The Tunneling Hybrid Monte-Carlo algorithm

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ABSTRACT

The hermitian Wilson kernel used in the construction of the domain-wall and overlap Dirac operators has exceptionally small eigenvalues that make it expensive to reach high-quality chiral symmetry for domain-wall fermions, or high precision in the case of the overlap operator. An efficient way of suppressing such eigenmodes consists of including a positive power of the determinant of the Wilson kernel in the Boltzmann weight, but doing this also suppresses tunneling between topological sectors. Here we propose a modification of the Hybrid Monte-Carlo algorithm which aims to restore tunneling between topological sectors by excluding the lowest eigenmodes of the Wilson kernel from the molecular-dynamics evolution, and correcting for this at the accept/reject step. We discuss the implications of this modification for the acceptance rate.
I. INTRODUCTION

The domain-wall-fermion (DWF) \cite{1, 2} formulation of lattice QCD is based on a hermitian, four-dimensional, super-critical Wilson-like kernel $H_W = \gamma_5 D_W$, which can be interpreted as governing propagation into an extra, fifth lattice dimension with coordinate \( s = 1, \ldots, L_5 \).\(^1\) For sufficiently large \( L_5 \), right-handed and left-handed four-dimensional quark fields live on walls opposite of each other across this fifth dimension, and are represented by wave functions which are bound to these walls. As long as \( L_5 \) is finite, the right-handed and left-handed quarks are coupled through a “residual” mass \( \beta \), an effective chiral-symmetry breaking mass term originating from the overlap of their wave functions.

In the free theory \cite{1, 6} or in perturbation theory \cite{5, 7} these wave functions are exponentially bound to the walls, and therefore the residual mass is exponentially small. It is proportional to \( e^{-\alpha_{\text{min}} L_5} \) where the gap of the transfer-matrix hamiltonian, \( \alpha_{\text{min}} \), is non-zero whenever the gap of the free \( H_W \) is. On realistic gauge field configurations, however, the super-critical \( H_W \) has a spectrum reaching all the way down to zero \cite{8, 9}, with a mobility edge that, by definition, separates a low-eigenvalue spectrum of localized modes from a high-eigenvalue spectrum of delocalized, or extended, modes. The near-zero modes are localized with a range of order the lattice spacing \( a \), provided that the bare gauge coupling \( g \) and domain-wall height \( M \) are chosen to be away from the region in the phase diagram where the mobility edge is less than order one in lattice units \cite{10}.

An additional contribution to the residual mass is coming from the near-zero modes. It can be approximated by the integrated spectral density \( \int_{-1/L_5}^{1/L_5} d\lambda \rho(\lambda) \), where \( \rho(\lambda) \) is the ensemble-average spectral density of \( H_W \) (see Appendix C of Ref. \[5\]). If the near-zero spectral density depends only mildly on \( \lambda \), this contribution is roughly equal to \( \rho(0)/L_5 \). Therefore, as \( L_5 \) is increased, eventually the slowly falling contribution of the near-zero modes becomes dominant. Much effort has been directed toward finding methods to suppress their presence, i.e., to make \( \rho(\lambda) \) as small as possible for \( |\lambda| \lesssim 1/L_5 \). The same goal is relevant for overlap simulations, where suppression of near-zero modes is equally important in order to make it affordable to compute the sign function \( \epsilon(H_W) = H_W/|H_W| \), which is at the heart of the construction of the overlap operator \cite{11}, to high precision.

A “surgical” method for suppressing the near-zero modes consists of modifying \( B \), the original domain-wall or overlap Boltzmann weight, to \( B \det(H_W^2) \) \cite{12, 13}. The first thing to note is that introducing the auxiliary determinant of \( H_W^2 \) into the Boltzmann weight does not change the universality class. Indeed, apart from a change in the lattice spacing, this modification does not affect the long-distance physics, because in itself the Wilson kernel \( H_W \) is a Dirac operator with a mass \( m_0 \) of the order of the cutoff, \( |am_0| = O(1) \).

It has been demonstrated that, after re-adjusting the lattice spacing to the same value, the inclusion of \( \det(H_W^2) \) in the path integral results in a significant reduction in the near-zero mode density \cite{12, 13}. This is easily understood at an intuitive level because the Boltzmann weight now contains an extra factor of \( \lambda^2 \) for each eigenmode of \( H_W \), including in particular the low-lying, localized ones. Provided we stay away from the region where

\(^1\) There is much freedom in choosing the super-critical kernel, and the detailed form is not important for this paper. For simplicity, we will assume the common choice that \( D_W \) is the standard Wilson operator with bare mass \( m_0 \) in the region \(-2 < am_0 < 0\). The domain-wall height is \( M = |am_0| \).
the mobility edge is too small, the near-zero modes of $H_W$ are associated with lattice-scale dislocations in the gauge field \[9\]. One may expect the inclusion of $\det(H_W^2)$ to deplete the near-zero modes efficiently because this method suppresses selectively only those—relatively rare—dislocations that happen to support a near-zero mode. In other words, once we re-adjust the bare coupling such that the gauge field regains the same average “roughness” as before the insertion of $\det(H_W^2)$, and hence the lattice spacing is unchanged, we find that only the “troublesome” dislocations leading to exceptionally small eigenmodes of $H_W^2$ have been removed. The new spectral density behaves like $\rho(\lambda) \sim \lambda^2$ at small $\lambda$, and the contribution to the residual mass is of order $\int_{-1/L_5}^{1/L_5} d\lambda \rho(\lambda) \sim 1/L_5^3$, to be compared with a $1/L_5$ suppression for a spectral density that does not vanish at $\lambda = 0$.

In spite of their largely negative role discussed above, the near-zero modes also play what might be called a positive role. The gauge-field configuration space is divided into topological sectors whose boundaries are defined by configurations where $\det(H_W) = 0$. If we continuously follow a curve in the gauge-field space, it follows that the topological charge, as measured through the index of the overlap operator, changes by one unit precisely when one of the eigenvalues of $H_W$ changes sign \[14\].

To date, the Hybrid Monte Carlo (HMC) algorithm \[15\] is the de facto algorithm for dynamical fermion simulations. The question is whether the trajectories generated by the HMC algorithm, or by one of its variants, will sample all topological sectors. Having fewer, even much fewer, near-zero eigenvalues would not constitute a problem all by itself, so long as these eigenvalues could move around and cross zero relatively freely. Unfortunately, the inclusion of $\det(H_W^2)$ not only reduces the near-zero spectral density significantly, but also completely suppresses the transitions between topological sectors. The reason is that, during the molecular-dynamics (MD) evolution phase of the HMC algorithm, the surfaces of co-dimension one where $\det(H_W) = 0$ constitute infinite-energy barriers. As a result, only one topological sector is sampled, typically the sector with zero topological charge. This constitutes a breakdown of ergodicity. In other words, the effect of adding in $\det(H_W^2)$ while using the standard HMC algorithm is to generate an ensemble according to the Boltzmann weight $\mathcal{B} \det(H_W^2) \delta(Q - q)$, where $Q$ is the topological charge operator, and $q$ the topological charge of the initial configuration. Thus the correct weight $\mathcal{B} \det(H_W^2)$ is reproduced in just one topological sector, while the weight vanishes in all other sectors.\[2\]

Unlike $\theta$-vacua, fixed-topological-charge vacua do not cluster. This leads to enhanced finite-volume effects, which, already for single-particle masses, decrease only with an inverse power of the volume, and, moreover, increase with the inverse pion mass \[16\]. This must be compared with the usual exponential fall-off of finite-size effects in QCD with massive quarks.

