Improved Lattice Actions with Chemical Potential

W. Bietenholz, HLRZ c/o Forschungszentrum Jülich, D-52425 Jülich, Germany

We give a prescription how to include a chemical potential $\mu$ into a general lattice action. This inclusion does not cause any lattice artifacts. Hence its application to an improved – or even perfect – action at $\mu = 0$ yields an improved resp. perfect action at arbitrary $\mu$. For short-ranged improved actions, a good scaling behavior holds over a wide region, and the upper bound for the baryon density – which is known for the standard lattice actions – can be exceeded.

1. Introduction

At chemical potential $\mu \neq 0$, the action of QCD is complex (see subtitle of this workshop). With respect to lattice simulations, this means that the standard Monte Carlo techniques fail. In principle, it is possible to simulate at $\mu = 0$ and include the baryon density $n_B$ in the measured observables by a suitable re-weighting. However, in practice this is extremely tedious: the ratio of an observable at $\mu \neq 0$ divided by the observable at $\mu = 0$ is exponentially suppressed by the physical volume. Hence the absolute values of the statistical contributions tend to be many orders of magnitude larger than the ratio of interest, so that tremendous statistics are required (“sign problem”) \footnote{In principle, the complex Langevin algorithm is an alternative \cite{2}, but it has not lead to QCD results, again due to the limited statistics.}

In addition to the statistical error, lattice simulations are also plagued by systematic errors. The worst source of them are artifacts due to the finite lattice spacing $a > 0$. Improved lattice actions are designed to suppress these artifacts, i.e. the continuum scaling should persist to a good approximation down to a rather short correlation length in lattice units, $\xi/a$, or up to rather large values of $\mu a$ (below we use lattice units, $a = 1$).

As a particularly bad manifestation of lattice artifacts, there is an upper bound for $n_B$, resp. for the fermion density $n_f$. We will show that improved actions can weaken this unphysical saturation effect.

In simulations, chiral symmetry appears to be restored already at half the pion mass (“onset problem” \cite{4,5}). Usually quenching was blamed for that, but attempts to go beyond the quenched approximation have not really helped in this respect. The Glasgow group now assumes that this is an effect of low statistics, but it is also conceivable that lattice artifacts contribute to this problem. If this is true, then the use of dynamical fermions together with an improved action should help to obtain a more continuum-like chiral behavior.

The extreme case of improved actions are perfect actions: they eliminate all lattice artifacts. Unfortunately they tend to involve an infinite number of couplings, hence we
can only apply short-ranged approximations. A perfect action is constructed by block variable renormalization group transformations (RGTs) of the type

\[ e^{-S[\Psi', \Psi, U]} = \int D\bar{\Psi}D\Psi DU e^{-S[\Psi, \Psi, U]} \exp\{-T[\bar{\Psi}', \bar{\Psi}, \Psi', \Psi, U', U]\} . \]  (1)

We start from a fine lattice with action \( S[\bar{\Psi}, \Psi, U] \), and introduce a new lattice with a \( n \) times coarser lattice spacing, where the action is given by \( S'[\bar{\Psi}', \Psi', U'] \) according to eq. \([\square]\). The transformation term \( T \) relates the original lattice variables to the new ones by averaging in some way over the fine lattice sites close to a given coarse site. It has to provide the invariance of the partition functions, \( Z' = Z \), and of the expectation values, hence of the physical contents of the theory. The choice for \( T \) characterizes the RGT. After the RGT, the correlation length in lattice units is reduced by a factor \( n \), \( \xi'/a' = 1/n \cdot \xi/a \).

Assume a mass \( m \) and an inverse temperature \( \beta \). Now we start from a very fine lattice at mass \( m/nN \) and inverse temperature \( \beta nN \), and we perform \( N \) RGTs of block factor \( n \). This leads to the desired parameters \( m, \beta \). In the limit \( nN \to \infty \), this method yields a perfect action at the desired finite parameters \( m, \beta \).

