

Approximate analytic self-consistent solution of the Overhauser problem for $T \geq 0$

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Overhauser's suggestion that plane-wave orbitals, which yield a homogeneous-density fluid phase, may not correspond to the ground state of nuclear matter is investigated by an approximate analytic method. Wave functions constructed from so-called Overhauser orbitals, which lead to an oscillating-density crystalline solid phase, are shown to yield an energy gain over the plane wave orbitals only at densities well below the saturation density $\rho_0 \sim 0.17 \text{ fm}^{-3}$. This is in good agreement with previous numerical results. The analytic solution is then generalized to finite temperatures and it is found that the solid phase can survive up to temperatures of approximately 1.1 MeV only. Nuclear matter in the solid phase is similar to an intrinsic semiconductor with an energy gap occurring at the Fermi energy. The gap decreases with the rise in temperature until the melting point is reached where it discontinuously jumps to zero indicating that the transition is of first order.

I. INTRODUCTION

In 1960 Overhauser¹ questioned the assumption usually made that the ground state of nuclear matter (or any interacting Fermi fluid of infinite extent) is described by the familiar wave function constructed from plane-wave orbitals with the familiar sphere of occupied momentum states. Such a solution results in a uniform density whereas it is possible to construct other wave functions from so-called Overhauser orbitals that produce a periodically varying density and which can be shown, for certain interactions, to give an energy lower than the plane-wave solution and may thus describe the ground state of the infinite system of fermions. This problem is actually related to the question of whether there is a crystalline (i.e., solid) phase of nuclear matter as the Overhauser orbitals lead essentially to α -like clusters of four nucleons arranged on a lattice.

This problem has been investigated thoroughly since Overhauser's original work (see, e.g., Refs. 2-6) and it has been demonstrated in a numerical Hartree-Fock calculation⁶ employing a modern density-dependent Skyrme interaction⁷ that Overhauser's orbitals do not correspond to the ground state at the saturation density of nuclear matter. It was found, however, that there is a low-density region, well below saturation density, in which Overhauser's orbitals yield an energy gain over the plane-wave solution. All of these investigations have, however, been carried out at zero temperature and hence did not explore the behavior of nuclear matter at nonzero temperatures, especially the possibility of a solid-fluid phase transition in nuclear matter.

The purpose of this work is to obtain an approximate analytic solution for this problem equivalent to the numerical calculation done in Ref. 6, to generalize this analytic solution to finite temperatures, and to study the existence of the solid like phase for nuclear matter.

II. The Overhauser problem at zero K

We consider a system of $A \gg 1$ nucleons in a cubic box of volume $V = L^3$ with periodic boundary conditions, and

use the orthonormal orbitals from Ref. 6:

$$\phi_{\mathbf{k}}(\mathbf{r}) = \phi_{k_x}(x)\phi_{k_y}(y)\phi_{k_z}(z), \tag{2.1a}$$

$$\phi_{k_x}(x) = (u_{k_x} + v_{k_x} e^{-iq_x x}) e^{ik_x x/\sqrt{L}}, \tag{2.1b}$$

where

$$\begin{aligned} \text{sgn} q_x &= \text{sgn} k_x; -k_0 \leq k_x, k_y, k_z \leq k_0, \\ |q_x| &= 2k_0, u_{k_x}^2 + v_{k_x}^2 = 1, \end{aligned} \tag{2.1c}$$

with similar expressions for y and z . Because of the cubic symmetry of the problem we have $q_x = q_y = q_z$ and we set

$$q = |q_x| = |q_y| = |q_z| = 2k_0. \tag{2.1d}$$

The starting point for our solution is to assume that the nucleons move with an effective mass m^* in a periodic single-particle potential of the form:

$$U(\mathbf{r}) = U_0 + U_1(\cos qx + \cos qy + \cos qz), \tag{2.2}$$

where U_0 and U_1 are real constants to be determined by requiring self-consistency (i.e., solving the Hartree-Fock equations). The assumption of such a form for $U(\mathbf{r})$ is justified because the density resulting from the single-particle orbitals of Eqs. (2.1) has such a periodic variation [see Eq. (2.9a) below] with a relatively small amplitude as will be shown towards the end of this section and as indicated by the results of previous calculations.⁶ If the single-particle potential has the form given in Eq. (2.2) then the three-dimensional problem reduces to three identical one-dimensional problems, as is already anticipated in the form of $\phi_{\mathbf{k}}(\mathbf{r})$ assumed in Eq. (2.1a).

These one-dimensional problems are identical to the one-dimensional weak-binding theory of energy bands found in any standard textbook in solid state physics (see, e.g., Ref. 8). This allows us to determine the single-particle energy levels and wave functions [i.e., u_{k_i} and v_{k_i} in Eq. (2.1b)]:

$$u_{k_i}^{\pm} = \frac{|U_1|}{[4\{\varepsilon_{k_i}^{\pm} - \varepsilon_{k_i}\}^2 + U_1^2]^{1/2}}, \quad (2.3a)$$

$$v_{k_i}^{\pm} = \frac{2\{\varepsilon_{k_i}^{\pm} - \varepsilon_{k_i}\}}{[4\{\varepsilon_{k_i}^{\pm} - \varepsilon_{k_i}\}^2 + U_1^2]^{1/2}}, \quad (2.3b)$$

where

$$\varepsilon_{k_i} = \frac{\hbar^2 k_i^2}{2m^*}, \quad (2.4a)$$

is the single-particle energy corresponding to a plane-wave solution, and

$$\varepsilon_{k_i}^{\pm} = \frac{1}{2}(\varepsilon_{k_i} + \varepsilon_{k_i - q}) \pm \frac{1}{2}[U_1^2 + (\varepsilon_{k_i} - \varepsilon_{k_i - q})^2]^{1/2} \quad (2.4b)$$

is the single-particle energy corresponding to an Overhauser orbital (i.e., for $U_1 \neq 0$). The minus signs in Eqs. (2.3) and (2.4) refer to single-particle orbitals with

$|k_i| \leq k_0$ (the first Brillouin zone in the extended zone scheme), and the plus signs refer to orbitals with $|k_i| > k_0$. Only the orbitals with $|k_i| \leq k_0$ are occupied at $T=0$ K so that only $u_{k_i}^-$ and $v_{k_i}^-$ are needed in this section; the $u_{k_i}^+$ and $v_{k_i}^+$ are given here for completeness since they will be needed when discussing the $T > 0$ case in the coming sections. Note that $\varepsilon_{k_0}^{\pm} = \varepsilon_{k_0} \pm (|U_1|/2)$ so that an energy gap of magnitude $\varepsilon_{k_0}^+ - \varepsilon_{k_0}^- = |U_1|$ appears at the boundary between the first and second Brillouin zones, i.e., between the occupied and unoccupied orbitals at $T=0$.

