Numerical Simulations of Strongly Correlated Electron Systems

F. F. Assaad

published in

NIC Symposium 2020
M. Müller, K. Binder, A. Trautmann (Editors)

Forschungszentrum Jülich GmbH,
John von Neumann Institute for Computing (NIC),
Schriften des Forschungszentrums Jülich, NIC Series, Vol. 50,
ISBN 978-3-95806-443-0, pp. 265.
http://hdl.handle.net/2128/24435

Numerical Simulations of Strongly Correlated Electron Systems

Fakher F. Assaad

Institut für Theoretische Physik und Astrophysik and
Würzburg-Dresden Cluster of Excellence ct.qmat,
Universität Würzburg, Am Hubland, 97074 Würzburg, Germany
E-mail: assaad@physik.uni-wuerzburg.de

The richness of emergent phenomena that stem from the fundamental laws of quantum mechanics is astonishing. Topology, inherent to the integer Hall effect and Chern insulators, allows us to understand why a dirty two-dimensional electron gas can provide the most precise determination of fundamental constants. Electron correlations lead to the notion of fractionalisation and associated emergent lattice gauge theories widely studied in high energy physics. Finally, quantum engineering leads to amazing possibilities for designing novel materials and nanostructures that may very well define the building blocks of information technologies beyond silicon. Given this fascinating richness of phenomena, the natural question to ask for a numerically oriented researcher is: can one develop a flexible and efficient program package that allows one to define and simulate, at minimal programming cost, a wide set of model Hamiltonians? We have recently written an open source library, coined **A**lgorithms for **L**attice **F**ermions (ALF) that allows us to study a large variety of designer and realistic models. In this article, we will summarise aspects of the ALF-library, demonstrate its range of application and then concentrate on the case study of fractionalisation in a Falicov-Kimball model.

1 Introduction

Consider a single spin-1/2 degree of freedom defined in a two dimensional Hilbert space. The quantum mechanical state of N spin-1/2 degrees of freedom on a graph, that for instance provides a minimal model for undoped high temperature cuprate superconductors, corresponds to a vector in a 2^N dimensional Hilbert space. The temporal evolution of this state requires diagonalisation of a $2^N \times 2^N$ Hamiltonian matrix $\hat{H}$. Since for a macroscopic cuprate sample, $N = 10^{23}$ and the task is generically out of reach. How is it that we can nevertheless solve so called non-frustrated spin models in thermodynamic equilibrium on arbitrarily large lattices? The answer lies in the formulation of the partition function in terms of a Feynman path integral:

$$Z = \mathrm{Tr} e^{-\hat{H}/k_B T} = \int d\phi(\boldsymbol{x}, \tau) e^{-S(\phi)} \tag{1}$$

Here, T is the temperature, k_B the Boltzmann constant, $\boldsymbol{x}$ a site of the graph, τ the imaginary time running from 0 to $1/k_B T$ and finally S the action that is a functional of ϕ. For fermion systems, the action generically takes the form $S = S_0(\phi) - \log\det M(\phi)$ where S_0 is the action of the bosonic field and the determinant arises from the coupling of the scalar field to the fermionic degrees of freedom. The above equation is the basis for auxiliary field QMC[1] algorithms used in the lattice gauge and solid state communities. The key point is that for a given configuration of fields, one can calculate the action in polynomial time. In our implementation, we compute explicitly the determinant, and the computation

cost to evaluate the action for a single field configuration scales as $N^3/(k_BT)$. The functional integral can be computed stochastically. This can can be achieved in polynomial time only in special cases.

