example, Baños, Ref. 1.

¹⁰E. Wolf, Opt. Commun. 1, 153 (1969).

¹¹M. Born and E. Wolf, Principles of Optics (Pergamon, Oxford, 1970), 4th ed.

¹²W. Friedrick, P. Knipping, and M. Von Laue, Ber. Bayer. Akad. Wiss., 303 (1912). See also G. E. Bacon, *X-Ray and Neutron Diffraction* (Pergamon, Oxford, 1966), p. 89, for a translation of this paper as well as a reprinting of other early works. Two other early and important papers in this field have been translated within the past year: P. P. Ewald, Ann. Physik <u>49</u>, 1 (1916); <u>49</u>, 117 (1916); see Translation No. 84, AFCRL-70-0580, Air Force Cambridge Res. Labs., Bedford, Mass. (unpublished). ¹³The message conveyed by (5.10) is equivalent, in the inverse "reconstruction" problem (see, e.g., Ref. 10), to the following "inverse" message: If only nonevanescent waves are detected, then details of the scattering potential of dimensions Δx , Δy , and Δz may be reconstructed as long as

 $(\Delta x)^{-2} + (\Delta y)^{-2} + (\Delta z)^{-2} \le 4\lambda^{-2}.$

¹⁴See, for example, K. Gottfried, *Quantum Mechanics* (Benjamin, New York, 1966), Vol. I, p. 110; or L. I. Schiff, *Quantum Mechanics* (McGraw-Hill, New York, 1955), 2nd ed., p. 170.

¹⁵See, for example, A. Messiah, *Quantum Mechanics* (North-Holland, Amsterdam, 1961), Vol. II, p. 26.

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High-Density Nucleon Localization

Robert Lynn Coldwell*

Physics Department, University of Washington, Seattle, Washington 98105 (Received 8 April 1971)

A nucleon system interacting by means of the Reid soft-core potential is considered at the very high densities which would be found in the core regions of neutron stars. The question of nucleon localization is considered, first with a simple Wigner-type calculation and then with a variational calculation in which the degree of crystallization is used as a variational parameter. The conclusion is that for some range of densities between $r_0 = 0.2$ F and $r_0 = 0.8$ F ($V/N = 4\pi r_0^3/3$) nucleons should localize in the sense that a crystal-like wave function which introduces particle anticorrelations by localizing the particles with respect to a periodic lattice is preferable to a plane-wave type of wave function which has only statistical correlations and that this is probably not true outside this region. There is no attempt to distinguish liquids from crystals, merely a gas from a crystal. The energy upper bounds resulting from the variational calculation are also given.

I. INTRODUCTION

Densities in the central regions of neutron stars range from near nuclear to infinite. Somewhere in this range of densities it would seem likely that the system would crystallize. In one of the simplest high-density approximations, nucleons can be described as classical hard spheres with a 0.4-F radius. The computer simulations of this system by Wood *et al.*¹ indicate a gas-crystal phase change at $V_0/V = 0.667$ which corresponds to an interparticle spacing of $r_0 = 0.5 \text{ F} [N/V]$ $=3/(4\pi r_0^3)$]. This is not a realistic potential at these densities; a better one is $\sum_i V_i \exp(-\mu_i r)/r$ which at extremely high densities behaves like a Coulomb potential. Wigner² has shown that the electron system (to which this corresponds) also has a "crystalline" region at low density $(r_0 \gg a_B)$, the Bohr radius). The nuclear "Bohr radius" is of the order of 0.03 F (Reid³ soft-core potential), so that a relatively high-density nuclear system can still behave like a low-density electron gas. The picture which is here considered then, is of

a low-density region in which the nucleons make up essentially a hard-sphere gas, an intermediate region in which they make up either a highdensity crystal of the hard-sphere variety or a low-density electron crystal, and finally a very high-density region in which the system is like a high-density electron gas. The crystallization considered here is localization in the sense that no attempt is made to distinguish a liquid from a crystal. All comparisons are between gas and crystal.

This paper treats the question of nucleon localization in three sections: The first is a simple argument along the same lines as the Wigner² analysis of the low-density electron gas. The second is a variational calculation of the ground-state energy, first in the standard manner with plane waves and then with Mathieu functions which allow the degree of crystallization of the system to be a parameter. These variational calculations are strictly Hartree-Fock in that each particle is assumed to move in the average field of the others. The third section is an attempt to extrapolate from these results to deduce the direction further correlations might be expected to move the system. The electron system is treated in tandem with the nucleon system in order to provide both a check on the analysis and a better understood system to refer to. The Reid³ soft-core potentials after suitable averaging (see Appendix) were used as a kind of worst possible case. The only way that the system can escape crystallizing is for the hard-sphere gas region and the high-density electron gas region to overlap, and the Reid soft-core potentials represent as Coulomb-like a system as is consistent with nuclear data. Harder cores, by making it more advantageous for particles to avoid being close together, would be expected to make the system like localization even more.

II. LOCALIZATION IN A SIMPLE WIGNER-LIKE APPROXIMATION

The Wigner-Seitz approximation that the unit cell can be replaced by a sphere of radius r_0 with the same volume is used, the spheres are assumed not to interact, and it is assumed that the particle density outside a given sphere can be approximated by $\rho = 3/(4\pi r_0^{-3})$. Then the singleparticle Hartree wave function is $(\hbar = 2m = 1)$

$$[p^{2} + V(r_{j})]u_{i}(r_{j}) = e_{i}u_{i}(r_{j}),$$

$$V(r_{j}) = \sum_{k \neq j} |u_{k}(r)|^{2}v(r_{j} - r) d^{3}r$$

$$= \int_{|r| > r_{0}} v(r_{j} - r) d^{3}r.$$

$$(1)$$

For small displacements and Yukawa potentials $[v(r) = \exp(-\mu r)/r]$ this can be expanded as

$$V(r) = V(0) + \frac{1}{6} r^{2} (\nabla^{2} V)_{0},$$

$$V(0) = 3 \exp(-\mu r_{0})(1 + \mu r_{0})/(\mu^{2} r_{0}^{3}),$$
 (2)

$$(\nabla^{2} V)_{0} = \mu^{2} V(0) = \frac{3}{2} \omega^{2},$$

so that the single-particle equation becomes

$$[p^{2} + V(0) + \frac{1}{4}\omega^{2}r^{2}]u_{i}(r) = e_{i}u_{i}(r),$$

which is the equation for a harmonic oscillator with ground-state eigenvalues

$$e_i = V(0) + \frac{3}{2}\omega.$$

The energy of the system is then given by

$$E = \sum_{i} e_{i} - \frac{1}{2} \sum_{i \neq j} \int |u_{i}(r_{1})|^{2} |u_{j}(r_{2})|^{2} \\ \times v(r_{1} - r_{2}) d^{3}r_{1} d^{3}r_{2} \\ = \sum_{i} e_{i} - \frac{1}{2} \rho^{2} \Omega \int_{|r| > r_{0}} v(r) d^{3}r \\ = N [\frac{1}{2} V(0) + \frac{3}{2} \omega].$$
(3)

