$, Re TSC$_{32y}$, Im TSC$_{32y}$}	{Re TSC$_{02z}$, Re TSC$_z$, Im VBS$_z$, Re TSC$_{32x}$, Im TSC$_{32y}$}
{Im VBS$_x$, QSHE$_y$, Re VBS$_x$, Néel$_x$, QSHE$_z$}	{Re TSC$_{02z}$, Re TSC$_z$, Im TSC$_{32z}$, Re SSC, QSHE$_z$}
{Im VBS$_x$, Re TSC$_{32y}$, Im TSC$_{32z}$, Im TSC$_{02x}$, Im TSC$_x$}	{Re TSC$_{02z}$, Re TSC$_{32x}$, Re VBS$_x$, Im TSC$_{02y}$, Im TSC$_x$}
{Im VBS$_x$, Re TSC$_{32z}$, Re TSC$_{02x}$, Re TSC$_x$, Im TSC$_{32y}$}	{Re TSC$_{02z}$, Re VBS$_y$, Re TSC$_{02x}$, Re TSC$_y$, Im TSC$_{32y}$}
{Im VBS$_x$, Re TSC$_{32z}$, Im TSC$_{32z}$, Im VBS$_y$, QSHE$_z$}	{Re TSC$_{02z}$, Re VBS$_y$, Re VBS$_x$, Im TSC$_{02z}$, QSHE$_z$}
{Im VBS$_x$, Re TSC$_x$, Im TSC$_x$, CDW, Re VBS$_x$}	{Re TSC$_{02z}$, Re TSC$_y$, Im TSC$_x$, Néel$_z$, Im TSC$_{32z}$}
{QSHE$_y$, Im VBS$_z$, QSHE$_x$, Re VBS$_z$, Néel$_z$}	{Re TSC$_z$, Im VBS$_z$, Im TSC$_z$, Re VBS$_z$, CDW}
{QSHE$_y$, Re TSC$_{02y}$, Re TSC$_y$, Im SSC, Im TSC$_{32y}$}	{Re TSC$_z$, Re TSC$_{02y}$, Re TSC$_x$, Néel$_y$, Im TSC$_{32y}$}
{QSHE$_y$, Re TSC$_{02y}$, Im TSC$_{02y}$, Re VBS$_x$, Re VBS$_z$}	{Re TSC$_z$, Re TSC$_{02y}$, Im TSC$_{02x}$, Im TSC$_{32z}$, Re VBS$_z$}
{QSHE$_y$, Re TSC$_{32y}$, Im TSC$_{02y}$, Im TSC$_y$, Re SSC}	{Re TSC$_z$, Re TSC$_{32x}$, Im TSC$_{02x}$, Im TSC$_y$, Néel$_x$}
{Re VBS$_y$, Néel$_y$, QSHE$_x$, Im VBS$_y$, QSHE$_z$}	{Re TSC$_{32z}$, Im SSC, Im TSC$_z$, Im TSC$_{02z}$, QSHE$_z$}
{Re VBS$_y$, Re TSC$_y$, Im TSC$_y$, CDW, Im VBS$_y$}	{Re TSC$_{32z}$, Re TSC$_x$, Im TSC$_y$, Néel$_z$, Im TSC$_{02z}$}
{Re VBS$_y$, Re TSC$_{32y}$, Im TSC$_y$, Im TSC$_{02z}$, Im TSC$_{02x}$}	{Re TSC$_{32z}$, Re TSC$_{32x}$, Im TSC$_y$, Im VBS$_y$, Im TSC$_{02y}$}
{Re VBS$_y$, Re TSC$_{02x}$, Im TSC$_{02x}$, QSHE$_x$, Re VBS$_z$}	{Re TSC$_{32z}$, Re TSC$_{02x}$, Im TSC$_{02y}$, Im TSC$_z$, Re VBS$_z$}
{Néel$_y$, Re TSC$_{32y}$, Im TSC$_{02y}$, Im TSC$_z$, Im TSC$_x$}	{Im SSC, Re TSC$_{32x}$, Im TSC$_{02x}$, QSHE$_x$, Im TSC$_x$}
{Im VBS$_z$, Re TSC$_{32y}$, Im TSC$_{02z}$, Im TSC$_z$, Im TSC$_{32x}$}	{Im VBS$_z$, Re TSC$_{32x}$, Im VBS$_y$, QSHE$_x$, Im TSC$_{32x}$}
{Re TSC$_{02y}$, Re TSC$_y$, Im TSC$_{32z}$, Im TSC$_{32x}$, Im VBS$_y$}	{Re TSC$_{02y}$, Re TSC$_x$, Re VBS$_x$, Im TSC$_{32x}$, Im TSC$_{02z}$}
{Re TSC$_y$, Re TSC$_{02x}$, Im TSC$_z$, Im TSC$_{32x}$, Néel$_x$}	{Re TSC$_x$, Re TSC$_{02x}$, QSHE$_x$, Im TSC$_{32x}$, Re SSC}

