Hartree-Fock states in the thermodynamic limit. II. Generalized Overhauser orbitals*

V. C. Aguilera-Navarro and M. de Llano†
Instituto de Física Teórica, São Paulo, Brasil

S. Peltier and A. Plastino
Departamento de Física, Universidade Nacional, La Plata and Conicet, Argentina

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Two infinite families of two-parameter generalized Overhauser orbitals are introduced and shown to satisfy explicitly, for occupied states, the self-consistent Hartree-Fock equations in the thermodynamic limit. For an attractive δ interaction, they give lower Hartree-Fock energy than the usual plane-wave solutions, even for relatively weak coupling and/or low density. The limiting members (possessing an infinite number of harmonics) of both families appear to tend to a "classical static lattice" state, via a second-order transition for one family and via first order for the other. The related density profiles and energy expressions are calculated as functions of the two new parameters. A direct variation with respect to these parameters was done numerically and results are presented graphically.

I. INTRODUCTION

In a recent paper,[1] hereafter referred to as I, several types of self-consistent Hartree-Fock (HF) Overhauser-like[2] orbital wave functions, with lower energy for sufficiently strong interparticle δ-potential coupling than the (so-called trivial) plane-wave orbitals, were studied mainly for the purpose of revealing the appearance of bifurcation points in the energy, the nature of the "transition" to a state with long-range order, etc. Their applicability to such problems as α-particle formation[3] and crystallization[4] in nuclear and neutron-star matter, as well as to the formation of a Wigner lattice[5] of point charges in a background of opposite charge, was mentioned.

In the present paper, we wish to report a similar analysis, but for two infinite families of orbitals which are, first, a considerable generalization of the previous ones, as they now contain any number of harmonics instead of only one as before, and, secondly, give *appreciably lower energy* than before. The results given herein refer only to the attractive δ potential between particles and as such might appear purely academic. However, the usefulness of these new self-consistent orbitals for N-body systems with realistic potentials can be visualized, and work along these lines is now in progress with the objective of establishing regimes where the HF plane-wave (PW) state is unstable against the appearance of HF states with long-range order. A (sufficient) condition for PW instability to occur is given in Appendix A; some of the states studied herein are found to occur at even *weaker* coupling than that predicted by that condition.

We consider a Hamiltonian for N particles,

$$H = -\frac{\hbar^2}{2M}\sum_{i=1}^{N}\nabla_i^2 + \sum_{i<j}^{N} v_{ij} \tag{1}$$

and the single Slater determinant

$$\Phi_0 = (N!)^{-1/2}\det[\,\phi_{\vec{k}}(\vec{r})\chi_\eta(\eta_3)\,], \tag{2}$$

where $\vec{k}$ labels the spatial and η the intrinsic (spin, isospin, ...) states. The variation, with respect to $\phi_{\vec{k}}^*(\vec{r})$,

$$\delta\{\langle\Phi_0|H|\Phi_0\rangle - \mu\langle\Phi_0|\Phi_0\rangle\} = 0, \tag{3}$$

where μ is a Lagrange multiplier, then leads to the HF equations

$$\langle\phi_k| - (\hbar^2/2M)\nabla_1^2 + U_1|\phi_{k'}\rangle = \epsilon_k\delta_{k'k}, \tag{4}$$

with the self-consistent single-particle field U_1 given by

$$\langle\phi_k|U_1|\phi_{k'}\rangle \equiv \sum_{h\ \mathrm{occ}}\langle\phi_k\phi_h|v_{12}|\phi_{k'}\phi_h - \phi_h\phi_{k'}\rangle. \tag{5}$$

[The last equation leads to the well-known result[6] that *only* the HF choice of $\sum_i U_i$—which is added to the kinetic energy in Eq. (1) to give an unperturbed Hamiltonian H_0, and subtracted from the potential energy to leave a perturbation H_1—allows for a complete cancellation of all U_1 ("external field") insertions in the Feynman-Goldstone diagrams for the exact ground-state energy, against the corresponding "bubble" and "exchange bubble" insertions.]

