Hadron thermodynamics with Wilson quarks

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We study hadron thermodynamics with Wilson quarks. The crossover curve between the high- and low-temperature phases is determined as a function of gauge coupling and hopping parameter on $8^3\times 4$ lattices. Screening lengths are calculated in the vicinity of the crossover region, and meson masses are calculated along the crossover curve on $8^2\times 16\times 4$ and $8^3\times 16$ lattices, respectively.

I. INTRODUCTION

The study of lattice QCD at high temperatures is important for an understanding of the theory, and has potential applications to cosmology and nuclear physics. A great deal of effort has gone into studies with Kogut-Susskind quarks,[1] but much less work has been devoted to high-temperature QCD with Wilson quarks.[2-6] In this paper we present results from a recent simulation with Wilson quarks.

For the study of hadron thermodynamics, Kogut-Susskind quarks have the advantage of retaining a remnant of chiral symmetry, a U(1) symmetry. Therefore, for zero quark mass, the lattice theory has a Goldstone boson in the broken-symmetry phase, and $\langle \bar\psi\psi \rangle$ is a bona fide order parameter. The chiral limit can be approached by simply decreasing the quark mass towards zero. However, for finite lattice spacing the flavor symmetry among the pion states is broken, and full chiral symmetry is achieved only in the continuum limit. By contrast, the Wilson quark action explicitly breaks chiral symmetry for finite lattice spacing. In order to identify the chiral limit one must search in the two-dimensional parameter space of the gauge coupling $6/g^2$ and hopping parameter κ for a one-dimensional manifold. Given the different types of behavior of the two formulations for finite lattice spacing, it is important to check that they approach the same continuum limit.

At present we are unable to study hadron thermodynamics in the continuum limit. An intermediate goal is to bring simulations with Wilson quarks to the same level as those for Kogut-Susskind quarks. As a step in that direction we report on a study of hadron thermodynamics with two flavors of Wilson quarks at a temperature of $1/4a$, where a is the lattice spacing. We have located the crossover curve between the high- and low-temperature phases as a function of the gauge coupling and the hopping parameter. We have measured hadron screening lengths in the vicinity of the crossover curve, and zero-temperature meson masses along it. Our results are in good agreement with earlier studies.[2-6] In particular our results for the crossover lie on a smooth curve with those of Bitar *et al.*,[6] Gupta *et al.*,[4] and Ukawa,[3] and our results for the screening lengths are in good qualitative agreement with Ukawa's.[3] Finally, we find that the zero-temperature pion mass is large in the entire region of $6/g^2$ and κ that we have scanned.

In Sec. II we describe our simulation, and in Sec. III we discuss our results.

II. THE SIMULATION

We have carried out simulations with two degenerate flavors of Wilson quarks using the hybrid Monte Carlo (HMC) algorithm.[7] After integrating out the fermion fields the effective action for the theory is

$$S_{\rm eff}=S_W+\Phi^*(M^\dagger M)^{-1}\Phi \ , \qquad (1)$$

where S_W is the pure gauge part of the Wilson action, Φ is the pseudofermion field introduced in integrating out the fermion fields, and M is the Wilson fermion matrix:

$$M_{i,j}=\kappa\sum_\mu [(\gamma_\mu+r)U_{i,\mu}\delta_{i,j-\mu} - (\gamma_\mu-r)U^\dagger_{i-\mu,\mu}\delta_{i,j+\mu}]-\delta_{i,j} \ . \qquad (2)$$

We take $r=1$. The statistical weight for the field configurations is $\exp(-H_{\rm eff})$, where

$$H_{\rm eff}=\sum_{i,\mu} P_{i,\mu}^2+S_{\rm eff}\ , \qquad (3)$$

and the $P_{i,\mu}$ are traceless anti-Hermitian matrices which play the role of momenta conjugate to the $U_{i,\mu}$.

The HMC algorithm is an exact algorithm, but care must be taken to avoid systematic errors. One step in the algorithm is the numerical integration of Hamilton's equations for $H_{\rm eff}$. This requires the introduction of a finite time step Δt. As long as the numerical integration algorithm is time-reversal invariant and area preserving, the errors due to a finite step size are eliminated by the Metropolis acceptance-rejection step at the end of each integration trajectory. The leapfrog method is used for this purpose. However, time-reversal invariance is violated if roundoff errors destroy the unitarity of the $U_{i,\mu}$ matrices. Our tests indicate that these errors can be made negligible by reunitarizing the $U_{i,\mu}$ after each time step Δt, and we have done so. In contrast, reunitarizing after every simulation time unit, that is, every $1/\Delta t$ steps, leads to observable systematic errors.

