Improved determination of the heavy-quark potential in lattice QCD

H.-Q. Ding
California Institute of Technology, Pasadena, California 91125
(Received 12 April 1991)

A new iterative procedure in fitting data is proposed which can properly correct small nonlinear effects. Applying this procedure to fit the Polyakov loop correlation functions previously obtained in lattice QCD simulations, we are able to eliminate the finite-size boundary effects and obtain the quark potential functions themselves, instead of just parameters for the potentials. The quality of the fits is improved significantly. The potential functions obtained at $\beta=6.0$–6.2 scale in fine detail, providing important further support of the scaling. The improved estimates of the string tension satisfy the asymptotic scaling within 97%. In comparison with experiments, the obtained value $\sqrt{\sigma}/\Lambda_L=79\pm3$ indicates $\Lambda_{\overline{\rm MS}}=449\pm17$ MeV, where MS denotes the minimal subtraction scheme. The coupling constant $\alpha=0.43\pm0.03$ agrees very well with experiments, and is also in excellent agreement with the theoretical value $\pi/8=0.39$, assuming that the long-distance behavior of QCD can be effectively described by the Neveu-Schwarz string theory.

One of the important aspects of lattice gauge theory is the calculation of a static quark potential between quark-antiquark pairs. Until very recently, the scaling violation of the string tension, the coefficient of the linear term which confines quarks, measured in Monte Carlo simulations, has prevented a unique determination of the potential in the continuum limit. Recently, we performed a series of extensive simulations [1,2] on large lattices and extracted the potential at large distances. As discussed there, our results indicate that the string tension is about 30% smaller than previous calculations [3] and the coupling constant of the Coulomb term is about twice as large as previous estimates. More importantly, these parameters satisfy the scaling relation within about 90% accuracy.

However, several aspects in the commonly used data-fitting method, which were adopted in Refs. [1] and [2], are not quite satisfactory. In lattice QCD simulations one measures the operator-operator connected correlations of the Polyakov loops:

$$C(R)=\mathrm{Re}\left\langle \sum_{x,y,z} P^{\dagger}(x,y,z)P(x,y,z+R)\right\rangle , \tag{1}$$

at $R=1,2,3,\ldots,N_z/2$, where N_t (N_z) is the lattice size in the t (z) direction. Since $\langle P\rangle=0$, the $\langle P\rangle^{\dagger}\langle P\rangle$ term has been dropped. The quark potential $V(R)$ is then extracted from the relation

$$C(R)=A(e^{-N_tV(R)}+e^{-N_tV(N_z-R)}) , \tag{2}$$

where A is a proportionality constant and the second exponential comes from the periodicity in the z direction. [There are an infinite number of *image* charges in the z direction, and in the x,y directions, too. But due to the exponential decay, only the closest one is accounted for in Eq. (2)]. Because of its highly nonlinear nature, $V(R)$ cannot be obtained directly [5]. Instead, the popular procedure is to assume a form for $V(R)$ and fit $C(R)$ to extract the parameters in $V(R)$ by minimizing $\chi^2=\sum_r\{[C(r)-C_m(r)]/e(r)\}^2$, where C_m is the measured value and $e(r)$ is the error [6]. The parameters thus obtained at each β are then compared with the asymptotic scaling. A drawback is that the potential function $V(R)$ itself cannot be determined. Moreover, the fitting is sensitive to short-distance points because $C(r)$ changes scale exponentially while the errors are of the same size, so that χ^2 is dominated by short-distance points. (In practice we found [1,2] that, dropping out $R=1$–3 data points, the fitting becomes stable. This is justified on the basis that only large-distance physics is described by the lattice theory.)

We now show that these two unsatisfactory features in data fitting can be eliminated or softened by an iterative procedure. The general idea is that if the nonlinear effects (terms) are small, one can estimate the effects and correct them iteratively. First assume the nonlinear effects are 0 and do a straight fit. Estimate the effects (this requires some knowledge about the form of the effect, usually available) and subtract them. Do the fit again. Repeat the procedure till convergence. This provides a set of data (and errors) with the small nonlinear effects corrected. The above procedure can be thought of as a direct generalization of the iterative methods in mathematics. If the nonlinear terms are "small," the convergence is very fast. In our case, typically two iterations lead to convergence at the 1% level.

