Basis States for Hamiltonian QCD with Dynamical Quarks

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Abstract
We discuss the construction of basis states for Hamiltonian QCD on the lattice, in particular states with dynamical quark pairs. We calculate the matrix elements of the operators in the QCD Hamiltonian between these states. Along with the “harmonic oscillator” states introduced in previous pure SU(3) work, these states form a working basis for calculations in full QCD.
1 Introduction

As detailed in papers with Bronzan [2, 3], we have been studying lattice QCD using an operator and states approach rather than the usual Monte Carlo simulation of the Feynman path integral. As we have emphasized, this requires the use of a suitable set of single degree-of-freedom (DOF) states on the SU(3) manifold. Here “suitable” means that matrix elements of the QCD Hamiltonian must be calculable in closed form using these states, and that the states have tunable parameters so they can model the QCD wave functions at all values of the coupling constant.

We have introduced a “harmonic oscillator” basis of states as one which satisfies the above criteria and is therefore useful in making calculations in Hamiltonian QCD. Since these states describe only gauge degrees of freedom, they are actually designed for studying only a pure SU(3) gauge theory.

In this paper we will introduce a similarly suitable set of dynamical-quark basis states to complement the harmonic oscillator states. We will discuss how we construct a quark ground state at arbitrary values of the coupling constant, create quark excitations, and calculate matrix elements of the QCD Hamiltonian between these states. Together with the harmonic oscillator states, then, we have a complete basis for the study of full QCD.

The layout of this paper is as follows. In Section 2 we briefly review our work on the construction of harmonic oscillator states. In Section 3 we describe the construction of the quark vacuum as well as the states which include virtual quark pairs. In Section 4 we discuss the combination of the harmonic oscillator states with the quark states to form a basis for simulating full QCD. In Section 5 we derive the matrix elements of the operators of the QCD Hamiltonian between these states. We conclude in Section 6 with a discussion of the usefulness of these states.

2 Review of pure gauge states

Each gauge degree of freedom (link variable on the lattice) can be described by a wave function which is a “harmonic oscillator” state on the SU(3) manifold. The harmonic oscillator states are derived from a “Gaussian” state on
the manifold. This Gaussian can be written
\[
\psi_{\alpha_1}(\alpha, t) = \sum_{p,q} d(p,q) e^{-t\lambda(p,q)} \chi^{(p,q)},
\]
where
\[
d(p,q) = (p + 1)(q + 1)(p + q + 2)/2
\]
is the dimension of the \((p,q)\) representation of SU(3), \(\lambda(p,q) = (p + q)^2/4 + (p - q)^2/12 + (p + q)\) is the quadratic Casimir eigenvalue, and \(\chi^{(p,q)}\) is the character. \(\alpha \equiv (\alpha^1, \alpha^2, \ldots, \alpha^8)\) is a parameterization of the adjoint representation of SU(3). The parameter \(t\) controls the width of the Gaussian, which is centered at \(\alpha_1\).

To make connection with a more familiar object, note that the corresponding wave function on the flat, three-dimensional manifold \(\mathbb{R}^3\) would be
\[
\psi_{x_1}(x, t) = \frac{e^{-(x - x_1)^2/4t}}{(4\pi t)^{4/2}},
\]
where \(x\) and \(x_1\) are ordinary vectors. On this flat manifold, harmonic oscillator states can be generated by applying a polynomial in the operators \(-i\frac{\partial}{\partial x_{1a}}\) to the wave function, then setting \(x_1\) to 0. On the SU(3) manifold, the corresponding operators are \(J_{L\alpha}(\alpha_1)\), the generators of SU(3) in differential form.

