Solidification of neutron matter

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A new parity-conserving equation of motion is used to evaluate the ground state of a system of high density neutrons in a quantum crystal. If one form of a purely repulsive *NN* potential is employed, the ground state energy has a minimum with respect to the localization parameter in the density range appropriate to neutron star interiors, whereas it does not if a realistic *NN* potential is used. However, the values of the localization parameters α_m^{-1} corresponding to the observed minima are very close to or even less than the separation Δ between neutrons. Since the method employed here for the solid is only reliable when $\alpha_m \Delta > 1$, one cannot definitely say that an equilibrium solid state exists even in this case.

[NUCLEAR STRUCTURE Neutron solidification, possibility of solidification of neutron star matter examined.]

I. INTRODUCTION

A letter with the same title was published by Canuto and Chitre[1] in 1973, which indicated how the Reid *NN* potential, used in the context of the *t* matrix, favored a solid arrangement of neutrons over a liquid structure at densities greater than 1.6×10^{15} g cm^{-3}.

Several authors have discussed the same problem with different answers. In particular, the phenomenological types of calculations indicated that arranging the neutrons in a solidlike structure would lower the energy, with respect to the liquid.[2] At the time of publication of Ref. 1, only one computation reported a negative answer.[3] However, it would be seriously incorrect to catalog Ref. 1 as one more, perhaps more sophisticated, computation indicating that a solid indeed exists and to make a case on a majority basis. The only significant comparison is between Ref. 1 and Ref. 3, leaving aside the results of Ref. 2 that, though very interesting, do not help in resolving the discrepancy between Ref. 1 and Ref. 3. In Ref. 3, both the solid and liquid computations were performed, whereas in Ref. 1 only the solid was computed. By comparing the solid energies found in Ref. 1 with the liquid energies of Ref. 3, the authors of Ref. 1 concluded in favor of a solid arrangement. Since it is methodologically unsatisfactory to compare energies obtained with different techniques, an alternative method was employed in Ref. 1, based on the study of the elastic properties of the solid arrangement. The result did not change. In order to resolve the discrepancy, H. A. Bethe suggested that the *NN* potential be taken the same for any angular momentum state and equal to the repulsive part of the $^1S_0$ Reid potential. We would like to stress that the Bethe problem is important in spite of its unrealistic appearance at first sight. In fact, the realistic *NN* potentials presently available are much more complex than that used in Refs. 4 and 5. However, if a solid does not set in with such a potential the extension to a more complicated form will bring more attraction, a feature that does not help solidification. The results obtained using the techniques of Refs. 1 and 3 did not agree, but the situation was soon clarified. The results, as reported in Refs. 4 and 5, can be summarized as follows:

(1) Both computations found that the energy per particle E/N has a clear minimum with respect to α^{-1}, the spread of the single-particle wave function.

(2) In Ref. 5, it was also found that the energy of the solid is lower than that of the liquid, thus indicating a phase transition.

(3) The absolute values of the energies for the solid phase were, however, different, those of Ref. 5 being much higher.

In conclusion, with respect to the Bethe potential, in Ref. 4 it was found that $E(\alpha)$ has a minimum with respect to α^2 and in Ref. 5 it was found that the solid is the minimum-energy state. At the same time, however, two other computations were performed with an almost equally repulsive potential as the one used in Ref. 4. The first, by Chakravarty, Miller, and Woo,[6] reached the following conclusions:

(1) As for the solid,[6] the values obtained were rather close to those of Ref. 4. However, the values of α^{-1} were unsatisfactorily large. We feel that the results cannot yet be considered certain and therefore we shall not make use of them.

(2) As for the liquid,[7] the energies obtained were much lower than those of Ref. 5, the dis-

crepancy increasing with density, being of the order of 200 MeV at around 10^{15} g cm^{-3}. From the results of Refs. 6 and 7, one cannot conclude that a solid exists, but only that there is a new discrepancy in the energy for the liquid state.

(3) The energies for the liquid state of Ref. 7 agreed very well with those found by Cochran and Chester,[8] who employed a Monte Carlo technique. More specifically:

(a) The energies of the liquid are within 25 MeV of those of Ref. 7. The agreement is very satisfactory.