We have used an integration trajectory length of one simulation time unit. At the end of each trajectory a Metropolis acceptance-rejection decision is made for the entire trajectory, and the $P_{i,\mu}$ and Φ fields are refreshed. Since it is necessary to evaluate $(M^\dagger M)^{-1}\Phi$ at each time step, one would like to make Δt as large as possible. However, the Metropolis acceptance probability declines as Δt is increased, which sets an upper limit on Δt. For the thermodynamics studies on $8^3\times 4$ lattices we have taken $\Delta T=0.05$ for all but the largest value of $\kappa=0.19$, and have obtained acceptance rates between 0.75 and 0.80. For $\kappa=0.019$ we required $\Delta t=0.04$ to obtain the same acceptance rate. For the zero-temperature calculations on $8^3\times 16$ lattices, Δt values in the range 0.05 to 0.025 were used, and yielded somewhat lower acceptance rates. Our simulation parameters for these two calculations are given in Table I. Those for the screening-length calculations are quite similar to the ones for the spectrum studies.

The vector $(M^\dagger M)^{-1}\Phi$ is calculated using the conjugate-gradient algorithm with incomplete lower upper (ILU) preconditioning by checkerboards.[8] The stopping criterion is $10^{-5}>\|r\|/\|\Phi\|$, where $\|r\|$ and $\|\Phi\|$ are the norms of the vectors r and Φ. Errors in the integration of Hamilton's equations arising from the finite stopping criterion do not lead to a violation of time reversal provided that the starting solution is time-reversal symmetric. As a result, they are eliminated by the Metropolis step. However, the acceptance-rejection step requires a calculation of the total energy, and therefore of $\|M^{-1}\Phi\|$. Errors in this quantity can lead to systematic errors in our results. Our production runs are carried out in 32-bit precision, with the global sums in 64-bit precision. (The ETA 32-bit precision is several bits less accurate than the IEEE standard.) We have made limited tests in full 64-bit precision which indicate that such errors are under control. The average number of conjugate-gradient iterations needed to satisfy our stopping criterion for the thermodynamics and spectrum calculations are given in Table I. We use the same criterion for the screening length and spectrum measurements with Φ replaced by an appropriate source vector.

Our thermodynamics studies were carried out on $8^3\times 4$ lattices. The primary aim of this phase of our work was to locate the crossover between the high- and low-temperature regimes as a function of $6/g^2$ and κ. To this end we monitored the real part of the Polyakov loop, the plaquette and $\langle\bar\psi\psi\rangle$. The Polyakov loop gave the clearest jump in all cases. We studied hopping parameters in the range $0.12\le\kappa\le 0.19$. For each value of κ studied we made a rough determination of the crossover point by scanning through different values of $6/g^2$. We generated 800 trajectories at each value of $6/g^2$, and made measurements at the end of each trajectory. The real part of the Polyakov loop for the scan at $\kappa=0.17$ is shown in Fig. 1. The location of the crossover points was then determined more accurately by making runs of 3000 trajectories for several values of $6/g^2$. The real part of the Polyakov loop for the long runs at $\kappa=0.17$ is shown in Fig. 2.

For $\kappa=0.16$ and 0.17 hadronic screening lengths were calculated on $8^2\times 16\times 4$ lattices for a range of values of $6/g^2$ in the vicinity of the crossover points. We also calculated zero-temperature masses on $8^3\times 16$ lattices at the values of κ and $6/g^2$ corresponding to the high-

TABLE I. The parameters for the thermodynamics studies on $8^3\times 4$ lattices and the spectrum calculations on $8^3\times 16$ lattices. Δt is the step size for the integration of Hamilton's equations, AC is the acceptance rate for the Metropolis step, and CG the number of conjugate-gradient iterations per inversion.