- **The sign problem.** To use Monte Carlo sampling we need a positive definite cost function. Hence the action has to be real. The path integral is by no means unique and one of the key questions is to ask if it is possible to find a formulation with real action that one can compute for a given field in polynomial time. This requirement defines a class of so called negative sign free problems. In this domain, tremendous progress has been achieved in terms of symmetry properties of the action that lead to negative sign free formulations.[2–5] Furthermore, and in the spirit of universality, the sign problem can be avoided by cleverly defining models that capture the relevant – negative sign free – physics and omits the irrelevant interactions that can generate negative sign problems. Such a designer model approach to study universal properties at criticality or to understand properties of specific phases is very much en vogue in the solid state community. A recent biased selection includes the following Refs. 6–10. If one is not able to find a negative sign free formulation, then one can use reweighing techniques to nevertheless formulate a Monte Carlo sampling. For a given precision the computational time will scale as $e^{\Delta N/k_BT}$ where Δ is a formulation dependent positive constant. There is a body of research that aims to find formulations of quantum many body problems that ease the negative sign problem by minimising the value of Δ. Here one can mention efforts based on the representation of the path integral in terms of a Lefschetz thimble decomposition.[11, 12] On each thimble the fermion sign is constant, but the problem is caused by the number of thimbles. The number of thimbles is however formulation dependent and optimal representations have recently been proposed.[13, 14]

- **Sampling.** The sign problem is only one of many issues. The action can be real, but the distribution can have fat tails that inhibit the very notion of Monte Carlo sampling.[15] Even for well defined distributions, critical slowing down remains an issue. For example there are many electron-phonon problems that are free of the negative sign problem but that suffer from very long autocorrelation times that inhibit precise calculations on large lattices. In the present version of the ALF library,[16] we are using discrete fields and global updating methods such as Langevin dynamics or Hybrid Monte Carlo are not applicable. We are planing to implement these updating schemes in a future release. We note that machine learning as a tool to propose global moves is presently en vogue.[17]

In the above, we have highlighted the challenges. There is nevertheless a number of model Hamiltonians that we can simulate efficiently. In what follows, we will briefly summarise the workings of the ALF-Library[16] and then concentrate on a case study of fractionalisation in a Falicov-Kimball model.

2 The ALF

The ALF-library is programmed following Fortran-2003 standard and comes with an MPI-implementation. We are only dependent on BLAS and LAPACK libraries and

all the heavy numerical calculations are done through calls to these libraries. Hence, if they are well optimised on the supercomputers we use, our code will perform well. For the program development, we have established a git software repository at `http://alf.physik.uni-wuerzburg.de` and a small steering committee meets regularly so as to discuss future developments and merge requests of feature branches into the master branch. On top of this, at each commit we run a series of tests, so as to at best track down bugs. For each project, we fork the master branch and if required implement the novel Hamiltonian. With this organisation, each run can be associated to a commit hash so that one can keep track of the version of the program that has produced the results. This organisation allows us to discuss and develop codes collaboratively, and has proven to be very efficient.

Being a Monte Carlo method, the ALF dumps the bins for a given observable on the disc. Although we have a feature branch aiming at using HDF5 file formats, the open source branch still prints out the data in scientific format. The ALF-library, comes with an independent error analysis suite that reads in the bins and produces final results. The path integral is formulated in imaginary time, so that to make contact with spectroscopic experiments, we have to carry out an analytical continuation. The present ALF-library comes with an implementation of the stochastic Maximum Entropy method[18] to carry out the continuation. This allows us to produce data that can be compared directly with experiment.

It is beyond the scope of this article to provide a detailed account of the ALF project, and the interested reader is referred to the documentation[16] and to our git instance at `http://alf.physik.uni-wuerzburg.de`. Here we will summarise one of the key points, namely the definition of the Hamiltonian on which the program package is based. Of course, the aim is to define a general Hamiltonian which can accommodate a large class of models. Our approach is to express the model as a sum of one-body terms, a sum of two-body terms each written as a perfect square of a one body term, as well as a one-body term coupled to an Ising field with dynamics to be specified by the user. The form of the interaction in terms of sums of perfect squares allows us to use generic forms of discrete approximations to the Hubbard Stratonovitch (HS) transformation.[19, 20] Symmetry considerations are imperative to enhance the speed of the code. We therefore include a *colour* index reflecting an underlying $SU(N)$ colour symmetry as well as a flavour index reflecting the fact that after the HS transformation, the fermionic determinant is block diagonal in this index.

