Lattice pseudoscalar-meson wave-function properties

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Using lattice gauge theory in the quenched approximation we calculate the decay constants and second moments of wave functions of pseudoscalar mesons containing nonstrange, strange, and charmed quarks. We find $f_D = 134(23)$ MeV and $f_{D_s} = 157(11)$ MeV. We use the methodology of two recent computations of the second moment of the pion wave function, and find that a nonperturbative treatment of operator mixing gives results consistent with calculations using sum rules.

I. INTRODUCTION

We report on a calculation of the decay constants and second moments of wave functions of nonstrange, strange, and charmed pseudoscalar mesons in lattice QCD in the quenched approximation. We compute the second moments using two choices for lattice operators which have been recently proposed.

The operators which we study were introduced by Brodsky and Lepage' in their study of exclusive processes in QCD, such as form factors or amplitudes for largeangle elastic scattering. Their calculation involves moments of the momentum-space wave function ϕ of the quark and the antiquark in a pseudoscalar meson, which are a function of the momentum transfer Q. The nth moment of the meson's wave function is

$$
\langle \xi^n \rangle = \int_{-1}^1 d\xi \, \xi^n \phi(\xi, Q^2) \tag{1.1}
$$

where ξ is the difference in the light-cone functions of the meson's momentum carried by the quark and the antiquark, $\xi = x_q - x_{\overline{q}}$. The normalization of ϕ is chosen so that $\langle \xi^0 \rangle = 1$.

The lowest twist operators which give these moments when sandwiched between a pseudoscalar meson M and the vacuum are

$$
O_{\mu_0\mu_1\cdots\mu_n} = (-i)^n \overline{\psi} \gamma_{\mu_0} \gamma_5 \overline{D}_{\mu_1} \overline{D}_{\mu_2} \cdots \overline{D}_{\mu_n} \psi \qquad (1.2)
$$

symmetrized over Lorentz indices, and
\n
$$
\langle 0 | O_{\mu_0\mu_1\cdots\mu_n} | M(p) \rangle
$$
\n
$$
= \sqrt{2} f_M p_{\mu_0} p_{\mu_1} \cdots p_{\mu_n} \langle \xi^n \rangle + \text{trace terms}, \quad (1.3)
$$

where f_M is the meson decay constant. These operators are the same ones used to calculate structure functions measured in deep-inelastic sattering. The difference between a moment of the wave function and of the structure function is that in the latter case one must compute expectation values of Eq. (1.2) between hadronic states, $\langle \hat{h}(p) | O_{\mu_0\mu_1\cdots\mu_n} | h(p) \rangle$. As in the case of structure functions, if $\langle \xi^n(Q_0) \rangle$ can be determined at sufficiently large Q_0 , one can compute it at higher Q using the perturbative renormalization group. Unfortunately, $\langle \xi^n(Q_0) \rangle$ cannot be computed using perturbation theory; one must have recourse to some nonperturbative calculational scheme, in this case, Monte Carlo simulation of lattice gauge theory.

Before we begin our discussion of the lattice calculation, we remind the reader of what is known from previous nonlattice work, mainly QCD sum rules. The most complete studies are due to Chernyak and Zhitnitsky, $2,3$ who find that the low moments are quite similar to what one would compute from the distribution

$$
\phi(\xi, Q^2) = \frac{15}{4}\xi^2(1 - \xi^2)
$$
\n(1.4)

at $Q = 0.5$ GeV, i.e., $\langle \xi^2 \rangle = 0.42$. Other studies give similar results at various low values of Q^2 (Refs. 4 and 5). The uncertainty in these determinations is about 15%. As Q^2 goes to infinity, ϕ approaches the limiting form $\phi_{\text{asym}} = \frac{3}{4}(1 - \xi^2)$ for which $\langle \xi^2 \rangle = 0.2$.

Computing matrix elements from the lattice is by no means straightforward at present. To begin with, one makes two severe approximations: first, that the size of the box containing the hadron (i.e., the lattice size) is very small (about one Fermi in diameter) and second, that space is coarse grained on a size scale of the lattice spacing, about 0.¹ F in present-day calculations. Next, many studies, including this one, neglect the effects of virtual quark-antiquark pairs (the so-called "quenched approximation"). Another uncertainty is the value of the lattice spacing itself, which is determined by equating some lattice quantity to its continuum value. It sets the overall scale of dimensionful continuum quantities. This problem is particularly serious for our calculation of decay constants, but not for the moments of the wave function since they are dimensionless. What is more important for them is whether or not the lattice spacing is small enough that a smooth extrapolation to continuum behavior is possible. Finally, lattice operators are related to their continuum analogs by finite multiplicative renormalizations. These renormalization constants have so far been computed only in perturbation theory or in a very few cases by Monte Carlo methods.