In this paper, we propose a modification of the HMC algorithm intended to restore ergodicity by allowing for zero crossings in the spectrum of $H_W$ even though $\det(H_W^2)$ is part of the Boltzmann weight. The generated ensemble will then reproduce the correct Boltzmann weight $\mathcal{B} \det(H_W^2)$ for configurations in all sectors. We will refer to this modification as the “Tunneling Hybrid Monte Carlo” or THMC algorithm.

The key idea is that, during the MD evolution, the usual HMC fermion force associated with $H_W^2$ is replaced by the force derived from a modified operator of the form of $H_W^2 + \alpha Q^\dagger Q$. The effect of the new term, $\alpha Q^\dagger Q$, is to lift the (lowest few) near-zero eigenvalues of $H_W^2$.

\[2\] We assume that there are no exactly massless quarks, and thus $\mathcal{B} > 0$ in all topological sectors.
This removes the infinite-energy barriers. As a result, the MD evolution can, and, we argue, will, visit all topological sectors. Using a trick reminiscent of renormalization-group blocking, the original determinant det$(H^2_W)$ can be factorized as det$(H^2_W + \alpha Q\dagger Q)$ times another term that corrects for the lifted near-zero modes. The original Boltzmann weight $B\det(H^2_W)$ is restored by incorporating the correcting factor in the accept/reject step that separates successive MD trajectories. While this procedure must lead to some reduction in acceptance, we will give arguments suggesting that that reduction may be affordable, given the physical merits of the generated ensemble. This paper does not as yet contain any numerical tests of the algorithms; these will have to be carried out in the future.

This paper is organized as follows. In Sec. II we set up the framework and explain the basic idea. In Sec. III we discuss the conceptually simplest realization of the algorithm, in which the new term that lifts the near-zero eigenvalues, $\alpha Q\dagger Q$, is chosen deterministically. The resulting implementation of the algorithm may not be very practical because of its cost. A more affordable implementation of the algorithm, introduced in Sec. IV, is based on a stochastic choice of the new term. In Sec. V we discuss reasonable choices for the parameters of the algorithm, and we end with our conclusions in Sec. VI. Some technicalities are relegated to two appendices.

II. THE BASIC IDEA

We will consider a lattice gauge theory with partition function

\begin{align}
Z &= \int DU \exp(-S_g(U)) \det(H^2_W(U)) \\
&= \int DU D\phi D\psi \exp(-S_g(U) - S_{pf}(U)) ,
\end{align}

where $S_g$ is the (unspecified) gauge action, and once again $H_W$ is the hermitian, super-critical Wilson operator. The QCD partition function should of course also include the physical domain-wall or overlap fermion determinant for each quark flavor. However, since we are concerned only with the effects of including the unphysical determinant det$(H^2_W)$, we have dropped the determinants representing the physical quarks. The continuum limit of the lattice theory (2.1) is thus a pure Yang-Mills theory.

In Eq. (2.1b) the determinant of $H^2_W$ has been rewritten as a pseudo-fermion partition function. If ergodicity were to hold, the HMC algorithm would generate an ensemble of configurations $U_i$ with a probability measure

$$
\mathcal{P}_g(U) = Z^{-1} \exp(-S_g(U)) \det(H^2_W(U)) ,
$$

by alternately updating the pseudo-fermion field $\phi$ and updating the gauge field $U$. As explained in the Introduction, the standard HMC algorithm in fact fails to be ergodic because of the zero modes of $H_W$, and this is what we seek to amend with the THMC variant.

Let us recall how the HMC algorithm normally works (for recent reviews, see Ref. [17]). An updating cycle begins by generating a new pseudo-fermion field via a heat bath. A random complex vector $\xi$ is drawn from a gaussian ensemble with unit width, that is, with probability distribution $P(\xi) \propto \exp(-\xi\dagger \xi)$, followed by setting

$$
\phi = H_W(U)\xi .
$$
Thus the probability distribution for $\phi$ is $\mathcal{P}(\phi) \propto \exp(-\phi^\dagger H^2_W(\mathcal{U})\phi)$. A set of fictitious momenta is similarly drawn, corresponding to the free action $S_\pi = \frac{1}{2} \sum_{x,\mu,a} \pi^2_{x,\mu,a}$. The gauge-field update then consists of two steps. First, the initial configuration of gauge field and conjugate momenta, $\{\mathcal{U}, \pi\}$, is evolved along an MD trajectory by numerically solving the classical Hamilton equations with some “guiding” hamiltonian $\mathcal{H}_{MD}$. In the most straightforward case, one takes as guiding hamiltonian

$$\mathcal{H}_{MD} = S_\pi(\pi) + S_g(\mathcal{U}) + S_{pf}(\mathcal{U}).$$

(2.4)

The gauge-field dependence of $S_{pf}$ comes from the operator $H^2_W(\mathcal{U})$ in Eq. (2.1c). We have suppressed the dependence of $S_{pf}$ on the pseudo-fermion field $\phi$, which is kept fixed during the MD evolution. Hamilton’s equations are numerically solved with some symmetric integrator with a non-zero step size $\delta \tau$, for a number of steps $n_{MD} = \tau_{MD}/\delta \tau$. This introduces “step-size” errors, which at the end of an MD trajectory are corrected for by a Metropolis test: the final configuration $\{\mathcal{U}', \pi'\}$ is accepted, which means that $\mathcal{U}'$ becomes the initial gauge-field configuration for the next cycle, or rejected, in which case the next cycle begins with the same initial gauge-field configuration $\mathcal{U}$, with probability

$$P_{\text{accept}} = \min\{1, \exp(\mathcal{H}(\pi, \mathcal{U}) - \mathcal{H}(\pi', \mathcal{U}'))\},$$

(2.5)

where we have taken $\mathcal{H} = \mathcal{H}_{MD}$. Assuming ergodicity, after thermalization the generated sets of configurations $\{\mathcal{U}_i, \pi_i, \phi_i\}$ follow the probability distribution

$$\mathcal{P}(\mathcal{U}, \pi, \phi) = Z^{-1} \exp(-\mathcal{H}(\mathcal{U}, \pi, \phi)),$$

(2.6)

which, upon integrating over the pseudo-fermions and fictitious momenta, reduces to the probability distribution (2.2).

In many applications, the randomness of the fictitious momenta and the pseudo-fermions at the start of each MD trajectory would be sufficient to make the algorithm ergodic [18]. However, in the case at hand this is hampered by the existence of zero modes of $H^2_W$. During the MD evolution $\mathcal{H}_{MD}(\mathcal{U}, \pi, \phi)$ plays the role of “energy.” The pseudo-fermion action, which is part of $\mathcal{H}_{MD}(\mathcal{U}, \pi, \phi)$, becomes infinite whenever $H^2_W(\mathcal{U})$ has an exact zero mode. Because the initial energy is always finite, and since it is (approximately) conserved during the (discretized) MD evolution, (in practice) the MD evolution never passes through any configuration where $\det(H^2_W(\mathcal{U})) = 0$. As explained in the introduction, this implies that only one topological sector is sampled.

What one would like to do is to somehow remove the infinite-energy barriers separating topological sectors during the MD evolution. The basic philosophy of the HMC algorithm allows for this option: one is free to choose $\mathcal{H}$ in Eq. (2.3) different from the guiding hamiltonian $\mathcal{H}_{MD}$. Eliminating the infinite-energy barriers necessarily means that $\mathcal{H}_{MD}$ cannot be given by Eq. (2.4) if $S_{pf}$ is given by Eq. (2.1c). But any “mistake” made by choosing a different guiding hamiltonian can be corrected for at the accept/reject step if the appropriate hamiltonian is used in Eq. (2.5). It should of course be anticipated that the discrepancy between the two hamiltonians will lead to reduced acceptance, an issue that we will return to below.