Is the transition from QSH to SC different than the one from AFM to VBS ?

AFM-VBS

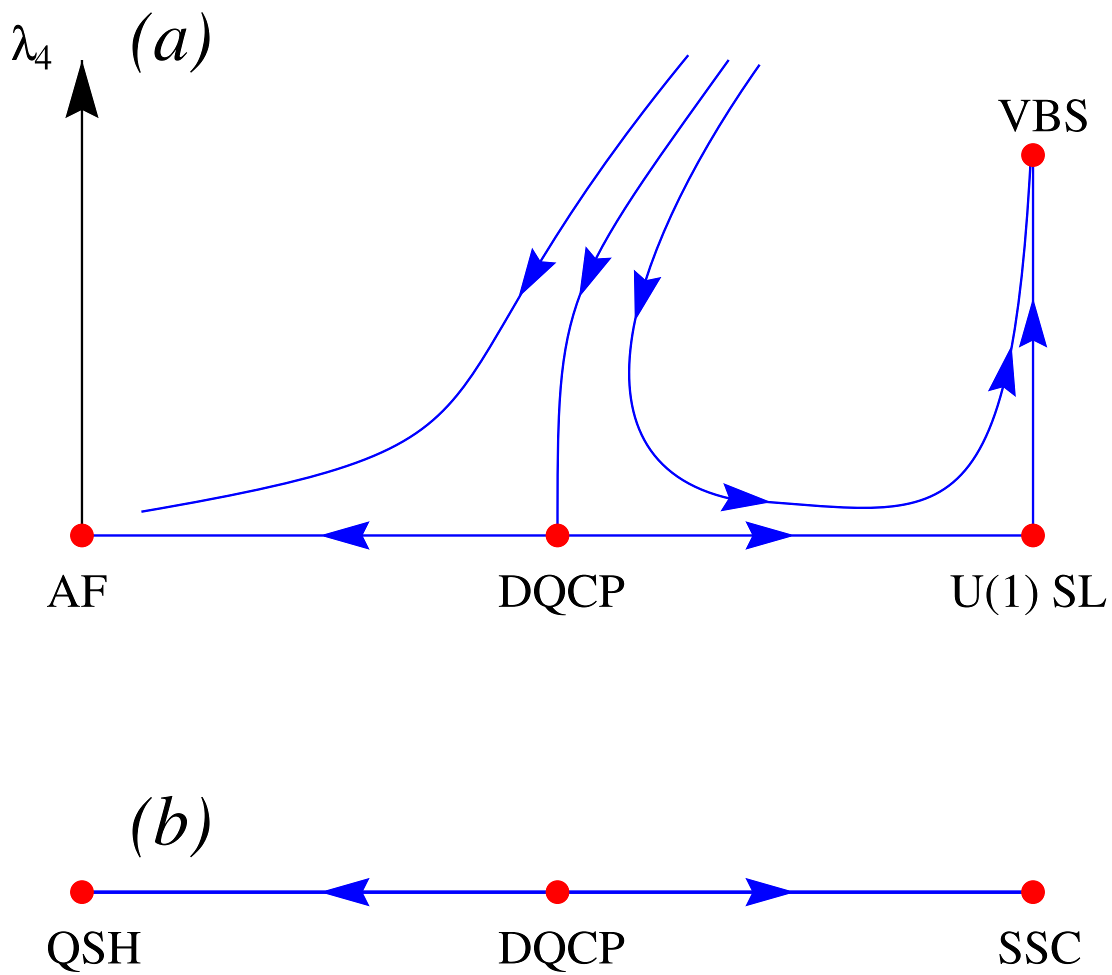
On the lattice the U(1) symmetry gives way to a C_4. This introduces a second length scales and complicates the analysis of the DQCP

QSH-SC

On the lattice the U(1) symmetry of the SC is conserved.

