Calculation of the heavy-quark potential at large separation on a hypercube parallel computer

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The static $q\bar{q}$ potential is measured on $24^3\times 10$, $24^3\times 12$, $12^3\times 24$, and $16^3\times 24$ lattices at $\beta=6.0$ with high statistics. Using Wilson line operator-operator correlations, we find $\sqrt{\sigma}/\Lambda_L \simeq 77$ and $\alpha \simeq 0.58$. This new result compares favorably with that obtained from charmonium experimental data, but is significantly different from many previous lattice calculations. Our calculations use a hypercube parallel computer which in its full configuration performs at 0.6 gigaflops on this application.

I. INTRODUCTION

Despite the large amount of CPU time spent on supercomputers, calculations[1-9] of static (heavy-)quark potentials in lattice QCD (Ref. 10) are far from conclusive: the string tension does not scale according the continuum scaling law of two-loop perturbation theory, so that this physical parameter cannot be uniquely determined. Moreover, the lattice data does not fit the charmonium experimental result.

One of the reasons often suggested for these failures is the presence of the deconfinement phase transition[11] near the β value where these simulations were carried out so that the static potential is strongly affected by the excitations of higher-energy states. This argument has difficulties in explaining the observed scaling violation in Refs. 3, 4, and 6 where the size of the lattices are so large that the effective temperature due to the finiteness of N_t (the shortest dimension on any lattice) is far below the transition temperature. Many of the large lattice high-temperature studies[12] show that the gauge field system behaves much like a zero-temperature system until β is very close to β_c. With β about 0.15 below the transition temperature β_c, the system is essentially in the low-temperature state. Thus, the finite-temperature effects in string tension calculations do not seen large enough to cause the scaling violation. For this and other reasons more complex operators have been developed. These "fuzzy"[8] or "smeared"[9] operators enhance the overlap of wave functions with the lowest-energy state; i.e., they enlarge c_1 in comparison with $c_2, c_3, \ldots$, in

$$\langle A(t)A(0)\rangle_c = \sum_i \langle 0|A|i\rangle\langle i|A|0\rangle e^{-(E_i-E_0)t} = c_1 e^{-(E_1-E_0)t} + c_2 e^{-(E_2-E_0)t} + \cdots , \quad (1)$$

where

$$E_1 - E_0 = V(R) + V_0 = -\frac{\alpha}{R} + \sigma R + V_0 \quad (2)$$

is the linear plus Coulomb potential. (V_0 is the self-energy of the quark and the antiquark and α is the coupling constant.) These enhancements, however, do not directly solve the difficulty of scaling[4] of the string tension σ.

A closer look at these studies reveals that most previous parameters were extracted from potentials at fairly short distances R in the range from $2a$ to $8a$, where a is the lattice spacing. In a lattice regularization, the momentum cutoff is π/a, so a distance of $2a$ is quite short. The wave functions at these distances are severely distorted by the lattice discretization of space-time. However, these short-distance points dominate the χ^2 fit because of the exponential decay of the correlation functions with increasing separation while the statistical errors remain fairly constant. Thus the extracted potential is dominated by the physics at $R=2a-4a$, rather than the desired long-distance physics.

These observations lead us to consider the possibility that previous estimates of the string tension may not correspond to the correct asymptotic value as larger distances are probed. [Here we mean the lattice potential $V(R)$ at large distance R, not just large lattice sizes.] In fact, looking back at the history of the value of the string tension, we see that it has decreased from the first estimate by Creutz *et al.*[1] in 1982 of $\sqrt{\sigma}/\Lambda_L = 167$ to about 90 presently[6,7] (at $\beta=6$).

By concentrating on the physics at $\beta=6$, and using data from four different large lattices with sufficiently long runs, we found that the asymptotic form Eq. (2) sets in at around $R=4a$. With these more stable fits, we have extracted reliable parameters.

II. THE SIMULATION

We have conducted a series of large-lattice pure gauge QCD simulations on a new generation of hypercube parallel supercomputer—the Mark IIIfp (Ref. 19) built by Caltech/JPL. In this first paper we concentrate on the physics at $\beta=6$. The lattices used in our simulations were $24^3\times 10$, $24^3\times 12$, $16^3\times 24$, and $12^3\times 24$ with runs of typically 20 000 sweeps (see the first two columns of Table I). We chose N_t as the shortest direction on the lattice and N_z as the longest. We used the Cabibbo-

TABLE I. Lattice sizes, number of sweeps, the string tension extracted from plane-plane correlation σ_{pp}, and the string tension and coupling constant extracted from line-line correlation σ_{ll} and α.

