

Outline

- 1) Monte Carlo
- 2) Auxiliary field QMC
- 3) Trotter
- 4) Hubbard Stratonovich
- 5) Integrating out the fermions
- 6) Measurements
- 7) Wicks theorem
- 8) Absence of sign problem
- 9) Organization of the code and fast updates.
- 10) Projective Approaches
- 11) Project suggestions
- 12) Global updating schemes → Langevin dynamics
- 13) Stabilization
- 14) ALF Examples
- 15) Supported Codes

- 1) Odd and even leg Hubbard models.

Predefined lattices: N_leg_lattice

■ ARTICLE

Surprises on the Way from One- to Two- Dimensional Quantum Magnets: The Ladder Materials

Elbio Dagotto and T. M. Rice

Science 271 (1996), no. 5249, 618–623.

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Surprises on the Way from One- to Two-Dimensional Quantum Magnets: The Ladder Materials

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- 1) Odd and even leg Hubbard models.

Predefined lattices: N_leg_lattice

- 2) Emergent SO(4) symmetry in the one-dimensional Hubbard model.

Up to logarithmic corrections:

Dimer-Dimer correlations are in predefined observables.

$$\langle \hat{S}_i \hat{S}_{i+r} \rangle \propto (-1)^r / r$$

$$\langle \hat{K}_i \hat{K}_{i+r} \rangle - \langle \hat{K}_i \rangle \langle \hat{K}_{i+r} \rangle \propto (-1)^r / r, \quad \hat{K}_i = \sum_{\sigma} \left(\hat{c}_{i,\sigma}^{\dagger} \hat{c}_{i+1,\sigma} + H.c. \right)$$

$$\langle \hat{D}_i \hat{D}_{i+r} \rangle - \langle \hat{D}_i \rangle \langle \hat{D}_{i+r} \rangle \propto (-1)^r / r, \quad \hat{D}_i = \hat{S}_i \hat{S}_{i+1}$$

Note: Field theory is O(4) non-linear sigma model in 1+1 dimensions with WZW term.

$$S[\hat{\varphi}] = \int dx d\tau \frac{1}{G} (\partial_{\mu} \hat{\varphi}(x, \tau))^2 + 2\pi i \Gamma[\hat{\varphi}], \quad \Gamma[\hat{\varphi}] = \frac{1}{\text{Area}(S^3)} \int_0^1 du \int dx d\tau \epsilon_{\alpha,\beta,\gamma,\delta} \hat{\varphi}_{\alpha} \partial_x \hat{\varphi}_{\beta} \partial_{\tau} \hat{\varphi}_{\gamma} \partial_u \hat{\varphi}_{\delta}$$

ALF simulations of O(5) non-linear sigma model in 2+1 d with WZW term → Z. Wang et al. Phys. Rev. Lett. 126 (2021), 045701

For an explicit calculation see supplemental material of
T. Sato, M. Hohenadler, T. Grover, J. McGreevy, and F. F. Assaad, Topological terms on topological defects: a quantum Monte Carlo study, arXiv:2005.08996 (2020).

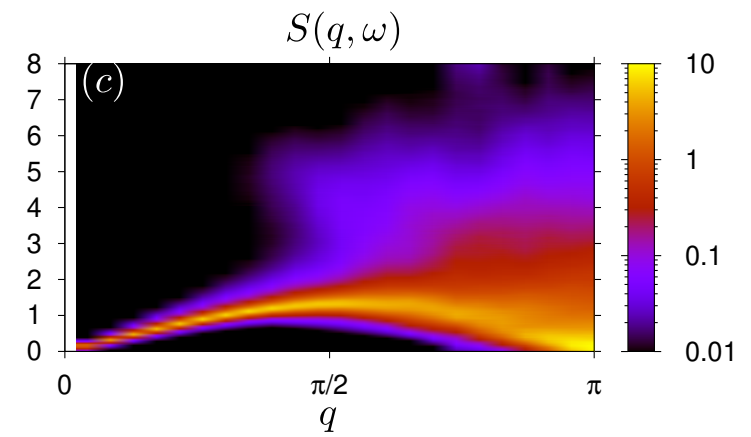
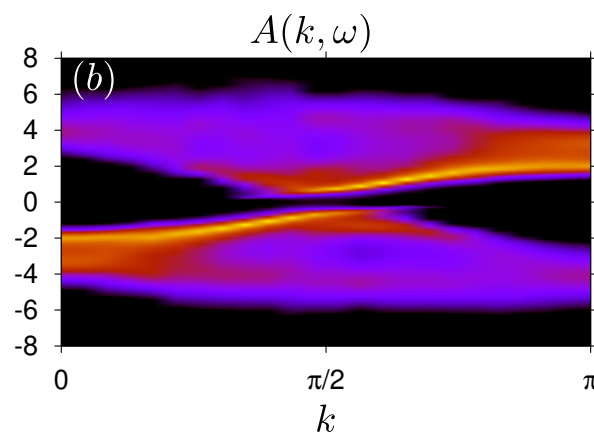
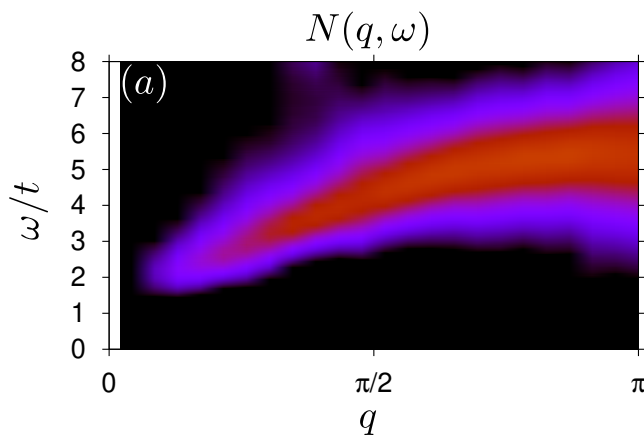
- 3) a) $SU(N)$ Hubbard model on the one-dimensional chain. Show that the ground state at $N = 4$ is dimerized.
- b) Can you write a program for the $SU(N)$ quantum antiferromagnetic in the self-adjoint antisymmetric representation? (See ALF 2.0 documentation, Section on the $SU(N)$ Kondo lattice.)

