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PHASE TRANSITIONS: THE LATTICE QCD APPROACH*

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Abstract

Recent results in the field of finite temperature lattice quantum chromodynamics (QCD) are presented with special emphasis on comparison of the different methods used to incorporate the dynamical fermions. Attempts to obtain a nonperturbative estimate of the velocity of sound in both the hadronic and quark-gluon phase are summarised along with the results.

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Recent results in the field of finite temperature lattice quantum chromodynamics (QCD) are presented with special emphasis on comparison of the different methods used to incorporate the dynamical fermions. Attempts to obtain a nonperturbative estimate of the velocity of sound in both the hadronic and quark-gluon phase are summarised along with the results.

1. INTRODUCTION

Quantum Chromo Dynamics (QCD) is now widely believed to be the theory of strong interactions. Many of its predictions, especially those stemming from its property called asymptotic freedom, have been verified experimentally. With the advent of lattice gauge theories, and the subsequent use of Monte Carlo techniques to simulate them on the powerful supercomputers of today, we may now be on our way to understand the low energy (low momentum transfer) strong interactions as well. Already, static properties, such as the masses of the stable hadrons or the chiral condensate $\langle\bar{\psi}\psi\rangle$, have been reliably obtained from QCD using these techniques, confirming thus a long-held view that chiral symmetry is broken dynamically in our world. A natural question to ask is whether the theory can tell us anything about what we should expect under extreme conditions such as high temperatures or densities. Such conditions could have occurred in the very early

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stages of our Universe and, interestingly enough, can perhaps be attained in the proposed heavy-ion experiments at Brookhaven National Laboratory and at CERN.

Lattice QCD at finite temperatures and finite densities offers us a way to obtain an answer to the question above. It may be emphasized that unlike many other approaches which too attempt to answer the same question, the lattice QCD approach is free of any arbitrary assumptions and does not need essentially any free parameters. The only parameters that enter are the quark masses and the scale of the theory Λ_{QCD}, all of which can be fixed by calculating hadron masses using the same methods.

Since the entire temperature domain of interest can be investigated using these methods, it is not a surprise that the very question of the existence of a phase transition has been pursued rather hotly in this field in the recent past. After a bit of controversy in the beginning, a consistent picture seems to be emerging now about the predictions of QCD with light, dynamical fermions, as I hope to show you later. Another interesting development in the past year or so has been the application of these techniques to obtain quantities such as the velocity of sound near the phase transition. Attempts to obtain a detailed space-time description of the evolution of the quark-gluon plasma would find such information quite useful. Before I present these results though, let me briefly review how one obtains them starting from first principles. I intend to give here only a broad idea; the interested reader may find it more rewarding to fill in the details from the literature[1)] elsewhere.

1.1 The Three Steps of Lattice Approach

The thermodynamic observables of a theory can be obtained in the canonical fashion from its partition function:

$$Z = \mathrm{Tr}\, \exp(-H/T) \ , \tag{1}$$

where H is the Hamiltonian of the theory and T is the temperature of the system. Tr denotes sum over all physical states of the theory. Usual thermodynamic formulae can be employed to obtain from Z the various physical quantities of interest, e.g., the energy density $\varepsilon = V^{-1}T^2\ \partial \ln Z/\partial T$. What we wish to do is to substitute the Hamiltonian of QCD in (1) and evaluate various physical quantities and order parameters as a function of temperature: a phase transition will show up as a nonanalytic behaviour. The lattice approach to do this consists of three major steps. First one rewrites the partition function in eq. (1) as a functional integral of the exponential of the euclidean action over all the fields of the theory. This essentially amounts to summing over all possible classical paths with a given boundary condition. Using a complete set of states $|i\rangle$ and dividing $1/T$ in n equal segments of length ε $(1/T = n\varepsilon)$, one can rewrite eq. (1) as below:

$$Z = \sum_{i,i_1,i_2\ldots} \langle i|e^{-\varepsilon H}|i_1\rangle \langle i_1|e^{-\varepsilon H}|i_2\rangle \ldots\ldots \langle i_{n-1}|e^{-\varepsilon H}|i\rangle\ . \qquad (2)$$

