Quark-hadron phase transition, QCD lattice calculations, and inhomogeneous big-bang nucleosynthesis

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We review recent lattice QCD results for the surface tension at the finite temperature quark-hadron phase transition and discuss their implications on the possible scale of inhomogeneities. In the quenched approximation the average distance between nucleating centers is smaller than the diffusion length of a proton, so that inhomogeneities are washed out by the time nucleosynthesis sets in. At present lattice results are inconclusive when dynamical fermions are included.

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I. INTRODUCTION

The density of luminous matter is $\Omega_L \sim 0.01$ (to within a factor of 2) and the density of clustered matter needed to account for the stability of galaxies or large-scale motions is $\Omega_G \sim 0.1 - 0.2$. Also, inflation predicts that $\Omega \sim \Omega_c = 1$, where Ω_c is the critical density for closure (Ω is the ratio of the present density to the critical density of the Universe). However, standard (homogeneous density) big-bang nucleosynthesis (BBN) calculations constrain the ratio of the present baryon density to Ω_c by $0.01 \leq \Omega_B \leq 0.09$ [1] (where uncertainties in the value of the Hubble parameter are included). While the value of Ω_B is consistent with Ω_G, if $\Omega \sim 1$ then the majority of matter in the Universe is nonbaryonic [consisting of, for example, axions, weakly interacting massive particles (WIMPS), massive neutrinos, etc.].

Recently the physics of the quark-hadron phase transition has been of much interest (cf. Reeves [2] and references therein). Of particular interest, from an astrophysical point of view, is the suggestion that (large) baryon density fluctuations are formed by QCD phase transitions, which occur in the early Universe [3], that will then affect BBN calculations [4]. In particular, initial calculations indicated that the upper bound on Ω_B from BBN might be relaxed and it was suggested that $\Omega_B \sim 1$ might be reconciled with observations [4]. We shall discuss inhomogeneous BBN in Sec. II.

However, many parameters of the quark-hadron phase transition are poorly known, and extensive QCD calculations on networks are necessary to determine the affects of inhomogeneous BBN more accurately. In Sec. III recent results from QCD lattice calculations will be reviewed. The consequences for BBN and the constraints on Ω_B will be briefly discussed in the concluding section.

II. PRIMORDIAL NUCLEOSYNTHESIS

The cosmological implications of the quark-hadron phase transition arises from the fact that it may induce baryon density inhomogeneities in the cosmic fluid, thereby producing inhomogeneities in the ratio of neutrons to protons, which then modify the abundances of the light elements obtained in the standard (homogeneous) BBN calculations. Larger values of Ω_B than in the baryon-homogeneous cosmologies are allowed, since in both proton-rich and neutron-rich regions the burning of neutrons and protons through D up to ^{4}He is less efficient (for larger baryon densities), and at later times (when sufficient neutrons have decayed) the temperature is lower and the subsequent burning of D is less efficient (than in the homogeneous case in both cases) resulting in relatively less ^{4}He being made in both neutron- and proton-rich regions but relatively greater amounts of D (and other heavier elements) being made in the neutron-rich regions.

Assuming that the phase transition is first-order, the new phase is not reached immediately; the system is cooled through the critical temperature T_c , but overcooling occurs in which fluctuations create small volumes of the new phase [5]. The nucleated bubbles of the hadronic phase then expand in the quark-gluon phase with the velocity of light in the quark-gluon plasma $v_s = 1/\sqrt{3}$. The shock wave will then reheat the plasma, so that no further nucleation occurs. The scale of the inhomogeneities produced at the quark-hadron phase transition within this simple bubble nucleation scenario is given by the mean separation of the nucleating centers l. Assuming that the phase transition occurs within thermodynamic equilibrium, the mean distance between nucleating centers has been estimated by Meyer *et al.* [6] to be (in terms of the inverse Hubble time H)

$$l \times H \approx 4.38 \frac{(0.4)^3\sqrt{3}}{32\pi} \left(\frac{\alpha}{T_c^3}\right)^{3/2} \left(\frac{L}{T_c^4}\right)^{-1}, \quad (1)$$

