Final report
Élvonal project KKP-126769

The Élvonal grant followed a previous ERC and Lendület grant and provided support for the lattice group at Eötvös University. During the supported period the group consisted of four senior researchers (the PI, Matteo Giordano, Tamás Kovács and Dániel Nógrádi) two postdocs (Attila Pásztor and Zoltán Tulipánt) for most of the grant period, a postdoc for a short period (Gergely Markó) and four graduate students (György Baranka, Kornél Kapás, Dávid Pesznyák and Zoltán Varga). It is an important achievement that by the end of the project one of the postdocs, Attila Pásztor received an assistant professor position at our institute. Ha was invited to give plenary talks on the QCD phase diagram at the two most important conferences of our field (Lattice 2023 and Quark Matter 2023). Kornél Kapás defended his PhD in 2023, Baranka and Pesznyák are still active students while Varga left the field of lattice QCD. The PI submitted two ERC Advanced grant applications during the project. In both cases the proposal was given a score of "B". In 2023 it barely missed the top 36% invited to the second step. Two group members (Matteo Giordano and Attila Pásztor) won OTKA grants in 2023 and Attila Pásztor was supported by a Bolyai fellowship.

The aim of the project was to perform lattice calculations of QCD at non-vanishing temperatures and chemical potentials and constrain the location of a possible critical point. The main challenge of such a project is the so-called complex action or sign problem which appears at non-vanishing chemical potentials. The partition function is $Z = \int \mathcal{D}U \det M(U) \exp(-S_g)$, where U are the gauge fields, $\det M$ is the fermion determinant and S_g is the gauge action. This, and its derivatives are usually calculated using importance sampling based Monte-Carlo which requires the integrand to be real and positive. Unfortunately, when we introduce a non-zero real chemical potential (μ for quarks of $\mu_B = 3\mu$ for baryons) the determinant becomes complex, thus spoiling importance sampling. This is the complex action problem. For the staggered discretization of fermions which we used for most of this project $\det M$ describes four fermions. Thus, in order to describe the two light quarks one has to take its square root (and fourth root for the strange quark). This introduces further problems which will be discussed below.

The original proposal had five sub-projects which were revised during the execution of the project. These changes were reported in the yearly reports and the panel accepted them. Here we briefly summarize the changes. The main reasons for changing two of the sub-projects (S3 and S5) were new ideas and techniques developed which made the original plans obsolete. In particular, the density of state method of S3 has been replaced by sign reweighting. While the density of states technique reduces the overlap problem of reweighting, sign reweighting (which was later also accompanied by phase reweighting) completely eliminates it. The complex Langevin technique which was proposed for S5 uses complexified fields to study finite chemical potentials. It has, however, unknown systematic uncertainties.

We replaced this method by contour deformation which also complexifies the gauge fields, but at the same time guarantees a correct result. In case of S2 (reweighting with chiral/overlap fermions) the reason for changing our research direction is a bit more involved. Overlap fermions are computationally very expensive. During the Covid19 pandemic we had a long shutdown of our GPU cluster due to broken air conditioning. This forced us to think of alternative strategies. Beyond the computational costs, overlap fermions have other disadvantages: (i) the introduction of the chemical potential is not unambiguous. One does not have the partition function as essentially a finite polynomial in fugacity. This makes the techniques we developed for staggered fermions in the first years of the project, i.e. the determination of Lee-Yang zeroes in the complex mu plane very difficult to apply for overlap fermions; (ii) overlap fermions are non-analytic in the gauge fields which makes contour deformation, which we will discuss later, inapplicable. The main motivation for the overlap fermion formulation was twofold: it has exact chiral symmetry on the lattice and no rooting of the fermion determinant is needed. We turned our interest towards the Karsten-Wilczek fermion discretization which also has a chiral symmetry (although similar to the staggered case) and describes two quarks, so no rooting is necessary for the light quarks. We started implementing this fermion formulation, first results are expected in the near future.

In the following we list the main results achieved during the six years of the project. We published 34 peer reviewed papers, three more are already submitted to journals. Furthermore, we have a review and a number of conference papers. One paper was published in Nature [1] (although not in the topic of the project), two in Phys.Rev.Lett. and the rest in Phys.Rev.D and JHEP, the top journals of the field. According to the inspire database the thermodynamics papers published during the six years of the project already received more than 750 independent citations (and the muon $g-2$ paper in Nature another 750). About half of the papers were published in collaboration with the Wuppertal lattice group.

