Prog. Theor. Phys. Vol. 72, No. 2, August 1984, Progress Letters

Further Study of the Nuclear Shape in High-Density Matter

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(Received April 18, 1984)

A refined argument is given which strengthens the previous conclusion that the stable "nuclear" shape in high-density matter successively changes from sphere to cylinder, board, cylindrical hole and spherical hole as the density of the matter increases in the neighborhood of 10^{14} g/cm^3.

In relation to the high-density matter in supernovae or in the crust of neutron star, Ravenhall et al.[1] and Hashimoto et al.[2] showed that atomic nuclei may not have spherical symmetry in high-density matter. These authors concluded that the stable nuclear shape changes from sphere to cylinder, board, cylindrical hole and spherical hole as the density of the matter increases from 10^{13}g/cm^3 to $10^{14.5}$g/cm^3 before nuclear continuum is formed. Although the conclusions of these two studies are essentially the same, there is a large difference in the argumentation: Ravenhall et al. assumed a specific Hamiltonian, while Hashimoto et al. took a general liquid-drop approach.

In this paper, we refine the argumentation of Hashimoto et al. [Ref. 2) is referred to as HSY hereafter.] In HSY, there were two uncertainties which led to ambiguity in determining the most stable shape. One is the inaccuracy of Coulomb energies due to the error in the Monte Carlo method, and the other is the insufficient criterion to single out the most stable shape. We remove these two uncertainties. First, we derive the Fourier series for the Coulomb energy considering several arrangements of "nuclei" in addition to the simple ones assumed in HSY. Second, we use a more effective criterion to single out the stable shape. As in HSY, we consider an infinite system composed of protons, neutrons and electrons of which the protons are distributed uniformly and the electrons are distributed uniformly in the whole volume. The neutrons are distributed inside as well as outside the "nuclei"; the distribution of each side is also uniform, but the density inside is generally different from the one outside. The average charge neutrality is assumed and the temperature is taken to be 0 K. As was done in HSY, we divide the whole volume into appropriate cells. This cell includes one nucleus in the case of spherical shape, and one hole in the case of spherical hole. The lattice constant a is defined as the cubic root of the cell volume. In the case of cylinder, the plane perpendicular to the cylinder is divided into two-dimensional cells, each of which includes one cross section of cylinder, and the lattice constant a is defined as the square root of the area of the two-dimensional cell. The case of cylindrical hole is similar. In the case of board, the lattice constant a is defined as the sum of the thickness of a board and the distance between the neighboring boards. For definiteness, we take the volume of the three-dimensional cell as a^3 for any shape.

The Coulomb energy per cell[3] is given by

$$W_C=\frac{1}{2}\int_{\text{cell}}\rho(\boldsymbol{r})\phi(\boldsymbol{r})d\boldsymbol{r}\,, \tag{1}$$

where the charge distribution $\rho(\boldsymbol{r})$ and the electrostatic potential $\phi(\boldsymbol{r})$ are both assumed to be periodic. Expanding $\rho(\boldsymbol{r})$ and $\phi(\boldsymbol{r})$ into Fourier series, and then eliminating $\phi(\boldsymbol{r})$ with the use of Poisson's equation, we obtain

$$W_C=2\pi(\rho_p{}^2/a^3)\sum_{hkl}{}'(I_{hkl}/|\boldsymbol{G}_{hkl}|)^2\,. \tag{2}$$

Here, ρ_p is the charge distribution of protons in nuclei, and $\boldsymbol{G}_{hkl}$ is the reciprocal lattice vectors given by

$$\boldsymbol{G}_{hkl}=h\boldsymbol{A}+k\boldsymbol{B}+l\boldsymbol{C}\,, \tag{3}$$

where h, k and l are integers, and $\boldsymbol{A}$, $\boldsymbol{B}$ and $\boldsymbol{C}$ are the primitive transformation vectors of the reciprocal lattice. The prime on the summation symbol means that the point $\boldsymbol{G}_{hkl}=0$ is excluded. I_{hkl} is given by

$$I_{hkl}=\int_{\Omega}\exp(-i\boldsymbol{G}_{hkl}\cdot\boldsymbol{r})d\boldsymbol{r}\,, \tag{4}$$

where Ω is the domain occupied by a nucleus.