which depends on the QCD parameters L (the latent heat) and α (the surface tension, which is the surface energy density of the hadronized bubbles). With the inclusion of the quark degrees of freedom the temperature-dependent Hubble time was estimated to be [7]

$$H^{-1} = \frac{3}{\sqrt{164\pi^3}} \frac{M_{\rm Pl}}{T^2}, \quad (2)$$

with the Planck mass $M_{\rm Pl} = 2 \times 10^{19}$ GeV, so that the scale of inhomogeneities becomes

$$l \approx 8 \times 10^5 m \left(\frac{\alpha}{T_c^3}\right)^{3/2} \left(\frac{L}{T_c^4}\right)^{-1} [T_c/(\text{MeV})]^{-2}. \quad (3)$$

QCD estimates indicate that $T_c = 200 \pm 50$ MeV in the quenched approximation [8] and $T_c = 80 \pm 20$ MeV with four flavors of light quarks [8]. Estimates for l have been discussed by various authors [6,9], although within the uncertainties of the QCD parameters in the original calculations l could range, in principle, from zero to relatively large values. Better estimates for l must therefore come from detailed QCD lattice calculations.

The Universe cools from the quark-hadron phase transition at T_c until the time of BBN at T_N ($t_N \sim 1$ sec), by which time antimatter has disappeared. Before t_N the neutron-to-proton ratio is governed by weak interactions (and given by the Boltzmann formula), but for $t > 1$ sec the weak processes are no longer in thermal equilibrium. Neutrons diffuse from high-baryon-density phases to low-density phases, changing both their density and their neutron-to-proton ratio, so that by T_N high-density proton-rich regions and lower-density neutron-rich regions would exist, thereby affecting nucleosynthetic yields [4]. The extent of neutron diffusion is a function of l (and the fractional volume of the high-density phase, f_v). The smaller the value of l the less the effect of inhomogeneities, and so for significant changes to nucleosynthetic yields a large value of l is necessary. For example, within a typical model one would need an l in the range of $l \sim 5 - 150$ m to get $\Omega \geq 0.15$ (cf. [6]).

Many authors [4,6,9] have estimated numerically the nucleosynthetic yields based on various physical models and approximations (e.g., 2–64 zone models, whether or not neutron and proton diffusion is taken into account before BBN, and so on) and various values for the QCD parameters, particularly to determine whether the observed abundance of the light nuclides D, ^{3}He, ^{4}He, and ^{7}Li [1] can be reconciled with a critical baryon density $\Omega_B \sim 1$. Although the various studies are in good agreement with each other, the ignorance of the exact values of many QCD parameters lead to corresponding uncertainties in the results.

III. CALCULATIONS FROM LATTICE QCD

Because of the lack of appropriate models and/or experimental knowledge of the quark-hadron transition, thermodynamic parameters of the transition have to be calculated directly from the underlying theory, which means that one has to consider QCD at the transition temperature. At very high physical temperature QCD can be treated by perturbation theory because the separation of quarks will be small and the effective coupling between quarks and gluons will be governed by the asymptotic freedom of QCD. However, as has been pointed out by Linde [10], perturbation theory will break down at $O(g^6)$ (here g is the QCD coupling constant) due to the infrared problem of the massless Yang-Mills theory. Therefore, nonperturbative calculational techniques such as Monte Carlo simulations of the latticized theory are the only known way to get reliable information on the hadron transition.

After discretizing the QCD action on a four-dimensional hypercubic lattice, the theory can be quantized due to Feynman's path integral formalism, where the lattice cutoff $\Lambda = \frac{1}{a}$ (a is the lattice spacing) regularizes the infrared singularities [11,12]. To remove the cutoff, the continuum limit has to be performed at a second-order phase transition of the equivalent statistical mechanics model, where the relevant scale on the lattice, the correlation length, diverges. In practice an ansatz of asymptotic scaling in the observables under consideration is enough to extrapolate reliably with the renormalization group to the continuum limit. A general method to calculate expectation values of the latticized theory is the numerical Monte Carlo simulation method. There, in addition to the discretization, the space-time dimensions have to be restricted to a finite volume. The simulations therefore should be done in a parameter range with a large correlation length and on large enough lattices compared to the correlation length, so that finite-size effects are under control.