With the u_{k_i} and v_{k_i} given by Eqs. (2.3) it is possible to calculate the density of the system:

$$\rho(\mathbf{r}) = g \sum_{k_x, k_y, k_z} |\phi_{\mathbf{k}}(\mathbf{r})|^2, \quad (2.5a)$$

where g is the spin-isospin degeneracy of each orbital ($g=4$ for symmetric nuclear matter), and the summation is over all occupied orbitals $|k_i| \leq k_0$. Therefore,

$$\begin{aligned} \rho(\mathbf{r}) &= \frac{g}{V} \sum_{k_x, k_y, k_z} (1 + 2u_{k_x}^- v_{k_x}^- \cos qx)(1 + 2u_{k_y}^- v_{k_y}^- \cos qy)(1 + 2u_{k_z}^- v_{k_z}^- \cos qz) \\ &= \rho_h (1 + 2\Delta \cos qx)(1 + 2\Delta \cos qy)(1 + 2\Delta \cos qz), \end{aligned} \quad (2.5b)$$

where

$$\rho_h = \frac{A}{V} = g \frac{(2k_0)^3}{(2\pi)^3} = g \frac{q^3}{(2\pi)^3} \quad (2.6)$$

is the homogeneous density of nuclear matter (i.e., if all the orbitals occupying the Fermi cube correspond to plane waves), and where we have introduced the dimensionless parameter [see the Appendix, Eqs. (A1)–(A8)]:

$$\begin{aligned} \Delta &= \frac{2\pi}{Lq} \sum_{k_i=-k_0}^{+k_0} u_{k_i}^- v_{k_i}^- \rightarrow \frac{2}{q} \int_0^{q/2} u_{k_i}^- v_{k_i}^- dk_i \\ &= \frac{-m^* |U_1|}{\hbar^2 q^2} \ln \left\{ \left[1 + \left[\frac{\hbar^2 q^2}{2m^* |U_1|} \right]^2 \right]^{1/2} + \frac{\hbar^2 q^2}{2m^* |U_1|} \right\}. \end{aligned} \quad (2.7)$$

Note that the last expression for Δ implies that Δ is always negative regardless of the sign of U_1 . This can also be inferred from Eqs. (2.3) since $u_{k_i}^- v_{k_i}^- < 0$. Equation (2.7) also implies that $|\Delta|$ must be small since $|U_1|$ is typically $\ll (\hbar^2 q^2 / 2m^*)$ so that

$$\Delta \approx \frac{m^* |U_1|}{\hbar^2 q^2} \ln \left[\frac{m^* |U_1|}{\hbar^2 q^2} \right].$$

It is also possible to evaluate the kinetic energy density:

$$\tau(\mathbf{r}) = g \sum_{k_x, k_y, k_z} |\nabla \phi_{\mathbf{k}}(\mathbf{r})|^2, \quad (2.8a)$$

where again the summation is over all occupied orbitals $|k_i| \leq k_0$. This leads after some straightforward but lengthy calculation to the result:

$$\begin{aligned} \tau(\mathbf{r}) &\approx \rho_h \left[\frac{q^2}{12} - \frac{q^2}{2} \Delta \cos qx \right] (1 + 2\Delta \cos qy)(1 + 2\Delta \cos qz) \\ &\quad + 2 \text{ corresponding terms obtained by permuting } x, y, \text{ and } z. \end{aligned} \quad (2.8b)$$

The details of evaluating $\tau(\mathbf{r})$ and obtaining Eq. (2.8b) are given in the Appendix [Eqs. (A9)–(A12)]. Linearizing Eqs. (2.5b) and (2.8b) in terms of Δ we get

$$\rho(\mathbf{r}) \approx \rho_h [1 + 2\Delta(\cos qx + \cos qy + \cos qz)], \quad (2.9a)$$

$$\tau(\mathbf{r}) \approx \frac{\rho_h q^2}{4} [1 - \frac{2}{3}\Delta(\cos qx + \cos qy + \cos qz)], \quad (2.9b)$$

where we have neglected terms of order Δ^2 and Δ^3 .

With $\rho(\mathbf{r})$ and $\tau(\mathbf{r})$ evaluated it is now possible to evaluate the single-particle potential $U(\mathbf{r})$. If we use a Skyrme interaction of the form

$$v(r_{12}) = t_0 \delta(\mathbf{r}_1 - \mathbf{r}_2) + \frac{1}{2} t_1 [\delta(\mathbf{r}_1 - \mathbf{r}_2) k^2 + k'^2 \delta(\mathbf{r}_1 - \mathbf{r}_2)] + t_2 \mathbf{k}' \cdot \delta(\mathbf{r}_1 - \mathbf{r}_2) \mathbf{k} + \frac{t_3}{6} \delta(\mathbf{r}_1 - \mathbf{r}_2) \rho \left[\frac{\mathbf{r}_1 + \mathbf{r}_2}{2} \right], \quad (2.10)$$

then the Hartree-Fock single-particle wave functions $\phi_{\mathbf{k}}(\mathbf{r})$ satisfy the equation⁷:

$$\left[-\nabla \cdot \frac{\hbar^2}{2m^*(\mathbf{r})} \nabla + U(\mathbf{r}) \right] \phi_{\mathbf{k}}(\mathbf{r}) = e_{\mathbf{k}} \phi_{\mathbf{k}}(\mathbf{r}), \quad (2.11)$$

where

$$U(\mathbf{r}) = \frac{3}{4} t_0 \rho(\mathbf{r}) + \frac{3}{16} t_3 \rho^2(\mathbf{r}) + \frac{1}{16} (3t_1 + 5t_2) \tau(\mathbf{r}) + \frac{1}{32} (5t_2 - 9t_1) \nabla^2 \rho(\mathbf{r}) \quad (2.12)$$

and

$$\frac{\hbar^2}{2m^*(\mathbf{r})} = \frac{\hbar^2}{2m} + \frac{1}{16} (3t_1 + 5t_2) \rho(\mathbf{r}). \quad (2.13)$$