- We determined the location of the critical point on coarse, $N_t = 4$ lattices for small smearing parameters which mimic a small move towards the continuum limit [2]. To this end we located the partition function zeroes in the complex gauge coupling plane (Fisher zeroes). We collected significant statistics and found that even a very small smearing makes Fisher zeroes move far from the real axis and difficult to find. We demonstrated that the overlap problem becomes much more severe with smearing. The findings discourage further search for Fisher zeroes on finer lattices, we turned our attention to zeroes in the complex mu plane (Lee Yang zeroes). This result was also the main motivation for our sign reweighting technique discussed below.

- The convergence radius of the Taylor expansion of the pressure is given by the closest singularity of $\log Z(\mu)$ to the origin in the complex μ plane. The partition sum Z is essentially a polynomial of the fugacity ($\exp(\mu/T)$) and therefore the singularities of $\log Z$ coincide with the zeroes of this polynomial. We implemented a technique to determine all zeroes of $Z(\mu)$ using the Aberth

method of polynomial root finding. This requires high precision arithmetic and a new way to perform staggered rooting which we dubbed "geometric matching". The latter we did by pairing the eigenvalues of the fermion matrix using a publicly available algorithm (Blossom V). Rooting then halves the number of eigenvalues by keeping only one from each pair. The closest zero of Z to the origin gives the convergence radius but it can also be used to locate the phase transition. Its infinite volume scaling tells the order of the transition. Since $Z(\exp(\mu/T))$ is always a polynomial the roots can be found for improved actions as well. It turns out that the closest root is stable and has a modest uncertainty for the 2 stout improved staggered action [3, 4]. The volume scaling does not suggest that a real phase transition would happen in the infinite volume limit.

- In a recent paper we showed that staggered rooting causes serious problems at large chemical potentials [5]. Since the determinant is complex at finite chemical potentials, there is an ambiguity in choosing among the Riemann-sheets when taking the square root of the determinant (at $\mu = 0$ this ambiguity is resolved by preferring the positive real root). Standard rooting methods at large chemical potential essentially choose a random root and thus correlation between the phase (sign) of the determinant and physical observables is lost. This problem does not show up in extrapolation techniques, however for direct simulations, such as sign reweighting, it becomes severe for large μ values. We have shown that the geometric matching technique discussed above, that we developed for rooting, behaves much better than standard rooting. This makes staggered fermions applicable also for large chemical potentials close to the continuum limit.

- Besides the complex action problem another difficulty arises for most reweighting methods: the overlap problem. The distribution of weights used for reweighting is long tailed and a finite Monte-Carlo statistics does not sample the tail well enough; there is no sufficient overlap between the generated configurations and the ones needed after reweighting. As mentioned above, to solve this problem, instead of the originally proposed density of states method, we developed a new technique called sign reweighting: one can in principle use $|\mathrm{Re}(\det M(\mu))|$ in Monte-Carlo simulations. This has various advantages: since $\mathrm{Re}(\det M)$ is always real (but not necessarily positive), there is no complex action problem but only a sign problem in this case. For small chemical potentials the phase of the determinant is still small, therefore the real part is mostly positive, i.e. the sign problem is mild. The most important advantage is that using the above weight in a Monte-Carlo study, we only have to reweight our configurations by ± 1 factors. Eventually, for large chemical potentials the $+$ and $-$ sectors will have comparable weights and a large cancellation will occur (thus the sign problem appears), but for all cases where this still does not happen the sign problem is under control and all results can be trusted. Since there is no long-tailed distribution in this case but only two sectors have to be sampled

by the Monte-Carlo, there is no overlap problem. Unfortunately, the proposed action is not analytic in the gauge fields, therefore we do not have an efficient simulation technique at the moment. It turned out, however, that a brute force Metropolis based algorithm is feasible up to quite large $(24^3 \cdot 12)$ lattices. We have applied this technique first on coarse lattices to reproduce our earlier results on the critical point [6]. Then we used our stout improved action and calculated thermodynamic observables using sign reweighting at finite chemical potentials [7]. We also used the same technique to study the equation of state of the quark gluon plasma and compare direct results with various extrapolation techniques [8]. This method made it possible to study finite density QCD up to $\mu_B/T \lesssim 3$ without any unknown systematic *for the first time in the literature.*