The class of solvable models includes Hamiltonians $\hat{\mathcal{H}}$ that have the following general form:

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_T + \hat{\mathcal{H}}_V + \hat{\mathcal{H}}_I + \hat{\mathcal{H}}_{0,I}, \text{ where} \tag{2}$$

$$\hat{\mathcal{H}}_T = \sum_{k=1}^{M_T} \sum_{\sigma=1}^{N_{\mathrm{col}}} \sum_{s=1}^{N_{\mathrm{fl}}} \sum_{x,y}^{N_{\mathrm{dim}}} \hat{c}^{\dagger}_{x\sigma s} T^{(ks)}_{xy} \hat{c}_{y\sigma s} \equiv \sum_{k=1}^{M_T} \hat{T}^{(k)} \tag{3}$$

$$\hat{\mathcal{H}}_V = \sum_{k=1}^{M_V} U_k \left\{ \sum_{\sigma=1}^{N_{\mathrm{col}}} \sum_{s=1}^{N_{\mathrm{fl}}} \left[\left(\sum_{x,y}^{N_{\mathrm{dim}}} \hat{c}^{\dagger}_{x\sigma s} V^{(ks)}_{xy} \hat{c}_{y\sigma s} \right) + \alpha_{ks} \right] \right\}^2 \equiv \sum_{k=1}^{M_V} U_k \left(\hat{V}^{(k)} \right)^2 \tag{4}$$

$$\hat{\mathcal{H}}_I = \sum_{k=1}^{M_I} \hat{Z}_k \left(\sum_{\sigma=1}^{N_{\mathrm{col}}} \sum_{s=1}^{N_{\mathrm{fl}}} \sum_{x,y}^{N_{\mathrm{dim}}} \hat{c}^{\dagger}_{x\sigma s} I^{(ks)}_{xy} \hat{c}_{y\sigma s} \right) \equiv \sum_{k=1}^{M_I} \hat{Z}_k \hat{I}^{(k)} \tag{5}$$

The indices and symbols have the following meaning:

- The number of fermion *flavours* is set by N_{fl}. After the HS transformation, the action will be block diagonal in the flavour index.

- The number of fermion *colours* is set by N_{col}. The Hamiltonian is invariant under $SU(N_{\mathrm{col}})$ rotations.

- N_{dim} is the total number of spacial vertices: $N_{\mathrm{dim}} = N_{\text{unit cell}} N_{\mathrm{orbital}}$, where $N_{\text{unit cell}}$ is the number of unit cells of the underlying Bravais lattice and N_{orbital} is the number of (spacial) orbitals per unit cell.

- The indices x and y label lattice sites where $x, y = 1, \cdots, N_{\mathrm{dim}}$.

- Therefore, the matrices $\boldsymbol{T}^{(ks)}$, $\boldsymbol{V}^{(ks)}$ and $\boldsymbol{I}^{(ks)}$ are of dimension $N_{\mathrm{dim}} \times N_{\mathrm{dim}}$.

- The number of interaction terms is labelled by M_V and M_I. $M_T > 1$ would allow for a checkerboard decomposition.

- $\hat{c}^{\dagger}_{y\sigma s}$ is a second quantised operator that creates an electron in a Wannier state centred around lattice site y, with colour σ, and flavour index s. The operators satisfy the anti-commutation relations:

$$\left\{\hat{c}^{\dagger}_{y\sigma s}, \hat{c}_{y'\sigma' s'}\right\} = \delta_{x,x'}\delta_{s,s'}\delta_{\sigma,\sigma'}, \text{ and } \left\{\hat{c}_{y\sigma s}, \hat{c}_{y'\sigma' s'}\right\} = 0 \tag{6}$$

The Ising part of the general Hamiltonian (Eq. 2) is $\hat{\mathcal{H}}_{0,I} + \hat{\mathcal{H}}_I$ and has the following properties:

- $\hat{Z}_k$ is an Ising spin operator which corresponds to the Pauli matrix $\hat{\sigma}_z$. It couples to a general one-body term.