Lattice	κ	Δt	AC	CG
$8^3\times 4$	0.12	0.05	0.76	6
$8^3\times 4$	0.14	0.05	0.79	11
$8^3\times 4$	0.16	0.05	0.79	22
$8^3\times 4$	0.17	0.05	0.80	36
$8^3\times 4$	0.18	0.05	0.76	55
$8^3\times 4$	0.19	0.04	0.75	110
$8^3\times 16$	0.16	0.05	0.60	25
$8^3\times 16$	0.17	0.04	0.70	36
$8^3\times 16$	0.18	0.04	0.65	64
$8^3\times 16$	0.19	0.025	0.55	132

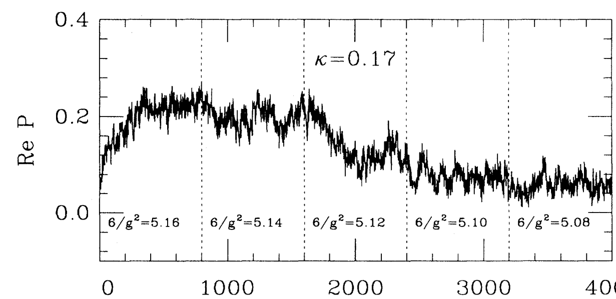

FIG. 1. Time history of the real part of the Polyakov loop. $6/g^2$ changes by 0.02 every 800 time units. Its values are indicated on the graph.

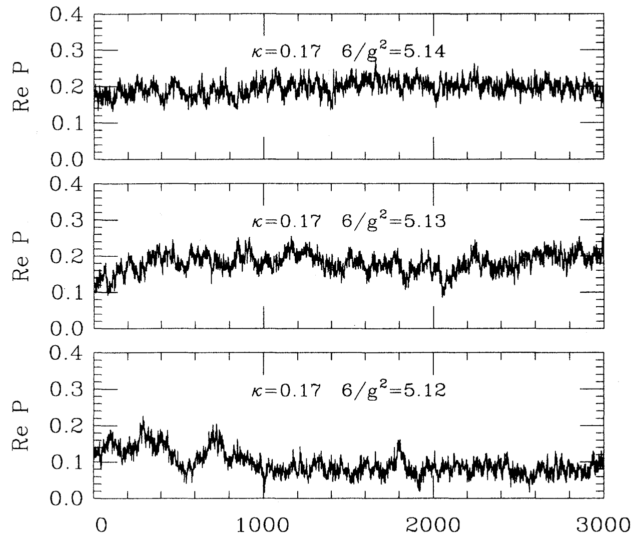

FIG. 2. Time history of the real part of the Polyakov loop for $\kappa=0.17$ and $6/g^2=5.12$, 5.13, and 5.14.

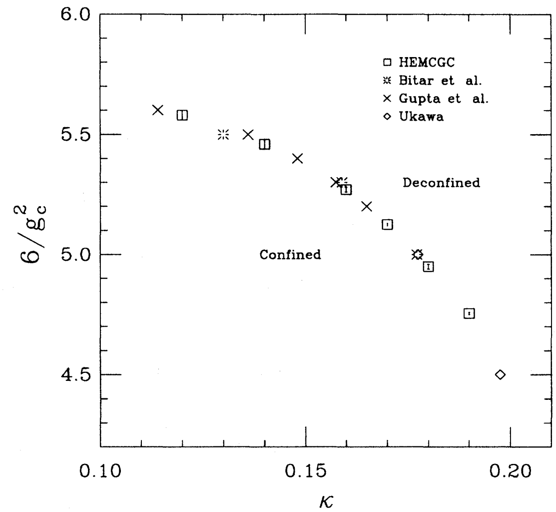

FIG. 3. The crossover value of $6/g^2$ as a function of κ on $8^3\times4$ lattices. The squares are the results from this study, the bursts are from the work of Bitar *et al.* (Ref. 6), the crosses from the work of Gupta *et al.* (Ref. 4), and the diamonds from Ukawa (Ref. 3).

temperature crossover on $8^3\times4$ lattices. For the screening length and spectrum calculations we used pointlike sources and sinks with the quantum numbers of the π, ρ, σ, and a_1 mesons. In all cases 2000 trajectories were generated, with measurements taken every ten trajectories. The correlation functions were blocked in units of two, and the masses and screening lengths were extracted using correlation fits as described in Ref. 9.