Finally, there are many purely computational problems. For example, one generally cannot calculate quark propagators for light quarks at the physical values of their masses; one is forced to extrapolate the results from heavier-quark masses. Generally, in these calculations the same gauge configurations are used for computing the different quark propagators. This introduces a systematic correlation between the results at these different masses and makes extrapolation dangerous. As we will see, these difficulties limit the precision of our lattice measurements to no better than about 20%. Nevertheless, where comparison is possible, our results show good agreement with the gross features of experimental data.

e gross reatures of experimental data.
The lattice analog of $O_{\mu_0\mu_1\cdots\mu_n}$ was first given by Kronfeld and Photiadis.⁶ The continuum derivative is replaced by a lattice nearest-neighbor difference operator. This introduces two possible complications. The first difficulty is that the lattice spacing may be so large that the finite difference is a poor approximation to the derivative. This problem is most serious for the higher moments of the wave function since they involve higher and higher derivatives; to date no one (including us) has calculated moments higher than the second. The second difficulty is more subtle. The lattice breaks rotational invariance, causing operators corresponding to high moments to mix with operators of lower dimension. The mixing coefficients contain power divergences of the form $1/aⁿ$, where *a* is the lattice spacing,

Two methods have been proposed for dealing with the mixing problem. The first proposal, made by Gottlieb and Kronfeld, is to calculate the mixing coefficients in perturbation theory and construct the appropriate operators to lowest order in the gauge coupling g. Gottlieb and Kronfeld took the mixing coefficients computed by Kronfeld and Photiadis⁶ and computed the second moment using the operator O_{000} . They worked at a lattice coupling of $\beta = 5.7$ with 19 configurations on a $6^{2} \times 12 \times 18$ lattice with $k = \frac{1}{2}$ fermions. They found

$$
\langle \xi^2 \rangle = 1.58 \pm 0.23 \tag{1.5}
$$

The second proposal was made by Martinelli and Sachrajda.⁸ They computed linear combinations of the operators of a given dimension which are members of irreducible representations of the group of discrete lattice rotations. This eliminates the problem of mixing of the desired operator with operators which are members of other representations. For the second moment, linear combinations of $O_{\mu\nu\nu}$ with $\mu \neq \nu$ are unaffected by mixing. A disadvantage of this method is that one must measure operators at nonzero values of the lattice momentum; in general, quantities measured at nonzero momentum are noiser than ones measured at zero momentum. They used a lattice coupling of $\beta = 6.0$ with 15 configurations on a $10^3 \times 20$ lattice with Wilson fermions. They found

$$
\langle \xi^2 \rangle = 0.26 \pm 0.13 \tag{1.6}
$$

These results are obviously quite different. However, one does not know a priori why they are different. Is the difference due to the choice of operators and subtraction scheme, or is it simply due to the fact that every lattice parameter which could be different between the two studies is different

We now present a third measurement of the second moment of the pion wave function. We have one-third

more data than Ref. 8 and our lattice is one-third larger. In order to determine the origin of the difference between the results of Refs. 7 and 8 we measure both perturbatively and nonperturbatively subtracted operators. There are two reasons for performing this study. The first is that one really does not know why the results of Refs. 7 and 8 are different until both operators are measured on the same lattice size at the same coupling. The second reason is that even if one has a prejudice that one method of measuring the operators is better than another, the calculation is so delicate that it is useful to have it checked by several independent groups.

Our results may be simply stated: we find that the two different operators measured on the same set of lattices have very different values. Our calculation of the second moment of the pion wave function using a nonperturbative subtraction agrees with the result of Martinelli and Sachrajda. The perturbatively subtracted operator gives results which are if anything worse at the weaker coupling of this study (β =6.0) than were seen by Ref. 7.

Finally, we make an important extension to the results of Ref. 8 by including strange and charmed mesons in addition to nonstrange ones. We compare our results to experiment whenever possible, as well as to other lattice and nonlattice calculationy of wave-function properties. We find that a simple quark model can reproduce our results.

We also present in Sec. III lattice determinations of the decay constants of the pion, kaon, D , and D_s mesons. These predictions are constant with the results of a more extensive calculation by Woloshyn, Draper, Liu, and Wilcox.

II. DETAILS OF THE LATTICE CALCULATION

The data set used in this simulation consists of 20 pure gauge configurations of an $11³ \times 20$ lattice with gauge coupling $\beta = 6.0$. The gauge fields were equilibrated using the Kennedy-Pendleton¹⁰ variation of the Cabibbo-Marinari¹¹ quasi-heat-bath algorithm. The resultant gauge configurations were stored at intervals of 1000 sweeps. We computed quark propagators using a conjugate residual algorithm with incomplete Cholesky decomposition.¹² We used skew-periodic boundary conditions for the gauge fields and skew-periodic spatial and open temporal boundary conditions for the fermions. Details of our methods will be described separately.¹³

We used Wilson fermions in this study. We took the hopping parameter for the light quark to be $\kappa = 0.150$, 0.152, and 0.153, and extrapolated our results to zero quark mass. In addition, we calculated quark propagators for heavy quarks, with hopping parameters $\kappa = 0.130$ and 0.145, and formed mesons using all possible pairs of heavy quarks as well as mesons made of heavy quarks and light quarks of each of the three hopping parameters listed above. Pseudoscalar mesons made of pairs of these heavy quarks have masses of 1540 and 2710 MeV, respectively (with the inverse lattice spacing taking a nominal value at this gauge coupling of $1/a = 1900$ MeV) and so these propagators will allow us to interpolate from the pion to the kaon, D, and D_s mesons. We found the critical hopping parameter, where the quark mass vanishes, is κ_c = 0.1566(4), which is in agreement with previous calculations on lattices of this size at β = 6.0 (Ref. 14).

