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Algorithms for Lattice Fermions (ALF) 2.0

a flexible package for the efficient simulation of lattice Hamiltonians

The **ALF Collaboration**: FF Assaad, M Bercx, F Goth, A Götz JS Hofmann, E Huffman, Z Liu, F Parisen Toldin, JSE Portela, and J Schwab

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Offers:

- ✓ Generic open-source package for auxiliary-field Monte Carlo simulations of fermion-boson lattice models
- ✓ Research platform (see examples below), also ideal for establishing benchmarks and golden standards
- ✓ Efficient implementation on modern HPC systems and ease of use through pyALF

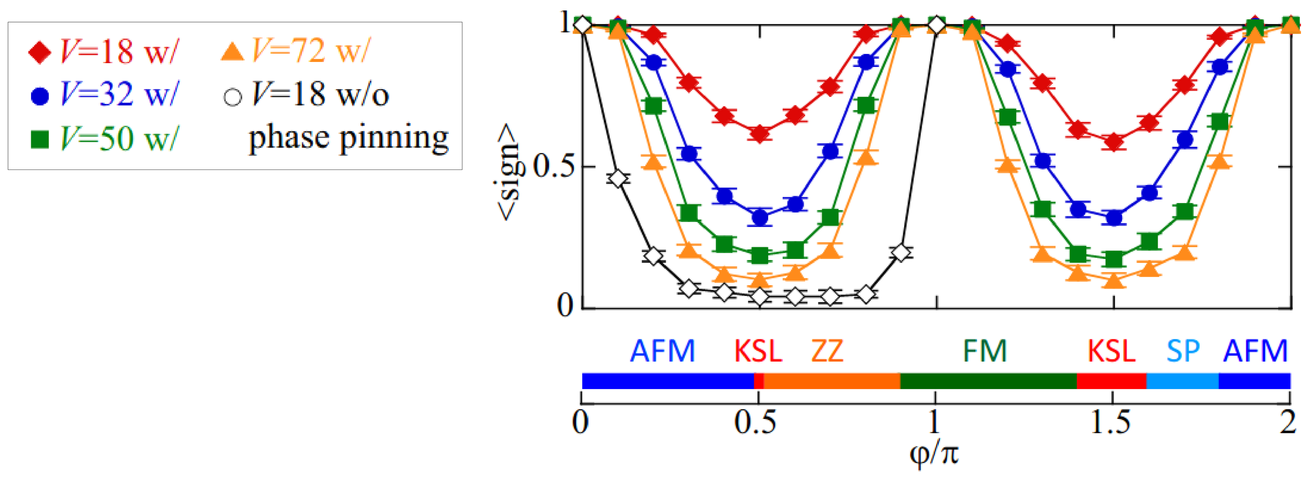
Tackling the sign problem through phase pinning

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

Quantum Monte Carlo simulation of generalized Kitaev models

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

$$\hat{H} = 2K \sum_{i\in A,\delta} \hat{S}_i^\delta \hat{S}_{i+\delta}^\delta + J \sum_{i\in A,\delta} \hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_{i+\delta}$$ with $$K = A\sin(\varphi),\ J = A\cos(\varphi)$$



Average sign 〈 sign 〉 as a function φ for various values of V. We can reach experimentally relevant energy scales: $\beta A \simeq 3 \ \rightarrow \ A \simeq 100$ meV $\simeq 100$ K, making the approach competitive for thermodynamics.