The harmonic oscillator states that we have formed on the manifold can be labeled by the number of SU(3) indices on the state. Thus, the zero-, one-, and two-color states are
\[
\begin{align*}
\phi &= \phi(\alpha, t) = \psi_{\alpha_1}(\alpha, t)|_{\alpha_1=0}, \\
\phi_a &= \phi_a(\alpha, t) = J_{L\alpha}(\alpha_1)\psi_{\alpha_1}(\alpha, t)|_{\alpha_1=0}, \\
\phi_{ab} &= \phi_{ab}(\alpha, t) = \{J_{L\alpha}(\alpha_1), J_{L\beta}(\alpha_1)\}\psi_{\alpha_1}(\alpha, t)|_{\alpha_1=0}.
\end{align*}
\]
For comparison, the analogous states on a flat manifold are
\[
\begin{align*}
\phi(x, t) &= e^{-x^2/4t}, \\
\phi_a(x, t) &= x_a e^{-x^2/4t}, \\
\phi_{ab}(x, t) &= x_a x_b e^{-x^2/4t}.
\end{align*}
\]
\[1\text{When applied to a representation of SU(3), } J_{L\alpha}(\alpha_1)\text{ has the effect of left-multiplying the representation by the } a^{th}\text{ generator. There are also operators } J_{R\alpha}(\alpha_1)\text{ which right-multiply the representation and could be used to generate a slightly different set of harmonic oscillator states.}\]
In the papers we have cited we described the orthogonalization of these states as well as the calculation of matrix elements of the QCD Hamiltonian between them. We will not need those details here, however.

These single-DOF wave functions must now be pieced together to form multi-DOF states suitable for computations in Hamiltonian QCD. Each multi-DOF state will be a product of single-DOF states. The most basic state is one with no excitations. Specifically, each degree of freedom is a zero-color state:

\[ |\Psi\rangle = |\phi\phi\phi\cdots\rangle. \] (2.5)

The next simplest states are those with just one excitation:

\[ |\Psi\rangle = |\phi_a\phi\phi\cdots\rangle. \] (2.6)

However, these states are not SU(3) singlets, as evidenced by the color index which is left hanging. In order to maintain global SU(3) invariance, we must sum over all indices. Therefore, the next possible states are

\[ |\Psi\rangle = \delta_{ab}|\phi_a\phi_b\phi\cdots\rangle, \] (2.7)

where \( \delta_{ab} \) is a Kronecker \( \delta \)-function. There are of course similar states where the excitations lie on different degrees of freedom. We call these one-pair states. In analogous fashion, we can form two-pair states, three-pair states, and so on.

Arbitrarily intricate states can be constructed by using highly colored, single-DOF states along with complicated coupling schemes. For instance, the following is a valid (that is, gauge-invariant) state:

\[ |\Psi\rangle = \delta_{ab}\text{Tr}(\lambda_c\lambda_d\lambda_e)|\phi_{ac}\phi_{bd}\phi_e\cdots\rangle, \] (2.8)

where the \( \lambda_i \)'s are Gell-Mann matrices.

The states described above provide the basis for a pure SU(3) gauge theory calculation, and they will likewise provide the basis for the gauge sector of our full QCD calculation. In the next sections we will describe how to form similar states that include dynamical quarks, to complete our basis.

3 Quark sector states

To formulate our quark states, we use staggered fermions \[ \square \]. (We follow closely the notation of Banks et al. \[ \square \]). Specifically, the quarks are created
and destroyed by applications of single-component fields $\chi_i^\dagger(s)$ and $\chi_i(s)$, where the index $i$ signifies color in the fundamental representation of SU(3), and the argument $s = (x, y, z)$ specifies a site on the lattice. The operators act on a simple Fock space, and any quark configuration can be specified by giving the location of the quarks on the lattice.

### 3.1 Strong-coupling quark vacuum

Just as we did for the gauge states, we would like to use quark states which are flexible enough to treat both the strong- and weak-coupling regimes. Toward this end, we will begin with a description of the strong-coupling vacuum, then discuss how to obtain the weak-coupling vacuum from it. We will then describe the excitations of the vacuum.

At very strong coupling the vacuum state is the “checkerboard” state, in which alternating sites are fully occupied $^1$. Two of these states can be formed, depending on which sublattice is filled (the “red” squares or the “black” squares of the checkerboard). The two states are

$$
|\psi_{\text{even}} > = \prod_{\text{even sites}} \frac{1}{6} \epsilon_{ijk} \chi_i^\dagger(s) \chi_j^\dagger(s) \chi_k^\dagger(s) |E > ,
$$

$$
|\psi_{\text{odd}} > = \prod_{\text{odd sites}} \frac{1}{6} \epsilon_{ijk} \chi_i^\dagger(s) \chi_j^\dagger(s) \chi_k^\dagger(s) |E > ,
$$

where $|E >$ is the empty lattice, and even/odd means that $x + y + z = \pm 1$. These two states transform into one another under a chirality transformation. We can form two degenerate vacua, the symmetric and antisymmetric combinations of these two states, which are eigenstates of the chirality operator. We have shown numerically that as we decrease the coupling constant, the true vacuum is the symmetric combination, so we use

$$
|0 >_{\text{strong}} = |\psi_{\text{even}} > + |\psi_{\text{odd}} >
$$

as the vacuum state at strong coupling.

