HADRON STRUCTURE IN LATTICE QCD: Exploring the Gluon Wave Functional

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The use of lattice QCD to understand hadron structure is described, with particular emphasis on exploring the role of glue.

1 Introduction

This conference on excited states of the nucleon emphasizes the wealth of information about hadron structure accessible empirically through clever experiments and frontier electromagnetic probes. For a theorist, it also highlights the concomitant need for understanding the remarkably rich structure of hadrons from first principles.

Lattice QCD is the only known way to solve, rather than model, QCD. Given the development of the tools of lattice field theory and advances in computer technology that now make Terascale lattice computation affordable, the time is right for a major initiative in hadronic physics. Thus, it is particularly noteworthy for participants at this conference at Jefferson Lab that Jefferson Lab, MIT, and the Lattice Hadron Physics Collaboration, representing twenty-two theorists at thirteen institutions, have undertaken such an initiative and proposed dedicated Lattice QCD clusters with a total capacity of 480 Gflops to study hadron structure. The understanding and support of the experimental community for such an initiative is crucial, and I hope to provide in this talk glimpses of some of the physics that will be possible.

One of the most striking features of the quark and gluon structure of the nucleon is the extremely important role of gluons as essential dynamical degrees of freedom. In most familiar many-body problems, the bosons whose exchange mediates the interaction between fermions may be subsumed into an effective two-body interaction and hence do not appear directly as essential degrees of freedom. In atomic physics, photon exchange is subsumed into a static Coulomb potential and one solves the Schrödinger equation in the presence of Coulomb forces. Similarly in nuclear physics, to a good approximation nuclear structure may be calculated as a many-body problem in the presence of a strong, state-dependent but static nucleon-nucleon potential. In both cases, the mass of an atom or nucleus comes overwhelmingly from the masses of the fermionic constituents.

Nucleons are strikingly different. We know experimentally that approximately half of the momentum and angular momentum of a nucleon is carried by its gluons. Furthermore, the mass of a nucleon would hardly be altered if the masses of its quarks decreased from their physical scale of the order of a few MeV to zero, so the mass arises almost completely from the gluonic interactions between fermions.
Hence, although we normally only think of the fermionic component of the atomic or nuclear wave function, in the case of the nucleon it is essential to understand the gluon component of the wave function. As I will describe below, lattice QCD provides an excellent framework to explore this physics.

In lattice QCD, an observable is evaluated by defining quark and gluon variables on the sites and links of a space-time lattice, writing a Euclidean path integral of the generic form

\[
\langle T e^{-\beta H} \bar{\psi} \gamma^\mu \gamma^\nu \psi \rangle = Z^{-1} \int \mathcal{D}(U) \mathcal{D}(\bar{\psi}) e^{-\beta M(U) \bar{\psi} \gamma^\mu \gamma^\nu \psi - S(U)} \psi \bar{\psi} \psi
\]

and evaluating the final integral over gluon link variables \(U\) using the Monte Carlo method. The link variable is \(U = e^{i g A_{\mu}(x)}\), the Wilson gluon action is

\[
S(U) = 2 n g^2 \sum_{\Box} (1 - \frac{1}{N} \text{Re} \text{Tr} U_\Box)
\]

where \(U_\Box\) denotes the product of link variables around a single plaquette, and \(M(U)\) denotes the discrete Wilson approximation to the inverse propagator such that in the continuum limit, \(M(U) \to m + \partial + igA\). For those unfamiliar with lattice QCD, an elementary introduction at the level required for this work is presented in ref. For our present purposes, it is useful to note that evolution in Euclidean time provides a convenient filter to extract the ground state from an arbitrary state of specified quantum numbers, since

\[
e^{-\beta H} |\Psi\rangle = \sum_n e^{-\beta E_n} c_n |\psi_n\rangle \to \text{const} \times |\psi_0\rangle + \mathcal{O}(e^{-\beta (E_1 - E_0)}).
\]

2 Lattice Wave Functions

The wave function plays a central role in our understanding of many-body systems. Familiar examples in nonrelativistic quantum mechanics include the shell model for nuclear and atomic systems, the BCS wave function for superconductivity and the phases of liquid He, and the Laughlin wave function for the quantum Hall effect. It is thus natural to seek analogous understanding of hadronic structure in terms of quark and gluon wave functionals, which become wave functions when defined on a discrete lattice.

