Structures of Metals (Pergamon, New York, 1964), Vol. 4.

[17]Assuming N = (number of valence *sd* electrons) − 1. (See Ref. 6.)

[18]L. Brewer and P. R. Wengert, Met. Trans. 4, 83 (1973).

[19]K. M. Myles, Trans. Met. Soc. 242, 1523 (1968).

[20]The relation between Miedema's *conceptual* approach and band theory is discussed by D. G. Pettifor and C. M. Varma, to be published.

[21]See, for example, the successful tight-binding explanation of the crystal structures of the transition-metal Laves phases by R. L. Johannes, R. Haydock, and V. Heine, Phys. Rev. Lett. 36, 372 (1976).

Cosmological Production of Baryons

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Departures from thermal equilibrium which are likely to occur in an expanding universe allow the production of an appreciable net baryon density by processes which violate baryon-number conservation. It is shown that the resulting baryon to entropy ratio can be calculated in terms of purely microscopic quantities.

It is an old idea[1] that the observed excess of matter over antimatter in our universe may have arisen from physical processes which violate the conservation of baryon number. Of course, the rates of baryon-nonconserving processes like proton decay are very small at ordinary energies, but if the slowness of these processes is due to the large mass of intermediate vector of scalar "X bosons" which mediate baryon nonconservation, then at very high temperatures with $kT \simeq m_X$, the baryon-nonconserving processes would have rates comparable with those of other processes. However, even if there are reactions which do not conserve C, CP, T, and baryon number, and even if these reactions proceed faster than the expansion of the universe, there can be no cosmological baryon production once the cosmic distribution functions take their equilibrium form, until the expansion of the universe has had a chance to pull these distribution functions out of equilibrium. This can easily be seen from the generalized Uehling-Uhlenbeck equation[2] for a homogeneous isotropic gas,

$$\begin{aligned} dn(p_1)/dt = \sum_{kl} \int dp_2 \cdots dp_k dp_1' \cdots dp_l' \\ \times \{\Gamma(p_1' \cdots p_l' \to p_1 \cdots p_k) n(p_1') \cdots n(p_l')[1 \mp n(p_1)] \cdots [1 \pm n(p_k)] \\ - \Gamma(p_1 \cdots p_k \to p_1' \cdots p_l') n(p_1) \cdots n(p_k)[1 \pm n(p_1')] \cdots [1 \pm n(p_l')]\}, \end{aligned} \tag{1}$$

where n is the single-particle density in phase space; p labels the three-momentum and any other particle quantum numbers, including baryon number; and Γ is a rate constant, equal, for $k = l = 2$, to the cross section times the initial relative velocity. The factors $1 \pm n(p)$ represent the effect of stimulated emission or Pauli suppression for bosons or fermions, respectively. If at any instant, $n(p)$ takes its equilibrium form, then $n(p)/[1 \pm n(p)]$ is an exponential of a linear combination of the energy and any other conserved quantities; so for any allowed reaction with $\Gamma \neq 0$, we have

$$n(p_1') \cdots n(p_l')[1 \pm n(p_1)] \cdots [1 \pm n(p_k)] = n(p_1) \cdots n(p_k)[1 \pm n(p_1')] \cdots [1 \pm n(p_l')]. \tag{2}$$

Under T invariance, Γ would be symmetric, and the two terms in the integrand of Eq. (1) would cancel. But even without T invariance, unitarity always gives

$$0 = \sum_l \int dp_1' \cdots dp_l' [1 \pm n(p_1')] \cdots [1 \pm n(p_l')][\Gamma(p_1 \cdots p_k \to p_1' \cdots p_l') - \Gamma(p_1' \cdots p_l' \to p_1 \cdots p_k)], \tag{3}$$

so that the p' integrals in (1) still cancel.[3] For an expanding gas there are also terms in Eq. (1) which represent the effects of dilution and red shift, and these terms can produce departures from equilibrium, but of course they have no direct effect on the baryon number per co-moving volume.

