Calculation of Weak Transitions in Lattice QCD

Richard C. Brower and Guillermo Maturana
Institute for Particle Physics, University of California, Santa Cruz, California 95064

and

M. Belén Gavela[(a)]
Department of Physics, Brandeis University, Waltham, Massachusetts 02254

and

Rajan Gupta
Department of Physics, Northeastern University, Boston, Massachusetts 02115
(Received 23 February 1984)

We propose the use of Monte Carlo simulations of QCD to evaluate hadronic matrix elements of local operators encountered in electroweak and grand-unified-theory transitions. Preliminary Monte Carlo estimates are made of the $\Delta S = 2$ matrix elements responsible for the K_L-K_S mass difference and the $\Delta S = 1$ operators believed to explain the $\Delta I = \frac{1}{2}$ enhancement.

PACS numbers: 11.15.Ha, 12.35.Eq, 13.25.+m, 14.40.Aq

In any attempt at an accurate estimate of the weak-interaction amplitudes, the difficulty lies in the hadronic matrix elements, not in the short-distance behavior of the gauge theory. The initial, intermediate, and final hadronic effects are the realm of nonperturbative QCD for which only intuitive and clever phenomenological estimates are known (quark models, bag models, etc.).

In principle, lattice gauge theories allow rigorous evaluation of nonperturbative QCD effects, when simulated by Monte Carlo techniques.[1] In this Letter we propose to extend the use of Monte Carlo simulations of lattice QCD to evaluate the hadronic matrix elements that arise in weak processes. For the lattice cutoff π/a between the W mass and the QCD scale Λ_{QCD} ($M_W >> \pi/a >> \Lambda_{\text{QCD}}$), the lattice provides a natural separation between hard- and soft-momentum physics. The renormalization group is used to sum the hard gluons into the coefficients of an effective theory, while the soft-gluon contribution to the matrix elements is summed to all orders by the lattice calculation.

Some of these matrix elements are known experimentally with high precision and their evaluation provides as good a test of QCD as the calculation of the hadronic spectrum.[2,3] Conversely, once confidence is gained in these techniques, it becomes possible to settle major questions in standard weak-interaction phenomenology such as the K_0-$\bar{K}_0$ mixing, the $\Delta I = \frac{1}{2}$ rule, etc., as well as to make new predictions for future measurements such as the ratio ϵ'/ϵ in CP-nonconserving decays, the proton lifetime in grand-unified theories (GUTs), etc. To make this program more precise, we give a brief description of the phenomenological picture for two cases.

$\Delta I = \frac{1}{2}$ *rule.*—The $\Delta I = \frac{1}{2}$ decay amplitudes for $K \rightarrow \pi\pi$ are known to dominate over the $\Delta I = \frac{3}{2}$ decay amplitudes by a factor of about 20. The effective Hamiltonian for the $\Delta S = 1$ weak interactions with four quark flavors and without strong-interaction corrections is, to first order,

$$(4G_F/\sqrt{2})\sin\theta_c\cos\theta_c[\bar{d}_L\gamma_\mu u_L\bar{u}_L\gamma_u s_L - \bar{d}_L\gamma_\mu c_L\bar{c}_L\gamma_\mu s_L], \tag{1}$$

where $G_F \sim 1/M_W^2$. In order to include the QCD effects down to a scale $\mu < M_W$, the renormalization group can be used to sum the leading logarithms between μ and M_W. Further, for $\mu < m_c$, the effective Hamiltonian after integration out of the effects of the charm quark is[4]

$$H_{\text{eff}}^{\Delta S=1} = \sum_\alpha C_\alpha(M_W/\mu, m_c/\mu)O_\alpha(x), \tag{2}$$

