Possibility of self-consistent long-range order in nuclear matter*

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Generalized Hartree-Fock Overhauser orbitals, corresponding to a (zero pressure) periodic structure of α particles, are shown to have lower energy than homogeneous nuclear matter with a Skyrme interaction, at subnuclear densities.

[NUCLEAR STRUCTURE Nuclear matter, Hartree-Fock approximation, cluster models.]

In a recent comment[1] the question of whether non-plane-wave Hartree-Fock (HF) states of the Overhauser[2] kind would give lower energy at some density in nuclear matter with a modern effective interaction was examined. The result, for a Skyrme-type interaction as parametrized by Vautherin and Brink,[3] was negative, contrary to Overhauser's original result, where an older such interaction (by Karplus and Watson[4]) was employed.

The possibility of lower-energy HF states with long-range order, however, of course, did not remain unambiguously excluded since variational (though non-self-consistent) calculations[5] have indicated their presence at densities *below* the nuclear saturation density of 0.17 fm^{-3}, and interpreted as α-particle formation at the nuclear surface—where the density is lower than the central nuclear density. An alternative and/or concomitant interpretation of the formation of such α particles (forming a periodic structure) might be the proposal by Clark, Chao, and Källman,[6] based on de Boer[7] scaling, that "α matter" at zero temperature *and pressure* should be crystalline (i.e., unlike typically *quantum* N-body systems like ^{3}He, ^{4}He, and, presumably, nuclear matter, which under similar conditions are liquid).

A difficulty for either of the above two interpretations is that all calculations to our knowledge, if at all, give *negative* pressure α matter, signifying an obvious instability.

We wish to report calculations which are: (i) self-consistent in the HF sense for occupied orbitals, based on generalized Overhauser orbitals, (ii) *ipso facto* variational, (iii) give *lower* energy than the (trivial) plane-wave HF orbitals at subnuclear densities (although with smaller binding than that *at* nuclear density), and (iv) correspond to zero pressure states.

The generalized HF Overhauser orbitals are, if α is a real (variational) parameter,

$$\phi_{k_x}(x) = C(\alpha)e^{ik_x x}[1+\alpha\cos qx]^n \quad (n=0,1,2,\ldots),$$
$$-k_0<k_x<k_0, \quad q=2k_0 m \quad (m=\pm1,\pm2,\ldots), \tag{1}$$
$$C(\alpha)=\left[L\sum_{i=0}^{n}\binom{2n}{2i}I_{2i}\alpha^{2i}\right]^{-1/2},$$
$$I_l \equiv L^{-1}\int_{-L/2}^{L/2}dx\,\cos qx = \frac{[1+(-)^l]}{2^{l+1}}\binom{l}{l/2},$$

(and likewise for y and z), and are orthonormalized in a cubic box of volume L^3. Further, they explicitly satisfy[8] the HF equations, for occupied orbitals, in the thermodynamic limit. (The parameter α is independent of k_x, contrary to Overhauser's original "ansatz," but the difference in energy has been shown[9] to be small.) The cosine term in Eq. (1) was found to give lower energy than Overhauser's original e^{iqx} term, partly because it clearly gives zero expectation value for the center of mass momentum. The associated single-particle density profile is, for quadruply occupied orbitals,

$$\rho(\vec{r}) = \rho f(x)f(y)f(z),$$
$$f(x) \equiv LC^2(\alpha)[1+\alpha\cos qx]^{2n}, \tag{2}$$
$$\rho \equiv 4(k_0/\pi)^3,$$

and defines a simple cubic lattice which smears out into spatially homogeneous density distribution as the "order parameter" $\alpha \to 0$. The limit

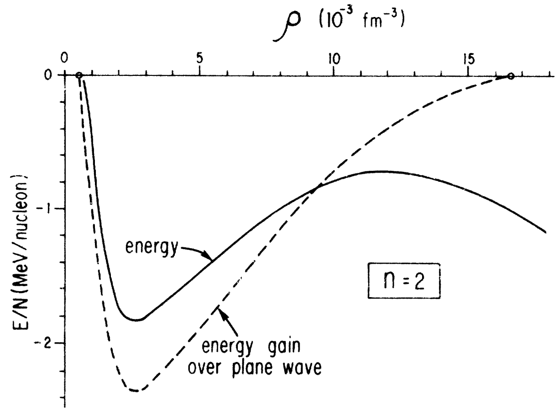

FIG. 1. The energy and energy gain over plane wave, Eq. (3) for $n=2$ and $\beta=\bar{\beta}$, where $\bar{\beta}$ minimizes the energy at fixed density, *versus* density ρ. Note that the energy minimum corresponds to zero pressure. Open circles are bifurcation points.

$n\to\infty$ in Eq. (2) leads[8] to a "classical static lattice" distribution, i.e., to a lattice of Dirac δ functions. Since the nearest-neighbor distance is $4(\rho/4)^{1/3}$, to each lattice point one may associate an α particle.