Note that $\exp(-\varepsilon H)$ is the time evolution operator in the euclidean space-time. Thus each term in the sum in eq. (2) can be thought as one corresponding to a path which takes the system from the state i to i_1, to i_2 ... and so on, and back to i. In the limit $\varepsilon \to o$ such that $1/T$ = constant, eq. (2) becomes

$$Z = \int_{bc} D\phi \exp\left(-L\left(\phi(x),\ \partial\mu\phi(x)\right)\right)\ . \qquad (3)$$

In the case of QCD, ϕ in eq. (3) denotes the gluon fields and the (anticommuting) quark, antiquark fields; L is the usual QCD Lagrangian, and bc denotes periodic boundary conditions for the gluon fields and antiperiodic ones for the fermions.

One way to handle the complicated integrals in eq. (3) is to introduce a space-time lattice. Then the lattice spacing a acts as a regulator for the theory. The lattice theory can be made to respect gauge invariance by appropriately choosing the field variables and the action on the lattice. A popular choice[1)] is to place the fermion fields $\psi(n)$ on the lattice sites $n = (n_1, n_2, n_3, n_4)$ and the gauge fields U_n^μ are then associated with the (oriented) bonds of the lattice. In terms of these variables eq. (3) takes the form

$$Z = \int_{bc} \prod_{\substack{n\\ \mu}} dU_n^\mu \prod_n d\psi(n)\ d\bar{\psi}(n) \exp\left(-S(\psi,\bar{\psi},U_n^\mu)\right) \qquad (4)$$

where the lattice action S in (4) is chosen by demanding a) gauge invariance, and b) proper classical continuum limit, i.e., $\lim S(\psi,\bar\psi,U_n^\mu) = L_{QCD}$. The gauge variables $U_n^\mu \sim \exp[ia\,g\,A^\mu(n)]$ in this limit, where $A^\mu(n)$ is the continuum gluon field which is an analogue of the photon field in QED. If the lattice has N_β sites in the temporal direction, and a_β is the lattice spacing in that direction, then the temperature $T = 1/N_\beta a_\beta$. Analoguous quantities in the three spatial direction determine the volume: $V = N_\sigma^3 a_\sigma^3$. In practice all the final expressions are evaluated for $a_\sigma = a_\beta$ for simplicity, making it necessary that $N_\sigma \gg N_\beta$. $(N_\sigma = N_\beta \to \infty$ would correspond to $T = 0)$. The expression in (4) looks very similar to those used in statistical mechanics, e.g. the partition function of the Ising model. It is thus natural to expect that the methods to obtain the expectation values of various observables from Z above are borrowed from those areas of physics. Monte Carlo simulations is one such technique. Its popular use is dictated by the third step we have to take.

Introduction of the lattice above was merely for calculational convenience. One must remove the lattice finally by taking the limit of vanishing lattice spacng a. Only those answers which are obtained in this limit are relevant to our original problem. Employing the Monte Carlo technique, Creutz[2)] showed how one can take this limit numerically. Asymptotic freedom of QCD tells us how the bare coupling g^2 must change as $a \to 0$. It goes to zero according to the following relation:

$$a\Lambda_L = (b_0 g^2)^{-b_1/2b_0^2} \exp(-1/2b_0^2 g^2)\,[1 + O(g^2)]\ , \qquad (5)$$

with $b_0 = 33-2N_f/48\pi^2$ (6)

and $b_1 = 153-19N_f/384\pi^2$. (7)

Here N_f is number of massless flavours in the theory. Creutz showed that for $N_f = 0$ eq. (5) holds true for rather small lattices and rather large couplings g^2. In the (asymptotic) scaling region, where above equation is satisfied, one can obtain continuum results for any physical quantity of interest by using eq. (5).