with known coefficient functions C_α and the six operators

$$\begin{aligned} &O_1=\bar{s}_L\gamma_\mu d_L\bar{u}_L\gamma_\mu u_L-\bar{s}_L\gamma_\mu u_L\bar{u}_L\gamma_\mu d_L, \quad O_2=\bar{s}_L\gamma_\mu d_L(\bar{u}_L\gamma_\mu u_L+2\bar{d}_L\gamma_\mu d_L+2\bar{s}_L\gamma_\mu s_L)+\bar{s}_L\gamma_\mu u_L\bar{u}_L\gamma_\mu d_L,\\ &O_3=\bar{s}_L\gamma_\mu d_L(\bar{u}_L\gamma_\mu u_L+2\bar{d}_L\gamma_\mu d_L-3\bar{s}_L\gamma_\mu s_L)+\bar{s}_L\gamma_\mu u_L\bar{u}_L\gamma_\mu d_L,\\ &O_4=\bar{s}_L\gamma_\mu d_L(\bar{u}_L\gamma_\mu u_L-\bar{d}_L\gamma_\mu d_L)+\bar{s}_L\gamma_\mu u_L\bar{u}_L\gamma_\mu d_L, \quad O_5=\bar{s}_L\gamma_\mu t^a d_L(\bar{u}_R\gamma_\mu t^a u_R+\bar{d}_R\gamma_\mu t^a d_R+\bar{s}_R\gamma_\mu t^a s_R),\\ &O_6=\bar{s}_L\gamma_\mu d_L(\bar{u}_R\gamma_\mu u_R+\bar{d}_R\gamma_\mu d_R+\bar{s}_R\gamma_\mu s_R). \end{aligned} \tag{3}$$

The subscripts L and R designate the left $[\frac{1}{2}(1-\gamma_5)]$ and right $[\frac{1}{2}(1+\gamma_5)]$ projected Dirac fields, respectively. The color SU(3) matrices t^a are normalized to $\mathrm{Tr}(t^a t^b)=2\delta^{ab}$. Shifman, Vainshtein, and Zakharov[4] have conjectured that the new $(V-A)(V+A)$ operator structure in O_5 and O_6 is responsible for the $\Delta I=\frac{1}{2}$ enhancement. On the basis of partial conservation of axial-vector current (PCAC) and vacuum insertion hypotheses, they find an enhancement factor of 70 for the ratio of matrix elements $\langle\pi|O_5|K\rangle/\langle\pi|O_1|K\rangle$. This is still too small to explain the $\Delta I=\frac{1}{2}$ rule because of the small coefficient O_5.

K_0-$\bar{K}_0$ mixing.—The second-order K_0-$\bar{K}_0$ matrix element is responsible for the K_L-K_S mass splitting. As a result of the Glashow-Iliopoulis-Maiani mechanism, the two-W-exchange graph gives zero except for a term proportional to $m_c^2-m_u^2$; for $\mu<m_c$ and up to leading logarithms the $\Delta S=2$ effective Hamiltonian leads to a mass difference[5]

$$m_{K_L}-m_{K_S}\simeq\frac{G_F}{\sqrt{2}}\frac{\alpha}{4\pi}\frac{m_c^2-m_u^2}{M_W^2\sin^2\theta_W}\cos^2\theta_c\sin^2\theta_c C\left(\frac{m_c}{\mu}\right)\langle\bar{K}_0|O^{\Delta S=2}|K_0\rangle, \tag{4}$$

where $O^{\Delta S=2}(x)=\bar{d}_L(x)\gamma_\mu s_L(x)\bar{d}_L(x)\gamma_\mu s_L(x)$. The effects of the heavier b and t quarks have again been neglected. Gaillard and Lee[5] estimated this matrix element and then made a remarkably good prediction of the charm quark mass before its discovery. However, Donoghue, Golowich, and Holstein[6] argue that the matrix element is about $\frac{1}{3}$ of the Gaillard and Lee value on the basis of PCAC and SU(3) symmetry.

Lattice formulation and evaluation of the matrix elements.—All lattice quantities are evaluated as a function of the bare coupling g_0 and the bare mass parameter κ for the Wilson $(r=1)$ fermions. For a given g_0 and κ the meson mass $m(\kappa,g_0)$ is calculated from the two-point correlation function as

$$\lim_{\tau\to\infty}\sum_{\vec{x}}\langle\phi_K^\dagger(\vec{x},\tau)\phi_K(\vec{0},0)\rangle=\frac{|\langle 0|\phi_K|K,0\rangle|^2 e^{-m_K\tau}}{2m_K(aL)^3}, \tag{5}$$

where $\sum_{\vec{x}}\phi_K(\vec{x},\tau)$ creates a zero-momentum meson state with the quantum numbers of the K meson. The meson correlation function is evaluated as a product of the quark propagators, $S(x,0;A)$, averaged over the gauge configurations, $A_\mu(x)$. On a lattice with spatial dimensions aL, the plane-wave–state normalization is taken to be $\langle K,\vec{p}|K,\vec{p}'\rangle=2E_p a^3L^3\delta_{\vec{p},\vec{p}'}$, where the momentum components are restricted to be discrete integer multiples of $2\pi/aL$ in the interval $-\pi/a<p<\pi/a$. We suggest that the K_0-$\bar{K}_0$ transition matrix element be calculated from the ratio of the vacuum processes

