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ON THE ACCURACY OF THE SINGLE-NUCLEUS APPROXIMATION IN THE EQUATION OF STATE OF HOT, DENSE MATTER

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ABSTRACT

We develop an analytical formalism for determining the errors committed in the entropy, free energy, pressure, and abundances of hot, dense matter in stellar collapse when it is assumed that all nuclei can be represented by a single isotope. This single-nucleus approximation is the standard *Ansatz*. We compare the properties of a mixture that contains a realistic spread of nuclei with those that contain a single nucleus and show that despite the wide spread of nuclei possible, thermodynamic functions deviate little from their single-nucleus conterparts. Further, we show that a sensible comparison must account for the variations in the free-baryon abundances due to the added degrees of freedom of the ensemble approach. We find that the fractional deviations of the free-particle abundances never exceed about 12%, that the realistic entropy is only 4%–7% higher than that of the simple approach, and that pressures, in the density range we focus on, are accurate to better than 0.8%. The general results of this paper can be easily used to correct the single-nucleus approximation predictions.

Subject headings: dense matter — equation of state — stars: collapsed

I. INTRODUCTION

The equation of state of matter at high densities and temperatures is of central importance to the study of the implosion and explosion of the cores of massive stars. In particular, the dependence of the pressure and adiabatic index on the density and entropy during collapse determines, in large measure, the outcome and energetics of the event (Lamb *et al.* 1978; Burrows and Lattimer 1983; Lattimer *et al.* 1984). Matter in this thermodynamic regime is composed of free neutrons and protons, electrons, neutrinos, photons, α-particles, and heavy nuclei, in proportions that depend on the values of three independent thermodynamic variables such as T, ρ, and Y_L, the lepton fraction per baryon. At the densities and temperatures relevant to this problem, the baryonic components are in nuclear statistical equilibrium. The photodissociation and recombination time scales are sufficiently rapid that an ensemble of nuclei with a spectrum of charges (Z_i) and atomic weights (A_i) exists in Saha equilibrium, subject to baryon and charge conservation constraints. The center of the distribution of nuclei would most naturally be that nucleus at the peak of the binding energy per nucleon curve. At electron fractions above 0.45 and the lower baryon densities, this nucleus would be iron or near iron, but at the lower electron fractions and higher densities encountered during collapse, exotic species with values of A between 100 and 1000 are favored. To include all nuclei present in a calculation of the equation of state would require detailed knowledge of the nuclear physics of nuclei, both known and unknown, and computational power of unreasonable magnitude. Considerable effort has gone into network calculations of the nuclear specifics at a few selected points in T-ρ-Y_L space (El Eid and Hillebrandt 1980; Mazurek, Lattimer, and Brown 1979), but in these calculations a great deal of nuclear physics is ignored. Additionally, this approach cannot be used in collapse simulations, which, by their nature, demand speed.

As a result, workers in the field have devised the so-called four-particle model for the equation of state (Epstein and Arnett 1975; Bethe *et al.* 1979). This approach restricts the baryons to reside in either free neutrons, free protons, α-particles, or a single representative heavy nucleus. Alpha-particles are included because, as a result of their high specific binding energy, their abundances generally dwarf those of other light ($A < 12$) nuclei and, in some instances, can exceed even those of nuclei near the nuclear peak. This method offers the tremendous advantage that realistic physical effects prevalent at high densities and temperatures, which can completely alter nuclear energies and partition functions, can be included (Lattimer 1981). Despite this simplification to a single heavy nucleus, the nuclear statistical equilibrium calculation for the abundances and other properties is still the choke point in any supernova hydrodynamical code. Nevertheless, with it, simulations can be performed (Burrows, Lattimer, and Yahil 1984; Van Riper 1982; Bowers and Wilson 1982; Hillebrandt 1982; Arnett 1977; Cooperstein 1983).

By suppressing the ensemble degree of freedom, one constrains the free energy (F) of the system above its true minimum and, hence, introduces errors in the internal energy, entropy, pressure, and abundances of the mixture. The purpose of this paper is to calculate the errors of the single-nucleus approximation in each of these important thermodynamical variables. For simplicity, α-particles are ignored. We develop an analytical formalism by which the accuracy of the single-nucleus approximation is easily determined. The numbers we obtain indicate that this approximation is highly accurate despite the fact that the width of the nuclear peak can be large.

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II. THE DEFINITION OF THE Δ'S

For the purposes of this paper, we concern ourselves with two thermodynamic configurations, which we label the x- and y-systems. In the x-system, the baryonic component consists of free neutrons and protons and a distribution, or "ensemble," of nuclei clustered about some average atomic weight. In the y-system, only one representative nucleus is allowed, in addition to the free baryons. The atomic weight, A_0, of this nucleus is determined by minimizing the nuclear free energy with respect to A in the standard manner (Lattimer 1981; Lattimer *et al.* 1984, hereafter LLPR). The y-system embodies the standard simplifying assumptions used in the collapse calculations mentioned above. The x-system, however, is more realistic, as the constraint of a representative nucleus has been discarded and the system is allowed to relax to a lower free energy with more degrees of freedom. We are interested in determining the errors in the various thermodynamic functions and abundances committed by substituting the y-system for the x-system at a given temperature, density, and lepton fraction.

