Hartree-Fock states in the thermodynamic limit*

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A two-parameter class of single-particle orbitals, giving rise to long-range order in the local (spatial and/or spin) density, is shown to satisfy the full Hartree-Fock (HF) equations for occupied states in the thermodynamic limit. For a δ interparticle potential, these states are stabler (have lower HF energy) than the usual plane-wave (or trivial) HF solutions, for sufficiently strong coupling and/or high density. Minimization of the energy with respect to the (new) free parameters leads to sometimes gradual (second-order transition) and sometimes abrupt (first-order transition) onset of order, accompanied by a "bifurcation" of the new energy state from the old. The existence of even lower-energy, nontrivial HF states is also mentioned. We discuss the relevance to neutron and nuclear matter, to the Pauling "close-packed spheron" model of nuclei, as well as to the electron-gas problem.

I. INTRODUCTION

In a previous set of papers[1] it was shown that the assumption that plane waves are the lowest-energy solutions to the Hartree-Fock (HF) equations in the thermodynamic limit breaks down whenever the interparticle potential is attractive enough to bind nuclear matter, for example, in first-order perturbation theory. This breakdown, commonly occurring at densities of 1% of the saturation density, is manifested by the appearance of a lower-energy determinantal state corresponding to an *inhomogeneous* single-particle density distribution. (It is further related to the onset[1,2] of unstable random-phase-approximation modes in the density-density correlation function.) The question arises then as to whether this inhomogeneity refers to (a) surface formation as the (homogeneous density) nonideal Fermi gas condenses within the normalization volume to one or more *droplets* of (also homogeneous-density) liquid *or* (b) formation of a state with inhomogeneous density structure (maybe with long-range order, as in a crystal) everywhere in the normalization volume. The present work is related only to point (b).

The importance of these possibilities is connected, in case (a), to a mechanism for the evolution of the (presumably) liquid droplet state of real (finite or infinite) nuclear matter and, in case (b) to (i) the possibility of a "close-packed spheron" structure in nuclei, as proposed by Pauling,[3] in explanation of, among other phenomena, the nuclear magic numbers, as well as (ii) the possibility of long-range crystalline order in nuclear and/or neutron star matter, as suggested by the observation of "star quakes".[4]

In the present paper we study the energetic behavior as a function of particle density and coupling of a class of two-parameter single-particle orbitals—resembling Overhauser[5] states—which *explicitly satisfy the HF equations for occupied states*. The analysis here is restricted to a δ-function interaction between pairs of nucleons. Although this potential can be very uncharacteristic of real physical systems, it drastically simplifies calculations. The stabler ordered states which the δ interaction yields with relative ease, however, are definitely present in a variety of physical cases, and it is this point which we feel lends this schematic study a wider significance. This study is presently being extended to both "effective," density-dependent potentials of the Skyrme kind,[6] as well as to "realistic" (adjusting empirical data) nuclear potentials on the one hand, and also to the electron-gas problem where the appearance of a "Wigner lattice" is widely believed.

II. "CORRUGATED-SHEET" DENSITY-WAVE (CSDW) STATE

Consider the determinantal state Φ_0 composed of $N \gg 1$ single-particle orbitals with spin and isospin,

$$\varphi_k(r) \equiv \varphi_{\vec{k}\sigma\tau}(\vec{r}\sigma_z\tau_z) = C(e^{i\vec{k}\cdot\vec{r}} + \alpha e^{i(\vec{k}+\vec{q})\cdot\vec{r}})\chi_\sigma(\sigma_z)\chi_\tau(\tau_z),$$
$$k < k_F, \quad q \geq 2k_F, \quad \alpha \text{ complex}, \tag{1}$$

which are orthonormalized in the cubic volume V, to which one applies periodic boundary conditions. For sufficiently large V

$$\int_V d^3r\, e^{i\vec{Q}\cdot\vec{r}} = V\delta_{\vec{Q},0}, \tag{2}$$

so that, since $\delta_{\vec{q},0}\equiv 0$,

$$\sum_{\sigma_z\tau_z}\int_V d^3r\,\varphi_k^*(r)\,\varphi_{k'}(r)=\delta_{k,k'}\,. \tag{3}$$

The constant C is then

$$C=[(1+|\alpha|^2)V]^{-1/2}, \tag{4}$$

and for $\alpha\to 0$, Eqs. (1) and (4) give the usual orthonormalized plane-wave states familiar in nuclear matter studies.