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1. One must be careful to maintain a fixed ordering for the product over the sites, lest minus sign errors creep in. Although we will not display it explicitly, we assume that the sites have been ordered in some appropriate manner.
3.2 Weak-coupling quark vacuum

We derive the weak-coupling vacuum from the strong-coupling vacuum by means of a projection operator. We write

\[ |0\rangle_{\text{weak}} = \lim_{\alpha \to \infty} e^{-\alpha H_w} |0\rangle_{\text{strong}}. \tag{3.3} \]

\(H_w\) is the weak-coupling limit of the quark Hamiltonian,

\[ H_w = \frac{1}{2a} \sum_{s,s'} \chi^\dagger(s) M_{ss'} \chi(s'), \tag{3.4} \]

where

\[ M_{ss'} = \sum_{\hat{n}} [\delta_{s,s'+\hat{n}} + \delta_{s,s'-\hat{n}}] \eta(\hat{n}), \tag{3.5} \]

\(\eta(x) = (-1)^x, \ \eta(y) = (-1)^y, \ \eta(z) = (-1)^y, \) and \(a\) is the lattice spacing. (There is a suppressed color index in this expression.) Note that in weak coupling the quarks decouple from the gauge degrees of freedom, and \(H_w\) is equal to the free-field quark Hamiltonian.

The projection works as follows. \(\alpha\) is an adjustable parameter which governs the strength of the projection. When \(\alpha = 0\), there is no projection, and we still have the strong-coupling vacuum. As \(\alpha\) becomes large, the projection operator damps out the pieces of \(|0\rangle_{\text{strong}}\) which have high energy in the weak-coupling limit, leaving intact the lowest energy weak-coupling state. So, for large \(\alpha\), this operator does exactly what we want: it projects out the weak-coupling vacuum.\[^{3}\] In practice, \(\alpha = 1\) will give nearly complete projection. As we vary \(\alpha\) from 0 to 1, we obtain a vacuum state which interpolates smoothly between the \(g \to \infty\) and \(g = 0\) vacua. We therefore hope to obtain a good approximate quark vacuum for arbitrary values of the coupling constant by using \(\alpha\) as a variational parameter in our simulations. We will designate this approximate vacuum \(|0_q\rangle\).

3.3 Quark excitations

Having established a quark-sector vacuum, we must now understand how to create excited quark states. This is much easier and more familiar than it

\[^{3}\text{Of course, we are assuming here that the strong- and weak-coupling vacua are not orthogonal to each other. This can be demonstrated a posteriori.}\]
was for the gluon states, where we were dealing with the complicated SU(3) manifold. Here, we have a simple Fock space, and we merely need to decide which states from that Fock space to include in our basis.

We can exclude a large number of states by observing that the “checkerboard” vacuum state is half filled and that the Hamiltonian preserves quark number. We are interested in studying the glueball spectrum, which has the same quantum numbers as the vacuum, so there is no reason to include any quark state that isn’t half-filled. If we wish to study the spectrum of particles with other quantum numbers, we likewise limit ourselves to those sectors.

We can obtain a new half-filled state directly from the vacuum state by applying one annihilation operator and one creation operator:

\[ |\Psi > = \chi_i^\dagger (s) \chi_i (s') |0_q > . \] (3.6)

Recall that the index \( i \) indicates color, in the fundamental representation of SU(3), reflecting the correct group properties of the quarks. Notice that we are summing over \( i \), thereby maintaining global gauge invariance in the quark sector in an analogous way to the gauge sector.

The state shown above corresponds to exciting one virtual quark pair out of the vacuum. Clearly, we can form states with an arbitrary number of virtual pairs by applying the appropriate number of creation and annihilation operators. One convenient feature of this scheme is that we can control how many such pairs we wish to have in the simulation simply by choosing which basis states to include. We will comment on this in the final section.