2. Inclusion of the chemical potential \( \mu \)

In the continuum, the chemical potential can be included by the substitutions \( \bar{\psi}(-p) \to \bar{\psi}(-\vec{p}, -p_4 + i\mu) \), \( \psi(p) \to \psi(\vec{p}, p_4 - i\mu) \) in the quark fields, or by replacing \( p_4 \to p_4 + i\mu \) in the Dirac operator. It is not trivial how to apply this substitution to the naive lattice Dirac operator \( i\gamma_\nu \sin p_\nu + m \). An early guess, \( \sin p_4 \to \sin p_4 + i\mu \) does not have the correct continuum limit. Instead one should use \( \sin(p_4 + i\mu) \) \([4]\). Also for the somewhat more complicated Wilson-Dirac operator, \( i\gamma_\nu \sin p_\nu + m + (r/2) \sum_\nu \tilde{p}_\nu^2 \), \( \tilde{p}_\nu = 2\sin(p_\nu/2) \), the substitution \( p_4 \to p_4 + i\mu \) works.

If we want to construct a perfect action, we can use a standard action (Wilson or staggered) on the finest lattice and incorporate \( \mu \) by this rule, which we call the standard procedure. In coordinate space, it amounts to the substitutions

\[ ^\mu\bar{\Psi}(\vec{x}, t) = e^{i\mu t}\bar{\Psi}(\vec{x}, t) , \quad ^\mu\Psi(\vec{x}, t) = e^{-i\mu t}\Psi(\vec{x}, t) . \]  (2)

Hence \( \mu \) is treated on the lattice consistently as an imaginary constant Abelian gauge potential \( A_4 = i\mu \). Therefore, \( ^\mu\bar{\Psi} \) and \( ^\mu\Psi \) are “parallel transported to \( t = 0 \)”, which confirms the gauge invariance of this procedure. This observation holds for all sorts of lattice actions, hence the standard procedure \([3]\) can always be applied.

We preserve this useful property also under the RGT by using the transformation term

\[ T^{[\mu\bar{\Psi}', \mu\bar{\Psi}, ^\mu\Psi', ^\mu\Psi, U', U]} , \quad ^\mu\bar{\Psi}'(\vec{x}', t') = e^{i\mu t'}\bar{\Psi}'(\vec{x}', t') , \quad ^\mu\Psi'(\vec{x}', t') = e^{-i\mu t'}\Psi'(\vec{x}', t') . \]  (3)

If \( t \in [0, \beta] \), then \( t' \in [0, \beta/n] \), and since distances are measured after the RGT in coarse lattice units, the transportation distance to \( t = t' = 0 \) is divided by \( n \). This is compensated by substituting \( n\mu \) in the coarse fields.

The result of the RGT is \( S'[\mu\bar{\Psi}', ^\mu\bar{\Psi}', U'] \), and it is easy to see that this is identical to the following construction: first let \( \mu = 0 \) and perform the RGT to arrive at \( S'[\bar{\Psi}', \Psi', U'] \). Now we include \( \mu \) in the blocked action again by the standard procedure \([2]\) (where \( \mu \) is multiplied by \( n \) due to the rescaling to the new lattice units).
Now the RGT can be iterated. In order to arrive at a chemical potential $\mu$ in the final action, we start with $\mu/nN$ on the finest lattice, and perform $N$ RGTs of block factor $n$, in analogy to the mass. The limit $nN \to \infty$ yields a perfect action with $\mu$.

From the analysis of one RGT we conclude that we can switch off $\mu$ in the beginning, iterate the RGT all the way to the perfect action, and then include $\mu$ again by the procedure (2). This leads to a perfect action at chemical potential $\mu$.\[\text{(4)}\]

The standard procedure to include $\mu$ preserves perfectness, it does not cause any lattice artifacts and it is therefore perfect itself.

In practice, such actions are hard to construct (for recent reviews, see [8]). What is more realistic is a classically perfect approximation, where the functional integral in eq. (1) is simplified to a minimization of the exponent on the right-hand side. A number of 2d studies suggest that classically perfect actions also suppress the lattice artifacts very strongly. Consideration of the transformation term shows that including $\mu$ in a classically perfect action by the procedure (2) leads again to a classically perfect action with $\mu$.

An alternative improvement program for lattice actions starts from a standard action and tries to eliminate the artifacts order by order in the lattice spacing (Symanzik’s program). Assume that this is realized to some order at $\mu=0$.\[\text{[8]}\] and we include $\mu$ once more by the standard procedure. The above properties suggest that we obtain an action with $\mu$, which is still free of lattice artifacts to the same order as it was the case at $\mu=0$.