In the quark-potential problem, we want to correct the small second term due to the boundary reflection in Eq. (2). We estimate the boundary term by assuming

$$V(R)=-\alpha/R+\sigma R . \tag{3}$$

Neglecting the boundary term and fitting Eq. (3) we obtain the first estimates of $\alpha^{(0)},\sigma^{(0)}$. Using these numbers, we can estimate the boundary term and eliminate it, i.e.,

$$C(R)/Z^{(0)}(R)=Ae^{-N_t V(R)}, \tag{4a}$$

$$Z^{(0)}(R)=1+e^{N_t[V^{(0)}(R)-V^{(0)}(N_z-R)]}, \tag{4b}$$

where $V^{(0)}(R)=-\alpha^{(0)}/R+\sigma^{(0)}R$ is used to calculate the correction $Z^{(0)}(R)$. [Or, equivalently, one can simply subtract the second term in Eq. (2).] We then extract the whole potential by

$$U(R)=\{\ln(A)-\ln[C(R)/Z^{(0)}(R)]\}/N_t , \tag{5a}$$

with errors estimated in the standard fashion:

$$\delta U(R)=\{\ln[C(R)+\delta C(R)]-\ln[C(R)]\}/N_t . \tag{5b}$$

$U(R)$ now has smaller variations and fitting $U(R)$ to Eq. (3) is more stable. With the improved estimates for $\sigma^{(1)},\alpha^{(1)}$, we can use them in Eq. (4b) and repeat the procedure iteratively. In practice, we find that the procedure converges after two iterations, because $Z^{(i)}$ varies very little from one iteration to the next due to the combined effects of σ and α. One can see that $Z^{(i)}(R)$ is a monotonic function ranging from 1 to 2. Neglecting these boundary effects will lead to systematic errors.

Once converged, the true potential function $U(R)$ and errors are readily obtained from Eq. (5); $U(R)=\text{const}-\ln[C(R)/Z(R)]/N_t$. We use $U(R)$ instead of $V(R)$ to emphasize that the true potential function can differ from the analytical form $V(R)$ in some fine details; $V(R)$ is only used to estimate the boundary term. This is justified if $V(R)$ is close to $U(R)$ and the boundary term is small.

With this new fitting procedure, we reanalyze the data previously published [1,2]. Figure 1 shows the Polyakov loop correlations $C(R)$ and the potential $V(R)$ obtained using the above method at $\beta=6.1$ on lattices $24^3\times 14$. One can see that the quality of the fits for the potential is better than that of the direct fit to the correlation functions $C(R)$. This is because the data points for $C(R)$ are drastically suppressed by the presence of N_t in the exponent in Eq. (2), and thus any deviation from the fitted line is correspondingly enlarged. This is especially clear for the short- and long-distance points. Clearly the new fitting method produces a more stable fit with clear physical content. The errors in the fitted parameters are also reduced. These features are shared by all the data for $\beta=6$, 6.1, and 6.2. In Fig. 2, the extracted potentials at $\beta=6$ and 6.2 are shown along with the fits. The fitted parameters are listed in Table I. Also listed is the dimensionless ratio $\sqrt{\sigma}/\Lambda_L$ calculated from the two-loop asymptotic scaling:

$$\sqrt{\sigma}/\Lambda_L=\sqrt{\sigma a^2}(8\pi^2\beta/33)^{-51/121}e^{4\pi^2\beta/33} . \tag{6}$$

The fact that $\sqrt{\sigma}/\Lambda_L$ at different β agrees within 97% accuracy indicates the scaling sets in around $\beta=6$. Simi-

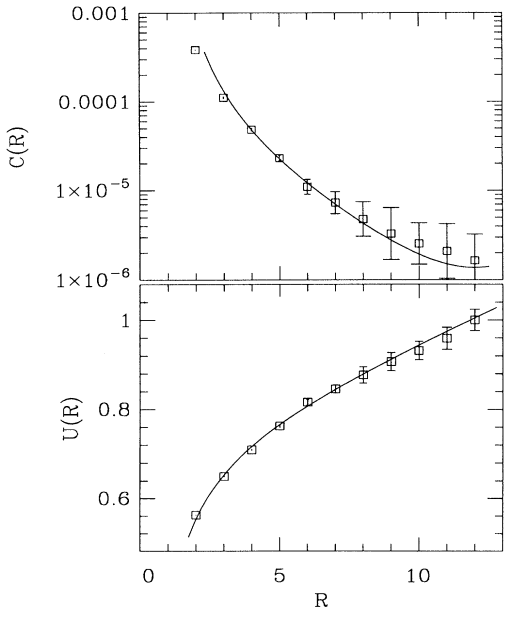

FIG. 1. The Polyakov loop correlation functions $C(R)$ (upper) and the extracted potential $U(R)$ (lower) at $\beta=6.1$ on the $24^3\times 14$ lattice.