$$\lim_{\tau_1,\tau_2\to\infty}\frac{\sum_{x,y}\langle\phi_K^\dagger(x,\tau_1)O_{\mathrm{latt}}^{\Delta S=2}(0)\phi_K(y,\tau_2)\rangle}{\sum_x\langle\phi_K^\dagger(x,\tau_1+\tau_2)\phi_K(0,0)\rangle}=\frac{a^3\langle\bar{K}_0|O^{\Delta S=2}|K_0\rangle}{4\kappa_s\kappa_d 2M_K}, \tag{6}$$

where O_{latt} is written in terms of the dimensionless lattice fermions $(a^3/2\kappa)^{1/2}\psi(x)$. This result and Eq. (6) are derived by inserting the eigenstates of the transfer matrix $e^{-\hat{H}\tau}$ between the operators; in the limit $\tau\to\infty$, only the lowest state survives. For off-diagonal matrix elements in Eq. (6) the wave functions do not cancel, but they can be calculated from Eq. (5). In the case of the $K\to\pi\pi$ amplitudes we shall simplify the calculation by using PCAC to remove one of the external pions, and consider the ratios of the expectation values of the $\Delta S=1$ operators, to avoid the problem of wave-function normalization.

Beyond the usual finite-lattice effects, there are corrections due to the mixing and rescaling of the matrix elements of the renormalized operators O_R^α relative to the bare operators O_{latt}^β with the lattice cutoff. For example, we have

$$\langle\bar{K}_0|O_R^\alpha|K_0\rangle=Z_{\alpha\beta}^{-1}(a\mu,g_0)\langle\bar{K}_0|O_{\mathrm{latt}}^\beta|K_0\rangle. \tag{7}$$

Renormalization-group scaling gives Z as a perturbation expansion in g_0,

$$Z_{\alpha\beta} \simeq \delta_{\alpha\beta}[1+\beta_0 g_0^2 \log(\pi^2/\mu^2 a^2)]^{\gamma_0/2\beta_0} + O(g_0^2), \quad (8)$$

and guarantees that the limit $a \to 0$ is finite and independent of the renormalization point μ for physical amplitudes. However, in practice, we have a nonzero lattice spacing. So we choose $\mu \simeq \pi/a$, cognizant of the fact that perturbative corrections to $Z=1$ in combination with better Monte Carlo data are important for accurate physical predictions.

Analysis and results.—Our numerical results were obtained on a $6^3 \times 10$ lattice with the bare coupling set equal to $g_0^2 = 1.0$.[3] Six independent gauge configurations, each separated by 600 sweeps after 5000 thermalization sweeps, were generated by use of the pure gauge action (quenched approximation). The quark propagators were calculated for periodic boundary conditions by the Gauss-Seidel method at $\kappa = 0.145$, 0.147, 0.1485, and 0.15. The Wilson parameter r was set equal to 1. The light u and d quarks were considered degenerate and we used the naive currents $J_\mu = \bar{q}_L(x)\gamma_\mu q_L(x)$.[7] On each of the six configurations the quark propagator was calculated for a single starting point selected at random. This restricts computations to matrix elements where all quark lines originate (or end) at this single point. For the K_0-$\bar{K}_0$ transition, the full operator can be evaluated but for the matrix elements $\langle \pi | O_\alpha | K\rangle$, we must normal order the operator $(:O:_\alpha)$ dropping the diagram with a contracted quark line,

$$\underbrace{\bar{\psi}\psi} = S(0,0;A),$$

because of the presence of a spectator quark going from K to π.