4 Combining the gauge and quark states

Sections 2 and 3 described our construction of states for the gauge and quark degrees of freedom in our simulations. The simplest way to form a combined state suitable for a full QCD simulation is to make a direct product of one state from the gauge sector with one from the quark sector. A typical state, then could be written

\[ |\Psi >= \delta_{ab} \delta_{cd} |\phi_a \phi_b \phi_c \phi_d \phi \ldots > \otimes \chi_i^\dagger (s_1) \chi_i (s_1') \chi_j^\dagger (s_2) \chi_j (s_2') |0_q > . \] (4.1)

Let us emphasize again that all of the SU(3) indices are contracted, ensuring that global gauge invariance is maintained. Note in particular that the indices
are summed separately within the two sectors, indicating that the gauge and quark sectors are separately invariant under the global SU(3) transformation.

There is a second way to form combined states, in which the two sectors are not separately invariant. To do this, we need an object which can intertwine the SU(3) adjoint representation of the gauge sector with the fundamental representation of the quark sector. The simplest way to do this is with the Gell-Mann matrices, which carry both three- and eight-dimensional indices. A simple state of this form is

\[ |\Psi \rangle = |\phi_a \phi \phi \phi \rangle \otimes \chi^a_I(s) \chi^e_{ij}(s') |0_q \rangle. \tag{4.2} \]

This completes the description of our basis states for full QCD calculations on the lattice. In the next section we will show how to compute the matrix elements necessary for our simulations.

## 5 Matrix elements

The matrix elements of our combined states are sums of products of gauge matrix elements with quark matrix elements. The results of our gauge sector calculations have already appeared in [3], and we will not repeat them here.

The most basic quark matrix element that we must calculate is the overlap of our projected vacuum, \(<0_q|0_q\>). This, in turn, can be broken down into sums of matrix elements of the projected checkerboard states:

\[
<0_q|0_q> = <\psi_{even}|e^{-2\alpha H_w}|\psi_{even}> + <\psi_{even}|e^{-2\alpha H_w}|\psi_{odd}>
+ <\psi_{odd}|e^{-2\alpha H_w}|\psi_{even} > + <\psi_{odd}|e^{-2\alpha H_w}|\psi_{odd}>. \tag{5.1}
\]

We will explicitly calculate only the first of these four nearly identical expressions. Recall that

\[
|\psi_{even} \rangle = \prod_{\text{even sites}} \frac{1}{6} \epsilon_{ijk} \chi^i(s) \chi^j(s) \chi^k(s) |E \rangle
\]

\[
= [\chi^i_1(s_1) \chi^j_1(s_1) \chi^k_1(s_1)] \cdots [\chi^i_M(s_M) \chi^j_M(s_M) \chi^k_M(s_M)] |E \rangle, \tag{5.2}
\]

where \( M = \frac{N^3}{2} \) is the number of even sites on our \( N \times N \times N \) lattice and \( s_1, \ldots, s_M \) specify the locations of those sites. First, we segregate the

\footnote{We assume \( N \) is an even number.}
creation operators by color. This involves an even number of permutations, so no minus sign is picked up.

$$|\psi_{\text{even}}> = [\chi_1^\dagger(s_1) \cdots \chi_M^\dagger(s_M)]|\psi_{\text{even}}>.$$  

Likewise, we can segregate $H_w$ into a product of single-color factors:

$$H_w \equiv H_1^w + H_2^w + H_3^w$$

$$= \frac{1}{2a} \sum_{s, s'} [\chi_1^\dagger(s) M_{ss'} \chi_1(s') + \chi_2^\dagger(s) M_{ss'} \chi_2(s') + \chi_3^\dagger(s) M_{ss'} \chi_3(s')] \] \] $$

Since the separate color factors commute, we can write

$$e^{-2\alpha H_w} = e^{-2\alpha H_1^w} e^{-2\alpha H_2^w} e^{-2\alpha H_3^w}$$

and thereby write our matrix element in color-factorized form:

$$<\psi_{\text{even}}|e^{-2\alpha H_w}|\psi_{\text{even}}> = \langle E|\chi_1(s_1) \cdots \chi_M(s_M)|e^{-2\alpha H_1^w} \chi_1^\dagger(s_1) \cdots \chi_M^\dagger(s_M)\] \] x [\chi_2(s_1) \cdots \chi_2(s_M)|e^{-2\alpha H_2^w} \chi_2^\dagger(s_1) \cdots \chi_2^\dagger(s_M)\] \] \] x [\chi_3(s_1) \cdots \chi_3(s_M)|e^{-2\alpha H_3^w} \chi_3^\dagger(s_1) \cdots \chi_3^\dagger(s_M)\] \] \] $$

