

## Toward a Ginsparg-Wilson lattice Hamiltonian

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To address quantum computation of quantities in quantum chromodynamics (QCD) for which chiral symmetry is important, it would be useful to have the Hamiltonian for a fermion satisfying the Ginsparg-Wilson (GW) equation. I work with a solution to the GW equation which is fractional linear in time derivatives. The resulting Hamiltonian is nonlocal and has ghosts, but is free of doublers and has the correct continuum limit. This construction works in general odd spatial dimensions, and I provide an explicit expression for the Hamiltonian in one spatial dimension.

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*Introduction.* There are a number of computations in quantum chromodynamics (QCD) that require a good realization of chiral symmetry. These include the color-flavor-locking phase [1] and the chiral symmetry restoring phase transition [2], both of which one would hope to be able to study on the lattice. The overlap operator [3,4] in the Euclidean Lagrangian formulation offers the ideal realization of lattice chiral symmetry in the form of Lüscher symmetry [5], a lattice symmetry which tends toward chiral symmetry in the continuum limit. However, computations using the path integral are afflicted by sign problems. A Hamiltonian approach on a quantum computer might be able to solve these issues, but there currently does not exist a Hamiltonian for Ginsparg-Wilson (GW) fermions.

Chiral symmetry can be expected to fail on the lattice because the lattice spacing introduces a mass scale, and masses violate chiral symmetry. This can be made more precise by the Nielsen-Ninomiya no-go theorem [6]; there is no lattice Dirac operator  $\mathcal{D}$  in four spacetime dimensions which has chiral symmetry, i.e., satisfies

$$\{\gamma_5, \mathcal{D}\} = 0, \quad (1)$$

and has other desirable features, namely the correct continuum limit, freedom from doublers, and locality [5]. Ginsparg and Wilson [7] suggested that this should be replaced by

$$\{\gamma_5, \mathcal{D}\} = a\mathcal{D}\gamma_5\mathcal{D}, \quad (2)$$

so that exact chiral symmetry fails at the order of the lattice spacing  $a$ . The first method for putting chiral fermions on the lattice involved edge states of a domain wall defect in one higher dimension [8]. Neuberger and Narayanan [3,4] found that this system could be studied in four dimensions via the “overlap” operator,

$$\mathcal{D} = \frac{M}{2}(1 + V), \quad V = \frac{D_w}{\sqrt{D_w^\dagger D_w}}, \quad (3)$$

where  $M = 1/a$  is the inverse lattice spacing, and  $D_w$  is the four-dimensional Wilson Dirac operator, which, in the absence of gauge fields, can be written in momentum space as

$$D_w = i \sum_{\mu=1}^4 \gamma^\mu \sin(p_\mu/M) - 1 + \sum_{\mu=1}^4 (1 - \cos(p_\mu/M)). \quad (4)$$

This operator has the correct continuum limit, and is not Hermitian, but is instead “ $\gamma_5$ -Hermitian”:

$$\gamma_5 \mathcal{D} \gamma_5 = \mathcal{D}^\dagger. \quad (5)$$

In fact, it can be quickly checked that any operator of the form

$$\mathcal{D} = \frac{M}{2}(1 + V); \quad \gamma_5 V \gamma_5 = V^\dagger, \quad V^\dagger V = I \quad (6)$$

satisfies Eq. (2) [9]. In this case, I say  $\mathcal{D}$  is an overlap operator, though in general it may not necessarily be constructed in terms of a state overlap. Lüscher [5] first observed that this operator has the following symmetry:

$$\delta\psi = \gamma_5 \left( \frac{1 - V}{2} \right) \psi, \quad \delta\bar{\psi} = \bar{\psi} \left( \frac{1 - V}{2} \right) \gamma_5. \quad (7)$$

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In the continuum limit, this becomes chiral symmetry. Lüscher noted that the Jacobian of this transformation produces the index of  $\mathcal{D}$ , a lattice version of the Fujikawa calculation [5,10] of the chiral anomaly. Indeed, there is a good deal of freedom in defining this Lüscher symmetry; hereafter I will refer to any symmetry

$$\delta\psi = \Gamma\psi, \quad \delta\bar{\psi} = \bar{\psi}\bar{\Gamma}, \quad (8)$$

for which

$$\lim_{M \rightarrow \infty} \Gamma = \lim_{M \rightarrow \infty} \bar{\Gamma} = \gamma_5, \quad (9)$$

as a Lüscher symmetry [5], provided its Jacobian reproduces the index of  $\mathcal{D}$ .

