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MIXED LATTICE PHASES IN COLD DENSE MATTER

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ABSTRACT

Over a wide density range, the ground state of cold neutral matter in the absence of external magnetic fields is a degenerate sea of electrons containing a lattice of nuclei. In certain density regions, a phase composed of interpenetrating cubic lattices of different nuclides is preferable to a body-centered cubic lattice of any single nuclide. The arguments supporting this result are first made assuming the electrons to be a uniform background; the qualitative features remain when screening and exchange effects are included.

Subject heading: dense matter

I. INTRODUCTION

The state of matter at densities from 10^4 g cm^{-3} to about 10^{11} g cm^{-3} is of interest in the study of white dwarfs and the crusts of neutron stars. As a first step in describing this matter, it is convenient to consider the ground-state properties of neutral matter in this density range for zero magnetic field. Salpeter (1961) found a succession of phases as the density increased, each a body-centered cubic (bcc) lattice of nuclei immersed in a sea of degenerate electrons. Each phase was characterized by the (Z, A) values of the nuclear species. Baym, Pethick, and Sutherland (1971) improved on this work by including the lattice energy in determining the equilibrium nuclear species present in the ground state phase, and they applied the results in discussing the structure of neutron stars.

Dyson (1971) investigated the possibility of heteronuclear compounds in cold matter. By investigating the ratio of lattice energy of the compound to the lattice energy of the individual lattice, he found that for certain ratios of nuclear charges a compound would be preferred. One such possibility is the compound FeHe. Witten (1974) has included zero-point and screening effects in this calculation.

A further possibility exists, however. Baym, Pethick, and Sutherland have not considered the possibility of heteronuclear compounds at high density, and Dyson and Witten have not allowed variations which can take advantage of the nuclear binding energy. In the present work, we pursue this possibility and find that between almost all phases considered by Baym, Pethick, and Sutherland there exists a phase composed of two interpenetrating cubic lattices. The nuclei at the lattice sites differ substantially from those found by Dyson and Witten, who were not considering nuclear equilibrium.

II. CALCULATIONS FOR THE MIXED PHASES

At a given pressure P, the ground state phase is the phase with the lowest chemical potential μ. In actual calculations, it is more convenient to start with the baryon number density, n_b, and the Z and A values for all nuclides to be considered. These determine directly the lattice spacing. Charge neutrality determines the electron density, which in turn gives the free electron Fermi energy. From the total energy per baryon, E/B, one then constructs $P = n_b^2 \partial(E/B)/\partial n_b$ and $\mu = E/B + P/n_b$. In these calculations, the nuclear mass energy as a function of (Z, A) competes with the electron Fermi energy and, in crystalline phases, with the Coulomb lattice energy. The nuclear masses are known or may be predicted, the free fermion equation of state is well known, and the Coulomb lattice energies are readily obtained. Zero-point motion, exchange, and screening effects play a secondary role and will be discussed later.

Baym, Pethick, and Sutherland found that at the low end of the density range, ^{56}Fe, with the minimum energy per nucleon, occupies bcc lattice sites. As the density increases, the electron Fermi energy increases rapidly and soon rises enough so that ^{62}Ni, even though its rest mass per baryon is larger than that of ^{56}Fe, becomes a more favorable tenant of the lattice sites. As the density rises still further, the ^{62}Ni gives way to a whole sequence of nuclei. In this progression, there is a delicate balance between nuclear energies and Coulomb energies, and it is this balance which may be exploited by a mixed lattice.

