Finite-Temperature Phase Transitions in SU(3) Lattice Gauge Theory with Dynamical, Light Fermions

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SU(3) lattice gauge theory with four light quark species is studied at finite temperature by microcanonical computer simulation techniques. An abrupt transition is found separating the hadronic-matter and the quark-gluon–plasma phases. Measurements of the critical temperature, latent heat, $\langle\bar{\psi}\psi\rangle$, Wilson line, and Wilson-line correlation function are presented and are compared to earlier calculations which ignored fermion vacuum polarization.

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The study, both theoretical and experimental, of quantum chromodynamics in extreme environments is attracting ever-increasing interest. Among the many reasons for this are these: (1) In hot and baryon-rich environments the confining and chiral-symmetry–breaking properties of quantum chromodynamics should disappear. (2) Models of cosmology use as input the sequence and character of the phase transitions which a gauge theory shows. (3) There are plans for creating extreme environments in the laboratory through the construction of a heavy-ion collider.

The quantitative study of the deconfining and chiral-symmetry–restoring transitions in quantum chromodynamics has been done earlier in the "quenched" approximation which neglects fermion vacuum polarization.[1] The results were very intriguing. At a temperature $T_c \approx 200$ MeV the system passes from a state of confined hadronic matter with dynamically generated quark masses (chiral-symmetry breaking) to a state of a quark-gluon plasma with vanishing quark masses.[2] The transition was first order with a large latent heat per unit volume, 1.50 ± 0.50 GeV/fm^3.[3]

However, theorists have questioned the relevance of quenched calculations to quantum chromodynamics, which has an almost massless ($m \approx 5$ MeV) isodoublet of quarks and a light ($m_s \approx 100$ MeV) strange quark, in addition to several heavy flavors. Because of vacuum polarization it was suggested that the transition between confined quarks (ordinary hadrons) and screened quarks (quark-gluon plasma) might not be abrupt. Model studies[4] and series expansions[5] support this view. It is clear, however, that the chiral-symmetry–restoring transition[6] must persist in the presence of vacuum polarization, but its impact on the bulk thermodynamics of the system has not been estimable in the past.

In this Letter we report a large-scale lattice gauge-theory simulation which addresses these physics issues. The inclusion of light dynamical fermions into computer simulations will be achieved here by use of the microcanonical formalism of Polonyi and co-workers.[7] As discussed there, this method has several advantages over series expansions[5] and pseudofermion stochastic techniques.[8] The description of the microcanonical method follows. Consider the classical system described by the coordinates $U_\mu(n)$ and $Q(n)$ whose Lagrangian is

$$L = \tfrac{1}{2} \textstyle\sum_{n,\mu} \mathrm{tr}\dot{U}_\mu^\dagger(n)\hat{P}\dot{U}_\mu(n) - \beta_{in}S[U] + \dot{Q}^\dagger A^\dagger[U]A[U]\dot{Q} - \omega^2 \textstyle\sum_n Q^\dagger(n)Q(n), \tag{1}$$

where S$[U]$ is Wilson's action for SU(3) lattice gauge theory and $A[U]$ is the hopping matrix of staggered fermions.[7] The matrix $\hat{P}$ is a projection operator, $\hat{P} = \mathrm{diag}(1,1,0)$. One can show that the thermal average of an observable $\theta[U]$ calculated at temperature T by the Gibb's canonical partition function

$$Z=\int D[U]\,D[p]\,D[Q]\,D[P]\exp(-T^{-1}H), \tag{2a}$$

$$H=\tfrac{1}{2}\textstyle\sum_{n,\mu}p_\mu^\dagger(n)\hat{P}p_\mu(n)+\beta_{in}S[U]+P(A^\dagger[U]A[U])^{-1}P^\dagger+\omega^2\sum_n Q^\dagger(n)Q(n), \tag{2b}$$

reproduces the expectation value,

$$\langle\theta[U]\rangle=\frac{\int D[U](\det A[U])^\gamma e^{-\beta S[U]}\theta[U]}{\int D[U](\det A[U])^\gamma e^{-\beta S[U]}}, \tag{2c}$$