Size	Sweep	σ_{pp}	σ_{ll}	α
$24^3\times 10$	16 600	0.034(3)	0.031(2)	0.69(6)
$24^3\times 12$	19 600	0.033(4)	0.033[a]	0.54(6)[a]
$12^3\times 24$	20 000	0.033(3)	0.036(4)	0.47(8)
$16^3\times 24$	16 000	0.035(5)	0.035[a]	0.54(10)[a]

[a]Because of the weakness of the signal, a reliable fit of the line-line correlations to obtain α and σ together is impossible. We instead fit them by fixing σ to the value obtained from fitting the plane-plane correlations and extracting these α values from the line-line correlations.

Marinari pseudo-heat-bath method for updating the lattices. By using the multihits variance reduction technique[13] for the measurements, we were able to determine the $q\bar{q}$ potential fairly accurately at large distances up to $R\simeq 10a$.

We calculated the Wilson line (line-line) correlation function

$$C_{ll}(R)=\mathrm{Re}\left\langle \sum_{x,y,z} W(x,y,z)W^{\dagger}(x,y,z+R)\right\rangle , \tag{3}$$

where the Wilson line $W(x,y,z)$ is the trace of the product of the gauge field links in the t direction. $C_{ll}(R)$ is then fitted to

$$C_{ll}(R)=\mathrm{const}\times(e^{-N_t V(R)}+e^{-N_t V(N_z-R)}) , \tag{4}$$

where the second exponential comes from the periodicity in the z direction. We also computed the zero-momentum (plane-plane) correlation function[13,14]

$$C_{pp}(R)=\mathrm{Re}\left\langle \sum_{x,y,z}\sum_{x',y'} W(x,y,z)W^{\dagger}(x',y',z+R)\right\rangle \tag{5}$$

and fit this to Eq. (4) with $\alpha=0$ in Eq. (2). This zero-momentum correlation gives a better fit, as can be seen in a simple analog with one-particle quantum mechanics. In the energy spectrum of the one-particle system, above the mass gap, there usually exists a continuum band of energy levels due to the non-zero-momentum states. This implies that $E_1, E_2, E_3, \ldots$ in Eq. (1) are close to each other, thus making a clean separation of the first term difficult. However, one can first sum over the spatial components of the wave function to project out the zero-momentum state, so that $c_2, c_3, \ldots$ in Eq. (1) become zero until the next discrete state is reached. Equation (1) then contains only terms from well-separated energy states and one can more easily isolate the first term.

Using Wilson line correlations to extract the potential has two advantages over the use of Wilson loops.[7] First, the fitting is straightforward and clean, as shown in Eq. (4). Second, the self-energy contribution V_0 to the correlations is a constant—because the quark loop length is a constant $(2N_t)$ for Wilson lines—and can therefore be clearly isolated from the potential contribution $V(R)$ as the separation R varies. The disadvantage with Wilson line correlations is that they are difficult to measure in practice because the loop sizes are large: $N_t\times z$, for $z=2-12$ on our lattices. Because of their exponential decrease in value, these large loops have a very small signal-to-noise ratio. To reduce this noise, sufficiently large statistics alone is not enough, since the noise, or statistical error, decreases only as $1/\sqrt{N}$, so that an order of magnitude longer run only reduces the noise by about a factor of 3. Therefore we used the variance reduction technique[13] and found that it works very well. The idea is simple. Given a fixed environment, instead of taking one random sample, one can take many samples and average them. This averaged quantity will have smaller random fluctuations. In our case, the variance reduction was achieved by doing multiple updates (hits) of a given link while keeping its environment fixed and then averaging these updated values as the measured link value. With a five-hit average, we found that the statistical errors decrease by about a factor of 5–10. This is equivalent to 25–100 times increase in computer simulation time. With this technique we were able to measure the line-line correlation at separation $R=12a$ with an accuracy of about 30%.