2. PROBLEMS WITH DYNAMICAL FERMIONS

The anticommuting nature of the fermion variables $\psi, \bar{\psi}$ in eq. (4) makes it difficult to apply the above procedure in a straightforward manner to obtain the thermodynamics of QCD. One finds it usually convenient to carry out the fermionic integrals explicitly since S in (4) is typically $S = S_G(U) + \sum_{n,n'} \psi(n) Q_{nn'} \psi_n$. This leads to the following expression for Z:

$$Z = \int_{bc} \prod_{\substack{n \\ \mu}} dU^\mu \exp\left(-S_G(U) \right) \cdot \det Q(U) \quad . \tag{8}$$

In a typical calculation, Q is a square matrix of dimension ~ 6000, and one needs to evaluate det Q about 1-10 million times. ($N_\sigma = 8$, $N_\beta = 4$ was assumed). Even with clever tricks which make use of the properties of Q such a calculation would need about three years on even a CRAY-XMP.

One therefore needs good approximation schemes which succeed in getting the essence of fermion loops contained in det Q with minimum computer time. The early calculations[3)] were done by dropping the determinant altogether, which can be thought of as the heavy quark limit of our world. There it was found that QCD had a strong first order deconfinement phase transition with a latent heat of about 1 GeV/fm^3. Research efforts in the past couple of years or so have

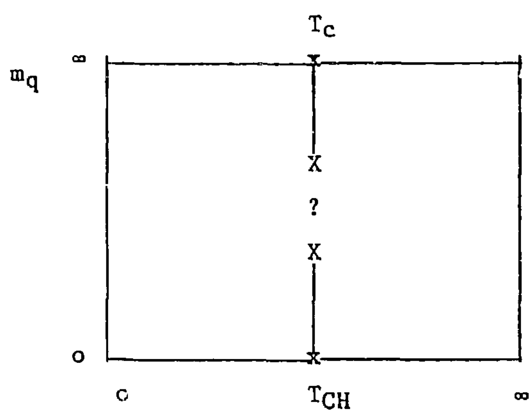

Fig. 1 Expected phase diagram of QCD.

been concentrated on the question of making those calculations more realistic by considering lighter quarks. Based on simple models which exploit only the symmetry aspects, one can argue what one would expect as the quark mass, m_q, is gradually lowered. These expectations are summarised in Fig. 1. The first order phase transition in the quenched or quarkless QCD is denoted there by T_c on the $m_q = \infty$ line. As m_q is lowered, one expects a line of first order phase transitions along which the latent heat decreases. The end of this line will be marked by a point where latent heat vanishes. It is not clear whether a second order line continues beyond this point. Starting from the other end, $m_q = 0$, one expects a chiral symmetry restoring phase transition there: we believe that chiral symmetry is broken in our world ($\langle\bar{\psi}\psi\rangle \neq 0$, $m_\pi^2 \to 0$ as $m_q \to 0$ etc.) and it can be shown[4] that at sufficiently high temperatures it must be restored. If this phase transition is also of first order, then as m_q is increased from zero, one expects an analogous scenario as that for the deconfinement phase transition.

The interesting question, of course, is about the positions of the two end points. Are they close to each other? or perhaps overlapping? Could one have two types of phase transitions for some value of m_q? These and other similar questions of details can only be answered after a good scheme to approximate the fermion determinant det Q is found. There are lots of proposals for such schemes in the literature, quite a few of which have been already used to study the full QCD thermodynamics, often leading to unfortunately confusing, sometimes even contradictory, results. In many cases the source of such a confusion is the method used to incorporate the fermion effects. Thus, one needs to test the methods rather thoroughly before drawing any firm conclusions. As I see, there are at least three necessary checks: i) one must study how stable the results are under variations of the parameters which keep the physics (i.e., temperature, number of flavours, quark mass, etc.) same, ii) one should compare results obtained by just varying the approximation schemes, and iii) one should compare the approximation with an exact numerical evaluation of the determinant in simpler situations.