- The dynamics of the Ising spins is given by $\hat{\mathcal{H}}_{0,I}$. This term is not specified here; it has to be specified by the user and becomes relevant when the Monte Carlo update probability is computed in the code.

Note that the matrices $\boldsymbol{T}^{(ks)}$, $\boldsymbol{V}^{(ks)}$ and $\boldsymbol{I}^{(ks)}$ explicitly depend on the flavour index s but not on the colour index σ. The colour index σ only appears in the second quantised operators such that the Hamiltonian is manifestly $SU(N_{\mathrm{col}})$ symmetric. We also require the matrices $\boldsymbol{T}^{(ks)}$, $\boldsymbol{V}^{(ks)}$ and $\boldsymbol{I}^{(ks)}$ to be Hermitian.

We are continuously developing the library. Although the open source public fork only contains single spin flip updates, our git repository for development, includes parallel tempering schemes, global updates, as well as continuous fields. Continuous fields were important so as to implement the long range Coulomb repulsion required to provide a realistic modelling of graphene.[21] Future developments include the implementation of hybrid molecular dynamics, Langevin dynamics as well as imaginary time dependent Hamiltonians.

3 A Case Study: Fractionalisation in a Falicov-Kimball Model

Here we will summarise work that was carried out in collaboration in M. Hohenadler and that was published in Refs. 9, 22. The Falicov-Kimball model is a simplification of the SU(2) Hubbard model in which one of the two fermion flavours acquires an infinite mass. One can generalise this notion to the case of the SU(3) Hubbard model, and the Hamiltonian reads:

$$\hat{H}^{cQ} = -t \sum_{\langle ij \rangle, \sigma} \left(\hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + \text{H.c.} \right) - U \sum_{i} \left(\hat{n}_{i\uparrow} - \tfrac{1}{2} \right) \left(\hat{n}_{i\downarrow} - \tfrac{1}{2} \right) \hat{Q}_i \tag{7}$$

We use the same notation as above, σ runs over the two spin components, and $\hat{Q}_i = \pm 1$ is an Ising variable. Importantly, $\hat{Q}_i$ is a locally conserved quantity $\left[\hat{H}^{cQ}, \hat{Q}_i \right] = 0$ and can be understood as a modulation of the sign of the Hubbard term depending upon the site occupation of the infinite mass third fermion. As it stands, it is highly non-trivial to see that this model has phases where the electron degree of freedom fractionalises into two entities:

$$\hat{c}^{\dagger}_{i\sigma} \mapsto \hat{f}^{\dagger}_{i\sigma} \hat{s}^{z}_{i} \,, \quad \hat{c}_{i\sigma} \mapsto \hat{f}_{i\sigma} \hat{s}^{z}_{i} \tag{8}$$

Here, the so called orthogonal fermion, $\hat{f}^{\dagger}_{i\sigma}$, carries an electron charge as well as a Z_2 charge and the Ising degree of freedom, $\hat{s}^{z}_{i}$, only a Z_2 charge. The composite object, the fermion, possesses the usual quantum numbers. Since the Hilbert space per site consists of a fermion degree of freedom, $\hat{c}^{\dagger}_{i\sigma}$, and the Ising field, $\hat{Q}_i$, the above substitution does not expand the Hilbert space so that no constraint is required. In the orthogonal fermion formulation, we can write the Ising variable as:

$$\hat{Q}_i = \hat{s}^{x}_{i} (-1)^{\sum_\sigma \hat{f}^{\dagger}_{i\sigma} \hat{f}_{i\sigma}} = \hat{s}^{x}_{i} (-1)^{\sum_\sigma \hat{c}^{\dagger}_{i\sigma} \hat{c}_{i\sigma}} \tag{9}$$