where the power γ which determines the number of fermion species is 2 for complex $A[U]$ with real determinant. In those cases where $A[U]$ is the sum of the identity and an anti-Hermitian nearest-neighbor hopping matrix, $A^\dagger[U]A[U]$ only connects sites with the same parity ($=x+y+z+t[\mathrm{mod}2]$). The determinant in Eq. (2c) is then the product of the determinants of $A^\dagger[U]A[U]$ restricted to even or odd sites: $\det A^\dagger[U]A[U]=\det(A^\dagger[U]A[U])_{\text{even}}\det(A^\dagger[U]A[U])_{\text{odd}}$. Therefore, setting $P(n)=0$ on even sites forces $\det(A^\dagger[U]A[U])_{\text{even}}$ to unity. Because of translation invariance we can interpret this thinning of the fermion degrees of freedom as the reduction of $\gamma=2$ to $\gamma=1$. Applying this scheme to four-dimensional staggered fermions we have $N_f=8$ or 4 flavors for $\gamma=2$ or $\gamma=1$, respectively.

To simulate the classical system of Eq. (1) we follow the molecular dynamics method.[7] Under the assumption that the classical system is ergodic, the time average

$$\langle\theta[U]\rangle_t=\lim_{T\to\infty}\frac{1}{T}\int_0^T d\tau\,\theta[U(\tau)]$$

is equivalent to the microcanonical average which itself agrees with the canonical average Eq. (2c) up to calculable power-behaved corrections $V^{-\alpha}$, $V=$ volume of the four-dimensional lattice. In order to obtain the time evolution of the classical system we discretize the time $\tau_k=k\Delta\tau$ and solve the resulting Euler-Lagrange equations,

$$U^{(k+1)}=2U^{(k)}-U^{(k-1)}+2(\Delta\tau)^2\left\{-\beta_{in}\frac{\partial S[U^{(k)}]}{\partial U^*}+\dot{Q}^{\dagger(k)}\frac{\partial A^\dagger[U^{(k)}]A[U^{(k)}]}{\partial U^*}\dot{Q}^{(k)}\right\}, \tag{3a}$$

$$A^\dagger[U^{(k+1)}]A[U^{(k+1)}]\dot{Q}^{(k+1)}=A^\dagger[U^{(k)}]A[U^{(k)}]\dot{Q}^{(k)}-(\Delta\tau)\omega^2Q^{(k+1/2)}, \tag{3b}$$

numerically. The conjugate-gradient method was used to solve Eq. (3b) for $\dot{Q}^{(k+1)}$. And finally, the coupling $\beta=6/g^2=\beta_{in}/T$ of the (3+1)-dimensional field theory is determined by the equipartition theorem,

$$\tfrac{1}{2}N^*T=\langle\tfrac{1}{2}\textstyle\sum_{n,\mu}\dot{U}_\mu^\dagger(n)\hat{P}U_\mu(n)+\dot{Q}^\dagger A^\dagger[U]A[U]\dot{Q}\rangle_t, \tag{4}$$

where N^* is the number of noncyclic coordinates which is $N_{\text{sites}}\times(28+3N_f/4)$ in our case.

Now we turn to our results. We simulated SU(3) gauge theory with four ($N_f=4$) light quark flavors. The lattice was chosen asymmetric, 4×8^3, to simulate finite temperature. Lattices of this size were used extensively in quenched studies and yielded physical results which have been modified by less than 20% as larger lattices have been studied.[9] Another technical point in the simulation method is the fact that a bare fermion mass term must be added to the theory's Lagrangian, and the full theory must be solved for several m values. The chiral limit ($m\to0$) of matrix elements is obtained by extrapolation. Recall from Kogut *et al.*[10] that for a given $\beta=6/g^2$ and lattice volume, there is a minimum m value below which finite-size effects become important. In this study mass values of $am=0.10$ and 0.08 were used ($a=$ lattice spacing).