Noting that $r_s = r_0/a_B = r_0(me^2/\hbar^2) = \frac{1}{2}e^2r_0$ and that 1 Ry = $me^4/(2\hbar^2) = \frac{1}{4}e^4$ in the customary electrongas units, it can be seen that, as $\mu \to 0$,

$$\omega^2 \to \frac{2}{3} \frac{3}{2} e^2 / r_0^3 = e^8 / 4 r_s^3, \tag{4}$$

so that

$$\frac{3}{2}\omega \rightarrow (3/r_s) \frac{1}{4}e^4$$

in agreement with the electron-crystal result⁴ although of course for the electron system the background is needed to cancel the infinity in V(0). In the nucleon system with $v(r) = \sum_i V_i \exp(-\mu_i r)/r$ and $\hbar^2/2m = 20.74$ MeV F², V(0) and ω^2 are given by

$$V(0) = (3/r_0) \sum_i V_i \exp(-\mu_i r_0) (1 + \mu_i r_0) / (\mu_i r_0)^2,$$
(5)
$$\omega^2 = (2/r_0^3) \sum_i V_i \exp(-\mu_i r_0) (1 + \mu_i r_0) / 20.74 \text{ MeV } \mathbf{F}^2.$$

The appropriate combinations of Reid potentials for use in the above is discussed in the Appendix. A measure of the spread of the single-particle wave function and hence of the self-consistency of this approximation is provided by $\langle r^2 \rangle / r_0^2 = 3 / (\omega r_0^2)$. This is shown in Fig. 1. As expected, there is a minimum at $r_0 \approx 0.4$ F and a region up to about 0.8 F for which the wave function can be reasonably well localized. The energy estimate is shown in Fig. 2. There is a mild dependence on whether the system is taken as normal (neutrons and protons of both spins), all neutron, or all neutron and ferromagnetic which enters into the determination of the potentials. Below $r_0 = 0.2$ F, the all neutron



FIG. 1. $\langle r^2 \rangle / r_0^2 \text{ vs } r_0$ from the simple Wigner-like calculation of Sec. II. Small values of $\langle r^2 \rangle / r_0^2$ are necessary for the calculation to be self-consistent.

FIG. 2. Energy bounds vs r_0 . ------ ferromagnetic all neutron plane-wave system, XXXXXX all neutron crystal, ---- normal crystal, ---- crystal in the Wigner-like approximation (not variational), 0000 all neutron normal plane-wave system, ----- normal plane-wave system.

system is slightly lower, while elsewhere the normal system is lowest. At $r_0 = 1.0$ F where $\langle r^2 \rangle / r_0^2$ indicates self-consistency problems, the energy estimate is 96 MeV/particle instead of -16 MeV/ particle which may give a handle on the expected accuracy. The estimates are not variational, and hence are not upper bounds to the energy; that comes in Sec. III.

III. VARIATIONAL CALCULATIONS

A. Plane Waves

A straightforward method of approximating the ground-state energy of a many-particle system is to assume that the single-particle wave functions are plane waves, to construct from these a properly symmetrized many-body wave function, and then to use this to calculate the expectation value of the Hamiltonian. This is the standard planewave Hartree-Fock approximation. Since the only approximations are made in the wave function, it is variational, which guarantees that the energy arrived at in this manner is an upper bound to the ground-state energy of the system. The game in this section will be to use, instead of plane waves, single-particle wave functions which reduce in one limit to plane waves and in another limit to crystallike wave functions, so that the expectation value of the energy can be minimized with respect to the degree of crystallization present in the trial wave function. It should be noted at the outset that the concept of a single-particle wave function implies that each particle moves in the average field of the others which is a serious limitation in the types of trial functions included in this method. In order to provide an example for the calculation to follow, let us first consider the plane-wave Hartree-Fock approximation.

The Hamiltonian and wave function are

$$H = \sum_{i} - \nabla_{i}^{2} + \frac{1}{2} \sum_{i \neq j} v(\mathbf{\tilde{r}}_{i} - \mathbf{\tilde{r}}_{j}),$$

$$\varphi = (1/N!)^{1/2} \det[\varphi_{+}(\mathbf{\tilde{r}}_{j})].$$
(6)

In these equations v(r) is the sum of Yukawa potentials mentioned earlier, and $\varphi_{\vec{k}}(\vec{r}_j)$ is the single-particle wave function

$$\varphi_{\vec{t}}(\vec{r}_{j}) = (1/\Omega)^{1/2} e^{i\vec{k}\cdot\vec{r}_{j}} \alpha(\xi) \gamma(\eta), \qquad (7)$$

with $\alpha(\frac{1}{2}) = \binom{1}{0}$ and $\alpha(-\frac{1}{2}) = \binom{0}{1}$ in spin space, and γ the same in isospin space. The largest value of k is related to the density through

$$k_F = \{9\pi/[2\times(2)\times(2)]\}^{1/3}/r_0 = \beta/r_0$$

with both (2)'s present for a system with both spins and both isospins, one (2) for a system with only one spin or isospin, and neither (2) present for a system of only one spin and only one isospin.

The expectation value of the kinetic energy and of the direct part of the potential energy can be found analytically as

$$\langle \Phi | T | \Phi \rangle / N = \frac{3}{5} \beta^2 / r_0^2,$$

$$\langle \Phi | V_d | \Phi \rangle / N = [3/(2r_0^3)] \sum_i V_i / u_i^2,$$
(8)

while the exchange part of the potential can be given as

$$\langle \Phi | V_{\text{ex}} | \Phi \rangle / N = -(3/\pi r_0) \beta \sum V_i f_{\text{HF}}(u_i r_0 / \beta).$$
 (9)

The indicated function is an integral which was evaluated numerically for a number of values of y, and the results fit to an inverse polynomial which reproduced them to three significant figures for y = 1.25 and somewhat less accurately beyond that:

$$f_{\rm HF}(y) = \int_0^\infty dx \, x e^{-yx} [(\sin x - x \cos x)/x^3]^2$$

$$\approx 1/(4.000 + 7.996y + 3.948y^2 + 1.432y^3).$$
(10)

With $\hbar^2/2m = 20.74 \text{ MeV F}^2$ and E in MeV and r_0 in



F, this yields expectation values of the energy for the following three possible cases:

Normal (neutrons and protons, both spins),

$$\langle \Phi | H | \Phi \rangle / N = 28.9 / r_0^2 + 320.4 / r_0^3$$

- $(1.455 / r_0) \sum_i V_i f_{\rm HF} (0.6565 r_0 u_i);$ (11)

neutron (all neutrons, both spins),

$$\langle \Phi | H | \Phi \rangle / N = 45.8 / r_0^2 + 313.4 / r_0^3$$

- $(1.833 / r_0) \sum_i V_i f_{\rm HF} (0.5211 r_0 u_i);$ (12)

ferromagnetic (all neutron, spins aligned),

$$\langle \Phi | H | \Phi \rangle / N = 72.8 / r_0^2 + 415.1 / r_0^3$$

- $(2.309 / r_0) \sum_i V_i f_{\rm HF} (0.4133 r_0 u_i).$ (13)

The differences in the values of the direct part of the potential are due to the different potentials implied by the different spins present. Of course, since the exchange effect is only between particles of the same spin and isospin, and since the kinetic energy does not depend on the potentials used, these terms change only because of the (2)'s discussed above. The results are plotted in Fig. 2. The normal wave function does not give the lowest upper bound to the ground-state energy anywhere in the region shown $(0.2 < r_0 < 1.2 \text{ F})$; instead the lowest bound is given by the ferromagnetic wave function. This is somewhat tentative evidence in itself in favor of nuclear crystallization as it is analogous to the situation in the crystal region of the electron gas where the lowest bound to the energy in a similar calculation is given by the physically unreasonable ferromagnetic wave function instead of by the normal wave function, the difficulty there being resolved by the fact that the true wave function is a crystal wave function.

B. Mathieu Functions

In order to use the above method with a crystalline wave function, a method is needed for generating orthonormal single-particle wave functions from which a many-body wave function can be constructed. To that end, let $V_g(c, x) = c \sin^2(\pi x/a)$ be a generating potential whose sole purpose is to generate crystal-like wave functions. c is an arbitrary parameter which will ultimately be varied to find the energy minimum. The single-particle wave function then is

$$\varphi(\vec{\mathbf{k}}, c, \vec{\mathbf{x}}) = \prod_{i=1}^{3} \varphi(k_i, c, x_i) \alpha(\eta) \gamma(\xi),$$

with $\varphi(k, c, x)$ the solution to

$$\left[-\frac{\partial^2}{\partial x^2} + V_g(c, x)\right]\varphi(k, c, x) = E(k, c)\varphi(k, c, x),$$
(14)

and it will be noted that by virtue of being nondegenerate eigenfunctions of the same equation $\varphi(k, c, x)$ and $\varphi(k', c, x)$ are orthogonal.

In the limit as c goes to zero, $\varphi(k, 0, x) = e^{ikx}$, and the wave function becomes the plane-wave one above. For $c \neq 0$, near the origin the generating potential is given by

$$V_{e}(c, x) = c[(\pi x/a)^{2} - \frac{1}{3}(\pi x/a)^{4} + \cdots];$$

near any other point, substitute x - na in the above. For particles sufficiently localized that $x/a \ll 1$, this reduces to a harmonic-oscillator potential so that the generating potential will give a harmonic-oscillator – or crystal-type single-particle wave function in this limit.

With a little manipulation, the equation for φ becomes

$$\left[-\frac{\partial^2}{\partial y^2} + \overline{a}(k, q) - 2q\cos(2y)\right] \varphi(k, q, ay/\pi) = 0,$$
(15)

with

$$q = (-a^2/\pi^2)^{\frac{1}{4}}c$$
 and $\overline{a}(k, q) = a^2 E(k, q)/\pi^2 + 2q$,

which is Mathieu's equation. A solution to this equation is

$$\varphi(k, q, ay/\pi) = (1/L)^{1/2} e^{iky} \sum_{r} c(r, k, q) e^{i2ry}$$
. (16)

Periodic boundary conditions imply that k = 2na/Lwhich in turn implies that for large L, $\sum_{k} (L/2a) \int dk$. The functions are automatically

 $\sum_{k} (L/2a) \int dk$. The functions are automatically orthogonal and will be orthonormal when we require the $\sum_{r} c^2(r, k, q) = 1$.

The only difference between these functions and the Mathieu functions normally encountered is that k is not integral. The method of solution using successive approximations and continued fractions described in McLachlan⁵ and elsewhere is still applicable. This method was incorporated into a set of computer subroutines which for a given value of q and k rapidly calculated the value of $\overline{a}(k, q)$ and of the c(r, k, q)'s for as many r values as desired. In practice the series was rapidly convergent so that only five to ten values of r were ever needed.

In addition to the orthogonality produced by the differential equation, there is that due to spin and isospin. These were utilized by an arbitrary fixing of the lattices around which the generating potentials are built. The case with all spins parallel, of course, has the simple cubic-lattice structure of the generating potential in three dimensions; with both spins but only one isospin the structure is that of two generating-potentialsupplied cubic lattices of opposite spins, one in the body-centered position of the other (bcc lattice); for the case with both spins and both isospins there are four cubic lattices, three of them in the face-centered positions of the fourth (fcc lattice), where in each case a is the lattice constant. The reason for fixing the spins in this manner is that it allows us to fill each set of states up to the same value of k_F , and therefore to use the same numerical work for all three cases. In the plane-wave limit where each single-particle state occupies the entire volume, this fixing of the lattices has no meaning and no effect on the energies calculated, while in the crystal limit these are not unreasonable ways to fix the spins. The obvious overlapping of the generating potentials in the bcc and fcc lattices emphasizes the fact that these are

not physical potentials, but rather enter the problem only to produce the wave functions.

Proceeding now in the same way as for plane waves, the expectation value of N is found from

$$\langle N \rangle = \sum_{\xi, \eta} \sum_{\tilde{\chi}} \langle \varphi(\mathbf{k}, q, \tilde{\mathbf{x}}) | \varphi(\mathbf{k}, q, \tilde{\mathbf{x}}) \rangle$$

= $\frac{1}{8} (L^3/a^3) \sum_{\xi, \eta} \int d^3 k.$ (17)

Using $(L/a)^3 = N_s$, the number of particles of a particular spin then becomes

$$N = N_s \sum_{\xi, \eta} \frac{1}{8} \int d^3k,$$

which implies that the Fermi volume must be 8. This fixing of the Fermi volume at a definite value means that the connection with r_0 now comes from the relation between a and r_0 , rather than through k_F and r_0 as above.