If we now use the linearized forms for $\rho(\mathbf{r})$ and $\tau(\mathbf{r})$ (i.e., Eqs. 2.9) in Eq. (2.12) we get $U(\mathbf{r})$ in the desired form given by Eq. (2.2) with

$$U_0 = \frac{3}{4} t_0 \rho_h + \frac{3}{16} t_3 \rho_h^2 + \frac{(3t_1 + 5t_2)}{64} \rho_h q^2 \quad (2.14a)$$

and

$$U_1 = \left[\frac{3}{2} t_0 \rho_h + \frac{3}{4} t_3 \rho_h^2 + \frac{51t_1 - 35t_2}{96} \rho_h q^2 \right] \Delta \equiv f_1(\rho_h, q) \Delta. \quad (2.14b)$$

Moreover, if we neglect the oscillatory part of $m^*(\mathbf{r})$ by putting $\rho(\mathbf{r}) \approx \rho_h$ into Eq. (2.13) we get a constant effective mass independent of position as has been assumed throughout.

With these approximations our solution of the Hartree-Fock equations is self-consistent up to terms linear in Δ , except for the term of order Δ we neglected in $m^*(\mathbf{r})$. If Δ turns out to be small then this solution should be satisfactory as will be demonstrated below. The only task remaining now is the simultaneous solution of Eqs. (2.7) and (2.14b) in order to obtain the self-consistent value of U_1 . To solve these equations we first note by inspecting Eqs. (2.2) and (2.9a) that U_1 and Δ must have opposite signs so that the maxima of $\rho(\mathbf{r})$ fall at the positions of the minima of $U(\mathbf{r})$ in order to obtain an energy lower than that due to the homogeneous density solution. From Eq. (2.14b) this implies that

$$f_1(\rho_h, q) \text{ must be } < 0. \quad (2.15)$$

This condition can also be obtained by inspecting the total energy of the system $E = \int H(\mathbf{r}) d^3r$ where the energy density $H(\mathbf{r})$ for the Skyrme interaction of Eq. (2.10) is given by⁷

$$H(\mathbf{r}) = \frac{\hbar^2}{2m} \tau + \frac{3}{8} t_0 \rho^2 + \frac{1}{16} t_3 \rho^3 + \frac{1}{16} (3t_1 + 5t_2) \rho \tau + \frac{1}{64} (9t_1 - 5t_2) (\nabla \rho)^2, \quad (2.16)$$

where $\rho(\mathbf{r})$ and $\tau(\mathbf{r})$ are given by Eqs. (2.5b) and (2.8b). This leads to an energy per particle:

$$\begin{aligned} \frac{E}{A} &= \frac{\hbar^2 q^2}{8m} + \frac{3}{8} t_0 \rho_h (1 + 2\Delta^2)^3 + \frac{1}{16} t_3 \rho_h^2 (1 + 6\Delta^2)^3 \\ &+ \frac{\rho_h q^2}{64} (3t_1 + 5t_2) (1 - 6\Delta^2) (1 + 2\Delta^2)^2 \\ &+ \frac{3}{32} \rho_h q^2 \Delta^2 (9t_1 - 5t_2) (1 + 2\Delta^2)^2 \\ &= \frac{\hbar^2 q^2}{8m^*} + \frac{3}{8} t_0 \rho_h + \frac{1}{16} t_3 \rho_h^2 + \frac{3}{2} \Delta^2 f_2(\rho_h, q) + O(\Delta^4), \end{aligned} \quad (2.17a)$$

where

$$f_2(\rho_h, q) = \frac{3}{2} t_0 \rho_h + \frac{3}{4} t_3 \rho_h^2 + \frac{6t_1 - 5t_2}{12} \rho_h q^2. \quad (2.17b)$$

Neglecting the terms of order Δ^4 (assuming $|\Delta| \ll 1$), and neglecting the small difference between

$$\frac{\hbar^2 q^2}{8m^*} = 1.9584 \frac{\hbar^2 \rho_h^{2/3}}{m^*}$$

and the corresponding term

$$\frac{3}{10} \frac{\hbar^2 k_F^2}{m^*} = 1.8088 \frac{\hbar^2}{m^*} \rho_h^{2/3}$$

for the usual plane-wave Fermi fluid (k_F = Fermi momentum), Eq. (2.17a) implies that the total energy with Overhauser's orbitals is lower than that obtained with plane-wave orbitals ($\Delta=0$) if the coefficient of Δ^2 is negative, i.e., if

$$f_2(\rho_h, q) < 0. \quad (2.18)$$

This is essentially the condition (2.15) except for a small term of magnitude $(3t_1 + 5t_2/96)\rho_h q^2$ that can be traced back to the neglect of the oscillatory part of $m^*(\mathbf{r})$, Eq. (2.13) [this is the only term of order Δ that has been neglected in deriving (2.14)]. In the actual calculation the difference between f_1 and f_2 is small enough that it can be safely neglected.

Since Δ is always negative [see Eq. (2.7) and the discussion following it], it follows from Eq. (2.14b) and the condition (2.15) that U_1 must be positive. We can therefore remove the absolute value sign in Eq. (2.7) and substitute it into Eq. (2.14b) to get

$$U_1 = -\frac{m^* U_1}{\hbar^2 q^2} f_1(\rho_h, q) \ln \left\{ \left[1 + \left[\frac{\hbar^2 q^2}{2m^* U_1} \right]^2 \right]^{1/2} + \frac{\hbar^2 q^2}{2m^* U_1} \right\}. \quad (2.19)$$

This can be readily solved for U_1 :

$$U_1 = -\frac{\hbar^2 q^2}{2m^*} / \sinh[f_3(\rho_h, q)], \quad (2.20a)$$

where

$$f_3(\rho_h, q) = \frac{\hbar^2 q^2}{m^*} / f_1(\rho_h, q). \quad (2.20b)$$

Similarly, using Eq. (2.14b), one gets for Δ :

$$\Delta = U_1 / f_1(\rho_h, q) = -\frac{1}{2} f_3(\rho_h, q) / \sinh[f_3(\rho_h, q)]. \quad (2.21)$$

It must be pointed out that in the above expressions ρ_h and q are not independent variables since they are related by Eq. (2.6).