The (global) particle density $\rho\equiv N/V$ is given by

$$N=\sum_k 1=4\sum_{\vec{k}}1\to 4\frac{V}{(2\pi)^3}\int_{k<k_F}d^3k=V\frac{2}{3\pi^2}k_F^3;$$

therefore,

$$\rho\equiv N/V=(2/3\pi^2)k_F^3\,. \tag{5}$$

The (local) density distribution $\rho(\vec{r})$ is

$$\begin{aligned}\rho(\vec{r})&\equiv\sum_k|\varphi_k(r)|^2\\&=\rho\{1+[2/(1+|\alpha|^2)]\\&\qquad\times[(\mathrm{Re}\alpha)\cos\vec{q}\cdot\vec{r}-(\mathrm{Im}\alpha)\sin\vec{q}\cdot\vec{r}]\}\end{aligned} \tag{6}$$

and evidently corresponds to an oscillating density wave of wavelength

$$\lambda=2\pi/q\leqslant\pi/k_F\,. \tag{7}$$

A result, to our knowledge new (since Overhauser's[5] problem was restricted to the one-dimensional Hartree case), is that the N occupied orbitals [Eq. (1)] explicitly satisfy the full HF equations

$$\langle k|-(\hbar^2\nabla_1^2/2m)|k'\rangle+\sum_{l\,(\mathrm{occ})}\langle kl|v_{12}|k'l-lk'\rangle=\epsilon_k\delta_{kk'} \tag{8}$$

for any translation-invariant [i.e., independent of center-of-mass $\vec{R}=\frac{1}{2}(\vec{r}_1+\vec{r}_2)$] two-body potential v_{12}. This is immediately seen by noting that, from Eq. (1),

$$\delta_{\vec{k}',\vec{k}\pm n\vec{q}}=0\quad(n=1,2,\ldots;\ k,k'<k_F;\ q\geqslant 2k_F)$$

so that

$$\begin{aligned}\left\langle k\left|-\frac{\hbar^2\nabla_1^2}{2m}\right|k'\right\rangle&=\delta_{\sigma\sigma'}\delta_{\tau\tau'}\frac{\hbar^2k^2}{2m}(1+|\alpha|^2)^{-1}\left[\delta_{\vec{k},\vec{k}'}\left(1+\frac{|\alpha|^2(\vec{k}+\vec{q})^2}{k^2}\right)+\delta_{\vec{k}',\vec{k}-\vec{q}}\alpha+\frac{\delta_{\vec{k}',\vec{k}+\vec{q}}\alpha^*(\vec{k}+\vec{q})^2}{k^2}\right]\\&=\delta_{kk'}[\cdots];\\\sum_{l\,(\mathrm{occ})}\langle kl|v_{12}|k'l-lk'\rangle&=\delta_{kk'}[\cdots]+(\text{terms containing }\delta_{\vec{k}',\vec{k}\pm\vec{q}}\text{ and }\delta_{\vec{k}',\vec{k}\pm 2\vec{q}})\,.\end{aligned} \tag{9}$$

The sum of the two brackets $[\cdots]$ then gives the constant ϵ_k. Q.E.D.

The HF energy will be

$$\begin{aligned}E&\equiv\left\langle\Phi_0\left|-\frac{\hbar^2}{2m}\sum_{i=1}^N\nabla_i^2+\sum_{i<j}^N v_{ij}\right|\Phi_0\right\rangle\\&=\sum_{k\,(\mathrm{occ})}\left\langle k\left|-\frac{\hbar^2\nabla_1^2}{2m}\right|k\right\rangle\\&\quad+\frac{1}{2}\sum_{k_1k_2\,(\mathrm{occ})}\langle k_1k_2|v_{12}|k_1k_2-k_2k_1\rangle\,.\end{aligned} \tag{10}$$

For the present we utilize only the interaction

$$v_{12}=v_0\delta(\vec{r}_{12}),\quad v_0=\text{const.} \tag{11}$$

Then, Eq. (10) reduces to

$$\begin{aligned}\epsilon(\tilde{q},\beta)&\equiv\frac{2mE}{\hbar^2k_F^2N}\\&=\frac{3}{5}\left(1+\frac{20}{3}\frac{\beta}{1+\beta}\tilde{q}^2\right)+\frac{3}{4}\frac{mv_0\rho}{\hbar^2k_F^2}\left(1+\frac{2\beta}{(1+\beta)^2}\right),\\&\qquad\beta\equiv|\alpha|^2,\quad\tilde{q}\equiv q/2k_F\geqslant 1\,.\end{aligned} \tag{12}$$