where $\hat{f}^{\dagger}_{i\sigma} \hat{f}_{i\sigma} = \hat{c}^{\dagger}_{i\sigma} \hat{c}_{i\sigma}$ follows from Eq. 8. Here, $\hat{s}^{z}_{i}$ and $\hat{s}^{x}_{i}$ are represented by Pauli matrices acting on the Ising spin at site i. Using the identity

$$(-1)^{\sum_\sigma \hat{f}^{\dagger}_{i\sigma} \hat{f}_{i\sigma}} = \prod_{\sigma} (2 \hat{n}_{i\sigma} - 1) \tag{10}$$

we can rewrite Eq. 7 as

$$\hat{H}^{fs} = -t \sum_{\langle ij \rangle, \sigma} \left(\hat{f}^{\dagger}_{i\sigma} \hat{f}_{j\sigma} \hat{s}^{z}_{i} \hat{s}^{z}_{j} + \text{H.c.} \right) - \frac{U}{4} \sum_{i} \hat{s}^{x}_{i} \tag{11}$$

Finally, one can explicitly check that $\left[\hat{H}^{fs}, \hat{Q}_i \right] = 0$ so that $\hat{H}^{fs}$ and $\hat{H}^{cQ}$ are dual. The above Hamiltonian is not amenable to simulations with the ALF library and a further transformation has to be carried out. Consider the bond variable

$$\hat{s}^{z}_{i} \hat{s}^{z}_{j} \mapsto \hat{Z}_{ij} \tag{12}$$

Because a spin flip on a single site i under the action of $\hat{s}^{x}_{i}$ affects all four bond variables, the dual representation involves a so-called star operator,

$$\hat{s}^{x}_{i} \mapsto \hat{X}_{i,i+x} \hat{X}^{x}_{i,i-x} \hat{X}^{x}_{i,i+y} \hat{X}^{x}_{i,i-y} \tag{13}$$

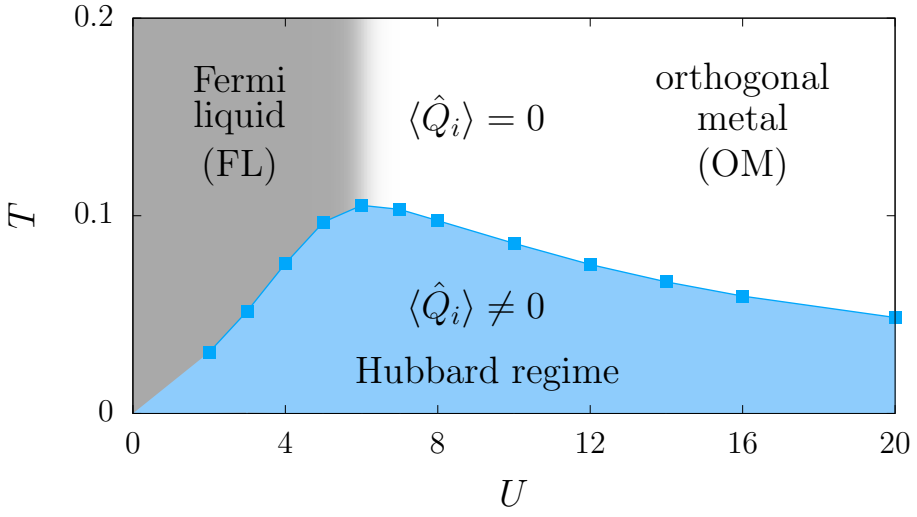

Figure 1. Phase diagram of the dual Hamiltonians (Eqs. 7, 11, and 14). A phase transition of the Ising variables $\hat{Q}_i$ at T_Q separates the low-temperature Hubbard regime from the high-temperature phase. Here, T_Q was determined from data for $L = 8$, see Ref. 22. The two metallic regimes at $T > T_Q$ appear to be separated by a crossover, as indicated by the colour gradient. Adapted from Ref. 9.