In nonrelativistic quantum mechanics, we define an N-particle wave function as the overlap between a state in which the positions of N particles are specified and the state \(|\psi\rangle\), \(\langle x_1, \ldots, x_N |\psi\rangle = \psi(x_1, \ldots, x_N)\). When it is impractical to deal with the exact wave function, one may alternatively study a variational wave function specified by some set of variational parameters \(\{\alpha_1, \ldots, \alpha_n\}\) and evaluate the inner product \(\psi_{\text{trial}}(\alpha_1, \ldots, \alpha_n) |\psi\rangle\). The “best” approximation is obtained by varying the \(\alpha\)’s to maximize the overlap. A familiar nuclear physics example is approximating a light nucleus by a harmonic oscillator wave function, and varying the size parameter to obtain the maximum overlap.

For pure Yang-Mills gauge theory on a lattice, we specify the gauge field \(A_{\mu}(x_n)\) for each space-time direction \(\mu\) and site \(x_n\), so the lattice wave function is the overlap \(\langle A_0(x_1), \ldots, A_4(x_N) |\psi\rangle\) corresponding to the wave functional \(\psi[A_{\mu}(x)]\) in the continuum limit. In QCD, it is convenient to use occupation number representation for the quarks, and indicate the lattice sites that contain quarks or antiquarks,
so that the wave function is written: 
\[ \langle q(x_1), \ldots, q(x_n), \bar{q}(y_1), \ldots, q(y_m), A_0(x_1), \ldots, A_4(x_N) | \psi \rangle. \]
Whereas it will be straightforward to examine components of the wave function involving a small number of quarks and antiquarks at specified positions, it will not be practical to keep track of all the components of the gauge field \( A_\mu(x_n) \) (which exceed \( 10^5 \) on a small \( 16^4 \) lattice). Hence, in general, we will need to consider some simple or physical Ansatz for \( A_\mu(x_n) \), and I will give illustrative examples below.

Given the form of a trial wave function
\[ \langle q(x_1), \ldots, q(x_n), \bar{q}(y_1), \ldots, q(y_m), A_0(x_1), \ldots, A_4(x_N) \rangle \]
the overlap with the ground state hadron wave functions is calculated on the lattice as sketched schematically in Fig. 1. A source with the quantum numbers of the desired meson is placed at the leftmost time \( t_l \), and propagation to time \( t \) near the middle of the lattice filters out the ground state. On time slice \( t \), one constructs an operator corresponding to the trial wave function. In the case considered in Fig. 1, a quark and antiquark are separated by distance \( \vec{y} \), the cm variable \( \vec{x} \) is integrated to project onto zero momentum, and the gluon wave function is the ground state vacuum configuration of gluons multiplied by a string of flux created by a Polyakov line as shown. Summing over an ensemble of gluon configurations then yields the quantum mechanical result for the overlap.

To elucidate the role of the gluon component of the hadron wave functional, it is instructive to display the results for several alternative approximations to the gluon field. To highlight the basic ideas, I will show some pedagogical results calculated previously in the meson sector by Kien Boon Teo. With the current interest in nucleon structure and the resources presently available, analogous calculations should certainly be carried out for nucleons. In particular, it is instructive to consider the following three definitions of variational wave functions.
2.1 Axial gauge or string wave function $\psi_s$

The conventional gauge-invariant wave function, which corresponds to the Bethe-Salpeter amplitude in the axial gauge $A_y = 0$, is given by

$$\psi_s(y) = \langle 0 | \bar{q}(0) \Gamma e^{\int_0^\gamma dz A_y(z)} q(y) | h \rangle$$

where $\Gamma$ depends on the Dirac structure of the ground state hadron $| h \rangle$. The exponential corresponds to a product of U links as shown in Fig. 1 and the implied gluonic component of $\psi_s$ is that of an infinitely thin string of glue. The square of the resulting wave function specifies the probability that a $q\bar{q}$ pair is separated by a distance $y$ and that the glue forms a narrow string connecting them.

2.2 Coulomb gauge-fixed amplitude $\psi_c$

Gauge fixing to Coulomb gauge surrounds each quark with the gluons corresponding to the static Coulomb field. In the Abelian case we can write down the following explicit expression:

$$\psi_c(y) = \langle 0 | \bar{q}(0) \Gamma e^{\int d^3 \bar{E}_{\text{static}}(\vec{z}).\vec{A}(\vec{z})} q(y) | h \rangle$$

where $\bar{E}_{\text{static}}$ is the static Coulomb field of an $e^+e^-$ pair separated by distance $y$. Since

$$\int \vec{A} \cdot \bar{E}_{\text{static}} = \int \vec{A} \cdot \nabla \phi = - \int (\nabla \cdot \vec{A}) \phi$$

it is evident that the exponent vanishes in Coulomb gauge.

