Appendix B

Algorithmic details

B.1 Even/odd preconditioning

In this appendix we describe how even/odd [106, 170] preconditioning can be used in the HMC algorithm in presence of a twisted mass term. By setting the twisted mass parameter to zero, even/odd preconditioning for the Wilson-Dirac operator can easily be recovered from the formulae presented in the following.

We start with the lattice fermion action in the hopping parameter representation in the χ-basis written as

$$\begin{aligned} S[\chi,\bar{\chi},U] = \sum_x \Bigg\{ & \bar{\chi}(x)[1+2i\kappa\mu\gamma_5\tau^3]\chi(x) \\ & - \kappa\bar{\chi}(x)\sum_{\mu=1}^{4}\Big[U(x,\mu)(r+\gamma_\mu)\chi(x+a\hat{\mu}) \\ & + U^\dagger(x-a\hat{\mu},\mu)(r-\gamma_\mu)\chi(x-a\hat{\mu})\Big]\Bigg\} \\ \equiv & \sum_{x,y}\bar{\chi}(x)M_{xy}\chi(y)\ . \end{aligned} \tag{B-1}$$

similar to Eq. (1-46) in section 1.2.4. For convenience we define $\tilde{\mu} = 2\kappa\mu$. Using the matrix M one can define the hermitian (two flavor) operator.

$$Q \equiv \gamma_5 M = \begin{pmatrix} Q^+ & \\ & Q^- \end{pmatrix} \tag{B-2}$$

where the sub-matrices $Q^{\pm}$ can be factorized as follows:

$$\begin{aligned} Q^{\pm} = \gamma_5 \begin{pmatrix} 1 \pm i\tilde{\mu}\gamma_5 & M_{eo} \\ M_{oe} & 1 \pm i\tilde{\mu}\gamma_5 \end{pmatrix} = \gamma_5 \begin{pmatrix} M_{ee}^{\pm} & M_{eo} \\ M_{oe} & M_{oo}^{\pm} \end{pmatrix} \\ = \begin{pmatrix} \gamma_5 M_{ee}^{\pm} & 0 \\ \gamma_5 M_{oe} & 1 \end{pmatrix} \begin{pmatrix} 1 & (M_{ee}^{\pm})^{-1} M_{eo} \\ 0 & \gamma_5 (M_{oo}^{\pm} - M_{oe} (M_{ee}^{\pm})^{-1} M_{eo}) \end{pmatrix} . \end{aligned} \tag{B-3}$$

Note that $(M_{ee}^{\pm})^{-1}$ can be computed to be

$$(1 \pm i\tilde{\mu}\gamma_5)^{-1} = \frac{1 \mp i\tilde{\mu}\gamma_5}{1 + \tilde{\mu}^2}. \tag{B-4}$$

Using $\det(Q) = \det(Q^+) \det(Q^-)$ the following relation can be derived

$$\begin{aligned} \det(Q^{\pm}) \propto \det(\hat{Q}^{\pm}) \\ \hat{Q}^{\pm} = \gamma_5 (M_{oo}^{\pm} - M_{oe} (M_{ee}^{\pm})^{-1} M_{eo}) \, , \end{aligned} \tag{B-5}$$

where $\hat{Q}^{\pm}$ is only defined on the odd sites of the lattice. In the HMC algorithm the determinant is stochastically estimated using pseudo fermion field ϕ_o: Now we write the determinant with pseudo fermion fields:

$$\begin{aligned} \det(\hat{Q}^+ \hat{Q}^-) = \int \mathcal{D}\phi_o \, \mathcal{D}\phi_o^{\dagger} \, \exp(-S_{\mathrm{PF}}) \\ S_{\mathrm{PF}} \equiv \phi_o^{\dagger} \left(\hat{Q}^+ \hat{Q}^- \right)^{-1} \phi_o \, , \end{aligned} \tag{B-6}$$

where the fields ϕ_o are defined only on the odd sites of the lattice. In order to compute the force corresponding to the effective action S_{PF} we need the variation of S_{PF} with respect to the gauge fields (using $\delta(A^{-1}) = -A^{-1} \delta A A^{-1}$):

$$\begin{aligned} \delta S_{\mathrm{PF}} &= -[\phi_o^{\dagger} (\hat{Q}^+ \hat{Q}^-)^{-1} \delta \hat{Q}^+ (\hat{Q}^+)^{-1} \phi_o + \phi_o^{\dagger} (\hat{Q}^-)^{-1} \delta \hat{Q}^- (\hat{Q}^+ \hat{Q}^-)^{-1} \phi_o] \\ &= -[X_o^{\dagger} \delta \hat{Q}^+ Y_o + Y_o^{\dagger} \delta \hat{Q}^- X_o] \end{aligned} \tag{B-7}$$

