Some recent advances in numerical algorithms for quantum many body problems

Simulation of interacting fermions with entanglement renormalization
P. Corboz, G. Evenbly, F. Verstraete, and G. Vidal
arXiv:0904.415

Fermionic Projected Entangled Pair States
C.V. Kraus, N. Schuch, F. Verstraete, J.I. Cirac
arXiv:0904.4667

Fermionic multi-scale entanglement renormalization ansatz
P. Corboz and G. Vidal
arXiv:0907.3184

Recommended with a Commentary by Matthias Troyer, ETH Zürich

Numerical simulations play a crucial role in the investigation of strongly interaction quantum many body systems. While analytical approaches, such as mean-field studies or perturbative methods can give insight into possible phases and their properties, numerical simulations are often essential in confirming the existence of exotic phases, establishing accurate phase diagrams and the nature of phases and phase transitions.

While for quasi- one dimensional systems such as chains or ladders consisting of a few coupled chains, the density matrix renormalization group method (DMRG) provides a reliable and accurate method to calculate static and dynamic properties, no such universal method exists in two and higher dimensions. Quantum Monte Carlo (QMC) simulations work amazingly well for bosonic models and unfrustrated quantum magnets, but in the case of fermions they suffer from the "negative sign problem": negative weights in the Monte Carlo sampling causing an exponential scaling of the computational complexity with system size. While there has been recent progress in QMC methods for fermions, this shall be left for another commentary.

The papers recommended here are on another approach: generalizations of DMRG to fermionic models in two dimensions. While DMRG works extremely well in one dimension, the straight-forward application to higher dimensions has remained limited due to an exponential growth of the complexity with the width of the system. DMRG can be understood as a variational method operating on *matrix product states* (MPS): an $M \times M$ matrix $A^{(i)}[\sigma_i]$, whose entries depend on the local state $|\sigma_i\rangle$, is associated with each lattice site, and the two indices of the matrix connect to the neighbors, leading to an ansatz wave function:

$$\sum_{\alpha_1,\ldots,\alpha_N} A^{(1)}_{\alpha_N\alpha_1}[\sigma_1]A^{(2)}_{\alpha_1\alpha_2}[\sigma_2]\cdots A^{(N)}_{\alpha_{N-1}\alpha_N}[\sigma_N]|\sigma_1,\sigma_2,\ldots,\sigma_N\rangle. \qquad (1)$$

Over the past years insights from quantum information theory have led to an understanding of the success of DMRG and the MPS ansatz wave function in terms of entanglement of the ground state. It can be regarded as a low-entanglement ansatz for the ground state: the entanglement that can be encoded is bounded by $S \leq \log M$. Since for one-dimensional systems the entanglement grows at most logarithmically with system size, a small number of states M is sufficient to make DMRG extremely accurate.

In two dimensions, however, the entanglement entropy usually follows an area law and grows proportional to the cross section A of the system: $S \sim A$ and hence an exponential number of states $M \sim \exp A$ is needed. With this insight in mind, the solution to the entanglement scaling problem is to find an ansatz that is not a one-dimensional chain like the matrix product states but a two-dimensional network built from higher-ranked tensors instead of matrices – similar to the *spin networks* invented by Penrose in 1971 and used in the context of loop quantum gravity. Such ansatz wave functions have appeared in various proposals over the past decade. First suggested by G. Sierra and M. A. Martin-Delgado under the name of vertex matrix product ansatz and published in a conference proceedings [arXiv:cond-mat/9811170] and used by T. Nishino for classical systems, the method became popular when it was reinvented by Verstraete and Cirac [arXiv:cond-mat/0407066] under the name of *projected entangled-pair states* (PEPS). A related proposal building on real-space renormalization ideas and tree-like tensor networks, called *multiscale entanglement renormalization ansatz* (MERA), has been proposed by G. Vidal [Phys. Rev. Lett. **99**, 220405 (2007)].