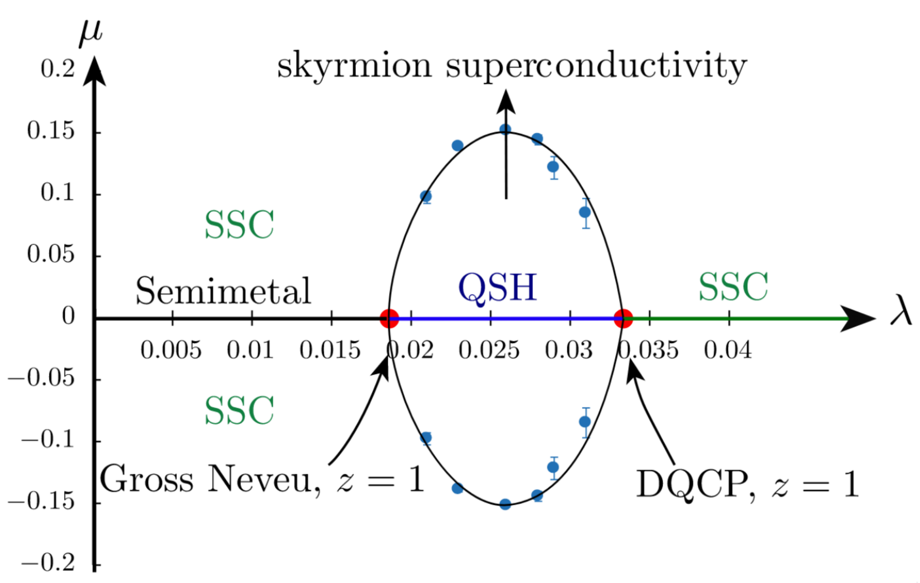
Finding new routes to superconductivity via the condensation of skyrmions

PHYSICAL REVIEW LETTERS **126**, 205701 (2021)

Doping-Induced Quantum Spin Hall Insulator to Superconductor Transition

Zhenjiu Wang,[1,*] Yuhai Liu,[2,3] Toshihiro Sato,[1] Martin Hohenadler,[1] Chong Wang,[4] Wenan Guo,[3,2] and Fakher F. Assaad[1,5,†]

$$\hat{H} = -t\sum_{\langle ij\rangle}(\hat{c}_i^\dagger \hat{c}_j + \mathrm{H.c.}) - \lambda \sum_{\hexagon}\left(\sum_{\langle\langle ij\rangle\rangle\in\hexagon} \hat{J}_{ij}\right)^2$$



Phase diagram in the interaction strength λ versus chemical potential plane. The critical chemical potential μ_c for the transition from the quantum spin Hall (QSH) to the *s*-wave superconductor (SSC) is computed by measuring the pairing gap at half-filling.

The ALF package

Kinetic | Potential (sum of perfect squares) | Coupling of fermions to Ising field

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

- Model specification at minimal programming cost + Python interface
- MPI/OpenMP implementation + near-optimal single-core performance
- Arbitrary Bravais lattice and observables, continuous fields
- Different updating schemes (e.g. global updates, Langevin dynamics)
- Parallel tempering, projective and finite *T* approaches
- Cotunneling for Kondo models, Rényi Entropy

Future/ongoing developments

- Time-dependent Hamiltonians
- Additional fermion algorithms (e.g. CT-INT)
- improved IO (e.g. HDF5 support)

- ALF Collaboration, **arXiv:2012.11914** [cond-mat.str-el] (2021) ALF 2.0
- M. Bercx, F. Goth, J. S. Hofmann and F. F. Assaad, SciPost Phys. 3 (2017), 013

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Landau level regularization of continuum field theories

PHYSICAL REVIEW LETTERS **126**, 045701 (2021)

Phases of the (2+1) Dimensional SO(5) Nonlinear Sigma Model with Topological Term

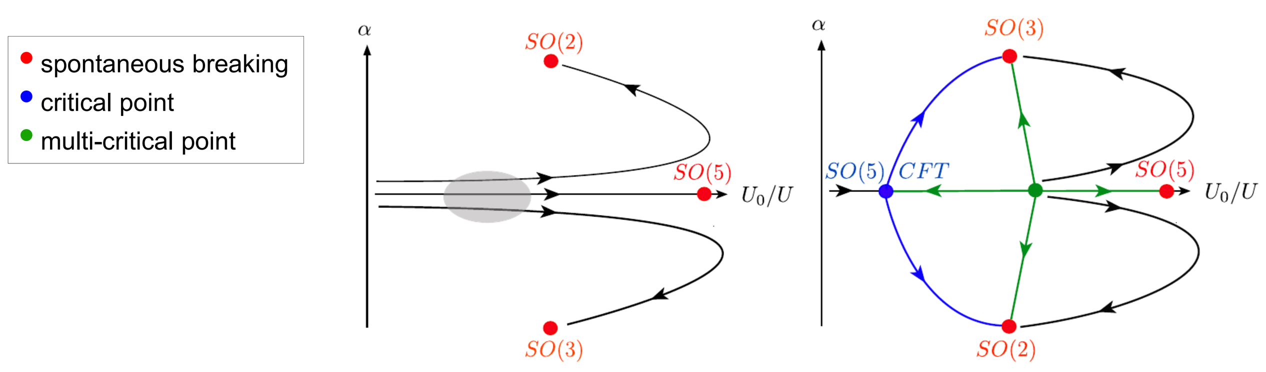
Zhenjiu Wang,[1,*] Michael P. Zaletel,[2] Roger S. K. Mong,[3] and Fakher F. Assaad[1,4,†]