We now want to commute the exponential factors all the way to the left, where we will be able to take advantage of the fact that

$$<E|e^{-2\alpha H_w} = <E|.$$ 

To do this, we will need the relation

$$\chi(s)e^{-\sigma H_w} = \sum_{s'} K_{s, s'}(\sigma) e^{-\sigma H_w} \chi(s'),$$

where

$$K_{s, s'}(\sigma) = \sum_{k, i} \phi(s; k, i) e^{\sigma \lambda(k, i)} \phi(s'; k, i)$$

and the functions $\phi(s; k, i)$ are the eigenfunctions of $M_{ss'}$. We prove this relation in the Appendix.
Commuting each of the exponential factors to the left gives

\[
< \psi_{\text{even}} | e^{-2\alpha H_w} | \psi_{\text{even}} > = < E | \prod_{i=1}^{M} \left( \sum_{s'_i} K_{s_i,s'_i} \chi_1(s'_i) \chi_1^\dagger(s_1) \cdots \chi_1^\dagger(s_M) \chi_2(s_1) \cdots \chi_2^\dagger(s_M) \right) \times \prod_{i=1}^{M} \left( \sum_{s'_i} K_{s_i,s'_i} \chi_3(s'_i) \chi_3^\dagger(s_1) \cdots \chi_3^\dagger(s_M) \right) | E > .
\]

(5.10)

The \( M \) sites \( s'_1, \ldots, s'_M \) can be chosen in any way from the even sites, but unless they are a permutation of \( s_1, \ldots, s_M \), the contribution to the matrix element is zero. Thus, we get

\[
< \psi_{\text{even}} | e^{-2\alpha H_w} | \psi_{\text{even}} > = < E | \sum_{\text{perms} P} K_{s_1,s_{P(1)}} \cdots K_{s_M,s_{P(M)}} \epsilon_{P(1) \cdots P(M)} \chi_1(s_1) \cdots \chi_3^\dagger(s_M) \chi_1(s_1) \cdots \chi_3^\dagger(s_M) | E > .
\]

(5.11)

Introduce the \( M \times M \) matrix \( L^{EE}(\alpha) \), whose \((m,n)\)th element is given by

\[
L^{EE}_{mn}(\alpha) = K_{s_m,s_n}(2\alpha).
\]

(5.12)

The EE refers to the fact that we are calculating the even-even matrix element. We can then write our even-even matrix element in its final, deceptively compact form:

\[
< \psi_{\text{even}} | e^{-2\alpha H_w} | \psi_{\text{even}} > = [\det L^{EE}(\alpha)]^3.
\]

(5.13)

The even-odd, odd-even, and odd-odd pieces of \(< 0_q | 0_q >\) can be calculated in analogous fashion, the only difference being the composition of the corresponding \( L \) matrix. We therefore have completed the calculation of the norm of the quark vacuum:

\[
< 0_q | 0_q >= [\det L^{EE}(\alpha)]^3 + [\det L^{EO}(\alpha)]^3 + [\det L^{OE}(\alpha)]^3 + [\det L^{OO}(\alpha)]^3.
\]

(5.14)
Now that the machinery is set up, the remaining matrix elements require much less effort. The next simplest matrix element to calculate is

\[ \langle 0_q | \chi_i(s_0) \chi_j^\dagger(s'_0) | 0_q \rangle. \]  

(5.15)

We need not consider operators \(\chi \chi\) or \(\chi^\dagger \chi^\dagger\), which change quark number and therefore have trivially vanishing matrix elements. (As we have mentioned already, the QCD Hamiltonian preserves quark number, and therefore does not include operators of this type.) Similarly, if \(i \neq j\), then the matrix element vanishes because there would be a mismatch in the number of quarks of a given color.