3. Scaling behavior of a free fermion gas as an example

A perfect lattice action for free fermions with mass $m$ at $\mu=0$ reads [8]

$$S^*[\bar{\Psi}, \Psi] = \int_{-\pi}^{\pi} \frac{d^4p}{(2\pi)^4} \bar{\Psi}(-p) \Delta^{-1}(p) \Psi(p), \quad \Delta(p) = \sum_{l \in \mathbb{Z}} \frac{\prod_{\sigma=1}^{4} \hat{p}_\sigma^2/(p_\sigma + 2\pi l_\sigma)^2}{i\gamma_\nu(p_\nu + 2\pi l_\nu) + m + \frac{1}{\alpha}}, \quad \text{(4)}$$

where $\alpha$ is a free RGT parameter. At $m=0$, $\alpha = \infty$ the action is chirally symmetric but non-local. For any finite $\alpha$ the action is local: its couplings in coordinate space decay exponentially. Since the limit $nN \to \infty$ relates the system directly to the continuum, there is still chiral symmetry in the observables [8]. Furthermore, the action itself also keeps a remnant continuous chiral symmetry [10].

For applications, it is important to optimize the locality, so that the truncation of the usual couplings is not too harmful. This is achieved by choosing $\alpha = (e^{m} - m - 1)/m^2$ [8].

According to section 2, the corresponding perfect action at finite $\mu$ is characterize by $\Delta(\vec{p}, p_4 + i\mu)$. A successful and yet applicable approximation is a truncation to the couplings in a unit hypercube by means of periodic boundary conditions. The corresponding couplings at $\mu=0$ for various masses are given in Ref. [11].

The RGT used for the above perfect action for Wilson-type fermions is based on the usual block average (BA) scheme. If one constructs the analogous perfect action for staggered fermions [12], then the truncation to the same number of degrees of freedom as before (couplings distance components $\pm1, \pm3$ resp. $0, \pm2$ at $m=0$) is not satisfactory. The locality – and hence the quality after truncation – can be improved significantly by using instead a blocking scheme that we call “partial decimation” (PD) [13].

---

2What has been achieved – to a good accuracy – is the $O(\alpha)$ improvement of QCD with Wilson fermions [8]. However, going beyond that is not realistic in the foreseeable future.
We now focus on $m = 0$ and temperature $T = 0$. The pressure and baryon density of the free fermion gas are given by

\[ P = \frac{\mu^4}{6\pi^2}, \quad n_B = \frac{2\mu^3}{9\pi^2} \] in the continuum, and obtained from

\[ P = \int_{-\pi}^{\pi} \frac{d^4p}{(2\pi)^4} \log \frac{\det \Delta(\vec{p}, p_4)}{\det \Delta(\vec{p}, p_4 + i\mu)}, \quad n_B = \frac{1}{3\partial_\mu} P \] on the lattice. \hfill (5)

For comparison, we insert a number of lattice fermion propagators $\Delta$. For Wilson-type fermions, we probe the Wilson fermion with Wilson parameter $r = 1$, a Symanzik improved version thereof called D234 with additional couplings on the axes \cite{14}, and the truncated perfect "hypercube fermion" (HF). For staggered fermions we insert the staggered standard action, the Naik fermion \cite{15} (which is Symanzik improved in the same way as the D234 fermion), and again the truncated perfect actions for the BA and the PD scheme. Fig. 1 shows the scaling ratios $P/\mu^4$ and $n_B/\mu^3$ for this set of fermions. Of course, they all reproduce the correct continuum values at $\mu \to 0$. As $\mu$ increases, the standard actions deviate very soon, the Symanzik improved actions do well up to a certain $\mu$ and then collapse completely, but the truncated perfect actions keep close to the continuum value up to remarkably large $\mu$. Their scaling region is extended by one order of magnitude compared to the standard actions.

One could also consider $\chi_B/\mu^2$, where $\chi_B = \partial/\partial_\mu n_B$ is the baryon number susceptibility, but in all these cases the qualitative behavior is very similar, and it is also in agreement with the scaling of $P/T^4$ at $\mu = 0$ \cite{11,13}, hence it is manifestly systematic.