In transforming from the y-system to the x-system, a certain fraction of the free nucleons will be absorbed into the then more favorable nuclei. We parameterize this fractional change in the free neutron and proton abundances by Δ_n and Δ_p, respectively, defined by

$$n_n^x = (1 + \Delta_n)n_n^y \tag{1a}$$

and

$$n_p^x = (1 + \Delta_p)n_p^y \,. \tag{1b}$$

In equations (1), $n_n^{x,y}$ and $n_p^{x,y}$ are the baryon densities of the free neutrons and protons. We also define a weighted average, Δ, by

$$\Delta = (1 - x_0)\Delta_n + x_0 \Delta_p \,, \tag{2}$$

where $x_0 = Z_0/A_0$. Note that all variables with subscript 0 refer to the y-system. The Δ's are expected to be small and negative, since a larger fraction of matter is in nuclei in the x-system. It is a remarkable and useful fact that the difference between the x- and y-systems in all the thermodynamic functions can be written simply and succinctly in terms of the Δ's. As a trivial illustration of this, we note that, as long as the free-nucleon density is not too large,

$$\mu_{n,p} = T \ln (an_{n,p}/2) \,, \tag{3}$$

where $\mu_{n,p}$ stands for either the neutron or the proton chemical potential and a equals $(h^2/2\pi m_n T)^{3/2}$ (we work in units such that $k_B = 1$). This is the standard formula for the chemical potential of noninteracting, nondegenerate particles, and, since both neutrons and protons are in equilibrium with their bound conterparts, it represents the chemical potential of these bound nucleons as well. Using equations (1) and setting $\ln(1 + \Delta_{n,p}) \approx \Delta_{n,p}$, we obtain

$$\delta\mu_{n,p} = \mu_{n,p}^x - \mu_{n,p}^y = T\Delta_{n,p} \,, \tag{4}$$

where $\delta\mu_{n,p}$ is the difference between the chemical potential of the subscripted species in the x- and y-systems. Henceforth, δ's will denote such a difference between the two systems and will represent the "error" of making the single-nucleus approximation.

Before proceeding to the calculation of these deviations in other functions, the formulae for baryon conservation and charge balance need to be stated. They are

$$n = n_n^x + n_p^x + \Sigma n_i A_i = n_n^y + n_p^y + n_0 A_0 \tag{5}$$

and

$$n_p^x + \Sigma n_i Z_i = nY_e^x \,, \qquad n_p^y + n_0 Z_0 = nY_e^y \,, \tag{6}$$

where n_i is the number density of a nucleus in the x-system with atomic weight A_i and charge Z_i, n_0 is the number density in the y-system of the representative nucleus with atomic weight A_0 and charge Z_0, n is the total baryon density, which is the same in both systems, and $Y_e^{x,y}$ is the total charge per baryon in the x- or y-system. Y_e^x does not, in general, equal Y_e^y. We have elected to perform our calculations not for $\delta Y_e = 0$ but for $\delta Y_L = 0$, i.e., by maintaining beta equilibrium at a fixed Y_L. The condition for beta equilibrium is that

$$\mu_n - \mu_p = \hat{\mu} = \mu_e - \mu_\nu \,, \tag{7}$$

where ν refers to the neutrinos ($Y_L = Y_e + Y_\nu$). Therefore,

$$\delta\hat{\mu} = \delta\mu_e - \delta\mu_\nu \,,$$

which implies, if $\Delta_{n,p} \ll 1$, that

$$(\Delta_n - \Delta_p) = (\mu_e/Y_e + \mu_\nu/Y_\nu)\delta Y_e/3T \equiv \theta\delta Y_e \,. \tag{8}$$

We have ignored the neutron-proton mass difference. Thus, although beta equilibrium implies $\delta Y_e \neq 0$, δY_e can be readily determined from the Δ's.

Equation (5) can be arranged to read

$$\Sigma n_i A_i - n_0 A_0 = -n_p^y \Delta_p - n_n^y \Delta_n \,, \tag{9}$$

or

$$\Sigma n_i A_i/n_0 A_0 = 1 - (Y_n \Delta_n + Y_p \Delta_p)/X_H > 1 \,, \tag{10}$$

where $X_H = n_0 A_0/n$ is the mass fraction in nuclei (heavies) in the y-system and $Y_{n,p}$ is the mass fraction in either free neutrons or protons in the y-system. The sign $>$ in equation (10) is just a statement of the fact that the x-system keeps a few more of its nucleons in nuclei.

Equation (6) can be combined to yield

$$\Sigma n_i Z_i - n_0 Z_0 = -n_p^y \Delta_p + n\delta Y_e \, , \tag{11}$$

which, with equation (9), tells that

$$\delta Y_e = (1 - x_0)\Delta_p Y_p - x_0 \Delta_n Y_n + X_H \delta x \, , \tag{12}$$

where $x_i = Z_i/A_i$ and $\delta x = \Sigma n_i A_i(x_i - x_0)/nX_H$. The last term in equation (12) is a measure of the deviation of the average x_i in the x-system from that in the y-system, x_0. We will calculate this term in § IV*c* after more of the formalism is developed. Equations (12) and (8) can then be used to obtain a linear relation between Δ_n and Δ_p. Since we will show in § IV that the combination, Δ, can be derived using other arguments, we can obtain Δ_n and Δ_p individually for any thermodynamic state.

In § III, we derive the errors in the total free energy, internal energy, pressure, and entropy as functions of the Δ's. Section IV contains the full formalism of the ensemble and attendant considerations. Finally, in § V, we discuss the numerical results for a sequence of densities along $s = 1$ and $s = 2$ isentropes at $Y_L = 0.4$ and draw some general conclusions.

III. THE DEVIATIONS OF THE THERMODYNAMIC FUNCTION

The change in the Gibbs free energy in the $y \rightarrow x$ transformation is the sum of the individual changes in the neutron, proton, and lepton sectors. These are given by

$$\begin{aligned}\delta G &= \mu_n^x(1 - Y_e^x) + (\mu_p^x + \mu_e^x)Y_e^x + \mu_\nu^x Y_\nu^x - \mu_n^y(1 - Y_e^y) - (\mu_p^y + \mu_e^y)Y_e^y - \mu_\nu^y Y_\nu^y \\ &= \mu_n^x + \mu_\nu^x Y_L - \mu_n^y - \mu_\nu^y Y_L \, , \end{aligned} \tag{13}$$

where beta equilibrium (eq.[7]) was invoked. By using the definition of Δ (eq. [2]) and mass and charge conservation, equation (13) may be written

$$\delta G \approx T(X_H \Delta + Y_p \Delta_p + Y_n \Delta_n) + \hat{\mu}^y \delta Y_e/3 \, , \tag{14}$$

where $\hat{\mu}^x$ was set equal to $\hat{\mu}^y$, since their difference introduces a term of second order in the Δ's and can be ignored.