Using the so-called pseudo-fermion method[5], I have studied the full QCD from the standpoint of these checks. Along with Karsch[6], I

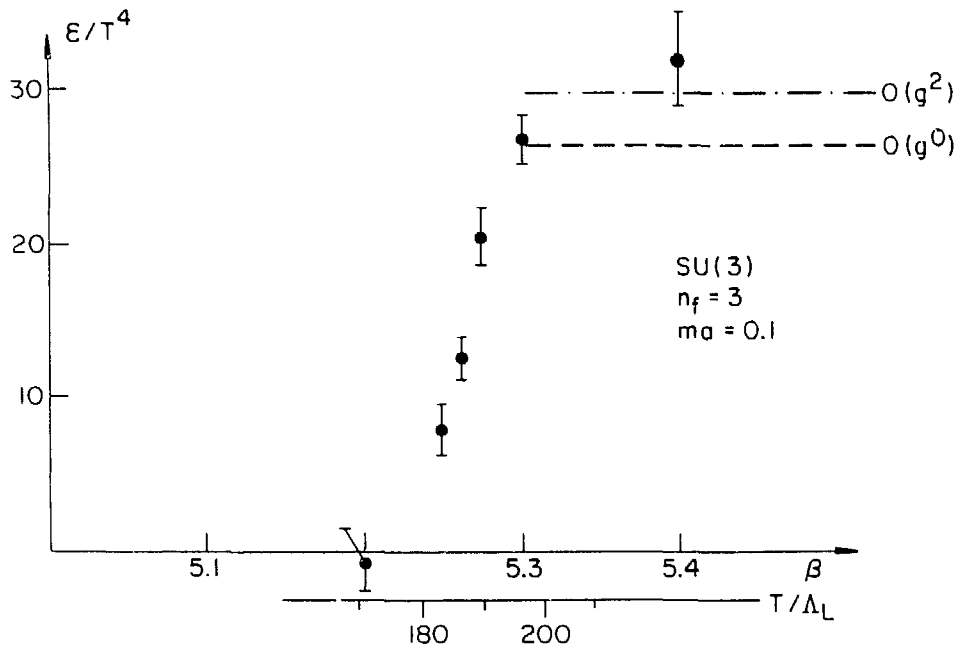

Fig. 2 Energy density as a function of β (=6/g^2) for QCD with three flavours of mass 0.1 on an $8^3 \times 4$ lattice. The temperature scale has been obtained by assuming the validity of eq. (5).

simulated the theory with three light dynamical flavours. Figures 2 and 3 show the energy density ε, and the order parameters $\langle\bar{\psi}\psi\rangle$ and $\langle L\rangle$ as a function of $\beta = 6/g^2$ or equivalently temperature on an $8^3 \times 4$ lattice. $\langle\bar{\psi}\psi\rangle$, the chiral condensate, can be thought of as a direct measure of the constituent mass of the quarks while $\langle L\rangle$ can be loosely described as the deconfinement order parameter: $\langle L\rangle \simeq o$ corresponds to a confining phase, and $\langle L\rangle \neq o$ to a deconfined phase.

One sees clearly that all these quantities undergo a rapid variation in a small range of temperature. The energy density jumps from a small value (~ 0.) to a value corresponding to that of an ideal gas of quarks and gluons. The constituent mass of the quarks becomes very small at the phase transition, and deconfinement seems to take place coincident with chiral symmetry restoration. We made attempts to look for the characteristic two state signal of a first order phase transi-