The kinetic energy for any one spin is

$$\langle \Phi | T | \Phi \rangle = (\pi/a)^2 \sum_{\vec{k}} 3 \langle \varphi(k_1, q, x_1) | - \partial^2 / \partial (x\pi/a)^2 | \varphi(k_1, q, x_1) \rangle,$$

which, using the equation for φ , becomes

$$= -3(\pi/a)^{2} \sum_{\vec{k}} [\langle \varphi(k_{1}, q, x_{1}) | 2q \cos(2\pi x_{1}/a) - \overline{a}(k_{1}, q) | \varphi(k_{1}, q, x_{1}) \rangle]$$

$$= -3(\pi/a)^{2} \sum_{\vec{k}} \sum_{r,s} c(r, k_{1}, q) c(s, k_{1}, q) \int_{-L/2}^{L/2} dx (e^{+i2x\pi/a} + e^{-i2x\pi/a}) e^{i2(s-r)x\pi/a},$$
(18)

which with the fact that $\int_{-L/2}^{L/2} dx e^{imx\pi/a} = L\delta_{m,0}$ and a little manipulation becomes

$$\langle \Phi | T | \Phi \rangle = 3(\pi/a)^2 \sum_{\mathbf{k}} \left[\overline{a}(k_1, q) - 2q \sum_{\mathbf{r}} c(\mathbf{r}, k_1, q) c(\mathbf{r}+1, k_1, q) \right],$$
(19)

and numerical methods will be used to go further.

The potential energy from the interactions between particles on the same cubic lattice is given by

$$\langle \Phi | V | \Phi \rangle = \frac{1}{2} \sum_{\vec{k}, \vec{k}'} [\langle \varphi(\vec{k}, q, \vec{r}) \varphi(\vec{k}', q, \vec{r}') | v(\vec{r} - \vec{r}') | \varphi(\vec{k}, q, \vec{r}) \varphi(\vec{k}', q, \vec{r}') \rangle - \langle \varphi(\vec{k}, q, \vec{r}) \varphi(\vec{k}', q, \vec{r}') | v(\vec{r} - \vec{r}') | \varphi(\vec{k}', q, \vec{r}) \varphi(\vec{k}, q, \vec{r}') \rangle].$$

$$(20)$$

Consider the first, the direct, part of the potential first:

$$\langle \Phi | V_{\mathrm{d}} | \Phi \rangle = \frac{1}{2} \int d^3 r \int d^3 r' v(\vec{\mathbf{r}} - \vec{\mathbf{r}}') \int \int \prod_i |\varphi(k_i, q, r_i)|^2 |\varphi(k_i', q, r_i')|^2 d^3 k \, d^3 k'.$$

Using the fact that the integral over r + r' is $L\delta_{m,0}$ as above, this can be put in the form

$$\langle \Phi | V_{\rm d} | \Phi \rangle = (N_{\rm s}/2 \times 64) \int d^3x \, v(xa) \int d^3k \int d^3k' \prod_i f(k_i, k_i', x_i), \tag{21}$$

where

$$f(k, k', x) = \sum_{v} e^{i 2x \pi v} F(v, k) F(v, k'), \qquad (22)$$

or equivalently for spherically symmetric potentials,

 $=\sum_{v}\cos(2\pi xv)F(v, k)F(v, k'),$

with

$$F(v, k) = \sum_{s} c(s, k, q) c(v + s, k, q);$$
(23)

and again this will be treated further.

In a similar manner the exchange part of the potential can be written as

$$\langle \Phi | V_{ex} | \Phi \rangle = -\frac{1}{2} \sum_{\vec{k}, \vec{k}'} \int d^3 x \, v(\vec{x}) \prod_i \int_{-L/2}^{L/2} \frac{dR_i}{L^2} \{ \sum_{s, t, u, v} c(s, k_i, q) c(t, k'_i, q) c(u, k_i, q) c(v, k'_i, q) \\ \times \exp[(-i\pi x_i/a)(k_i - k'_i + s - t + u - v)] \exp[i\pi R_i(-2s - 2t + 2u + 2v)] \},$$

$$(24)$$

which simplifies much as did the direct potential on using the Kronecker δ function with supplementary functions somewhat more involved than in the direct potential defined as

$$\overline{F}(v, k'_i, k_i) = \sum_i c(t, k'_i, q)c(t+v, k_i, q)$$

and

$$f_{\rm ex}(k_i, k_i', x_i) = \sum_{v} \exp\{i2\pi x_i [-v + \frac{1}{2}(k_i' - k_i)]\} \overline{F}^2(v, k_i', k_i),$$
(25)

which, using spherically symmetric potentials, is equivalent to

$$f_{\rm ex}(k, k', x) = \frac{1}{2} \sum_{v} \left(\cos\{2\pi x \left[-v + \frac{1}{2} (k'-k) \right] \right\} \overline{F}^2(v, k', k) + \cos\{2\pi x \left[-v + \frac{1}{2} (k'+k) \right] \right\} \overline{F}^2(v, k', -k) \right), \tag{26}$$

so that

$$\langle \Phi | V_{\text{ex}} | \Phi \rangle = -(N_s/2 \times 64) \int d^3x \, v(\bar{\mathbf{x}}a) \int d^3k \int d^3k' \prod_i f_{\text{ex}}(k_i, \, k_i', \, x_i), \tag{27}$$

which will be treated further.

In principle, now the functions f and f_{ex} can be determined and a numerical scheme found to do the necessary integrals so that, for example,

$$G_{\rm ex}(r) = {\rm const} \int d\Omega \int d^3k \int d^3k' \prod_i f_{\rm ex}(k_i, k_i', x_i)$$
(28)

can be found which would give

$$\langle \Phi | V_{\text{ex}} | \Phi \rangle = \int_0^\infty dr \ v(ra) G_{\text{ex}}(r) r^2.$$

In fact, the limits of the k integrations have not been determined, only that the volume is 8. Also the various functions have discontinuities at k = n, where n is any integer, and in particular they have discontinuities at $k=\pm 1$. These discontinuities are the mathematical manifestations of the energyband gaps found in crystals and, as might be expected, the single-particle states with $k=1^+$ are higher in energy by an amount proportional to the degree of crystallization than those with $k=1^{-}$. This leads to the suspicion, confirmed by Monte Carlo integrations of the above for the case of an electron system, that for q values large enough to be evidence for crystallization, the appropriate Fermi surface is a cube with $-1 < k_i < +1$. It should be noted that, while this is the only choice for the system with only one spin and isospin, it is our lattice choice which makes it also the choice for the other cases. In addition to the obvious simplification in making the three cases have the same

Fermi surface, there is a suspicion that the maximum gain from crystallization is for those singleparticle states just below the discontinuity which will get the most filling with these lattices.