The values of U_1 and Δ obtained from Eqs. (2.20) and (2.21) are plotted in Fig. 1 for the density region $\rho_h \lesssim 0.095$ nucleons/fm³ in which condition (2.15) is satisfied. It is seen that U_1 can be as large as ~ 8 MeV,

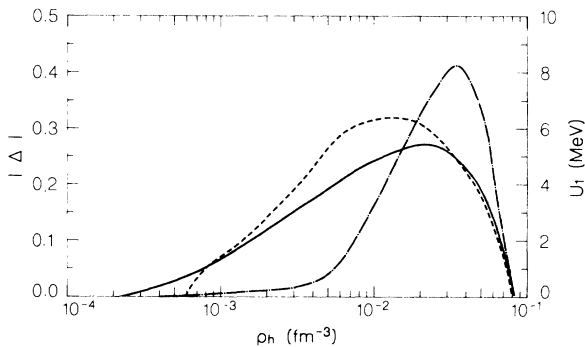


FIG. 1. Values of U_1 and $|\Delta|$ at $T=0$ as functions of nuclear matter density. Note that the density has a logarithmic scale. The continuous curve gives the magnitude of Δ obtained in this work while the dot-dashed curve gives the corresponding U_1 . Note that U_1 has a maximum ≈ 8.2 MeV at $\rho \approx 0.035$ nucleons/fm³. The dashed curve gives $|\Delta|$ obtained by Döhnert *et al.* (Ref. 6).

and that Δ is generally small ($|\Delta| \lesssim 0.27$) as anticipated so that the approximations made are justifiable. Also shown in Fig. 1 are the values of Δ obtained by Döhnert *et al.*⁶ in their numerical solution of the Hartree-Fock equations for the same problem. Both the present results and those of Ref. 6 are obtained with the use of Vautherin and Brink's parametrization I of the Skyrme interaction given in Ref. 7. We notice that there is an overall agreement between the two sets of results for Δ . The largest discrepancy occurs in the neighborhood of the maximum value of $|\Delta|$. This is understandable since the present results depend on the approximation that Δ is small. There is also some disagreement about the ends of the density region in question. Whereas in Ref. 6 Δ is different from zero for the region $0.0006 \lesssim \rho_h \lesssim 0.08$, this work indicates that Δ is nonzero for $\rho_h \lesssim 0.095$. This can best be understood by noting that f_1 and Δ tend to zero at the end of the region so that the gain in energy obtained with Overhauser's orbitals [see Eq. (2.17)] becomes smaller than the terms that have been neglected like, for instance, the excess kinetic energy referred to following Eq. (2.17). Thus the plane-wave orbitals should give a lower energy near the ends of the region as in Ref. 6. In any case, both calculations indicate that the Overhauser solution provides a lower energy than the plane-wave solution only in a density region well below the saturation density of nuclear matter: $\rho_0 \sim 0.17$ nucleons/fm³. The general agreement between the two sets of results indicates that the method developed in this work provides a good approximation to the exact Hartree-Fock solution and may be expected to yield dependable results when extended to finite temperatures.

III. THE OVERHAUSER PROBLEM FOR NONZERO TEMPERATURES

At finite temperatures the occupation of the single-particle orbitals is not confined to the Fermi cube $|k_i| \leq k_0$. This effect appears explicitly in the calculation of the density and kinetic energy density which have to be generalized from the expressions given in Eqs. (2.5a) and (2.8a):

$$\rho(\mathbf{r}) = g \sum_{\mathbf{k}} n_{\mathbf{k}} |\phi_{\mathbf{k}}(\mathbf{r})|^2, \quad (3.1a)$$

$$\tau(\mathbf{r}) = g \sum_{\mathbf{k}} n_{\mathbf{k}} |\nabla \phi_{\mathbf{k}}(\mathbf{r})|^2, \quad (3.1b)$$

where

$$n_{\mathbf{k}} = \{ \exp[\beta(e_{\mathbf{k}} - \mu)] + 1 \}^{-1} \quad (3.1c)$$

is the occupancy of the orbital \mathbf{k} whose self-consistent single-particle energy is $e_{\mathbf{k}}$. Here $\beta = 1/T$ where T is the temperature in energy units, and μ is the chemical potential. Apart from this, the finite-temperature Hartree-Fock equation is identical to the one for $T=0$.⁹ In particular, Eqs. (2.11)–(2.13) are still applicable but with the finite-temperature effects included in $\rho(\mathbf{r})$ and $\tau(\mathbf{r})$.

The only consequence of this is, therefore, to modify Eq. (2.7) for Δ . For example, in evaluating $\rho(\mathbf{r})$ to the same approximation as in Eqs. (2.9) we get:

$$\begin{aligned}\rho(\mathbf{r}, T) &= \frac{g}{V} \sum_{\mathbf{k}} n_{\mathbf{k}} (1 + 2u_{k_x} v_{k_x} \cos qx + 2u_{k_y} v_{k_y} \cos qy \\ &\quad + 2u_{k_z} v_{k_z} \cos qz) \\ &= \rho_n (1 + 2\Delta_x \cos qx + 2\Delta_y \cos qy \\ &\quad + 2\Delta_z \cos qz) \cdots, \end{aligned} \quad (3.2)$$

where

$$\Delta_x = \frac{\sum_{\mathbf{k}} n_{\mathbf{k}} u_{k_x} v_{k_x}}{\sum_{\mathbf{k}} n_{\mathbf{k}}} \quad (3.3)$$

with similar expression for Δ_y and Δ_z . By symmetry, $\Delta_x = \Delta_y = \Delta_z = \Delta(T)$, where the temperature dependence of Δ is shown explicitly in order to distinguish it from its value at $T=0$. We now proceed to evaluate $\Delta(T)$ assuming that the temperature is very low. It will be seen later that this assumption is justified and that it is not necessary to consider higher temperatures.