The simulations were done by generating a thermalized field configuration at large $\beta=6/g^2$ and then increasing the kinetic energy of the microcanonical ensemble in order to decrease the β of the system and probe the critical region $\beta\approx5.0$. Typically 5000 steps with $\Delta\tau=0.01$ were taken at each β, and matrix elements were measured every 50 or 100 steps. All the matrix elements were quickly convergent and required far fewer sweeps than we ran except for the gluonic internal energy. This matrix element showed long-wavelength oscillations versus step number (waves of length 500 steps were typical) with amplitudes of 50% of the mean value in the quark-gluon phase. The origin of these long-time correlations are not known to us, but they may have physical significance (unexpected low-mass modes?).

In Fig. 1 we show the resulting curve of the internal energy density ϵ/T^4 versus temperature for a quark mass of $am = 0.08$. We note the dramatic rise of ϵ/T^4 from zero to a value consistent with the free-field Stefan-Boltzmann result expected on a 4×8^3 lattice.[11] This rise occurs within a temperature interval of $T_c/\Lambda_L = 280 \pm 10$. The temperature axis on this figure was obtained from our data by use of asymptotic freedom. In particular, the temporal lattice size N_t, the lattice spacing a, and the physical temperature are related by $aT = N_t^{-1}$. The lattice spacing a can be eliminated by use of asymptotic freedom,

$$a\Lambda_L = \left(\frac{8\pi^2}{25}\beta\right)^{231/625} \exp(-4\pi^2\beta/25) \quad \text{(4 flavors)}, \tag{5}$$

and the T/Λ_L axis in the figure results. In terms of $\Lambda_{\overline{\rm MS}}$, Eq. (5) corresponds to[12]

$$T_c/\Lambda_{\overline{\rm MS}} = 3.65 \pm 0.30 \quad \text{(4 flavors)}. \tag{6a}$$

It is interesting to compare these results with those of earlier quenched simulations. There it was found that[3]

$$T_c/\Lambda_{\overline{\rm MS}} = 2.77 \pm 0.30 \quad \text{(quenched)}, \tag{6b}$$

and the transition was first order with a latent heat which came within 75%–85% of saturating the Stefan-Boltzmann limit. Including four light fermions we see that T_c has increased in units of $\Lambda_{\overline{\rm MS}}$ by roughly 30% and the latent heat per T^4 has increased roughly 25%. Our computer simulation data for the internal energy did not show a strong dependence on the fermion bare mass for $am = 0.10$ and 0.08. Since the physical temperature T is given by $aT = N_t^{-1} = 0.25$ and since $am = 0.10$ or 0.08, the fermion masses are $m/T = 0.40$ or 0.32 in physical units. In Fig. 2 we show the fermionic and gluonic contributions to the internal energy at the larger fermion mass $am = 0.10$ as a function of $\beta = 6/g^2$ for comparison. It is intriguing that the gluonic internal energy exceeds the Stefan-Boltzmann value for β values between 5.00 and 7.00.

Finally consider $\langle\bar\psi\psi\rangle$ and the Wilson line. Recall that $\langle\bar\psi\psi\rangle$, the order parameter for chiral symmetry breaking, and the Wilson line, the exponential of minus the free energy of a static quark, are both measures of dynamical mass generation. In the quenched approximation the Wilson line vanishes identically in the confining phase, but with fermion vacuum polarization one expects it to be nonzero at all temperatures because of screening. In Fig. 3 we show the zero-mass–extrapolation[13] results for both $\langle\bar\psi\psi\rangle$ and the Wilson line. Note that the Wilson line turns on exactly where the internal energy did, and exactly where $\langle\bar\psi\psi\rangle$ vanishes. These relationships suggest that chiral symmetry restoration is responsible for our results.

Our measurements of the Wilson-line correlation function showed linear confinement below the transition and Debye screening above it and will be discussed at length elsewhere.

