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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. 43.
http://hdl.handle.net/2128/24435

Heavy Quarks, Multi-Level Algorithms and Tensor Networks: Developing Methods for Non-Perturbative Aspects of Quantum Field Theories

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The particle physics group at the John von Neumann Institute for Computing (NIC) is concerned with quantum field theories, in particular with their non-perturbative aspects. Here we describe recent efforts of the group to develop and consolidate methods and concepts to reach the goal to understand non-perturbative phenomena in quantum field theories and to calculate observables with a high precision.

1 Introduction

The group covers a large range of topics, from the exploration of new strategies to treat quantum field theories non-perturbatively (Tensor networks, quantum computations) to the development of ever more efficient algorithms for Markov chain Monte Carlo to high precision applications concerning the determination of fundamental parameters of QCD, the muon anomalous magnetic moment, or weak decays of hadrons. In this contribution we give a short summary of recent work on three subjects: Tensor network methods, multilevel Monte Carlo and heavy sea quarks (quantum effects of heavy quarks).

2 Tensor Network Methods

Nowadays, the path integral is clearly the method of choice to evaluate lattice quantum field theories (LQFT). Still, in the beginning of LQFT it has been the Hamiltonian formalism which was used frequently. In practice, this approach was abandoned, due to the untractably large size of the Hilbert space. However, it has been realised in the last years that it is only a small set of all possible states which is relevant to obtain ground state properties. This small corner of the Hilbert space is build by states which obey the so called area law. These states can, in general, be constructed through tensor network states which become matrix product states (MPS) in one dimension. In this approach, the very high dimensional coefficient tensor needed in the Hamilton formalism is replaced by a product of complex matrices. By systematically increasing the size of these matrices and computing their entries through a variational method, minimising the energy as a cost function, ground state properties can be computed very precisely. In fact, mathematical theorems state that this procedure converges exponentially fast to the ground state of the considered Hamiltonian. In practice, the size of the used matrices are of order 100 which make such computations completely feasible and tensor networks have been used for condensed matter systems very successfully, see *e. g.* Ref. 1 for an introduction into tensor network techniques.

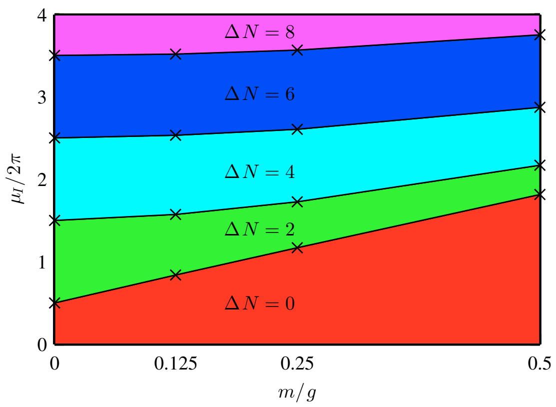

Figure 1. Phase diagram in the m/g - $\mu_I/2\pi$ plane with m denoting the fermion mass, g the coupling and μ_I the chemical potential. The black X's mark the computed data points, the different colours indicate the different phases.

As one of the first, the NIC group has adapted this approach of the Hamilton formalism using MPS for models in high energy physics, see Ref. 2 for a recent review. Since the Hamilton formalism is free of the sign problem, it offers the exciting possibility to study, in principle, questions where conventional Monte Carlo (MC) methods fail and which include non-zero baryon density as relevant for understanding the early universe; topological terms for the matter anti-matter asymmetry and real time evolutions of physical systems.