The pressure deviation can be easily derived by noting that it results from changes in the ideal gas pressure of the baryons, the Coulomb lattice pressure P_c, and the degeneracy pressure of the leptons. We find

$$\delta P = \delta P_b + \delta P_c + \delta P_{e+\nu} \, , \tag{15a}$$

where

$$\delta P_b = nT(Y_p \Delta_p + Y_n \Delta_n) + T(\Sigma n_i - n_0) \, , \tag{15b}$$

and

$$\delta P_{e+\nu} = (\mu_e \delta Y_e + \mu_\nu \delta Y_\nu)n/3 = \hat{\mu}^y n \delta Y_e/3 \, . \tag{15c}$$

The change in the lattice pressure, δP_c, is the dominant term at high densities and will be discussed later.

We now use the standard thermodynamic relation for the Helmholtz free energy per baryon,

$$\delta F = \delta G - \delta P/n \, , \tag{16}$$

to obtain

$$\delta F = TX_H \Delta - \delta P_c/n - T(\Sigma n_i - n_0)/n \, . \tag{17}$$

This equation is, in fact, more general than the above derivation suggests. It can also be derived from equations (20), (24), (10), and (11). Note that the $\hat{\mu}^y$ term has canceled. In general the first two terms on the right-hand side of equation (17) are the most important, and we combine them in the form

$$\delta F \approx TX_H \Delta^* \, , \tag{18}$$

where $\Delta^* = \Delta - \delta P_c/nX_H T$. This is a surprisingly simple and powerful result, and it emphasizes the central role played by the quantity Δ^* in these considerations. Δ^* is a direct measure of the accuracy of the single-nucleus representation. Since the x-system allows more degrees of freedom, we expect that $\delta F < 0$ and, therefore, that $\Delta^* < 0$. We shall see below that this expectation is borne out.

We may use the relation $\delta S = -\partial(\delta F)/\partial T$ to find the entropy variation. We show in § IV that Δ^* varies with T as A_0^{-1} ln (constant $\times$ T). Ignoring variations with T of X_H and using equation (18), we therefore see that

$$\delta S \approx -X_H(\Delta^* - 1/A_0) \, . \tag{19}$$

Not only is Δ^* a direct measure of the free-energy error, but it is also approximately equal to the entropy error. Since Δ^* is negative, δS will be positive, as expected.

We have seen in this section how the thermodynamic deviations between the x- and y-systems can be simply, and sometimes surprisingly, related to the Δ's. We now proceed to the physics of the ensemble and the analytic formalism for the calculation of Δ^*.

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IV. THE PHYSICS OF THE ENSEMBLE

a) The Saha Equation and the Expression for n_i/n_0

The free energy per baryon of a nucleus in the x-system can be written as

$$F_i = f_i + f_t \,, \tag{20a}$$

where

$$f_i = E_0 - a_T T^2 + S_V(1-2x_i)^2 + [a_S - S_S(1-2x_i)^2]A_i^{-1/3} + a_C x_i^2 A_i^{2/3} \tag{20b}$$

and

$$f_t = (T/A_i)[\ln(n_i a/A_i^{3/2}) - 1] \,. \tag{20c}$$

In these equations, f_i is simply one form of the standard semiempirical mass formula for nuclei, with the usual bulk, surface, Coulomb, and asymmetry terms. The term $a_T T^2$ is included to account for the thermal excitation of nuclear levels, and f_t is the translational free energy. (See Lattimer 1981 and LLPR for more details.) For the purposes of this work, the constants of equation (20b) are

$$E_0 = -16 \,, \quad S_V = 30 \,, \quad S_S = 43.6 \,, \quad a_T = 1/8 \,, \quad a_S = 19 \,, \quad a_C = 0.756(1 - 1.5u^{1/3} + u/2) \,, \tag{20d}$$

all in MeV. Here, the u in a_C is the volume occupied by nuclei ($u \approx nX_H/0.155\ \mathrm{F}^{-3}$). The Coulomb energy in equation (20b) is not generally correct for a nucleus in a lattice comprised of an ensemble of nonidentical nuclei. It is a good approximation, however, if fluctuations in $Z^2/A^{1/3}$ dominate fluctuations in a_C. It will be seen (cf. eqs. [10] and [35]) that $\delta u/u = \delta X_H/X_H \ll \delta A/A_0$. In the y-system, we have

$$F_0 = f_0 + f_t^y \,; \qquad f_t^y = (T/A_0)[\ln(n_0 a/A_0^{3/2}) - 1] \,. \tag{20e}$$

We expand f_i in a Taylor series around A_0 and x_0, the weight and Z/A, respectively, for the representative nucleus in the y-system:

$$f_i = f_0 + (\partial f_i/\partial x)_0 \Delta x + (\partial f_i/\partial A)_0 \Delta A + (\partial^2 f_i/\partial A^2)_0 (\Delta A)^2/2 + (\partial^2 f_i/\partial A \partial x)_0 \Delta A \Delta x + (\partial^2 f_i/\partial x^2)_0 (\Delta x)^2/2 + (\partial^3 f_i/\partial A^3)_0 (\Delta A)^3/6 + \dots \,, \tag{21}$$

where $\Delta A = A_i - A_0$ and $\Delta x = x_i - x_0$. The value of A_0 is determined by minimizing the total free energy in the y-system with respect to A, at fixed X_H (LLPR), which in our case is the same as setting the derivative of F_0 with respect to A, evaluated at fixed $n_0 A_0$, equal to zero. Note that f_0 is not itself minimized, but the translational term, which is A-dependent, must be included. Along the $s = 1$ isentrope, at densities in excess of 10^{11} g cm^{-3}, it generally decreases the predicted A_0 by 10–20 units. From this minimization condition we also obtain an expression for $(\partial f_i/\partial A)_0$:

$$(\partial f_i/\partial A)_0 \approx (\partial f_t^y/\partial A)_0 = f_t^y/A_0 + 5T/2A_0^2 \,, \tag{22}$$

where we have neglected the variation of u in f_i. The first derivative with respect to x, $(\partial f_i/\partial x)_0$, is simply $-\hat{\mu}^y$.