Finite physical temperatures can be taken into account (as in perturbation theory) by taking finite lattice extensions in the time direction. In finite-temperature lattice calculations, however, the number of lattice points N_t in the time direction have to be large enough to be in the asymptotic scaling region of the observables under investigation. Whether this can be realized is mainly a question of the available computer time and how fast the scaling of the observables sets in.

Monte Carlo simulations of lattice QCD have established a phase transition between a chiral symmetric quark-gluon plasma phase at high physical temperatures with no color confinement and the hadron phase at low temperatures where quarks are confined in hadrons and the chiral symmetry is broken spontaneously as proposed by McLerran and Svetitzky [13] (see [12] for details). The lattice calculations have established a first-order phase transition in the quenched approximation, where the quarks are infinitely heavy and therefore only the gauge degrees of freedom have to be treated dynamically. Also, in the case of at least four flavors of dynamical light fermions lattice results indicate a weak first-order phase transition [8]. Therefore, there exists the possibility that hadronization takes place through nucleation of hadronic droplets in a supercooled plasma. In addition, since nucleation is a dynamical process it is governed by equilibrium parameters of the transition such as the surface free energy and the latent heat, which can be calculated in lattice QCD.

A. The interface tension in quenched QCD

The interface tension is given by the free energy of the interface between coexisting phases normalized to the area of the interface [14], $\alpha = \frac{F}{A}$, and is usually given in units of the critical temperature T_c. The free energy of the interface accounts only for the small difference of the free energies of bulk phases. Therefore, the interface tension is difficult to calculate in Monte Carlo simulations. Reliable results have been derived until now only in the quenched approximation, on which we will concentrate in this subsection.

Several methods have been used over the past 3 yr to extract the surface tension in quenched QCD. Most of the results are obtained on lattices with the small time extent $N_t = 2$, but the first results on $N_t = 4$ and $N_t = 6$ lattices are now being quoted. We have collected recent results for the surface tension together in Table I.

Kajantie *et al.* [15] have used a surface tension operator derived from the partition function by derivation of the partition function with respect to the area of the interface. In this method some parameters have to be estimated by perturbative methods and thus reliability can be questioned at the transition temperature. Potvin *et al.* [16,17] have used integral methods, where the average action is integrated in the space of the gauge coupling parameter. The interface is thereby generated by a temperature difference of two parts of the lattice or by applying different external fields to the two sublattices. The main difficulty in this principally exact method is the extrapolation of the numerical results to the zero difference limit of the temperatures or the external fields of the sublattices. This method has been recently used to calculate the surface tension in simulations of $N_t = 4$ lattices [17]. An elegant transfermatrix method has been applied to quenched QCD in [18]. In this method, finite-size effects of the spectrum of states are used to extract the surface tension. With this method very precise results have been obtained for $N_t = 2$ lattices; however, due to the lack of global updating algorithms it has not been applied to lattices with larger time extents.

The most recent results have been derived by an histogram method proposed some time ago by Binder [19], where finite-size effects in histograms of different operators due to interface effects are used to calculate the surface tension. The reason for a renaissance of this method is that the recently proposed multicanonical algorithm produces more statistics of interface configurations and that the analysis method is easy to apply to existing high statistical data of the QCDPAX Collaboration. Grossmann and Laursen [20] have analyzed multicanonical data on $N_t = 2$ lattices with finite-size formulas, where fluctuations of the interface have been taken into account by a capillary wave model and interfacial interactions have been reduced by the use of rectangular lattices. These authors have also analyzed $N_t = 4$ data of the QCDPAX Collaboration [21] with the capillary wave improved finite-size formulas. Preliminary analysis of the QCDPAX data by Iwasaki *et al.* [22] lead to preliminary estimates for $N_t = 6$ data also.

