Progress in Diagrammatic Monte Carlo Methods for Quantum Field Theories in Particle-, Nuclear-, and Condensed Matter Physics

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Monte Carlo simulations are among the most powerful tools for obtaining non-perturbative results in quantum field theories. They are used for a wide range of applications in particle-, nuclear-, and condensed matter physics. In these different fields of physics applications, Monte Carlo techniques developed significantly in recent years. With new ideas like rewriting the systems in terms of new degrees of freedom, serious challenges were overcome such as problems related to the sign problem. Exchanging ideas and discussing the new Monte Carlo approaches used in the various communities will certainly speed up the development of the new techniques. More specifically, the central goal of the scientific program was to explore recent advances in Monte Carlo methods, especially those that use the Monte Carlo sampling of diagrams. The specific topics covered were organized in the following fields: (i) techniques for fermions, (ii) weak coupling diagrammatic Monte Carlo, (iii) dual variables in lattice field theories, (iv) tensor networks, (v) special topics.

Different formats for structuring the scientific program were used: conventional lectures, tutorial lectures, moderated discussions as well as a poster session. In addition, there was ample time for discussions and work in smaller groups. To make sure that all areas of interest were met in our scientific program, an opening discussion at the beginning of each of the two weeks took place in which the participants chose the relevant scientific topics.

In the context of techniques for fermions, Uwe-Jens Wiese led a moderated discussion on the significance of the sign problem. It also dealt with the question whether it is really a problem for general fermionic systems. He tried to clarify his work in which they had claimed that the problem was considered to be NP hard.

Based on diagrammatic Monte Carlo methods, Nikolay Prokofiev argued that general fermionic systems can be solved in polynomial time, although success seemed to depend on the convergence of the diagrammatic series. The conclusion was that the sign problem in Monte Carlo methods sampling the partition function may be qualitatively different from those in diagrammatic Monte Carlo methods sampling the effective action.

Shailesh Chandrasekharan gave two tutorial type lectures on the fermion bag approach. He discussed how the idea is based on rewriting the fermionic path integral in the lattice

Lagrangian approach, namely as a sum over fermion world lines and then regrouping the sum differently than it is traditionally done. He discussed how this approach could be combined with the world line approach for bosons to solve new sign problems. He then showed how these ideas could also be extended to lattice Hamiltonian formulations. He argued that this extension leads to fermion algorithms which are faster than conventional methods.

Timo Lähde gave an overview of recent advances in Monte Carlo methods for graphene and carbon nanotubes. This led to some lively discussions, as there were several others in the workshop also working on auxiliary field simulations of graphene. He discussed the advantages of the hexagonal lattice simulations, the incorporation of physical lattice effects, and the difference between Hubbard-like interactions and Coulomb interactions. Calculations are now underway to determine the energy gap in carbon nanotubes with radii up to 1 nanometer.

Fakher Assaad led a discussion on fermion algorithms. He presented some of his recent results and thoughts on the comparison between hybrid Monte Carlo (HMC) and the auxiliary field Monte Carlo (AFMC) methods. He concluded that while the HMC method scales well for a class of problems, the AFMC continues to perform better for another class of problems - at least for lattice sizes that are currently studied. While electron-phonon models fall in the former class, Hubbard models seem to fall in the latter class. Assaad later also led a discussion on the recent excitement related to phase diagrams in 2+1 dimensional Dirac systems. Using a specific example, he explained that there are new predictions of non-Landau type second order phase transitions between phases with two different mass order parameters. These transitions are related to the presence of topological terms in the action. Later, Toshihiro Sato presented specific results in a conventional talk entitled Dirac fermions with competing mass terms and emergent symmetry.

In the framework of weak coupling diagrammatic Monte Carlo, Boris Svistunov discussed the Bose-Hubbard system tuned to the Wilson-Fisher fixed point with a single-site impurity potential. Since the impurity potential is varied, the number of particles localized by the impurity relative to the uniform background is typically an integer number. However, worm algorithm simulations show that there is a special point at which the number of localized particles is a half integer. This feature is called a halon, a polaron with half-integer charge.

Pavel Buividovich gave a talk entitled diagrammatic Monte-Carlo for non-abelian lattice field theory at weak coupling. He outlined the strategies and techniques for setting up the diagrammatic Monte Carlo approach in the weak-coupling regime. The talk discussed simple examples in detail so that not only Pavel's work, but also the method itself became clear to a broader audience. This turned out to be very helpful for appreciating the talks by Nikolay Prokofiev and Felix Werner. They gave two back-to-back blackboard talks on dealing with the sign problems through diagrammatic Monte Carlo evaluations of the perturbative series in the thermodynamic limit.