At low temperatures the chemical potential μ can be taken to be independent of the temperature and equal to the Fermi energy ε_F . The latter can be determined by noting that the highest occupied orbital at $T=0$ corresponds to $k_x = k_y = k_z = k_0^-$ with a single-particle energy:

$$e_0 = 3\varepsilon_{k_0}^- = \frac{3\hbar^2 q^2}{8m^*} - \frac{3|U_1|}{2}, \quad (3.4a)$$

where e_0 is measured from the bottom of the potential U_0 . The first excited state would then correspond to removing a particle from this orbital and putting it in an orbital like $k_x = k_0^+$, $k_y = k_z = k_0^-$ with a corresponding energy:

$$e_1 = \varepsilon_{k_0}^+ + 2\varepsilon_{k_0}^- = \frac{3\hbar^2 q^2}{8m^*} - \frac{|U_1|}{2} \quad (3.4b)$$

which leads to an energy gap $= e_1 - e_0 = |U_1|$. The Fermi energy ε_F lies at the midpoint of the gap so that we have

$$\mu = \varepsilon_F = \frac{3\hbar^2 q^2}{8m^*} - |U_1|. \quad (3.4c)$$

In order to evaluate both summations in Eq. (3.3) for $\Delta(T)$ at low temperatures it is noted that the main contributions come from the single-particle orbitals below the edge of the Fermi cube where $n_{\mathbf{k}} \approx 1$ so that the sums in (3.3) would be close to their values at $T=0$ up to $O(T^2)$ since the terms linear in T vanish for a Fermi system at low temperatures (see, e.g., Ref. 10). It then follows that [cf. Eq. (A2) in the Appendix]:

$$\sum_{\mathbf{k}} n_{\mathbf{k}} \approx \left[\frac{Lq}{\pi} \right]^3 + O(T^2). \quad (3.5a)$$

In evaluating $\sum_{\mathbf{k}} u_{k_x} v_{k_x} n_{\mathbf{k}}$ it is necessary to be more careful since $|u_{k_x} v_{k_x}| \ll 1$ except near the edge of the Fermi cube ($k_x \approx k_0$), i.e., near the gap region:

$$\begin{aligned} \sum_{\mathbf{k}} u_{k_x} v_{k_x} n_{\mathbf{k}} &= \sum_{|k_x| \leq k_0} u_{k_x}^- v_{k_x}^- n_{\mathbf{k}} + \sum_{|k_x| \geq k_0} u_{k_x}^+ v_{k_x}^+ n_{\mathbf{k}} \\ &= \sum_{|k_x| \leq k_0} u_{k_x}^- v_{k_x}^- - \sum_{|k_x| \leq k_0} (1 - n_{\mathbf{k}}) u_{k_x}^- v_{k_x}^- + \sum_{|k_x| \geq k_0} u_{k_x}^+ v_{k_x}^+ n_{\mathbf{k}} \\ &= \left[\frac{Lq}{2\pi} \right]^2 \sum_{|k_x| \leq k_0} u_{k_x}^- v_{k_x}^- - \sum_{|k_x| \leq k_0} \frac{u_{k_x}^- v_{k_x}^-}{e^{-\beta(e_{\mathbf{k}} - \mu)} + 1} + \sum_{|k_x| \geq k_0} \frac{u_{k_x}^+ v_{k_x}^+}{e^{\beta(e_{\mathbf{k}} - \mu)} + 1}. \end{aligned}$$

In the second summation it is noted that the main contribution comes from the region $k_x \approx k_y \approx k_z \approx k_0^-$ so that $e_{\mathbf{k}} \approx e_0$. Similarly in the last summation the main contribution comes from the region $k_x \approx k_0^+$, $k_y \approx k_z \approx k_0^-$ so that $e_{\mathbf{k}} \approx e_1$. Utilizing Eqs. (3.4) we can then use the approximation:

$$\sum_{\mathbf{k}} u_{k_x} v_{k_x} n_{\mathbf{k}} \approx \left[1 - \frac{1}{\exp\left[\frac{\beta|u_1|}{2}\right] + 1} \right] \sum_{|k_x| \leq k_0} u_{k_x}^- v_{k_x}^- + \left[\frac{1}{\exp\left[\frac{\beta|u_1|}{2}\right] + 1} \right] \sum_{|k_x| \geq k_0} u_{k_x}^+ v_{k_x}^+. \quad (3.5b)$$

Noting that [see Eq. (A15)]

$$\sum_{|k_x| \geq k_0} u_{k_x}^+ v_{k_x}^+ = - \sum_{|k_x| \leq k_0} u_{k_x}^- v_{k_x}^-, \quad (3.6)$$

we finally get with the help of Eq. (2.7)

$$\begin{aligned} \Delta(T) &= \Delta_0(T) \tanh \left[\frac{|U_1|}{4T} \right] \\ &= \frac{-m^* |U_1|}{\hbar^2 q^2} \ln \left\{ \left[1 + \left[\frac{\hbar^2 q^2}{2m^* |U_1|} \right]^2 \right]^{1/2} + \frac{\hbar^2 q^2}{2m^* |U_1|} \right\} \tanh \left[\frac{|U_1|}{4T} \right]. \end{aligned} \quad (3.7)$$

Note that $\Delta_0(T)$ is identical to Δ given in Eq. (2.7) for the $T=0$ case except that in Eq. (3.7) $U_1 = U_1(T)$ which is different from $U_1 = U_1(0)$ its value at $T=0$ that occurs in Eq. (2.7).