3) a) SU(N) Hubbard model on the one-dimensional chain. Show that the ground state at $N = 4$ is dimerized.

b) Can you write a program for the SU(N) quantum antiferromagnetic in the self-adjoint antisymmetric representation? (See ALF 2.0 documentation, Section on the SU(N) Kondo lattice.)

4) Dynamics of one-dimensional Hubbard chains. Understand how to use Maxent (see Documentation Chapter 10) to produce:

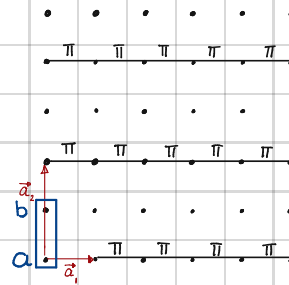
$$\langle n \rangle = 1, U/t = 4, \beta t = 10, L = 46$$



5) Correlation effects in Chern bands.

No sign problem for negative U, and arbitrary filling.

For positive U, no sign problem only at half-filling ($\mu = 0$)



$$H = H_{\text{Dirac}} + H_{\text{QSH}} + U \sum_i \left[\sum_{\mathbb{V}} (a_{i,\mathbb{V}}^\dagger a_{i,\mathbb{V}} - \frac{1}{2}) \right]^2 + U \sum_i \left[\sum_{\mathbb{V}} (b_{i,\mathbb{V}}^\dagger b_{i,\mathbb{V}} - \frac{1}{2}) \right]^2 - \mu \sum_{i,\mathbb{V}} (a_{i,\mathbb{V}}^\dagger a_{i,\mathbb{V}} + b_{i,\mathbb{V}}^\dagger b_{i,\mathbb{V}})$$

$$H_{\text{Dirac}} = -t \sum_{i,\mathbb{V}} \left[a_{i,\mathbb{V}}^\dagger (-a_{i+a_1,\mathbb{V}} + b_{i,\mathbb{V}}) + b_{i,\mathbb{V}}^\dagger (a_{i+a_2,\mathbb{V}} + b_{i+a_1,\mathbb{V}}) + h.c. \right]$$

$$H_{\text{QSH}} = \lambda \sum_{i,\mathbb{V}} i \mathbb{V} (a_{i,\mathbb{V}}^\dagger b_{i+a_1,\mathbb{V}} + b_{i,\mathbb{V}}^\dagger a_{i+a_1,\mathbb{V}} - b_{i,\mathbb{V}}^\dagger a_{i+a_1+a_2,\mathbb{V}} - a_{i,\mathbb{V}}^\dagger b_{i-a_2+a_1,\mathbb{V}}) + h.c.$$

PHYSICAL REVIEW B **102**, 201112(R) (2020)

Rapid Communications

Editors' Suggestion

Superconductivity, pseudogap, and phase separation in topological flat bands

Johannes S. Hofmann ¹, Erez Berg ^{1,*} and Debanjan Chowdhury ^{2,†}

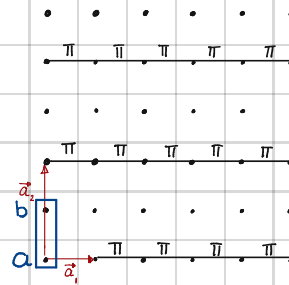
¹Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot 76100, Israel

²Department of Physics, Cornell University, Ithaca, New York 14853, USA

5) Correlation effects in Chern bands.