One of the significant new developments was an algorithm to sum all connected diagrams for fixed positions of the vertices by Riccardo Rossi. Prokofiev gave some computational time estimates for reaching set error tolerances under some general assumptions about diagrammatic convergence, and Werner discussed the resummation of divergent series and the large-order behavior of diagram amplitudes. Markus Wallerberger gave a tutorial talk in which he explained how one can convert many interesting quantum many-body problems into a quantum impurity problem and solve the quantum impurity problem using diagrammatic Monte Carlo methods. Approximations such as the dynamical mean field theory (DMFT) are based on this connection. Wallerberger also discussed some limitations of the method.

Falk Bruckmann, Christof Gattringer and Tin Sulejmanpasic organized a moderated discussion entitled sign problems from topological terms. The first part of this session was used to outline the strategy for mapping lattice field theories to a dual representation in terms of world lines and world sheets. The role of topological terms in relativistic quantum field theories was discussed by comparing this role to the one in quantum field theories in condensed matter theory. In the second part examples were discussed in which the complex action problem from the topological term is overcome by a dualization. Bruckmann gave a talk entitled dual variables in O(N) / CP(N-1) and in QCD with scalar quarks. For the two spin models, dualizations in terms of worldlines were presented which allow for a Monte Carlo simulation at arbitrary values of the chemical potential. The representation is correct at all orders of the strong coupling expansion. For QCD with scalar quarks only the leading terms of the strong coupling expansion are accessible but hopefully these terms already reveal some of the structure expected for non-abelian gauge theories coupled to matter fields.

Maria-Carmen Banuls and Roman Orus gave two pedagogical reviews on tensor network theory. Banuls focused on basics and introduced the concepts that go into the construction of tensor network states. Ideas of matrix product states and connections to density matrix renormalization group (DMRG) were introduced. Banuls also discussed an application of the method to the Schwinger Model, the simplest model example of lattice gauge theory. Orus then discussed extensions to higher dimensions, especially focusing on projected entangled pairs (PEP) and on multiscale entanglement renormalization ansatz (MERA). In the afternoon Maria-Carmen Banuls and Roman Orus led another discussion session where attempts were made to synthesize the lectures and make connections with other approaches like quantum Monte Carlo methods. An interesting question that came up was whether there was a way to combine the two ideas. It was pointed out that the loop cluster algorithm for quantum spin systems precisely accomplishes this connection. In terms of physics, questions about the lattice Schwinger model and the need to explore two different mass terms were discussed.

Anders Sandvik analyzed some recent developments in computing time correlations and spectral functions, going beyond the usual maximum entropy approach. He discussed the stochastic analytic continuation method which includes a sampling temperature, but encounters problems when configurational entropy becomes dominant. He then presented an improved stochastic analytic continuation method that can incorporate sharp edge features in the spectrum by using a distribution of delta functions with equal weight. Dean Lee gave a tutorial on lattice effective field theory simulations relevant for few-body systems. The topics discussed were the implementation of chiral effective field theory at leading order on the lattice, the adiabatic projection method for scattering and reactions, and the pinhole method for calculations of density distributions.

Ribhu Kaul presented a tutorial lecture on deconfined critical points. He argued that such points were more ubiquitous than earlier thought and were related to topological excitations that arise naturally in quantum systems. He later gave a more conventional talk on the physics of critical points in quantum spin systems, especially spin-one systems, relating them to CP(N-1)models. Tin Sulejmanpasic gave a talk in which he explained how some of the physics of quantum spin systems were related to anomalies in gauge theories through ‘t Hooft’s anomaly matching conditions. Thomas Lang presented an overview of the recent applications of machine learning to quantum many body physics. He explained that while the method was promising, there were also many hurdles to overcome before it could be used as a viable alternative to quantum Monte Carlo methods.

The poster session was held on Wednesday of the second week and the following posters were presented: Stefan Beyl, revisiting the hybrid quantum Monte Carlo method for Hubbard and electron-phonon models; Mario Giuliani, condensation thresholds and scattering data; Daniel Göschl, worldline simulation of the Schwinger model; Emilie Huffman, fermion bag approach to Hamiltonian lattice field theories in continuous time; Carla Marchis, a test for dynamical stabilization in complex Langevin simulations: the XY-model; Francesco Parisen Tolden, Entanglement properties of the Hubbard chain model; Zhenjiu Wang, spin and valence bond dynamics across a DQCP in a fermionic SU(3) Model; Manuel Weber, directed-loop quantum Monte Carlo method for retarded interactions; Savvas Zafeiropoulus, Complex Langevin simulations of a finite density matrix model for QCD.

The scientific program successfully fostered of fostering the exchange of methods and techniques in the area of diagrammatic Monte Carlo among the three communities represented at the scientific program, high energy physics, nuclear physics and condensed matter.