This note will describe a mechanism for production of a cosmic baryon excess, based on the departures from thermal equilibrium which are likely to have occurred in the early universe. It is assumed here that all particles have masses below (though not necessarily far below) the Planck mass $m_P \equiv G^{-1/2} = 1.22\times 10^{19}$ GeV. For simplicity, it will be assumed that the only superheavy particles with masses above 1 TeV or so are the X bosons which mediate baryon nonconservation; however, it would not be difficult to incorporate superheavy fermions with masses $m \simeq m_X$ in these considerations. Aside from gravitation itself, all interactions are supposed to have dimensionless coupling constants. For the interaction of X bosons with fermions, this coupling is denoted g_X. Finally, it will also be assumed that $\alpha_X{}^2 N \ll 1$, where $\alpha_X = g_X{}^2/4\pi$, and N is the number of helicity states of all particle species. Under these assumptions, we can trace the following chain of events[4]:

(1) At very early times, when $kT \approx m_P$, the interactions of gravitons were so strong that thermal equilibrium distributions would have been established at least approximately for all particle species; for instance, by graviton-graviton collisions.[5] (Of course, we do not know how to calculate detailed reaction rates at these times, but we can be confident that gravitational interactions were strong, because this is indicated by lowest-order calculations, and it is only the strength of the interactions that invalidates such calculations.) If gravitational interactions conserved baryon number at $kT \gtrsim m_P$, then the universe could have begun with a nonvanishing value for the baryonic chemical potential; I assume here that this is not the case.

(2) As kT fell below m_P, gravitational interactions became ineffective. The rates for X-boson decay, baryon-nonconserving collisions (or, for $kT \gtrsim m_X$, all collisions) and cosmic expansion may be estimated as[6]

$$\Gamma_X \simeq \alpha_X m_X{}^2 N/[(kT)^2 + m_X{}^2]^{1/2}, \tag{4}$$

$$\Gamma_C \simeq \alpha_X{}^2 (kT)^5 N/[(kT)^2 + m_X{}^2]^2, \tag{5}$$

$$\dot{R}/R \equiv H = 1.66(kT)^2 N^{1/2}/m_P. \tag{6}$$

With $\alpha_X{}^2 N \ll 1$ and $m_X < m_P$, both Γ_X and Γ_C were much less than H at $kT \simeq m_P$. However, as long as kT remained above all particle masses, the expansion preserved the equilibrium form of all particle distributions, with red-shifted temperature $T \propto 1/R$.

(3) The X bosons began to decay when $\Gamma_X \simeq H$. If at this time $kT > m_X$, the collisions of the decay products with each other or with ambient particles would have rapidly recreated the X bosons through the inverse of the decay process, thus reestablishing equilibrium distributions. In order to produce any appreciable baryon excess, it is necessary that $kT \lesssim m_X$ when $\Gamma_X \simeq H$, so that the Boltzmann factor $\exp(-m_X/kT)$ could block inverse decay. Equation (4) then gives $\Gamma_X \simeq H$ at a temperature

$$kT_D \simeq (N^{1/2}\alpha_X m_X m_P)^{1/2}, \tag{7}$$

so that the condition $m_X \gtrsim kT_D$ yields a lower bound on m_X

$$m_X \gtrsim N^{1/2}\alpha_X m_P. \tag{8}$$

(For gauge bosons we expect $\alpha_X \simeq \alpha$, so (8) requires $m_X \gtrsim 10^{17} N^{1/2}$ GeV, while for Higgs bosons α_X is presumably in the range of 10^{-4} to 10^{-6}, and the lower bound on m_X would be of order 10^{13} to $10^{15} N^{1/2}$ GeV.) Note also that (5), (6), and (8) give $\Gamma_C \ll H$ for all temperatures. This justifies the neglect of X-boson production or annihilation in reactions other than X decay and its inverse, and insures that any baryon excess produced when the X bosons decayed would have survived to the present time.