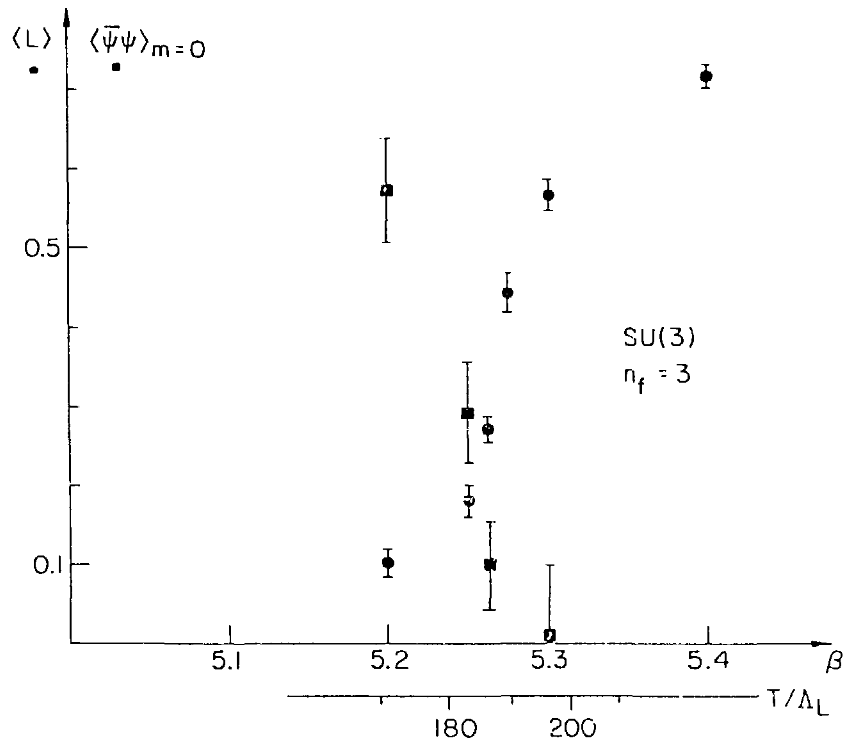

Fig. 3 The order parameters ⟨L⟩ and $\langle\bar{\psi}\psi\rangle_{m=0}$ versus $\beta(=6/g^2)$ and T/Λ_L. All the input parameters are the same as in Fig. 2 except that an additional quark mass of 0.075 was used to obtain a linear extrapolation to $\langle\bar{\psi}\psi\rangle_{m=0}$.

tion with negative results. While our results agree with the previous results[7] obtained on smaller lattices and with lesser statistics quantitatively, both sets of authors obtained $\beta_c \sim 5.25$, ref. 7 did find a first order phase transition. Our study suggests that the nature of the phase transition is sensitively dependent on the choice of parameters pertaining to the method. In particular, the signal observed in ref. 7 was washed out in higher statistics studies. Nonetheless, a safe conclusion would perhaps be that even in the phase transition in the full theory is indeed of first order, the latent heat (and similar discontinuities) is much smaller than was estimated in the earlier studies of quenched (or heavy quark) QCD. Phenomeno-