Although the scattering of the $N_t = 2$ results show how difficult the extraction of the surface tension is, the data indicate at least the order of magnitude of α to be expected at the finite-temperature phase transition of gluonic matter. The decrease of the values with increasing N_t indicate that the region of asymptotic scaling has not yet been reached.

Lattice results for the latent heat at the finite-temperature phase transition in quenched QCD can be estimated from [21] to be $L/T_c^4 = 3.10(6)$ on the $N_t = 4$ lattice and $L/T_c^4 = 1.98(5)$ on the $N_t = 6$ lattice. With the largest value of the surface tension on $N_t = 2$ lattices together with the lowest estimate of 150 MeV for the transition temperature and $L/T_c^4 = 1.98$ for the latent heat, we obtain an estimate for an upper bound on the average distance between nucleating centers of $l \approx 0.93$ m. However, with the estimate of $\alpha/T_c^3 = 0.025$ on $N_t = 4$ lattices, which is closer to the continuum limit, and with the same values of L and T_c as used above, we obtain the more realistic estimate of $l \approx 0.07$ m. Therefore, the average distance of nucleating centers is likely to be smaller than the diffusion length of protons (~ 0.5 m) and neutrons (~ 30 m), so that inhomogeneities created at the finite-temperature phase transition of pure gluonic matter are washed out by the time primordial nucleosynthesis sets in. These conclusions are consistent with those of Ref. [7].

Also, a large fraction of supercooling seems to be unlikely in quenched QCD. At the finite-temperature phase transition of the pure SU(3) gauge theory three different deconfinement phases can coexist with the confinement phase, because the $Z(3)$ center symmetry of the SU(3) gauge symmetry is spontaneously broken at $T > T_c$ [13]. As pointed out in [18] it is then most likely that a layer of the confined phase will completely wet the network of interfaces between deconfinement phases, which is rather different to the bubble nucleation scenario. However, this is only true in pure gluonic matter.

TABLE I. The surface tension in quenched QCD calculated with different methods on lattices with different time extent N_t.

Refs.	α/T_c^3 $N_t = 2$	$N_t = 4$	$N_t = 6$
[15]	0.08(2)		
[16,17]	0.12(2)	0.027(4)	
[18]	0.139(4)		
[20]	0.092(4)	0.025(4)	
[22]		0.029(2)	0.022(4)

B. The influence of dynamical fermions on the hadronization

Although the quenched approximation of QCD can give a rough idea of the behavior of strongly interacting matter, the influence of the fermion dynamics has to be taken into account in a real world QCD calculation. Unfortunately the simulation of dynamical fermions is not only beset with technical difficulties but is also very consuming of computer time, so that these studies have until now not reached the quality of quenched simulations.

Although it has not yet been demonstrated that there exists a finite-temperature phase transition with a realistic fermion spectrum (see [23] for a discussion), it is now widely accepted that in full QCD a weak first-order phase transition also exists with at least two light and one not-too-heavy quark flavors. The transition temperature is, however, flavor dependent and drops from the above quoted 200 MeV in the pure gauge theory to $T_c \approx 100$ MeV for four degenerate quark flavors [8]. The quark degrees of freedom also breaks the $Z(3)$ symmetry of the pure SU(3) Lagrangian, so that complete wetting will no longer inhibit supercooling. It has been estimated by Ignatius *et al.* [24] that a metastable $Z(3)$ phase will convert into a stable one by a temperature of $T \approx 10$ TeV.

Lattice results for the surface tension with dynamical fermions are not yet available. The only simulations of Markum *et al.* [25] lead to an inconsistent negative value of the surface tension and show only that it seems not to be considerably larger than in the quenched approximation. On the other hand, the transition is weaker than in the quenched approximation leading to a larger correlation length and a smaller latent heat. Together with the reduction of the critical temperature, these factors might lead to a larger average separation of nucleating centers as indicated by Eq. (3). Whether these would result in significant inhomogeneities by the time primordial nucleosynthesis sets in is unclear, however. More calculations on the lattice with dynamical fermions need to be done.