The calculation of this matrix element proceeds exactly as the overlap calculation, except that one of the colors (suppose it’s color 1) will have the extra operators \(\chi_1(s_0)\) and \(\chi_1^\dagger(s'_0)\) to commute through the exponential. This gives color 1 a contribution of

\[ \sum_{s_0, s'_0} K_{s_0, s_0'}(-\alpha) K_{s_0, s_0'}(-\alpha) < E | [\chi_1(s_M) \cdots \chi_1(s_1) \chi_1(s_0)] \times e^{-2\alpha H_0} [\chi_1^\dagger(s'_0) \chi_1^\dagger(s_1) \cdots \chi_1^\dagger(s_M)] | E >. \]  

(5.16)

If we define the extended \((M + 1) \times (M + 1)\) matrix

\[
L^{EE}(s_0, s'_0) = \begin{pmatrix}
\delta_{s_0, s'_0} & K_{s_0, s_1}(\alpha) & \cdots & K_{s_0, s_M}(\alpha) \\
K_{s_1, s'_0}(\alpha) & K_{s_1, s_1}(2\alpha) & \cdots & K_{s_1, s_M}(2\alpha) \\
\vdots & \vdots & \ddots & \vdots \\
K_{s_M, s'_0}(\alpha) & K_{s_M, s_1}(2\alpha) & \cdots & K_{s_M, s_M}(2\alpha)
\end{pmatrix},
\]

(5.17)

then we can again write a compact expression for our matrix element,

\[ \langle 0_q | \chi_i(s_0) \chi_j^\dagger(s'_0) | 0_q \rangle = \delta_{ij} \det L^{EE}(s_0, s'_0) [\det L^{EE}(\alpha)]^2 + \text{EO + OE + OO contributions}. \]  

(5.18)

The factors of \(\det L^{EE}(\alpha)\) are the contribution of the two unmodified colors.

Matrix elements involving more \(\chi \chi\) pairs can be calculated in analogy with the above derivation. Each additional pair requires the introduction of a further extended matrix, for the case in which all the \(\chi\)’s act on the same color. For instance, the next extension of the matrix comes from

\[
\langle 0_q | \chi_1(s_0) \chi_1(s_{00}) \chi_1^\dagger(s'_0) \chi_1^\dagger(s'_{00}) | 0_q \rangle = \det L^{EE}(s_0, s'_0; s_{00}, s'_{00}) [\det L^{EE}(\alpha)]^2 + \text{EO + OE + OO contributions},
\]

(5.19)
where
\[
L^{EE}(s_0, s'_0; s_{00}, s'_{00}) = \begin{pmatrix}
\delta_{s_{00}, s'_0} & \delta_{s_{00}, s'_0} & K_{s_{00}, s_1}(\alpha) & \cdots & K_{s_{00}, s_M}(\alpha) \\
\delta_{s_{00}, s'_0} & \delta_{s_{00}, s'_0} & K_{s_{00}, s_1}(\alpha) & \cdots & K_{s_{00}, s_M}(\alpha) \\
K_{s_{1}, s_{00}}(\alpha) & K_{s_{1}, s_0}(\alpha) & K_{s_{1}, s_1}(2\alpha) & \cdots & K_{s_{1}, s_M}(2\alpha) \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
K_{s_{M}, s_{00}}(\alpha) & K_{s_{M}, s_0}(\alpha) & K_{s_{M}, s_1}(2\alpha) & \cdots & K_{s_{M}, s_M}(2\alpha)
\end{pmatrix}
\]

We have calculated matrix elements of this type for up to four \(\chi\chi^\dagger\) pairs, which is the requirement for simulations with two dynamical quark pairs.

6 Summary

We have introduced a set of basis states that is suitable for making calculations in an “operator and states” approach to the study of lattice QCD. The previous section detailed the computation of matrix elements of the quark-sector states. In previous work we calculated matrix elements for pure gauge simulations. Taken together, these matrix elements provide us the tools to construct a Hamiltonian matrix on a basis of states in full QCD. The eigenvalues of this matrix are then estimates of masses in the QCD spectrum.

We would like to emphasize the particular power that this method has with respect to testing the quenched approximation. Unlike Monte Carlo simulations of the Feynman path integral, dynamical quarks pose no particular problems to our method. The states which include quark pairs are “just another configuration.” Moreover, by choosing which states to include, we can limit the simulation to having as many virtual quark pairs as we wish. By comparing runs with and without quark pairs, we hope to be able to provide some insight into the quenched approximation.

We would like to acknowledge the contributions made to this work by J. B. Bronzan.