To the same approximation, i.e., neglecting terms of order T^2 , the expressions for $\rho(r)$ and $\tau(r)$ are identical to Eqs. (2.9) except that Δ is replaced by $\Delta(T)$. Consequently Eq. (2.14b) remains formally unaffected by the finite temperature so that:

$$U_1(T) = f_1(\rho_h, q) \Delta(T). \quad (3.8)$$

We are therefore left with the solution of the simultaneous Eqs. (3.7) and (3.8) for $U_1(T)$ and $\Delta(T)$. Eliminating $\Delta(T)$ from both equations leads for positive U_1 to the equation:

$$\begin{aligned} \frac{-m^* U_1}{\hbar^2 q^2} \ln \left\{ \left[1 + \left[\frac{\hbar^2 q^2}{2m^* U_1} \right]^2 \right]^{1/2} + \frac{\hbar^2 q^2}{2m^* U_1} \right\} \\ = \frac{U_1}{f_1(\rho_h, q) \tanh \frac{U_1}{4T}}. \end{aligned} \quad (3.9)$$

This reduces to Eq. (2.19) as $T \rightarrow 0$. Unlike (2.19), however, it is not possible to obtain an analytic solution for (3.9) similar to Eq. (2.20a). Values of $U_1(T)$ obtained by solving Eq. (3.9) numerically are given in Fig. 2. The resulting $\Delta(T)$ can be evaluated with the help of Eq. (3.8). A general feature of the results, true at any density, is that $U_1(T)$ and, consequently, $|\Delta(T)|$ decrease as the temperature increases until a certain temperature T_m is reached such that for $T > T_m$ Eq. (3.9) does not have any solution. This implies that above T_m only the homogeneous-density fluid phases can exist and therefore T_m is to be identified with the temperatures of melting. Typical values for T_m are given in Table I where it is observed that the highest value for T_m is ≈ 1.12 MeV which occurs at $\rho_h \approx 0.035$. This corresponds to the triple point for nuclear matter. Since the temperatures involved are much lower than the corresponding Fermi energies and also much lower than the energy gap as shown in Table I, the use of the low-temperature approximation in this section is therefore justified.

Although Eq. (3.9) cannot be solved analytically, it can be used to derive an upper limit for T_m . The first step is to note that both sides of Eq. (3.9) are negative monotonically decreasing functions of U_1 since $f_1(\rho_h, q)$ is negative in the region of interest. The left-hand side [which is really Δ_0 of Eq. (3.7)] decreases from 0 at $U_1=0$ to -0.5 as $U_1 \rightarrow \infty$ while the right-hand side decreases from $4T/f_1(\rho_h, q)$ at $U_1=0$ to $U_1/f_1(\rho_h, q)$ as $U_1 \rightarrow \infty$ and the two sides will intersect (if at all) at $U_1(T) < U_1(0)$

where each side will have the magnitude $|\Delta_0(T)| < |\Delta_0(0)|$. Equation (3.9) will then definitely not have a solution if

$$\left| \frac{4T}{f_1(\rho_h, q)} \right| \geq |\Delta_0(0)|.$$

This can be very easily seen by plotting both sides of Eq. (3.9). Therefore, the temperature of melting satisfies

$$T_m < \frac{|\Delta_0(0)| |f_1(\rho_h, q)|}{4} = \frac{\Delta_0(0) f_1(\rho_h, q)}{4} = \frac{U_1(0)}{4}, \quad (3.10)$$

where the last step comes from using Eq. (2.14b). This upper limit for T_m can be easily calculated and is given in the last column of Table I. It is seen by comparison with the values of T_m also given in Table I that this upper limit tends to overestimate T_m by about a factor of 2 so that $T_m \approx U_1(0)/8$.

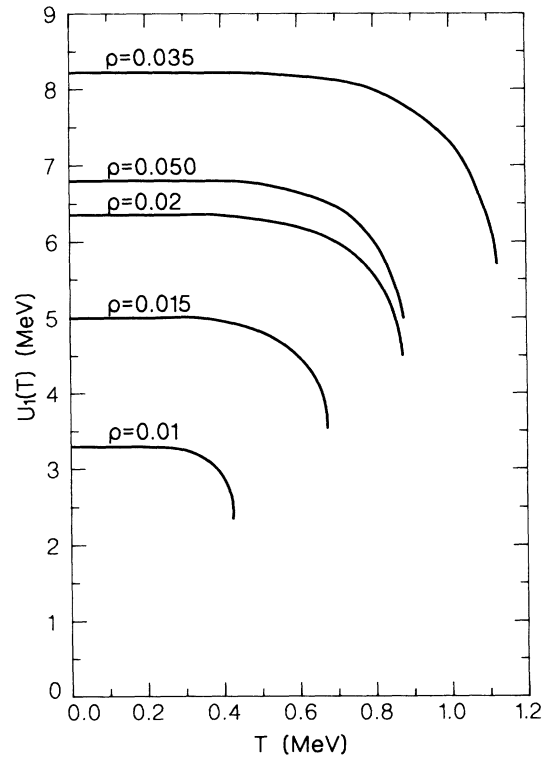


FIG. 2. The variation of U_1 with temperature for various representative densities. At low temperatures U_1 is almost independent of temperature but then drops rather quickly with rising temperature until the melting point is reached. The maximum $U_1(T)$ occurs for $\rho \approx 0.035$ nucleons/fm³.

TABLE I. Values of the temperature of melting T_m , the Fermi energy ε_F , the energy gap $U_1(0)$, and the function f_1 of Eq. (2.14b) for various representative values of the average density ρ_h . Note that T_m is much less than both ε_F and $U_1(0)$. The function f_1 can be used to calculate $\Delta(T)$ from $U_1(T)$ through Eq. (3.8). The upper limit for T_m given in Eq. (3.10) is listed in the last column.

ρ_h (fm^{-3})	T_m (MeV)	ε_F (MeV)	f_1 (MeV)	$U_1(0)$ (MeV)	$U_1(0)/4$ (MeV)
0.005	0.18	5.72	-7.29	1.41	0.35
0.01	0.44	8.05	-13.60	3.31	0.83
0.02	0.88	11.78	-23.64	6.36	1.59
0.03	1.10	15.92	-30.47	7.99	2.00
0.035	1.12	18.34	-32.73	8.24	2.06
0.04	1.08	21.04	-34.22	8.11	2.03
0.05	0.87	27.20	-34.98	6.82	1.70
0.06	0.54	34.20	-32.80	4.46	1.11
0.07	0.20	41.28	-27.73	1.82	0.46
0.08	0.022	47.18	-19.80	0.21	0.053

IV. DISCUSSION AND CONCLUSION

In this work a simple analytic approximate solution of the Hartree-Fock equations for nuclear matter has been obtained at $T=0$ with Overhauser's orbitals. The solution was then generalized to finite temperatures. The results for $T=0$ agree reasonably well with the numerical results obtained in previous calculations, and the extension to finite temperatures is straightforward. These results indicate the existence of a crystalline-like phase of nuclear matter at very low temperatures ($\lesssim 1.1$ MeV) and at densities well below that of saturated cold nuclear matter.