with X_o and Y_o defined on the odd sides as

$$X_o = (\hat{Q}^+ \hat{Q}^-)^{-1} \phi_o, \quad Y_o = (\hat{Q}^+)^{-1} \phi_o = \hat{Q}^- X_o \, , \tag{B-8}$$

where $(\hat{Q}^{\pm})^{\dagger} = \hat{Q}^{\mp}$ has been used. The variation of $\hat{Q}^{\pm}$ reads

$$\delta \hat{Q}^{\pm} = \gamma_5 \left(-\delta M_{oe} (M_{ee}^{\pm})^{-1} M_{eo} - M_{oe} (M_{ee}^{\pm})^{-1} \delta M_{eo} \right) , \tag{B-9}$$

and one finds

$$\begin{aligned} \delta S_{\mathrm{PF}} &= -(X^{\dagger} \delta Q^+ Y + Y^{\dagger} \delta Q^- X) \\ &= -(X^{\dagger} \delta Q^+ Y + (X^{\dagger} \delta Q^+ Y)^{\dagger}) \end{aligned} \tag{B-10}$$

where X and Y are now defined over the full lattice as

$$X = \begin{pmatrix} -(M_{ee}^{-})^{-1} M_{eo} X_o \\ X_o \end{pmatrix}, \quad Y = \begin{pmatrix} -(M_{ee}^{+})^{-1} M_{eo} Y_o \\ Y_o \end{pmatrix}. \tag{B-11}$$

In addition $\delta Q^+ = \delta Q^-$, $M_{eo}^\dagger = \gamma_5 M_{oe} \gamma_5$ and $M_{oe}^\dagger = \gamma_5 M_{eo} \gamma_5$ has been used. Since the bosonic part is quadratic in the ϕ_o fields, the ϕ_o are generated at the beginning of each molecular dynamics trajectory with

$$\phi_o = \hat{Q}^+ R, \tag{B-12}$$

where R is a random spinor field taken from a Gaussian distribution with norm one.

Inversion

In addition to even/odd preconditioning in the HMC algorithm as described above, it can also be used to speed up the inversion of the fermion matrix.

Due to the factorization (B-3) the full fermion matrix can be inverted by inverting the two matrices appearing in the factorization

$$\begin{pmatrix} M_{ee}^{\pm} & M_{eo} \\ M_{oe} & M_{oo}^{\pm} \end{pmatrix}^{-1} = \begin{pmatrix} 1 & (M_{ee}^{\pm})^{-1} M_{eo} \\ 0 & (M_{oo}^{\pm} - M_{oe}(M_{ee}^{\pm})^{-1} M_{eo}) \end{pmatrix}^{-1} \begin{pmatrix} M_{ee}^{\pm} & 0 \\ M_{oe} & 1 \end{pmatrix}^{-1}.$$

The two factors can be simplified as follows:

$$\begin{pmatrix} M_{ee}^{\pm} & 0 \\ M_{oe} & 1 \end{pmatrix}^{-1} = \begin{pmatrix} (M_{ee}^{\pm})^{-1} & 0 \\ -M_{oe}(M_{ee}^{\pm})^{-1} & 1 \end{pmatrix}$$

and

$$\begin{aligned} &\begin{pmatrix} 1 & (M_{ee}^{\pm})^{-1} M_{eo} \\ 0 & (M_{oo}^{\pm} - M_{oe}(M_{ee}^{\pm})^{-1} M_{eo}) \end{pmatrix}^{-1} \\ &= \begin{pmatrix} 1 & -(M_{ee}^{\pm})^{-1} M_{eo} (M_{oo}^{\pm} - M_{oe}(M_{ee}^{\pm})^{-1} M_{eo})^{-1} \\ 0 & (M_{oo}^{\pm} - M_{oe}(M_{ee}^{\pm})^{-1} M_{eo})^{-1} \end{pmatrix}. \end{aligned}$$

The complete inversion is now performed in two separate steps: First we compute for a given source field $\phi = (\phi_e, \phi_o)$ an intermediate result $\varphi = (\varphi_e, \varphi_o)$ by:

$$\begin{pmatrix} \varphi_e \\ \varphi_o \end{pmatrix} = \begin{pmatrix} M_{ee}^{\pm} & 0 \\ M_{oe} & 1 \end{pmatrix}^{-1} \begin{pmatrix} \phi_e \\ \phi_o \end{pmatrix} = \begin{pmatrix} (M_{ee}^{\pm})^{-1} \phi_e \\ -M_{oe}(M_{ee}^{\pm})^{-1} \phi_e + \phi_o \end{pmatrix}.$$