![Figure 2: Lattice calculation of the meson wave function, $\psi_c$, corresponding to the overlap between the meson ground state (left) with a vacuum gluon configuration in Coulomb gauge (right).](image)

For QCD, the implied gluonic component of $\psi_c$ is obtained by the lattice measurement shown in Fig. 2 with the gluon field at time slice $t$ fixed to Coulomb
Gauge. As discussed later, the Coulomb gauge result has a well-behaved continuum limit.

2.3 Adiabatic Wave Function $\psi_a$

A more physical definition of a gluon wave function is the adiabatic wave function obtained by letting the gluonic component be the ground state distribution of gluons in the presence of a $q\bar{q}$ pair at separation $y$:

$$
\psi_a(y) = \lim_{n \to \infty} \frac{\langle 0 | \mathcal{P}(0) \Gamma S_y(t, n) q(y) | h \rangle}{W(y, 2n)^{1/2}} \quad (3)
$$

where $S_y(t, n) = U^{(0, t \to 0, t+n)}_y \cdot U^{(0, t+n \to y, t+n)}_y \cdot U^{+ \text{ } (y, t \to y, t+n)}_0$ and $W(y, 2n)$ is a Wilson loop of size $y \times 2n$. When the temporal links are extended (by increasing $n$) far enough, the gluons in the vacuum adjust themselves to the presence of the $q\bar{q}$ pair, forming the ground state of a flux tube connecting two fixed color charges.

![Figure 3: Lattice calculation of the adiabatic meson wave function, $\psi_a$, corresponding to the overlap between the meson ground state on the left with a configuration containing a static $q\bar{q}$ pair connected by a ground state flux tube on the right.](image)

3 Density-Density Correlation Functions

Since the density-density correlation function is a gauge-invariant quantity that describes the distribution of quarks in a hadron and reduces to the square of the wave function in nonrelativistic quantum mechanics, we have for comparison also calculated

$$
\langle \rho(x) \rho(0) \rangle = \langle h | \mathcal{P} \gamma_0 u(x) \mathcal{P} \gamma_0 d(0) | h \rangle \quad (4)
$$

and its projection $\langle \rho \rho \rangle_{q\bar{q}}$ onto the $q\bar{q}$ subspace. Computationally the projection is performed by using hard-wall boundary conditions to exclude those paths in which
the propagators can cross the time slice \( t \) at which \( \langle \rho \rho \rangle \) is evaluated. Figure 4 shows representative time histories corresponding to the density-density correlation function in the \( \bar{q}q \) sector, diagram (a), where only one quark and antiquark propagator cross time slice \( t \), and a general contribution, diagram (b), containing multiple quark-antiquark excitations at time \( t \).

4 Lattice Calculation of Meson Wave Functions and Correlation Functions

Figures 5–7 show the results of calculating the three wave functions and two density-density correlation functions described above in quenched lattice QCD.

Figure 5: Pion \( \psi_s \) and \( \psi_c \) for \( \beta = 5.7 \) (Teo and Negele\(^2\)) and \( \beta = 6.0 \) (extracted from Hecht and DeGrand\(^4\)) versus \( q\bar{q} \) separation \( y \). The lines are to guide the eye.
Figure 6: Comparison of $|\psi|^2$ and density-density correlation functions for the pion as a function of the $q\bar{q}$ separation in units of 0.2 fm. Lines connecting Monte Carlo results are to guide the eye.

All propagators were calculated with twenty quenched configurations at $\beta = 5.7$ on a $16^3 \times 16$ lattice using the Wilson action for both gluons and quarks and quark masses of 40, 95, and 170 MeV. We computed $\psi_s$ using a string of links and explicitly fixing to Coulomb gauge for $\psi_c$. $\Gamma = \gamma_5$ and $\Gamma = \gamma_i$ are used for $\pi$ and $\rho$ mesons respectively.

Figure 5 compares $\psi_s$ and $\psi_c$ calculated on the lattice for two different values of $\beta$ with a quark mass 170 MeV. The $\psi_c$'s agree to within error bars, indicating a well-behaved continuum limit. In contrast, $\psi_s$ decreases with increasing $\beta$ because of lattice artifacts that diverge as the lattice spacing approaches zero. As discussed below, the small overlap between a thin string of glue and the gluons in the ground state hadron accounts for much of the falloff of $\psi_s$ with $q\bar{q}$ separation.