The second derivatives can be obtained from equation (20b):

$$(\partial^2 f_i/\partial A^2)_0 = 2a_C x_0^2 A_0^{-4/3}/3 - 4(f_t/T + 5/2A_0)T/3A_0^2 = 2T[Q_A - (f_t^y/T + 5/2A_0)/A_0^2] \,, \tag{23a}$$

$$(\partial^2 f_i/\partial x^2)_0 = 2a_C A_0^{2/3} + 8(S_V - S_S A_0^{-1/3}) = 2TQ_x \,, \tag{23b}$$

and

$$(\partial^2 f_i/\partial A \partial x)_0 = [4a_C x_0 - 8(0.5 - x_0)S_S/A_0]/3A_0^{1/3} = TQ_{Ax} \,. \tag{23c}$$

These equations define the Q's. The definition of Q_A in equation (23a) will simplify some subsequent expressions.

The Saha equation, which is a statement of the chemical equilibrium between a nucleus and free nucleons in the mixture, is written

$$N_i \mu_n^x + Z_i \mu_p^x = F_i A_i + T + P_c^x V_i \,, \tag{24a}$$

which holds for each nucleus in the distribution in the x-system, and

$$N_0 \mu_n^y + Z_0 \mu_p^y = F_0 A_0 + T + P_c^y V_0 \tag{24b}$$

in the y-system. P_c is the Coulomb lattice pressure, and in the y-system it is

$$P_c^y = nX_H u(\partial f_0/\partial u) = -0.378 nX_H u^{1/3}(1 - u^{2/3})x_0^2 A_0^{2/3} \,. \tag{24c}$$

In the x-system, as with the Coulomb energy, no such generalization exists, and we just write $P_c^x = P_c^y + \delta P_c$. The form of δP_c is considered in § IV*d*. The essential point is that P_c^x must be the same for all nuclei in the x-system, because of pressure equilibrium. V_i is the nuclear cell size, and we assume it is proportional to the nuclear mass:

$$V_i = A_i/\Sigma n_i A_i \,; \qquad V_0 = A_0/nX_H \equiv 1/n_0 \,. \tag{24d}$$

Note that $V_i \neq 1/n_i$. Since the translational term in the free energy, f_t, contains n_i, we can employ the Saha equations to find the number density of a nucleus with a given (A_i, x_i) in the x-system or the number density, n_0, of the representative nucleus in the

y-system. By normalizing n_i with respect to n_0, we can eliminate a variety of distracting parameters. After some tedious algebra, involving equations (20)–(24), we find

$$\begin{aligned} n_i/n_0 &= (A_i/A_0)^{3/2}(1+\Delta_n)^{N_0}(1+\Delta_p)^{Z_0} \exp\,(L - P - A_0\,\delta P_c/nX_H T) \\ &\approx (A_i/A_0)^{3/2}(1+\Delta^*)^{A_0} \exp\,(L-P)\,. \end{aligned} \tag{25a}$$

The last expression was obtained with the aid of equation (2) and the definition of Δ^*. L and P, which are linear and quadratic terms, respectively, are given by

$$L = \alpha\Delta A + \beta\Delta x\,, \tag{25b}$$

where

$$\alpha = \Delta^* - 1.5/A_0\,, \qquad \beta = A_0(\Delta_p - \Delta_n)\,, \tag{25c}$$

and

$$P = Q_A A_0(\Delta A)^2 + Q_{Ax} A_0\,\Delta A\Delta x + Q_x A_0(\Delta x)^2\,. \tag{25d}$$

We have assumed that $Q_{Ax} A_0 \gg \Delta_p - \Delta_n$. Note that we have dropped third- and higher-order terms. It can be shown that these terms have very small coefficients. However, the cross-term in equation (25d) must be retained.

Interesting quantities are the widths of the distributions represented by equation (25a) at A_0 and x_0. Since equation (25a) is nearly a Gaussian, we easily find

$$\sigma_A^2 = Q_x/(2A_0 \text{ dis } Q) \approx (2Q_A A_0)^{-1} \tag{26a}$$

and

$$\sigma_x^2 = Q_A/(2A_0 \text{ dis } Q) \approx (2Q_x A_0)^{-1}\,, \tag{26b}$$

where dis Q is the discriminant of Q (cf. eq. [A8]). The sign $\approx$ reflects the fact that, in practice, $Q_{Ax}^2/4 \ll Q_A Q_x$. Straightforward manipulation yields the corresponding spreads in N_i and Z_i:

$$\sigma_N^2 = (1-x_0)^2\sigma_A^2 + A_0^2\sigma_x^2 + Q_{Ax}(1-x_0)/(2 \text{ dis } Q) \tag{26c}$$

and

$$\sigma_Z^2 = x_0^2\sigma_A^2 + A_0^2\sigma_x^2 - Q_{Ax}x_0/(2 \text{ dis } Q)\,. \tag{26d}$$

Equation (25a) is a central expression of our investigation. It states, not unexpectedly, that the distribution of nuclei in the x-system is approximately Gaussian. The fact that it is written in terms of Δ^* can be exploited to great advantage, as we now show.