Ordinary liquid nuclear matter has a saturation density of about 0.17 nucleons/ fm^3 while solid nuclear matter exists at densities $\lesssim 0.08$ fm^{-3} so that nuclear matter should have a phase diagram similar to that for substances, like water, which expand on freezing. This is consistent with the fact that nuclear matter exists at $T=0$ in the liquid phase and that the solid state does not exist above the triple-point temperature.

The present results also indicate the existence of an energy gap at the Fermi energy. It must be pointed out, however, that this energy gap is not related to the energy gap associated with the second-order superconducting phase transition predicted by a recent calculation¹¹ to possibly occur in nuclear matter at very low temperatures. In fact the solid-fluid phase transition is, as it should be, a first-order phase transition with an associated latent heat of transformation corresponding to the change in energy (or, to be exact, enthalpy) resulting from the difference between the densities of the two phases. The actual calculation of the latent heat, however, requires the evaluation of the equation of state for

both phases and determining the coexistence densities. This has not been attempted here. The energy gap for solid nuclear matter is also different from that for a superconductor in that it does not tend to zero continuously as the transition temperature is approached. This is obvious from Fig. 2. Actually the energy gap of solid nuclear matter is analogous to that due to an intrinsic semiconductor.

This work has also been limited to the use of the simple-cubic lattice structure. It may well turn out that other lattice structures, like the face-centered cubic lattice, are more stable over the same or different density regions and that more than one solid phase exists so that the phase diagram is more complicated than assumed above.

Finally, it would be interesting to investigate whether it is possible to detect any phenomena that can be related to the existence of the solid phase or to the solid-fluid phase transition. However, because nuclear matter occurs only in the form of finite nuclei it may not be possible to detect a clear signature corresponding to the phase transition. Another possibility is the existence of α clusters at the surface of nuclei where the nuclear density is comparable to that at which the solid phase exists. As an extreme case it may well be that the α -particle model of the nucleus is really a reflection of the existence of a solid phase.

APPENDIX

We now proceed to give the details of evaluating $\rho(\mathbf{r})$ and $\tau(\mathbf{r})$ at $T=0$ with the Overhauser orbitals of Eq. (2.1). Only the orbitals whose energy lies below the Fermi energy will contribute:

$$\begin{aligned}
 \rho(\mathbf{r}) &= g \sum_{\mathbf{k}} |\phi_{\mathbf{k}}(\mathbf{r})|^2 \\
 &= \frac{g}{V} \sum_{\mathbf{k}} (1 + 2u_{k_x}^- v_{k_x}^- \cos qx)(1 + 2u_{k_y}^- v_{k_y}^- \cos qy)(1 + 2u_{k_z}^- v_{k_z}^- \cos qz) \\
 &= \frac{g}{V} \left[\sum_{k_x=-k_0}^{+k_0} (1 + 2u_{k_x}^- v_{k_x}^- \cos qx) \right] \left[\sum_{k_y=-k_0}^{+k_0} (1 + 2u_{k_y}^- v_{k_y}^- \cos qy) \right] \left[\sum_{k_z=-k_0}^{+k_0} (1 + 2u_{k_z}^- v_{k_z}^- \cos qz) \right] \cdots \quad (\text{A1})
 \end{aligned}$$

By changing the summations into integrations in the standard way:

$$\sum_{k_i=-k_0}^{+k_0} \rightarrow \frac{L}{2\pi} \int_{-k_0}^{+k_0} dk_i, \quad (\text{A2})$$

we get

$$\sum_{k_i=-k_0}^{+k_0} 1 = \frac{L}{\pi} \int_0^{q/2} dk_i = \frac{L}{\pi} \frac{q}{2} \quad (\text{A3})$$

and

$$\rho(\mathbf{r}) = \rho_h (1 + 2\Delta_x \cos qx) (1 + 2\Delta_y \cos qy) (1 + 2\Delta_z \cos qz), \quad (\text{A4})$$

where ρ_h is given by Eq. (2.6) and, by cubical symmetry,

$$\Delta_x = \Delta_y = \Delta_z = \Delta = \frac{2\pi}{Lq} \sum_{k_x=-k_0}^{+k_0} u_{k_x}^- v_{k_x}^- \rightarrow \frac{2}{q} \int_0^{q/2} u_{k_x}^- v_{k_x}^- dk_x. \quad (\text{A5})$$

The integration in Eq. (A5) can be carried out by introducing the variable ω defined for $|k_x| \leq k_0$ by the relation:

$$\cot \omega = (\varepsilon_{k_x-q} - \varepsilon_{k_x}) / |U_1| = \left[\frac{\hbar^2 q^2}{2m^*} - \frac{\hbar^2 k_x q}{m^*} \right] / |U_1|. \quad (\text{A6a})$$

Noting that

$$u_{k_x}^- v_{k_x}^- = -\left(\frac{1}{2}\right) \sin \omega \quad (\text{A6b})$$

and

$$dk_x = \frac{m^* |U_1|}{\hbar^2 q} (\csc^2 \omega) d\omega, \quad (\text{A6c})$$

it follows that

$$\Delta = -\frac{m^* |U_1|}{\hbar^2 q^2} \int_{\omega_0}^{\pi/2} \csc \omega d\omega \quad (\text{A7a})$$

with ω_0 given by

$$\cot \omega_0 = \frac{\hbar^2 q^2}{2m^* |U_1|}, \quad (\text{A7b})$$

which corresponds to $k_x = 0$ in Eq. (A6a).

The integral in (A7a) can be easily evaluated leading to

$$\begin{aligned} \Delta &= \frac{m^* |U_1|}{\hbar^2 q^2} \ln \left\{ \left[\left(\frac{\hbar^2 q^2}{2m^* |U_1|} \right)^2 + 1 \right]^{1/2} - \frac{\hbar^2 q^2}{2m^* |U_1|} \right\} \\ &= -\frac{m^* |U_1|}{\hbar^2 q^2} \ln \left\{ \left[\left(\frac{\hbar^2 q^2}{2m^* |U_1|} \right)^2 + 1 \right]^{1/2} + \frac{\hbar^2 q^2}{2m^* |U_1|} \right\} \end{aligned} \quad (\text{A8})$$

which is Eq. (2.7).