→ No dangerously irrelevant operator.

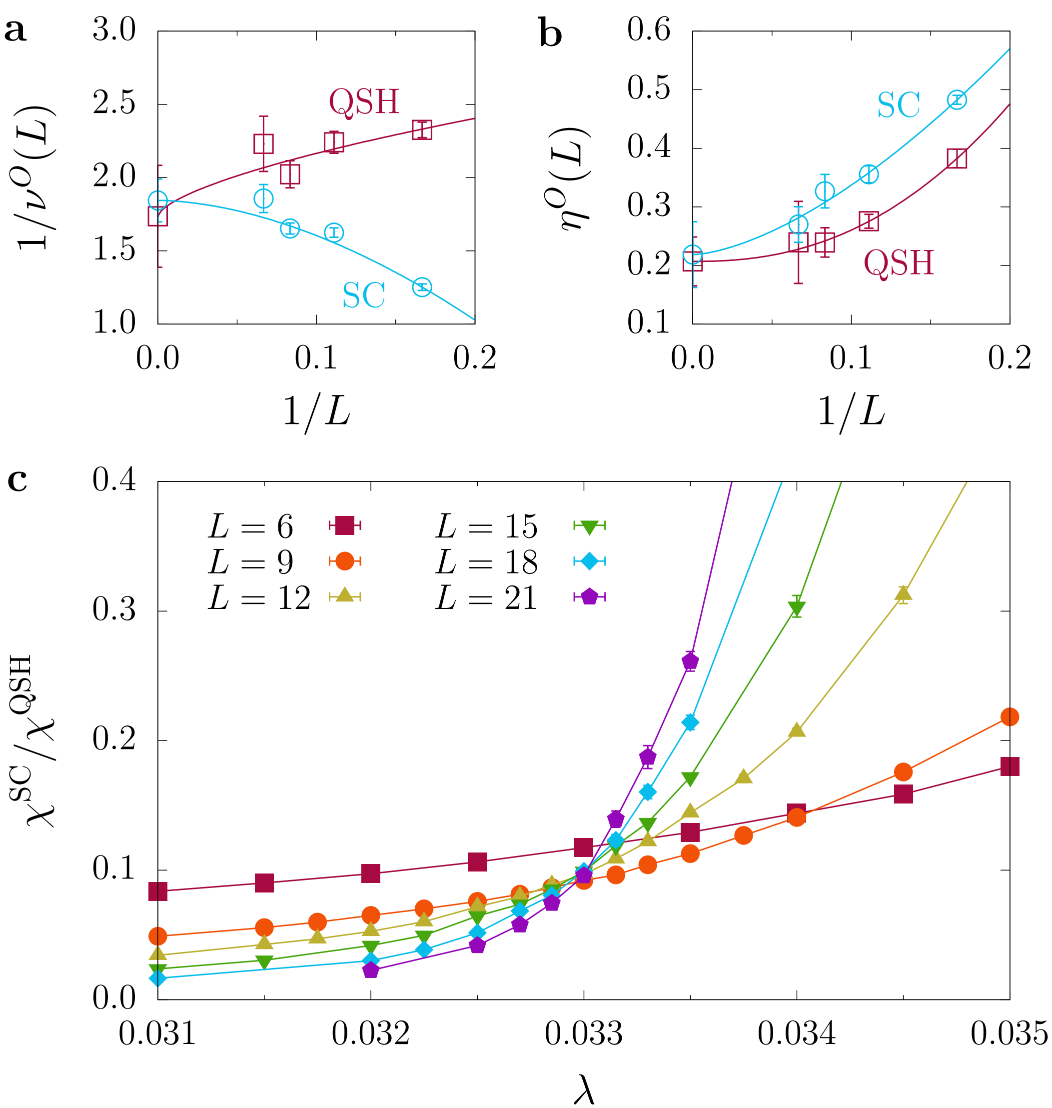
→ Improved model for DQCP



Picture from W. Guo

Superconductivity from condensation of topological defects in QSH insulator

Critical exponents



$$\eta^{QSH} = 0.21(5), \quad \eta^{SC} = 0.22(6)$$