For a cubical Fermi surface, the above integral is considerably simplified owing to its separability. For example,

$$\int d^{3}k \int d^{3}k' \prod_{i} f(k_{i}, k'_{i}, x_{i})$$

$$= \prod_{i} \int_{-1}^{1} dk_{i} \int_{-1}^{1} dk'_{i} f(k_{i}, k'_{i}, x_{i})$$

$$= \prod_{i} \sum_{v} \cos(2\pi x_{i}) \left(\int_{-1}^{1} dk F(v, k) \right)^{2},$$
(29)

or defining

$$F(v) = \int_{-1}^{1} F(v, k),$$
(30)

we find

$$\langle \Phi | V_{\rm d} | \Phi \rangle = (N_s/2) \int r^2 dr \, v(ra) \int d\Omega \prod_i G(r_i), \quad (31)$$

where

$$G(r_i) = \frac{1}{4} \sum_{v} \cos(2\pi r_i v) F^2(v).$$
(32)

Similarly

$$\langle \Phi | V_{\text{ex}} | \Phi \rangle = (-N_s/2) \int r^2 dr \, v(ra) \int d\Omega \prod_i G_{\text{ex}}(r_i),$$
(33)

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where

$$G_{\rm ex}(r_i) = \frac{1}{4} \int_{-1}^{1} dk \int_{-1}^{1} dk' f_{\rm ex}(k, k', r_i), \qquad (34)$$

which is somewhat more difficult in that it involves a double numerical integration instead of the single one for the direct term above.

The potential energy is now in the form

$$\langle \Phi | V | \Phi \rangle = (N_s/2) \int r^2 dr v(ra)$$

$$\times \left(\int d\Omega \prod_i G(r_i) - \int d\Omega \prod_i G_{ex}(r_i) \right).$$
(35)

Since the terms coming from the interactions of one lattice with another can be shown to be trivially related to $G(r_i)$, the above is the potential in the form of a single-particle potential times a correlation function which is the result of doing the angular integrations. Correlation functions, which will be of interest in the extrapolation section, are shown for the normal (fcc) nucleon system along with that for ferromagnetic plane waves in Fig. 3. These show the expected oscillations typical of crystalline wave functions, and it is fortunate that all of the separability coming from the type of wave function and cubical Fermi surface has not yet been exploited, since the r integration with these correlation functions would converge only for very large values of r.

The spatial integral for $\langle \Phi | V | \Phi \rangle$ is already in separable form except for the part involving v(ra). For Yukawa potentials this can be made separable by using the fact that

$$\int_{0}^{\infty} d\alpha \, e^{-r^{2} \alpha^{2}} e^{-u^{2}/4 \alpha^{2}} = \pi^{1/2} e^{-ru}/2r, \qquad (36)$$

so that, for example, with $v(ra) = \sum_i V_i e^{-u_i ra} / ra$,

$$\langle \Phi | V_{d} | \Phi \rangle = \sum_{i} V_{i} (2/\pi^{1/2})^{3} \int_{0}^{\infty} d\alpha \ e^{-u_{i}^{2} a^{2}/4\alpha^{2}} \times \left[\int_{-\infty}^{\infty} dx \ e^{-x^{2} \alpha^{2}} G(x) \right]^{3}.$$
(37)

Furthermore

$$\int_{-\infty}^{\infty} dx \, e^{-x^2 \alpha^2} G(x) = \frac{1}{4} \sum_{v} F^2(v) \int_{-\infty}^{\infty} dx \, e^{-x^2 \alpha^2} \cos(2\pi x v)$$
$$= \frac{1}{4} (\pi^{1/2} / \alpha) \sum_{v} F^2(v) e^{[-(2\pi v)^2/4]^2},$$
(38)

so that letting $y = 1/\alpha$, defining

$$\overline{v}(y) = \sum_{i} V_{i} e^{-(u_{i}y/2)^{2}}$$
(39)



FIG. 3. Correlation functions for the normal (fcc) nucleon crystal for various values of q along with that of the ferromagnetic plane-wave system. ferromagnetic plane wave, ------ q = 1.0, ----- q = 2.0, ------ q = 3.0 (gives minimum energy bound for $r_0 = 0.6$ F).

and

$$F_{\rm d}(y) = \frac{1}{4} \sum F^2(v) e^{-(\pi v y)^2}$$
(40)

gives

$$\langle \Phi | V_{\rm d} | \Phi \rangle = N_{\rm s}(\pi/a) \int_0^\infty dy \, y \, \overline{v}(y \, a) F_{\rm d}^{3}(y). \tag{41}$$

The interaction of a lattice with one displaced from it differs from its interaction with itself only by a $\frac{1}{2}a$ which appears in $\varphi^2(k_i, q, r_i + \frac{1}{2}a)$ and then in $G(r_i + \frac{1}{2})$ which finally results in

$$G(r_{i} + \frac{1}{2}) = \sum_{v} [\cos(\pi v) \cos(2\pi r_{i} v)F^{2}(v) + \sin(\pi v) \sin(2\pi r_{i} v)F^{2}(v)], \qquad (42)$$

where the sine terms will integrate to zero for any symmetric potential and the $\cos(\pi v)$ is just $(-1)^{\nu}$, so that

$$F_{I}(y) = \frac{1}{4} \sum_{v} (-1)^{v} F^{2}(v) e^{-(\pi v y)^{2}}.$$
(43)

Then for the interaction of the direct lattice with the bcc lattice

$$\langle \Phi | V_{\rm bcc} | \Phi \rangle = N_s(\pi/a) \int_0^\infty dy \, y \,\overline{v}(ya) F_I^3(y), \qquad (44)$$

5



FIG. 4. The transform of the exchange part of the correlation function, $f_{ex}(q, y)$.

and with the fcc lattice

$$\langle \Phi | V_{\text{fcc}} | \Phi \rangle = N_s(\pi/a) \int_0^\infty dy \, y \,\overline{v}(y \, a) F_{\text{d}}(y) F_I^2(y).$$
(45)

Then the same transformation applied to the ex-

with

$$F_{\rm ex}(y) = \int_0^1 dk \int_0^1 dk' \sum_{v} \{ \exp(-\pi^2 y^2 [-v + \frac{1}{2}(k'-k)]^2 F^2(v,k',k)) + \exp(-\pi^2 y^2 [-v + \frac{1}{2}(k'+k)]^2 F^2(v,k',-k)) \}.$$
(47)

 $F_{\rm ex}(y)$ is the most difficult to evaluate. To evaluate it we must find and integrate over F(v, k', k), a function of three variables. Furthermore, the convergence as a function of y is not exponential as it might seem at first owing to the fact that for some values of k and k' the arguments of the exponentials go to zero. It can be shown, however, that $F_{ex}(y)$ goes rapidly to $2\pi^{1/2}/y$ as y becomes large, and furthermore that owing to the vanishing of the derivatives which would appear in an error analysis of the trapezoidal-rule integration over k and k', a simple-minded midpoint trapezoidalrule integration for small values of y (those for which the asymptotic limit does not hold) converges