In the, by now, conventional way we extract operators from measurements of correlation functions of operators a time slice t apart and averaged over all spatial sites, with a possible Fourier transform:

$$
C_{ij}(\mathbf{k},t) = \sum_{\mathbf{x}} e^{i\mathbf{k}\cdot\mathbf{x}} \langle O_i(\mathbf{x},t)O_j(0,0) \rangle .
$$
 (2.1) and

With skew-periodic boundary conditions on an $N_s^2 \times N_t$ lattice a point at a location (x, y, z, t) is labeled by an integer

$$
r = x + N_s y + N_s^2 z + N_s^3 t \t . \t\t(2.2)
$$

When one Fourier transforms on this lattice, the discrete momenta are labeled by

$$
k = \left[\frac{2\pi}{N_s^3 N_t a}\right],\tag{2.3}
$$

where *m* is an integer running from 0 to $N_s^3 N_t - 1$. The skew-periodic momentum most peaked in the z direction 1s

$$
k_z = (2\pi/N_s a)m_z,
$$

where

$$
m = N_t N_s^2 m_z \tag{2.4}
$$

with $m_z = 0$ to $N_s - 1$. For this choice of m, k_v and k_x are suppressed by factors of N_s and N_s^2 , respectively, relative to k_z . We took $m_z = 0,1,2$ in (2.4) for nonperturbative operators in this study. We found that the cancellations due to Fourier transforming at $m_z > 1$ introduced a great deal of noise. Consequently, we could obtain no useful results, other than to check the energy-momentum dispersion relation, at $m_z=2$.

Inserting a complete set of relativistically normalized states, Eq. (2.1) becomes

$$
C_{ij}(\mathbf{k},t) = \sum_{n} \frac{1}{2E_n(k)} \langle 0 | O_i | n \rangle \langle n | O_j | 0 \rangle e^{-E_n(k)t},
$$
\n(2.5)

where

$$
E_n(k)^2 = m_n^2 + q^2
$$
 (2.6)

 $(m_n$ and t are the mass and time separation in lattice units) and

$$
q^2 = 2(1 - \cos k_z a)
$$
 (2.7) and

because of finite-lattice-spacing effects.

We are of course only interested in the lightest meson states and so we must determine the range of t for which Eq. (2.5) is dominated by a single exponential:

$$
C_{ij}(\mathbf{k},t) = \frac{1}{2E_h(k)} \langle 0 | O_i | h \rangle \langle h | O_j | 0 \rangle e^{-E_h(k)t}
$$

$$
\equiv B_{ij} \epsilon^{-E_h(k)t}.
$$
 (2.8) or

We did this by varying the lowest-t value used in a fit,

 t_{min} , until the fitted mass changed by less than a standard deviation when t_{min} increased by one time slice. We found that taking $t_{\text{min}} = 7$ was always a safe choice for beginning our fits.

The operators which we measured in this study were

$$
O_5 = \sum_{\text{color}} \bar{\psi} \gamma_5 \psi \tag{2.9}
$$

$$
O_{05} = \sum_{\text{color}} \bar{\psi} \gamma_0 \gamma_5 \psi , \qquad (2.10)
$$

and the operators appropriate for the second moment, described as follows: The second moment of the wave function in either subtraction method is given by an expectation value of combinations of the operator

$$
(2ia)^{2}O_{\mu\nu\nu}^{2} = (1+t_{\nu})^{2}\overline{\psi}i\gamma_{\mu}\gamma_{5}(U_{\nu}U_{\nu}+H.c. - 2)\psi,
$$
\n(2.11)

where $t_v = \exp(ik_v a)$. In the perturbative subtraction scheme (with Wilson fermions)

$$
O_p = O_{000}^2 - \text{trace term}
$$

-C_f $\frac{\alpha_s}{4\pi}$ $\left[0.76 \frac{i}{a^2} \bar{\psi} \gamma_0 \gamma_5 \psi + 3.49 \frac{1}{ia} \frac{\delta}{\delta t} \bar{\psi} \gamma_5 \psi + \frac{1.17}{a} \bar{\psi} \sigma_{0a} \gamma_5 \vec{\Delta}^a \psi \right],$ (2.12)

where the trace term is given explicitly in Ref. 6, $C_f = \frac{4}{3}$, $\delta/\delta t$ is a lattice time derivative, and Δ^{α} is a lattice covariant derivative.

