Non-plane-wave Hartree-Fock states and nuclear homework potentials

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It is shown that non-plane-wave single-particle Hartree-Fock orbitals giving rise to a "spin-density-wave-like" structure give lower energy than plane waves beyond a certain relatively low density in both nuclear and neutron matter with homework pair potentials v_1 and v_2.

[NUCLEAR STRUCTURE Nuclear matter, Hartree-Fock: nuclear structure.]

In a recent series of papers[1] the plausibility of non-plane-wave (PW) Hartree-Fock (HF) orbitals was studied in the thermodynamic limit for many-fermion systems interacting via *simplified* two-body interactions, such as attractive and repulsive delta functions. Subsequently, *effective* two-body (Skyrme type) interactions were introduced and shown[2] to lead to such nuclear effects as alpha-particle clustering at subnuclear densities. The question still remained whether the various non-PW HF orbitals would be relevant when employed with realistic (i.e., bare) two-body forces. The work of Calogero *et al.*[3] unfortunately omits the repulsive cores in the nucleon-nucleon force, whereas the importance of these repulsions (hard or soft) for the establishment of long-range order in the form of crystallization is well accepted both classically[4] and quantally.[5] The present note reports on the use of several new non-PW HF orbitals with two of the most common "homework" potentials, so-called v_1 and v_2,[6] used for both neutron-star and balanced nuclear matter. We establish that the new HF states have lower energy for densities beyond a certain, relatively low, value and may thus play an important role not only in the understanding of pion condensation and other "exotic" nuclear states, but also in providing a nontrivial unperturbed vacuum state upon which to base correlation energy calculations by either perturbation (ladder summations, hole-line expansions, etc.) or variational schemes.

The non-PW HF orbitals considered here are a somewhat modified and superior version of those found in Ref. 1 under the name "corrugated-sheet-spin-density waves" (CSSDW), which now include higher-order harmonics. They are orthonormal, obey periodic boundary conditions in a box of volume V, and are given by

$$\varphi_{\vec{k}\sigma\tau}(\vec{r},\sigma_3,\tau_3)=\left[V\sum_{m=1}^{2n+1}\left|P_m(\alpha)\right|^2\right]^{-1/2}e^{i\vec{k}\cdot\vec{r}}(1+\alpha S_\sigma\cos\vec{q}\cdot\vec{r})^n\chi_\sigma(\sigma_3)\chi_\tau(\tau_3) \tag{1}$$

$$n=1,2,3,\ldots;\quad k<k_F;\quad q\geq 2k_F;\ S_\sigma=\pm 1 \text{ for } \sigma=\pm\tfrac{1}{2},$$

while α and q are two additional variational parameters. The coefficients $P_m(\alpha)$ are defined by the expansion

$$(1+\alpha\cos\vec{q}\cdot\vec{r})^n\equiv\sum_{m=1}^{2n+1}P_m(\alpha)e^{-i(n+1-m)\vec{q}\cdot\vec{r}}. \tag{2}$$

The global density is just

$$\rho_0\equiv N/V=\nu k_F^{\,3}/6\pi^2, \tag{3}$$

with $\nu=2$ for neutron and $\nu=4$ for nucleon matter. On the other hand, the local density (sum of orbitals modulus squared which are occupied in the HF states determinant) is

$$\rho(\vec{r})/\rho_0=1+\left[\sum_{m=1}^{2n+1}\left|P_m\right|^2\right]^{-1}\sum_{m_1>m_2=1}^{2n+1}\left[1+(-)^{m_1+m_2}\right]\mathrm{Re}\left[P_{m_1}^*P_{m_2}^*e^{i(m_2-m_1)\vec{q}\cdot\vec{r}}\right]$$