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3 We note that it is not possible to regain tunneling by choosing $\delta \tau$ to be very large because this must lead to significant drop in acceptance and ultimately to integrator instabilities [17].
We thus wish to split the hamiltonian of the metropolis test into two parts:

\[ \mathcal{H} = \mathcal{H}_{MD} + \mathcal{H}_{\text{corr}} \quad , \]

where contributions of near-zero modes are kept out of the guiding hamiltonian \( \mathcal{H}_{MD} \), and are accounted for by the correction \( \mathcal{H}_{\text{corr}} \), to be added in the accept/reject step. This can be done as follows. Borrowing from the way ultra-violet modes are integrated out in a Renormalization-Group (RG) block transformation for a bilinear action, one can show that the fermion determinant can be split as

\[ \text{det}(H_W^2) = \alpha^{-n} \text{det}(\mathcal{M}) \text{det}(\mathcal{A}) \quad , \]

\[ \mathcal{M} = H_W^2 + \alpha Q^\dagger Q \quad , \]

\[ \mathcal{A}^{-1} = \alpha^{-1} + Q H_W^{-2} Q^\dagger \quad . \]

Here \( H_W \) and \( \mathcal{M} \) are \( N \times N \) matrices, \( \mathcal{A} \) is an \( n \times n \) matrix, and \( Q \) is an \( n \times N \) matrix, usually referred to as the blocking kernel in the RG context. For a proof of Eq. (2.8), see App. A.

Here we will choose the kernel \( Q \) such that \( Q^\dagger Q \) projects onto the lowest \( n \) eigenmodes of \( H_W^2 \), either exactly or approximately. Let \( |\psi_i\rangle \), \( i = 1, \ldots, n \), be the eigenvectors of the first-order operator \( H_W \) with eigenvalues \( \lambda_i \) chosen such that \( \{\lambda_i^2\}_{i=1}^n \) is the set of \( n \) smallest eigenvalues of \( H_W^2 \). Now choose another set of \( n \) vectors \( |\chi_i\rangle \) such that

\[ \mathcal{I}_{ij} = \langle \psi_i | \chi_j \rangle \approx \delta_{ij} \quad , \]

\[ i, j = 1, \ldots, n \quad . \]

and define \( Q^\dagger \) to be the \( N \times n \) matrix whose \( i \)-th column is the vector \( |\chi_i\rangle \). Equations (2.8b) and (2.8c) then turn into

\[ \mathcal{M} = H_W^2 + \alpha \sum_{i=1}^{n} |\chi_i\rangle \langle \chi_i| \quad , \]

\[ (\mathcal{A}^{-1})_{ij} = \alpha^{-1} \delta_{ij} + \langle \chi_i | H_W^{-2} | \chi_j \rangle \quad . \]

Assuming Eq. (2.9), the rightmost term in Eq. (2.10a) lifts the \( n \) lowest eigenvalues of \( H_W^2 \), and the corresponding eigenvalues of \( \mathcal{M} \) are of order \( \alpha \). All the remaining eigenvalues of \( H_W^2 \) are more or less unaffected, if we choose \( \alpha \) to be of order \( \lambda_{n+1}^2 \).

Using Eq. (2.8a) we may write

\[ \text{det}(H_W^2) = \text{det}(\mathcal{A}) \int D\phi^\dagger D\phi \ exp(-S_{pf}) \quad , \]

\[ S_{pf} = \phi^\dagger \mathcal{M}^{-1} \phi \quad . \]

The THMC algorithm is based on choosing \( \mathcal{H}_{MD} \) as in Eq. (2.4) with \( S_{pf} \) given by Eq. (2.11a). In order to recover the desired Boltzmann weight (2.2), we will include \( \text{det}(\mathcal{A}) \)

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4 Equation (2.8) is true for an arbitrary choice of the kernel matrix \( Q \) and of the parameter \( \alpha \neq 0 \). There is no restriction on \( n \) and \( N \) (curiously, it is valid even for \( n > N \)). Furthermore, Eq. (2.8) holds in a limiting sense even if \( H_W \) has an exact zero mode.

5 As discussed later in detail, we have in mind choosing \( n \) very small and, thus, \( n \ll N \).

6 Following common practice to leave unspecified the overall normalization of a path-integral measure, we disregard from now on the normalization factor \( \alpha^{-n} \) in Eq. (2.8a).
in the correction term \( \exp(-H_{\text{corr}}) \), cf. Eqs. (2.7) and (2.5). The definition of the THMC algorithm is not complete until a method for choosing the vectors \( |\chi_i\rangle \) is specified. There are two basic options: the \( |\chi_i\rangle \) can be chosen deterministically or stochastically, and this leads to the concrete implementations of THMC presented in Sec. III and Sec. IV, respectively. In the latter case, \( \exp(-H_{\text{corr}}) \) is not precisely equal to \( \det(A) \), as we will see. In both implementations the gauge field will be distributed according to the probability measure (2.2).

Using only the new form of the guiding hamiltonian, it is easy to see that all topological sectors will now be sampled. Any configuration at a crossing point between two adjacent topological sectors has an exact zero mode of \( H_W \). But, so long as Eq. (2.9) holds, Eq. (2.10a) implies that the spectrum of \( \mathcal{M} \) has an \( O(\alpha) \) gap, even if \( H_W \) happened to have an exact zero mode. Thus, the excess MD energy associated with a crossing is of order \( 1/\alpha \). This is a finite number, because of our choice of \( \alpha \). This means that the initial MD energy has a considerable probability of being larger than the minimal MD energy needed for the crossing. As a result, the MD trajectory can pass through configurations where \( H_W \) has an exact zero mode. Typically, both at the start and end points of an MD trajectory the gauge-field configuration will be well inside some topological sector, so that neither \( \det(A(U)) \) nor \( \det(A(U')) \) will be exceedingly small. This already suggests that there is no inherent reason that the acceptance rate should be intolerably small. We will discuss the issue of acceptance when introducing concrete implementations in the next two sections.

III. DETERMINISTIC IMPLEMENTATION

In this section we present the conceptually simplest implementation of THMC. It is defined by setting

\[
|\chi_i\rangle = |\psi_i\rangle ,
\]

at each time step during the MD evolution, where \( |\psi_i\rangle \) are the \( n \) lowest eigenmodes of \( H_W^2 \) on the updated gauge field. It follows that \( I_{ij} = \delta_{ij} \) in Eq. (2.9), and also that

\[
\mathcal{M} = H_W^2 + \alpha \sum_{i=1}^{n} |\psi_i\rangle\langle\psi_i|,
\]

\[
(A^{-1})_{ij} = \left( \alpha^{-1} + \lambda_i^{-2} \right) \delta_{ij}.
\]

The representation of the partition function which is being simulated is thus

\[
Z = \int DU DU' D\phi D\phi' \det(A) \exp(-S_g - S_{pf}) ,
\]

with \( S_{pf} \) given by Eq. (2.11b). The guiding hamiltonian is given by Eq. (2.4), and the accept/reject step is done with

\[
P_{\text{accept}} = \min \left\{ 1, \exp(\mathcal{H}_{\text{MD}}(\pi, U) - \mathcal{H}_{\text{MD}}(\pi', U')) \frac{\det(A(U'))}{\det(A(U))} \right\} .
\]

Comparing to Eqs. (2.5) and (2.7), we see that this amounts to choosing \( H_{\text{corr}} = -\log \det(A) \). We note that since \( \mathcal{M} \) cannot be written in the form \( X^\dagger X \) with \( X \) local,
one updates the pseudo-fermions via $\phi = r(\mathcal{M}(U))\xi$ with some high-accuracy rational approximation\(^7\) $r(x) \simeq \sqrt{x}$.