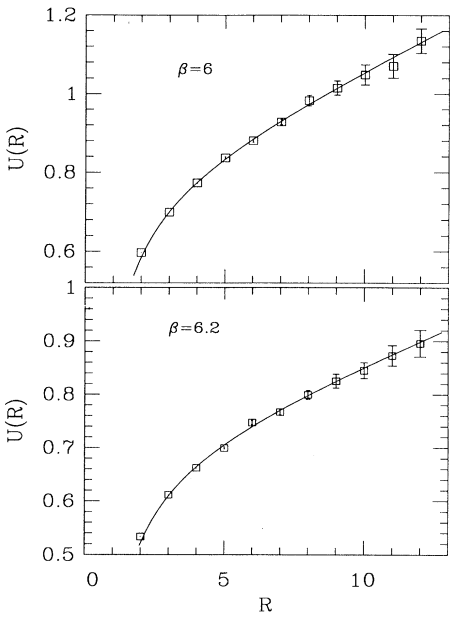

FIG. 2. Quark potentials at $\beta=6$ on the $24^3\times 12$ lattice (upper) and at $\beta=6.2$ on the $24^3\times 16$ lattice (lower).

TABLE I. σ and α obtained from the iterative procedure. The scaling ratio $\sqrt{\sigma}/\Lambda_L$ is also listed.

β	σ	α	$\sqrt{\sigma}/\Lambda_L$
6.0	0.0343(27)	0.48(6)	78.9(3.1)
6.1	0.0267(24)	0.46(4)	77.9(3.5)
6.2	0.0215(18)	0.41(5)	78.8(2.7)

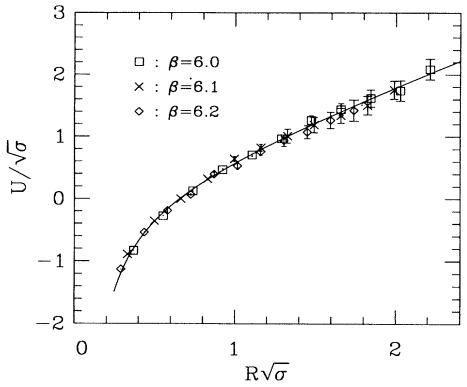

FIG. 3. Potential functions from Figs. 1 and 2, scaled as in Eq. (7). All data points collapse into a single universal curve. This indicates the scaling of potential functions.

lar onset of scaling around $\beta=6$ is also observed in the quark deconfinement transition temperature T_c [7,8] and latent heat L [8].

Scaling is a central issue in lattice QCD simulations because it ensures a unique continuum limit. The scaling observed in σ, T_c, L so far is only single-parameter scaling. Stronger evidence of scaling would be the scaling of a continuous function at each β. The quark-potential function at each β obtained from these new fits provides such a function. This is in fact the motivation of this work. In Fig. 3 we plot the scaled potentials

$$U(R)/\sqrt{\sigma}=-\alpha/(\sqrt{\sigma}R)+\sqrt{\sigma}R \tag{7}$$

at each β with dimensionless distance $x=\sqrt{\sigma}R$. The data points nicely collapse into a single curve. This fact indicates that the potential functions at each β scale *in fine detail,* a significant further support for scaling.