4. The fermion density

We now consider the fermion density $n_f$. It is well known that the standard lattice actions suffer from an upper bound for $n_f$. We choose the normalization such that naive fermions saturate at $n_f = 32$. This corresponds to an occupation of each site by $2^d$ species, each with spin up and down.

For Wilson fermions the doublers are heavier, hence $\mu$ must be larger to exceed their masses, and the saturation is delayed. However, for $r \neq 1$ this is unimportant in the limit $\mu \to \infty$, so we have again $n_f,\text{max} = 32$. The case of $r = 1$ is special: here the mass of the time-like doublers diverges, hence $n_f,\text{max} = 16$.

From Pauli’s principle one might be tempted to conclude that $n_f = 32$ is an absolute upper bound for all lattice actions. However, since this bound is a lattice artifact, this leads to a puzzle about the behavior of a perfect action. The solution is that the above argument is wrong. Considering

\[ S[\bar{\Psi}, \Psi] = \sum_{\vec{x},t} \sum_{\vec{y},s} \bar{\Psi}_{\vec{x},t} e^{\mu(t-s)} \Delta^{-1}(\vec{x} - \vec{y}, t - s) \Psi_{\vec{y},s}, \] \hfill (6)

we recognize that the exponential growth of the factor containing $\mu$ is limited by the maximal coupling distance in the temporal direction, which occurs in $\Delta^{-1}$. (In fact, such a saturation limit also exists for bosons.) For the perfect action this distance is infinite, hence $n_f$ has no upper bound, in agreement with the absence of artifacts. To turn it the other way round, we can conclude that (in infinite volume) no perfect action with

\footnote{At this point I thank especially M.-P. Lombardo, who suggested to me to consider also $n_f(\mu)$ itself.}
Figure 1. The scaling of Wilson-type fermions (on top) and staggered fermions (below), both in a number of variants discussed in the text. The D234 and the Naik fermion are Symanzik improved, and the fermions denoted as HF, BA and PD are truncated perfect.

couplings only in a finite range can exist, and this is indeed correct. For the hypercube fermion we have again \((t-s)_{\text{max}} = 1 \rightarrow n_{f,\text{max}} = 32\), but the saturation is significantly delayed. The D234 action has \((t-s)_{\text{max}} = 2\), so one could expect \(n_{f,\text{max}} = 64\). But there is a cancelation going on, similar to the Wilson fermion at \(r = 1\), which reduces \(n_{f,\text{max}}\) again to 32. If we keep that structure and vary the couplings, then \(n_f\) does rise up to 64. But in both cases, the saturation occurs at practically the same value of \(\mu\) as it happens for the \(r = 1\) Wilson fermion. This behavior is shown in Fig. 2, which also illustrates the Wilson fermion at various values of \(r\). For instance at \(r = 2\), \(n_f(\mu)\) rises quite steadily to 32. If \(r\) decreases towards 1, then half of the particles in the spectrum turn very heavy. The curve reaches a first plateau at 16, and when \(\mu\) catches up with this heavy species, it performs a second jump up to 32. This looks similar if we approach \(r = 1\) from below. If \(r\) is exactly 1, then the plateau at 16 extends to infinity.

We also show these curves for various types of staggered fermions. The standard bound is 8, but if couplings over temporal distance 3 are involved, then this bound is amplified by a factor of 3. Here we also show some Symanzik improved actions with diagonal couplings from Ref. [16]. One type called p4 has maximal temporal coupling distance

\(^4\)The only exception for matter fields is the case \(d = 1\), which does, however, not lead to a contradiction.
2 and saturates at $n_f = 16$, the others couple over distance 3 like the truncated perfect fermions. Also here the saturation is delayed, and we mention that especially the p6 action is doing very well in the scaling tests too.

5. Generalizations

A number of generalizations are straightforward, for instance the steps to finite temperature and finite mass. The latter has been considered in Ref. [17] for naive fermions, and the behavior is similar in all other cases: the saturation is delayed as $m$ grows, but the upper bound is not affected.