TABLE I. Coefficients A_{mn} in the polynomial expansion $f_{ex,d}(q, y) = \sum_{n=0}^{6} \sum_{n=1}^{6} A_{mn}(q/5)^m(y/2)^n$ valid in the region $0 \le q \le 5$, $0 \le y \le 2$. The standard deviation of the polynomial from the points to which it was fitted is $\sigma \le 0.02$ in the region $0 \le y \le 0.4$, $0 \le q \le 5$; $\sigma \le 0.08$ in the region $0.4 \le y \le 1.0$, $0 \le q \le 5$; $\sigma \le 0.15$ in the region $1.0 \le y \le 2.0$, $0 \le q \le 5$. This is the $f_{ex,d}$ of Eq. (51), and the energy may be obtained from it by doing the one-dimensional integration indicated there. The sum of terms is 7.47.

	m = 0	<i>m</i> = 1	<i>m</i> = 2	m = 3	<i>m</i> =4	<i>m</i> = 5	<i>m</i> = 6
<i>n</i> = 1	15,93	-0.60	24.20	-45.38	72.53	-99.13	51.18
n=2	2,36	-2.98	-252.62	-275.42	1264.82	-941.27	135.19
n=3	-52,25	-160.20	998.49	3492.57	-11842.68	11062.66	-3283.88
n=4	57.46	794.73	-3015.89	-3438.79	17485.41	-17647.76	5498.40
n = 5	-20.99	-957.39	3599.61	-1695.23	-5615.97	6956.61	-2135.09
n = 6	1.60	334.20	-1311.57	1689.40	-782.88	129.31	-81.22



FIG. 5. The transform of the direct part of the correlation function for an all neutron system, $f_d(q, y)$.

change potential yields

$$\langle \Phi | V_{\rm ex} | \Phi \rangle = -N_s(\pi/a) \int_0^\infty dy \,\overline{v}(ya) F_{\rm ex}{}^3(y), \qquad (46)$$

n = 6

804.23

gion $0 \le y \le 0.4$, $0 \le q \le 5$; $\sigma \le 0.08$ in the region $0.4 \le y \le 2$, $0 \le q \le 5$; the sum of terms is -1.41.						
	<i>m</i> = 1	<i>m</i> = 2	<i>m</i> = 3	<i>m</i> = 4	<i>m</i> = 5	<i>m</i> = 6
n = 1	-82.58	-144.02	1723.02	-4161.87	4115.43	-1466.76
n=2	-148.66	1920.77	-7692.94	14 626.38	-13211.60	4525.82
n = 3	1089.55	-10 936.86	34 714.55	-54 257.45	42 137.80	-12896.35
n=4	-1403.49	$20\ 697.47$	-66899.73	99201.36	-71053.32	19862.81
n=5	470.30	-15277.80	50 975.86	-71401.62	45798.54	-10929.96

-12 670.65

15695.34

TABLE II. Coefficients A_{mn} in the polynomial expansion $f_i(q, y) = \sum_{m=1}^{6} \sum_{n=1}^{6} A_{mn} (q/5)^m (y/2)^n$ valid in the region $0 \le q \le 5$, $0 \le y \le 2$. The standard deviation of the polynomial from the points to which it was fitted is $\sigma \le 0.03$ in the region $0 \le y \le 0.4$, $0 \le q \le 5$; $\sigma \le 0.08$ in the region $0.4 \le y \le 2$, $0 \le q \le 5$; the sum of terms is -1.41.

very well for reasonable numbers of points. In the numerical work it was convenient to use

76.51

$$f_{\text{ex,d}}(q, y) = y[-F_{\text{ex}}^{3}(q, y/\pi) + F_{\text{d}}^{3}(q, y/\pi) - 1],$$
 (48)

3704.02

$$f_i(q, y) = y[F_i^{3}(q, y/\pi) - 1],$$
(49)

 $f_{\rm fcc}(q, y) = y [F_i^2(q, y/\pi) F_{\rm d}(q, y/\pi) - 1].$ (50)

This means that $\langle V_b \rangle = \frac{1}{2}\rho \int_{\Omega} d^3 r v(r)$ has been explicitly subtracted out and must be added on later to get the total energy so that, for example, the potential energy's expectation value in the case where there is a single isospin and both spins is

$$\begin{split} \langle \Phi | V_{\text{bcc}} | \Phi \rangle &= -(1/8\pi) \int_0^\infty dy [\overline{v}_1(y a/\pi) f_{\text{ex, d}}(q, y) \\ &+ \overline{v}_2(y a/\pi) f_i(q, y)] + \langle V_b \rangle, \end{split}$$

(51)

where some of the spin and isospin dependence of the soft-core nucleon potential fits can be taken into account through differences in \overline{v}_1 and \overline{v}_2 . Examples of these functions are shown in Figs. 4 and 5 and polynomial fits to them are given in Tables I-IV. This was done as follows: The c's and \overline{a} 's were generated for some given value of q and for as many k's as were needed in the integrations which were all done by the midpoint trapezoidal rule (the only exception to this was in the integrals needed for the correlation functions which were done by five-point Gaussian integration), then for about twenty different values of y, the integrals needed for $F_{ex}(y)$, $F_{d}(y)$, and $F_{i}(y)$ were performed, and these results printed out. From these the functions which actually are needed could be determined for various values of q and y. The accuracy of these points was determined by decreasing the mesh size for selected ones. As expected from the nature of the integrand, the accuracy was either not at all or very good for F_{ex} as mentioned above and much better than that for F_d and F_i which were determined at the same time. The polynomials were fitted to these points by a two-dimensional least-squares fitting routine in which the points at y = 0.1 and 0.3 were weighted 10, those at 0.5 were weighted 3, at 0.7 were weighted 2, at 0.9 were weighted 1.5, and for larger values of y were weighted 1. This weighting was done so that the products of f and \overline{v} would have as constant an error as possible; the points themselves were an order of magnitude more accurate than the fit: they were just too few to be used directly. The tables are the result of fitting 156 data points with 42 or fewer constants. Beyond y=2, only $f_{ex}(y) = yF_{ex}^{3}(y)$ is needed since the others go exponentially to zero.

-7505.51

The kinetic energy was determined using Eq. (19) at the same time as the F's above with the result that

$\langle \varphi | T | \varphi \rangle = (31.25/r_0^2) K(q) \text{ MeV } F^2$

(normal nucleon crystal fcc),

TABLE III. Coefficients A_{nm} in the polynomial expansion $f_{fcc}(q, y) = \sum_{m=1}^{6} \sum_{n=1}^{6} A_{nm} (q/5)^m (y/2)^n$ valid in the region $0 \le q \le 5$, $0 \le y \le 2$. The standard deviation of the polynomial from the points to which it was fitted is $\sigma \le 0.01$ in the region $0 \le y \le 0.4$, $0 \le q \le 5$; $\sigma \le 0.03$ in the region $0.4 \le y \le 1.0$, $0 \le q \le 5$; $\sigma \le 0.07$ in the region $1.0 \le y \le 2.0$, $0 \le q \le 5$. The sum of terms is 0.32.