(b) These energies are considerably lower than those of Ref. 5.

(c) The energies for the solid are considerably higher than those of Ref. 4.

(d) Within the same Monte Carlo technique, the energies for the solid are higher than the energies for the liquid.

One can therefore conclude, for the liquid

(i) The LOCV technique, in itself, as employed in Ref. 5 cannot be trusted, since it yields too high energies. The results of a full variational technique[9] are however in good agreement with those of Refs. 7 and 8.

(ii) As far as the solid arrangement is concerned, the solid energies of Refs. 1 and 4 must be reevaluated.

It was realized by the present authors that within the t-matrix approach as previously employed,[1,4] a most serious deficiency was the lack of symmetry under parity inversion of the two-body Hamiltonian

$$[T_1 + T_2 + U(1) + U(2) + V_{12}]\psi_{12} = E_{12}\psi_{12}, \tag{1}$$

where $\hat{T}_1$ and $\hat{T}_2$ are the kinetic-energy operators for particles 1 and 2, respectively, $U(1)$ and $U(2)$ are their respective self-consistent Hartree potentials, and V_{12} is the two-body potential. $U(i)$ is taken to be of the form of a simple harmonic oscillator

$$U(i) = U(0) + \tfrac{1}{2}M\omega^2(\vec{r}_i - \vec{R}_i)^2, \tag{2}$$

where $\vec{R}_i$ is the coordinate of the ith lattice site, when the center of mass is eliminated, Eq. (1) reads

$$H(\vec{r})\psi(\vec{r}) = \epsilon\psi(\vec{r}), \tag{3}$$

where

$$H(\vec{r}) = -\frac{\hbar^2}{M}\nabla_r^2 + \tfrac{1}{4}M\omega^2(\vec{r} - \vec{\Delta})^2 + V(\vec{r}) \tag{4}$$

and $\vec{\Delta} \equiv \vec{R}_2 - \vec{R}_1$. Since $\hat{H}(\vec{r}) \neq \hat{H}(-\vec{r})$, ψ has no definite parity and when a full angular momentum decomposition is performed, unwanted waves like $^3S_1$ and $^1P_1$ appear. In Ref. 1 the potential for such waves was taken to be repulsive, thus introducing an unjustified amount of repulsion.

II. SYMMETRIC TWO-BODY HAMILTONIAN

Recently, a parity conserving two-body Hamiltonian analogous to Eq. (4) has been derived. This can be accomplished by requiring that Eq. (1) for two particles in the $V_{12} = 0$ case be

$$[T_1 + T_2 + U_s(1,2)]\phi^{\pm}(1,2) = E_0^{\pm}\phi^{\pm}(1,2), \tag{5}$$

where $\phi^{\pm}(1,2)$ are properly antisymmetrized wave functions for the two particles and $U_s(1,2)$ is the Hartree potential for the two particles. The above antisymmetrized wave functions require $U_s(1,2)$ to be symmetric under particle exchange. Since the equation of motion for each particle is given by

$$(T_i + U_i)\varphi_i(i) = [\tfrac{3}{2}\hbar\omega + U(0)]\varphi_i(i), \tag{6}$$

where $U(i)$ is given by Eq. (2) and $\phi_i(i)$ is a Gaussian function of the form

$$\varphi_i(i) = \varphi_{R_i}(\vec{r}_i) = \frac{\alpha^{3/2}}{\pi^{3/4}}\exp[-\tfrac{1}{2}\alpha^2(\vec{r}_i - \vec{R}_i)^2]. \tag{7}$$

$\alpha^{-1} \equiv (\hbar/M\omega)^{1/2}$ is a measure of the spread of the wave function about the lattice site $\vec{R}_i$. We now choose the eigenvalue of Eq. (5) for the two-body equation in the case $V_{12} = 0$ to be simply twice that of the one-body equation given in Eq. (6), i.e.,

$$E_0^{\pm} = 3\hbar\omega + 2U(0). \tag{8}$$

This choice amounts to neglecting exchange effects. Similarly, $\phi^{\pm}(1,2)$ is chosen to be the properly symmetrized and antisymmetrized product of Gaussians

$$\varphi^{\pm}(1,2) = 2^{-1/2}[\varphi_1(1)\varphi_2(2) \pm \varphi_2(1)\varphi_1(2)]; \tag{9}$$

