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Algorithms for lattice fermions (ALF): a flexible package for the efficient simulation of lattice Hamiltonians

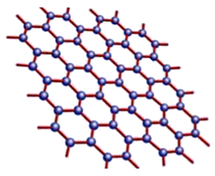
The ALF collaboration (F. F. Assaad, M. Bercx, F. Goth, J. S. Hofmann, J. Portela, and J. Schwab)

https://git.physik.uni-wuerzburg.de/ALF

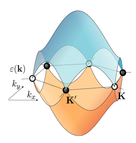
Goals:

- ✓ Generic package for auxiliary field Monte Carlo simulations of fermion-boson lattice models
- ✓ Efficient implementation on modern HPC systems
- ✓ Benchmarking and golden standards

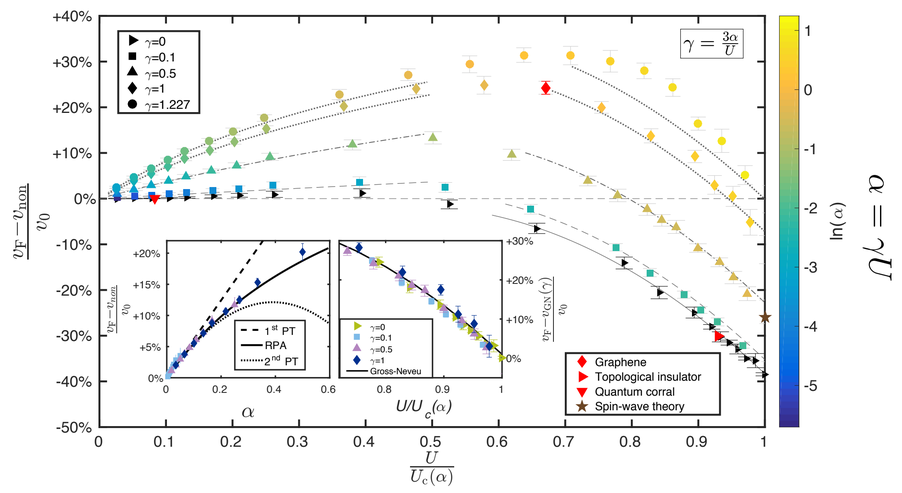
The role of electron-electron interactions in two dimensional Dirac fermions



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



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



Ho-Kin Tang, J. N. Leaw, J. N. B. Rodrigues, I. F. Herbut, P. Sengupta, F. F. Assaad, and S. Adam, Science 361 (2018), no. 6402, 570–574.

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

Quantum Monte Carlo Simulation of Frustrated Kondo Lattice Models

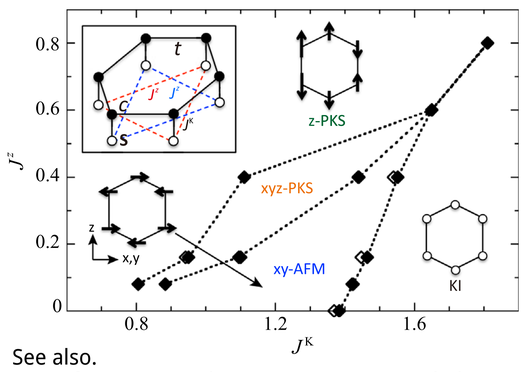
Toshihiro Sato,[1] Fakher F. Assaad,[1] and Tarun Grover[2]

$$\hat{H} = \hat{H}_{\text{Spin}} + \hat{H}_{\text{Fermion}} + \hat{H}_{\text{Kondo}}$$

$$\hat{H}_{\text{Spin}} = \sum_{i,j} [J^{z}_{ij}\hat{S}^{z}_{i}\hat{S}^{z}_{j} + J^{\perp}_{ij}(\hat{S}^{+}_{i}\hat{S}^{-}_{j} + \text{H.c.})],$$

$$\hat{H}_{\text{Fermion}} = \sum_{x,y,\sigma} \hat{c}^{\dagger}_{x\sigma} T_{x,y} \hat{c}_{y\sigma} + \sum_{x} U \left(\hat{n}_{x,\downarrow} - \frac{1}{2}\right)\left(\hat{n}_{x,\uparrow} - \frac{1}{2}\right),$$

$$\hat{H}_{\text{Kondo}} = \sum_{i,x} \frac{J^{K}_{i,x}}{2} \hat{\boldsymbol{c}}^{\dagger}_{x}[\sigma^{z} \cdot \hat{S}^{z}_{i} - (-1)^{x}(\sigma^{+}\hat{S}^{-}_{i} + \sigma^{-}\hat{S}^{+}_{i})]\hat{\boldsymbol{c}}_{x}.$$



Interplay of Kondo, RKKY and geometric frustration

See also.
J. S. Hofmann, FFA, and T. Grover, PRB 2019, FL* phase in Kondo lattice model. BFG model Kondo coupled to electrons.