Although Z and A must change discretely in going from one phase to another, we might expect still further phases if Z and A could be changed more continuously. Since this cannot be done directly, we instead simulate this action by constructing a mixed lattice with nuclei corresponding to both (Z, A) and (Z', A'). We consider four mixed lattice structures: face-centered cubic (fcc) with (Z, A) on the faces and (Z', A') at the corners; simple cubic (sc) with each (Z, A) surrounded by (Z', A'); bcc with (Z, A) at the corners and (Z', A') in the middle (interpenetrating cubic lattices); hexagonal close-packed (hcp) with alternating layers of (Z, A) and (Z', A'). In the last three cases, there is complete symmetry between (Z, A) and (Z', A'). The unscreened Coulomb lattice energy per baryon may be written as:

$$E_L/B = -\left(e^2 n_b^{1/3}/\bar{A}^{1/3}\right) \times C\left[\alpha Z^2 + \beta Z'^2 + (1-\alpha-\beta)ZZ'\right], \quad (1)$$

where $\bar{A}$ is the mean A for the given structure, and the coefficients C, α, and β were computed using the methods of Coldwell-Horsfall and Maradudin (1960) and are given in Table 1.

Starting with a homogeneous lattice of charge $\bar{Z}$, the Coulomb attraction of the lattice given in equation (1) will be increased if Z and Z' are slowly changed, provided that their weighted average remain $\bar{Z}$. This is basically because the nearest neighbor repulsion is reduced by making the charges unequal. In general, this is at the expense of the nuclear Coulomb energy, which is of order e^2Z^2/R, where R is a nuclear radius. However, it is possible that the other contributions to the nuclear binding energy and the change in electron Fermi energy can decrease enough to provide a more stable phase with different charges Z and Z'. Such a circumstance is likely to occur when the bcc phases corresponding to (Z, A) and (Z', A') are nearly in equilibrium.

We first treat the electrons as a uniform background, neglecting exchange energies, atomic binding energies in the nuclear masses, and screening energies. We then find between almost every pair of phases given by Baym, Pethick, and Sutherland a new mixed bcc phase, which is stable over a narrow pressure range. For each phase characterized by $(Z, A;\ Z', A')$, the entries in Table 2 give the lowest pressure, P, at which the phase first occurs and the pressure range, ΔP, over which it occurs.

TABLE 1

Coulomb Lattice Energy Parameters

Lattice	C	α	β	$(1-\alpha-\beta)$
bcc	1.444231	0.389821	0.389821	0.220358
fcc	1.444141	0.654710	0.154710	0.190580
hcp	1.444083	0.345284	0.345284	0.309433
sc	1.418649	0.403981	0.403981	0.192037

TABLE 2

Pressure P and Pressure Range ΔP for Different Phases

Z	A	Z'	A'	P(dyn cm^{-2})	ΔP(dyn cm^{-2})
26	56	26	56	...	...
26	56	28	62	5.5×10^{23}	1.5×10^{19}
28	62	28	62	5.5×10^{23}	6.9×10^{25}
28	62	28	64	6.9×10^{25}	2.7×10^{17}
28	64	28	64	6.9×10^{25}	4.5×10^{26}
28	64	34	84	5.2×10^{26}	3.2×10^{22}
34	84	34	84	5.2×10^{26}	5.2×10^{27}
34	84	32	82	5.8×10^{27}	8.8×10^{22}
32	82	32	82	5.8×10^{27}	1.5×10^{28}
32	82	30	80	2.1×10^{28}	3.6×10^{23}
30	80	30	80	2.1×10^{28}	3.6×10^{28}
30	80	28	78	5.7×10^{28}	1.1×10^{24}
28	78	28	78	5.7×10^{28}	2.1×10^{29}
28	78	26	76	2.7×10^{29}	5.4×10^{24}
26	76	26	76	2.7×10^{29}	2.0×10^{28}
42	124	42	124	2.9×10^{29}	6.1×10^{27}
42	124	40	122	2.9×10^{29}	2.1×10^{24}
40	122	40	122	2.9×10^{29}	1.6×10^{29}
40	122	38	120	4.5×10^{29}	3.9×10^{24}
38	120	38	120	4.5×10^{29}	2.2×10^{29}
38	120	36	118	6.8×10^{29}	6.8×10^{24}
36	118	36	118	6.8×10^{29}	...