- In collaboration with the Wuppertal group we used extrapolation techniques to determine the phase diagram, the equation of state of QCD as well as cumulants of conserved charges in the continuum limit. These quantities are of direct relevance for heavy ion experiments. Extrapolations are usually done from imaginary chemical potentials where the sign problem is absent. We determined the phase diagram up to fourth order in the chemical potential [9]. We calculated the equation of state using a new resummation scheme [10, 11]. Cumulants and cross-correlations of conserved charges were calculated in the continuum limit in Refs [12, 13, 14].

- Even though sign reweighting provides reliable results at $\mu > 0$, this method is still suffering from the sign problem: the required statistics grows exponentially with the volume and chemical potential. In the original proposal the use of complex Langevin dynamics was suggested to penetrate chemical potential regions inaccessible by standard reweighting methods. Complex Langevin dynamics is based on complexifying the original field of the theory (in case of QCD $SU(3)$ is complexified to $SL(3, C)$). Unfortunately, complex Langevin can give incorrect results. Even though the criteria for correctness are known in principle, they consist of infinitely many conditions and are therefore impossible to check in practice. There is, however an alternative way to exploit the complexification of fields. The path integral is a product of integrals over the fields of the theory at each lattice site. These integrals can be redefined as contour integrals in the complexified space of the fields. If one deforms the periodic integral contours such that no singularities are crossed, the integral is guaranteed to remain constant according to Cauchy's theorem. The integrand, however changes, and thus the severity of the sign problem may be reduced in principle (there are simple examples where the sign problem can be completely eliminated by choosing an appropriate contour). Since there are many integration variables (proportional to the volume) and arbitrary contours can be used, there is a vast number of possible integration manifolds. Reducing the sign problem becomes an optimization problem over the possible integration manifolds. This idea has been around in the literature for a few years but has

not been applied to QCD yet. We also started our studies with two simpler systems, the 3D XY model [15] and a chiral random matrix model [16]. The results are quite encouraging. By using a simple ansatz for the new contours and optimizing its parameters, the strength of the sign problem can be significantly reduced. Even though it is not completely eliminated, the necessary Monte-Carlo statistics for a given accuracy can be reduced by two orders of magnitude. The reduction was shown to be exponential both in the chemical potential and the volume. A similar improvement would be a game changer in QCD and this is one of the most promising directions for the future.

- The low lying eigenvalues of the Dirac-operator are responsible for chiral symmetry breaking and thus the emergence of the chiral condensate at low temperatures. The exact zero modes or near zero modes are related to the non-trivial topology of gauge field configurations. Interestingly, at high temperatures, just above the transition the low eigenvalues have a highly non-trivial behavior. They become independent and thus follow a Poisson-statistics and the corresponding eigenvectors are localized. The detailed study of these properties, their connection to the phase transition in various systems has been carried out by our group in the past years. Besides QCD, various gauge theories have been studied: the centers of $SU(2)$ and $SU(3)$: Z_2 [17] and Z_3 [18], respectively; as well as $SU(2)$ directly [19] and low dimensional SU(3) [20]. The connection between localization and Goldstone's theorem has been studied in [21]. In the case of QCD the continuum behavior of the mobility edge (where localized eigenvalues end in the spectrum) was investigated [22]. Since chiral symmetry is essential for the low modes, pilot studies with overlap fermions were also done [23]. Two group members wrote a review on the localization of Dirac eigenmodes [24].

Even though we did not locate the critical point, the results listed above greatly contributed to our understanding of QCD at nonzero chemical potentials and also constrain the location of a possible critical point. For the first time in the literature we were able to go beyond extrapolations and calculate thermodynamic observables directly at finite μ. Since no sign of criticality has been observed, we can safely exclude the critical point for $\mu_B/T \lesssim 3$. The new methods also paved the way for larger chemical potentials. In the coming years the combination of sign reweighting, Karsten-Wilczek fermions and contour deformation will take us to uncharted regions of the phase diagram, possibly even close to regions which are already relevant for neutron star mergers.

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