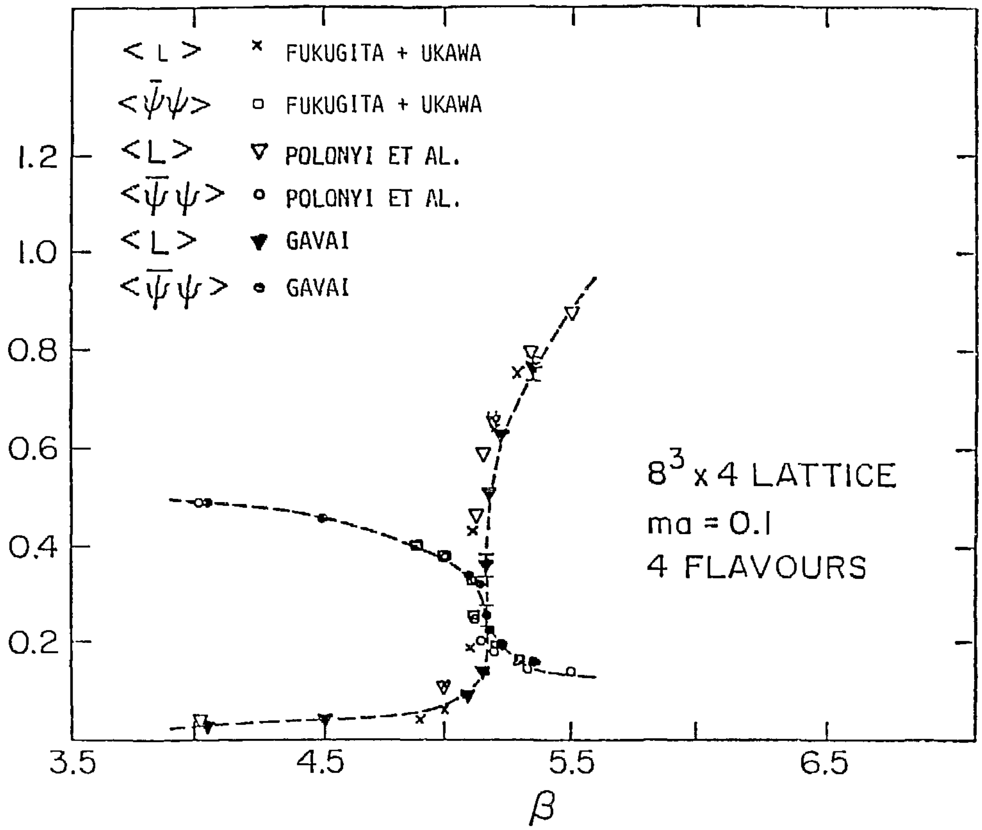

Fig. 4 <L> and $<\bar{\psi}\psi>_{ma=0.1}$ as a function of β. All the data have been obtained for QCD with four light flavours of mass 0.1 on an $8^3 \times 4$ lattice. The dashed curves are drawn to guide the eye. Data from ref. 9, 10, and 11.

logical implications of this conclusion could be significant, especially in the studies of space-time evolution of the plasma and the experimental signatures to detect the plasma. Our lattice was perhaps not big enough to allow a good estimate of T_c in MeV. A rough estimate can, however, be obtained by using the recent spectroscopic calculations[8)] to set the scale Λ_L: $T_c \sim 200\text{-}250$ MeV.