Our results are certainly not precise enough to distinguish rapid crossover dynamics from real first-order transitions. We plan, however, to use

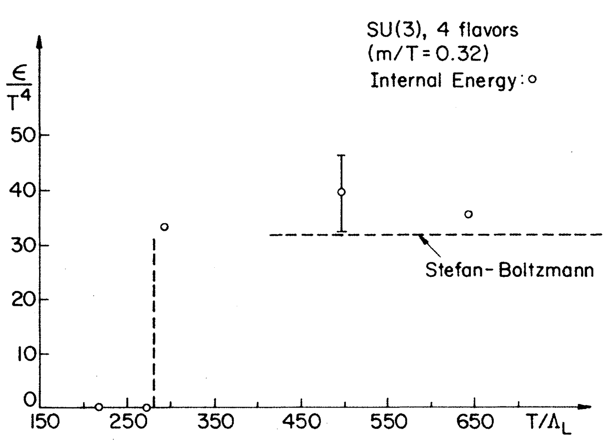

FIG. 1. Internal energy vs temperature. The fermion mass is $am = 0.08$. A characteristic error bar is shown. The Stefan-Boltzmann line for a 4×8^3 lattice is taken from Ref. 11.

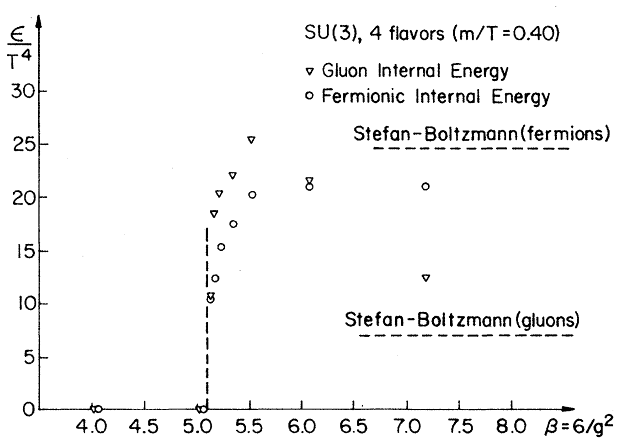

FIG. 2. Gluonic and fermionic internal energies (following the notation of Ref. 3) vs $\beta = 6/g^2$ for a bare fermion mass of $am = 0.10$. The gluonic (fermionic) internal energy is uncertain by $\pm 50\%$ ($\pm 10\%$).

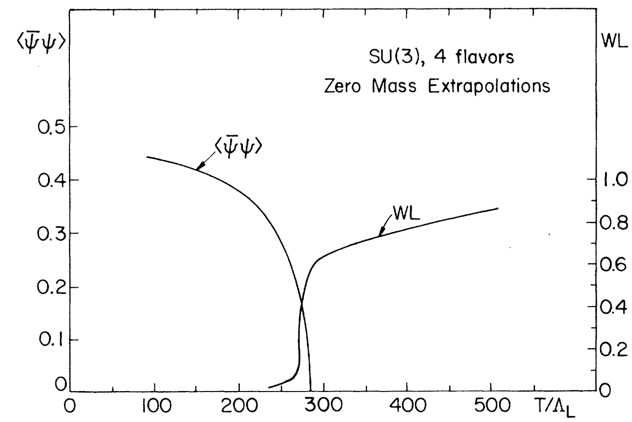

FIG. 3. $\langle\bar{\psi}\psi\rangle$ and the Wilson line (WL) vs temperature. The curves are the results of a mass $\rightarrow 0$ extrapolation. Error bars are at the several percent level.

microcanonical methods of investigating metastable states[14] to clarify this point. We will also measure hadron masses in the four-flavor theory so that the scale of T_c can be established more precisely ($\Lambda_{\overline{\mathrm{MS}}}$ is not known accurately). In this study we have assumed that asymptotic freedom is relevant to our data. The position and size of a scaling window in simulations which include light fermions has yet to be determined. Only after asymptotic freedom is verified and after several mass scales in addition to T_c are determined in a given simulation shall we be able to quote physical quantities in gigaelectronvolt units with confidence.

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