b) *The Calculation of* Δ^*

Since Y_n and Y_p are small, and both Δ_n and Δ_p will be shown to be small, we can use equation (10) to state that

$$J = \Sigma n_i A_i/n_0 A_0 \approx 1\,. \tag{27a}$$

Since n_i/n_0 is given in equation (25a) as a function of the Δ's equation (27a) can be used to find an additional relation between them. The sum in equation (27a), which is a sum over neutron and proton number in the x-system, can be approximated by a 2-dimensional integral over N_i and Z_i. We are led directly to the expression

$$J = (1+\Delta^*)^{A_0}K\,, \tag{27b}$$

where

$$K = A_0 \int (A_i/A_0)^{7/2} \exp\,(L-P)dA_i\,dx_i\,. \tag{27c}$$

In equation (27c) we have used the fact that $dN_i\,dZ_i = A_i\,dA_i\,dx_i$. The exponential can be transformed into a double Gaussian by rotating away the cross-term and shifting away the linear terms by completing the square. The rotation requires that we map (ΔA, Δx) onto (ΔA^*, Δx^*). The algebra of the rotation is set down in the Appendix. Since the x^* integration is trivial, we obtain for K the result

$$\begin{aligned} K &= A_0 G \int (A_i/A_0)^{7/2} \exp\,\{-A_0[Q_A^*(\Delta A^* - S_A^*)^2 + Q_x^*(\Delta x^* - S_x^*)^2]\}dA^*dx^* \\ &= (\pi A_0/Q_x^*)^{1/2} G \int (A_i/A_0)^{7/2} \exp\,[-A_0\,Q_A^*(\Delta A^* - S_A^*)^2]dA^*\,, \end{aligned} \tag{28a}$$

where

$$S_A^* \approx (\alpha - \beta Q_{Ax}/2Q_x)/2Q_A A_0 \approx \alpha/2Q_A A_0\,, \tag{28b}$$

$$S_x^* \approx (\beta + \alpha Q_{Ax}/2Q_x)/2Q_x A_0\,, \tag{28c}$$

and

$$G = \exp\,[A_0(Q_x^* S_x^{*2} + Q_A^* S_A^{*2})]\,. \tag{28d}$$

Q_A^* and Q_x^* are related to Q_A and Q_x through equations (A4) and (A5). It should be noted that $Q_A^* \approx Q_A$ and $Q_x^* \approx Q_x$, because the rotation angle ϕ, defined by equation (A7), is generally small ($< 10^{-3}$). S_A^* and S_x^* are the shifts in ΔA^* and Δx^* obtained by completing the square in the exponent after the rotation and are not the physical shifts of the x-system averages from the A_0 and x_0 of the y-system. We address the physical shifts, S_A and S_x, a bit later.

The integration over A^* can be done numerically, or, to a very good approximation, analytically by the method of steepest descent. Equation (27b) can then be written

$$1 = (1 + \Delta^*)^{A_0} \Lambda \pi / (\text{dis } Q)^{1/2}\,, \tag{29}$$

where Λ, a weak function of Δ^*, is a complicated numerical factor of order unity. Thus, equation (29) is an implicit equation for the combination Δ^*, since no lone Δ_n's or Δ_p's have survived. As we showed in § II, it is just Δ^* that figures so prominently in δF and δS, not Δ_n or Δ_p individually. Solving equation (29) for Δ^*, we have

$$\Delta^* = \Delta_1 - (1/A_0) \ln \Lambda \approx \Delta_1\,, \tag{30a}$$

where

$$\Delta_1 = \ln\,[(\text{dis } Q)^{1/2}/\pi]/A_0 \approx -\ln\,(2\pi A_0 \sigma_A \sigma_x)/A_0\,. \tag{30b}$$

In practice, the value of Λ is always between $\frac{1}{2}$ and 1, so the approximation in equation (30a) is a good one. We note here that equation (30a), when combined with equation (18), yields $\delta F \approx X_H T \Delta_1$. This result was found earlier by Mackie (1976), using a completely different technique.

Equation (30a) is another central result of this paper. We see from it that Δ^* is a simple function of A_0 and the Q's, which are y-system parameters. In principle, equation (24b), charge and baryon conservation, and beta equilibrium can be used in a Newton-Raphson procedure to solve for all the thermodynamic particulars of the y-system at any given combination of temperature or entropy, density, and lepton fraction. Specifically, x_0, A_0, Y_n, Y_p, X_H, and u can be found. We have, instead, chosen to use the LLPR equation of state to obtain these y-system numbers. We continue to use equations (23) to evaluate the Q's which are the only derived quantities we need. The accuracy of this scheme depends only slightly on the accuracy of equations (20b) and (20c), as well as equation (3), which can be viewed as approximations to the LLPR equation of state. Since the Q's are second derivatives, this procedure is acceptable. Alternatively, one could difference the LLPR equation of state to find the Q's, but this would perceptibly alter our results only at the highest densities (Appendix D of LLPR pursues this approach).

Table 1 contains some of the relevant LLPR raw numbers for $s = 1$ and 2 isentropes for $Y_L = 0.4$, at four density points. Table 2 contains the Q's derived from equations (23) and the resulting widths (sigmas) of the distributions at the appropriate values of A_0 and x_0. In Figure 1 we graph the x-system distributions in A_i (after integrating over x_i) for the $s = 1$ isentrope. These curves are normalized to unit area. Finally, in Table 3, we present the corresponding values of Δ^*, Δ, Δ_n, Δ_p, the shift (S_A) in the average A_i of the x-system from A_0, δS, δF, $\delta P/P$, and the Coulomb pressure deviation $\delta P_c/nX_H T$. The values of Δ^* in this table come from the numerical solution of equations (27a), (27b), and (28a), after the x^* integration is first performed analytically. The analytical formula, equation (30a), is in excellent agreement with the numerical results even at the high-entropy, high-density point ($s = 2$, $n = 0.01$ F^{-3}), where deviations due to the significant breadth and distortion of the distribution might have been expected to introduce an appreciable error. In all cases, the analytical theory is good to better than 6%. The following subsection deals with the calculation of Δ_n and Δ_p.