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\[5\] If one fixes the gauge by our current method, the QCD Hamiltonian can contribute up to two pairs of operators, rather than just one. In this case we would need two more “extensions” of the \(L\) matrix to do the equivalent simulations.
A Appendix

To prove the relation
\[ \chi(s)e^{-\sigma H_w} = \sum_{s'} K_{s,s'}(\sigma)e^{-\sigma H_w}\chi(s'), \]  
we first need to diagonalize \( H_w \). Recall that \( H_w \) is bilinear in the quark creation and annihilation operators:
\[ H_w = \frac{1}{2a} \sum_{s,s'} \chi^\dagger(s)M_{ss'}\chi(s'), \]
where
\[ M_{ss'} = \sum_n [\delta_{s,s'+\hat{n}} + \delta_{s,s'-\hat{n}}]\eta(\hat{n}). \]
Diagonalizing \( M_{ss'} \) amounts to solving the Dirac equation on the lattice. We introduce quark mode operators, which annihilate “plane-wave” states:
\[ \chi(k,i) = \sum_s \chi(s)\phi(s; k, i). \]
The \( \phi(s; k, i) \) are the eigenfunctions of \( M_{ss'} \):
\[ \sum_{s'} M_{ss'}\phi(s'; k, i) = \lambda(k, i)\phi(s'; k, i), \]
where \( k \) is the lattice momentum, \( i \) enumerates the modes, and \( \lambda(k, i) \) is the eigenvalue of the mode. On a lattice with \( N \times N \times N \) sites, \( 1 \leq k_x, k_y, k_z \leq \frac{N}{2} \) and \( 1 \leq i \leq N^3 \). The derivation of the eigenfunctions is straightforward but rather tedious. We have carried it out explicitly only for a \( 2 \times 2 \times 2 \) lattice.

The weak-coupling quark Hamiltonian is (by design) diagonal using these new operators:
\[ H_w = 1 \frac{1}{2a} \sum_{s,s'} \chi^\dagger(s)M_{ss'}\chi(s') \]
\[ = 1 \frac{1}{2a} \sum_{k,k',i,i'} \chi^\dagger(k, i)\phi(s; k, i)M_{ss'}\phi(s'; k', i')\chi(k', i') \]
\[ = 1 \frac{1}{2a} \sum_{k,i} \lambda(k, i)\chi^\dagger(k, i)\chi(k, i). \]

6The plane-wave operators also have a color index, which we suppress here.
Next, we define the expression

\[ S(\sigma) = e^{\sigma H_w} \chi(k, i) e^{-\sigma H_w}. \]  \hspace{1cm} (A.7)

Then

\[ \frac{dS(\sigma)}{d\sigma} = e^{\sigma H_w} [H_w, \chi(k, i)] e^{-\sigma H_w}. \]  \hspace{1cm} (A.8)

Substituting the diagonal form of \( H_w \) we just derived, we have

\[ [H_w, \chi(k, i)] = -\lambda(k, i) \chi(k, i). \]  \hspace{1cm} (A.9)

Therefore,

\[ \frac{dS(\sigma)}{d\sigma} = -\lambda(k, i) S(\sigma), \]  \hspace{1cm} (A.10)

which implies that

\[ S(\sigma) = \text{constant} \times e^{-\sigma \lambda(k, i)}. \]  \hspace{1cm} (A.11)

Noting that \( S(0) = \chi(k, i) \), we have

\[ S(\sigma) = e^{-\sigma \lambda(k, i)} \chi(k, i), \]  \hspace{1cm} (A.12)

giving us the relation

\[ e^{\sigma H_w} \chi(k, i) e^{-\sigma H_w} = e^{-\sigma \lambda(k, i)} \chi(k, i). \]  \hspace{1cm} (A.13)

If we now multiply both sides of this by \( \phi(s; k, i) \), sum over \( k \) and \( i \), and change back to configuration space variables \( \chi(s) \), we obtain

\[ e^{\sigma H_w} \chi(s) e^{-\sigma H_w} = \sum_{s'} \sum_k \phi(s; k, i) e^{-\sigma \lambda(k, i)} \phi(s'; k, i) \chi(s'). \]  \hspace{1cm} (A.14)

Substituting the variable \( K \), and left-multiplying by \( e^{-\sigma H_w} \), we get the relation we set out to prove,

\[ \chi(s) e^{-\sigma H_w} = \sum_{s'} K_{s, s'}(\sigma) e^{-\sigma H_w} \chi(s'). \]  \hspace{1cm} (A.15)
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