To find a Hamiltonian describing a GW fermion, one may try to compute the transfer matrix of Eq. (3) directly, but this involves square roots of the time derivative and is therefore challenging. Creutz *et al.* [11] considered the following construction. First, define the three-dimensional overlap operator,

$$d = \frac{M}{2}(1+v), \quad v = \frac{d_w}{\sqrt{d_w^\dagger d_w}}, \quad (10)$$

where  $d_w$  is the three-dimensional analog of Eq. (4):

$$d_w = i \sum_{i=1}^3 \gamma^i \sin(p_i/M) - M + \sum_{i=1}^3 (1 - \cos(p_i/M)), \quad (11)$$

and  $\gamma^i$  are  $4 \times 4$  Clifford algebra matrices. Then by analogy with the continuum Hamiltonian,

$$H_\psi^c = \int d^3x \bar{\psi}^\dagger i\gamma^0 \gamma^i D_i \psi \quad (12)$$

(where  $D_i$ ,  $H_\psi^c$  denote the continuum covariant derivative and continuum Hamiltonian, respectively), it is reasonable to identify  $\gamma^i D_i$  with the three-dimensional Dirac operator, and formulate a lattice prescription for a Hamiltonian via the replacement  $\gamma^i D_i \rightarrow d$ :

$$H_\psi \equiv \bar{\psi}^\dagger i\gamma^0 d \psi. \quad (13)$$

This system has the symmetry of Eq. (7), and associated to that symmetry is the charge

$$Q_5 = \bar{\psi}^\dagger \gamma_5 \left( \frac{1-V}{2} \right) \psi. \quad (14)$$

This chiral charge is conserved with respect to  $H_\psi$ , i.e.,  $[H_\psi, Q_5] = 0$ , but upon introduction of the gauge field Hamiltonian,

$$H_g = \frac{1}{2}(E^2 + B^2), \quad (15)$$

one finds  $[H_g, Q_5] \neq 0$ , since  $E^2$  involves derivatives with respect to the gauge fields in the quantized theory, and the  $V$  appearing in  $Q_5$  involves link variables.

It is important to note that the Hamiltonian considered by Creutz *et al.* is not derived from a GW fermion in the Euclidean Lagrangian; it is simply an ansatz. If it were, it would enjoy a full Lüscher symmetry that descends to the Hamiltonian formulation, even in the presence of gauge fields.

Therefore it is sensible to start at the level of the Lagrangian, with a modified overlap operator which still solves the GW equation, but from which the extraction of a Hamiltonian is considerably easier. It is simpler to consider a theory which is fractional linear in time derivatives, i.e., a rational expression linear in time derivatives. The feasibility of such an approach will become clear by construction of an overlap operator in the continuum with ghosts, namely a Pauli-Villars regulated fermion.

In the section titled *Pauli-Villars as overlap*, I will describe the way in which Pauli-Villars fermions satisfy the GW relation, and the Hamiltonian and Lüscher symmetry associated to them. In *Overlap Lagrangian*, I will derive a Lagrangian describing a GW fermion in discrete space and continuous time, and generalizing the arguments of *Pauli-Villars as overlap*, I will derive a Hamiltonian describing the system. In *Overlap Hamiltonian*, I will describe the properties of this Hamiltonian.

*Pauli-Villars as overlap.* In a recent paper generalizing the GW relation [12], it was found that the GW equation holds for a Pauli-Villars regulated fermion in the continuum. I will derive the Hamiltonian for this example, as it is instructive for generalization to the lattice.

A Pauli-Villars regulated fermion is equivalent to a Lagrangian with the following Dirac operator:

$$\mathcal{L} = \bar{\psi} \mathcal{D} \psi, \quad \mathcal{D} = M \frac{\not{D}}{\not{D} + M}, \quad (16)$$

where  $\not{D}$  is the usual Euclidean Dirac operator,  $\not{D} = \gamma^\mu D_\mu$ . This may be rewritten

$$\mathcal{D} = \frac{M}{2}(1+V), \quad V = \frac{\not{D}/M - 1}{\not{D}/M + 1}. \quad (17)$$