where $i \pm \alpha$ is a compact notation for the site at $\boldsymbol{r}_i \pm \hat{e}_\alpha$ and $\hat{X}$, $\hat{Z}$ corresponds to the x- and y-Pauli matrices acting on the bond variables. These steps lead to the Hamiltonian

$$\hat{H}^{fZ} = -t \sum_{\langle ij \rangle, \sigma} \left(\hat{f}^\dagger_{i\sigma} \hat{f}_{j\sigma} + \text{H.c.} \right) \hat{Z}_{ij} - \frac{U}{4} \sum_i \hat{Z}_{i,i+x} \hat{Z}_{i,i-x} \hat{Z}_{i,i+y} \hat{Z}_{i,i-y} \tag{14}$$

This Hamiltonian (Eq. 14) with bond Ising variables takes the form familiar of Ising lattice gauge theories coupled to matter. Here, there are important differences that lead to the unique properties of the phase diagram. Firstly, in Ising lattice gauge theories the Gauss law $\hat{Q}_i = \pm 1$ is imposed. Secondly, since $\hat{Z}_{i,i+y} \mapsto \hat{s}^z_i \hat{s}^z_j$ visons (a π-fluxes of the Z_2 field) are absent. In the above formulation, the model can be simulated with the ALF-library without encountering the negative sign problem.

The phase diagram of the model is plotted in Fig. 1 and contains three phases that one can understand very transparently when considering the slave spin formulation. Since $\hat{Q}_i$ commutes with the Hamiltonian, we expect this Ising variable to show a finite temperature transition akin to the two dimensional Ising universality class. Below the transition temperature $\hat{Q}_i$ orders ferromagnetically, such that at $T = 0$ we can replace $\hat{Q}_i$ by unity in Eq. 7 and recover the physics of the generic half-filled Hubbard model. At $U = 0$, the Ising field $\hat{Z}_{ij}$ has no quantum fluctuations, and with the vison-less constraint, $\hat{Z}_{i,i+a_x} \hat{Z}_{i+a_x,i+a_x+a_y} \hat{Z}_{i+a_x+a_y,i+a_y} \hat{Z}_{i+a_y,i} = 1$, one can show with a gauge transformation that any Ising bond configuration will be equivalent to the choice $\hat{Z}_{i,j} = 1$, or equivalently to the choice $\hat{s}^z_i = 1$. The model then reduces to a simple Fermi liquid. At finite values of U above Ising transition temperature, one cannot solve the model exactly,

but one can carry out educated guesses based on a mean-field analysis that breaks the local Z_2 symmetry inherent to the model.[23] At weak coupling, we can set $\langle \hat{s}_i^z \rangle = s > 0$ and $\langle \hat{s}_i^x \rangle = 0$ such that we recover the Fermi liquid state. On the other hand, at strong coupling, temporal fluctuations of the Ising field will be quick such that we expect the Ising correlations to decay exponentially in time and space, but the short ranged ones to remain finite. In a mean field picture we would hence set $\langle \hat{s}_i^z \rangle = 0$ but $\langle \hat{s}_i^z \hat{s}_{i+a_x}^z \rangle > 0$. Fractionalisation of the electron into an orthogonal fermion and a Z_2 field means that it can propagate coherently – in this mean-field vertex free picture – only if both constituents have a coherent propagation. Hence, in the disordered state of the Ising variable, the physical electron is localised and the single particle spectral shows no Fermi surface. Consider on the other hand a charge degree of freedom. The propagation of such an electron-hole pair does not depend on the coherent motion of the Z_2 field. Hence, charge fluctuations are gapless.

Our numerical calculations published in Refs. 9, 22 confirm the above mean field picture of the orthogonal metallic state in the Falicov-Kimball model. Seen from the perspective of particle-hole quantities the OM is a metallic (not superconducting) state. Seen from the perspective of the single particle, it is an insulator. Showing that this state of matter can emerge in a Falikov-Kimball model is one of the highlights of the work we recently carried out using the computational resources at the NIC.