III. RESULTS

The time histories shown in Figs. 1 and 2 are typical of our results for other values of κ. In particular, we did not observe any tunnelings in our long runs at fixed coupling. From Fig. 2 it is clear that for $\kappa=0.17$ the crossover value of $6/g^2$ is between 5.12 and 5.13. In Fig. 3 we show the crossover values of the gauge coupling, $6/g_c^2$, for our entire data set on $8^3\times4$ lattices. We include on this graph earlier results of Bitar *et al.*,[6] Gupta *et al.*,[4] and Ukawa.[3]

We have performed spectrum calculations on $8^3\times16$ lattices for $0.16\le\kappa\le0.19$ with the gauge coupling set equal to $6/g_c^2$. We have measured only meson masses, and our results for the π, ρ, σ, and a_1 are given in Table II. All masses are given in lattice units. The results for the σ and a_1 masses should be treated cautiously as we did not obtain a plateau in the effective mass plots for these heavy particles.

In Fig. 4 we plot m_π^2 as a function of κ. The pion masses that we have measured on $8^3\times16$ lattices are not small. Thus, if one defines the chiral limit as the vanishing of the pion mass on zero-temperature lattices, this limit is not reached in the low-temperature phase on $8^3\times4$ lattices for the values of κ and $6/g^2$ that we have studied. However, other definitions of κ_c on finite-volume lattices have been proposed.[6,10,11] Bitar, Kennedy, and Rossi have suggested that κ_c be determined by the location of zeros in the fermion determinant.[6] They showed that these zeros are configuration dependent, so it is not surprising that this definition of κ_c leads to a different result on a finite lattice than a measurement of the zero-temperature pion mass, which is necessarily an

TABLE II. Zero-temperature masses in lattice units. The last column gives χ^2 per degree of freedom for the correlated fit which is quoted in the table.

Particle	Mass	$\chi^2/N_{\rm DF}$
	$\kappa=0.16$, $6/g^2=5.28$	
π	1.213±0.004	9.1/3
ρ	1.287±0.0005	2.8/2
σ	2.24±0.05	0.6/1
a_1	2.23±0.04	2.5/1
	$\kappa=0.17$, $6/g^2=5.12$	
π	1.088±0.003	2.1/2
ρ	1.210±0.005	3.0/2
σ	2.36±0.09	1.1/1
a_1	2.33±0.09	0.2/1
	$\kappa=0.18$, $6/g^2=4.94$	
π	0.934±0.003	1.0/3
ρ	1.117±0.005	2.0/2
σ	2.9±0.3	2.5/2
a_1	2.5±0.1	2.0/2
	$\kappa=0.19$, $6/g^2=4.76$	
π	0.722±0.003	0.3/2
ρ	1.020±0.009	5.3/3
σ	2.1±0.2	0.6/1
a_1	2.2±0.1	2.8/1

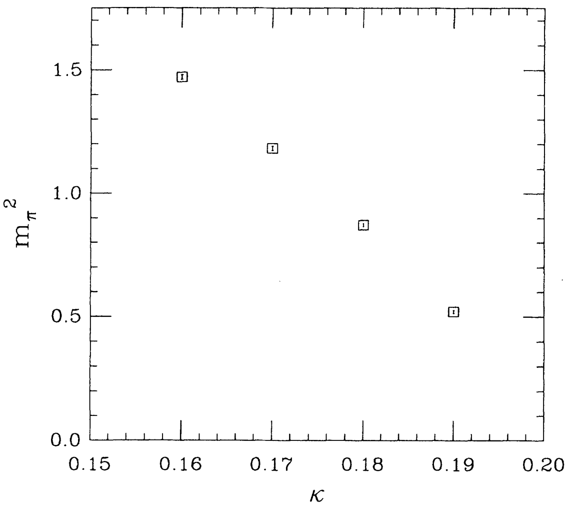

FIG. 4. m_π^2 as a function of κ for points along the crossover curve on $8^3\times16$ lattices.

