LIQUID AND CRYSTALLINE NEUTRON MATTER*

L. H. Nosanow⁺ and L. J. Parish

School of Physics and Astronomy
University of Minnesota
Minneapolis, Minnesota 55455

425 7000

and

School of Mathematical and Physical Sciences
University of Sussex
Falmer, Brighton, England

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⁺ Senior Visiting Fellow at the University of Sussex for the 1971-72 academic year.

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Abstract

Results of calculations of the ground-state energies of liquid and crystalline neutron matter are presented. It is found that neutron matter will crystallize at a density near normal nuclear density. This results indicates that a large fraction of the interior of a neutron star consists of crystalline neutron matter. An intuitive physical discussion is given to illuminate this result. Furthermore, it is suggested that, contrary to the usual point of view, low density matter should be regarded as a "quantum liquid" which is "almost" a "quantum crystal".

Since the identification of pulsars as rapidly rotating neutron stars¹, there have been many studies^{2,3} of the ground-state properties of neutron matter because an accurate knowledge of these properties is basic to the understanding of neutron stars.^{4,5} The purpose of this letter is twofold: to present the initial results of our calculations of the ground-state properties of neutron matter and to give an intuitive physical discussion of these results. We have calculated the ground-state energy of both the liquid and crystalline phases of neutron matter for densities in the range 0.17 nucleons/fm³ (normal nuclear density) to 0.4 nucleons/fm³. The results are summarized and compared with those for helium-three in Fig. 1. We find that neutron matter will begin to crystallize at a density of about 0.23 nucleons/fm³ with a solidification pressure of about 7.1 MeV/fm³ (1.1×10^{28} atm). Although this result is consistent with recent intuitive arguments,^{6,7,8} it differs from that of Canuto and Chitre⁹ (who find solidification at a much higher density) and from that of Pandharipande¹⁰ (who does not find solidification at all). If this result is confirmed in future more refined calculations, we believe that it may modify the present conceptual picture of nuclear matter, which is often¹¹ regarded as a low-density liquid which is "almost" a gas. On the contrary, our results indicate that nuclear matter should be thought of as a "quantum liquid" which is "almost" a "quantum crystal."

It is worthwhile to discuss neutron matter and helium-three in parallel because there are many similarities between the two systems. In both cases the Hamiltonian is well approximated by the same form

$(H = \sum_i (-\hbar^2/2m)\nabla_i^2 + \sum_{i<j} v_{ij})$, where each pair potential has a strong, short-range repulsion with a core diameter r_c and a weak attraction of longer range as shown in Fig. 2. Of course, the neutron-neutron interaction is more complicated because of its spin and angular momentum dependence. An important feature of both systems is that they are quantum systems; i.e., the magnitude of the zero-point kinetic energy is comparable to the magnitude of the potential energy. This causes both systems to exist at anomalously low densities. If we define Δ as an average nearest-neighbor distance for the liquid, then we can see from Fig. 2 that for liquid helium-three $\Delta_L \simeq 1.5 r_{\min}$ whereas for normal nuclear matter $\Delta_N \simeq 2 r_{\min}$. In our opinion, it is most illuminating to view this low density as a quantum-mechanical effect arising from the particles behaving as if they had an "effective core diameter" $r_c^{\text{eff}} > r_c$, which is due to the relatively large amplitude zero-point motion. A crude estimate of this effect can be obtained by considering each particle to be in an oscillator well and estimating the mean-square deviation from the well-known result $\langle u^2 \rangle = 3\hbar^2/2m\langle t \rangle$, where $\langle t \rangle$ is the average kinetic energy per particle. Taking $\langle t \rangle \simeq 20$ deg for helium-three and $\langle t \rangle \simeq 30$ MeV for nucleons, we find $\sqrt{\langle u^2 \rangle} \simeq 1.1 \text{ \AA}$ for helium-three and $\sqrt{\langle u^2 \rangle} \simeq 1.4 \text{ fm}$ for nucleons. Thus, for helium-three r_c^{eff} should be of the order of 50% greater than r_c , whereas for neutrons, it should be several times larger. From this point of view, it is easy to understand not only why nuclear matter has been thought analogous to a low-density gas but also why it is really more analogous to a quantum liquid such as liquid helium-three.