IV. CONCLUSIONS

Original studies, based on a simple two-zone model in which back diffusion of neutrons are neglected during BBN suggested that an $\Omega \sim 1$ model might be consistent with light element observations. The importance of neutron diffusion during BBN was emphasized [4], leading to numerical codes treating nucleosynthesis and diffusion simultaneously [9,26]. Neutron diffusion also leads to an overestimation of the neutron number density in the low-density region in a simple two-zone model, resulting in more realistic multizone calculations [9]. These calculations led to upper limits on Ω_B lower than the critical value. Finally, a large nuclear reaction network including very neutron-rich nuclei and heavy elements were included in the multizone calculations [26] (using various values of the QCD parameters), leading to a considerably lower upper limit on Ω_B and ensuring that an $\Omega_B \sim 1$ model is inconsistent with the observed abundances of the light elements even if the Universe is inhomogeneous.

Recently [27] the yields of primordial light elements from baryon-inhomogeneous BBN have been recalibrated using new "improved" diffusion coefficients calculated from relativistic kinetic theory, with the result that the yields previously obtained using more crudely derived diffusion coefficients (e.g., Refs. [4,6,9]) remain virtually unchanged. The various results are essentially consistent and in basic agreement with Reeves' [2] quoted limits of $0.01 < \Omega_B < 0.2$ (a range that is somewhat larger than that in the standard BBN scenario) based on the then allowable ranges of the QCD parameters.

To date there are no lattice calculations available with a realistic fermion spectrum close to the continuum limit, so that definitive conclusions for the quark-hadron transition cannot be made yet. Further research in this field is necessary to get a better understanding of the phase transitions in the early Universe. However, in the models studied so far there is *no evidence at all* for a strong supercooling and a cosmologically relevant scale for the inhomogeneities created at the quark-hadron transition.

The most detailed studies of the surface tension have been done in the quenched approximation of QCD, where the fermion dynamics have been neglected. In this approximation only a small surface tension was found. Although the results are still not in the asymptotic scaling region close to the continuum limit, the trend is that for larger lattices even smaller values of the surface tension result, leading to scales of inhomogeneities which are irrelevant for primordial nucleosynthesis.

With dynamical fermions included no value for the surface tension has so far been extracted. However, the lattice calculation indicates that the phase transition is weaker than in the quenched approximation. A strong increase in the surface tension seems not to be likely, but the latent heat can drop significantly when dynamical quarks are considered. However, it has not been demonstrated yet that this, together with the decrease of the transition temperature, could lead to an increase in the scale of inhomogeneities, which would then affect primordial nucleosynthesis. Indeed, it has been argued that this possibility is unlikely [7].

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[1] M.S. Smith, L.H. Kawano, and R.A. Malaney, Astrophys. J. Suppl. **85**, 219 (1993); R.A. Malaney and G.J. Mathews, Phys. Rep. **229**, 145 (1993).

[2] H. Reeves, Phys. Rep. **201**, 335 (1990).

[3] E. Witten, Phys. Rev. D **30**, 272 (1984).

[4] J.H. Applegate and C. Hogan, Phys. Rev. D **31**, 3037 (1985); J.H. Applegate, C. Hogan, and R.J. Sherrer, Astrophys. J. **329**, 572 (1988); C.R. Alcock, G.M. Fuller, and G.J. Mathews, *ibid.* **320**, 439 (1987); R.A. Malaney and W.A. Fowler, *ibid.* **333**, 14 (1988); see also K. Jedamzik and G.M. Fuller, *ibid.* **423**, 33 (1994); K. Jedamzik, G.M. Fuller, and G.J. Mathews, *ibid.* **423**, 50 (1994).

[5] K. Kajantie and H. Kurki-Suonio, Phys. Rev. D **34**, 1719 (1986).

[6] B.S. Meyer, C.R. Alcock, G.J. Mathews, and G.M. Fuller, Phys. Rev. D **43**, 1079 (1991).

[7] B. Banerjee and R.V. Gavai, Phys. Lett. B **293**, 157 (1992).

[8] H. Satz, in *Proceedings of the Strasbourg Symposium on Quark-Hadron Phase Transition*, Strasbourg, 1985 (World Scientific, Singapore, in press); R.V. Gavai *et al.*,

Phys. Lett. B **241**, 567 (1990).