The HF energy for the Skyrme potential, as parametrized in Ref. 3 and called "I" there, is (by inspection) minimum in the parameter m of Eq. (1) for $|m|=1$, and gives, letting $\alpha^2=\beta$, the only remaining parameter to be varied,

$$
\begin{aligned}
E_n(\beta;\rho)/N = {} & \frac{\hbar^2\pi^2}{2M}\left(\frac{\rho}{4}\right)^{2/3}\left[1+6n^2\beta\,\frac{Q_{n-1}}{P_n}\right] \\
& + \frac{3}{2}t_0\left(\frac{\rho}{4}\right)\left(\frac{P_{2n}}{P_n^{\,2}}\right)^3 + t_3\left(\frac{\rho}{4}\right)^2\left(\frac{P_{3n}}{P_n^{\,3}}\right)^3 \\
& + \frac{\pi^2}{4}(3t_1+5t_2)\left(\frac{\rho}{4}\right)^{5/3}\left(\frac{P_{2n}}{P_n^{\,2}}\right)^3\left[1+6n^2\beta\,\frac{Q_{2n-1}}{P_{2n}}\right] \\
& + \tfrac{3}{2}(9t_1-5t_2)n^2\left(\frac{\rho}{4}\right)^{5/3}\pi^2\beta\left(\frac{P_{2n}}{P_n^{\,3}}\right)^2 Q_{2n-1}\,;
\end{aligned} \tag{3}
$$

$$E_n(0;\rho)/N \equiv E_{\rm PW}(\rho)/N\,;$$

$$P_n(\beta)\equiv\sum_{i=0}^{n}\binom{2n}{2i}I_{2i}\beta^i\,;\quad Q_n(\beta)\equiv\sum_{i=0}^{n}\binom{2n}{2i}\frac{I_{2i}}{(i+1)}\,\beta^i\,.$$

The force constants t_0, t_1, t_2, and t_3 are the set *I* of Ref. 3. The plane-wave determinant HF expectation energy is $E_{\rm PW}(\rho)$, and corresponds to $\beta=0$ in the general formula.

We carried out a numerical direct variation of Eq. (3), in the parameter β for different ρ, for $n=1, 2, \ldots, 12$. For $n=1$ there are indeed $\beta\neq 0$ states with lower energy than the PW state, but always with *negative* pressure $P=\rho^2\partial(E/N)/\partial\rho$. It is for $n\geq 2$ that $P=0$ states appear for the first time. Results are displayed in Figs. 1 to 3. For $n>2$ the behavior is qualitatively similar to the $n=2$ case, namely, there is an energy minimum in ρ (i.e., $P=0$) for the non-PW state and the "order parameter" β which minimizes the energy at each ρ grows as

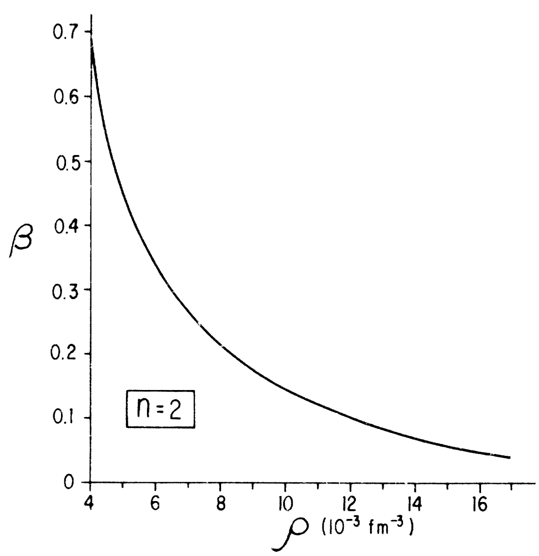

FIG. 2. The "order parameter" $\beta\equiv\alpha^2$ *versus* density ρ, which minimized the energy Eq. (3) at different densities, for $n=2$. Larger β signifies (Ref. 8) smaller overlap between "α sites" and thus more clearly individuated α particles.

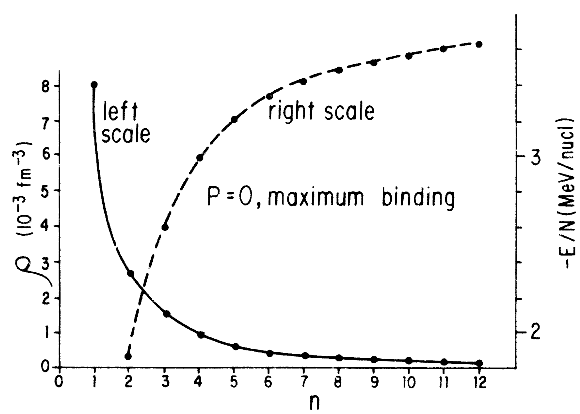

FIG. 3. Density values (in *nucleons*/fm^3) at which the energy Eq. (3) took its minimum (negative) value, as well as the binding energy/nucleon at that density, *versus* the parameter n. Only for $n=1$ was the α crystal unstable (pressure $P<0$). An extrapolation of energy *versus* n^{-1} gives -4 MeV/nucleon for $n^{-1}=0$, to be compared with the empirical -7 MeV/nucleon. Center of mass delocalization will reduce this discrepancy.

ρ decreases (showing a tendency of each "α particle" to become more and more individuated).

These stable (zero pressure), self-consistent, periodic states found to emerge from homogeneous nuclear matter may be considered as "embryonic" states of the α (crystalline) matter[6] and/or α-particle formation[10] presumably occurring at subnuclear densities.

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