TABLE 1

LLPR Raw Numbers of Relevance, for $Y_L = 0.4$

n (F^{-3})	A_0	x_0	T (MeV)	Y_n	Y_p	u
			a) $s = 1$			
10^{-5}..........	60.16	0.4317	0.8564	0.0256	8.800($-$6)	5.621($-$5)
10^{-4}..........	65.87	0.4243	1.177	0.05277	2.314($-$5)	5.454($-$4)
10^{-3}..........	80.79	0.41	1.787	0.08432	6.213($-$5)	5.281($-$3)
10^{-2}..........	137.0	0.3868	3.28	0.08549	3.345($-$4)	5.391($-$2)
			b) $s = 2$			
10^{-5}..........	54.69	0.4413	1.106	0.09479	9.537($-$4)	4.667($-$5)
10^{-4}..........	56.84	0.4361	1.61	0.1536	2.359($-$3)	4.341($-$4)
10^{-3}..........	60.39	0.4282	2.75	0.2118	7.363($-$3)	3.997($-$3)
10^{-2}..........	70.56	0.4081	5.747	0.2142	1.945($-$2)	4.294($-$2)

TABLE 2

Q and σ Values for $Y_L = 0.4$

n (F^{-3})	Q_A	Q_x	Q_{Ax}	σ_A	σ_x
		a) $s = 1$			
10^{-5}..........	2.02($-$4)	100.93	0.0838	6.4	0.009
10^{-4}..........	1.15($-$4)	74.46	0.0509	8.1	0.010
10^{-3}..........	4.46($-$5)	50.44	0.0229	11.8	0.011
10^{-2}..........	6.30($-$6)	29.09	0.0049	24.0	0.011
		b) $s = 2$			
10^{-5}..........	1.78($-$4)	76.27	0.0705	7.2	0.011
10^{-4}..........	1.02($-$4)	52.52	0.0418	9.3	0.013
10^{-3}..........	4.02($-$5)	30.70	0.0177	14.3	0.016
10^{-2}..........	4.50($-$6)	14.65	0.0022	39.7	0.022

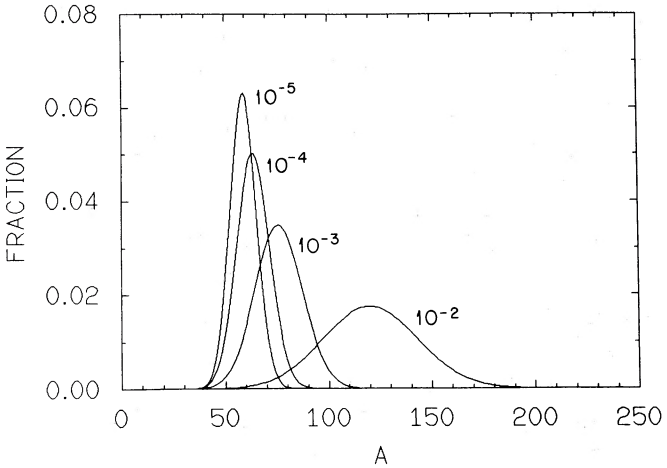

FIG. 1.—Distribution of nuclei for $s = 1$ and $Y_L = 0.4$ for baryon densities of 10^{-5}, 10^{-4}, 10^{-3}, and 10^{-2} F^{-3} [1 F$^{-3} \approx 1.675(15)$ g cm^{-3}]

c) Formulae for Δ_n and Δ_p

We are now in a position to calculate the last term of equation (12):

$$\begin{aligned}\delta x &= \Sigma n_i A_i \Delta x / n_0 A_0 \\ &\approx (A_0 G/K) \int (A_i/A_0)^{7/2} \Delta x \exp\left[-Q_A^*(\Delta A^* - S_A^*)^2 - Q_x^*(\Delta x^* - S_x^*)^2\right] dA^* dx^* \, . \qquad (31)\end{aligned}$$

Taking Δx from equation (A1) of the Appendix, we obtain

$$\delta x \cos \phi \approx S_x^* - \sin \phi \Sigma n_i A_i \Delta A / n_0 A_0 \, . \qquad (32)$$

Using the fact that $\phi \ll 1$ and expanding the (A_i/A_0) term in the integral, we have

$$\begin{aligned}\delta x &\approx S_x^* - (S_A^* + 7/4 Q_A A_0^2) Q_{Ax}/2Q_x \\ &\approx [\Delta_p - \Delta_n - \sigma_A^2(\Delta^* + 2/A_0) Q_{Ax}]/2Q_x \, . \qquad (33)\end{aligned}$$

Generally, δx is positive. We can derive S_A, the shift in the average A_i from A_0, by a similar procedure. The result is

$$S_A = \Sigma n_i \Delta A / n_0 \approx S_A^* + 5/4 Q_A A_0^2 \approx \sigma_A^2(\Delta^* + 1/A_0) \, . \qquad (34)$$

The S_x^* term, which is multiplied by $\sin \phi$, has been dropped. For S_x, the shift in the average x_i from x_0, we find

$$S_x = \Sigma n_i \Delta x / n_0 \approx [\Delta_p - \Delta_n - \sigma_A^2(\Delta^* + 1/A_0) Q_{Ax}]/2Q_x \, . \qquad (35)$$

In general, S_x is positive and $\ll \sigma_x$. Using the approximation $S_x^* \approx (\Delta_p - \Delta_n)/2Q_x$, we can substitute equation (33) in equation (12), and, using equations (2) and (8), we can find relations for Δ_n and Δ_p:

$$\Delta_n = \{\Delta[\xi + (1 - x_0)Y_p] - x_0 \Gamma\}/[\xi + (1 - x_0)^2 Y_p + x_0^2 Y_n] \, , \qquad (36)$$

and

$$\Delta_p = [\Delta(\xi + x_0 Y_n) + (1 - x_0)\Gamma]/[\xi + (1 - x_0)^2 Y_p + x_0^2 Y_n] \, , \qquad (37)$$