No sign problem for negative U, and arbitrary filling.

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$$H = H_{\text{Dirac}} + H_{\text{QSH}} + U \sum_i \left[\sum_{\nu} (a_{i,\nu}^\dagger a_{i,\nu} - \frac{1}{2}) \right]^2 + U \sum_i \left[\sum_{\nu} (b_{i,\nu}^\dagger b_{i,\nu} - \frac{1}{2}) \right]^2 - \mu \sum_{i,\nu} (a_{i,\nu}^\dagger a_{i,\nu} + b_{i,\nu}^\dagger b_{i,\nu})$$

$$H_{\text{Dirac}} = -t \sum_{i,\nu} \left[a_{i,\nu}^\dagger (-a_{i+a_1,\nu} + b_{i,\nu}) + b_{i,\nu}^\dagger (a_{i+a_2,\nu} + b_{i+a_1,\nu}) + h.c. \right]$$

$$H_{\text{QSH}} = \lambda \sum_{i,\nu} (a_{i,\nu}^\dagger b_{i+a_1,\nu} + b_{i,\nu}^\dagger a_{i+a_1,\nu} - b_{i,\nu}^\dagger a_{i+a_1+a_2,\nu} - a_{i,\nu}^\dagger b_{i-a_2+a_1,\nu}) + h.c.$$

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6) Edge physics.

Consider the above model with open boundary conditions in the y-direction. Along the edge you should be able to investigate the physics of a helical Luttinger liquid.

PRL **106**, 100403 (2011)

PHYSICAL REVIEW LETTERS

week ending
11 MARCH 2011

Correlation Effects in Quantum Spin-Hall Insulators: A Quantum Monte Carlo Study

M. Hohenadler, T. C. Lang, and F. F. Assaad

7) Sticking issues. Consider the doped attractive Hubbard model. Both HS decompositions based on

$$H_U = -\frac{U}{2} (n_{i,\uparrow} - n_{i,\downarrow})^2 \quad M_z = \text{True in Hubbard Hamiltonian.}$$

$$H_U = \frac{U}{2} (n_{i,\uparrow} + n_{i,\downarrow} - 1)^2 \quad M_z = \text{False in Hubbard Hamiltonian.}$$

are free of the negative sign problem. Check autocorrelation times (see Documentation Sec. 4) for the particle number as a function of doping for *large* values of $|U|$ and assess which choice the HS transformation is more efficient.

- 8) Investigate the spinless t-V model on a π -flux lattice. As a function of V, you should observe a transition in the Gross-Neveu Ising universality class to a charge density wave state.

PHYSICAL REVIEW D **101**, 074501 (2020)

**Fermion-bag inspired Hamiltonian lattice field theory
for fermionic quantum criticality**

Emilie Huffman¹ and Shailesh Chandrasekharan²

- 9) Consider the half-filled Kondo lattice model on the Honeycomb lattice. Show that there is direct magnetic order disorder transition as a function of J. The transition is a consequence of the competition between the RKKY and Kondo interactions.

PHYSICAL REVIEW B, VOLUME 63, 155114

**Spin and charge dynamics of the ferromagnetic and antiferromagnetic
two-dimensional half-filled Kondo lattice model**

S. Capponi and F. F. Assaad

10) Dzyaloshinskii-Moriya

$$\hat{H} = \sum_{\langle i,j \rangle} \left(J \hat{S}_i^{\alpha} \hat{S}_j^{\alpha} + \vec{D}_{i-j} \cdot \hat{S}_i^{\alpha} \times \hat{S}_j^{\alpha} \right) = \sum_{\langle i,j \rangle} \left[J \hat{S}_i^{\alpha} \hat{S}_j^{\alpha} + |\varepsilon_{\alpha\beta\gamma} D_{i-j}^{\alpha}| \left(\hat{S}_i^{\beta} + \text{sign}(\varepsilon_{\alpha\beta\gamma} D_{i-j}^{\alpha}) \hat{S}_j^{\gamma} \right)^2 \right]$$

Fermionize. $\hat{S}_i^{\alpha} = \sum_{s,s'} \hat{F}_{i,s}^{\alpha} \frac{\mathbb{1} - \tau_{s,s'}}{2} \hat{F}_{i,s'}$ and impose the constraint, $\sum_s \hat{F}_{i,s}^{\dagger} \hat{F}_{i,s} = 1$, by including a Hubbard U .

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

Letter

Quantum Monte Carlo simulation of generalized Kitaev models

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11) Define your own problem