The energy is independent of the *direction* of $\vec{q}$; hence the density-wave distribution [Eq. (6)] is analogous to a "corrugated-sheet," the energy [Eq. (12)] being degenerate with respect to the orientation of the "sheet." Moreover, as the energy depends only on the *magnitude* of α, there is no loss of generality in taking α real in Eq. (6). Finally, $\epsilon(\tilde{q},\beta)$ is obviously minimized in $\tilde{q}$ for $\tilde{q}=1$, so that the density oscillations, from Eq. (7), have the familiar π/k_F wavelength. The energy is then

$$\epsilon(\beta)=\tfrac{3}{5}+4\beta/(1+\beta)+\lambda(1+A)\,, \tag{13}$$

$$A\equiv 2\beta/(1+\beta)^2,\quad\lambda\equiv v_0k_Fm/2\pi^2\hbar^2\,, \tag{14}$$

where Eq. (5) was used in defining the dimensionless coupling constant λ. To minimize with respect to β one has, first

$$\epsilon'(\beta)=0\Rightarrow\beta=(\lambda+2)/(\lambda-2)\geqslant 0\Rightarrow\lambda\leqslant -2\ \text{ or }\ \lambda>2\,, \tag{15}$$

the last inequality ensuring that β is finite; secondly, we must impose

$$0 < \epsilon''(\beta)(1+\beta)^4 = \frac{8\lambda - 4\lambda^2}{\lambda - 2} \Rightarrow \lambda \leq -2\,, \tag{16}$$

where the right-hand side of the first inequality [Eq. (15)] for β was used *after* doing the second differentiation. Eliminating β from Eq. (13), again via Eq. (15), leaves

$$\epsilon(\lambda) = \tfrac{13}{5} + 2/\lambda + \tfrac{3}{2}\lambda \tag{17}$$

which is to be compared with the plane-waves result, Eq. (13) with $\beta = 0$, namely,

$$\epsilon_{\rm PW}(\lambda) = \tfrac{3}{5} + \lambda\,. \tag{18}$$

Finally one has that

$$\Delta\epsilon \equiv \epsilon(\lambda) - \epsilon_{\rm PW}(\lambda) = 2 + 2/\lambda + \tfrac{1}{2}\lambda \leq 0 \quad \text{for } \lambda \leq -2 \tag{19}$$

(attractive interaction) with equalities coinciding. Figure 1 shows that the equality alluded to corresponds to a "bifurcation point," since the function $\epsilon(\lambda)$ violates the basic condition $\beta \equiv |\alpha|^2 \geq 0$ to the left of that point (dashed curve). We also note that the new (self-consistent) lower-energy, determinantal state appears at a critical coupling ($\lambda_{\rm crit} = -2$) somewhat stronger than that found in Ref. 1 ($\lambda_{\rm crit} = -\frac{1}{3}$) to signal the instability of the PW determinant, i.e., beyond which the *existence* of a non-PW state can be established. The appearance

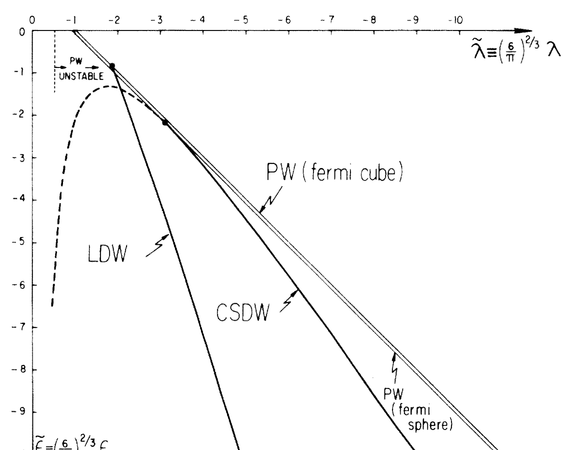

FIG. 1. Dimensionless HF energies, as functions of the dimensionless coupling $\tilde{\lambda}$ defined in Eq. (24), for the (simple cubic) lattice density-wave (LDW) state and the "corrugated-sheet" density-wave (CSDW) state compared to their respective relevant plane-wave (PW) states with Fermi cube and sphere fillings. Dashed portion of CSDW curve violates condition $\beta \equiv |\alpha|^2 \geq 0$. Dashed vertical line indicates critical $\tilde{\lambda}$ beyond which the PW state was found unstable according to methods of Ref. 1.

of a new, lower-energy state, from the old (trivial) state, at a "bifurcation point" *with* tangency is characteristic of a *second-order transition* wherein the corresponding "order parameter" sets in *gradually* from the value zero. Here, the order parameter is the amplitude of the density oscillation

$$\frac{2\alpha}{1+|\alpha|^2} = (1 - 4/\lambda^2)^{1/2} \underset{\substack{\lambda = -2-\eta,\\ \eta \to 0^+}}{\longrightarrow} \sqrt{\eta}\ .$$

A good example of this in an empirically observed instance is the experimental free energy vs temperature for both normal and superconducting phases, at low temperatures, showing[7] two branches joined at a bifurcation point at critical temperature.

The corrugated-sheet density-wave (CSDW) state treated here may be related to the concentric-shell density oscillations arising from Pauling's concentric packing of "spherons" (alphas or tritons) in his model[3] of nuclear structure. Pauling's packing, however, is apparently limited to *finite* aggregates, whereas the states considered here are for the (essentially) infinite-particles limit. The spherically-invariant state studied above, though, is *not* the stablest state, as will be seen in Sec. III.