In the nonperturbative subtraction scheme one takes linear combinations of the $O_{\mu\nu\nu}$'s which suffer no mixing with lower-dimensional operators. The choice in this study was to take $m_z = 1$ (see above) and measure

$$
O_{np} = O_{033}^{(2)} - \frac{1}{2} (O_{022}^{(2)} + O_{011}^{(2)}) \tag{2.13}
$$

We always take the operator at the origin to be O_5 and the operator at time slice t is one of the operators appropriate to the desired physics: O_5 , O_{05} , O_p , or O_{nn} . For the second moment it is more direct to measure ratios of operators. For future reference we define

$$
R_{np}(\mathbf{k},t) = \frac{\sum_{\mathbf{x}} e^{i\mathbf{k}\cdot\mathbf{x}} \langle O_{np}(\mathbf{x},t)O_5(0,0) \rangle}{\sum_{\mathbf{x}} e^{i\mathbf{k}\cdot\mathbf{x}} \langle O_0(\mathbf{x},t)O_5(0,0) \rangle}
$$
(2.14)

$$
R_p(t) = \frac{\sum_{\mathbf{x}} \langle O_p(\mathbf{x}, t) O_5(0,0) \rangle}{\sum_{\mathbf{x}} \langle O_{50}(\mathbf{x}, t) O_5(0,0) \rangle} .
$$
 (2.15)

One can extract the second moment from

$$
R_p = \frac{1}{2}m^2 \langle \xi^2 \rangle \tag{2.16}
$$

$$
R_{np} = q^2 \langle \xi^2 \rangle \tag{2.17}
$$

There are two possible ways to determine the lattice pseudoscalar-meson decay constant f^L_M . The most direct way involves O_{05} :

$$
\langle 0 | O_{05} | M \rangle = \sqrt{2} f_M^L m_M \tag{2.18}
$$

Alternatively, one can determine f_{π} from current algebra which gives

$$
\sqrt{2}m_{\pi}^{2}f_{\pi} = (m_{u} + m_{d})\langle 0 | O_{5} | \pi \rangle . \qquad (2.19)
$$

We choose the direct measurement of f_M^L via Eq. (2.18) for all mesons for two reasons. First, since the naive relation between the hopping parameter κ which we input, and the quark mass which we need in (2.19}, $m = \frac{1}{2}(1/\kappa - 1/\kappa_c)$, is not preserved in the interacting system, it must also be computed (for a discussion of this point, cf. Ref. 15}. Second we are interested in mesons containing a heavy quark, for which PCAC (partial conservation of axial-vector current) is probably not trustworthy.

One difficulty marred our extraction of f_M^L . Our lattice has skew periodic boundary conditions except at the ends of the lattice, where we set the fermion propagator to zero. This modifies the correlation function in time slices near the ends of the lattice and invalidates Eq. (2.5) there. Unfortunately, we set our source for matrix inversion one time slice away from the boundary. This distorts the coefficient B_{ij} from its true value. We corrected our data by recomputing all propagators for one-quarter of the gauge configurations (5) with the source set in the center of the fourth time slice. The masses we measured were the same as in our full data set, within errors. We computed the corrected B_{ij} 's by taking ratios of extracted B_{ij} 's between the same gauge configurations and multiplying the B_{ij} 's computed from the whole data set by that ratio. In the absence of rerunning the whole data set, this is the appropriate approach to take because different operators on the same lattices are highly correlated and the error obtained from taking a ratio of averages is a considerable overestimate of the uncertainty. The factor ranged from $R = 2.83(25)$ for two $\kappa = 0.153$ quarks to $R = 2.36(26)$ for a $\kappa = 0.153$, $\kappa = 0.130$ meson, so that while the overall renormalization is large, its ffuctuation from lattice to lattice (as shown by the error in R) is small. It small variation is also small. Since we are extracting $\langle \xi^2 \rangle$ from ratios of operators, the particular choice of operator we take at $t = 0$ is not important for it.

We would also like to remark that there is an extra trivial lattice-to-continuum renormalization factor of 2κ for fermion bilinears for the form of Wilson fermions which we are using. In that action the lattice field ψ is rescaled by a factor of $\sqrt{2\kappa}$ so that the $\bar{\psi}\psi$ part of the action appears with unit coefficient and the derivative terms appear multiplied by the hopping parameter κ .

III. PSEUDOSCALAR-MESON DECAY CONSTANTS

Our results for f_L^M are shown in Fig. 1 as a function of the light-quark hopping parameter for the three cases: quark and antiquark hopping parameter equal, antiquark hopping parameter equal to 0.145, and antiquark hop-

FIG. 1. Meson decay constant f_M^L in lattice units as a function of the hopping parameter κ . Squares label points for which the quark and antiquark hopping parameters are equal, crosses and diamonds the points for which the antiquark hopping pararneter is 0.145 and 0.130, respectively. The data points at κ = 0.1566 are the results of a linear extrapolation in κ to κ_c .

ping parameter equal to 0.130.