Note.—For each phase characterized by $(Z, A;\ Z', A')$, the entries give the lowest pressure P at which the phase first occurs and the pressure range ΔP over which it occurs.

Typically, the pressure range, ΔP, for a mixed bcc phase is about a hundredth of a percent of the pressure at which the transition occurs. This range is small because the advantage obtained in the mixed phase is a fraction of the Coulomb lattice energy, which in turn is only part of the total energy. The other possible mixed lattice structures never arise in the ground state. This is obvious for the fourth structure (see Table 1) since its Coulomb energy is already rather repulsive compared with the others.

Since small terms in the energy appear to be important in determining the phase, the other small terms should not be neglected. We include the atomic binding, screening, exchange, and zero-point motion corrections estimated by Salpeter in our final calculations. Qualitatively, the results are unchanged. The same phases appear, but at different pressures. The complete set of phases found and the corresponding pressures are given in Table 2. These numbers are based on the nuclear binding energies given by Myers and Swiatecki (1965) and used by Baym, Pethick, and Sutherland. Using the tables of Garvey *et al.* (1969), we find that the (26,76) phase is replaced by a (44,126) phase and that there is an extra (36,86) phase after (34,84). In addition, the (28,62; 28,64) phase disappears and a small (42,126; 44,126) phase appears. The existence of the mixed phases is insensitive to the nuclear data, although the details are rather sensitive to it. Note that the (28,62; 28,64) phase does not follow from the arguments given above, since $Z = Z'$. The appearance of this phase depends not on the Coulomb lattice energy but on the other contributions to the energy. It is interesting to note that its range of pressures is about 10^{-4} that which would be expected for a phase benefiting from the mixed-phase Coulomb lattice energy. This aspect of this phase reflects the relatively minor role played in a mixed-phase state by the other small corrections to the energy.

III. DISCUSSION

At this stage, we should stress that we are investigating a bulk effect and not the interface formed between two slabs of different composition. That surface problem would be appreciably more difficult. Whether the thickness of the new phase is large or small compared with a reasonable number of lattice spacings will depend on the density gradient in a star. It should also be pointed out that these phases are completely different from normal alloys because there are no core electrons.

Do these phases exist and play any important role in real stars? First, consider white dwarfs. The maximum density in a white dwarf, as found by Baym, Pethick, and Sutherland, is about 1.4×10^9 g cm^{-3}. Such a star could have a noticeable fraction of its mass tied up in such a phase if the phase occurred near the center of the star. It is doubtful that normal evolution would result in a star in complete nuclear equilibrium. However, by considering a more restricted set of nuclei, those actually expected to be present in such a star, one would expect to obtain similar mixed phases. These mixed phases are likely to exist in white dwarfs.

In neutron stars, these phases again play a minor role in the structure of a star, because the equation of state is not sensitive to the phase of the matter. For the more massive stars, say above 1.3 $M_\odot$, the fraction of mass tied up in the outer crust is small and the density gradient there is large. A typical thickness of one of these phases would be about a millimeter. While small on the stellar scale, this still represents a large number of interparticle spacings. Another hope for observing a mixed phase would be if similar phases occurred in the inner crust, where the electron sea around nuclei is joined by a sea of neutrons. The Z values must change discretely in this region too, and magic Z values seem favored. Hence there is a possibility that a mixed phase will be present in this region as well. The chief problem in the inner crust is the strong competition between the Coulomb lattice energy and the neutron sea–nucleus surface energy, and it is substantially harder to determine in this case what a change in the lattice structure would do to the total energy. Assuming that such a phase did exist, it would be most likely to be noticeable in a low-mass star with appreciable crust or even a 1.3 $M_\odot$ star with a stiff equation of state. The existence of three nearly degenerate phases of matter could result in crustal regions with very large impurity levels, which might be reflected in the critical angle for stresses in the region. On the whole, it is unlikely that these phases will be directly observed.

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