Similarly, using the Overhauser orbitals of Eq. (2.1), the kinetic energy density is given by

$$\begin{aligned} \tau(\mathbf{r}) &= g \sum_{\mathbf{k}} |\nabla \phi_{\mathbf{k}}(\mathbf{r})|^2 = g \sum_{\mathbf{k}} \left| \frac{\partial \phi_{\mathbf{k}}(\mathbf{r})}{\partial x} \right|^2 + \left| \frac{\partial \phi_{\mathbf{k}}(\mathbf{r})}{\partial y} \right|^2 + \left| \frac{\partial \phi_{\mathbf{k}}(\mathbf{r})}{\partial z} \right|^2 \\ &= g \sum_{\mathbf{k}} \left| \frac{\partial \phi_{k_x}(x)}{\partial x} \right|^2 |\phi_{k_y}(y)|^2 |\phi_{k_z}(z)|^2 \\ &\quad + 2 \text{ similar terms obtained by permuting } x, y, \text{ and } z. \end{aligned} \quad (\text{A9})$$

Again the summation is over orbitals below the Fermi energy: $|k_i| \leq k_0$. Denoting the first term of (A9) by $\tau_x(\mathbf{r})$ we get

$$\tau_x(\mathbf{r}) = \rho_h \left[\frac{2\pi}{Lq} \right] \left[\sum_{k_x} k_x^2 + 2k_x(k_x - q_x) u_{k_x}^- v_{k_x}^- \cos qx + (q^2 - 2k_x q_x) v_{k_x}^{-2} \right] (1 + 2\Delta \cos qy)(1 + 2\Delta \cos qz) \quad (\text{A10})$$

with similar expressions for $\tau_y(\mathbf{r})$ and $\tau_z(\mathbf{r})$ obtained by permuting x, y , and z .

Each of the summations in (A10) can be evaluated by changing it into an integral:

$$\sum_{k_x} k_x^2 \rightarrow \frac{L}{\pi} \int_0^{q/2} k_x^2 dk_x = \frac{L}{\pi} \frac{q^3}{24}, \quad (\text{A11a})$$

and

$$2 \sum_{k_x} k_x(k_x - q_x) u_{k_x}^- v_{k_x}^- \rightarrow \frac{2L}{\pi} \int_0^{q/2} k_x(k_x - q) u_{k_x}^- v_{k_x}^- dk_x \approx \frac{2L}{\pi} \left[-\frac{q^2}{4} \right] \int_0^{q/2} u_{k_x}^- v_{k_x}^- dk_x = -q^2 \left[\frac{Lq}{4\pi} \right] \Delta. \quad (\text{A11b})$$

The approximation used in (A11b) depends on the fact that $u_{k_x}^- v_{k_x}^- \ll 1$ except near $|k_x| \approx q/2$ and also that $k_x(k_x - q)$ has its maximum value at $|k_x| = q/2$. The remaining sum in (A10) is very small and can be safely neglected:

$$\sum_{k_x} (q^2 - 2k_x q_x) v_{k_x}^{-2} \rightarrow \frac{L}{\pi} \int_0^{q/2} (q^2 - 2k_x q) v_{k_x}^{-2} dk_x \approx 0, \quad (\text{A11c})$$

since $v_{k_x}^{-2} \ll 1$ except when $k_x \approx q/2$, i.e., when $(q^2 - 2k_x q) \approx 0$. Actually the integrals in (A11b) and (A11c) can both be evaluated exactly by using the variable ω of Eq. (A5). However the difference between the exact and approximate results turns out to be small. Moreover, the approximations involved in (A11b) and (A11c) are consistent with other approximations used throughout this work.

Substituting Eqs. (A11) into (A10) we get

$$\tau_x(\mathbf{r}) \approx \rho_h \left[\frac{q^2}{12} - \frac{q^2}{2} \Delta \cos qx \right] (1 + 2\Delta \cos qy)(1 + 2\Delta \cos qz) \quad (\text{A12})$$

with similar expressions for $\tau_y(\mathbf{r})$ and $\tau_z(\mathbf{r})$. By adding these three terms we get Eq. (2.8b).

For $|k_x| \geq k_0$ the variable ω' is introduced by the definition:

$$\cot \omega' = (\varepsilon_{k_x} - \varepsilon_{k_x - q}) / |U_1| = \left[\frac{\hbar^2 k_x q}{m^*} - \frac{\hbar^2 q^2}{2m^*} \right] / |U_1|, \quad (\text{A13a})$$

which yields

$$u_{k_x}^+ v_{k_x}^+ = +\left(\frac{1}{2}\right) \sin \omega', \quad (\text{A13b})$$

$$dk_x = -\frac{m^* |U_1|}{\hbar^2 q} \csc^2 \omega' d\omega', \quad (\text{A13c})$$

and finally

$$\frac{2\pi}{Lq} \sum_{|k_x| \geq k_0} u_{k_x}^+ v_{k_x}^+ = \frac{4\pi}{Lq} \sum_{k_x = +q/2}^{+q} u_{k_x}^+ v_{k_x}^+ \rightarrow \frac{2}{q} \int_{q/2}^q u_{k_x}^+ v_{k_x}^+ dk_x = +\frac{m^* |U_1|}{\hbar^2 q^2} \int_{\omega'_0}^{\pi/2} \csc \omega' d\omega', \quad (\text{A14a})$$

where the summation over k_x has been restricted to the second Brillouin zone. Here ω'_0 is defined by

$$\cot \omega'_0 = \frac{\hbar^2 q^2}{2m^* |U_1|}, \quad (\text{A14b})$$

which corresponds to $k_x = q$ in Eq. (A13a). By comparison with Eq. (A7b) it is found that $\omega'_0 = \omega_0$ and, hence, from Eqs. (A7) and (A14), it follows that

$$\frac{2\pi}{Lq} \sum_{|k_x| \geq k_0} u_{k_x}^+ v_{k_x}^+ = -\Delta = -\frac{2\pi}{Lq} \sum_{|k_x| < k_0} u_{k_x}^- v_{k_x}^-, \quad (\text{A15})$$

which proves Eq. (3.6).

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