We must continue our results for the π, K , and D to zero light-quark mass. Realizing that our three data points for each value of the antiquark hopping parameter are strongly correlated, but not having any better procedure to follow, we fit them to a linear dependence in $\kappa - \kappa_c$ [a linear fit in $(1/\kappa_c - 1/\kappa)$ gives identical results]. These values are shown in Fig. 1 as the points at $\kappa = \kappa_c$.

Finally we convert f_M^L 's to continuum numbers by

$$
f_M^{\text{contin}} = f_M^L \frac{1}{a} Z_A \tag{3.1}
$$

where the multiplicative factor Z_A is a renormalization constant which converts from lattice to continuum regularization. Neither a nor Z_A is precisely known. Let us discuss our choices for each of them.

We begin with the lattice spacing. There are several possible choices. First, we can fix the lattice spacing from our calculation of the mass of the ρ meson. We find $m_a a = 0.37(1)$ at zero light-quark mass: $\kappa = \kappa_c$. This gives $1/a = 2081(56)$ MeV. Second, we can use the perturbative β function and the string tension. Taking the square root of the string tension $\sqrt{\sigma} = 400$ MeV and $\sqrt{\sigma}/\Lambda_L$ = 95 from lattice string tension studies, ¹⁶ we have $\Lambda_L = 4$ MeV and $1/a = 1800$ MeV. Third, Fukugi $ta¹⁷$ has made a compilation of quenched approximation fits to the π and ρ mass and finds $\Lambda_L = 4.7$ MeV and $1/a = 1800$ MeV. Finally, in the quenched approximation calculations done on lattices of similar size to ours, the proton mass is generally too high. For example, in the simulation of Lipps *et al.*¹⁴ $m_p = 1.25(15)$ GeV. There is no very good reason to assume that the quenched approximation is better than the ρ than for the proton; if we chose to fit the lattice spacing to the proton we would find $1/a = 1650$ MeV. Finally, we do not know how all these numbers are changed when one relaxes the quenched approximation. In what fo1lows we will take the uncertainty in the lattice spacing from all of these different determinations into effect of choosing $1/a$ to nominally equal 1900 MeV.

Next we turn to Z_A . In perturbation theory at $\beta = 6.0$ several groups¹⁸ have computed $Z_A = 0.87$. Z_A has also been calculated on the lattice at β =6.0 by Maiani and Martinelli;¹⁵ they find $Z_A = 0.7(1)$. It is not too surprising that the two calculations do not agree since β =6.0 corresponds to a lattice coupling $g^2 = 1.0$. When we convert our f_{π}^{L} into a continuum number using Z_{A} =0.87 we find f_{π} =76(31) MeV. Using the Z_A of Ref. 15, f_{π} =61(27) MeV. The physical number is 93 MeV.

Decay constants for mesons containing at least one massless quark, using the perturbative Z_A , are shown in Fig. 2. We linearly interpolate our light-quark and κ =0. 145 heavy-quark results to the physical kaon mass; we find $f_K = 103(22)$ MeV, where the error comes only from the extrapolation. This is within one σ of the experimental number, 112 MeV. The D-meson decay constant can also be read off from Fig. 2: $f_D = 134(32)$ MeV. With our choice for lattice spacing, the vector meson whose mass is closest to the physical ϕ mass is made of two $\kappa = 0.152$ quarks. We can interpret the D_s as a κ = (0.152,0.130) bound state. Referring to Fig. 1 we find $f_{D_e} = 157(11)$ MeV.

Finally, we can eliminate all Z_A dependence by computing ratios of the different decay constants. We find

$$
f_K/f_{\pi} = 1.35(62) , \qquad (3.2)
$$

$$
f_D/f_K = 1.31(36) , \t(3.3)
$$

$$
f_D/f_K = 1.31(36) , \t\t(3.3)
$$

$$
f_{D_s}/f_D = 1.17(22) . \t\t(3.4)
$$

Most of the error comes from the extrapolation to $\kappa = \kappa_c$; the fractional errors on the unextrapolated decay constants are only about 10%.

Woloshyn, Draper, Liu, and Wilcox 9 have recently carried out an extensive study of the decay constants of heavy mesons. They studied both Wilson and staggered fermions, and instead of the local axial-vector current O_{05} used the point-split operator

$$
\hat{O}_{\mu 5} = \frac{1}{2} (\bar{\psi} \gamma_{\mu} \gamma_5 U_{\mu} \psi + \text{H.c.}) \tag{3.5}
$$

They infer that f_D is 2–3 times f_π . Our results appear to be consistent with theirs, but the errors are large.

FIG. 2. Meson decay constant versus mass in physical units using $1/a = 1900$ MeV and $Z_A = 0.87$. The crosses show the known value for the pion and kaon.

There are a number of more conventional calculations of f_D . In a nonrelativistic quark model Suzuki¹⁹ predicts $f_D = 83$ MeV. Bag models give $f_D = 220$ to 240 MeV (Ref. 20) or f_D = 120 MeV (Ref. 21). Recent QCD sumrule calculations give $f_D = 1.31f_\pi$ (Ref. 22) and $f_D = 1.71 f_\pi$ (Ref. 23).