This  $\mathcal{D}$  satisfies Eq. (6), so it is an overlap operator. For reasons that will become clear shortly, is helpful to define  $A = \not{D}/M - 1$ , and note  $V$  is of the form

$$V = -A^{-1}A^\dagger; \quad \gamma_5 A \gamma_5 = A^\dagger. \quad (18)$$

In order to make this theory look familiar, I introduce ghost fields  $\phi, \bar{\phi}$  with opposite statistics to the action, so that the full Lagrangian is

$$\mathcal{L}_{\text{tot}} = \bar{\psi} \frac{M}{2} A^{-1} (A - A^\dagger) \psi + \bar{\phi} \phi. \quad (19)$$

I perform the simultaneous change of variables,

$$\bar{\psi}' = \bar{\psi} A^{-1}, \quad \bar{\phi}' = \bar{\phi} A^{-1}. \quad (20)$$

This change of variables has trivial Jacobian in the path integral because of the opposite statistics. Under this change of variables the Lagrangian becomes

$$\mathcal{L}_{\text{tot}} = \bar{\psi}' \not{D} \psi + \bar{\phi}' (\not{D} + M) \phi. \quad (21)$$

Consider how a Lüscher symmetry  $\Gamma, \bar{\Gamma}$  on  $\psi, \bar{\psi}$  is affected by this change of variables.  $\Gamma$  is unaffected, while the new  $\bar{\Gamma}$  is related to the original by

$$\bar{\Gamma}' = A \bar{\Gamma} A^{-1}. \quad (22)$$

In particular, consider the choice

$$\Gamma = \gamma_5, \quad \bar{\Gamma} = -V \gamma_5. \quad (23)$$

Since  $V$  is of the form of Eq. (18), Eq. (22) becomes

$$\bar{\Gamma}' = A^{-1} A^\dagger \gamma_5 A^{-1} = A^\dagger \gamma_5 A^{-1} = \gamma_5 A A^{-1} = \gamma_5. \quad (24)$$

In summary, the Pauli-Villars fermion described in Eq. (16), with the Lüscher symmetry of Eq. (23) descends to a massless fermion with ordinary chiral symmetry and a heavy ghost fermion where the symmetry acts trivially. The Hamiltonian of the theory is thus

$$H^c = H_\psi^c + H_\phi^c, \quad (25)$$

where

$$H_\psi^c = \int d^3x \psi^\dagger i \gamma^0 \gamma^i D_i \psi, \quad (26)$$

$$H_\phi^c = \int d^3x \phi^\dagger i \gamma^0 \gamma^i D_i \phi - \phi^\dagger \gamma^0 M \phi. \quad (27)$$

In order to study the dynamics of  $H_\psi^c$  alone, one must work in the vacuum to vacuum sector of the ghost theory. Excitations with energy less than the regulator mass  $M$  (later taken to infinity) do not contribute to scattering amplitudes involving the  $\psi$  field. Further discussion on Pauli-Villars fermions can be found in any introductory text on quantum field theory (e.g., [13]). They are not typically dealt with in a Hamiltonian formalism. In this Letter, the Pauli-Villars regularization prescription is simply a helpful

tool, as it allows one to regulate the UV divergence that comes from the introduction of a continuous time coordinate, and subsequently describe the low energy modes in a simple effective way.

*Combined overlap.*

Overlap Lagrangian: Now I work in continuous time and latticized space. Since the Pauli-Villars and overlap solutions apply to continuum and lattice cases of an overlap operator respectively, it is reasonable to try to write an ansatz for  $\mathcal{D}$  which combines the forms of Eqs. (17) and (3). Such an operator is determined by a choice of unitary and  $\gamma_5$ -Hermitian  $V$ . Recall the three-dimensional analog  $v$  in Eq. (10). Since the low energy spectrum of  $v$  is  $-1 + i\vec{p}/M$  in the free theory, a reasonable ansatz incorporating Pauli-Villars regularization might be

$$V = \frac{\gamma^0 \partial_t + Mv}{\gamma^0 \partial_t - Mv^\dagger}. \quad (28)$$