Compares well with

$$\eta^{AFM} = 0.259(6), \quad \eta^{VBS} = 0.25(3)$$

A. Nahum et. al. Phys. Rev. X 5 (2015), 041048.

From conformal bootstrap:

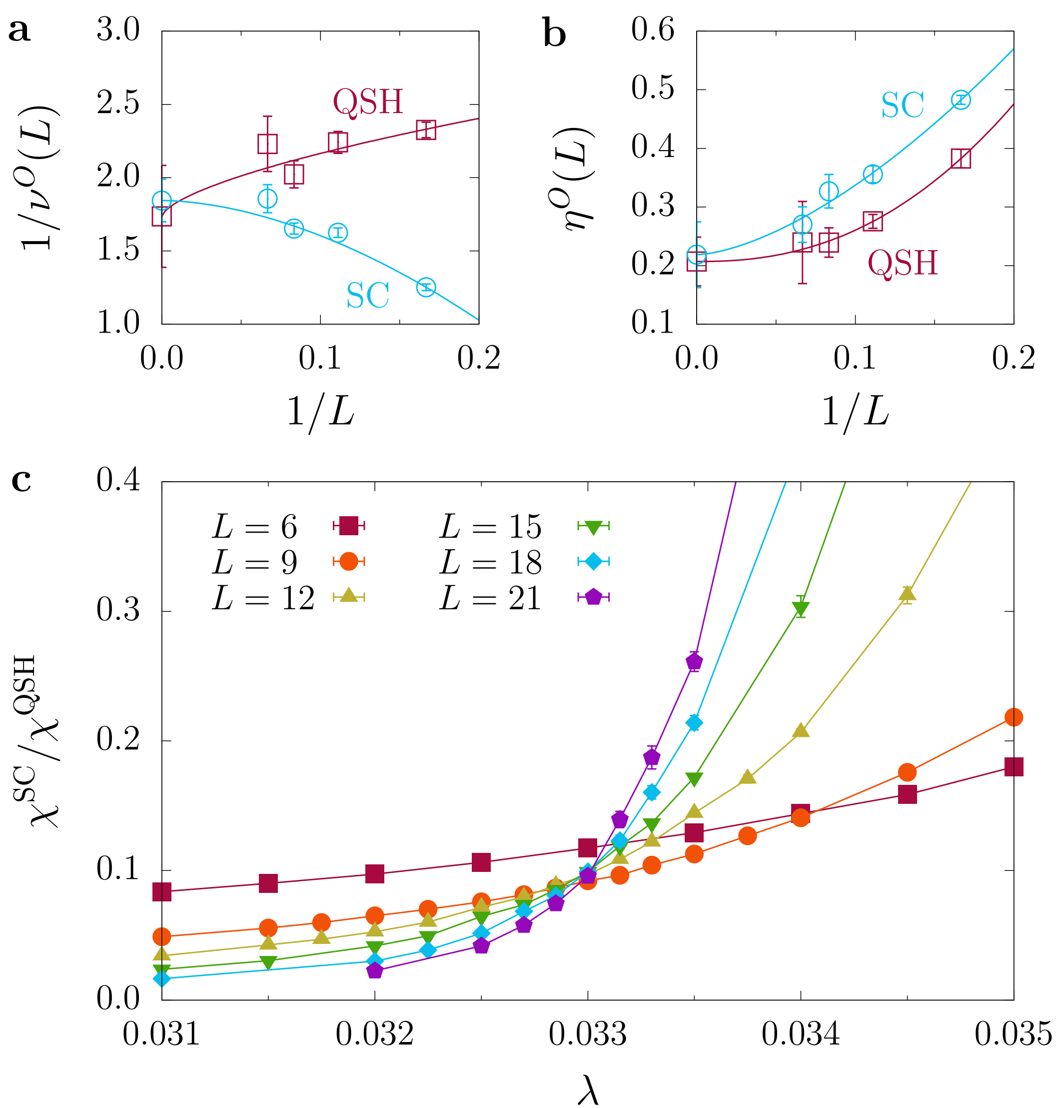
$\eta > 0.52$

for emergent SO(5) symmetry.