The concept of the large "effective core size" is also important

in understanding the formation of a "quantum crystal." After all, helium-three crystallizes at a very low density as shown by the value of Δ_x (the nearest-neighbor distance in the crystal at the lowest pressure at which it exists) from Fig. 2. This result can be understood simply in terms of the packing of these "quantum mechanical spheres." On this basis, it is to be expected that neutrons will also crystallize at a low density with a Δ slightly less than Δ_N and this is what we find in our calculations.

For the initial phase of our calculations, we have assumed a simple form for the neutron-neutron interaction; i.e.,

$$v_{ij} = \sum_{s=0,1} v_s(r_{ij}) P_s(ij), \quad (1)$$

where P_0 and P_1 are the singlet and triplet spin-projection operators and $v_0(r)$ and $v_1(r)$ are, respectively, the 1S_0 and the central part of the 3P_2 potentials as given by Reid.¹² These two potentials reproduce the neutron-neutron phase shifts¹² up to center-of-mass energies of about 50 MeV. In addition, (1) gives the general characteristics of the nucleon-nucleon interaction; namely, that it is strongly attractive in spatially symmetric states and weakly attractive in spatially antisymmetric states.

Our calculation is patterned after those of McMillan,¹³ Schiff and Verlet¹⁴ and Hansen and Levesque¹⁵ because their approach has yielded the best calculation of the ground-state energies of liquid and crystalline helium-three. The essential feature of this approach is the use of Monte-Carlo integration techniques to calculate the many-body effects of the short-range correlations. The problem

is formulated as a variational calculation of the ground-state energy of both liquid and crystalline phases using similar approximations for each phase. The trial function is chosen to have the form $\Psi = F \Phi$, where $F = \prod_{i < j} f(r_{ij})$ and $\Phi = A(\prod_i \varphi_i(r_i) \xi_i)$, where A is the antisymmetrizer and ξ_i is the spin function for particle i . For the liquid $\varphi_i(r_i) = \exp(i \underline{k}_i \cdot \underline{r}_i)$, where the wave vectors $\underline{k}_i$ and spin functions ξ_i are chosen to fill the Fermi sea; whereas, for the crystal $\varphi_i(r_i) = \exp(-\frac{1}{2} A(\underline{r}_i - \underline{R}_i)^2)$, where $\underline{R}_i$ is the i th lattice vector and A is a variational parameter which characterizes the mean-square deviation of a particle from its lattice site and we chose an antiferromagnetic arrangement of spins on a body-centered cubic lattice. In most of our calculations we chose $f(r) = \exp(-(b/r)^\eta)$, where b and η are variational parameters.

In order to make the calculation computationally feasible, those correlations arising from antisymmetrization have been approximated by evaluating the leading term in a statistical cluster expansion.^{16,17} This expansion is known to converge rapidly for helium-three.¹⁴ With all of the above, the ground-state energies for the liquid and crystalline phases to leading order in the exchange are given as follows:

$$\begin{aligned}
 E_{\text{liquid}} = & (3/5)\epsilon_F \\
 & + 12 \rho \epsilon_F \int_0^1 dy y^4 (1 - \frac{3}{2}y + \frac{1}{2}y^3) \int d^3r g_B(r) \cos(2 \underline{k}_F \cdot \underline{r} y) \\
 & + (\rho/8) \sum_{S=0,1} (2 - (-1)^S) \int d^3r g_B(r) \tilde{v}_S(r) (1 + \\
 & \quad (-1)^S (3 J_1(k_F r)/k_F r)^2) , \quad (2)
 \end{aligned}$$

where

$$\tilde{v}_S(r) = v_S(r) - (\hbar^2/2m)\nabla^2 \ln f(r)$$

$$g_B(r) = N(N-1) \int d^3r_3 \dots \int d^3r_N F^2 / \rho^2 \int d\tau F^2,$$

and $d\tau = d^3r_1 \dots d^3r_N$, and

$$\begin{aligned} E_{\text{crystal}} = & 3 \hbar^2 A/4m + (\hbar^2 A^2/8m) \sum_{j>1} \Delta_j^2 P_j/(1-P_j) \\ & + (\rho/4) \sum_{S=0,1} \sum_{j>1} (1 - (-1)^S \delta_{m_1 m_j}) \int d^3r \tilde{v}_S(r) \\ & \times (F_j(r) + (-1)^S F_{jx}(r))/(1-P_j), \end{aligned} \quad (3)$$