The papers recommended here are recent generalizations of these methods to fermions. Unlike in one-dimensional DMRG calculations where the extension to fermions is trivial, fermions in two dimensions cannot be as easily mapped to bosons. The papers by Corboz *et al.* present a fermionic version of MERA. In their first paper fermionic statistics is taken into account using a Jordan-Wigner transformation and counting the number of fermionic permutations needed for every fermion that hops on the lattice, while the second paper offers a conceptually simpler way of contracting the tensor directly taking into account fermionic statistics.

The other proposal by Kraus *et al.* uses a PEPS ansatz built from fermionic degrees of freedom. In bosonic PEPS each of the M states on a bond between two sites can be viewed as a maximally entangled state of two auxiliary spins on each of the sites. In fermionic PEPS (fPEPS) these auxiliary spins are replaced by fermions, which automatically anti-symmetrizes the many-body fermionic wave function.

Both methods promise the chance to finally study two-dimensional fermionic systems, including the two-dimensional Hubbard model, using a method without uncontrolled approximations – in the limit $M \to \infty$ these methods accurately describe any physically relevant quantum state. Have we finally found a way to solve two-dimensional strongly correlated fermion systems? Unlike DMRG which has been shown to be accurate in one dimension, these methods are still mostly uncharted territory. There are two important open questions: can

interesting states of strongly correlated systems be well described by such tensor network states with low dimensions M? If the answer is yes, are there efficient algorithms to compute those states? Current implementations scale with a high power of M, such as about M^{12} for PEPS or M^{16} for two-dimensional MERA, restricting simulations to low values of M, e.g. $M \approx 5$ in a PEPS simulation. This seems small compared to DMRG where typically $M = 100 \ldots 1000$ is used, but a rank-4 tensor has more degrees of freedom than a matrix. One can further argue that two-dimensional systems should be more mean-field like than one-dimensional systems and for a mean-field product state $M = 1$ is sufficient.

While there may be doubts or optimism, the only way to really tell the accuracy of these algorithms is to perform benchmark simulations on known problems and see where they excel and where problems appear. Both PEPS and MERA have been shown to work extremely well for the transverse field Ising model, other models with discrete symmetries. They correctly predict the first-order nature of the superfluid to solid transition for hard-core boson models on a square lattice [arXiv:0905.4880] – without an intervening supersolid phase that is incorrectly seen in mean-field calculations. However, for Heisenberg models with SU(2) symmetry PEPS is less accurate: while the energies are still pretty good the magnetization of the square lattice antiferromagnet is off by about 10%. It is unclear whether this is due to inefficient algorithms that fail to find the optimal tensor network state, or if much larger dimensions M are needed for models with continuous symmetries.

The fermionic methods are much less tested. Corboz *et al.* present benchmark results for non-interacting spinless fermions, and some results with interactions. Ground state energies come out accurately to up to six digits! However, there are few results for correlation functions, which are much harder to get right in any variational method. Whether the new fermionic algorithms will be able to solve the phase diagram of the Hubbard model is thus still an open question. One will have to be careful not to jump straight to the most ambitious problems without learning more about strengths, limitations and potential pitfalls of these methods first.

While the final verdict is still undecided, especially in the case of the new fermionic algorithms, one might be cautiously optimistic. These new algorithms are definitely interesting and they work well for models with little entanglement in the ground state wave function. What this means in terms of physical properties is still unclear – we are not yet used to classifying states according to their entanglement properties. The algorithms to contract, evaluate and optimize the tensor networks are also still in their infancy. Substantial improvements are certainly possibly and new ideas are being brought up every month, such as a combination with variational Monte Carlo to reduce the complexity of the tensor contractions, or new variants of tensor networks like the tensor renormalization group method. I can only reiterate the final sentence Steve White wrote in a commentary about the original PEPS paper several years ago: "Perhaps the holy grail, reliable, accurate, and unbiased simulations of large 2D fermion clusters, is coming within reach!"