D. Poland, S. Rychkov, and A. Vichi
ArXiv:1805.04405 (2018).

Superconductivity from condensation of topological defects in QSH insulator

Critical exponents



$$1/\nu^{QSH} = 1.7(4), \quad 1/\nu^{SC} = 1.8(2)$$

Compares with

$$1/\nu = 2.24(4)$$

H. Shao, W. Guo, and A. W. Sandvik,
Science 352 (2016), no. 6282, 213–216.

From conformal bootstrap

$$1/\nu < 1.957$$

for continuous transition
(Unitary CFT with one relevant scalar).

Y. Nakayama and T. Ohtsuki,
Phys. Rev. Lett. 117 (2016), 131601.

How should one reconcile conformal bootstrap and numerical results?

1) Pseudo criticality

Unitary CFT with SO(5) emergent symmetry lies "close" to accessible parameter space (e.g. $D_c = (2+1+\epsilon)$). In this case the cited bootstrap bounds are not valid, and the RG flow is very slow in the proximity of the fixpoint. Correlation length is greater than accessible lattice sizes and the phase transition is ultimately first order.

C.Wang, A. Nahum, M. A. Metlitski, C. Xu, and T. Senthil, PRX 7, (2017), 031051.
P. Serna and A. Nahum, arXiv:1805.03759.

2) Continuous transition

Unitary CFT without SO(5) symmetry. The bound $1/\nu < 1.957$ is satisfied. Should be checked with our *improved* model.

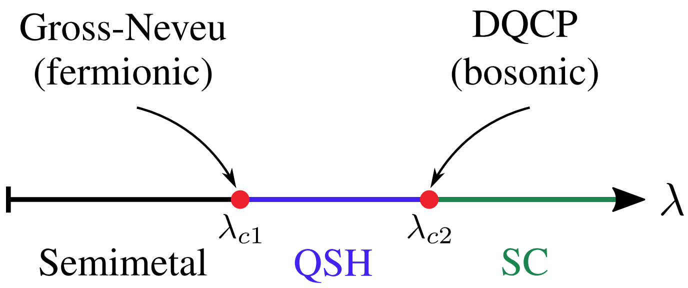
3) ....

Summary

- Competing mass terms in Dirac fermions → Route to generate exotic phase transition (topological terms).

Y. Liu, Z. Wang, T. Sato, M. Hohenadler, C. Wang, W. Guo, FFA, arXiv:1811.02583

$$\hat{H} = -t \sum_{\langle ij \rangle} (\hat{c}_i^\dagger \hat{c}_j + \hat{c}_j^\dagger \hat{c}_i) - \lambda \sum_{\hexagon} \left(\sum_{\langle\langle i,j \rangle\rangle \in \hexagon} \nu_{i,j} i \left(\hat{c}_i^\dagger \boldsymbol{\sigma} \hat{c}_j - \hat{c}_j^\dagger \boldsymbol{\sigma} \hat{c}_i \right) \right)^2$$



- Novel route to superconductivity

Skyrmions of the QSH order parameter carry charge 2e. When they condense they disorder to QSH state and create an s-wave superconductor.

- Improved model to study deconfined quantum critical points (DQCP)

U(1) charge conservation is not broken by lattice → only a single length scale.

- Doping? Thermodynamics? Additional attractive U terms ?

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 Ising field 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
- Parallel tempering, projective and finite T approaches
- Long range Coulomb


F. Goth


M. Bercx


J. Hoffmann


M. Ulybyshev

KONWIHR

DFG Wissenschaftliche Literaturversorgungs und Informationssysteme (LIS)

M. Bercx, F. Goth, J. S. Hofmann and F. F. Assaad, SciPost Phys. 3 (2017), 013