TABLE 3

Δ'S AND THERMODYNAMIC DEVIATIONS FOR $Y_L = 0.4$

n (F^{-3})	$-\Delta^*$	$-\Delta$	$-\Delta_n$	$-\Delta_p$	$-S_A$	δS	$-\delta F$	$\delta P/P$	$\delta P_c/nX_H T$
				a) $s = 1$					
10^{-5}..........	0.050	0.049	0.042	0.058	1.3	0.065	0.041	4.1(−4)	9.3(−4)
10^{-4}..........	0.052	0.050	0.034	0.071	2.3	0.064	0.057	8.2(−4)	2.1(−3)
10^{-3}..........	0.051	0.046	0.024	0.078	4.9	0.058	0.082	1.8(−3)	5.1(−3)
10^{-2}..........	0.040	0.028	0.012	0.054	16.7	0.043	0.117	3.7(−3)	1.3(−2)
				b) $s = 2$					
10^{-5}..........	0.058	0.057	0.041	0.077	1.9	0.069	0.057	−1.4(−3)	1.0(−3)
10^{-4}..........	0.064	0.062	0.034	0.099	3.6	0.069	0.085	−3.7(−4)	2.4(−3)
10^{-3}..........	0.072	0.066	0.029	0.115	9.1	0.069	0.149	8.1(−4)	6.4(−3)
10^{-2}..........	0.083	0.061	0.037	0.096	31.6	0.074	0.338	7.8(−3)	2.3(−2)

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where

$$\xi = 1/\theta + X_H/2Q_x \tag{38}$$

and

$$\Gamma = X_H \sin \phi \Sigma n_i A_i \Delta A/n_0 A_0 \approx X_H \sigma_A^2(\Delta^* + 2/A_0)Q_{Ax}/2Q_x \, . \tag{39}$$

To obtain the corresponding relation with the $\delta Y_e = 0$ constraint, we merely set $\theta = \infty$. However, the beta-equilibrium assumption made above is much more useful and illuminating. Up to densities of 10^{-3} F^{-3}, the approximations of the sums in equations (34) and (39) are accurate to within 20%. The values of S_A, Δ_n, and Δ_p tabulated in Table 3, however, were computed by performing the summations $\Sigma n_i \Delta A$ and $\Sigma n_i A_i \Delta A$ numerically.

d) Variations in the Coulomb Pressure

In this subsection we evaluate, very approximately, the variation in the Coulomb lattice pressure. The thermodynamic relation $\delta P = n^2[\partial(\delta F)/\partial n]\,|_T$, when applied to equation (18), is

$$\partial(\delta P_c)/\partial n \approx n[\partial(T X_H \Delta^*)/\partial n]\,|_T \, , \tag{40}$$

where we have retained only the Coulombic contribution to the pressure. This approximation is valid particularly at high densities, where $\delta P_c \gg \delta P_b, \delta P_{e+\nu}$. The derivative of X_H is small compared to that of Δ^*, and we neglect it. Using equations (30), we derive

$$\partial \Delta^*/\partial n \approx (-\Delta^*/A_0 + 2/3A_0^2)\partial A_0/\partial n \, , \tag{41}$$

where we have assumed that dis $Q \propto A_0^{-4/3}$ (cf. eq. [23]). Neglecting translational terms, the minimization of the nuclear free energy gives a simple formula for A_0 which can be used to obtain

$$\partial A_0/\partial n \approx 0.378 A_0 u^{1/3}(1 - u^{2/3})/(n a_C) \, . \tag{42}$$

Using the fact that Δ^* is approximately proportional to $1/A_0$, which is also proportional to a_C, we can integrate equation (40). We find

$$\delta P_c/n X_H T \sim -(3/8)(\Delta^* - 2/3A_0)u^{1/3}(1 - 2u^{2/3}/3)/(1 - 3u^{1/3}/2 + u/2) \, . \tag{43}$$

This result is tabulated in Table 3. Note that δP_c is always positive. A qualitatively similar formula for δP_c can be found from the relation

$$\delta P_c \sim (\partial P_c/\partial A)\delta A \approx (2/3)(P_c^y/A_0)S_A \, , \tag{44}$$

if use is made of equations (24c) and (34).

V. DISCUSSION

As Figure 1 and Table 2 indicate, the spread in A of a realistic distribution can be large. The value of σ_A is a steadily increasing function of both density and entropy, becoming a significant fraction of the mean A at the higher densities. It is interesting that this width is roughly proportional to temperature along isentropes. The spread in x, σ_x, however, is small and relatively independent of density at the lower entropy and only a weakly increasing function of density at the higher, simply doubling between $n = 10^{-5}$ F^{-3} and $n = 0.01$ F^{-3}. From equations (26c) and (26d), we note that $\sigma_Z \approx x_0 \sigma_A$ and $\sigma_N \approx (1 - x_0)\sigma_A$, since $\sigma_A \gg A_0 \sigma_x$. At all times, σ_x is significantly larger than the shift S_x. However, S_A, the shift in A, can become large, and, as Table 3 shows, it is a sensitive function of both density and entropy. It should be noted that when $|S_A/A_0|$ becomes large, as it does for the highest density considered, the approximations we have used are not quantitatively accurate, although they are still qualitatively useful. Although we have not addressed in this paper the characteristics of matter at densities above 0.01 F^{-3}, we have every reason to believe that, despite the increased complications of nuclear interaction and Coulomb lattice effects, not to mention the effects of nuclear asphericity, the general character of our results may be extrapolated fairly well as the phase transition to nuclear matter is approached (Bonche and Vautherin 1981).