Before the X bosons decayed, at temperatures just above T_D, their number density was $n_{XD} = \zeta(3)(kT_D)^3 N_X/\pi^2$, where N_X is the total number of X (and $\bar{X}$) spin states. Also, the total entropy density of all other particles was $s_D = 4\pi^2 k(kT_D)^3 \times N/45$, with N now understood to include factors of 7/8 for fermion spin states. If the mean net baryon number produced in X or $\bar{X}$ decay is ΔB per decay, and if one can ignore the entropy released in X-boson decay, then the ratio of baryon number to entropy after the X bosons decayed was

$$kn_B/s = kn_{XD}\Delta B/s_D = 45\zeta(3)(N_X/N)\Delta B/4\pi^4. \tag{9}$$

If one assumes the subsequent expansion to be adiabatic, both n_B and s would have scaled as R^{-3}, so that Eq. (9) would give the ratio of baryon number to entropy of the present universe.

Strictly speaking, one should take into account the entropy contributed by the X-boson decay products when they finally thermalize. This increases the energy density by a factor

$$\lambda = 1 + \frac{m_X n_{XD}}{\pi^2 (kT_D)^4 N/30} = 1 + \frac{30\zeta(3) N_X m_X}{\pi^4 N k T_D}$$
$$\simeq 1 + (N_X/N)(m_X/N^{1/2}\alpha_X m_P)^{1/2}, \tag{10}$$

and so decreases the ratio of baryon number to entropy by a factor $\lambda^{-3/4}$. However, this effect can be ignored if $N \gg N_X$.

The crucial quantity ΔB in Eq. (9) can be determined from the branching ratios for X-boson decay. For instance, suppose that an X boson decays into two channels with baryon numbers B_1 and B_2 and branching ratios r and $1-r$. The antiparticle will then decay into channels with baryon numbers $-B_1$ and $-B_2$, with the same total rate, but with different branching ratios $\bar{r}$ and $1-\bar{r}$. The mean net baryon number produced when X or $\bar{X}$ decays is then

$$\Delta B = \tfrac{1}{2}[rB_1 + (1-r)B_2 - \bar{r}B_1 - (1-\bar{r})B_2]$$
$$= \tfrac{1}{2}(r-\bar{r})(B_1 - B_2). \tag{11}$$

CPT invariance gives $r=\bar{r}$ in the Born approximation. If the leading contribution to $r-\bar{r}$ arises from an interference of graphs with a total of l loops, then one expects $r-\bar{r}$ to be of order $\epsilon(\alpha_X/2\pi)^l$, where ϵ is whatever small angle characterizes CP violation. Of course, to be more definite, a detailed model of baryon nonconservation is needed. However, in any given model, Eqs. (9) and (11) give a precise prediction for the ratio of baryon number to entropy kn_B/s, which may be compared with the observed value[7] 10^{-8} to 10^{-10}.

The above discussion has assumed a homogeneous isotropic expansion, in which the entropy stays fixed except for the small effects of bulk viscosity.[7] However, it is also possible to deal with gross departures from thermal equilibrium that might be produced by cosmic inhomogeneities. As any part of the universe relaxes toward equilibrium, the rate at which its entropy increases will be proportional to the difference between the entropy and its maximum value $S_{\max}$. Baryon production vanishes in the equilibrium configuration with $S=S_{\max}$, so the rate of increase of baryon number will also be proportional to $S-S_{\max}$. Thus, the ratio of the baryon-number production to the entropy production will be given by the ratio of the coefficients of $S-S_{\max}$ in dB/dt and dS/dt, and independent of the amount of the initial departure from thermal equilibrium. If most of the entropy and baryon number of the universe were created in this way, then it is this ratio that would have to be compared with the experimental value of 10^{-8} to 10^{-10}.