We have calculated the Coulomb energies for three lattice types in the case of spherical nuclei, and two lattice types in the case of the cylindrical nuclei; for spheres, they are simple cubic (sc), body-centered cubic (bcc) and face-centered cubic (fcc), and for cylinders, they are two-dimensional square (sq) and two-dimensional hexagonal (hex). We have also calculated the Coulomb energy of boards. For simplicity, we express W_C in terms of $w_{C1}(u)$ as follows:

$$W_C=\rho_p{}^2a^5w_{C1}(u), \tag{5}$$

where u is the volume ratio of the nucleus to the cell. For spheres, $w_{C1}(u)$ are given as

$$\text{sc: } w_{C1}(u)=C_1u^{4/3}\sum_{hkl}{}'[j_1(u^{1/3}C_2R_{sc})/R_{sc}^2]^2, \tag{6}$$

$$\text{bcc: } w_{C1}(u)=C_1(2u)^{4/3}\times\sum_{hkl}{}'[j_1(u^{1/3}2^{-1/3}C_2R_{bcc})/R_{bcc}^2]^2, \tag{7}$$

$$\text{fcc: } w_{C1}(u)=C_1(4u)^{4/3}\times\sum_{hkl}{}'[j_1(u^{1/3}4^{-1/3}C_2R_{fcc})/R_{fcc}^2]^2, \tag{8}$$

with

$$C_1=3(4\pi^2)^{-1}(6/\pi)^{1/3},\quad C_2=\pi(6/\pi)^{1/3},$$
$$R_{sc}=(h^2+k^2+l^2)^{1/2},$$
$$R_{bcc}=[(h+k)^2+(k+l)^2+(l+h)^2]^{1/2},$$
$$R_{fcc}=[(h+k-l)^2+(h-k+l)^2+(-h+k+l)^2]^{1/2}.$$

Here j_1 is the first-order spherical Bessel function. For cylinders,

$$\text{sq: } w_{C1}(u)=\frac{u}{2\pi^2}\sum_{hk}{}'[J_1(2\sqrt{\pi u}R_{sq})/R_{sq}^2]^2, \tag{9}$$

$$\text{hex: } w_{C1}(u)=\frac{2u}{3\pi^2}\times\sum_{hk}{}'[J_1((2\sqrt{3}\pi u)^{1/2}R_{hex})/R_{hex}^2]^2, \tag{10}$$

with

$$R_{sq}=(h^2+k^2)^{1/2},$$
$$R_{hex}=\left[h^2+\frac{1}{3}(h-2k)^2\right]^{1/2}.$$

Here J_1 is the first-order cylindrical Bessel function, and the prime on the summation symbol means that the point $(h, k)=(0, 0)$ is excluded. We have numerically calculated the series (6) ~(10) up to the accuracy of 0.01 %. For boards,

$$\text{board: } w_{C1}(u)=\pi u^2(1-u)^2/6, \tag{11}$$

which was already given in Ref. 1). The expressions of $w_{C1}(u)$ for the lattice types of holes are obtained by replacing u by $1-u$. The function $w_{C1}(u)$ is illustrated in Figs.1 and 2. In Fig. 1 the curves for bcc and fcc are hardly distinguishable from each other, but that of bcc is slightly lower, and bcc is the most stable shape in the spherical nuclei. From Fig. 2 we see that hex is more stable than sq.

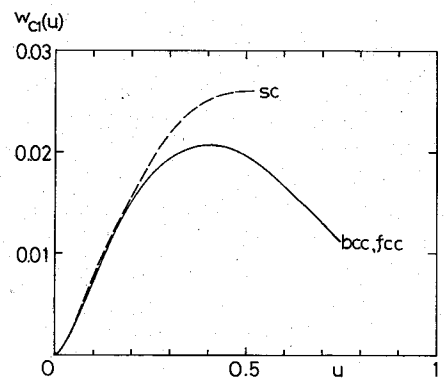

Fig. 1. Relative Coulomb energy $w_{C1}(u)$ for the matter with spherical nuclei. The curves correspond to three lattice types. The curve for bcc is actually lower than the one for fcc only by an indistinguishable amount. The range of u for bcc is $0\leqq u\leqq 0.6802$, which is narrower than that for fcc.