The Monte Carlo results for the $K \leftrightarrow \pi$ transitions are summarized in Fig. 1. A large enhancement of $\langle \pi | :O_5: | K\rangle$ over $\langle \pi | :O_1: | K\rangle$ is observed. Before these results are extrapolated to the physical quark mass, i.e., κ_{physical}, the difference between the normal-ordered and the full operators has to be taken into account. In the limit $m = m_K = m_\pi \to 0$, PCAC implies that the matrix elements of all operators O_α vanish as m^2.[8] This same behavior is also required of the $(V-A)(V-A)$ normal-ordered operators $:O_1:$ to $:O_4:$, since both the original and the Fierz-transformed expression have vector indices. By Lorentz invariance the matrix elements of these normal-ordered operators are proportional to $p\cdot k$, which in our analysis is evaluated at $p=(\vec{0},m_\pi)$, $k=(\vec{0},m_K)$ to give a factor $m_\pi m_K$. For the $(V-A)(V+A)$ operators O_5 and O_6 the relation between the full and the normal-ordered part is[9]

$$\langle \pi | O_5 | K\rangle = \langle \pi | :O_5: | K\rangle + \langle \pi | \underbrace{\bar{\psi}\psi} ds | K\rangle. \quad (9)$$

Apparently the second term goes to a constant in the chiral limit. In this case the normal-ordered part also has a leading constant piece, and the ratios $\langle :O_5:\rangle / \langle :O_1:\rangle$ and $\langle :O_6:\rangle / \langle :O_1:\rangle$ will diverge like $1/m_\pi m_K$ in the chiral limit.[9] This effect, which is evident in our data (Fig. 1), is also exactly reproduced in strong-coupling calculations. Therefore the extrapolation in the pion mass, i.e., a multiplicative factor of 4 coming from the ratio of the pion mass at $\kappa = 0.15$ to its physical value,[3] results in a ratio $\langle :O_5:\rangle / \langle :O_1:\rangle \sim 200$. On the other hand, the direct extrapolation of our data for $\langle :O_5:\rangle / \langle :O_1:\rangle$ by fitting to $m_\pi \sim (\kappa_c - \kappa)^{1/2}$ yields $\kappa_c = 0.153$, which is in disagreement with the value $\kappa_c \simeq 0.156$

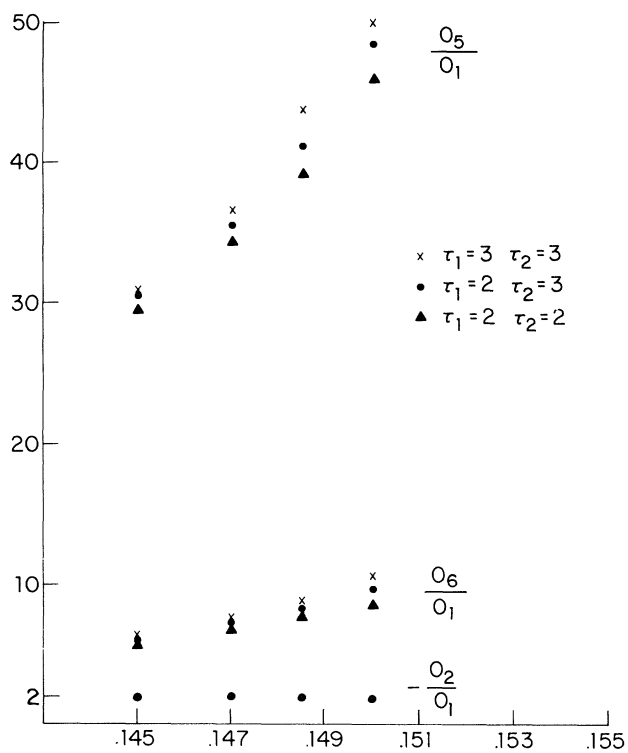

FIG. 1. The ratios of the $\langle \pi | :O_{2,5,6}: | K\rangle$ amplitudes relative to $\langle \pi | :O_1: | K\rangle$ as a function of the light-quark mass parameter κ extracted from the time intervals $\tau_1 = 2$ and $\tau_2 = 3$ (circles), $\tau_1 = \tau_2 = 2$ (triangles), and $\tau_1 = \tau_2 = 3$ (crosses). The amplitudes for O_3 and O_4 are identical to O_2.

TABLE I. Lattice results for the K^0-$\bar{K}^0$ transition elements [left-hand side of Eq. (6)] as a function of the light-quark mass parameter κ and the time separation. The finite-size corrections for the propagator in the denominator $1+\exp\{-m[L-2(\tau_1+\tau_2)]\}$ have been included.