$$\hat{H} = \int_V d^2\boldsymbol{x} \left(\frac{U_0}{2} [\hat{\boldsymbol{\psi}}^\dagger(\boldsymbol{x})\hat{\boldsymbol{\psi}}(\boldsymbol{x}) - C(\boldsymbol{x})]^2 - \frac{U}{2}\sum_{i=1}^{5} [\hat{\boldsymbol{\psi}}^\dagger(\boldsymbol{x}) O^i \hat{\boldsymbol{\psi}}(\boldsymbol{x})]^2 \right),$$

which maps to

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

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



Compatible RG flows in U_0 ("stiffness") vs. α (which breaks SO(5) into SO(3)×SO(2)): (left) 1st order transition with slow flow (shaded); and (right) ordered and critical phases with multi-critical point. At small U_0 the correlation length exceeds the system size.

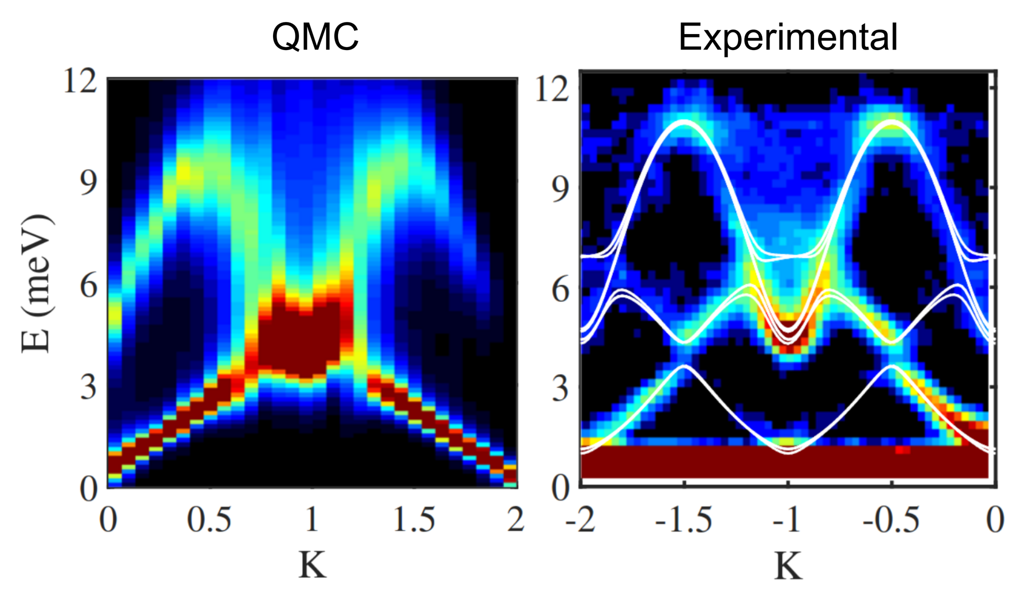
Understanding magnon-spinon interactions

PHYSICAL REVIEW LETTERS **125**, 037204 (2020)

Coexistence and Interaction of Spinons and Magnons in an Antiferromagnet with Alternating Antiferromagnetic and Ferromagnetic Quantum Spin Chains

H. Zhang,[1] Z. Zhao,[2] D. Gautreau,[3] M. Raczkowski,[4] A. Saha,[3] V. O. Garlea,[5] H. Cao,[5] T. Hong,[5] H. O. Jeschke,[6] Subhendra D. Mahanti,[1] T. Birol,[3] F. F. Assaad,[4,7] and X. Ke[1,*]

$$\hat{H} = \sum_{i,j} J_{ij} \vec{S}_i \cdot \vec{S}_j$$



Magnetic excitation spectra: (left) quantum Monte Carlo simulations considering intrachain couplings J1, J2 and antiferromagnetic interchain coupling J3; and (right) neutron scattering intensity map measured at T=5K (minus 100K background).