+ corresponds to spin antisymmetric ($S = 0$) case and − to the spin symmetric ($S = 1$) case. In terms of relative and center of mass coordinates $\vec{r}$ and $\vec{R}$, respectively, Eq. (9) reads

$$\phi^{\pm}(1,2) = 2^{-1/2}\Phi(\vec{R})[\varphi_d(\vec{r}) \pm \varphi_x(\vec{r})], \tag{10}$$

where $\Phi(\vec{R})$ is the center of mass wave function given by

$$\Phi(\vec{R}) = \frac{\alpha^{3/2}}{(\frac{1}{2}\pi)^{3/4}}\exp\{-\alpha^2[\vec{R} - \tfrac{1}{2}(\vec{R}_1 + \vec{R}_2)]^2\}, \tag{11}$$

and

$$\varphi_d(\vec{r}) = \frac{\alpha^{3/2}}{(2\pi)^{3/4}}\exp[-\tfrac{1}{4}\alpha^2(\vec{r} - \vec{\Delta})^2],$$
$$\varphi_x(\vec{r}) = \frac{\alpha^{3/2}}{(2\pi)^{3/4}}\exp[-\tfrac{1}{4}\alpha^2(\vec{r} + \vec{\Delta})^2]. \tag{12}$$

In terms of $\vec{r}$ and $\vec{R}$ Eq. (5) now reduces to

$$\left[-\frac{\hbar^2}{4M}\nabla_R^2-\frac{\hbar^2}{M}\nabla_r^2+U_s(1,2)\right]\phi^{\pm}(1,2)=[3\hbar\omega+2U(0)]\,\phi^{\pm}(1,2). \quad (13)$$

If we write $U_s(1,2)\equiv U_s(\vec{R})+U_s(\vec{r})$, Eq. (13) becomes

$$\left[-\frac{\hbar^2}{M}\nabla_r^2+U_s(\vec{r})+\tfrac{3}{2}\hbar\omega\right]\varphi^{\pm}(\vec{r})=[3\hbar\omega+2U(0)]\varphi^{\pm}(\vec{r}), \quad (14)$$

where

$$U_s(\vec{R})=M\omega^2[\vec{R}-\tfrac{1}{2}(\vec{R}_1+\vec{R}_2)]^2. \quad (15)$$

Now

$$\nabla_r^2\varphi^{\pm}(\vec{r})=-\frac{\alpha^2}{2\sqrt{2}}\{[3-\tfrac{1}{2}\alpha^2(\vec{r}-\vec{\Delta})^2]\varphi_d(\vec{r})\pm[3-\tfrac{1}{2}\alpha^2(\vec{r}+\vec{\Delta})^2]\varphi_x(\vec{r})\},$$

so we can solve Eq. (14) for $U_s(\vec{r})$ to get

$$U_s^{\pm}(\vec{r})=2U(0)+\tfrac{1}{4}M\omega^2(r^2+\Delta^2-2\vec{r}\cdot\vec{\Delta})\begin{cases}[\tanh(\frac{1}{2}\alpha^2\vec{r}\cdot\vec{\Delta})], & S=0\\ [\coth(\frac{1}{2}\alpha^2\vec{r}\cdot\vec{\Delta})], & S=1,\end{cases} \quad (16)$$

so that the proper parity-conserving two-body equation of motion for two neutrons now becomes

$$\left[-\frac{\hbar^2}{M}\nabla_r^2+\tfrac{1}{4}M\omega^2\left((r^2+\Delta^2-2\vec{r}\cdot\vec{\Delta})\begin{cases}[\tanh(\frac{1}{2}\alpha^2\vec{r}\cdot\vec{\Delta})]\\ [\coth(\frac{1}{2}\alpha^2\vec{r}\cdot\vec{\Delta})]\end{cases}\right)+V(r)\right]\psi(\vec{r})=\epsilon\psi(\vec{r}). \quad (17)$$

This new form of $U(r)$ is (a) symmetric with respect to space inversion, thus ensuring the inclusion of only the right waves; (b) has a hump at $r=0$, the height being Δ^2, (c) is zero at $r\sim\pm\Delta$, i.e., it has the form of a double humped harmonic oscillator; and, finally, (d) it follows directly from requiring that the properly symmetrized ψ_{12} should reduce to the free wave function ϕ_{12}, when V_{12} vanishes. The healing property of ψ_{12} is automatically satisfied.