κ	$\tau_1=1, \tau_2=1$	$\tau_1=2, \tau_2=2$	$\tau_1=2, \tau_2=3$
0.145	0.86	0.32	0.22
0.147	0.79	0.29	0.2
0.1485	0.73	0.25	0.17
0.15	0.68	0.21	0.16

obtained from the pion-mass calculations.[2,3] In spite of the obvious shortcoming of our restriction to normal-ordered diagrams, we are encouraged by the evidence for a strong dynamical enhancement in these contributions to the penguin diagrams. A complete evaluation of the matrix element is being pursued for future publication.

An error estimate is as follows: In Fig. 1 we show the effect of changing the time separation between the operator and the states. In a large lattice (required for convergence in time separation) the absolute numbers will change but we feel that the large enhancement will survive. We also binned the six configurations into two sets of three each. The individual matrix elements had up to 50% variation but the ratios were stable up to 10%.

The results for the dimensionless K^0-$\bar{K}^0$ matrix element [left-hand side of Eq. (6)] are shown in Table I. The numbers are very sensitive to both κ and the time separation. For illustration purposes, we quote the result for $\kappa=0.15$ and $\tau_1=\tau_2=2$:

$$\langle \bar{K}_0 | O^{\Delta S=2} | K_0 \rangle = 0.04 m_K/a^3. \tag{10}$$

With the lattice parameter a satisfying $am_K \sim 1$ at $\kappa=0.15$, this value is not inconsistent with the phenomenological estimates of $0.08m_K^4$ (Gaillard and Lee[3]) or $0.025m_K^4$ (Donoghue, Golowich, and Holstein[6]). Obviously, our prediction for $m_{K_L} - m_{K_S}$ is very uncertain as a result of large systematic errors from finite-size effects, as well as the strong sensitivity on κ and a^3 dependence of the mass scale.

To conclude, our preliminary analysis of the $\Delta I = \frac{1}{2}$ rule and the K_L-K_S mass difference shows how Monte Carlo techniques can be used to compute weak effects in hadronic processes without recourse to phenomenological models. It is important to extend this approach to GUT-scale physics to compute, for example, proton decay from first principles.

We wish to thank Larry Abbott, Enrique Alvarez, Edouard Brézin, John Ellis, Roscoe Giles, Howard Georgi, Toni Gonzalez-Arroyo, Apoorva Patel, Michael Peskin, A. Le Yaouanc, L. Oliver, O. Pene, and J. C. Raynal for discussions. Also, we acknowledge the generous assistance of colleagues at Brandeis and Harvard Universities and Richter Seismological Laboratory, University of California at Santa Cruz, for their generous help with the computations. When this work was completed we received a preprint by N. Cabibbo, G. Martinelli, and R. Petronzio describing similar work. This work was supported in part by the National Science Foundation through Grants No. NSF PHY81-115541, No. PHY-83-05734, and No. PHY-82-15249, and in part by the U.S. Department of Energy through Grant No. DEAC02-76-ER0220.

(a)Present address: Laboratoire de Physique Theorique et Hautes Energies, University of Paris-Sud, F-91405 Orsay, France.

[1]K. J. Wilson, Phys. Rev. D **10**, 2445 (1974).

[2]D. Weingarten, Phys. Lett. **109B**, 57 (1982), and Nucl. Phys. **B215** [FS7], 1 (1983); H. Hamber and G. Parisi, Phys. Rev. D **27**, 208 (1983); C. Bernard, T. Draper, and K. Olynyk, Phys. Rev. D **27**, 223 (1983); H. Hamber, E. Marinari, G. Parisi, and C. Rebbi, Nucl. Phys. **B225** [FS9], 475 (1983), and references therein.

[3]R. Gupta and A. Patel, Nucl. Phys. **B226**, 152 (1983).

[4]M. A. Shifman, A. I. Vainshtein, and V. J. Zakharov, Nucl. Phys. **B120**, 315 (1977).

[5]M. K. Gaillard and B. W. Lee, Phys. Rev. Lett. **33**, 108 (1974).

[6]J. F. Donoghue, E. Golowich, and B. R. Holstein, Phys. Lett. **119B**, 412 (1982).

[7]In all subsequent discussions κ_s was held fixed at 0.147 and κ refers to the light u and d quarks only. The raw numbers showed a 10% variation when $\kappa_s=0.1485$ but the ratios were more stable.

[8]Y. Dupont and T. N. Pham, Ecole Polytechnique Report No. A533.1283 (unpublished).

[9]J. F. Donoghue, E. Golowich, W. Ponce, and B. R. Holstein, Phys. Rev. D **21**, 186 (1980).