We make measurements of both the line-line correlation C_{ll} and the plane-plane correlation C_{pp} every five sweeps of updates. In order to check the statistical independence of these successive measurements we computed the autocorrelation length[15]

$$\lambda=1+\sum_{t=1}^{M} 2\left(1-\frac{t}{M}\right)\xi(t) , \tag{6}$$

$$\xi(t)=\frac{\sum_i [A(t+i)-\bar{A}][A(i)-\bar{A}]}{\sum_i [A(i)-\bar{A}]^2} \tag{7}$$

using all M data points. For the single Wilson line $\langle W\rangle$, λ is about 100 measurements, or 500 sweeps. For the line-line correlations $\lambda\simeq 15$ sweeps and for the plane-plane correlations $\lambda\simeq 50$. The larger λ for the plane-plane correlation results from the larger extent of these operators. All the errors below are calculated by first computing the standard uncorrelated error and then multiplying by $\sqrt{\lambda}$ to take into account the autocorrelation.

The reason that the line-line correlation, which is of the form $\langle W^{\dagger}(x)W(y)\rangle$, is much less autocorrelated than the single Wilson line can be explained by their different physical interpretations: the former relates to self-energy, i.e., the quark world line absorbing virtual gluons emitted by itself, while the latter has in addition the exchange of gluons between the two opposite-going (quark and antiquark) lines. The slow oscillations of $W(x)$ and $W(y)$ could be nearly phase coherent—they are highly correlated—so that these fluctuations cancel out in $\langle W^{\dagger}(x)W(y)\rangle$ allowing the latter to progress with the faster dynamics of multiple-gluon exchanges.

The data points are plotted in Fig. 1. Two general features are clear. (1) As N_t gets bigger, the signal-to-noise ratio gets smaller because the quark self-energy diverges, leading to $\langle W\rangle\sim\exp(-\text{self-energy})\to 0$. (2) The plane-plane correlations have better signal/noise