In a nonrelativistic quark model a pseudoscalar meson of mass m has a decay constant

$$
f_M = \left(\frac{6}{m}\right)^{1/2} |\psi(0)| \quad , \tag{3.6}
$$

where $|\psi(0)|$ is the wave function at the origin. If one assumes a linear potential then $|\psi(0)|$ scales like $\sqrt{\mu}$ where μ is the reduced mass. In that limit that one mass is much greater than the other, we expect from (3.6) that f_M rises as the lighter mass rises but falls as they heavy mass rises. Figure 1 shows the first effect and a flattening of the decay constants as the heavy-quark mass increases. Of course, for the π , K, and D mesons there is no reason to assume that a nonrelativistic quark model might be applicable because the motion of the light quark is certainly relativistic.

IV. SECOND MOMENT OF MESON WAVE FUNCTIONS A. The pion

We begin our evaluation of the second moment by first verifying that the individual $O_{\mu\nu}$'s showed the same exponential decay as O_5 and O_{05} . Since the different operators are strongly correlated, it is better to divide them before averaging than vice versa. Therefore in this analysis we measured the ratios of operators using Eqs. (2.14) and $(2.15).$

We fit for the second moment using the following four procedures: We measured the two ratios R_{np} and R_p lattice by lattice and then computed an error by either (a) averaging over all 20 configurations or by (b) breaking the data into four bins of five lattices and assigning an error from the bin-to-bin fiuctuations. (The averages will be the same but the errors will be different.) Next (c) we averaged the numerators and denominators of R_{np} and R_p separately over groups of five lattices, computed the ratio of these averaged quantities, and took an error from the bin-to-bin fiuctuations of these quantities. Finally (d) we fit R to each of our four bins using Eqs. (2.14) and (2.15) and computed an error from the bin-to-bin fluctuations in the fits. We performed a least-squares fit to a constant to each of these data sets, varying the initial and final time slices of the fit. The fits to R_{np} were generally stable from $t_{\text{min}}=6$ to 8 (but not at $t_{\text{min}}=5$ in contrast with the results of Ref. 8) and t_{max} extending to about 12; the signal above $t_{\text{max}} = 12$ usually disappeared into the noise. Fits to the three choices of R_{np} agreed to within one standard deviation of each other. As an example of our data, we present in Fig. 3 the time dependence of O_{np} and $O_{.05}$ with $m_z = 1$ and $\kappa = 0.153$. In Fig. 4 we show $\langle \xi^2 \rangle_L$ extracted from the same data using method (b) above.

The fits to the perturbative operator were performed similarly. Once again, the values of R obtained from the

FIG. 3. Time dependence of O_{np} (labeled by squares) and O_{05} (labeled by crosses) with $m_z = 1$ and $\kappa = 0.150$.

four fitting methods agreed with each other within two standard deviations.

Finally, we converted the measurement of R to one for $\langle \xi^2 \rangle$ using Eqs. (2.16) and (2.17). The results are shown in Fig. 5 (where we take the first fitting choice described above for R) with $t_{\min} = 7$, $t_{\max} = 12$. The results are clearly quite different. In Fig. 6 we replot the nonperturbatively subtracted operator together with the results from Ref. 8. They appear to be in good agreement with one another. Our results are also displayed in Table I.

Extrapolation to the limit $\kappa = \kappa_c$ is not very meaningful for our data since the results for different κ values are known to be correlated, and they are all equal within errors. Nevertheless, we find $\langle \xi^2 \rangle = 0.30(13)$ at $\kappa = \kappa_c$ after extrapolating (and assuming a linear dependence in $\kappa - \kappa_c$) to be contrasted with $\langle \xi^2 \rangle = 0.31(3)$ from a simple least-squares fit to a constant to the three κ values.

This result was obtained using a lattice regularization. In order to pass to the continuum, one must renormalize it:

$$
\langle \xi^2 \rangle_{\overline{\text{MS}}} = \frac{Z_0}{Z_A} \langle \xi^2 \rangle_L \tag{4.1}
$$

Here Z_0 is the ratio of renormalization constants in the

FIG. 4. $\langle \xi^2 \rangle_L$ extracted using method (c) described in the text, with $m_z = 1$ and $\kappa = 0.153$. The three horizontal lines show a least-squares fit to a constant and its one σ error bar over the range $7 \le t \le 12$.

FIG. 5. The second moment of the pion wave function as a function of the quark hopping parameter κ : Open squares, nonperturbatively subtracted operators; circles, perturbatively subtracted operator.

modified minimal subtraction (MS) and lattice schemes. In view of the difficulty in extrapolating to $m_q = 0$ it would be inappropriate to attempt to convert our lattice number into a continuum one. Nevertheless, as long as these renormalization factors are not too large the second moments we are measuring will be in good agreement with the results of Chernyak and Zhitnitsky.³ The uncertainties are still too large to give a result which is really interesting phenomenologically.