Note added.—(1) Any X bosons which can mediate baryon-nonconserving reactions are necessarily much heavier than the Z^0 or $W^{\pm}$; so their interactions can be analyzed using the weak and electromagnetic gauge group $SU(2)\otimes U(1)$ as well as the strong gauge group $SU(3)$ as if they were all unbroken symmetries. In this way one finds in general there are just three kinds of bosons which can couple to channels consisting of a pair of ordinary fermions, with these channels not all having equal baryon numbers: They are an SU(3) triplet SU(2) singlet X_S of scalar bosons with charge $-\frac{1}{3}$; an SU(3) triplet SU(2) doublet X_V of vector bosons with charges $-\frac{1}{3}$, $-\frac{4}{3}$; and an SU(3) triplet SU(2) doublet of X_V' of vector bosons with charges $\frac{2}{3}$, $-\frac{1}{3}$; plus their corresponding SU(3)-$\bar{3}$ antibosons. For all these bosons, the decay channels are $X\to gl, \overline{qq}$ and $\bar{X}\to \overline{gl}, qq$, with q and l denoting general quarks and leptons. Hence $B_1=+\frac{1}{3}$ and $B_2=-\frac{2}{3}$ in Eq. (11). This analysis incidentally shows that lowest-order baryon-number–nonconserving interactions always conserve baryon number *minus* lepton number, so nucleons may decay in lowest order into antileptons, but not leptons.

(2) Detailed calculations have been carried out with Nanopoulos[8] to estimate the difference in the branching ratios $r,\bar{r}$ for $X\to gl$ and $X\to \overline{gl}$ that arises from the interference of tree graphs with one-loop graphs. In general, a difference between r and $\bar{r}$ could arise from one-loop graphs in which a scalar or vector boson is exchanged between the final fermions, even when all fermion masses are negligible compared with the temperature, provided that CP invariance is violated in the Lagrangian, or is already spontaneously broken at these high temperatures. In various grand unified theories there are relations among the various couplings of Higgs or gauge bosons to fermions, which eliminate most of these contributions to $r-\bar{r}$. However, there will still be a contribution to $r-\bar{r}$ in X_S decay from the exchange of X_S bosons of different species. Since Higgs-boson exchange is naturally weaker than $W^{\pm}$ or Z^0 exchange at ordinary energies, it is possible that the CP-invariance violation is maximal in the coupling of fermions to Higgs bosons, including X_S bosons. In this case, $r-\bar{r}$ is of order $\alpha_H/2\pi \approx 10^{-6}$. With $B_1-B_2=1$ and $N_X/N\approx 10^{-2}$, Eqs. (11) and (9) then give a ratio of baryon number to entropy of order 10^{-9}.

(3) The masses of superheavy gauge bosons were estimated in grand unified gauge theories to be of order 10^{16} GeV, by Georgi, Quinn, and Weinberg.[9] (As shown there, this estimate applies for arbitrary simple grand unified gauge groups, under reasonable general assumptions on the spectrum of fermions. The same assumptions yielded a Z^0-γ mixing angle with $\sin^2\theta \simeq 0.2$.) Presumably the Higgs-boson masses are of the same order. Decay and inverse-decay processes arising from the gauge coupling of vec-

tor bosons to each other and to Higgs bosons and fermions will bring all these particles into thermal equilibrium at a temperature given by Eq. (7) [with $N \approx 100$, $\alpha_X \approx 10^{-2}$, $m_X \approx 10^{16}$ GeV] as of order 10^{17} GeV. Hence there is no need to invoke gravitational processes at the Planck temperature to establish initial equilibrium distributions, and any preexisting baryon imbalance would have been wiped out at $kT \simeq 10^{17}$ GeV. As the temperature dropped below 10^{16} GeV all superheavy gauge bosons and some of the superheavy Higgs bosons would have disappeared. However, if the lightest superheavy bosons happen to be X_S bosons, then these bosons would have survived as the temperature fell below their mass, because the only decay channels open then would have been two-fermion states, and $\alpha_X \ll \alpha$ for Higgs-fermion couplings. The decay of these scalar bosons when the temperature finally dropped to $kT_D \approx 10^{14}$ GeV $\ll m(X_S)$ would then produce the baryon excess estimated in Note (2).