Equation (17) has been used in Ref. 10 to compute the ground state energy for solid He^3 and the results are the closest to the experimental data obtained so far.

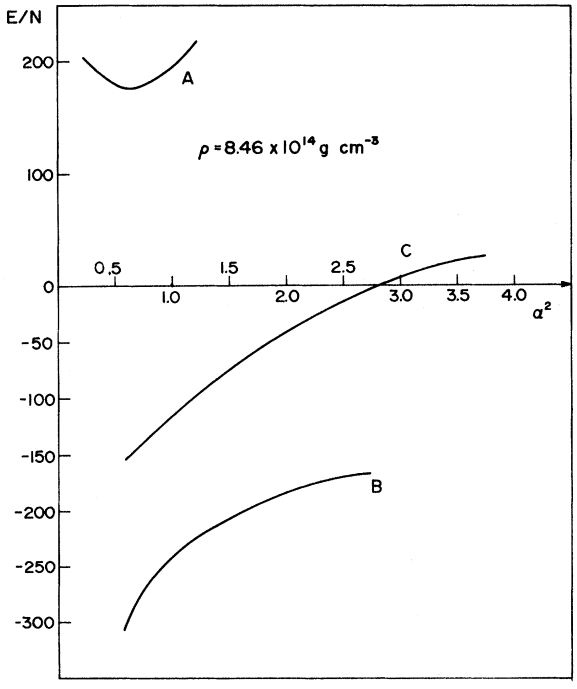

FIG. 1. Energy per particle, E/N (MeV) vs α^2 (fm^{-2}) at a density of 8.43×10^{14} g cm^{-3}, for different choices of the NN potential as specified in Eq. (18).

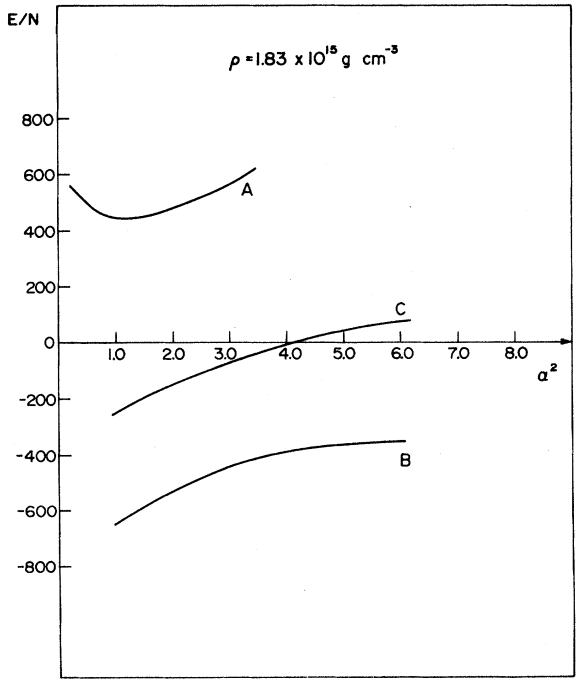

FIG. 2. Same as Fig. 1 for $\rho=1.83\times10^{15}$ g cm^{-3}.

III. RESULTS FOR NEUTRON SOLID

Having solved the main difficulty of Eq. (4) and having tested the results in the sensitive He^3 case, we have applied the t-matrix technique, as fully explained in Ref. 1, to the neutron case.