B. Results for mesons containing one heavy quark

We have also collected data for other mesons. We will present our results only for nonperturbatively subtracted operators, since they are the ones which give physically reasonable results for the pion. In the case of one light and one heavy quark our results extrapolate smoothly to zero light-quark mass and we show our results after extrapolation [using method (a) described above] in Fig. 7. One can see that the second moment shows little change from the second moment of the pion. That is to be expected from simple quark models, as we now demonstrate.

First, Chernyak and Zhitnitsky³ have presented a sum-rule calculation of the second moment of the kaon

FIG. 6. The nonperturbatively subtracted second moment of the pion's wave function (open squares) compared with the results of Ref. 8 (crosses).

TABLE I. Second moment of pseudoscalar wave function: nonperturbative and perturbative subtraction.

	Nonperturbative	Perturbative
0.150	0.31(4)	0.004(10)
0.152	0.34(6)	0.64(5)
0.153	0.29(6)	1.47(10)

wave function: $\langle \xi^2 \rangle = 0.17$.

Second, as one of the quarks becomes much heavier than the other, the wave function becomes more and more asymmetric in ξ . However, this asymmetry may not be reflected in a large change in $\langle \xi^2 \rangle$. For example, a simple model for ϕ , inspired by the so-called Peterson²⁴ form of quark fragmentation function, is

$$
\phi = N \left(\Delta E p_{\parallel}\right)^{-1},\tag{4.2}
$$

where ΔE is the energy difference in the infinitemomentum frame of an initial state consisting of the meson with mass M and a final state consisting of a quark meson with mass *m* and a final state consisting of a qual
of mass m_1 , transverse momentum **k**, and momentu fraction x_1 plus an antiquark of mass m_2 , transverse momentum $-k$, and longitudinal-momentum fraction $x_2 = 1-x_1$:

$$
\Delta E p_{\parallel} = M^2 - \frac{(m_1^2 + k^2)^{1/2}}{x_1} - \frac{(m_2^2 + k^2)^{1/2}}{x_2} \ . \tag{4.3}
$$

This wave function does not have the "dimple" at $\xi = 0$ of the Chernyak-Zhitnitsky pion wave function, but that is not necessary for this simple exercise. Recalling that $2\xi - 1 = x_1$, we can compute $\langle \xi^2 \rangle$. Taking $M = m_2 + 100$ MeV, $k = 300$ MeV, and $m_1 = 0$ gives the solid curve shown in Fig. 7. It qualitatively resembles the Monte Carlo data, although the errors are very large.

We also measured the second moment of mesons containing two heavy quarks, to see if their wave functions approached the expected nonrelativistic limit of $\delta(\xi)$. The meson made of two $\kappa=0.145$ quarks has $\langle \xi^2 \rangle$ = 0.19(3) and the meson made of two κ = 0.130 quarks has $\langle \xi^2 \rangle = -0.11(3)$. The first result goes in the right direction but the second is clearly absurd. We do not believe that we are seeing continuum physics in this number; rather, we think the size of the bound state has become small compared to the lattice spacing so that lattice effects have become important: in particular, that the replacement of a derivative by a finite difference can no longer be justified. For $\bar{q}Q$ mesons the variation in size of the wave function with changing heavy-quark mass is expected to be small since the relevant parameter is the reduced mass μ . In the nonrelativistic limit $\langle r^2 \rangle$ scales like $\mu^{-1/3}$ for a linear potential using Quigg Rosner²⁵ scaling laws. Going from the pion to the D meson the reduced mass changes by at most a factor of 2, and since the pion radius has been measured at about 0.4 F at $\beta = 5.7$ (Ref. 26), the lattice spacing should still be small relative to the D diameter.

FIG. 7. Second moments of mesons containing one heavy and one light quark, as a function of the meson mass (taking the lattice spacing to be $1/a = 1900$ MeV). The light-quark mass has been continued to zero. The line is the prediction of the simple model described in the text.

V. CONCLUSIONS

We have calculated decay constants and second moments of light, strange, and charmed pseudoscalar mesons. The calculations of f_{π} and f_{K} are in agreement with experiment (although with large errors). When a nonperturbative subtraction is used to eliminate operator mixing due to the effects of a finite lattice spacing, the second moment of the pion is in good agreement with the results of QCD sum rules and with the earlier Monte Carlo study in Ref. 8. The second moment of mesons containing one heavier quark shows very little dependence on the heavy-quark mass, at least as far as charm. This is in accord with simple quark-model ideas.

Using perturbation theory to eliminate operator mixing due to lattice artifacts is a common practice in the calculation of hadronic matrix elements.²⁷ However, as $a \rightarrow 0$ the coupling constant vanishes logarithmically while the denominator of a typical term vanishes like a raised to a power. This means that at best many terms in the perturbation expansion would be needed as the $a \rightarrow 0$ limit is approached. At worst, the powers of a^{-1} imply that nonperturbative contributions to the mixing coefficients might not vanish as $a \rightarrow 0$ (Ref. 28). Based on a comparison of our results with those of Ref. 7, perturbative subtraction does not appear to be converging for the operators appropriate to $\langle \xi^2 \rangle$ for β in the range 5.7—6.0. It appears that for the sizes of lattices and lattice spacings which may be attainable in the foreseeable future, nonperturbative subtraction is the only method which can be used to give reliable QCD predictions from the lattice.