While conceptually the simplest, the deterministic implementation of THMC involves several costly ingredients. The $n$ smallest eigenvalues of $H_W^2$ and the corresponding eigenmodes must be re-calculated after each MD step. For the calculation of the fermion force we have to monitor for level crossings during each MD time increment.\(^8\) If no level crossings occurred, the calculation of the fermion force requires

$$\delta_{x,\mu} (|\psi_i\rangle\langle\psi_i|) = (\delta_{x,\mu}|\psi_i\rangle\langle\psi_i| + |\psi_i\rangle\langle\psi_i|\delta_{x,\mu}|\psi_i\rangle) ,$$

$$\delta_{x,\mu}|\psi_i\rangle = - (H_W - \lambda_i)^{-1} (1 - |\psi_i\rangle\langle\psi_i|) (\delta_{x,\mu}H_W) |\psi_i\rangle ,$$

where the last equality follows from first-order perturbation theory, and

$$\delta_{x,\mu} = i \left( U_{x,\mu} \frac{\partial}{\partial U^T_{x,\mu}} - \text{h.c.} \right ) .$$

The numerical evaluation of $\delta_{x,\mu}|\psi_i\rangle$ using Eq. (3.5a) may be difficult in the vicinity of a level-crossing point. For a practical solution to this problem, see e.g. Ref. [19].\(^9\)

The situation is different if level crossing occurs between levels $n$ and $n + 1$. In this case the set of $n$ lowest eigenmodes changes discontinuously which, according to Eq. (3.2a), results in a discontinuity in the operator $\mathcal{M}$. The discontinuous change in $S_{pf}$ and, by Eq. (2.4), in the MD energy, gives rise to a $\delta$-function singularity in the fermion force. This singularity must be handled by a reflection/refraction step analogous to that discussed in Ref. [21]. The discussion of Ref. [21] addresses specifically the discontinuity of the overlap operator arising from a zero crossing in the spectrum of the corresponding kernel operator, here assumed to be $H_W$. But the recipe of Ref. [21] is actually rather general, and can be easily adapted to the case at hand. This completes the definition of the deterministic implementation of THMC.

We comment in passing that one might be tempted to consider the alternative of evolving continuously the $n$ eigenmodes that were the lowest levels on the initial configuration. This, however, would constitute a breakdown of reversibility of the MD evolution whenever the set of $n$ lowest eigenmodes on the final configuration is different from the $n$ states that have evolved continuously from the initial set.\(^10\) Thus, reflection/refraction steps are unavoidable.

The cost of the deterministic implementation of THMC involves two components: first, the extra cost of each MD step, and second, the reduction in acceptance due to the omission of $\det(A)$ from the MD evolution. We discuss them in turn.

In a dynamical overlap simulation,\(^11\) in order to improve the accuracy of the evaluation of the sign function of $H_W$ one usually computes $n_{oo}$ of the lowest eigenvalues of $H_W^2$, alongside

\(^7\) By construction, $\mathcal{M}$ does not have any extremely small eigenvalues, and we expect that an accurate rational approximation of $\sqrt{\mathcal{M}}$ is feasible with relatively few poles.

\(^8\) We assume that for some $n' > n$, the $n'$ lowest eigenmodes evolve slowly enough that one can track their evolution from time $\tau$ to $\tau + \delta \tau$.

\(^9\) In an overlap simulation, it is known that the presence of roughly degenerate near-zero eigenvalues of $H_W$ may lead to large fermion forces and to low acceptance rates. Using THMC may help indirectly, because the presence of $\det(H_W^2)$ will lead to much reduced density of low-lying eigenvalues. For a direct approach to solving this problem, see Ref. [20].

\(^10\) We thank Urs Heller for this observation.

\(^11\) For a recent review, see Ref. [22].
with their eigenfunctions and the variations defined in Eq. (3.5). Thus, so long as we choose \( n \) in Eq. (2.10) to be less than or equal to \( n_{ov} \), there is no extra cost involved in using them for the deterministic THMC algorithm.

The exception is the occurrence of level crossing between eigenvalues \( n \) and \( n + 1 \) of \( H^2_W \), as explained above, must be handled by a reflection/refraction step. This new reflection/refraction step represents an additional cost not present in an ordinary dynamical overlap simulation. We stress that the discontinuity encountered here results directly from the breakup of \( \det(H^2_W) \) in Eq. (2.8a). The discontinuity in \( \det(M) \) is matched by a discontinuity in \( \det(A) \), such that \( \det(H^2_W) \) as a whole is continuous. Also, clearly, in this case there is no discontinuity in the corresponding overlap operator, because no eigenvalue of \( H_W \) has crossed zero. The cost of this new reflection/refraction step could be more tolerable than in the familiar overlap case, because the eigenfunctions of the crossing eigenvalues are both expected to be well localized, hence the cost of the necessary computation is likely to be independent of the volume. In addition, also the number \( n \) of eigenmodes kept out of the MD evolution is held fixed and small, independent of the volume (see also Sec. VI).

Omitting \( \det(A) \) from the MD evolution, or equivalently, performing the metropolis test with a hamiltonian \( H \) which is different from the guiding hamiltonian \( H_{MD} \), will in general decrease the acceptance. In App. B we consider a crude model to estimate this effect. According to this model, when a single eigenmode is omitted from the MD evolution, the drop in acceptance is expected to be in the range of \( 1/3 \) to, at most, \( 1/2 \). When two eigenmodes are omitted, the drop in acceptance is in the range of roughly 50\% to 65\%. It is thus desirable to keep the number of eigenmodes relegated to \( \det(A) \) as small as possible, perhaps even \( n = 1 \). We return to this issue in Sec. V. In order to avoid confusion, we stress that in the stochastic implementation discussed in the next section there is an additional source for a reduction in acceptance.

### IV. STOCHASTIC IMPLEMENTATION

We now turn to a different version of THMC in which the vectors \( |\chi_i\rangle \) are kept fixed during the MD evolution. As we will see, a valid algorithm exists provided that the vectors \( |\chi_i\rangle \) are chosen stochastically. While the \( n \) lowest eigenmodes of \( H^2_W \) will have to be computed at the beginning and the end of each trajectory, this implementation avoids the costly operations of re-computing these eigenmodes and their gauge-field derivatives at every MD step. Also, no reflection/refraction steps are needed for the trivial reason that the vectors \( |\chi_i\rangle \) are not to be evolved.\(^{12}\) The stochastic implementation is thus more suitable for domain-wall fermion simulations, where these calculations are normally not done.

Before we proceed, we need to address a technical issue. Eigenfunctions of \( H_W \) are determined only up to an arbitrary overall phase. In Sec. III the undetermined overall phase dropped out (see in particular Eq. (3.2)), and this ambiguity thus was of no concern. For the stochastic implementation introduced below, the phase ambiguity will have to be resolved. If \( |\psi_i\rangle \) is an eigenmode with some arbitrary overall phase, we may for example

\(^{12}\) Of course, in an overlap simulation a reflection/refraction step is in principle still needed at a zero crossing of an eigenvalue of the kernel \( [22] \).
choose

\[ |\psi_i\rangle = \frac{\langle \hat{\psi}_i | 1 \rangle}{|\langle \hat{\psi}_i | 1 \rangle|} |\hat{\psi}_i\rangle . \tag{4.1} \]

Here \(|1\rangle\) stands for the vector with all component equal to one.\(^{13}\) It is easily seen that \(|\psi_i\rangle\) is still a normalized eigenvector, and that it is unchanged if we multiply \(|\hat{\psi}_i\rangle\) by some arbitrary phase.