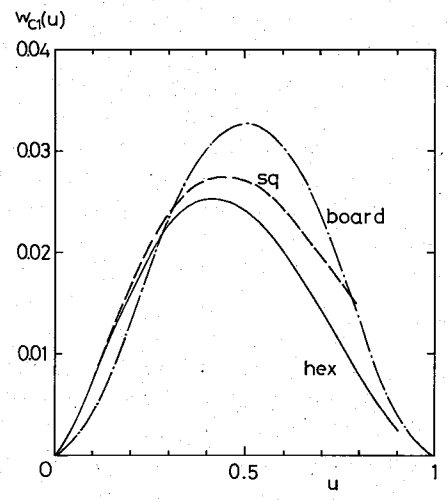

Fig. 2. Relative Coulomb energy $w_{C1}(u)$ for the matter with board-shaped or cylindrical "nuclei". Two lattice types are assumed for the latter.

Now we refine the criterion to be used to single out the stable shape. We compare the average energy densities of the two kinds of matter which have the nuclear shapes A and B and have the same microscopic intensive variables (u, n, x and n_{out} in HSY) but do not necessarily have the same lattice constant.*) Let shape A be in equilibrium, and let us denote its surface energy per cell by $W_s^A(a)$ and its Coulomb energy per cell by $W_c^A(a)$, in which the lattice constant a is explicitly written. With the same values of the same variables, shape B is not generally in equilibrium, but we define both $W_s^B(a)$ and $W_c^B(a)$ similarly. For shape A, we have the equilibrium condition[2] $W_s^A(a)=2W_c^A(a)$. Then, the energy density for shape B with a lattice constant μa is, apart from the bulk energy, written as

$$[W_s^B(\mu a)+W_c^B(\mu a)]/(\mu a)^3 = \lambda_1^{AB}(\mu) W_s^A(a)/a^3, \tag{12}$$

where

$$\lambda_1^{AB}(\mu)=\mu^{-1}[W_s^B(a)/W_s^A(a)] + \mu^2[W_c^B(a)/2W_c^A(a)]. \tag{13}$$

The minimum of $\lambda_1^{AB}(\mu)$ with respect to variation of μ is given by

$$\lambda_{10}^{AB}=\frac{3}{2}[W_s^B(a)/W_s^A(a)]^{2/3} \times [W_c^B(a)/W_c^A(a)]^{1/3}. \tag{14}$$

Then, we get a very simple criterion to determine the stable shape: If $\lambda_{10}^{AB}<3/2$, then shape B is more stable than shape A. Obviously this criterion uniquely determines the most stable nuclear shape for a given u. The results are shown in Fig. 3. We have taken bcc for spherical nuclei and hex for cylindrical nuclei. If we compare Fig. 3 with Fig. 4 of HSY, we see that the ambiguities in the latter are completely removed in the former.

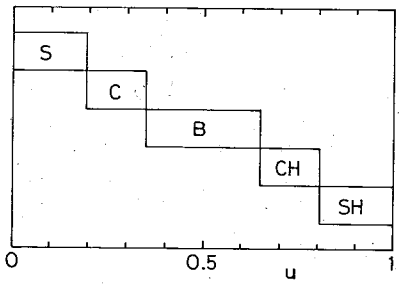

Fig. 3. The stable nuclear shapes to be realized with various values of the nuclear volume fraction u. S: sphere (bcc lattice), C: cylinder (hexagonal lattice), B: board, CH: cylindrical hole (hexagonal lattice), SH: spherical hole (bcc lattice).

In conclusion, we have improved the argument and results of HSY[2] and strengthened the conclusion that the nuclear shape in high-density matter successively changes from sphere to cylinder, board, cylindrical hole and spherical hole as the density of the matter increases before nuclear continuum is formed.

1) D. G. Ravenhall, C. J. Pethick and J. R. Wilson, Phys. Rev. Lett. **50** (1983),2069.
2) M. Hashimoto, H. Seki and M. Yamada, Prog. Theor. Phys. **71** (1984), 320.
3) C. Kittel, *Introduction to Solid State Physics* (John Wiley and Sons, New York, 1956), p. 571.

*) In HSY, comparison was made between two shapes with the same lattice constant, which led to a less effective criterion.