This step requires only the application of M_{oe} and $(M_{ee}^{\pm})^{-1}$, the latter of which is given by Eq (B-4). The final solution $\psi = (\psi_e, \psi_o)$ can then be computed with

$$\begin{pmatrix} \psi_e \\ \psi_o \end{pmatrix} = \begin{pmatrix} 1 & (M_{ee}^{\pm})^{-1} M_{eo} \\ 0 & (M_{oo}^{\pm} - M_{oe}(M_{ee}^{\pm})^{-1} M_{eo}) \end{pmatrix}^{-1} \begin{pmatrix} \varphi_e \\ \varphi_o \end{pmatrix} = \begin{pmatrix} \varphi_e - (M_{ee}^{\pm})^{-1} M_{eo} \psi_o \\ \psi_o \end{pmatrix},$$

where we defined

$$\psi_o = (M_{oo}^{\pm} - M_{oe}(M_{ee}^{\pm})^{-1}M_{eo})^{-1}\varphi_o\,.$$

Therefore the only inversion that has to be performed numerically is the one to generate ψ_o from φ_o and this inversion involves only an operator that is better conditioned than the original fermion operator.

B.2 Multiple mass solver for twisted mass fermions

In this appendix we show that within the Wilson twisted mass fermion formulation it is possible to apply the multi mass solver (MMS) [171, 172, 173] method to the conjugate gradient (CG) algorithm. We will call this algorithm CG-M and give here the details of the implementation.

The advantage of the MMS is that it allows the computation of the solution of the following linear system

$$(A + \sigma)\, x - b = 0 \tag{B-13}$$

for several values of σ simultaneously, using only as many matrix-vector operations as the solution of a single value of σ requires.

We want to invert the Wilson twisted mass operator at a certain value of the twisted mass μ_0 obtaining automatically all the solutions for other values μ_k (with $|\mu_k| \geq |\mu_0|$). We use the twisted mass operator $D_{\rm tm}$ as defined in Eq. (1-47) and denote the number of additional twisted mass values with N_m. The operator can be split up as

$$D_{\rm tm} = D_{\rm tm}^{(0)} + i(\mu_k - \mu_0)\gamma_5\tau^3, \qquad D_{\rm tm}^{(0)} = D_{\rm W} + m_0 + i\mu_0\gamma_5\tau^3\,. \tag{B-14}$$

The trivial observation is that

$$D_{\rm tm}D_{\rm tm}^{\dagger} = D_{\rm tm}^{(0)}D_{\rm tm}^{(0)\dagger} + \mu_k^2 - \mu_0^2\,, \tag{B-15}$$

where we have used $\gamma_5 D_W \gamma_5 = D_W^{\dagger}$. Now clearly we have a shifted linear system $(A+\sigma_k)x - b = 0$ with $A = D_{\rm tm}^{(0)}D_{\rm tm}^{(0)\dagger}$ and $\sigma_k = \mu_k^2 - \mu_0^2$. In the following we describe the CG-M algorithm in order to solve the problem $(A + \sigma_k)x - b = 0$. The lower index indicates the iteration steps of the solver, while the upper index k refers to the shifted problem with σ_k.

$$
\begin{aligned}
&\mathrm{CG-M\ \ Algorithm}\\
&x_0^k = 0, r_0 = p_0^k = b, \alpha_{-1} = \zeta_{-1}^k = \zeta_0^k = 1, \beta_0^k = \beta_0 = 0\\
&\text{for}\ \ i = 0, 1, 2, \cdots\\
&\quad \alpha_n = \frac{(r_n, r_n)}{(p_n, Ap_n)}\\
&\quad \zeta_{n+1}^k = \frac{\zeta_n^k \alpha_{n-1}}{\alpha_n \beta_n (1 - \frac{\zeta_n^k}{\zeta_{n-1}^k}) + \alpha_{n-1}(1 - \sigma_k \alpha_n)}\\
&\quad \alpha_n^k = \alpha_n \frac{\zeta_{n+1}^k}{\zeta_n^k}\\
&\quad x_{n+1}^k = x_n^k + \alpha_n^k p_n^k\\
&\quad x_{n+1} = x_n + \alpha_n p_n\\
&\quad r_{n+1} = r_n - \alpha_n A p_n\\
&\quad \text{convergence check}\\
&\quad \beta_{n+1} = \frac{(r_{n+1}, r_{n+1})}{(r_n, r_n)}\\
&\quad p_{n+1} = r_{n+1} + \beta_{n+1} p_n\\
&\quad \beta_{n+1}^k = \beta_{n+1} \frac{\zeta_{n+1}^k \alpha_n^k}{\zeta_n^k \alpha_n}\\
&\quad p_{n+1}^k = \zeta_{n+1}^k r_{n+1} + \beta_{n+1}^k p_n^k\\
&\text{end for}
\end{aligned}
$$

We give here the algorithm explicitly again, since it has a different definition of ζ_{n+1}^k compared to the one of Ref. [173]. This version allows to avoid roundoff errors when $\sigma_k = \mu_k^2 - \mu_0^2$ becomes too large.

We remind that when using a MMS the eventual preconditioning has to retain the shifted structure of the linear system. This means for example that it is not compatible with even/odd preconditioning.