But before closing this section, we mention a rather curious example of an HF state which, for the δ interaction studied here, has *higher* energy than the PW HF state. This is formed by orbitals [Eq. (1)] where the vector $\vec{q}$ is assumed parallel (or antiparallel) to the vector $\vec{k}$, over which one then sums. The resulting density distribution is

$$\rho(\vec{r}) = \rho\left[1 + {\rm Re}\left(\frac{\alpha}{\pi(1+|\alpha|^2)}\right)\frac{\sin qr}{qr}\right] \tag{20a}$$

and the HF energy per particle, for interaction Eq. (11), and $q = 2k_F$ as before, is then

$$\frac{E}{N} = \frac{3}{5}\frac{\hbar^2 k_F^2}{2m}\left(1 + \frac{35}{3}\frac{|\alpha|^2}{1+|\alpha|^2}\right) + \tfrac{3}{8}v_0\rho[1 + O(N^{-2/3})]\,, \tag{20b}$$

which is clearly never lower than the $\alpha = 0$ case. The conclusion does not necessarily hold for a finite-range interaction, but this case is considerably more complicated and may merit closer study, particularly in connection with the Pauling nuclear model mentioned before.

III. LATTICE DENSITY-WAVE (LDW) STATE

We now form a (simple cubic) lattice configuration for $\rho(\vec{r})$ by introducing the orthonormal orbitals

$$\varphi_k(\vec{r}) = \phi_{k_x}(x)\phi_{k_y}(y)\phi_{k_z}(z)\chi_\sigma(\sigma_z)\chi_\tau(\tau_z)\,,$$
$$\phi_{k_x}(x) = D(e^{ik_x x} + \alpha e^{i(k_x+q)x}),\quad \text{same for } y \text{ and } z,$$
$$-k_0 < k_x, k_y, k_z < +k_0,\quad q \geq 2k_0, \tag{21}$$
$$D \equiv [(1+|\alpha|^2)V^{1/3}]^{-1/2}.$$

These give rise to global ρ, and local $\rho(\vec{r})$, densities.

$$\rho = N/V = 4(k_0/\pi)^3\,,$$
$$\rho(\vec{r}) = \sum_{\sigma\tau}\sum_{k_x}|\phi_{k_x}(x)|^2\sum_{k_y}|\phi_{k_y}(y)|^2\sum_{k_z}|\phi_{k_z}(z)|^2$$
$$\equiv \rho f(x) f(y) f(z)\,, \tag{22}$$
$$f(x) \equiv \{1 + 2(1+|\alpha|^2)^{-1}[(\mathrm{Re}\,\alpha)\cos qx - (\mathrm{Im}\,\alpha)\sin qx]\}\,.$$

The above orbitals also satisfy the full HF equations, as is seen similarly as in Eqs. (9). Because the δ interaction [Eq. (11)] is separable in x, y, and z, one readily finds the HF energy per particle

$$\frac{E}{N} = \frac{\hbar^2 k_0^2}{2m}\left(1 + 12\frac{\beta}{1+\beta}\tilde{q}^2\right) + \frac{3}{8}v_0\rho(1+A)^3\,,$$
$$A \equiv \frac{2\beta}{(1+\beta)^2},\quad \tilde{q} \equiv \frac{q}{2k_0} \geq 1,\quad \beta = |\alpha|^2\,, \tag{23}$$

which is clearly minimum in $\tilde{q}$ for $\tilde{q} = 1$, so that

$$\tilde{\epsilon}(\rho) \equiv \frac{2mE}{\hbar^2 k_0^2 N} = 1 + \frac{12\beta}{1+\beta} + \tilde{\lambda}(1+A)^3\,,$$
$$\tilde{\lambda} \equiv \frac{3mv_0k_0}{\hbar^2\pi^3} = \left(\frac{6}{\pi}\right)^{2/3}\lambda\,, \tag{24}$$

the last equality coming from the relation

$$k_F = (6/\pi)^{1/3}k_0\,. \tag{25}$$

The plane-wave energy, corresponding to filling a Fermi *cube* (to make the appropriate comparison later) of sides $2k_0$, is then

$$\tilde{\epsilon}(0) \equiv \tilde{\epsilon}_{\mathrm{PW}} = 1 + \tilde{\lambda}\,. \tag{26}$$

The conditions for a minimum in $\tilde{\epsilon}(\beta)$ with respect to β are

$$\tilde{\epsilon}'(\beta) = 0 \Rightarrow \tilde{\lambda} = \frac{2(1+\beta)}{(\beta-1)[1+2\beta/(1+\beta)^2]}$$
$$\xrightarrow[\beta\ll 1]{} -2 + O(\beta)\,, \tag{27}$$
$$\tilde{\epsilon}''(\beta) = -\frac{24}{(1+\beta)^3} + 6\tilde{\lambda}\,\frac{1+2\beta/(1+\beta)^2}{(1+\beta)^4}$$
$$\times\left[(2\beta-4)\left(1+\frac{2\beta}{(1+\beta)^2}\right) + 4\frac{(1-\beta)^2}{(1+\beta)^2}\right] > 0\,. \tag{28}$$

We note, however, that by eliminating $\tilde{\lambda}$ from Eq.