By computing the low-lying particle spectrum of the Schwinger model,[3] which has one space dimension, as a benchmark, a proof of principle could be provided that MPS can be used also for gauge theories. Followed by a calculation in this model at non-zero temperature,[4] the Schwinger model for two flavours of fermions was studied with a non-zero (isospin) chemical potential.[5] Addressing this question by conventional Monte Carlo methods is impossible due to a severe sign problem. It has therefore been very important to test, whether MPS can overcome this difficulty, or, whether the sign problem re-appears in a different way. Indeed, it was shown that the technique of MPS performs very well also in the situation with a non-zero chemical potential. Working first with a zero fermion mass, MPS results could be confronted with an analytically known expression and a complete agreement was found, demonstrating that MPS solves the problem of a non-zero chemical potential. Switching on a fermion mass, the phase diagram in the plane of chemical potential and fermion mass could be established,[5] see Fig. 1. Here no analytical result is available and only the usage of MPS made it possible to obtain this phase diagram making MPS or tensor networks the most promising tool to address important and so far intractable problems in high energy physics. Tensor network techniques were also used for non-abelian theories[6] and for studying the Schwinger model in presence of a topological term.[7] Still, a warning is in order since the computational cost of calculations for higher than one (space) dimension is presently too large to study systems of realistic size. However, there is a substantial amount of research ongoing to find better techniques for high dimensions as discussed in a recent workshop[a] co-organised by the NIC group. There, sev-

[a] `https://indico.desy.de/indico/event/21941/overview`

eral new ideas were presented which have the potential to make tensor networks practical also in higher dimensions.

3 Towards Multilevel Monte Carlo Methods for QCD

In this section we directly consider three space dimensions and remain within the framework of Monte-Carlo importance sampling methods for lattice field theory computations. In this framework, a major obstacle to progress is the deterioration of the signal of n-point correlation functions with increasing distance of these points. Large distances are needed to effectively study the ground state properties of the theory. Since lattice computations employ Monte Carlo sampling, uncertainties decrease with the inverse square root of the number of measurements – an expensive technique in the face of a noisy signal. By using the locality of the underlying theory, and designing algorithms where this fundamental property is manifest even in the presence of fermions, sampling strategies can be devised which have an improved convergence: depending on the number of regions, a convergence with the inverse number of measurements, or even a higher power becomes possible.

Such methods have been available since some time for pure gauge theory, where the formulation is manifestly local and also observables are typically easily decomposed into products of local contributions.[8, 9] Each of these local components can then be averaged over independently, leading to an exponential speed-up in the size of the observable.

Fermions are fundamentally different from bosons. They are integrated out analytically before formulating the Monte Carlo and thus lead to non-local contributions. Using domain decomposition techniques, we managed to propose a strategy that these multilevel methods become amenable to theories with fermions.[10, 11] In order to achieve this, the hadronic two-point functions as well as the contributions from the fermion sea to the path integral had to be factorised, such that the independent averages of each of the factors can be taken.

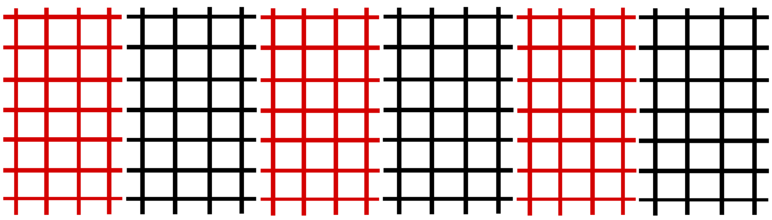

Figure 2. One-dimensional decomposition of the lattice into regions. If the thickness of the black regions is chosen sufficiently large, the red regions can be updated independently.

Contrary to the pure gauge case, the regions in which the independent updates are performed need to be separated by a certain distance, given by the correlation length (the inverse of the pion's mass). An illustration of the geometry is found in Fig. 2, where one envisions independent updates in the red regions, with the field variables in the black regions kept fixed. If one thinks of fermionic contributions in terms of paths on the lattice, it is obvious that as long as the quark does not travel between the red regions forth and back, such a path is trivially factorised in contributions which can be associated to a single red region, together with the neighbouring black ones. Since longer paths typically contribute less than shorter ones, good approximations can be found which fulfil this property.

It becomes more difficult once we have to consider quark loops, as is necessary for the determinant. Here we managed to rewrite the corresponding terms using integrals over scalar fields, an idea which has already been used in the multiboson algorithm[12] and could demonstrate that the idea works in dynamical simulations.