We are now ready to introduce the stochastic implementation of THMC. At the start of an MD trajectory we compute, as before, the lowest \(n\) eigenvectors \(|\psi_i(U)\rangle\), which are now free of any phase ambiguity by virtue of Eq. (4.1). We then draw \(n\) random vectors \(|\eta_i\rangle\) from a gaussian ensemble with probability \(\exp(-\gamma \eta \overline{\eta})\), and set

\[ |\chi_i\rangle = |\psi_i(U)\rangle + |\eta_i \rangle . \tag{4.2} \]

Equivalently, the vectors \(|\chi_i\rangle\) can be thought of as \(n\) new complex bosonic fields (each carrying the same set of indices as a Wilson-fermion field) with their own Boltzmann weight \(\exp(-S_{ker})\), with kernel action

\[ S_{ker} = \gamma \sum_{i=1}^{n} \langle \chi_i - \psi_i(U) | \chi_i - \psi_i(U) \rangle . \tag{4.3} \]

With the proper (gauge-field-independent) normalization we then have

\[ \int D\chi D\chi^\dagger \exp(-S_{ker}) = 1 , \tag{4.4} \]

which we may thus insert into the original partition function Eq. (2.1), obtaining (with Eqs. (2.8a) and (2.11))

\[ Z = \int DUD\phi D\phi D\chi D\chi^\dagger \exp(-S_g - S_{pf} - S_{ker}) \det(A) . \tag{4.5} \]

The relation between the representation (4.5) of the partition function and the stochastic implementation of THMC parallels the relation between the representation (3.3) and the deterministic implementation. At the beginning of each trajectory a new set of pseudo-fermions \(\phi\), vectors \(|\chi_i\rangle\), and fictitious momenta \(\pi\) are drawn, each from the corresponding heat bath. The MD evolution is then carried out with the same guiding hamiltonian as before, cf. Eq. (2.4). Finally, the metropolis test (2.5) is done with the hamiltonian

\[ H = H_{MD} + S_{ker} - \log \det(A) . \tag{4.6} \]

Note that both \(H_{MD}\) and \(\det(A)\) are now functions of the (fixed) vectors \(|\chi_i\rangle\), but not directly of any eigenmode of \(H_U^2\). The initial and the final lowest \(n\) eigenmodes, \(|\psi_i(U)\rangle\) and \(|\psi_i(U')\rangle\), are only required for the evaluation of \(S_{ker}\).

The stochastic implementation of THMC generates the correct equilibrium distribution (2.2), for the same reasons that the original HMC algorithm works \(^{13}\). The algorithmic

\(^{13}\) Other choices for the reference vector can be made in case that the inner product \(|\langle \psi_i | 1 \rangle|\) would happen to be numerically unstable.
role of the new stochastic degrees of freedom, $|\chi_i\rangle$, parallels the role of the pseudo-fermions $\phi$ in the standard HMC algorithm (or, for that matter, in the deterministic implementation of THMC). In particular, satisfying the detailed balance condition \cite{15} requires that the classical MD evolution be reversible. This means that if $\{\mathcal{U}, \pi\}$ is evolved into $\{\mathcal{U}', -\pi'\}$ then $\{\mathcal{U}', \pi'\}$ is evolved into $\{\mathcal{U}, -\pi\}$, when all other degrees of freedom are held fixed. This now includes both $\phi$ and $|\chi_i\rangle$. Just like in ordinary HMC, using a symmetric integrator ensures the reversibility of the MD evolution in the stochastic implementation of THMC.

According to Eq. (4.2) the vectors $|\chi_i\rangle$ drawn from the heat bath depend on the initial gauge field. One might infer from this equation the erroneous conclusion that “reversibility is not satisfied.” If this were true, reversibility would not be satisfied in the original HMC algorithm in the first place, because according to Eq. (2.3) the pseudo-fermion field drawn from the heat bath depends on the initial gauge field as well. What drives this confusion is that, as a whole, the HMC algorithm is not reversible; it generates a Markov chain that converges to a specified probability distribution irrespective of initial conditions, hence irreversibly \cite{15, 17, 18}. The same goes for both versions of THMC. Reversibility is only required for the classical MD evolution, where, as stated above, it amounts to the interchangeability of $\{\mathcal{U}, \pi\}$ and $\{\mathcal{U}', -\pi'\}$ for any given, fixed set of values of the remaining degrees of freedom. Thus, reversibility of the MD evolution is guaranteed by the use of a symmetric integrator in the two versions of THMC, just like in standard HMC.

V. CHOICE OF PARAMETERS

The THMC algorithm has not been tested yet, and at present it is not known how well it works in practice. Assuming some particular choice of the physical-sector action (including the gauge action and some action (domain-wall or overlap) for the physical quarks) there are five parameters that determine the performance of the stochastic implementation of the algorithm: $n$, $\alpha$, $\gamma$, $\tau_{MD}$ and $\delta\tau$. In Sec. II we already argued that the “blocking” parameter $\alpha$ should be chosen equal to a typical small eigenvalue of $H_W^2$. In this section we discuss the remaining parameters of the stochastic implementation.

We begin with the parameter $\gamma$ occurring in $S_{ker}$, and explain why this parameter should be chosen to be of order one. We will assume that the initial and final low eigenmodes are all localized and, thus, that their components are of order one within their region of support. The norm\footnote{ Because $|\eta\rangle$ is not localized, the magnitude of its individual components is of order $1/\sqrt{V}$, where $V$ is the number of lattice sites.} of the random vector $|\eta\rangle$ is of order $1/\sqrt{\gamma}$. We immediately see that one cannot choose $\gamma$ too small, if we want $|\chi_i\rangle$ to be a reasonable approximation of $|\psi_i(U)\rangle$. If not, there would be no reason for the $n$ lowest eigenvalues of $H_W^2$ to be lifted by the addition of $\alpha \sum_i |\chi_i\rangle\langle\chi_i|$, cf. Eq. (2.10a).

The parameter $\gamma$ cannot be chosen arbitrarily large either. In fact, in the limit $\gamma \to \infty$ acceptance will vanish. For $\gamma \gg 1$ the vectors $|\chi_i\rangle$ drawn from the heat bath at the beginning of the trajectory will satisfy $|\chi_i\rangle = |\psi_i(U)\rangle + O(1/\sqrt{\gamma})$. At the end of the trajectory we will thus have

$$\gamma \langle\chi_i - \psi_i(U')|\chi_i - \psi_i(U')\rangle = \gamma \langle\psi_i(U) - \psi_i(U')|\psi_i(U) - \psi_i(U')\rangle,$$  \hspace{1cm} (5.1)

where we have neglected subleading terms in $1/\gamma$. The accumulated discrepancy
We note that Refs. [13, 23] actually used $\det(H^2_W)$ is a function of various simulation parameters (in particular the total MD time $\tau_{MD}$), but it is independent of $\gamma$. On the final configuration we would thus have $S_{\ker} \to \infty$ for $\gamma \to \infty$, implying that every trial configuration would be rejected. Combining both requirements, we must therefore choose $\gamma$ of order one.

There are three more parameters to discuss: the number of “lifted” eigenvalues $n$, the total MD time per trajectory $\tau_{MD}$, and the MD time increment $\delta \tau$. While existing numerical simulations of the super-critical $\det(H^2_W)$ using the ordinary HMC algorithm are confined to the sector with topological charge zero, the results can guide us in the choice of the remaining parameters. Our conclusion is that we advocate first trying THMC with values of $\tau_{MD}$ and $\delta \tau$ similar to those used in Refs. [12, 13, 23], and with a very small value of $n$, perhaps even $n = 1$.