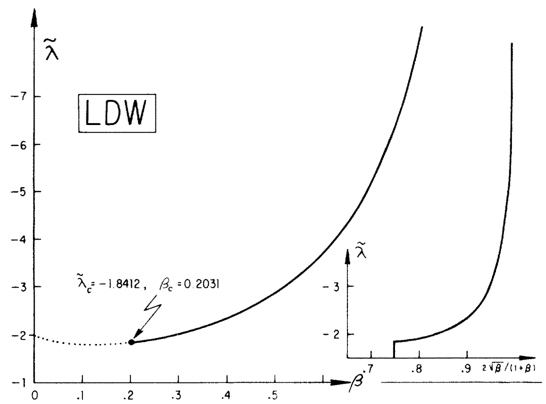

FIG. 2. Extremum condition for the lattice density-wave (LDW) [Eq. (27)] relating $\tilde{\lambda}$ to β. The three conditions [Eqs. (27), (28), and (30)] are simultaneously satisfied only along full portion of curve. [Inset: Oscillation amplitude, as in Eq. (22), as function of coupling, showing its abrupt appearance at critical coupling $\tilde{\lambda}_{\mathrm{crit}}$.]

(28) one has

$$\tilde{\epsilon}''(\beta) \xrightarrow[\beta\ll 1]{} -24 + O(\beta) < 0 \tag{29}$$

meaning that, if a solution to Eqs. (27) and (28) and to

$$\Delta\tilde{\epsilon} \equiv \tilde{\epsilon}(\beta) - \tilde{\epsilon}_{\mathrm{PW}} \leq 0 \tag{30}$$

exists, it must correspond to *nonzero* β, or that the transition must be a *sudden* one to a finite oscillation amplitude (first-order transition).

Indeed, detailed calculations show that the above-mentioned three conditions are satisfied simultaneously for $\beta \geq 0.2031$ corresponding to an oscillation amplitude $2\sqrt{\beta}/(1+\beta) \simeq 0.75$ (cf. Figs. 1 and 2). Thus, the lattice density-wave (LDW) state energy is *not* tangent to the PW state energy (upper straight line curve in Fig. 1) at the corresponding bifurcation point. Evidently, the LDW state is *stabler* than the previous CSDW state.

IV. "CORRUGATED-SHEET" SPIN-DENSITY-WAVE (CSSDW) STATE

The states considered so far are found to be stabler than the plane-waves state only for (sufficiently strong) *attractive* forces. In Secs. V and VI we take up states which become stabler for *repulsive* forces—these are of the "spin-density-wave" kind, in which spin-up and -down populations oscillate out of phase, creating an antiferromagnetic structure.

Define the orthonormalized orbitals

$$\varphi_k(r) = C(e^{i\vec{k}\cdot\vec{r}} + \alpha S_\sigma e^{i(\vec{k}+\vec{q})\cdot\vec{r}})\chi_\sigma(\sigma_z)\chi_\tau(\tau_z);$$
$$k < k_F;\quad q \geq 2k_F;\quad C = [(1+|\alpha|^2)V]^{-1/2} \tag{31}$$

with $S_\sigma = +1(-1)$ for spin up (down).

The local density distribution

$$\rho(\vec{r}) = \sum_k |\varphi_k(r)|^2$$
$$= \frac{1}{4}\rho \sum_{\sigma\tau}\left(1 + S_\sigma \frac{2}{1+|\alpha|^2} \times [(\mathrm{Re}\,\alpha)\cos\vec{q}\cdot\vec{r} - (\mathrm{Im}\,\alpha)\sin\vec{q}\cdot\vec{r}]\right) = \rho\,, \tag{32}$$

where the last equality follows from $\sum_\sigma S_\sigma = 0$, so that there is a "corrugated-sheet" density oscillation, similar to the CSDW state studied before, except that it is now for spins up (down) separately, and these two basic oscillations are out of phase so as to cancel completely, leaving a homogeneous net particle density with underlying long-range ordering in spins (anti-ferromagnetic-like).