However, despite the large widths and shifts, as we can see in Table 3, all the Δ's remain small. At $s = 1$, Δ^* has a constant value of roughly -0.05. At $s = 2$, it varies weakly from -0.06 to -0.08 as n increases from 10^{-5} F^{-3} to 0.01 F^{-3}. Similarly, Δ_n and Δ_p remain small. Δ_n is the smaller of the two (in absolute value), and Δ_p is a mildly increasing function of both density and entropy. It must be remembered, however, that $Y_p \ll Y_n$, so that, although Δ_p is greater than Δ_n in absolute value, the decrease in the free-neutron abundance is generally larger than that of the free protons. Some of the neutrons that are incorporated into the nuclei of the x-system change through β-decay into bound protons to maintain beta equilibrium; the nuclei are slightly less neutron-rich than the single-nucleus approximation predicts. Incidentally, equation (8) shows that $\delta Y_e/Y_e$ is less than $\frac{1}{2}$% for the cases discussed in this paper.

Using equation (19), we derive the values of δS shown in Table 3, which range between 0.04 and 0.07. Note that the *fractional* change in entropy decreases with increasing entropy. All in all, δS is comfortably small.

With the aid of the relevant numbers in Tables 1 and 3, equation (15) can be used to show that the absolute value of $\delta P/P$ varies from less than 0.1% at $s = 1$ and $n = 10^{-5}$ F^{-3} to its largest value of about 0.8% at $s = 2$ and $n = 0.01$ F^{-3}. Since pressure is the most hydrodynamically relevant variable, this small variation is reassuring. In general, δP is positive because δP_c is the largest term, but at higher entropies when the density is small, δP_b becomes more important, and there δP is negative. The derived values of $\delta P/P$ are included in Table 3.

Similarly, equation (17) can be used to show that δF is indeed negative and, for $s = 1$, varies between -0.041 MeV at $n = 10^{-5}$ F^{-3} and -0.12 MeV at $n = 0.01$ F^{-3} (see Table 3). For $s = 2$, the absolute value of δF is somewhat larger, and δF is -0.06 MeV and -0.34 MeV for these same two densities.

We conclude, therefore, that relaxing the single-nucleus constraint changes the thermodynamical functions in ways that can be calculated and are found to be small, except possibly near the critical point. Obviously, as one approaches the critical point (according to LLPR, for $Y_L = 0.4$ it lies near $n \sim 0.03$ F^{-3} and $T \sim 18$ MeV) the effects of fluctuations become relatively large. Nevertheless, the ensemble corrections never dominate the thermodynamics of the system. However, the single-nucleus approximation may still lead to significant errors in other quantities of physical interest, such as the net electron capture rate during infall. Since electron capture strength functions vary from nucleus to nucleus, assuming the presence of a single nucleus instead of a distribution is likely to alter the rate. The electron capture rate is, in general, not a simple function of A and Z. Hence it is not possible to determine, *a priori*, from thermodynamic arguments the magnitude or sign of the effect. Attempts have been made to estimate the effective electron capture rate with an ensemble (Fuller 1982; Cooperstein and Wambach 1984). These preliminary studies indicate that the overall effect is small.

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APPENDIX

In this appendix, we present some of the details of the rotation of the bilinear form in ΔA and Δx. Our purpose is to eliminate the cross-term and derive some useful consequences of the transformation. We set

$$\Delta x = \Delta x^* \cos \phi - \Delta A^* \sin \phi \tag{A1}$$

and

$$\Delta A = \Delta A^* \cos \phi + \Delta x^* \sin \phi \ , \tag{A2}$$

where ϕ is the rotation angle and the asterisk refers to the transformed frame. Note that the Jacobian of this transformation is 1. Next, we demand

$$Q_x^*(\Delta x^*)^2 + Q_A^*(\Delta A^*)^2 = Q_x(\Delta x)^2 + Q_A(\Delta A)^2 + Q_{Ax}\Delta A \Delta x \ . \tag{A3}$$

Using equations (A1) and (A2) in equation (A3), we derive

$$Q_x = Q_x^* \cos^2 \phi + Q_A^* \sin^2 \phi \ , \tag{A4}$$

$$Q_A = Q_x^* \sin^2 \phi + Q_A^* \cos^2 \phi \ , \tag{A5}$$

and

$$Q_{Ax} = (Q_x^* - Q_A^*) \sin 2\phi \ . \tag{A6}$$

Combining the last three equations provides an equation for ϕ:

$$\tan 2\phi = Q_{Ax}/(Q_x - Q_A) \ . \tag{A7}$$

With the help of equations (A4)–(A6), we arrive at the result

$$\mathrm{dis}\ Q = Q_A^* Q_x^* = Q_A Q_x - Q_{Ax}^2/4 \ . \tag{A8}$$

Equation (A8) is simply a statement of the invariance of the discriminant. Since $Q_x \gg Q_A$ and $Q_{Ax} \ll Q_x$ (Table 2), we see that ϕ is very small and is of the order 10^{-3}–10^{-4}.

The linear term L (eq. [25b]) becomes, after the rotation,

$$\begin{aligned} \alpha \Delta A + \beta \Delta x &= \Delta A^*(\alpha \cos \phi - \beta \sin \phi) + \Delta x^*(\beta \cos \phi + \alpha \sin \phi) \\ &= \alpha^* \Delta A^* + \beta^* \Delta x^* \ , \end{aligned} \tag{A9}$$

which defines α^* and β^*. From equations (27b), (28a), and (A9), it is easy to derive

$$S_A^* = \alpha^*/2Q_A^* A_0 \ ; \qquad S_x^* = \beta^*/2Q_x^* A_0 \ . \tag{A10}$$

Since ϕ is small, we obtain equations (28b) and (28c).

It should be noted that terms such as $(A_i/A_0)^{7/2} \approx (1 + \Delta A^*/A_0)^{7/2}$ in equation (27c) in the text are hardly affected by the rotation, but the rotation can appreciably mix ΔA^* into Δx^* in the expression for Δx. This fact is important when one is seeking the shifts in § IV*c*.

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