	<i>m</i> = 1	<i>m</i> = 2	<i>m</i> = 3	<i>m</i> = 4	<i>m</i> =5	m = 6
n = 1	-18.22	-388.16	1826.64	-3435.37	2974.53	-975.71
n=2	-0.81	-284.82	1341.60	-2165.50	1484.29	-360.84
n =3	19.71	5256.14	-28686.11	56 537.24	-49173.46	15 907.02
n = 4	209.39	-11 821.09	70 162.07	-145430.93	130 748.48	-43298.79
n = 5	-415.61	11 226.69	-70 618.04	151 406.23	-138 963.05	46 648.11
n = 6	206.41	-4009.05	26092.66	-57171.64	53 174 .08	-18 003.77

TABLE IV. Coefficients A_{mn} in the polynomial expansion $g_{ex}(q, y) = \sum_{m=0}^{3} \sum_{n=1}^{3} A_{mn} (q/5)^m (2/y)^n$ valid in the region $0 \le q \le 5$, $y \ge 2$ with a standard deviation from the calculated points of $\sigma = 0.5$. In the region $y \ge 2$, $0 \le q \le 5$, f_{ex} is given by $f_{ex}(q, y) = -44.545/y^2 + g_{ex}(q, y)/y^2$. The sum of terms is 8.5.

	m = 0	<i>m</i> =1	<i>m</i> = 2	<i>m</i> = 3
n = 1	18.8	-143.2	280.6	-157.6
n=2	33.6	3.1	-131.5	104.2
n = 3	-24.0	74.1	-64.9	15.3
				1. Contract (1997)

$$\langle \varphi | T | \varphi \rangle = (49.60/r_0^2) K(q) \text{ MeV } \mathbf{F}^2$$

(all neutron crystal bcc),

 $\langle \varphi | T | \varphi \rangle = (78.68/r_0^2) K(q) \text{ MeV } \mathbf{F}^2$

(ferromagnetic all neutron crystal cubic), with

 $K(q) = 0.9771 + 1.8210(\frac{1}{5}q) + 35.7420(\frac{1}{5}q)^{2}$ $-116.0312(\frac{1}{5}q)^{3} + 177.7894(\frac{1}{5}q)^{4}$

 $-134.5125(\frac{1}{5}q)^5 + 40.0941(\frac{1}{5}q)^6 \pm 0.0025$

valid in the region $0 \le q \le 5$.

The energy upper bounds are given in Fig. 2. An estimate of the accuracy found by assuming that the first neglected polynomial times σ is the error in the functions being integrated gives an error estimate of about 2 MeV which is negligible compared to the energies being calculated. A sample of the integrand actually used in Eq. (51) is shown in Fig. 6.

The energy bounds have also been calculated for the electron gas system with the results shown in Fig. 7. The values of q_{\min} for both the nucleon and electron systems are shown in Fig. 8. In the electron system, it is possible to use perturbation theory to take into account the differences between the generating potential and a harmonicoscillator potential and calculate explicitly the value of q expected to minimize the energy of an electron crystal (dashed line in Fig. 8).

IV. CONCLUSIONS (EXTRAPOLATIONS)

The correlation function of the normal (fcc) system for various values of the crystallization parameter, q, along with that for ferromagnetic plane waves is shown in Fig. 3. The correlation functions are not particularly useful for computation owing to their slow damping with r; however, they do give us some ideas about what the wave functions are trying to say about the particles and how to extrapolate beyond Hartree-Fock. The first expected change in going beyond Hartree-Fock is that since we are dealing with repulsive po-



FIG. 6. Sample of the functions appearing in Eq. (51). $\overline{V}(y) = \sum_i V_i \exp[-(u_i y a/2)^2]$ as in Eq. (39). V_i and u_i are from the Reid potential and a is the lattice constant determined by r_0 . $V_{int}(y) = f_{ex,d}(q=1.0, y)V(y)/8$, and is the first of the integrands in Eq. (51), shown here for q=1.0. $----r_0=1.0$ F, $----r_0=0.5$ F.

tentials, the particles will try to stay out of each other's way, and hence lower the value of the correlation function for small separations. The normal plane-wave function (not shown) is 0.75 for zero separation and therefore stands to make, and certainly needs, the most improvement. This is too much for us to guess at, so the ferromagnetic wave function whose correlation function is zero at zero separation will be considered to represent the system as a gas despite the fact that the correct wave function is probably not ferromagnetic. The comparison of interest is then between the energy bound given by the ferromagnetic wave function and that given by the crystal wave function for the normal system with $q \approx 3$ (see Fig. 9 for the energy comparison). The change expected in the ferromagnetic system upon going beyond Hartree-Fock is that it will become a normal system thereby lowering the kinetic energy (~200 MeV/ part at $r_0 = 0.6$ F) towards the kinetic energy of the normal plane-wave system (80 MeV/part at r_0 = 0.6 F) and a slight lowering of the correlation function for small separations, $r/a \approx 0.2$, but not much else. The change expected in the crystal wave function with q=3 is a lowering of the correlation function between r/a=0 and r/a=0.3. Since the potential in this region is on the order of 1000 MeV and since the crystal correlation



function shows the most room for improvement, it would be expected that calculations going beyond Hartree-Fock would lower the potential energy of the crystal wave function more than that of the ferromagnetic wave function by enough extra to more than account for the fact that the ferromagnetic wave function's kinetic energy would also be lowered. In short, one would expect the crystal-wave-function energy bounds and the gas-wave-function energy bounds as represented by the ferromagnetic wave function to be both lowered, but roughly by the same amounts. Especially in extrapolating, it should be noted that liquids are a lot like crystals. The long-range correlations may well be the first to go in any subsequent improvements of the wave function. The comparison is really between the type of correlations in a liquid or a crystal, here represented by a crystal-like wave function, and the statistical plus, on extrapolating, the purely repulsive correlations of a gas of plane waves.

For r_0 greater than 1.0 F, the lowest energy bound is given by the ferromagnetic wave function. This agrees with the crude crystal calculation which showed that the value of $\langle r^2 \rangle / r_0^2$ becomes large in this region. For r_0 greater than 1.0 F, the system is undoubtedly not crystal-like.