The results of this study, as those of Ref. 8, can only be considered to be exploratory. In order to see the renormalization-group evolution of the moment or the dependence of the second moment with quark mass, the statistical errors must be reduced to the level of a few percent. This will require a minimum of several hundred lattice configurations. One also needs larger lattices to avoid possible finite-size effects as well as similar lattice spacings to better approximate the continuum derivatives which are what one really wants to measure. Finally, one needs to include the effects of dynamic fermions. (However, even an exploratory study including dynamic fermions would be interesting.) On the positive side, these operators involve very little computational overhead and can be readily measured as part of any large spectroscopy project.

The other obvious next steps in an exploratory program are to extend wave-function results to the baryon sector and to compute moments of the structure functions of hadrons. A recent study of Martinelli and

- ¹S. Brodsky and G. P. Lepage, Phys. Lett. 87B, 359 (1979); Phys. Rev. D 22, 2157 (1980).
- V. L. Chernyak and A. R. Zhitnitsky, Nucl. Phys. B201, 492 (1982).
- 3V. L. Chernyak and A. R. Zhitnitsky, Phys. Rep. 112, 173 (1984).
- 4M. J. Lavelle, Z. Phys. C 29, 203 (1985).
- 5D. Johnston and H. Jones, Imperial College Report No. TP/85-86/28, 1986 (unpublished).
- 6A. Kronfeld and D. Photiadis, Phys. Rev. D 31, 2939 (1985).
- ⁷S. Gottlieb and A. Kronfeld, Phys. Rev. D 33, 227 (1985).
- G. Martinelli and C. Sachrajda, Phys. Lett. B 190, 151 (1987).
- ⁹R. Woloshyn, T. Draper, K. Liu, and W. Wilcox, TRIUMF report, 1987 (unpublished).
- 10A. Kennedy and B. Pendleton, Phys. Lett. 156B, 393 (1985).
- ¹¹N. Cabibbo and A. Marinari, Phys. Lett. 119B, 387 (1982).
- ¹²Compare with Y. Oyanagi, Comput. Phys. Commun. 42, 333 (1986).
- ¹³R. Loft and T. DeGrand (in preparation).
- ¹⁴H. Lipps, G. Martinelli, R. Petronzio, and F. Rapuano, Phys. Lett. 126B, 250 (1983).
- ¹⁵L. Maiani and G. Martinelli, Phys. Lett. B 178, 265 (1986).
- ¹⁶M. Flensberg and C. Peterson, Nucl. Phys. **B283**, 141 (1987).
- ¹⁷M. Fukugita, in Lattice Gauge Theory Using Parallel Processors, proceedings of CCASI Symposium, Beijing, China, 1987, edited by X. Li, Z. Qiu, and H.-C. Ren (Gordon and Breach, New York, 1987), p. 198.

Sachrajda for the pion²⁹ indicates that the latter calculation is within reach of present-day computing power.

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- ¹⁸B. Meyer and C. Smith, Phys. Lett. **123B**, 62 (1983); G. Martinelli and Y.-C. Zhang, ibid. 123B, 433 (1983); R. Groot, J. Hock, and J. Smit, Nucl. Phys. 8237, 111 (1984).
- ¹⁹M. Suzuki, Phys. Lett. **162B**, 392 (1985).
- ²⁰D. Izatt, C. DeTar, and M. Stephenson, Nucl. Phys. **B269**, 269 (1982).
- ²¹M. Claudson, Harvard Report No. HUTP-81/A016 (unpublished).
- ²²S. Narison, Phys. Lett. B 198, 104 (1987).
- 23 C. Dominguez and N. Paver, Phys. Lett. B 197, 423 (1987).
- ²⁴S. Brodsky, C. Peterson, and N. Sakai, Phys. Rev. D 23, 2745 (1981).
- 25C. Quigg and J. Rosner, Phys. Rep. 56, 167 (1979).
- ²⁶See, for example, S. Gottlieb, in Advances in Lattice Gauge Theory, edited by D. Duke and J. Owens (World Scientific, Singapore, 1985).
- 27 For a discusssion in a related context, see the contribution by C. Bernard, in Lattice Gauge Theory 1986, proceedings of the International Workshop, edited by H. Satz, I. Harrity, and J. Potvin {Plenum, New York, 1987).
- ²⁸M. Bochicchio et al., Nucl. Phys. **B262**, 331 (1985); C. Bernard, in Field Theory of the Lattice, proceedings of the International Symposium, Seillac, France, 1987, edited by A. Billoire et al. (Nucl. Phys. B. Proc. Suppl., Vol. 1) (North-Holland, Amsterdam, 1988).
- ²⁹G. Martinelli and C. Sachrajda, Phys. Lett. B 196, 184 (1987).