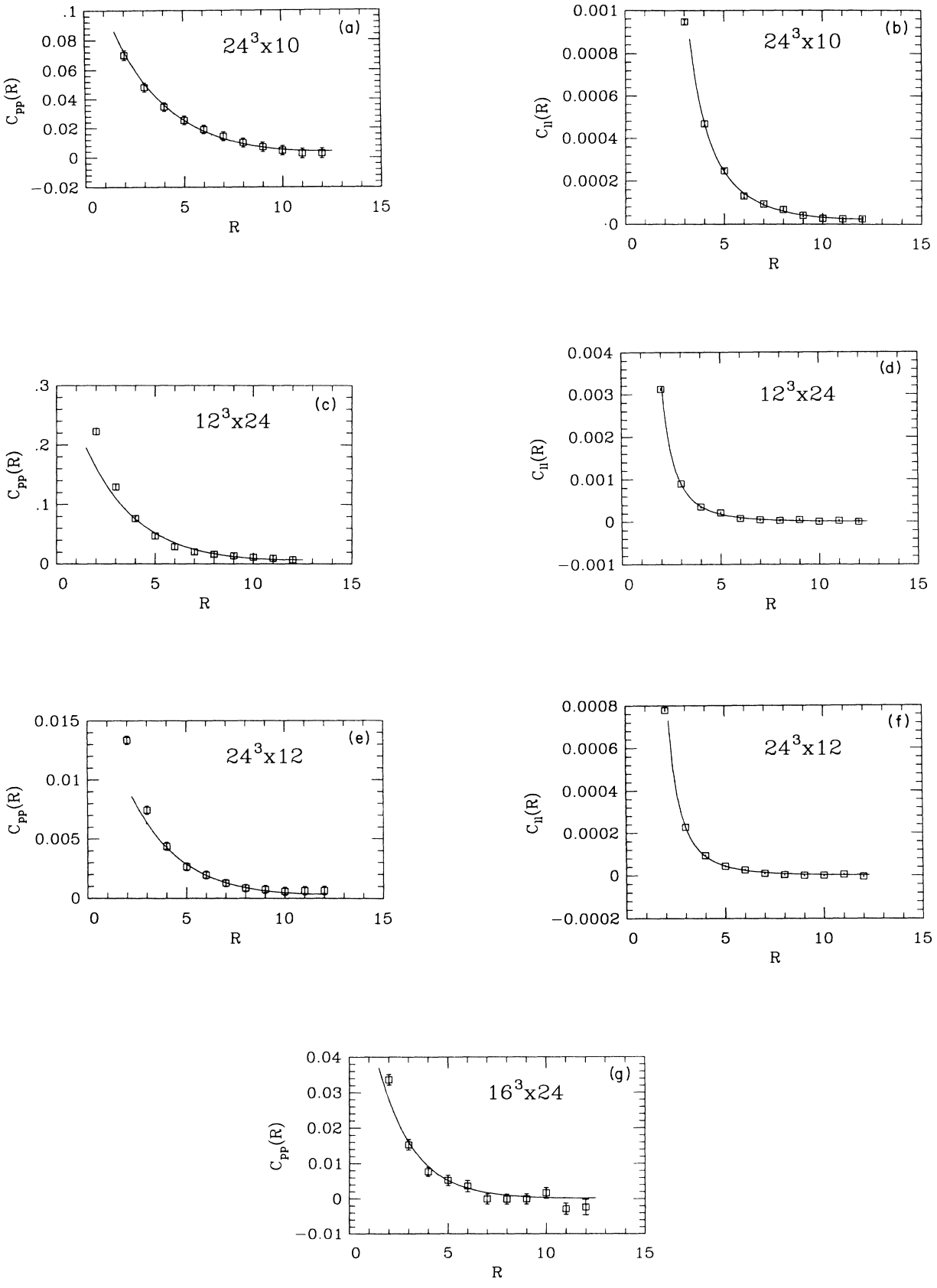

FIG. 1. The line-line, $C_{ll}(R)$, and plane-plane, $C_{pp}(R)$, correlation functions are shown as points and the fit as a line for various lattice sizes.

than the line-line correlations because more components are involved in the average.

III. DATA ANALYSIS

As we generate more and more data with high statistics on many different lattices, fitting this data to the theoretical model becomes a challenge—consistency and parameter stability have to be systematically examined. Consistency means that the same fit criteria is applied on different sized lattices. Parameter stability means that the fitted parameters should be stable against dropping short-distance points from the fit.

It should be noted that the data points at different R's are correlated. We performed the χ^2 fit which included correctly these correlations;[14] i.e., we minimized

$$\chi^2_{\text{correlated}}=\sum_{j,k}(\gamma^{-1})_{jk}[C_t(j)-C_s(j)][C_t(k)-C_s(k)] , \quad (8)$$

where C_t are the theoretical predictions from Eq. (4) and C_s are measured in the simulation. The error matrix, γ_{jk}, is related to the errors e_j, e_k of $C(j), C(k)$ through $\gamma_{jk}=\rho_{jk}e_j e_k$. ρ_{jk} are the standard correlation coefficients between $C(j), C(k)$:

$$\rho_{jk}=\frac{\sum_i[C^{(i)}(j)-C(j)][C^{(i)}(k)-C(k)]}{\left[\sum_i[C^{(i)}(j)-C(j)]^2\sum_i[C^{(i)}(k)-C(k)]^2\right]^{1/2}} , \quad (9)$$

where $C^{(i)}(R)$ stands for the ith measurement of $C(R)$. The fit is good in general, with the χ^2 per degree of freedom ~ 1.5. We also tried the usual χ^2 fit by ignoring the correlation between $C(j), C(k)$ so $\gamma_{jk}=\delta_{jk}e_j e_k$. The fitted parameters change less than 1%, which is completely within the error bars. In fact, the errors increase from $\sim 2\%$ to $\sim 10\%$. When we systematically drop short-distance points from the fit, the fitted parameters fluctuate in the range of 10%. Thus this systematic error is more realistic and is quoted in Table I.

We first consider C_{pp} on the $24^3\times 10$ lattice, Fig. 1(a), because it has the best signal/noise ratio and because only two adjustable parameters (string tension and the normalization constant) are involved in the fit. The fit is quite stable as we drop $R=1,2,3,4$ points from it; see Table II. Plane-plane correlations on other lattices exhibit similar fitting stability; Figs. 1(c), 1(e), and 1(g). For the line-line correlations, the fits start becoming reasonably stable around $R=4$. One can see that on the two lattices $24^3\times 10$ and $12^3\times 24$ where the signal/noise ratio is good, the values of σ obtained from C_{pp} and C_{ll} are fairly close (Table I). This is significant, because in most previous calculations of quark potential using Wilson line correlations the authors *assume* that at these distances simulated ($R=3-10$) the asymptotic behavior of $\sigma_{ll}=\sigma_{pp}$ sets in (where σ_{ll} is obtained from C_{ll} and σ_{pp} from C_{pp}). The signal/noise ratio for C_{ll} on the $24^3\times 12$ lattice is as good but the fitted parameters drift quite a bit as short-distance points are dropped. For the $16^3\times 24$ lattice, C_{ll} is very noisy and reliable fits could not be obtained. Fortunately, good fits for C_{pp} are obtained on these two lattices. To extract the coupling constant α, we fit C_{ll} by fixing σ to the value obtained from the C_{pp} fit. The best-fitted parameters are listed in Table I.