It is fashionable to use anisotropic lattices in thermodynamic simulations. In particular, $\xi = a_{\text{spatial}}/a_{\text{temporal}} > 1$ is useful, because it provides a better resolution of a decay in the temporal direction. Remarkably, the couplings in a perfect action are independent of $\xi$. This property still holds after truncation by periodic boundary conditions. In the previous plots, we would reproduce the same curves, and the horizontal axes now means $a_{\text{temporal}} \cdot \mu$. However, the lattice units are defined by $a_{\text{spatial}}$, so $\mu$ is multiplied by $\tilde{\xi}$.

6. Conclusions

So far, $\mu$ has only been included in standard lattice actions. We have seen how to do this in general. Of interest are applications to improved actions, and there the improved quality (perfectness, classical perfectness, or Symanzik improvement to some order) is
preserved under the inclusion of \( \mu \).

We have shown that an improved action allows us to go beyond the standard limits for the baryon resp. fermion density (in spite of a widespread believe that this is impossible).

Applicable truncated perfect actions extend the scaling region of a free fermion gas by one order of magnitude, which suggests that simulations with them can be carried out on very coarse lattices. This is not a direct remedy of the sign problem mentioned in the introduction (because that is a problem of statistics, whereas the improved action cures systematic errors), but it helps indirectly, because larger physical volumes can be handled.

For the fermion-gauge couplings and for the pure gauge part, there is much work going on to construct Symanzik improved or approximately perfect actions \([7,6]\). If this is achieved at \( \mu = 0 \), then the extension to \( \mu \neq 0 \) is solved by the prescription shown here.

Hopefully this is a step towards more conclusive simulations for \( n_B \neq 0 \).


Most of this talk is based on Ref. \([4]\); I am indebted to U.-J. Wiese for his collaboration. I also thank M.-P. Lombardo and F. Karsch, both, for organizing this workshop and for instructive discussions.

REFERENCES

1. Talks presented at this workshop by I. Barbour and A. Galante.
2. H. Gausterer, talk presented at this workshop.
3. S. Morrison, talk presented at this workshop.
4. P. Hasenfratz and F. Karsch, Phys. Lett. B125 (1983) 308. J. Kogut, H. Matsuoka, M. Stone, H. Wyld, S. Shenker, J. Shigemitsu and D. Sinclair, Nucl. Phys. B225 [FS] (1983) 93.
5. W. Bietenholz and U.-J. Wiese, hep-lat/9801022, to appear in Phys. Lett. B.
6. P. Hasenfratz, hep-lat/9803027, W. Bietenholz, hep-lat/9802014, F. Niedermayer, Nucl. Phys. B (Proc. Suppl.) 60A (1998) 257.
7. Proceedings of LATTICE 97, Nucl. Phys. B (Proc. Suppl.) 63 (1998).
8. W. Bietenholz and U.-J. Wiese, Nucl. Phys. B464 (1996) 319.
9. W. Bietenholz and U.-J. Wiese, Phys. Lett. B378 (1996) 222; Nucl. Phys. B (Proc. Suppl.) 47 (1996) 575.
10. M. Lüscher, hep-lat/9803016.
11. W. Bietenholz, R. Brower, S. Chandrasekharan and U.-J. Wiese, Nucl. Phys. B (Proc. Suppl.) 53 (1997) 921.
12. W. Bietenholz and U.-J. Wiese, Nucl. Phys. B (Proc. Suppl.) 34 (1994) 516. H. Dilger, Nucl. Phys. B490 (1997) 331. W. Bietenholz, R. Brower, S. Chandrasekharan and U.-J. Wiese, Nucl. Phys. B496 (1997) 285.
13. W. Bietenholz and H. Dilger, hep-lat/9803018.
14. M. Alford, T. Klassen and G.P. Lepage, Nucl. Phys. B496 (1997) 377.
15. S. Naik, Nucl. Phys. B316 (1989) 238.
16. A. Peickert, B. Beinlich, A. Bicker, F. Karsch and E. Laermann, Nucl. Phys. B (Proc. Suppl.) 63 (1998) 895.
17. I. Barbour, N. Behilil, E. Dagotto, F. Karsch, A. Moreo, M. Stone and H. Wyld, Nucl. Phys. B275 [FS17] (1986) 369.