Here when I write the quotient, I mean left multiplication by the inverse of the denominator, as in Eq. (18). Note that the  $V$  of Eq. (28) also satisfies the relations of Eq. (18). Furthermore  $V$  is  $\gamma_5$ -Hermitian, unitary, and has the correct low energy spectrum. However, this  $V$  has doublers: Note that zero modes of  $\mathcal{D}$  correspond to  $-1$  modes of  $V$ , and therefore generally an overlap operator has doublers if there are any  $V = -1$  modes away from the origin in the Brillouin zone. Note that at  $v = 1$ ,  $V = -1$ , and so the free theory already has doublers at  $\vec{p}_i = \pi/a$ . This is because at  $\partial_t = 0$ ,  $V = -v/v^\dagger$ . Since complex conjugation treats the  $v = \pm 1$  modes identically, doublers arise at  $\partial_t = 0$ . Therefore, in order to find a  $V$  without doublers, the  $v = \pm 1$  modes need to be treated differently under conjugation. One way to do this is to replace

$$v \rightarrow -\sqrt{-v} \equiv \xi. \quad (29)$$

Then  $V$  becomes instead

$$V = \frac{\frac{1}{2} \gamma^0 \partial_t - M\xi}{\frac{1}{2} \gamma^0 \partial_t + M\xi^\dagger}. \quad (30)$$

I define the square root  $\sqrt{u}$  of a unitary matrix  $u$  generally as the unique matrix whose log spectrum lies in the interval  $(-i\pi/2, i\pi/2]$ , and which squares to  $u$ ; this can be equivalently defined as the matrix whose eigenvalues are the square root of the eigenvalues of  $u$ , with the same eigenvectors. Such a definition involves choosing a branch cut, namely  $\sqrt{-1} = i$ , and therefore a discontinuity at the edge of the Brillouin zone (which introduces nonlocality). Note  $\sqrt{u^\dagger} \neq \sqrt{u}^\dagger$ , but instead

$$\sqrt{u^\dagger} = \sqrt{u^\dagger} + 2iP_{-1}, \quad (31)$$

where  $P_{-1}$  is the projector onto the  $-1$  modes of  $u$ .

It is worth noting the denominator is not invertible at  $v = 1$  and  $\partial_t = 2iM$ . However, it can be seen that  $V = 1$  in this limit. In the free case, this guarantees  $\mathcal{D}(p)$  is continuous at the edge of the Brillouin zone, but higher order derivatives are discontinuous, so this theory is non-local. It should be noted this nonlocality is not so severe that it precludes definition of a gauge theory entirely, as one can still simply replace the free derivative with the covariant derivative in the operator Eq. (4) (in the position space representation).

In most cases, the complication which arises in Eq. (31) can simply be ignored, and the  $V = 1$  case can be treated separately. In particular, I will simply write

$$\gamma^5 \xi \gamma^5 = \gamma^0 \xi \gamma^0 = \xi^\dagger. \quad (32)$$

The operator  $V = -A^{-1}A^\dagger$  in Eq. (30) is, in general, not unitary. Unitarity of  $V$  follows from normality of  $A$ . However, for time dependent gauge fields,

$$A^\dagger A - AA^\dagger = \frac{1}{2} \gamma^0 \partial_t (\xi + \xi^\dagger) \neq 0. \quad (33)$$

Furthermore,  $V$  is not in general  $\gamma_5$ -Hermitian. Instead, note that the weaker statement

$$\gamma^5 A \gamma^5 = A^\dagger \quad (34)$$

still holds, so that for general gauge fields it holds that

$$\gamma^5 V \gamma^5 = V^{-1}. \quad (35)$$

As noted in [12], the operator  $\mathcal{D} = \frac{1}{2}(1 + V)$  still satisfies the relation Eq. (2), and still enjoys Lüscher symmetries, e.g., Eq. (23). Under the Lüscher symmetry, the anomalous symmetry violation of the expectation value of an observable  $\mathcal{O}$  is given by (cf. [5])

$$\langle \delta \mathcal{O} \rangle = (-\text{tr} \gamma_5 \mathcal{D} + \text{tr} \gamma_5) \langle \mathcal{O} \rangle. \quad (36)$$

The quantity  $\text{tr} \gamma_5 \mathcal{D}$  can be evaluated using the arguments of [5];

$$\text{tr} \gamma_5 \mathcal{D} = \text{tr} \gamma_5 + 2\text{ind} \mathcal{D}, \quad (37)$$

therefore,

$$\langle \delta \mathcal{O} \rangle = 2\text{ind} \mathcal{D} \langle \mathcal{O} \rangle \quad (38)$$

and so this operator has the correct anomaly in the Lagrangian formulation. It is worthwhile to note that evaluation of  $\text{tr} \gamma_5 \mathcal{D}$  in [5] relies on the point 0 being an

isolated point of the spectrum of  $\mathcal{D}$ . This can clearly be done when the spacetime lattice is finite, since the operator  $\mathcal{D}$  only has a finite number of eigenvalues. In the present case, the eigenvalues  $\omega$  of  $\partial_t$  have no UV cutoff. However, an IR cutoff is sufficient: the eigenvalues  $\omega$  become discrete. For very large  $\omega$ ,  $V \sim 1$ . Therefore the lack of a UV cutoff in time adds a dense set of eigenvalues near  $\mathcal{D} = 1$ . Any eigenvalues at  $\mathcal{D} = 0$  remain isolated.