The first interesting lesson is that, even at rather large lattice spacings (with $a^{-1}$ as low as 1.5 GeV), near-zero eigenvalues of $H_W$ were efficiently suppressed by the inclusion of $\det(H^2_W)$ in the Boltzmann weight. What this means is that, even if we were to choose an unrealistically large value for $n$ (e.g., $n = 100$), topology change during a given MD trajectory should still take place mostly through the zero crossing of just one, or very few, eigenvalues. In principle, then, THMC will restore ergodicity even if we allow for just one crossing per trajectory, which, in turn, is made possible by choosing any non-zero value for $n$. Because multiple crossings per trajectory should be much less frequent, a plausible strategy is to make no special effort to allow for them.

The next question is about the effect of the number $n$ of eigenmodes kept out of the MD evolution on the acceptance rate. As explained in Sec. III when using the THMC algorithm the acceptance rate will be less than one even in the limit $\delta \tau \to 0$ where $H_{MD}(\pi', U') = H_{MD}(\pi, U)$. In the deterministic implementation of Sec. III acceptance is controlled by the ratio $\det(A(U'))/\det(A(U))$ in the limit $\delta \tau \to 0$. Based on the model of App. B we have concluded that the acceptance rate is likely to go down with increasing $n$, and thus it is desirable to keep $n$ as small as possible.

In the stochastic implementation, the metropolis test involves the additional factor $\delta S_{\ker} = S_{\ker}(U') - S_{\ker}(U)$ (cf. Eq. (4.6)). Let us discuss the role of $\delta S_{\ker}$ at a qualitative level, considering first the case $n = 1$. Because $\gamma = O(1)$, we clearly have $S_{\ker}(U) = O(1)$ at the beginning of the trajectory. During the MD evolution the shape and location of the (localized) eigenmode $|\psi_1\rangle$ changes by an unknown amount, and at the end of the trajectory $S_{\ker}(U')$ will assume another $O(1)$ value. If we would now allow for larger values of $n$, the size of the interval containing the most probable values of $\delta S_{\ker}$ will increase. Positive values of $\delta S_{\ker}$, which one expects to occur a fraction of the time, will thus tend to further decrease the acceptance rate with increasing $n$. We conclude that one should indeed try to keep $n$ as small as possible.

This brings us to the trade-off between tunneling and acceptance. While it remains to be tested, we think that it is not implausible that THMC with values as small as $n = 1$ or $n = 2$ will produce an appreciable tunneling rate. Many of the results of Refs. [12, 13] are relevant for this question, but particularly illuminating is Fig. 2 of Ref. [23] which reports the results of an experimental two-flavor simulation. We consider the left panel, generated with $\det(H^2_W)$ in the Boltzmann weight. This plot shows the lowest few eigenvalues of $H_W$ as a function of MD time. The MD time interval corresponding to one trajectory was $\tau_{MD} = 0.5$, and with a very small value of $n$, perhaps even $n = 1$.

\footnote{We note that Refs. [13, 23] actually used $\det(H^2_U)/\det(H^2_W + \mu^2)$ with $\mu = O(1)$, in order to reduce the contribution of the large eigenvalues of $H^2_W$ to the fermion force.}
with $\tau_{MD}/\delta \tau = O(20)$. We learn from the plot that, frequently, $H_W$ has a small eigenvalue that changes by nearly 100% over a one-trajectory interval. This is an encouraging result, suggesting that if one would switch from HMC to THMC, there is a good change that zero crossings will take place.

Two worries immediately come to mind. Consider those trajectories where one eigenvalue has changed by a relatively large amount and became exceptionally small toward the end of the trajectory. As already noted, such trajectories are relatively frequent in the data. However, it is often true that that particular eigenvalue is not the smallest, nor even the next-smallest (in absolute value), at the beginning of the trajectory. If we would now re-run the trajectory from the same starting point with THMC, but use only $n = 1$ or $n = 2$ and no higher value, our selection of the initial lowest eigenvalue(s) would miss that particular eigenvalue, which is the best candidate for crossing. In such a case, THMC would not do its job, because the $|\chi_i\rangle$ would likely not have much overlap with the eigenvector corresponding to this eigenvalue, cf. Eq. (2.9). Nevertheless, for some fraction of the configurations the best-candidate eigenvalue did actually start as the smallest one. Thus, even $n = 1$ should produce a non-vanishing tunneling rate.

A related worry is that when an eigenvalue became exceptionally small at the end of the trajectory, often the final configuration was rejected. Once again, part of the answer is that some configurations were accepted even though they had one exceptionally small eigenvalue. If we would switch to THMC for the next trajectory, that eigenvalue would now be selected even with $n = 1$, and would have an appreciable chance to cross zero.

However, more importantly, with ordinary HMC, any eigenvalue must eventually be deflected away from zero because of the unboundedly growing fermion force. In contrast, with THMC any large repelling force originating from one of the $n$ eigenvalues which were the lowest ones at the beginning of the trajectory is eliminated. An eigenvalue motion that, with standard HMC, had been slowed down by the unboundedly growing repelling force, will speed up under THMC. Therefore, we expect that many of the eigenvalue flows that ended up very close to zero (but with, invariably, no crossing) when HMC was used, would move more rapidly when we switch to THMC. In fact, they may well cross zero during the same MD time interval, and end up with the opposite sign and well away from being exceptionally small by the end of the trajectory, thus increasing considerably the acceptance probability of the configuration at the end of the trajectory.

Finally, we consider how the location of an initially low-lying mode evolves. If the eigenmode would “drift” appreciably away from its original location, this would give rise to increased $S_{ker}$ on the final configuration, and once again decrease the acceptance rate. Worse, the overlap between the $|\chi_i\rangle$ and this mode would rapidly decrease, thus possibly decreasing the smallest eigenvalues of $\mathcal{M}$, and hence re-introducing barriers in the MD evolution. This, however, is unlikely to happen for the following reason.

Having an exceptionally low eigenvalue requires two things: values for some plaquettes substantially different from one, as well as a certain “fine tuning” of the link variables relative to each other. This picture, put forward in Ref. [9], is corroborated by the fact that large plaquette values are far more frequent compared to exceptionally low eigenvalues. Now, because the momenta conjugate to each link variable are basically uncorrelated with each

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16 This can be seen from the discontinuities in the spectral flows at integer values of the horizontal axis ("traj"): when a configuration was rejected the next trajectory was started with the same initial configuration as the previous one.
other, the likely outcome of the MD evolution is that any finely-tuned relation between local plaquettes will be quickly destroyed. Once again this expectation is supported by Fig. 2 of Ref. [23], which shows that exceptionally-low eigenvalues tend to evolve much more rapidly compared to the “bulk” of (not-so-small) eigenvalues. This supports the conjecture that indeed the necessary fine-tuned dislocations only exist for a relatively short MD time, in agreement with the general observation that dislocations supporting exceptionally low eigenvalues are rare. In contrast, a “drift” of the location of the eigenmode (in which the eigenvalue is kept very small) would require an orchestrated motion of the dislocation with almost no change in its shape, something which is very unlikely to happen.

The picture that emerges, then, is that of a localized eigenvector that remains more or less in place and localized, with a rapidly changing eigenvalue and, presumably, correspondingly rapid changes in its detailed shape. This implies that \( \langle \psi_i | \chi_i \rangle \) remains of order one, and thus no MD barrier is re-generated. We emphasize, as above, that this picture only needs to hold for a sizable fraction of the low-lying eigenmodes that exist at the start of the MD evolution trajectories.