A fit to the data points in Fig. 3 gives

$$\alpha=0.43\pm0.03\ , \tag{8}$$

quite consistent with those obtained in individual fits (Table I), and is in excellent agreement with the potential-model analysis [9,10] on the heavy-quark systems $c\bar{c}$ ($\alpha=0.48$) and $b\bar{b}$ ($\alpha=0.38$). The value for the string tension from Table I,

$$\sqrt{\sigma}/\Lambda_L=79\pm3\ , \tag{9}$$

compared with $\sigma=0.18$ GeV^2 from the analysis [9,10] of $c\bar{c}$ and $b\bar{b}$ systems, implies

$$\Lambda_{\overline{\rm MS}}=\frac{83.5}{79\pm3}\sqrt{0.18}\ \text{GeV}=449\pm17\ \text{MeV}\ , \tag{10}$$

where MS denotes the minimal subtraction scheme. (See Table 3 in Ref. [2] for some details.) From this QCD scale, we can learn some basic physics. At $\beta=6$–6.2, the lattice spacing $a=0.07$–0.09 fm [via Eq. (6)]. Thus the range of potential we measured is 0.2–1 fm, which is about the size of these $c\bar{c}$ ($R_{\rm avg}\gtrsim0.5$ fm) and $b\bar{b}$ ($R_{\rm avg}\gtrsim0.2$ fm) systems.

It has been suggested that the long-distance behavior of QCD can be effectively described by string theory [11,12]. The effective coupling term, the second term in Eq. (3), originated from the "flux-tube" fluctuations, and has different coefficients in different strings. For the scalar strings [11], $\alpha=\pi/12=0.26$. For the Ramond and the Polyakov strings, $\alpha=0$ [12]. For the Neveu-Schwarz strings [13], $\alpha=\pi/8=0.39$ [12]. Our results therefore strongly favor the Neveu-Schwarz string.

Finally, we point out that this iterative approach is quite general. In particular, the iterative procedure outlined in Eqs. (2), (4), and (5) can be directly applied in simulations on finite-size systems to eliminate finite-size boundary effects.

This research was supported in part by DOE Grant No. DE-FG03-85ER-25009.

[1] H.-Q. Ding, C. F. Baillie, and G. C. Fox, Phys. Rev. D **41**, 2912 (1990).

[2] H.-Q. Ding, Phys. Rev. D **42**, 2350 (1990).

[3] For a recent review, see C. Michael, in *Lattice '89,* Proceedings of the International Symposium, Capri, Italy, 1989, edited by R. Petronzio *et al.* [Nucl. Phys. B (Proc. Suppl.) **17**, 59 (1990)]. We note that on their largest lattice at $\beta=6.2$, Michael and Teper [4] obtained $\sqrt{\sigma}/\Lambda_L=82\pm2$, consistent with our value $\sqrt{\sigma}/\Lambda_L=79\pm3$, although their values at $\beta=6$ are substantially higher than ours. This difference could be due to our emphasis on large-distance points. We used $24^3\times12$ whereas they used 16^4.

[4] C. Michael and M. Teper, Nucl. Phys. **B314**, 347 (1989).

[5] Since Eq. (2) defines $N_z/2$ equations for $R=1,\ldots,N_z/2$, one might attempt to invert them numerically to obtain $V(R)$'s. However, $C(R)$ comes with errors and their scales change exponentially with R; a small error in $C(R)$ will be amplified at $V(R)$ so that direct inversion is ill defined. A similar situation occurs in the analytical continuation from imaginary time to real time. See, for example, S. R. White, D. J. Scalapino, R. L. Sugar, and N. E. Bickers, Phys. Rev. Lett. **63**, 1523 (1989).

[6] A more complete fit should include the correlation matrix, as discussed in Ref. [1]. However, the qualitative feature discussed here remains unchanged.

[7] A. D. Kennedy *et al.*, Phys. Rev. Lett. **54**, 87 (1985); S. A. Gottlieb *et al., ibid.* **55**, 1958 (1985).

[8] N. H. Christ and H.-Q. Ding, Phys. Rev. Lett. **60**, 1367 (1988).

[9] E. Eichten *et al.*, Phys. Rev. D **21**, 203 (1980).

[10] S. N. Gupta, S. F. Radford, and W. W. Repko, Phys. Rev. D **26**, 3305 (1982); **34**, 201 (1986).

[11] M. Lusher, K. Symanzik, and P. Weisz, Nucl. Phys. **B173**, 365 (1981); J. Stack and M. Stron, Phys. Lett. **100B**, 476 (1981).

[12] P. Olesen, Phys. Lett. **160B**, 144 (1985).

[13] A. Neveu and J. Schwarz, Nucl. Phys. **B31**, 86 (1971).