Figures 4 and 5 exhibit the same quantities as in Figs. 2 and 3

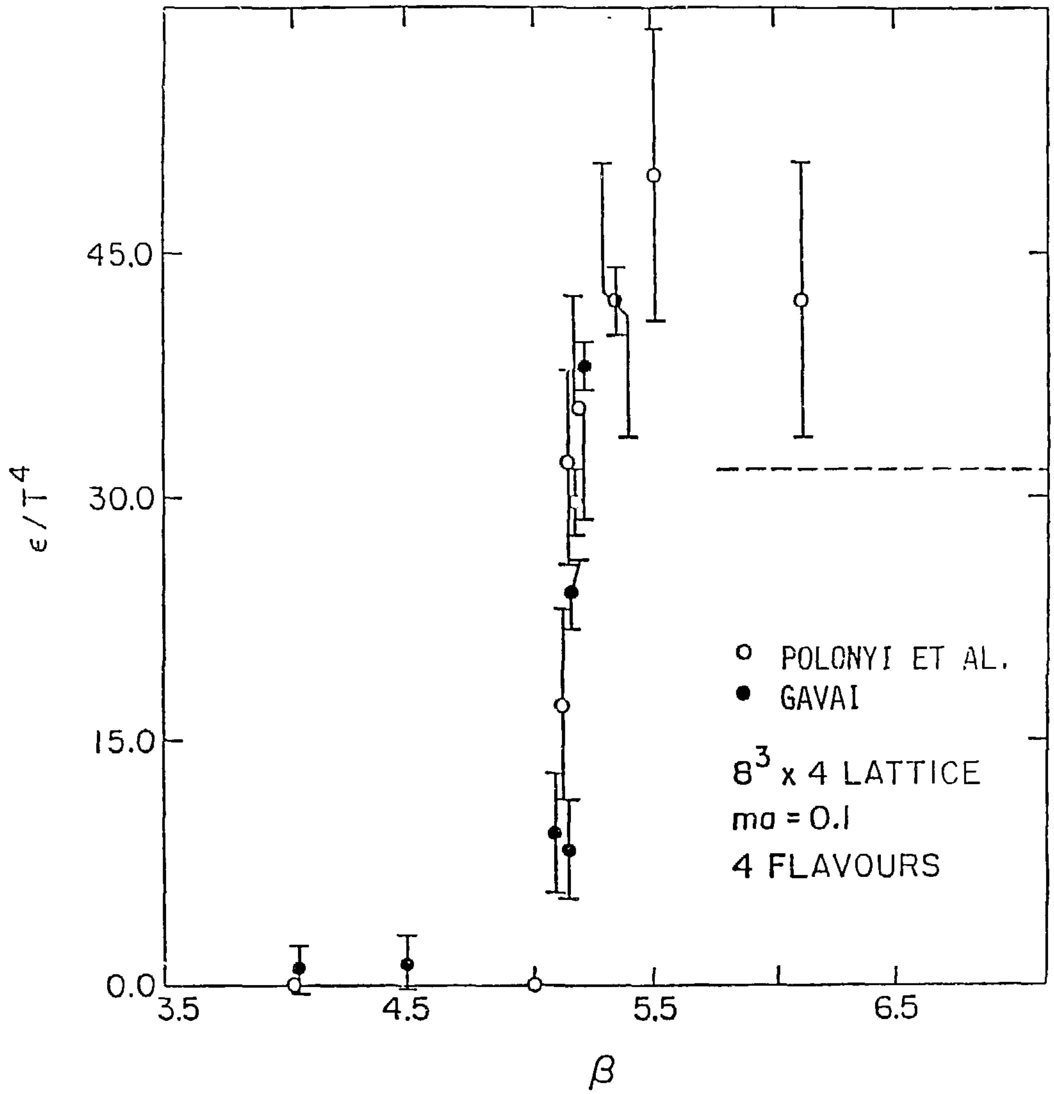

Fig. 5 The energy density ε versus β for the same theory as in Fig. 4. The dashed line represents the value for a corresponding ideal gas of 8 gluons and 12 quarks.

but calculated[9)] for four light flavours, again by using the pseudo-fermion method, in order to compare with a very different scheme to include the fermions, namely the microcanonical method[10)]. All the parameters which govern the physics, such as m_q or N_f were chosen to be the same for the two cases. A good quantitative agreement is evident in each of the three observables over the entire temperature range studied. I received a preprint[11] very recently where yet another method, called Langevin method, was used to study the same problem.

Table I: COMPARISON OF THE PSEUDO-FERMION METHOD WITH AN EXACT METHOD

Physics Parameters: Lattice size = 4^4, $N_f = 4$, $m_q a = 0.1$

	Observables						
METHOD	$\langle\bar{\psi}\psi\rangle$	W(1,1)	W(1,2)	W(1,3)	W(2,2)	W(2,3)	W(3,3)
Exact	0.402 ±0.006	0.415 ±0.003	0.177 ±0.003	0.074 ±0.003	0.035 ±0.003	0.008 ±0.002	-0.001 ±0.002
Pseudo-fermion	0.413 ±0.009	0.404 ±0.002	0.168 ±0.002	0.070 ±0.001	0.030 ±0.001	0.006 ±0.001	0.001 ±0.001

Their results also agree quantitatively with those discussed above, as one can see in Fig. 4. This is indeed very encouraging, and leads one to believe that these results are perhaps stable and reliable. Finally, Table I shows the comparison of the pseudo-fermion method with a method[12] using an exact numerical evaluation of the fermion determinant, but on a smaller lattice[13]. The physical observables labelled by W are relevant in the determination of hadron masses or the heavy quark potential. Once again, one finds an impressive agreement.

3. VELOCITY OF SOUND IN LATTICE GAUGE THEORIES

A popular approach to obtain a detailed space-time picture of the quark-gluon plasma produced in the relativistic heavy ion collisions is to employ the equations of relativistic hydrodynamics. One needs an equation of state to solve these equations. It is therefore of some interest to know the velocity of sound in the quark-gluon "fluid" in the non-perturbative region around the phase transition. Since $V_s^2 = (\partial P/\partial \varepsilon)_S$, one can use the lattice approach to obtain it. Unfortunately both ε and P are hard to obtain since both are dominated by two terms of about the same magnitude but opposite sign. It turns out[14], however, that one can relate it to another quantity which involves less of these uncertainties, and some preliminary results[14,15] have thus been obtained.