Using the same methods as before, the HF energy per particle (after minimizing in q to find $q = 2k_F$) is finally seen to be

$$\epsilon(\beta) \equiv \frac{2mE}{\hbar^2 k_F^2 N} = \frac{3}{5} + \frac{4\beta}{1+\beta} + \lambda\left(1 - \frac{1}{3}A\right),$$
$$A \equiv \frac{2\beta}{(1+\beta)^2}, \quad \beta \equiv |\alpha|^2, \quad \lambda \equiv m v_0 k_F / 2\pi^2\hbar^2\,. \tag{33}$$

As before, minimizing with respect to β now yields

$$\epsilon'(\beta) = 0 \Rightarrow \beta = (\lambda - 6)/(\lambda + 6) \geq 0 \Rightarrow \lambda \geq 6 \quad \text{or} \quad \lambda < -6 \tag{34}$$

as well as

$$\epsilon''(\beta) = [(\lambda+6)^3/(2\lambda)^4](\tfrac{4}{3}\lambda^2 + 8\lambda) > 0\,, \tag{35}$$

where Eq. (34) was substituted *after* the second differentiation. The parameter β as given by Eq. (34) is easily eliminated from Eq. (33) leaving

$$\epsilon(\lambda) = \tfrac{13}{5} - 6/\lambda + \tfrac{5}{6}\lambda \tag{36}$$

and, as before

$$\epsilon(\beta = 0) \equiv \epsilon_{\mathrm{PW}} = \tfrac{3}{5} + \lambda\,. \tag{37}$$

Thus

$$\Delta\epsilon(\lambda) \equiv \epsilon(\lambda) - \epsilon_{\mathrm{PW}}(\lambda) = 2 - 6/\lambda - \lambda/6 \leq 0 \quad \text{for } \lambda \geq 6 \tag{38}$$

with equalities coinciding. Note that *all* three Eqs. (34), (35), and (38) are satisfied for $\lambda \geq 6$ (repulsive δ). Moreover, for $\lambda = 6$, $\epsilon(\lambda) = \epsilon_{\mathrm{PW}}$, and $\beta = 0$—hence this point corresponds to bifurcation of energies with $\epsilon(\lambda)$ tangent to ϵ_{PW} (second-order transition).

V. LATTICE SPIN-DENSITY-WAVE (LSDW) STATE

Analogous to the LDW state of Sec. III, this case is also constructed by taking separate orbitals for each Cartesian coordinate, viz.,

$$\varphi_{k_x\sigma}(x) = C(e^{ik_x x} + \alpha S_\sigma e^{i(k_x+q)x}); \quad \text{same for } y, z\,.$$
$$-k_0 < k_x, k_y, k_z < +k_0; \quad q \geq 2k_0;$$
$$S_\sigma = +1(\text{spin up}) \text{ or } -1(\text{spin down}),$$
$$C = [(1+|\alpha|^2)V^{1/3}]^{-1/2} \tag{39}$$

giving rise to the global density

$$\rho = N/V = 4(k_0/\pi)^3 \tag{40}$$

and the local density distribution

$$\rho(\vec{r}) = \sum_{\sigma\tau}\sum_{k_x}|\varphi_{k_x\sigma}(x)|^2 \sum_{k_y}|\varphi_{k_y\sigma}(y)|^2 \sum_{k_z}|\varphi_{k_z\sigma}(z)|^2$$
$$= \tfrac{1}{4}\rho\sum_{\sigma\tau}[1 + S_\sigma h(x)][1 + S_\sigma h(y)][1 + S_\sigma h(z)]$$
$$= \rho[1 + h(x)h(y) + h(y)h(z) + h(z)h(x)]\,, \tag{41}$$
$$h(x) \equiv \frac{2}{1+|\alpha|^2}[(\mathrm{Re}\,\alpha)\cos qx - (\mathrm{Im}\,\alpha)\sin qx]\,,$$

which is *not* spatially homogeneous but has a net (simple cubic) lattice structure, where each lattice site has an associated spin up (down) surrounded by spin down (up) nearest-neighbor sites (anti-ferromagnetic structure).

A somewhat tedious calculation, which nonetheless exploits the separability in x, y, and z of the interaction Eq. (11), leads to the HF energy

$$\frac{E}{N} = \frac{\hbar^2 k_0^2}{2m}\left(1 + \frac{12\beta}{1+\beta}\tilde{q}^2\right) + \frac{3\rho v_0}{8}\left(1 + 3A^2 - A - \frac{A^3}{3}\right);$$
$$\beta \equiv |\alpha|^2; \quad \tilde{q} \equiv q/2k_0 \geq 1; \quad A \equiv 2\beta/(1+\beta)^2\,, \tag{42}$$

which is again clearly minimum in $\tilde{q}$ for $\tilde{q} = 1$. Thus

$$\tilde{\epsilon}(\beta) \equiv \frac{2mE}{\hbar^2 k_0^2 N} = 1 + \frac{12\beta}{1+\beta} + \tilde{\lambda}\left(1 + 3A^2 - A - \frac{A^3}{3}\right),$$
$$\tilde{\lambda} \equiv 3 m v_0 k_0 / \pi^3\hbar^2\,, \tag{43}$$

