The Algorithms for lattice fermions(ALF) project

The ALF collaboration, speaking: Florian Goth

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16. March 2023

Algorithms
Lattice
Fermions

General, open source implementation of auxiliary field quantum Monte Carlo algorithms

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


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SFB1170 ToCoTronics
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NIC
lrz Leibniz-Rechenzentrum der Bayerischen Akademie der Wissenschaften
GCS Gauss Centre for Supercomputing
KONWIHR

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Laughlin, Pines: The theory of everything, 28-31, PNAS, Jan. 4 2000

$$H = -\sum_{j}^{N_e} \frac{\hbar^2}{2m} \nabla_j^2 - \sum_{\alpha}^{N_i} \frac{\hbar^2}{2M_\alpha} \nabla_\alpha^2 - \sum_{j}^{N_e} \sum_{\alpha}^{N_i} \frac{Z_\alpha e^2}{|\vec{r}_j - \vec{R}_\alpha|} + \sum_{j \ll k}^{N_e} \frac{e^2}{|\vec{r}_j - \vec{r}_k|} + \sum_{\alpha \ll \beta}^{N_j} \frac{Z_\alpha Z_\beta e^2}{|\vec{R}_\alpha - \vec{r}_\beta|}$$

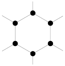
$\vec{r}_j$: electrons, $\vec{R}_\alpha$: ions

Thermodynamics

$$\langle O \rangle = \frac{\mathrm{Tr}\left(e^{-\beta H} O\right)}{\mathrm{Tr}\left(e^{-\beta H}\right)}, \quad \beta = \frac{1}{k_B T}$$

Our Model Hamiltonian

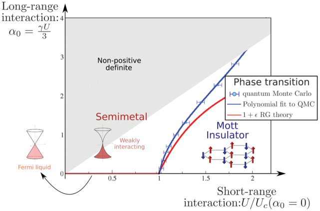
$$H = \sum_{x,y} T_{x,y} c_x^\dagger c_y + \frac{1}{2} \sum_{x,y,w,z} V_{x,y,w,z} c_x^\dagger c_y^\dagger c_w c_z, \quad \{c_x^\dagger, c_y\} = \delta_{x,y}, \{c_x, c_y\} = 0$$

low energy effective models: e.g. graphene, consider only the $2p^z$ atomic states. 

Toy models

$$H = -t \sum_{\langle i,j \rangle, \sigma=1}^{2} \left(c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma} \right) + \sum_{i,j} (n_i - 1) V_{i,j} (n_j - 1)$$

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



H.K. Tang et al. Science 2018; 361:570-574

The most generic Hamiltonian

$$H = H_0 + H_V + H_I + H_{0,\mathrm{I}}$$

$$H_0 = \sum_{k=1}^{M_T} \sum_{\sigma=1}^{N_{col}} \sum_{s=1}^{N_{fl}} \sum_{x,y}^{N_{dim}} c^{\dagger}_{x\sigma s} T^{(ks)}_{x,y} c_{y\sigma s}$$

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

$$H_I = \sum_{k=1}^{M_I} Z_k \left(\sum_{\sigma=1}^{N_{col}} \sum_{s=1}^{N_{fl}} \sum_{x,y}^{N_{dim}} c^{\dagger}_{x\sigma s} I^{(ks)}_{x,y} c_{y\sigma s} \right)$$

Symmetries

$$c^{\dagger}_x = c^{\dagger}_{x=(i,n),\sigma,s}$$

- $x = (i, n)$: Unit cell i and orbital n, encodes point group and translation symmetry.
- σ: Matrices T, V, and I are σ independent, corresponding to an $SU(N_col)$ symmetry.
- s: Block diagonal in flavour index. $\rightarrow$ Flavour is conserved.

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Finite Temperature Algorithm

$$
\begin{aligned}
Z &= \mathrm{Tr}\, e^{-\beta H} \\
&= \mathrm{Tr}\left(\prod_{\tau=1}^{L_\tau} e^{\Delta\tau(H_0+H_I+H_{0,\mathrm{I}})} e^{\Delta\tau H_V}\right) + \mathcal{O}(\Delta\tau^2) \\
&= \sum_{C\in\mathcal{C}} P(\Phi(C)) + \mathcal{O}(\Delta\tau^2) \\
&= \underbrace{\sum_{C\in\mathcal{C}} D[\Phi(C)]}_{\text{High dimensional sum}} \quad \underbrace{e^{-S[\Phi(C)]}}_{1-\text{body problem}} + \mathcal{O}(\Delta\tau^2)
\end{aligned}
$$

- $\Delta\tau$: imaginary time discretization, $\beta = \Delta\tau L_\tau$.
- $\Phi(C)$: value of Hubbard Stratonovitch fields for a configuration $C \in \mathcal{C}$.
- Markov-chain by spin flips on to C.

R.Blankenbecler, D.J. Scalapino, and R.L. Sugar, Phys. Rev. D 24 (1981), 2278

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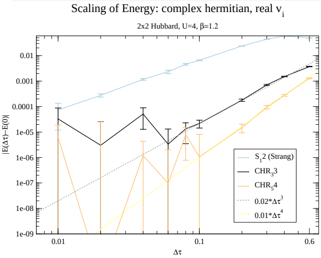
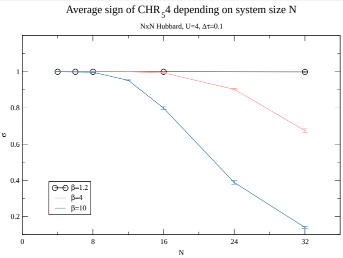
Modern Splitting techniques

- Algorithm inherits a second order discretization error due to the use of a Trotter decomposition.
- Operator splitting methods enable a higher approximation order.
- Goldman-Kaper bound requires the use of negative or complex step sizes.
- in arXiv:2009.04491 we introduced a new family of hermitian splitting methods with one set of real coefficients
- 3. order example: $t_1 = (3 - i\sqrt{3})/24$, $t_1 = (3 + i\sqrt{3})/8$, $v_1 = 1/3$
- generates a mild sign problem...