[9] H. Kurki-Suonio, Phys. Rev. D **37**, 2104 (1988); H. Kurki-Suonio, R.A. Matzner, K.A. Olive, and D.N. Schramm, Astrophys. J. **353**, 406 (1990); G.J. Mathews, B.S. Meyer, C.R. Alcock, and G.M. Fuller, *ibid.* **358**, 36 (1990); H. Reeves, J. Richer, K. Sato, and N. Terasawa, *ibid.* **355**, 18 (1990); K. Sato and N. Terasawa, Prog. Theor. Phys. **81**, 254 (1989); Phys. Rev. D **39**, 2893 (1989).

[10] A.D. Linde, Phys. Lett. **96B**, 289 (1980).

[11] K.G. Wilson, Phys. Rev. B **4**, 3184 (1971).

[12] H.J. Rothe, *Lattice Gauge Theory: An Introduction* (World Scientific, Singapore, 1992).

[13] L.D. McLerran and B. Svetitsky, Phys. Rev. D **24**, 450 (1981).

[14] L.D. Landau and E.M. Lifschitz, *Statistical Physics*, 3rd ed. (Pergamon, New York, 1980).

[15] K. Kajantie and L. Kärkkäinen, Phys. Lett. B **214**, 595 (1988); K. Kajantie, L. Kärkkäine, and K. Rummukainen, Nucl. Phys. **B333**, 100 (1990); **B357**, 693 (1991).

[16] J. Potvin and C. Rebbi, Phys. Rev. Lett. **62**, 3062 (1989); in *Lattice '89*, Proceedings of the International Symposium, Capri, Italy, edited by R. Petronzio *et al.* [Nucl. Phys. B (Proc. Suppl.) **17**, 223 (1990)]; S. Huang, J. Potvin, C. Rebbi, and S. Sanielevici, Phys. Rev. D **42**, 2863 (1990); Phys. Rev. D **43**, 2056(E) (1991).

[17] R. Brower, S. Huang, J. Potvin, and C. Rebbi, Phys. Rev. D **46**, 2703 (1992).

[18] B. Grossmann, M.L. Laursen, U.-J. Wiese, and T. Trappenberg, Nucl. Phys. **B397**, 431 (1993); T. Trappenberg, Int. J. Mod. Phys. C **3**, 947 (1992).

[19] K. Binder, Z. Phys. B **43**, 119 (1981); Phys. Rev. A **25**, 1699 (1982).

[20] B. Grossmann and M.L. Laursen, Nucl. Phys. **B408**, 637 (1993); see also B. Grossmann, M.L. Laursen, U.-J. Wiese, and T. Trappenberg, Phys. Lett. B **293**, 175 (1992); in *Lattice '92*, Proceedings of the International Symposium, Amsterdam, The Netherlands, edited by J. Smit and P. van Baal [Nucl. Phys. B (Proc. Suppl.) **30**, 869 (1993)].

[21] M. Fukugita, M. Okawa, and U. Ukawa, Phys. Rev. Lett. **63**, 1768 (1989); Nucl. Phys. **B337**, 181 (1989); Y. Iwasaki *et al.*, Phys. Rev. D **46**, 4657 (1992).

[22] L. Kärkkäinen (private communication); Y. Iwasaki, K. Kanaya, L. Kärkkäinen, and K. Rummukainen (unpublished).

[23] F.R. Brown *et al.*, Phys. Rev. Lett. **65**, 2491 (1990).

[24] J. Ignatius, K. Kajantie, and K. Rummukainen, Phys. Rev. Lett. **68**, 737 (1992).

[25] M. Hackel, M. Faber, H. Markum, and M. Müller, Phys. Rev. D **46**, 5648 (1992).

[26] K. Sato and N. Terasawa, Astrophys. J. Lett. **362**, L47 (1990); Phys. Scr. **T36** (1991).

[27] H. Kurki-Suonio *et al.*, Phys. Lett. B **289**, 221 (1992).