$$\equiv\rho_\uparrow(\vec{r})/\rho_0+\rho_\downarrow(\vec{r})/\rho_0, \tag{4}$$

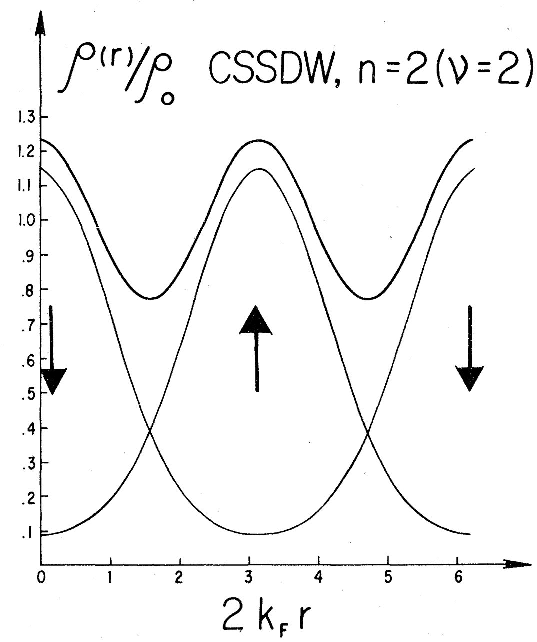

FIG. 1. The local density Eq. (4) (thick curve) arising from the non-PW orbitals considered here Eq. (1), for $n=2$ and $\nu=2$ (neutron matter) shown along the direction of $\vec{q}$. Along perpendicular directions the density is space independent. Also seen are the contributions from spin-up and spin-down matter (thin curves).

where $\rho_\uparrow(\vec{r})/\rho_0$ comes from the unity in the first (square) bracket and from *half* of the first unity on the right-hand side, and clearly corresponds to a corrugated-sheet density wave, in the direction of $\vec{q}$, of spin-up particles. Out of phase with this wave is that of $\rho_\downarrow(\vec{r})/\rho_0$ of spin-down particles, but the total density *is still spatially inhomogeneous*

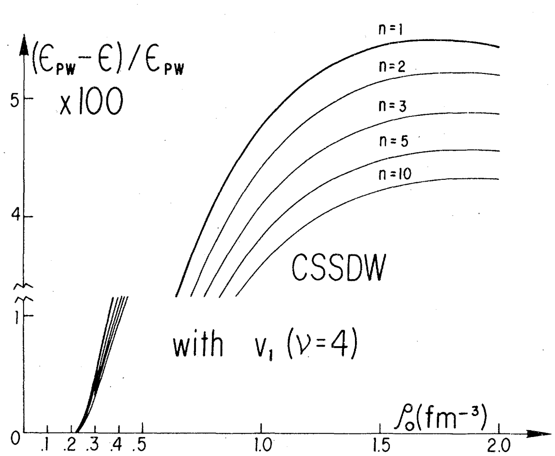

FIG. 2. Energy lowering of CSSDW HF state of orbitals Eq. (1), with respect to the PW orbital, as a function of nuclear matter density ρ_0 for the v_1 homework potential. Energy gain begins at about $\rho_0 \simeq 0.22$ fm^{-3}.

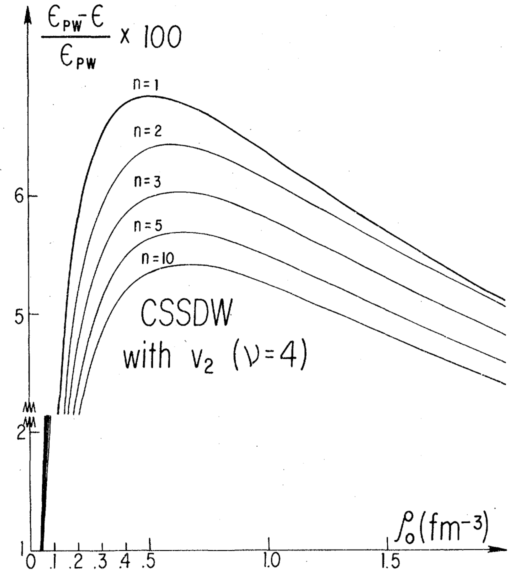

FIG. 3. Same as Fig. 2 but for the v_2 homework potential. Here the energy gain begins at $\rho_0 \simeq .024$ fm^{-3}, probably due to the fact that the v_2 repulsion is larger than that of v_1.

(cf. Fig. 1) unlike the original Overhauser[7] spin-density wave (SDW).

The energy-per-particle difference between HF determinants of orbitals (1) and those of the usual PW orbitals is tedious though straightforward to calculate. It is

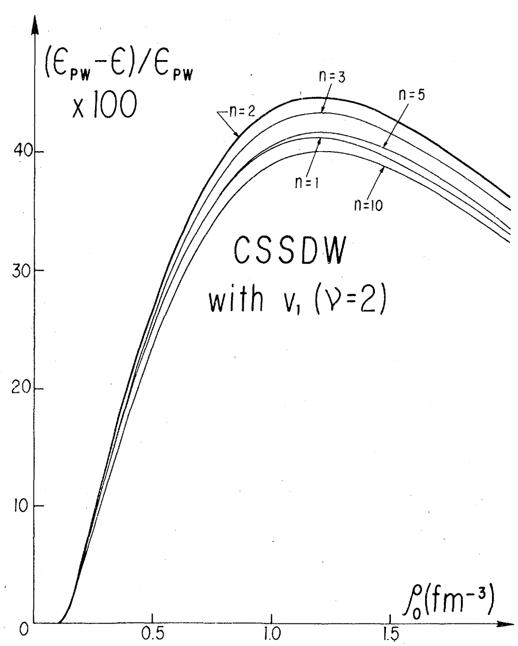

FIG. 4. Same as Fig. 2 but for neutron matter. Note that the $n=2$ orbitals give the lowest energy. Energy gain begins at $\rho_0 \simeq 0.12$ fm^{-3}.