Ordinary Monte Carlo simulations lead to uncertainties which are reduced with the inverse square root of the number of measurements $1/\sqrt{N}$. In the ideal case, for updates in n independent regions, such a method leads to a scaling with $1/N^{n/2}$. However, as we have seen, for fermions such regions will have to be sufficiently thick in order to profit from this technique. It needs to be seen if for a given observable a decomposition into sufficiently many regions can be found to profit from this algorithm.

4 Effects of Heavy Fermions on Low-Energy Physics and High-Energy Strong Coupling

The discretisation of space-time on a regular lattice leads to a Brilloin zone just like in crystals. Thus the high momentum, high energy behaviour is distorted. Also particles with large masses can't be simulated properly. For this reason lattice simulations include up, down and strange quarks, while the bottom and top quarks with masses above 4 GeV are excluded since they would contribute more distortion effects than physical effects. The charm quark with a mass of around our $M_{\rm charm}$=1.6 GeV is in between the typical scale of hadronic physics $E_{\rm had} \approx$ 0.5 GeV and the achievable cutoffs (the edge of the Brilloin zone) of $E_{\rm cut} \approx$ 4 GeV. It is thus a good question whether it is better to include the charm quark (often called $2+1+1$ simulations) or not $(2+1)$ and what are the uncertainties introduced by leaving it out.

In general, the answer to this question will depend on many details, from how one discretised QCD to which process one wants to predict from the simulations. Fortunately, there are also some rather universal statements which can be made. These have been the subject of our recent investigations and we give a brief account of them here.

4.1 The Effective Theory: decQCD

At low energies and momenta, say at $E_{\rm had}$ and below, there is a systematic expansion in terms of $y = E/M_{\rm charm}$, given in terms of an effective field theory, which excludes the charm quark, but has a few additional terms in its Lagrangian with coefficients proportional to $1/M^2_{\rm charm}$.

The leading order low energy effective theory is QCD_{n_ℓ}, where n_ℓ is the number of quarks in the Lagrangian. So far we had talked about $n_\ell = 3$. Next-to-leading order terms in the local effective Lagrangian are gauge-, Euclidean- and chiral-invariant local fields. These invariances allow only for fields, $\Phi_i(x)$, of at least dimension six. The Lagrangian may then be written as

$$\mathcal{L}_{\rm dec} = \mathcal{L}_{\mathrm{QCD}_{n_\ell}} + \frac{1}{M^2}\sum_i \omega_i \Phi_i + \mathrm{O}(\mathrm{M}^{-4}) \tag{1}$$

with dimensionless couplings ω_i which depend logarithmically on the mass M.

At the lowest order in $1/M$, a single coupling[b], $\bar{g}_{\rm dec}$, is adjusted such that the low energy physics of QCD_{n_ℓ} and $\mathrm{QCD}_{n_\mathrm{f}}$ match for energies $E \ll M$. It then suffices to require one physical low-energy observable to match, *e. g.* a physical coupling. Discussing the issue in perturbation theory,[13] Bernreuther and Wetzel chose the MOM-coupling as a physical coupling and worked out the matching of the $\overline{\mathrm{MS}}$ coupling. Meanwhile, the latter is known to high perturbative order,[14–20] which we use.

4.2 Non-Perturbative Investigation for $n_\mathrm{f} = 2 \ \rightarrow \ n_\ell = 0$

The main question is now, whether the effective theory is accurate at values of the quark mass around the charm mass, *i. e.* around 1.6 GeV. A direct test would require to simulate the $2{+}1{+}1$ theory which would be very expensive because of the light quarks.

We therefore investigated a very closely related model, namely QCD with $n_\mathrm{f} = 2$ heavy, mass-degenerate quarks.[21, 22] The decoupling is then $2 \rightarrow 0$ and the Lagrangian of the effective theory, $\mathcal{L}_{\rm dec}$, is the Yang-Mills one up to $1/M^2$ corrections. in $n_\mathrm{f} = 2$ we use quark mass values up to 1.8 GeV, slightly above the charm.

In principle any low-energy hadronic scale $\mathcal{S}(M)$ can be used to test decoupling, but in practice some choices are far superior to others. We want them to have good precision in the MC and have controllable lattice artifacts. In our purely gluonic effective theory, very good scales are defined in terms of the gradient flow.[23, 24] Here we report on two scales explicitly, which probe the theory in the low energy region at $E \approx 1/\sqrt{8t_0} \approx 0.5$ GeV and $E \approx 1/\sqrt{8t_c} \approx 0.7$ GeV.