is minimum also in β if

$$\tilde{\epsilon}'(\rho) = 0 \Rightarrow \tilde{\lambda} = \frac{6(1+\beta)}{(1-\beta)(1+A^2-6A)} \xrightarrow[\beta \ll 1]{} 6 + O(\beta) \tag{44}$$

and

$$\tilde{\epsilon}''(\beta) = -\frac{24}{(1+\beta)^3} + \frac{\tilde{\lambda}}{(1+\beta)^3} \times \left(\frac{4(\beta-2)}{1+\beta}(6A - A^2 - 1) + \frac{4(1-\beta)^2}{(1+\beta)^3}(6 - 2A)\right) > 0\,. \tag{45}$$

Inserting Eq. (44) into Eq. (45) one finds that

$$\tilde{\epsilon}''(\beta) \xrightarrow[\beta \ll 1]{} 168 + O(\beta) > 0 \tag{46}$$

so that, provided solutions exist simultaneously for Eqs. (44), (45), as well as for

$$\Delta\tilde{\epsilon} \equiv \tilde{\epsilon}(\beta) - \tilde{\epsilon}_{PW} \leq 0,$$

where (47)

$$\tilde{\epsilon}_{PW} \equiv \tilde{\epsilon}(0) = 1 + \tilde{\lambda} ,$$

at least one of those solutions will correspond to a $\beta = 0$ bifurcation point with tangency (second-order transition).

Numerical calculations show that *three* branches occur which simultaneously satisfy Eqs. (44), (45), and (47): branch "*a*" is second order, whereas "*b*" and "*c*" are first order, as seen in Figs. 3 and 4. We note from Fig. 3 that the LSDW state (branch "*a*") is stabler than both the PW and CSSDW state for $\tilde{\lambda} \geq 6$, but that the latter state becomes the stablest at larger coupling: such a "crossing," barely appreciable in Fig. 3, and which did not occur for the attractive case, can be associated with a first-order transition of LSDW to the CSSDW state.

VI. EXISTENCE OF OTHER LOWER-ENERGY HF STATES WITH LONG-RANGE ORDER

The PW state used in all previous discussions corresponds to a *paramagnetic* spin state, i.e., spins are spatially at random but cancel out to a net spin $\mathcal{S} = 0$ (for even number of particles N). A lower-energy PW state, for repulsive δ interaction, can be obtained[8] which has a net spin $\mathcal{S} = \frac{1}{2}N$ (*ferromagnetic* state) with HF energy per particle [compare Eq. (26)]

$$\tilde{\epsilon}_{PW\ ferro} = 2^{2/3} + \tfrac{1}{3}\tilde{\lambda} . \tag{48}$$

This is also included in Fig. 3, where the cross-point between PW (paramagnetic) and PW (ferromagnetic) occurs at $\tilde{\lambda}_{crit} = \frac{3}{2}(2^{2/3} - 1) = 0.8811$ (for *cubic* Fermi-surface filling) and is a first-order transition.

The *existence* of even lower-energy non-PW HF states can be established by just constructing non-PW determinants (not necessarily satisfying the HF equations) which have lower expectation energy. For the δ interaction, there are *localized* single-particle states which give *zero* potential energy in one[9] as well as three[10] dimensions, so that

$$\tilde{\epsilon}_s = s^2 g^{2/3} \quad (s = 1, 2, 3, \cdots ; \; g = 2 \text{ or } 4) \tag{49}$$

independent of coupling $\tilde{\lambda}$. Here, g is the number of intrinsic degrees of freedom and the integer index s characterizes the single-particle local density, cf. Ref. 10, i.e., $s = 1$ is homogeneous but $s \geq 2$ are periodic (simple cubic). The first few such cases of Eq. (49) are graphed in Fig. 3. The lowest-energy one corresponding to $s = 1$ and $g = 2$ (homogeneous; ferromagnetic with *localized* spins, in contrast to the PW case above). The next lowest state has $s = 1$ but $g = 4$ (homogeneous; net spin $\mathcal{S} = 0$ allowing for para- or even antiferromagnetic, but with localized spins). Successively higher states have $s \geq 2$ and thus are spatially nonhomogeneous (periodic) in local density. Note that for sufficiently strong (repulsive) coupling, all of these are lower in energy than the PW states, since only the latter depend on $\tilde{\lambda}$.

These comments serve only to emphasize that HF states with still lower energy than those discussed in this paper are yet to be found.