For r_0 between 0.2 F and 1.0 F, the lowest energy bound is given by the normal crystal. For example, at $r_0 = 0.6$ F, the crystal wave function

gives an energy bound of 640 MeV/particle, while the ferromagnetic wave function gives 900 MeV/ particle. Comparing this with the better-understood electron system at $r_s = 20$, where it is commonly believed to be crystalline, the crystal bound there is -0.040 Ry, the ferromagnetic bound -0.035 Ry, and Carr's⁶ calculation of the actual energy -0.044 Ry. There is far more change in the nuclear system's energy bound than for the electron system. Furthermore, the energy lowering is more than could be accounted for by giving the ferromagnetic wave function the kinetic energy of the normal wave function. The energy lowering has come about because the system has been able to pay the price in kinetic energy to lower the value of the correlation function between r/a=0.2 and r/a=0.6 and still show a profit. The system is undoubtedly trying to localize itself in this region. It is worth noting that the peak improvement (Fig. 3) is at the value of r_0 for which classical hard spheres would crystallize.1

For $r_0 \approx 0.2$ F, the lowest energy bound is still given by the crystal wave function although this is rapidly changing, but more ominously the ferromagnetic system is no longer lower than the normal plane-wave system. The normal system, moreover, stands to gain a lot when calculations beyond Hartree-Fock are included. The trading of kinetic energy (going as $1/r_0^2$) for potential



FIG. 8. q_{\min} vs r_0 and r_s for the nucleon and electron systems.

energy [now going as about $7000 \exp(-4.9r_0)/r_0$] may no longer lower the energy. This is the condition for the beginning of the region corresponding to the dense electron gas, not crystalline.

The energies compared here are all variational, and hence upper bounds to the true energy. They have been fit to polynomials so that in the region $0.2 \le r_0 \le 1.0$ F with r_0 in F the energy bounds are

normal nucleon gas (fcc),

$$\frac{E}{N} \leq \left(-\frac{3550}{r_0} + \frac{10367}{r_0^{3/2}} - \frac{10317}{r_0^2} + \frac{3793}{r_0^{5/2}} - \frac{152}{r_0^3} \pm 0.5\%\right) \text{ MeV};$$
(52)

normal all-neutron gas (bcc),

$$\frac{E}{N} \leq \left(-\frac{2196}{r_0} + \frac{6371}{r_0^{3/2}} - \frac{6055}{r_0^2} + \frac{1844}{r_0^{5/2}} + \frac{184}{r_0^3} \pm 0.5\%\right) \text{ MeV}.$$
(53)



FIG. 9. Energy bound for the normal nucleon crystal, E_{C} , compared with that for the ferromagnetic plane-wave system, E_{F} .

APPENDIX

To get numbers, it is necessary to have a potential. The potential used here is the Reid soft-core potential.³ This potential is state-dependent which for nonsymmetric states means that it has a nonsymmetric part which will average to zero in the many-body problem considered here. For example, between particles with parallel spin and isospin, $T_z = 1$ and $S_z = 1$, the relevant potentials are $V({}^{3}P_0)$, $V({}^{3}P_1)$, and $V({}^{3}P_2 - {}^{3}F_2)$. The dependence on S_{12} and $\vec{L} \cdot \vec{S}$ was removed from the first two by assuming it to be that explicitly given in the third, and the results averaged to give

$$V(^{3}A) = (3.488e^{-x} - 36.04e^{-2x} + 134.32e^{-3x} - 573.74e^{-4x} - 690.1e^{-6x} + 6887.3e^{-7x})/x,$$

$$x = r \times 0.7 \ \mathbf{F}^{-1}.$$
 (54)

For particles with parallel isospin and antiparallel spin, $T_z = 1$ and $S_z = 0$, the states are half tripleantisymmetric and half singlet-symmetric. The triplet potential is $V({}^{3}A)$, while the singlet is either Reid's $V({}^{1}S)$ or $V({}^{1}D)$:

$$V({}^{1}S) = (-10.463e^{-x} - 1650.6e^{-4x} + 6484.2e^{-7x})/x,$$
(55)
$$V({}^{1}D) = (-10.463e^{-x} - 12.322e^{-2x} - 1112.6e^{-4x} + 6484.2e^{-7x})/x.$$
(56)

For particles with parallel spin and antiparallel isospin, $T_z = 0$ and $S_z = 1$, the space state may be symmetric or antisymmetric so that the potential is half $V(^3A)$ and half $V(^3S - ^3D)$,

$$V(^{3}S - {}^{3}D) = (-10.463e^{-x} + 102.012e^{-2x} - 2915e^{-4x})$$

$$-7800e^{-6x})/x.$$
 (57)

For particles with antiparallel spin and isospin, $T_z = 0$ and $S_z = 0$, the potential is an average of $V(^3A)$ $V(^1P_1)$, $V(^3S - ^3D)$, and $V(^1S)$ or $V(^1D)$.

$$V({}^{1}P_{1}) = (31.389e^{-x} - 634.39e^{-2x} + 2163.4e^{-3x})/x.$$

Owing to the fact that for a crystal system $4 \approx k_F a$, the $V(^1D)$ potentials were used for the crystal calculations, while the $V(^1S)$ potentials were used with plane waves. This was not found to affect significantly the results, those with $V(^1D)$ being only about 10% higher than those with $V({}^{1}S)$.

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*Present address: Physics Department, Northwestern University, Evanston, Ill. 60201.

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Gravitation Theory and Oscillating Universe

Itzhak Goldman and Nathan Rosen

Department of Physics, Technion-Israel Institute of Technology, Haifa, Israel (Received 19 August 1971)

The field equations of a noncovariant theory of gravitation, based on the existence of a preferred frame of reference in the universe, are applied to the homogeneous isotropic cosmological model. One is naturally led to a particular value of the previously undetermined constant present in the equations. The second-order equation determining the radius of the universe can be integrated to give a first-order equation similar to that of general relativity, but with an additional term that can lead to oscillations without any singular state. One obtains a conservation law for the total energy, which is found to be positive definite.

I. INTRODUCTION

Recently a noncovariant theory of gravitation was proposed by one of the authors,^{1,2} based on the idea that there exists a preferred frame of reference in the universe, determined by the distribution of matter and energy. The field equations chosen were associated with a variational integral which depended on three constants. By considering the case of a weak, static field and comparing the field equations with those of Newton and Einstein one could fix two of the constants, while the third remained undetermined. However, it turned out that, in the case of a static, spherically symmetric field in empty space, the theory agreed with the general relativity theory to the accuracy required for comparison with the wellknown crucial tests, for arbitrary values of this constant.

In principle, the remaining constant could be determined from observations on gravitational waves. However, it would be desirable to fix this constant by means of theoretical considerations. The purpose of the present paper is to attempt to do this by applying the field equations to a model of the universe. Aside from the question of the value of the constant, such an application is of interest since, after all, the theory was arrived