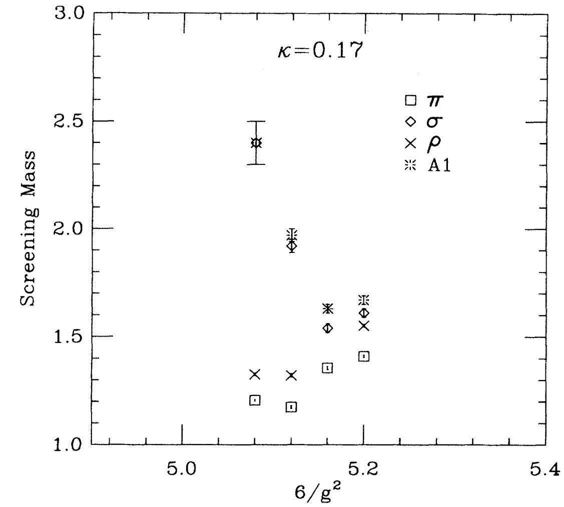

FIG. 6. Hadron screening lengths as a function of $6/g^2$ for $\kappa=0.17$.

average over many configurations. They concluded that the chiral limit is reached in the low-temperature phase on $8^3\times4$ lattices for $6/g^2<5.0$.[6]

Hadron screening lengths have proven to be a useful tool for the study of chiral-symmetry restoration in the high-temperature phase.[12,3] We have calculated screening lengths in the channels with the quantum number of the π, ρ, σ, and a_1, on $8^2\times16\times4$ lattices. In Figs. 5 and 6 we plot the inverse screening lengths, or screening masses, as a function of $6/g^2$ for $\kappa=0.16$ and 0.17, respectively. The screening masses are given in units of $1/a=4T$. The crossover values of $6/g^2$ for these two values of κ are 5.27±0.01 and 5.125±0.005. Here the temperature increases with $6/g^2$. Thus, we see that the π and σ screening masses tend toward each other as the system is heated above the crossover temperature, as do the ρ and a_1 masses. The effect is not as dramatic as for Kogut-Susskind fermions[12] since we are not close to the chiral limit. Note the dip in the π screening mass at the crossover point. The σ and a_1 screening masses are larger in the low-temperature phase. As a result, the correlation functions fall off very rapidly with distance, and a plateau is not found in the effective mass. Just as in

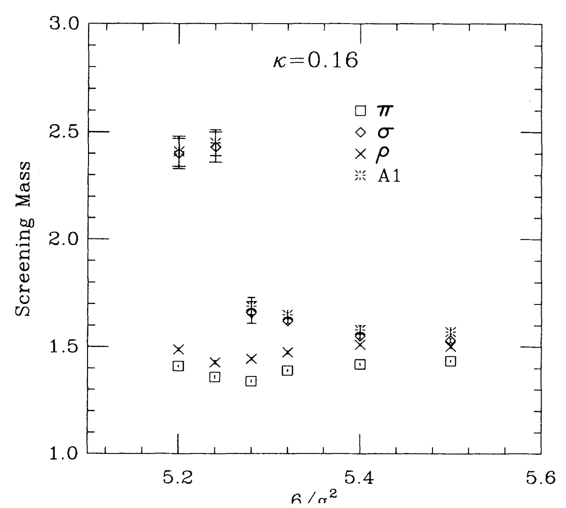

FIG. 5. Hadron screening lengths as a function of $6/g^2$ for $\kappa=0.16$.

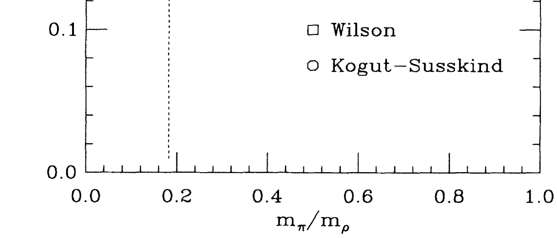

FIG. 7. The dimensionless ratio T_c/m_ρ as a function of m_π/m_ρ along the crossover curve. The squares are from the present work with Wilson quarks, and the circles are from a previous study with Kogut-Susskind quarks also at $N_t=4$ (Ref. 13). Reading from left to right the Wilson points are for $6/g^2$ and κ values (4.76,0.19), (4.94,0.18), (5.12,0.17), and (5.28,0.16), while the Kogut-Susskind points are for $6/g^2$ and quark mass values (5.2875,0.025), (5.32,0.05), and (5.375,0.1).

the case of the zero-temperature masses, our results for these quantities should be treated cautiously.

It is well known that the crossover coupling for four time slices, $N_t=4$, corresponds to a lattice spacing that is far too large to be in the scaling region. As a result, it is not surprising that at this lattice spacing Kogut-Susskind and Wilson quarks give significantly different results. Spectrum calculations have been carried out for two flavors of Kogut-Susskind quarks at the crossover coupling for $N_t=4$ with quark masses 0.1, 0.05, and 0.025 in lattice units.[13] In Fig. 7 we plot the dimensionless ratio $T_c/m_\rho=1/4am_\rho$ as a function of m_π/m_ρ from that study (circles), and from our present work with Wilson quarks (squares). The statistical errors are smaller than the plotting symbols. The dotted line is the physical value of m_π/m_ρ to which we would extrapolate these results. The strong difference between the two quark formulations is evident.