VI. CONCLUSION

In this paper we proposed a new variant of the HMC algorithm. The aim of the tunneling HMC algorithm is to allow for eigenvalue crossings through zero even in situations where the determinant containing such eigenvalues is included in the Boltzmann weight. The application we considered explicitly is lattice QCD with domain-wall or overlap fermions and with the auxiliary determinant of \( H_2^W \). The THMC algorithm may find other applications as well.\(^{17}\)

A major issue is the competition between tunneling rate and acceptance. We have discussed in some detail why we believe that appreciable tunneling is not incompatible with reasonably high acceptance. Setting aside the details, the underlying reason why this can be true is that the difference between the guiding and metropolis hamiltonians, \( \mathcal{H} - \mathcal{H}_{MD} \), is not an extensive quantity. For any lattice volume, in order to allow for tunneling between topological sectors, we only need to keep a fixed, and very small, number of degrees of freedom outside of the guiding hamiltonian. Once ergodicity is restored via THMC, the correct Boltzmann weight will automatically be reproduced, in all topological sectors. Therefore, the cost of THMC does not grow with volume. We stress that our semi-quantitative conclusions will have to be tested numerically.

We discussed two concrete implementations of THMC, a deterministic and a stochastic one. We believe that the stochastic implementation of THMC is likely to be the most practical interest (especially for domain-wall simulations), because of its smaller computational overhead. For this to be the case, any further decrease in acceptance coming from the extra element present in the stochastic implementation, \( S_{\text{ker}} \), should not be too large.

In comparison to standard HMC, the extra cost of THMC comes partly from its more elaborate structure. For example, it takes more operations to perform a single multiplication of a vector by \( \mathcal{M} \), as compared to \( H_2^W \). However, it is likely that the major extra cost of THMC will come from reduced acceptance: if acceptance is a factor of two smaller, this

\(^{17}\) For example, we envisage using THMC as an ingredient in the simulation of the ghost sector of equivariantly gauge-fixed Yang-Mills lattice theories [24].
immediately translates into a factor of two extra cost. Any extra cost of THMC will have to be weighed against the physical merits of the generated ensemble. For example, the fixed-topology simulations of JLQCD \cite{13} give rise to enhanced finite-volume effects proportional to $1/(m_*^2 V)$ \cite{16}. Ultimately, the only way to keep such enhanced finite-size effects under systematic control is to simulate bigger lattice volumes, something that carries its own price tag. Clearly, it is the cost for “equal-quality” physics output which must be compared. For domain-wall fermion simulations, the extra cost of THMC must be balanced against the improvement of chiral symmetry.

Are there possible alternatives to THMC? The answer is yes. A simple approach is to replace $\det(H^2_W)$ by $\det(H^2_W + \epsilon^2)$ as the auxiliary determinant, where presumably $\epsilon^2$ would be chosen comparable to a typical small eigenvalue of $H^2_W$, much like the parameter $\alpha$ introduced in Eq. (2.8). Because there are no exact zero modes any more, one can simulate $\det(H^2_W + \epsilon^2)$ using ordinary HMC. \cite{18} In comparison with THMC, this avoids altogether any drop in acceptance associated with a non-zero $H - H_{MD}$. At the same time, if $\epsilon$ is chosen small enough, the low-lying eigenvalues of $H^2_W$ would still be suppressed. An additional benefit of simulating $\det(H^2_W + \epsilon^2)$ is that no new code needs to be written, and there are fewer new parameters that one has to experiment with for optimal performance.

In spite of the obvious advantages of this alternative, we believe that it is an open question which solution is better. When using $\det(H^2_W + \epsilon^2)$ one will have to compromise the value of $\epsilon$ between two conflicting requirements: the basic need to suppress the low-lying eigenvalues, and the need not to suppress them too much so as to allow for tunneling. In contrast, the advantage of THMC is that it solves one problem at a time: the reduction of an abundance of low-lying eigenvalues comes from $\det(H^2_W)$, while the restoration of tunneling comes from the modification of the algorithm.

While in this paper we have assumed that the auxiliary determinant is $\det(H^2_W)$, the THMC algorithm evidently generalizes to other even powers as this determinant. If the auxiliary determinant is $\det(H^{2k}_W)$, the near-zero spectral density will behave like $\rho(\lambda) \sim \lambda^{2k}$. In a domain-wall simulation, the residual mass will thus scale like $1/L_5^{2k+1}$. This constitutes a bigger pay-back for any increase of $L_5$ in the region where the residual mass is dominated by the near-zero modes.

The choice of the JLQCD collaboration to run fixed-topology dynamical overlap simulations stems from several technical advantages arising from the introduction of $\det(H^2_W)$. The (much!) smaller near-zero spectral density leads to a smaller range for $1/|H_W|$, and an affordable cost for an adequate approximation of the sign function $H_W/|H_W|$. The costly reflection/refraction step is not needed by design, because no eigenvalue of $H_W$ ever reaches zero during the MD evolution. With THMC, the same reduction in the near-zero spectral density is achieved, with all the ensuing advantages. Of course, reflection/refraction steps cannot be avoided if we want topology to change. \cite{19} But the number of attempted topology changes will remain small, and will not grow with the volume, because it is controlled by the number $n$ of eigenvalues which are relegated to $\det(A)$. As we have argued above, this number can be chosen to be very small. The cost of reflection/refraction steps should thus be tolerable.

Some of the difficulties in achieving a satisfactory topology-changing rate are inherent. While too-many small eigenvalues of $H_W$ is the problem at relatively large lattice spacing,
when the lattice spacing gets smaller eventually the situation changes, because the near-zero mode density decreases rapidly with the bare coupling. This means that tunneling becomes rare, even without the auxiliary determinant in the Boltzmann weight. For other difficulties associated with tunneling from the \( Q = 0 \) sector to sectors with a higher topological charge, see e.g. Ref. \[22\]. It is an open question whether THMC can help in creating a bigger interval of lattice-spacing values where the tunneling rate is satisfactory.

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APPENDIX A: PROOF OF EQ. (2.8)

We represent \( \det(H_W^2) \) as a Grassmann integral over \( \psi \) and \( \bar{\psi} \), multiply the integrand by unity written as a new Grassmann integral over \( \Psi \) and \( \bar{\Psi} \), and perform the integration first over \( \psi \) and \( \bar{\psi} \) and then over \( \Psi \) and \( \bar{\Psi} \). Keeping all normalization factors the result is

\[
Z \equiv \det(H_W^2) = \int D\psi D\bar{\psi} \exp(-\bar{\psi}H_W^2\psi) \tag{A1}
\]

\[
= \alpha^{-n} \int D\psi D\bar{\psi} \prod_{i=1}^{n} d\Psi_i d\bar{\Psi}_i \exp\left(-\bar{\psi}H_W^2\psi - \alpha(\Psi - \bar{\psi}Q)(\Psi - Q\bar{\psi})\right)
\]

\[
= \alpha^{-n} \det(\mathcal{M}) \int \prod_{i=1}^{n} d\Psi_i d\bar{\Psi}_i \exp(-\bar{\Psi} \tilde{A} \Psi)
\]

\[
= \alpha^{-n} \det(\mathcal{M}) \det(\tilde{A}),
\]

where \( \mathcal{M} \) is given by Eq. (2.8b) and

\[
\tilde{A} = \alpha - \alpha^2 Q \mathcal{M}^{-1} Q^\dagger. \tag{A2}
\]

We next consider the two-point function

\[
\tilde{A}^{-1}_{ij} = \langle \Psi_i \bar{\Psi}_j \rangle = Z^{-1} \alpha^{-n} \int D\psi D\bar{\psi} \prod_{i=1}^{n} d\Psi_i d\bar{\Psi}_i \times \exp\left(-\bar{\psi}H_W^2\psi - \alpha(\Psi - \bar{\psi}Q)(\Psi - Q\bar{\psi})\right) \Psi_i \bar{\Psi}_j
\]

\[
= Z^{-1} \int D\psi D\bar{\psi} \exp(-\bar{\psi}H_W^2\psi) \left(\alpha^{-1} \delta_{ij} + (Q\psi)_i (\bar{\psi}Q^\dagger)_j\right).
\]