where, if $\psi_e = F \prod_{i=1}^N \phi_i(r_i)$ and P_{ij} permutes i and j ,

$$F_j(r) = \int d\tau \delta(r-r_{1j}) \psi_e^2 / 4\pi r^2 \int d\tau \psi_e^2$$

$$F_{jx}(r) = \int d\tau \delta(r-r_{1j}) \psi_e P_{ij} \psi_e / 4\pi r^2 \int d\tau \psi_e^2$$

$$P_j = \delta_{m_1 m_j} \int d\tau \psi_e P_{1j} \psi_e / \int d\tau \psi_e^2$$

Equations (2) and (3) reduce to the well-known equations for liquid¹⁴ and crystalline¹⁷ helium-three if $v_0(r)$ and $v_1(r)$ are taken to be equal.

Our results are given in Fig. 1b and in Table I. From the figure, we see that neutron matter is a liquid for densities lower than ≈ 0.23 neutrons/fm³ and a crystal for densities higher than ≈ 0.30 neutrons/fm³.

At intermediate densities both phases coexist and the pressure is constant at approximately 7 MeV/fm^3 . Thus, we find that for neutron matter $\Delta_x = 1.6 \text{ fm}$. So that for neutron matter $\Delta_x/\Delta_N = 0.8$; whereas, $\Delta_x/\Delta_L = 0.85$ for helium-three. In Table 1, we show some of the numerical results for a density of $0.3 \text{ nucleons/fm}^3$. The main point illustrated here is the insensitivity of our results to different correlation functions.¹⁸ It is readily seen that, not only is the energy difference between the liquid and solid phases insensitive to the form of the correlation function, but the value of the localization parameter A is also unchanged. This result gives us confidence that our calculation of the solidification pressure is unlikely to be qualitatively affected by the choice of the correlation function.

Still, we believe that there are many points to be studied before the results we have reported here can be regarded as firmly established. In the first place, it is clearly necessary to ascertain the effects of spin dependence in the Jastrow factor. Secondly, it remains to test, in detail, the convergence of the cluster expansion. In addition, it is a formidable problem to include the effect of the angular momentum dependence of the potential and of the correlation function. Although all of these effects could have a bearing on the final results, it is our opinion that they will only shift the absolute value of the liquid and crystal energies by about the same amount so that our conclusion regarding the solidification density and pressure would remain basically unchanged. Our results indicate that the entire interior of a neutron star inside the crust is a giant quantum crystal. The possible implications of this result should merit careful study.

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18. We are indebted to Dr. V. Pandharipande for suggesting the second form that we used.

Table Caption

Table 1. The liquid and crystalline energy/particle(MeV) at a density of $0.3 \text{ neutrons/fm}^3$ for two different correlation functions.. The energies are the correlational and total kinetic energies, the potential energy, and the total energy. The values of the variational parameters b (in fm) and A (in fm^{-2}) are also given.

Table I

Correlation function		T_F	T	V	E	b	A
$f(r) = \text{Exp}(-(b/r)^4)$	Liquid	25.9	78.9	-38.0	41.0	.425	-
	Crystal	27.6	94.9	-55.7	39.2	.45	.80
$f(r) = \begin{cases} \frac{1}{2}(1 - \cos(\pi r/b)), & r < b \\ 1 & , r > b \end{cases}$	Liquid	25.9	76.7	-41.4	35.3	1.11	-
	Crystal	23.0	90.8	-56.8	34.0	1.11	.75

Figure Captions

1. The calculated equation-of-state for helium-three (Fig. 1a) and neutron matter (Fig. 1b). The curves for helium-three were taken from references (14) and (15). The arrows on Fig. 1b indicate the density regime in which liquid and crystalline neutron matter coexist.
2. A schematic comparison of the helium-helium (Fig. 2a) and neutron-neutron (Fig. 2b) interactions. Only the central part of the $^3P_2 - ^3F_2$ is given.

ENERGY (DEG/PARTICLE)

Fig. 1a

ENERGY (MeV/NEUTRON)

Fig. 1b

Fig. 2a

$v(r)$ (100 MeV/PARTICLE)