M. Raczkowski and FFA, PRL 2019, B. Danu, FFA. and F. Mila, arXiv:1903.08622 Nano-Kondo systems.

The ALF package

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

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

- Model can be specified at minimal programming cost
- MPI/OpenMP implementation
- Fortran 2003 standard
- SU(N_{col}) symmetric in colors N_{col}
- Arbitrary Bravais lattice for d=1, 2
- Block diagonal in flavors, N_{fl}
- Parallel tempering, projective and finite T approaches

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

Future/ongoing developments

- Continuous fields
- Hybrid molecular dynamics
- Langevin dynamics
- Imaginary time dependent Hamiltonians

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SFB1170 ToCoTronics

Lattice gauge theories

PNAS

Confinement transition of $\mathbb{Z}_2$ gauge theories coupled to massless fermions: Emergent quantum chromodynamics and *SO*(5) symmetry

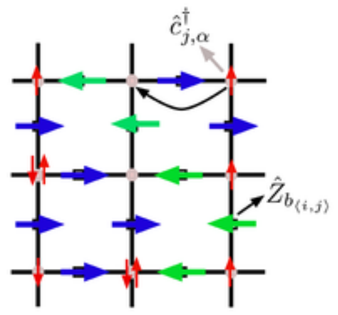
Snir Gazit[a,1], Fakher F. Assaad[b], Subir Sachdev[c,d,1], Ashvin Vishwanath[c], and Chong Wang[c]

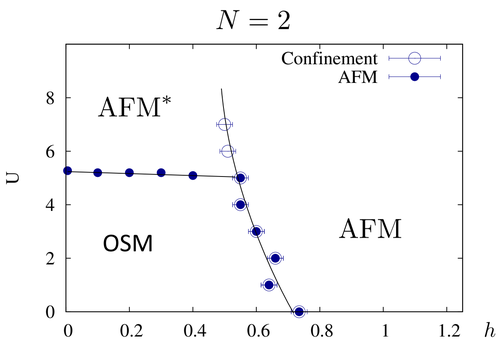
PHYSICAL REVIEW X **6,** 041049 (2016)

Simple Fermionic Model of Deconfined Phases and Phase Transitions

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

$$\hat{H} = \sum_{\langle i,j\rangle} \hat{Z}_{\langle i,j\rangle} \left(\sum_{\alpha=1}^{N} \hat{c}^{\dagger}_{i,\alpha}\hat{c}_{j,\alpha} + \text{H.c.} \right) - Nh \sum_{\langle i,j\rangle} \hat{X}_{\langle i,j\rangle}.$$





$$\hat{Q}_{\vec{i}} = (-1)^{\sum_{\sigma} \hat{c}^{\dagger}_{\vec{i},\sigma}\hat{c}_{\vec{i},\sigma}} \hat{X}_{\vec{i},\vec{i}+\vec{a}_x} \hat{X}_{\vec{i},\vec{i}-\vec{a}_x} \hat{X}_{\vec{i},\vec{i}+\vec{a}_y} \hat{X}_{\vec{i},\vec{i}-\vec{a}_y}, \quad \left[\hat{Q}_{\vec{i}}, \hat{H}\right] = 0$$

	Gauge Field	Particle-hole
OSM	De-confined	No binding
AFM	Confined	Condensed
AFM*	De-confined	Condensed

The c-orthogonal fermion carries global U(1) charge and local Z_2 charge

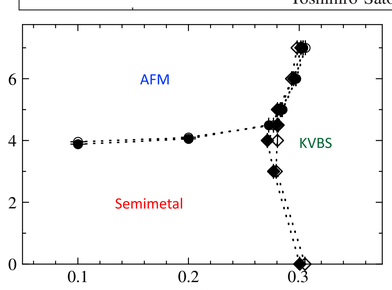
See also.
M. Hohenadler and FFA (arXiv:1906.11937, PRL 18), Orthogonal metal in Falicov-Kimball model.
S. Gazit, FFA, and S. Sachdev (arXiv:1906.11250), OSM → FL* transitions

Intertwined orders in Dirac fermions

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]



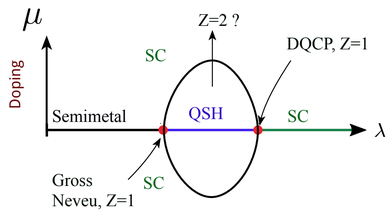
AFM (QSH) and VBS (SSC) from quintuplet of anticommuting Mass terms.

nature COMMUNICATIONS

ARTICLE
https://doi.org/10.1038/s41467-019-10372-0 OPEN

Superconductivity from the condensation of topological defects in a quantum spin-Hall insulator

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



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