Performing the integral over \( \psi \) and \( \bar{\psi} \) we arrive at Eq. (2.8c) with the identification \( \tilde{A} = A \).
APPENDIX B: ACCEPTANCE RATE IN THE DETERMINISTIC IMPLEMENTATION

In this appendix we discuss a simple model for the decrease in acceptance resulting from the omission of det(\(A\)) from the MD evolution, within the deterministic implementation of THMC. We will first consider the case \(n = 1\), namely, a single eigenmode is omitted from the MD evolution. We begin by writing down a general expression for the acceptance rate. At the beginning of a trajectory, \(x = \text{det}(A(U))\) follows a probability distribution \(P(x)\). At the end of the trajectory, \(y = \text{det}(A(U'))\) follows another distribution \(\hat{P}(y|x)\). This distribution is conditional on \(x\), because the initial and final gauge field configurations are not uncorrelated. Ignoring step-size errors, i.e., assuming that \(\mathcal{H}_{MD}(\pi, U) = \mathcal{H}_{MD}(\pi', U')\), Eq. (3.4) gives an acceptance rate

\[
P_{\text{accept}} = \int_0^1 dx \int_0^1 dy \, \hat{P}(y|x) \min\{1, y/x\}, \tag{B1}
\]

where have we rescaled the possible values of \(\text{det}(A)\) to a unit interval.

In order to estimate \(P_{\text{accept}}\) we need to make several assumptions. The initial configuration \(U\) is an equilibrated configuration of the ensemble generated by the Boltzmann weight \(\exp(-S_g(U)) \prod_i \lambda_i^2\), cf. Eq. (2.1). We assume that the eigenvalue \(\lambda_0\) with smallest absolute value is localized, and practically uncorrelated with the remaining eigenvalues. This suggests a probability distribution for this eigenvalue which is proportional to \(\lambda_0^2\) itself, for \(\lambda_0^2 \ll 1\). As for the support, we postulate a sharp-cutoff model, namely, we assume that the probability distribution for the smallest eigenvalue vanishes outside the interval \([0, C\alpha]\); inside this interval, it increases with \(\lambda_0^2\), starting from zero at \(\lambda_0^2 = 0\). Physically, \(C\alpha\) is the average of the second-smallest eigenvalue (squared). Our choice of \(\alpha\) (see Sec. II) ensures that \(C = O(1)\). Treating \(C\) as a free parameter thus allows us to get an idea on how sensitively the drop in acceptance depends on the details of the theory.

What enters Eq. (B1) is not directly the probability distribution for \(\lambda_0^2\) but, rather, that for the related quantity \(x = \text{det}(A(U))\). Treating \(x\) as the independent variable, we specify the probability distribution by postulating \(P(x) \propto \lambda_0^2(x) = x\alpha/(\alpha - x)\) over its support, where the last equality follows from Eq. (3.2b). Similarly using Eq. (3.2b) to obtain the \(x\)-range that corresponds to the previously selected range of \(\lambda_0^2\), followed by a rescaling to the unit interval, we obtain the probability distribution

\[
P(x) = N \frac{x}{C + 1 - Cx}, \quad 0 \leq x \leq 1, \tag{B2}
\]

where

\[
\frac{1}{N} = \frac{C + 1}{C^2} \log(C + 1) - \frac{1}{C}. \tag{B3}
\]

We next turn to the conditional probability \(\hat{P}(y|x)\). The small eigenvalues of \(H_W^2\) on a typical configuration are expected to be well below its mobility edge, and thus to be localized with a range of order \(a [10, 25]\). These eigenvalues are only sensitive to the details of the gauge field near the corresponding localized modes, and these gauge fields fluctuate on a short (MD) time scale. It is therefore not unreasonable to expect that, for typical values

\[\text{See below for more discussion of this crude approximation.}\]
of the MD time interval $\tau_{MD}$ for one complete trajectory, the variable $y$ actually becomes decorrelated from $x$, $\hat{P}(y|x) = \hat{P}(y)$. Moreover, the THMC algorithm is designed to remove the lowest eigenvalue from the MD force. This suggests that the probability distribution $\hat{P}(y)$ is rather flat. For the sake of simplicity we thus take $\hat{P}(y)$ to be constant, and have the same support as $P(x)$, which amounts to choosing $\hat{P}(y) = 1$ for $0 \leq y \leq 1$ (after a similar rescaling). Finally, plugging this into Eq. (B1) and using Eq. (B2) we obtain

$$P_{\text{accept}} = \frac{1}{2} + \frac{N - 2}{4C}. \quad (B4)$$

The limits $C \to 0$ and $C \to \infty$ give rise to $P_{\text{accept}} = 2/3$ and $P_{\text{accept}} = 1/2$, respectively.

Let us now generalize this model to the case that two eigenmodes are omitted from the MD evolution. We write $\det(A(U)) = x_1 x_2$, where $x_1$ and $x_2$ are related to the corresponding eigenvalues in the same way that $x$ was previously related to the smallest eigenvalue. These modes are expected to be localized, and uncorrelated, at the beginning of the trajectory. We may thus assume the same probability distribution as before, separately for $x_1$ and for $x_2$.\(^{21}\) Similarly, writing $\det(A(U')) = y_1 y_2$, we will assume the same flat distribution for $y_1$ and $y_2$ at the end of the trajectory prior to the metropolis test. The acceptance rate is then given by

$$P_{\text{accept}} = \int_0^1 dx_1 dx_2 \ P(x_1) P(x_2) \ \int_0^1 dy_1 dy_2 \ \min\{1, (y_1 y_2)/(x_1 x_2)\} , \quad (B5)$$

where $P(x)$ is given by Eq. (B2). Varying $C$ in the range of 0.01 to 100 we now find that $P_{\text{accept}}$ varies between roughly 50% and 35% respectively.

Returning to the case that just one eigenmode is omitted from the MD evolution, our model, the probability distribution $P(x)$ of Eq. (B2), neglects most factors in the Boltzmann weight. We have ignored the pure-gauge action, as well as all the remaining eigenvalues of $H_W$. In addition, we neglected the jacobian that arises if we treat $x = \det(A(U))$ as an independent integration variable. The motivation for neglecting all these factors is twofold. First, clearly, it would be difficult to incorporate all factors accurately. Also, while all the neglected factors are unlikely to be constant for the range where our chosen $P(x)$ is non-zero, they are also not expected to vanish. The most crucial feature of the exact, yet unknown, probability distribution is that it vanishes with $\lambda_0^2$. This essential feature is captured by our model. Of course, many other models with the same behavior for $\lambda_0^2 \ll 1$ could be conceived. The free parameter $C$ reflects to some extent the arbitrariness of the model. The fact that rather large changes in the value of $C$ do not lead to a dramatic change in the resulting acceptance is, we believe, an encouraging sign that the acceptance rate will indeed be roughly in the range predicted by our model. Of course, ultimately the only way to verify these expectations is through numerical tests of the THMC algorithm.

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\(^{21}\) Here we assume that the smallest and second-smallest eigenvalues are associated to $x_1$ or to $x_2$ based not on their magnitude but rather on some other criterion such as, for example, the location of the eigenmodes. This justifies using the same probability distribution for $x_1$ and $x_2$, because $x_2$ will correspond to the smallest eigenvalue just as often as $x_1$.\[18\]
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