From Table I one can see that the six independent σ's are close to each other. This suggests that finite-size effects on these fairly large lattices are small. The α's differ about 20%, reflecting the difficulty in an accurate determination.

TABLE II. String tension obtained as a function of fitting range R_0–$R_{\max}$. The data indicates that the fits become stable at $R_0\simeq 4$.

Size	$C(R)$	2–12	3–12	4–12	5–12
$24^3\times 10$	C_{pp}	0.0343(22)	0.0338(25)	0.0345(30)	0.0363(32)
$24^3\times 12$	C_{pp}	0.0428(35)	0.0376(33)	0.0333(38)	0.0344(41)
$12^3\times 24$	C_{pp}	0.0415(22)	0.0374(25)	0.0331(27)	0.0311(31)
$24^3\times 10$	C_{ll}	0.0413(15)	0.0383(17)	0.0311(18)	0.0303(23)

IV. CONCLUSION

By a systematic study of quark potentials at large distances at $\beta=6$, we find

$$\sigma a^2\simeq 0.033, \quad \alpha\simeq 0.58 . \quad (10)$$

These numbers were fairly insensitive to the lower cutoff in R and are consistent on all four different lattices we simulated. The string tension, converting to the dimensionless ratio

$$\frac{\sqrt{\sigma}}{\Lambda_L}\simeq 77$$

is about 20% smaller than previously estimated.[2–9] The coupling constant α is almost twice the transverse flux-tube calculation[16] result of $\pi/12=0.26$, which is the value obtained from previous simulations.[3,5–7] Thus, our result indicates, as also noted in Ref. 17, that the origin of the Coulomb term is perhaps more complicated than that provided by the transverse flux picture. These differences can be attributed to the larger distance points we have used in our fits. In fact, if we fit only $C_{pp}(2-8)$ or $C_{ll}(2-8)$ on the $24^3\times 10$ lattice, we obtain results con-

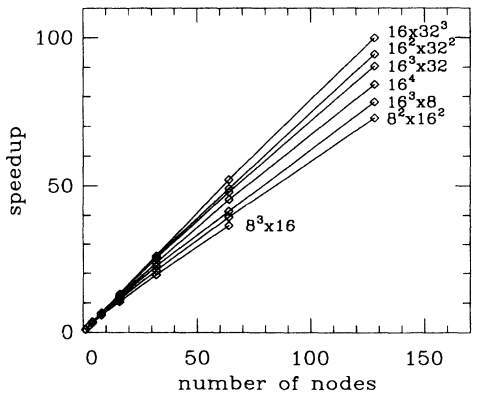

FIG. 2. Speedup of the program on the 128-node Mark IIIfp for fixed total lattice sizes.

sistent with the previous work.[2-9]

We can compare our calculations to the experimental measurements of α and σ. Charmonium is a natural system to look at since for it we expect the heavy-quark potential approach to be reasonable. In fitting charmonium data to a Coulomb plus linear potential, Eichten *et al.*[18] estimated that $\alpha=0.52$ and $\sigma=0.18$ GeV^2. This compares favorably with our estimate: $\alpha\simeq 0.58$ and $\sigma\simeq 0.15$ GeV^2, assuming $\Lambda_{\rm mom}=420$ MeV. Note that the previous simulations gave $\alpha\simeq 0.3$.

This work is based on about 1300 CPU hours on the 32-node Caltech/JPL Mark IIIfp hypercube[19] which has a performance roughly twice that of a Cray X-MP processor. The codes were first developed by Jon Flower and Steve Otto on the Mark II hypercube computers. After using Weitek assembly language for the matrix calculations and much of the update, and with the use of optimized communication routines,[20] the program updates a link matrix in 32 μsec, which is equivalent to a sustained speed of 150 megaflops on a 32-node hypercube. In Fig. 2 we present the performance of the 32- to 128-node Mark IIIfp hypercube as the speedup of the parallel system compared to a single processor node. A single node runs at 6 megaflops for our algorithm so the speedup of 100 in Fig. 2 for a $32^3\times 16$ lattice on 128-node system reflects a performance of 600 megaflops. The hypercube has been shown to be a general purpose scientific computer for many applications[21,22] and this figure illustrates the good performance it achieves on this particular computationally intensive application.

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