4.2.1 Simulations

In order to avoid the freezing of the topological charge for simulations with lattice spacings below $a = 0.05$ fm,[25] we adopt open boundary conditions in time and use the openQCD[c] package.[26]

Even after solving the topological charge problem, simulations remain difficult. An impression is given in Fig. 3. It shows the integrated autocorrelation times $\tau_{\rm int}^{O}$ of two observables, O. Their meaning is that (on average) after $2\tau_{\rm int}^{O}$ MC iterations a statistically independent value of the particular observable is obtained. $\tau_{\rm int}$ itself is difficult to obtain, but the trend in the figure is clear and confirms theoretical expectations, $\tau_{\rm int} \sim a^{-2}$. We then need many thousand MC iterations for reliable and precise results at the smallest a. Our error analysis adds a tail to the autocorrelation function as an estimate of the slow mode [d] contribution.[25] It is thus robust with respect to long autocorrelations.

Note also that due to the expensive nature of the simulations it is very important that projects with different physics goals coordinate and share resources, namely gauge configurations. In our case the group of F. Knechtli extended the simulations to larger quark masses in a separate NIC project whose gauge fields we were able to use.

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[b] Again we refer to the theoretical situation where the first n_ℓ flavours are mass-less. In general, also the light quark masses have to be matched.

[c] `http://luscher.web.cern.ch/luscher/openQCD/`

[d] `http://www-zeuthen.desy.de/alpha/public_software/UWerrTexp.html`

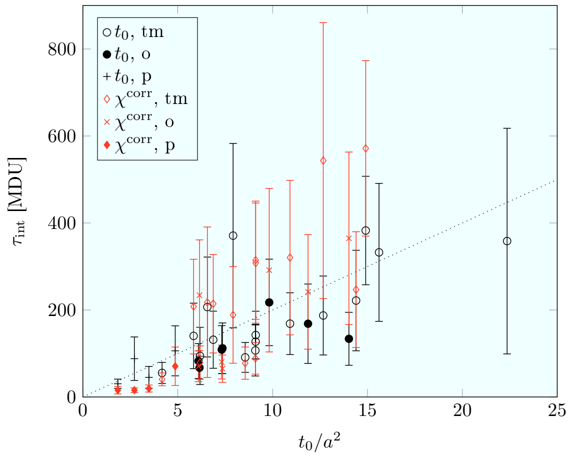

Figure 3. Autocorrelation times derived from observables which are expected to have large overlap with the slowest modes in the simulation are plotted as a function of $t_0(M)/a^2$.

4.3 Results

We turn to the results. The left part of Fig. 4 shows the ratio of two low energy scales in the $n_{\rm f} = 2$ theory as a function of the squared lattice spacing and for four different quark masses. The continuum extrapolated values are indicated at $a = 0$. In dimensionless ratios, such as the one shown, the value of the gauge coupling in the effective theory is irrelevant and as $M \to \infty$ they approach the $n_\ell = 0$ value. The corresponding behaviour is shown in the right part. Where the data are, a linear behaviour in $1/M$ looks more plausible than the prediction of the EFT, which is $\sim 1/M^2$ for large M. After our pioneering work, Knechtli