I am grateful for valuable conversations with J. Ellis, D. Nanopoulos, A. Salam, L. Susskind, F. Wilczek, C. N. Yang, and M. Yoshimura.

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[1]For one example, see S. Weinberg, in *Lectures on Particles and Fields*, edited by S. Deser and K. Ford (Prentice-Hall, Englewood Cliffs, N. J., 1964), p. 482. The subject has been considered in recent papers by M. Yoshimura, Phys. Rev. Lett. 41, 381 (1978); S. Dimopoulos and L. Susskind, Phys. Rev. D 18, 4500 (1978); B. Toussaint, S. B. Treiman, F. Wilczek, and A. Zee, Phys. Rev. D 19, 1036 (1979). After this work was completed I also became aware of a discussion by A. Yu. Ignatiev, N. V. Krosnikov, V. A. Kuzmin, and A. N. Tavkhelidze, Phys. Lett. 76B, 436 (1978); and new reports have appeared by S. Dimopoulos and L. Susskind, Stanford University Report No. ITP-616, (to be published), and J. Ellis, M. K. Gaillard, and D. V. Nanopoulos, CERN Report No. Ref. TH-2596 (to be published). The approach followed and the conclusions reached here differ from those of Yoshimura, for reasons indicated below; from Ignatiev *et al.* because they adopt a different picture of baryon nonconservation (without superheavy X bosons); and from Ellis, Gaillard, and Nanopoulos, for reasons indicated in their erratum (to be published). The assumptions and general approach followed here is similar in many respects to that of Dimopoulos and Susskind and Section 2 of Toussaint *et al.* A major difference is that by following the baryon production scenario in detail, a formula is obtained here, Eq. (9), which gives the ratio of baryon number to entropy in terms of purely microscopic quantities.

[2]E. A. Uehling and G. E. Uhlenbeck, Phys. Rev. 43, 552 (1933).

[3]A very general version of this argument in the context of the "master" equation was given about a decade ago in an unpublished work of C. N. Yang and C. P. Yang. Also see A. Aharony, in *Modern Developments in Thermodynamics* (Wiley, New York, 1973), pp. 95–114, and references cited therein. I first learned of this argument for the special case of massless distinguishable particles from the original version of the paper of Toussaint *et al.*, Ref. 1. For indistinguishable particles, the factors $1 \pm n(p')$ in Eq. (3) arise from the effects of the ambient bosons or fermions on identical virtual particles in these reactions; in old-fashioned perturbation theory, the ambient particles generate a product of $1 \pm n$ factors for each intermediate state. These factors were omitted in the unitarity relation as given by Aharony, so that it was not possible in his paper to see how the Uehling-Uhlenbeck equation yields a vanishing rate of change for equilibrium distributions. Equation (3) shows that the physical processes considered by Yoshimura (Ref. 1) cannot produce an appreciable net baryon density if all relevant channels are taken into account, as pointed out by Toussaint *et al.*, Ref. 1.

[4]This scenario was developed in the course of conversations with F. Wilczek, and is also discussed in Section 2 of Toussaint *et al.*, Ref. 1. I am very grateful to F. Wilczek for numerous discussions of these ideas.

[5]Horizon effects may prevent complete establishment of thermal equilibrium at $kT \simeq m_P$; G. Steigman, private communication.

[6]It we keep track of all factors of 2π from Fourier integrals and 4π from solid-angle integrals, but set all other numerical constants equal to unity, then factors 4 and $8/\pi$ would appear in the right-hand sides of Eqs. (4) and (5), respectively. The powers of $m_X^2/[(kT)^2 + m_X^2]$ in Eqs. (4) and (5) are inserted to take account of time dilation and the virtual X-boson propagator, respectively.

[7]See, e.g., S. Weinberg, *Gravitation and Cosmology–Principles and Applications of the General Theory of Relativity* (Wiley, New York, 1972), Chap. 15.

[8]S. Weinberg and D. V. Nanopoulos, to be published.

[9]H. Georgi, H. Quinn, and S. Weinberg, Phys. Rev. Lett. 33, 451 (1974).