4 Conclusions

The ALF implementation of the auxiliary field quantum Monte Carlo method provides us with a very flexible tool to simulate a variety of correlated electron systems. In the future, we will further develop this library and place emphasis on alternative sampling methods such as Hybrid Monte Carlo and Langevin dynamics as well as on time dependent Hamiltonians. The ALF-library and the associated git repository provide a documented and collaborative program development. It also allows to easily reproduce data since the output of each run includes the commit hash. As it stands, we have no efficient collaborative means to analyse the data of runs, and this is taken care of at the user level. Clearly each user stores data on tapes, but the access becomes very slow. Each run produces GBs of data in the forms of Monte Carlo bins such that a project cumulates to several TBs. Disc space is in principle not an issue but the challenge lies in defining the meta data as well as efficient tools that will allow us to navigate and search data bases and reanalyse, if required, the Monte Carlo time series. Such efforts will be pursued in the future. The pool of applications is very big. It ranges from toy models that capture interesting concepts such as fractionalisation, as described above, to realistic modelling of many body systems. In fact within the ALF-library we are able to consider long range Coulomb interactions,[21] a necessity for an accurate description of graphene. Furthermore, we are able to simulate very general spin systems embedded in a metallic environment.[24] This allows us to provide numerical support for a variety of magnetic nano-systems grown on metallic surfaces.[25, 26]

Acknowledgements

This work is a group effort. I would like to thank Martin Bercx, Florian Goth, Johannes Hofmann, and Jonas Schwab for the development of the ALF-Library and discussions, as

well as Stefan Beyl, Bimla Danu, Martin Hohenadler, Emilie Huffman, Yuhai Liu, Marcin Raczkowski, Toshihiro Sato, Francesco Parisen Toldin, Maksim Ulybyshev, and Zhenjiu Wang for many applications. We gratefully acknowledge the Gauss Centre for Supercomputing e.V. (`www.gauss-centre.eu`) for funding this project by providing computing time through the John von Neumann Institute for Computing (NIC) on the GCS Supercomputer JUWELS at Jülich Supercomputing Centre (JSC). We thank the DFG for financial support through the FOR 1807, SFB 1170 as well as through the Würzburg-Dresden Cluster of Excellence on Complexity and Topology in Quantum Matter - ct.qmat (EXC 2147, project-id 39085490). Finally we thank KONWIRH (Competence Network for Technical, Scientific High Performance Computing in Bavaria) for providing seed funding that enabled us to start the ALF project and secure further support from the DFG Scientific Library Services and Information Systems (LIS) program under the grant number AS 120/14-1.

References

1. R. Blankenbecler, D. J. Scalapino, and R. L. Sugar, *Monte Carlo calculations of coupled boson-fermion systems.*, Phys. Rev. D **24**, 2278–2286, 1981.
2. C. Wu and S.-C. Zhang, *Sufficient condition for absence of the sign problem in the fermionic quantum Monte Carlo algorithm*, Phys. Rev. B **71**, 155115, 2005.
3. E. Fulton Huffman and S. Chandrasekharan, *Solution to sign problems in half-filled spin-polarized electronic systems*, Phys. Rev. B **89**, 111101, 2014.
4. Z.-X. Li, Y.-F. Jiang, and H. Yao, *Majorana-Time-Reversal Symmetries: A Fundamental Principle for Sign-Problem-Free Quantum Monte Carlo Simulations*, Phys. Rev. Lett. **117**, 267002, 2016.
5. Z. C. Wei, C. Wu, Y. Li, S. Zhang, and T. Xiang, *Majorana Positivity and the Fermion Sign Problem of Quantum Monte Carlo Simulations*, Phys. Rev. Lett. **116**, 250601, 2016.
6. F. F. Assaad and T. Grover, *Simple Fermionic Model of Deconfined Phases and Phase Transitions*, Phys. Rev. X **6**, 041049, 2016.
7. T. Sato, M. Hohenadler, and F. F. Assaad, *Dirac Fermions with Competing Orders: Non-Landau Transition with Emergent Symmetry*, Phys. Rev. Lett. **119**, 197203, 2017.
8. S. Gazit, F. F. Assaad, S. Sachdev, A. Vishwanath, and C. Wang, *Confinement transition of Z2 gauge theories coupled to massless fermions: Emergent quantum chromodynamics and SO(5) symmetry*, Proceedings of the National Academy of Sciences **115(30)**, E6987-E6995, 2018.
9. M. Hohenadler and F. F. Assaad, *Fractionalized Metal in a Falicov-Kimball Model*, Phys. Rev. Lett. **121**, 086601, 2018.
10. Y. Liu, Z. Wang, T. Sato, M. Hohenadler, C. Wang, W. Guo, and F. F. Assaad, *Superconductivity from the condensation of topological defects in a quantum spin-Hall insulator*, Nature Communications **10**, 2658, 2019.
11. E. Witten, *A New Look At The Path Integral Of Quantum Mechanics*, 2010, arXiv:1009.6032 [hep-th].
12. E. Witten, *Analytic Continuation Of Chern-Simons Theory*, 2010, arXiv:1001.2933 [hep-th].