Another indication of the difference between the two quark formulations at the present lattice spacing can be seen by estimating T_c in physical units. From the data of Table II we can make a linear fit to m_ρ as a function of m_π^2. We find

$$m_\rho=(0.87\pm0.01)+(0.283\pm0.009)m_\pi^2 \quad (4)$$

with $\chi^2/N_{\rm DF}=0.6/2$. If we set the energy scale by taking m_ρ to have its physical value at $m_\pi=0.0$, then T_c is estimated to be 221 ± 3 MeV.[14] The same calculation for Kogut-Susskind quarks at $N_t=4$ yields $T_c=142\pm6$ MeV. Of course the errors quoted in Eq. (4) and for T_c are statistical only. If we make a linear fit of m_π^2 as a function of κ from the data of Table II, we find that $m_\pi=0.0$ for $\kappa=0.207\pm0.002$; however, the fit is a poor one with $\chi^2/N_{\rm DF}=25/2$. From Fig. 3 we see that if this value of κ is reached at all by the crossover curve, it is only in the strong-coupling regime. It is possible that our extrapolation has simply taken us to a point in the high-temperature phase. Clearly this calculation should be taken with great caution. We include it to illustrate the difference between the two lattice formulations of quarks at $N_t=4$.

It is essential to extend the study of Wilson thermodynamics to larger values of N_t in order to determine whether the chiral limit exists in the low-temperature phase, and in order to study the approach to the continuum limit. A start in this direction was made in Ref. 4, and we hope to return to this problem in the near future.

ACKNOWLEDGMENTS

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[1]For a recent review see A. Ukawa, in *Lattice '89,* proceedings of the International Symposium, Capri, Italy, 1989, edited by R. Petronzio *et al.* [Nucl. Phys. B (Proc. Suppl.) **17** (1990)].

[2]M. Fukugita, S. Ohta, and A. Ukawa, Phys. Rev. Lett. **57**, 1974 (1986).

[3]A. Ukawa, in *Lattice '88,* proceedings of the International Symposium, Batavia, Illinois, 1988, edited by A. Kronfeld and P. MacKenzie [Nucl. Phys. B (Proc. Suppl.) **9**, 463 (1989)].

[4]R. Gupta, A. Patel, C. Baillie, G. Guralnik, G. Kilcup, and S. Sharpe, Phys. Rev. D **40**, 2072 (1989).

[5]Y. Iwasaki and Y. Tsuboi, Phys. Lett. B **222**, 269 (1989).

[6]K. Bitar, A. D. Kennedy, and P. Rossi, Phys. Lett. B **234**, 333 (1990).

[7]S. Duane, A. D. Kennedy, B. J. Pendleton, and D. Roweth, Phys. Lett. B **195**, 216 (1987).

[8]T. DeGrand and P. Rossi, Comput. Phys. Commun. **60**, 211 (1990).

[9]D. Toussaint, in *From Actions to Answers—Proceedings of the 1989 Theoretical Advanced Summer Institute in Particle Physics,* edited by T. DeGrand and D. Toussaint (World Scientific, Singapore, 1990).

[10]M. Bochicchio, L. Maiani, G. Martinelli, G. Rossi, and M. Testa, Nucl. Phys. **B262**, 331 (1985).

[11]Y. Iwasaki, Y. Tsuboi, and T. Yoshie, Phys. Lett. B **220**, 602 (1989).

[12]C. E. DeTar and J. B. Kogut, Phys. Rev. Lett. **59**, 399 (1987); S. Gottlieb, W. Liu, R. L. Renken, R. L. Sugar, and D. Toussaint, *ibid.* **59**, 1881 (1987).

[13]S. Gottlieb, W. Liu, R. L. Renken, R. L. Sugar, and D. Toussaint, Phys. Rev. D **38**, 2245 (1988).

[14]A similar result for T_c with Wilson quarks was obtained from a thermodynamics study on $5^3\times4$ lattices (Ref. 5).