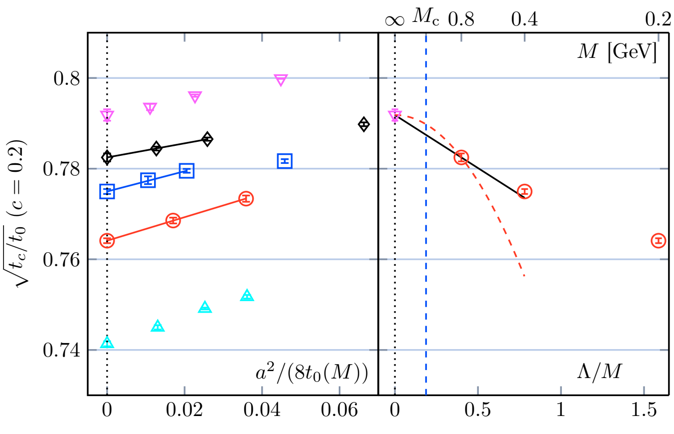

Figure 4. Left: The continuum extrapolation of the ratio $\sqrt{t_c/t_0}$ $(c = 0.2)$ at mass values (from top to bottom) $\Lambda/M = 0$, 0.4, 0.78, 1.59, ∞. Right: Its mass-dependence including a linear and quadratic fit in Λ/M between the largest mass and $N_{\rm f} = 0$ $(\Lambda/M = 0)$.

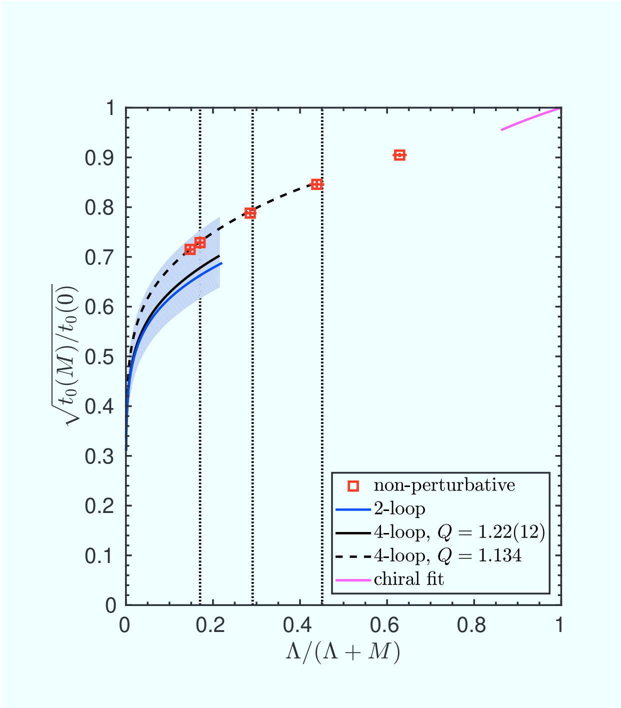

Figure 5. The mass-dependence of the ratio $\sqrt{t_0(M)/t_0(0)}$ in the theory with two mass-degenerate quarks. Monte Carlo data after continuum extrapolation are compared with the perturbative predictions for $1/(QP)$ at large M. The dashed line is the 4-loop curve adjusting the value of Q to go through the point at $M/\Lambda = 5.7781$. The vertical dotted lines mark the values of the quark mass M_c, $M_c/2$ and $M_c/4$.

et al.[27] extended the computation to larger mass and found agreement with $1/M^2$. But the most relevant result is that the corrections due to finite mass are very small, few per-mille level, when one rescales to the decoupling of *a single* quark. This holds for the scale ratios which were investigated, which are a few.[21, 27] It is justified to conclude that for low energy physics, also in QCD as realised in nature, one may safely leave out the charm quark and work with the $2{+}1$ theory.

Also the M-dependence of dimensionfull scales themselves are predictable by the effective theory. Now the matching of the coupling of the fundamental, n_f, theory and the n_ℓ theory is relevant. It turns out that for large M, the mass scaling function $\eta^\mathrm{M} = \frac{\mathrm{d}\log(\mathcal{S})}{\mathrm{d}\log(M)}$ is computable in perturbation theory and the perturbative series looks very well behaved. A comparison of the shape obtained in the fundamental theory to the one predicted by perturbative matching is given by the comparison of squares and dashed line in Fig. 5. The shape is very well reproduced by PT.

From this non-perturbative test of the quality of perturbative decoupling at the charm quark, we can deduce[22] two important things:

1. The effects of charm, bottom and top-quarks in the running coupling can indeed be added perturbatively as it has been done in Ref. 28 and a number of other works.

2. The heavy quark contribution to the coupling of “scalar dark matter” to hadrons is accurately given by perturbation theory and therefore known more accurately than previously thought.

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