Figures 6 and 7 show the results for the squares of wave functions and density-density correlation functions for $\pi$ and $\rho$ mesons, respectively. All quantities are
Figure 7: Comparison of $|\psi|^2$ and density-density correlation functions for the rho meson as a function of the $q\bar{q}$ separation in units of 0.2 fm. Lines connecting Monte Carlo results are to guide the eye.

normalized to 1 at zero $q\bar{q}$ separation. We display results for a quark mass of 40 MeV, where errors are in better control, instead of the extrapolated chiral limit which differs inconsequentially.

The dramatic difference between $\psi_a^2$, $\psi_c^2$, and $\psi_s^2$ shows that the gluon flux tube of the adiabatic wave function produces a much larger overlap with the gluons in the ground state hadron than does the Coulomb or string wave function. Beyond 1 fm, the adiabatic flux tube is favored by more than an order of magnitude. Physically, there is a substantial probability to find a quark-antiquark pair separated by 1 fm, connected by a physical adiabatic flux tube, but a very small probability to find them joined by an unphysically narrow string of flux. Also note, as mentioned in connection with Fig 5, that the string of flux becomes increasingly unfavorable as one approaches the continuum limit.
The role of multiple quark-antiquark excitations in the density-density correlation function is evident from the fact that \( \langle \rho \rho \rangle \) falls off more slowly than \( \langle \rho \rho \rangle_q \) at large distances. For both the pion and rho, \( \psi^2 \) is close to \( \langle \rho \rho \rangle_q \), suggesting that the adiabatic flux tube is a reasonable approximation to the full gluon wave function.

5 Overlap with Variational Wave Functions

A complementary means of studying the overlap of a trial gluon wave function with a hadronic ground state is through the calculation of two-point correlation functions.

\[
\psi(x) = \sum_{x'} \left( 1 + \alpha \sum_i [U_i(x) \delta_{x',x+i} + U_i^+(x-i) \delta_{x',x-i}] \right)^N q(x')
\]

where \( q(x) \) is the quark creation operator. The two-point function may be written

\[
\langle J(T)J^+(0) \rangle = c \sum_n \langle \psi_{\text{trial}} | n \rangle^2 e^{-E_n T}.
\]

At \( T = 0 \), the value of the correlation function is \( A = c \sum_n \langle \psi_{\text{trial}} | n \rangle^2 \). The large \( T \) behavior of the correlation function is \( c |\langle \psi_{\text{trial}} | 0 \rangle|^2 e^{-E_0 T} \), and extrapolating this behavior back to \( T = 0 \) yields \( B = c |\langle \psi_{\text{trial}} | 0 \rangle|^2 \). Hence one may study the overlap of
ψ_{trial} with the physical ground state by calculating $B/A = |\langle \psi_{\text{trial}} | 0 \rangle|^2$ and optimize it with respect to the variational parameters in $\psi_{\text{trial}}$.

Figure 8 shows the ratio of overlap with excited states to the overlap with the ground state, $(A - B)/B = \sum_{n > 0} |\langle \psi_{\text{trial}} | n \rangle|^2 / |\langle \psi_{\text{trial}} | 0 \rangle|^2$ for a nucleon created with Wuppertal smeared sources of different rms radii. The striking fact here is that, whereas for point sources the excited state content is $10^4$ larger than the ground state content, for the optimal smearing the overlap with the ground state, $B/A = |\langle \psi_{\text{trial}} | 0 \rangle|^2$, is approximately 65%. In other words, the sum of the sets of gauge-field links generated by the smearing provides a reasonable physical approximation to the behavior of the gauge fields in the nucleon. This suggests that a systematic study of variational wave functions has the potential to yield even larger overlaps and to provide a valuable tool for exploring the nucleon’s gluon wave function.

6 Conclusions

Lattice QCD provides a powerful tool for exploring hadron structure and, in particular, the gluon wave functional. The exploratory results for meson wave functions shown here display large effects of the gluonic components in three definitions of hadron wave functions, and the adiabatic flux tube wave function yielded the most physical results. Quantitative measurement of the overlap of a trial wave function with the ground state may be obtained from two-point correlation functions, providing the opportunity for quantitative study of variational wave functions.

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