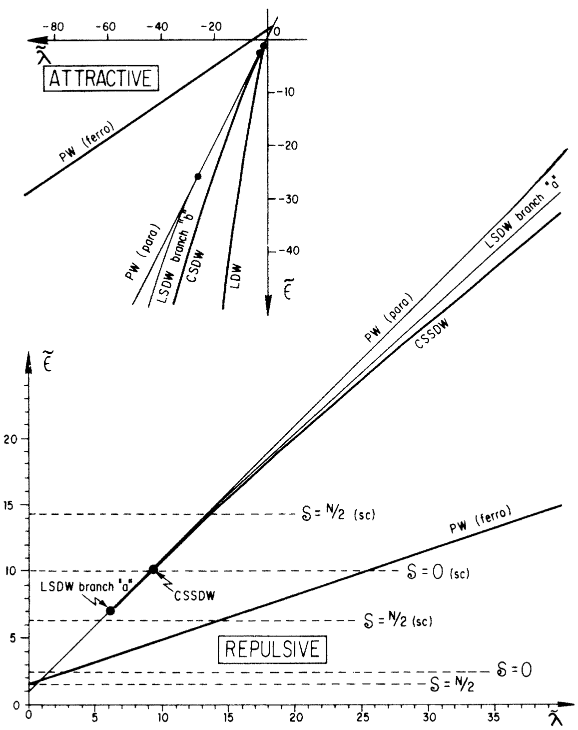

FIG. 3. Dimensionless HF energies (full curves) vs dimensionless coupling for all states examined in this paper. (Branch "*c*" of lattice spin-density-wave (LDSW) state lies outside graph.) Results are for "repulsive" and "attractive" (Inset) δ interaction between fermions. Dots are "bifurcation points". "Para" ("ferro") refer to paramagnetic and ferromagnetic spin configurations for the plane-wave (PW) states. Energy difference between Fermi cube and sphere fillings are not distinguishable graphically on this scale. Dashed (horizontal) curves refer to non-HF determinantal states labeled by net spin value $\mathcal{S}$ (even N); lowest two are spatially homogeneous, higher ones are periodic (simple cubic).

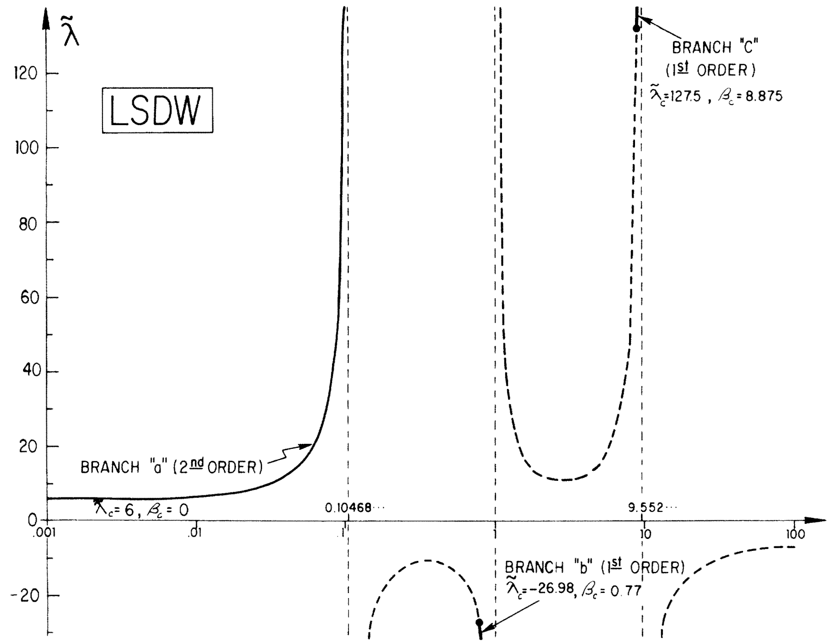

FIG. 4. Extremum condition for the lattice spin density-wave (LSDW) state [Eq. (44)] relating $\tilde{\lambda}$ to β, showing three distinct branches. The *three* conditions [Eqs. (44), (45), and (47)] are simultaneously satisfied only along the full portion of curves.

VII. DISCUSSION

The immediate purpose of this paper has not been to reach definite conclusions in regard to any specific physical system, but merely to analyze in some detail the behavior of a certain class of non-PW HF solutions for many-fermion systems interacting with a two-body δ potential. This has permitted relative ease of calculation, reducing to a minimum the numerical work, and thus clarifying the main features to be expected (energy bifurcations with and without tangency, first- and second-order transitions, presence of more than one branch, etc.) with more realistic interactions where computation is heavier. We wish to emphasize again, though, that all states referred to, up to and including Eq. (48), can be shown, as in Sec. II, *to satisfy explicitly the full Hartree-Fock equations in the thermodynamic limit*, for any translation-invariant two-body potential—and it is this aspect which we feel is of considerable interest.

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