$$\Delta\epsilon_n(\alpha, q; \rho_0) \equiv \epsilon_{\text{CSSDW}-n} - \epsilon_{\text{PW}}$$
$$= \frac{\hbar^2}{2m}\left[\sum_{m=1}^{2n+1}\left|P_m\right|^2\right]^{-1}\left[q^2\sum_{m=1}^{2n+1}(n+1-m)^2\left|P_m\right|^2\right]$$
$$+\left[\sum_{m=1}^{2n+1}\left|P_m\right|^2\right]^{-2}\sum_{\substack{m_1,m_2,m_3,m_4=1\\(m_1+m_2=m_3+m_4)}}^{2n+1} P_{m_1}P_{m_2}P^*_{m_3}P^*_{m_4}M(m_3-m_4, m_1-m_2) - M(0,0) \tag{5}$$

For the homework potentials, one has an interaction

$$\sum_\lambda a_\lambda e^{-\lambda x}/x, \quad x=\mu r, \quad \mu = 0.7 \text{ fm}^{-1},$$

where $\lambda = 1$, 4, and 7 for v_1, and 1, 2, 4, and 6 for v_2, while the coefficients a_λ are found, e.g., in Ref. 6. Then the terms $M(A,B)$ appearing in (5) are

$$M(A,B) = \frac{k_F}{3\pi\mu}\sum_\lambda a_\lambda\{\tfrac{1}{2}\nu(a^2+b^2)^{-1}[1+(-)^{(3A+B)/2}] - 9I_\lambda(A,B)\}, \quad a\equiv\lambda\mu/k_F, \quad b\equiv(B-A)q/2k_F, \tag{6}$$

$$I_\lambda(A,B) = \frac{1}{b}\int_0^\infty \frac{dx}{x^6}e^{-ax}\sin bx\,(\sin x - x\cos x)^2 \equiv \frac{1}{480b}\sum_{j=0}^{5} f_j b^j,$$
$$f_5 \equiv \tfrac{1}{2}\ln\left[1+\frac{8(a^2-b^2+2)}{(a^2+b^2)^2}\right],$$
$$f_4 \equiv 5A\left[\tan^{-1}\frac{b-2}{a} - 2\tan^{-1}\frac{b}{a} + \tan^{-1}\frac{b+2}{a}\right],$$
$$f_3 \equiv 4 - 10(2+a^2)f_5, \tag{7}$$
$$f_2 \equiv 20\ln\left[1-\frac{8b}{a^2+(b+2)^2}\right] - 2(6+a^2)f_4,$$
$$f_1 \equiv (88-12a^2) + (60a^2+5a^4)f_5 + 80a\left[\tan^{-1}\left(\frac{b-2}{a}\right) - \tan^{-1}\left(\frac{b+2}{a}\right)\right],$$
$$f_0 \equiv -(20a^2+16)\ln\left[1-\frac{8b}{a^2+(b+2)^2}\right] + \tfrac{1}{5}(a^4+20a^2)f_4.$$

The PW energy per particle is just

$$\epsilon_{\text{PW}} \equiv \frac{3}{5}\frac{\hbar^2}{2m}\left(\frac{6\pi^2}{\nu}\rho_0\right)^{2/3} + M(0,0). \tag{8}$$

For all two-body interactions examined in Refs. 1 and 2, the minimum with respect to $q \geq 2k_F$ occurred for the equality, i.e., $q = 2k_F$. Taking this choice here also we minimized Eq. (5) for each density ρ_0 with respect to α, for several $n = 1, 2, \cdots$. Some typical results are shown in Figs. 2—4 where a definite energy lowering is found for all densities above a certain value. From the variational principle one can expect even lower energy by having density oscillations along *all three* mutually perpendicular directions.

We finally note that the corrugated-sheet-density waves (CSDW), defined as in Eq. (1) but *without* the S_σ spin factor which dephases spin-up and spin-down populations, and which would be more akin to the "charge-density waves" (CDW) of Overhauser,[8] were also attempted as above with the two homework potentials but found *never* to have lower energy than the PW state.

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