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The Sign Problem

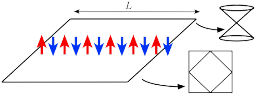
$$Z = \sum_{C \in \mathcal{C}} D[\Phi(C)] e^{-S[\Phi(C)]} + \mathcal{O}(\Delta\tau^2)$$

$$S[\Phi] = S_B[\Phi] - \log|\det(M[\Phi])| - i \arg\det M[\Phi]$$

- $\arg\det M[\Phi] = 0$, No sign problem, CPU $\propto V^3 \beta$
- $\arg\det M[\Phi] \neq 0$, sign Problem, CPU $\propto e^{\alpha\beta V}$
- Absence of the sign problem is often based on symmetry arguements. (e.g. time reversal + U(1) symmetries)

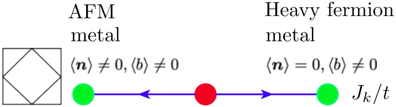
C. Wu and S.-C. Zhang, Phys. Rev. B, 71 (2005), 155115
E. Huffman and S. Chandrasekharan, Phys. Rev. B 89 (2014), 111101
Z.C. Wei, arXiv: 1712.09412

A model, e.g. CuN_2/Cu(100)



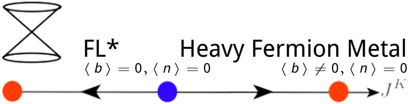
$$H = -t \sum_{<i,j>} (c_i^\dagger c_j + h.c.) + \frac{J_k}{2} \sum_r c_r^\dagger \vec{\sigma} c_r \bullet \vec{S}_r + J_h \sum_{r,r'} S_r S_{r'}$$ B.

Danu, F.Assaad, F. Mila, Phys. Rev. Lett. 123 (2019), 176601



- Dissipation vs. Kondo Screening
- Anti-ferromagnetic metal to heavy fermion metal QCP

B. Danu, M. Vojta, T. Grover, F. Assaad, Phys. Rev. B 106 (2022), L161103
M. Weber, D. J. Luitz, F. Assaad, Phys. Rev. Lett. 129 (2022), 056402



Spinons are deconfined Kondo break-down phase

Heavy-fermion phase Kondo screen

B. Danu, M. Vojta, F. Assaad, T. Grover, Phys. Rev. Lett. 125 (2020), 206602

PHYSICAL REVIEW LETTERS **128**, 087201 (2022)

Editors' Suggestion

Metallic and Deconfined Quantum Criticality in Dirac Systems

Zi Hong Liu ,[1] Matthias Vojta,[2] Fakher F. Assaad,[1] and Lukas Janssen [2]

Searching for new phases and exotic phase transitions

$$H = -t \sum_{<i,j>} c^{\dagger}_{i\sigma\lambda} c_{j\sigma\lambda} - J \sum_{i\alpha} \left(c^{\dagger}_{i\sigma\lambda} K^{\alpha}_{\sigma\sigma'} \tau^{z}_{\lambda\lambda'} c_{i\sigma'\lambda'} \right)^2$$

- $\lambda = 1, 2$ Layer index
- $(K^{\alpha})_{\sigma\sigma'} = -i\epsilon_{\alpha\sigma\sigma'}$ Generators of $SO(3)$
- $\alpha, \sigma, \sigma' = 1, 2, 3$ SO(3) index

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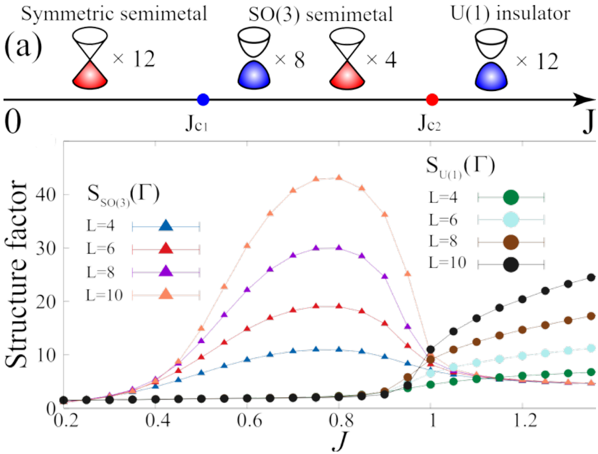

Novel Phases, Exotic Criticality

- Default Sampling is a single spin flip -> extend to HMC and Langvin updates(partially done)
- pyALF, python interface to the Fortran core
- Code is available at: alf.physik.uni-wuerzburg.de
- Regular schools and a youtube channel
- Integration into FAIRmat(NFDI consortia) database NOMAD.
- ALF nonprofit society founded

- Regular Software Carpentry workshops
- Classical Monte Carlo Code MARQOV, available at marqov.de
- Low-level optimization of the common routine $r < e^{-\beta \Delta E}$
- HackyHour, next 27.03, 5pm, physics department
- Wü-RSE, a local community for like-minded people working at the interplay between research and software: https://de-rse.org/chapter/wue/

Thank you for your attention!

Slides available at

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