13. M. Ulybyshev, C. Winterowd, and S. Zafeiropoulos, *Taming the sign problem of the finite density Hubbard model via Lefschetz thimbles*, 2019, arXiv:1906.02726 [cond-mat.str-el].
14. M. Ulybyshev, C. Winterowd, and S. Zafeiropoulos, *Lefschetz thimbles decomposition for the Hubbard model on the hexagonal lattice*, 2019, arXiv:1906.07678 [cond-mat.str-el].
15. M. Bercx, J. S. Hofmann, F. F. Assaad, and T. C. Lang, *Spontaneous particle-hole symmetry breaking of correlated fermions on the Lieb lattice*, Phys. Rev. B **95**, 035108, 2017.
16. M. Bercx, F. Goth, J. S. Hofmann, and F. F. Assaad, *The ALF (Algorithms for Lattice Fermions) project release 1.0. Documentation for the auxiliary field quantum Monte Carlo code*, SciPost Phys. **3**, 013, 2017.
17. X. Y. Xu, Y. Qi, J. Liu, L. Fu, and Z. Y. Meng, *Self-learning quantum Monte Carlo method in interacting fermion systems*, Phys. Rev. B **96**, 041119, 2017.
18. K. S. D. Beach, *Identifying the maximum entropy method as a special limit of stochastic analytic continuation*, 2004, arXiv:cond-mat/0403055.
19. Y. Motome and M. Imada, *A Quantum Monte Carlo Method and Its Applications to Multi-Orbital Hubbard Models*, Journal of the Physical Society of Japan **66**, 1872–1875, 1997.
20. F. F. Assaad, M. Imada, and D. J. Scalapino, *Charge and spin structures of a $d_{x^2-y^2}$ superconductor in the proximity of an antiferromagnetic Mott insulator*, Phys. Rev. B **56**, 15001–15014, 1997.
21. H.-K. 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**, 570–574, 2018.
22. M. Hohenadler and F. F. Assaad, *Orthogonal metal in the Hubbard model with liberated slave spins*, Phys. Rev. B **100**, 125133, 2019.
23. R. Nandkishore, M. A. Metlitski, and T. Senthil, *Orthogonal metals: The simplest non-Fermi liquids*, Phys. Rev. B **86**, 045128, 2012.
24. T. Sato, F. F. Assaad, and T. Grover, *Quantum Monte Carlo Simulation of Frustrated Kondo Lattice Models*, Phys. Rev. Lett. **120**, 107201, 2018.
25. M. Raczkowski and F. F. Assaad, *Emergent Coherent Lattice Behavior in Kondo Nanosystems*, Phys. Rev. Lett. **122**, 097203, 2019.
26. B. Danu, F. F. Assaad, and F. Mila, *Exploring the Kondo effect of an extended impurity with chains of Co adatoms in a magnetic field*, Phys. Rev. Lett. **123**, 176601, 2019.