First, let us consider what one expects from simple considerations. Approximating the confined phase at low temperatures by a non-relativistic ideal gas of hadrons, it is simple to obtain $V_s^2 = \gamma\, T/m_H$ where m_H is the (effective) hadron mass. At large temperatures, one ought to have an ideal relativistic gas of quarks and gluons, and hence $V_s^2 \to 1/3$. In the absence of a phase transition, one expects thus the dashed line to represent V_s^2 as a function of T in fig. 6. At the phase transition point V_s^2 goes to zero, and the solid line in fig. 6 then would depict the behaviour of V_s^2.

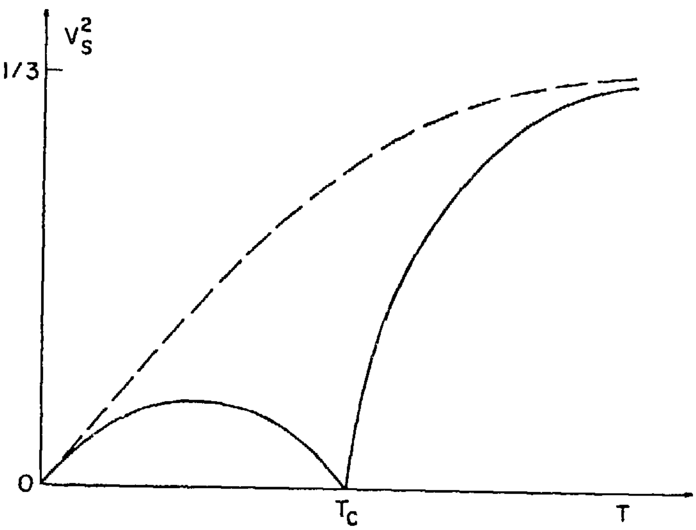

Fig. 6 A schematic representation of theoretical expectations for V_s^2 as a function of T.

Figure 7 shows the lattice evaluation of V_s^2 in the case of quenched QCD which is consistent with these naive expectations. Estimating the glueball mass from the low temperature relation above, one obtains m_G = 900 MeV which is certainly in the right ballpark. This calculation has now been performed with the dynamical fermions, and one again

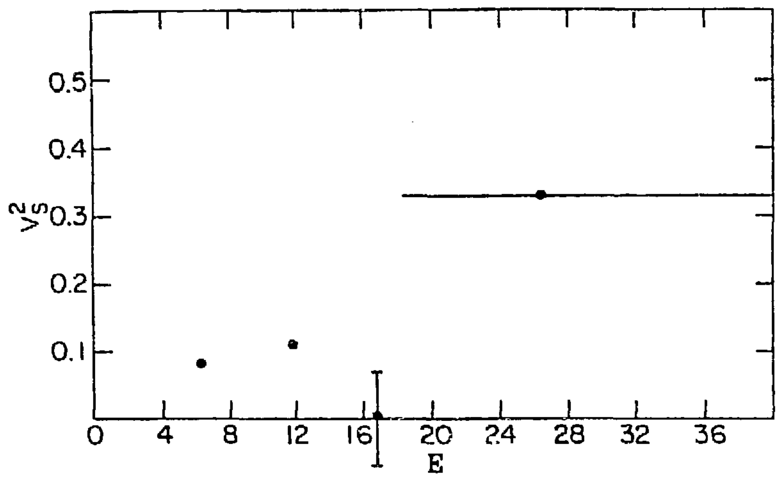

Fig. 7 The velocity of sound squared versus ε for the quenched QCD on an $8^3 \times 4$ lattice.

obtains a similar picture. Since the effective m_H is then expected to decrease, one should see the height of the maximum in the confined phase increase appreciably, which is what one finds in the Monte Carlo simulations[15)].

4. CONCLUSIONS

While we are still rather far away from obtaining the phase diagram in fig. 1 completely, especially the critical (end) points in the diagram, I feel rather optimistic that it will soon be done. We now have good approximation schemes to include the fermion determinant, which do satisfy some necessary checks. In particular, the results obtained by using pseudo-fermion method agree with those obtained by other methods, including an exact one. One has now begun to obtain quantities of phenomenological interest, such as the velocity of sound, using the lattice approach and the first set of results in this area appear quite encouraging.

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