The potentials were taken from the *NN* potential recently constructed by Bethe and Johnson.[11] The forms used were the following ($y = 0.7r$):

(A) for any L,

$$yV(r) = 4015.5e^{-5.5y}, \tag{18}$$

(B) for any L,

$$yV(^1S_0) = 4015.5e^{-5.5y} - 10.463e^{-y} - 1837.5e^{-3.8y},$$

(C)

$$yV(^1S_0) = \text{same as above},$$

$$yV(^1D_2) = 4015.5e^{-5.5y} - 10.463e^{-y} - 1441.2e^{-3.8y}$$

$$yV(L=1) = 4015.5e^{-5.5y} + 3.488e^{-y} - 1010.36e^{-3.8y}$$

$$yV(L=3) = 4015.5e^{-5.5y} + 3.488e^{-y} - 937.9e^{-3.49y}.$$

With the repulsive potential A, the curves of E/N vs α^2 had minima within the density range tested, viz., 5×10^{14} to 1.83×10^{15} g cm^{-3}. Two of these curves are shown in Figs. 1 and 2 and are labeled A.

Since the quantity $\alpha\Delta$ is a measure of the ratio of the lattice separation to the spread of the wave function, we require $\alpha_n\Delta > 1$ for this t-matrix method to be reliable, where α_n are the values of α at the minima. According to Figs. 1 and 2, the minima occur at $\alpha_n\Delta \lesssim 1$, so it cannot reliably be stated that an equilibrium solid state exists in the above density range for potential A. In Ref. 4, where the repulsive part of the Reid $^1S_0$ potential is used, minima in the E/N vs α^2 curves occurred at $\alpha_n\Delta \approx 2$, which is a more comfortable value. Even if an equilibrium solid state does exist for potential A, we cannot definitely say that it is the phase of lowest energy since we lack the corresponding energy for the liquid phase.

If one introduces some attraction and one uses the full $^1S_0$ potential for all angular momentum states, the minimum disappears, as shown by curves B.

Even more realistically, we can now use the full Bethe-Johnson potential for each partial-wave state, as shown by choice C. The E/N vs α^2 curves again have no minima. The negative energies of curves B and C are unphysical, and these curves clearly have no minima.

It is apparent then that the parity-conserving Hamiltonian used in the paper reduces the possibility of a solid structure in neutron stars by eliminating the repulsive unwanted waves. We have also checked that another purely phenomenological local potential[12] that fits the phase-shifts equally well does not change the previous results. As a matter of fact, the resulting energies are almost identical.

A few comments on both Fig. 1 and Fig. 2 concerning the negative values of E/N are in order. Potentials A and B are highly unrealistic. The first is repulsive for any internuclear distance and it therefore produces positive energy for any density. Potential B is equally unrealistic since it pretends to represent the *NN* potential in any LJ state as a $^1S_0$ potential. As we know, the $^1S_0$ potential is more attractive than any other potential in any LJ state. It reaches a minimum of about -80 MeV at $r \approx 0.7$ fm. The repulsive part of $^1S_0$ is not strong enough to overcome such an attraction except at high density. As a matter of fact, were the repulsive part more repulsive, the analogy with solid He^3 where a strong Lennard-Jones potential is operating, would have been instructive. The only realistic choice is actually potential C. The action of the extra repulsion with respect to $^1S_0$ brought in by high angular momentum waves is clearly discernible. Finally, the $^3P_1$ state is known to be always repulsive, whereas the $^1D_2$ potential, even though almost as attractive as $^1S_0$ has its action strongly curtailed by the strong centrifugal barrier $l(l+1)/r^2$.

For $\rho = 8.46\times10^{14}$ g cm^{-3}, the distance of the first neighbor is $\Delta = 1.358$ fm. Since each wave function[7] has a spread α^{-1}, the very fact that we use localized wave function of this type implies that the computation is not valid if $\alpha^{-1} \gtrsim \frac{1}{2}\Delta$, i.e., each wave function, localized at a lattice site R, should not have a spread larger than half the distance to the next particle.

For instance, only from $\alpha^2 = 2$, $\alpha^{-1} = 0.7$, and $\frac{1}{2}\Delta = 0.7$ do the results start to become meaningful. We have, however, reported values of E/N for lower values of α^2 to stress the importance of the interplay between attraction and repulsion.

We therefore conclude that if we employ the realistic form of the *NN* potentials the E/N vs α^2 curve does not possess a minimum, a condition necessary for a solid structure to exist.

Recently, Takemori and Guyer[13] have published computations on solid neutron matter using a t-matrix formalism similar to ours but with the corresponding Reid potentials to A, B, and C. Their results of E/N vs α^2 are quite close to those presented here for all three potentials.

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