Before proceeding with the prescription of *Pauli-Villars as overlap*, I integrate out in the path integral the modes at  $V = 1$ , since they are at high energy and contribute only to overall normalization. They come in chiral pairs and are thus also invariant under the Lüscher symmetry of Eq. (23) so cannot contribute to the anomaly.

Therefore, the operator  $\mathcal{D} = \frac{1}{2}(1 + V)$ , with the choice of  $V$  in Eq. (30) satisfies the Ginsparg-Wilson equation, and has a Lüscher symmetry which correctly realizes the anomaly.

Overlap Hamiltonian: The Hamiltonian following the prescription in *Pauli-Villars as overlap* can be seen to be

$$\begin{aligned} H &= H_\psi + H_\phi, \\ H_\psi &= \psi^\dagger h_\psi \psi, \quad H_\phi = \phi^\dagger h_\phi \phi, \end{aligned} \quad (39)$$

where

$$\begin{aligned} h_\psi &= M \gamma^0 (\xi^\dagger - \xi), \\ h_\phi &= 2M \gamma^0 \xi^\dagger, \end{aligned} \quad (40)$$

and repeated (suppressed) indices are summed over. The ghost fields here have been rescaled to be canonically normalized. The ghost Hamiltonian  $H_\phi$  is clearly gapped; since it is Hermitian and unitary its eigenvalues are all of magnitude  $2M$ . Therefore, I consider only ghost vacuum-to-vacuum amplitudes of the combined quantum system at energy scales much lower than the cutoff  $M$ , which are described by  $H_\psi$ .

Following the analysis in *Pauli-Villars as overlap*, the Lüscher symmetry in Eq. (23) descends once again to ordinary chiral symmetry, so that the chiral charge is

$$Q_5 = \psi^\dagger \gamma^5 \psi. \quad (41)$$

It is evident that both  $h_\psi$  and  $h_\phi$  are Hermitian matrices. Chiral charge is conserved for the  $\psi$  fermions, and violated for the ghost fermions:

$$[\gamma^5, h_\psi] = 0, \quad [\gamma^5, h_\phi] = 4M \gamma^5 \gamma^0 (\xi^\dagger - \xi). \quad (42)$$

This is consistent with anomalous chiral symmetry violation of Pauli-Villars fermions in the continuum, where the mass term in the ghost fermion violates chiral symmetry explicitly. The gauge field Hamiltonian in Eq. (15) trivially

commutes with  $\gamma_5$ , so that the chiral charge is conserved in the full theory describing the light  $\psi$  modes. This is in contrast to the Creutz *et al.* [11] Hamiltonian of Eq. (13), since the chiral charge in Eq. (41) no longer involves the overlap operator as in Eq. (14), but is in direct analogy with the continuum chiral charge.

It is easily checked that  $h_\psi$  has the right continuum limit, since  $v \rightarrow -1 + i\hat{p}$ . The same holds true in the presence of gauge fields which are sufficiently smooth.

It is illuminating to consider replicating this construction in  $d = 1 + 1$ . One finds  $v = -e^{-ip\gamma_1/2M}$ , and in this case the free Hamiltonian is explicitly

$$h_\psi = 2M\gamma_\chi \sin p/4M, \quad (43)$$

where  $\gamma_\chi = i\gamma_1\gamma_2$  is the three-dimensional analog of  $\gamma_5$ . This matches the continuum Hamiltonian for a free two-component Dirac spinor in the low energy limit.

*Conclusions.* I have derived a Hamiltonian for a massless fermion on a spatial lattice with exact chiral symmetry from a spatial-lattice plus continuous-time Lagrangian for a GW fermion, starting with an overlap operator with Lüscher symmetry and introducing ghosts. This came at the expense of locality.

One of the main motivations for this Letter is demonstrating the difficulty of the formulation of a consistent Hamiltonian describing GW fermions. I hope that this Letter either spurs interest in a local solution for a GW Hamiltonian, or in a no-go theorem that forbids the formulation of a local Hamiltonian for Ginsparg-Wilson fermions.

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