A (trivial) solution of the nonlinear equations (4) and (5) is given by the set of plane waves

$$\phi_{\vec{k}}(\vec{r}) = L^{-3/2}e^{i\vec{k}\cdot\vec{r}}, \quad -k_0 < k_x, k_y, k_z < k_0, \tag{6}$$

orthonormalized in the cubic volume L^3, and which fills the Fermi cube of sides $2k_0$ in k space, provided only that $L \gg$ range of v_{12}. The associated local density (if g particles occupy each space state) is then

$$\rho(\vec{r}) = g \sum_{\vec{k}\ \mathrm{occ}} |\phi_{\vec{k}}(\vec{r})|^2 = N/L^3 \equiv \rho_0 = g(k_0/\pi)^3, \qquad (7)$$

and thus spatially constant (homogeneous).

We consider an infinite family of orthonormal two-parameter orbitals given, for each space component, by

$$\phi_{k_x}(x) = Ce^{ik_x x}(1 + \alpha \cos^{n_1} qx\, e^{in_2 qx})^{n_3}, \quad \alpha \text{ complex},$$
$$-k_0 < k_x < k_0, \quad q \equiv 2k_0 m \ (m = \pm 1, \pm 2, \ldots), \qquad (8)$$
$$n_1, n_2, n_3 = 0, 1, 2 \ldots$$

where C is a normalization constant and m and α are the two parameters to be eventually varied. These states can be shown (cf. Appendix B) to explicitly satisfy the HF Eqs. (4) and (5), for any α and m, for *occupied* orbitals, for any two-body potential independent of the center of mass of the two particles and of range much shorter than the normalization length L. Only three sets of subfamilies of Eq. (8) are treated here, namely,

$$(n_1, n_2, n_3) = \begin{cases} (0,0,0) & \text{plane wave (PW)} \qquad (9) \\ (0,1,n) & \text{"density wave" (DW-}n\text{)} \qquad (10) \\ (1,0,n) & \text{"density standing wave"} \\ & \text{(DSW-}n\text{)} \qquad (11) \end{cases}$$

with $n = 0, 1, 2, \ldots$. The set of orbitals Eq. (9) coincides with Eq. (6): the first (nontrivial) member of Eq. (10), $n = 1$, was studied in I while the first member of Eq. (11), $n = 1$, was recently found to give α-clustering effects in the nuclear surface,[7] under the effects of a Skyrme interaction.

II. SELF-CONSISTENT ORBITALS AND DENSITY PROFILES

The family of orbitals called "density-wave" states, Eq. (10), is then given by

$$\phi_{k_x}(x) = Ce^{ik_x x}(1 + \alpha e^{iqx})^n \quad (\text{DW-}n); \quad n = 0, 1, 2, \ldots,$$
$$-k_0 < k_x < k_0, \quad q = 2k_0 m \ (m = \pm 1, \pm 2, \ldots), \qquad (12)$$
$$C^{-2} = L \sum_{i=0}^{n} \binom{n}{i}^2 |\alpha|^{2i}.$$

In three dimensions, it gives rise to a (local) density profile

$$\rho(\vec{r}) = g\rho(x)\rho(y)\rho(z), \qquad (13)$$

where, for α real (cf. below)

$$\rho(x) = \frac{(\rho_0/g)^{1/3}(1 + \alpha^2 + 2\alpha \cos qx)^n}{\sum_{i=0}^{n} \binom{n}{i}^2 \alpha^{2i}} \qquad (14)$$

where ρ_0 is the global density given in Eq. (7). Clearly, the expressions for $\rho(y)$ and $\rho(z)$ are similar.

The family denoted "density-standing-wave," Eq. (11), reduces to

$$\phi_{k_x}(x) = Ce^{ik_x x}(1 + \alpha \cos qx)^n \quad (\text{DSW-}n), \quad n = 0, 1, 2, \ldots,$$
$$-k_0 < k_x < k_0, \quad q = 2k_0 m \quad (m = \pm 1, \pm 2, \ldots), \qquad (15)$$
$$C^{-2} = L \sum_{i,j=0}^{n} \binom{n}{i} \binom{n}{j} I_{i+j} \alpha^{*i} \alpha^j,$$

where, for l non-negative integer,

$$I_l \equiv \frac{1}{\pi} \int_0^{\pi} dx \cos^l x = \tfrac{1}{2}[1 + (-)^l] \frac{(l-1)!!}{l!!}$$
$$= \tfrac{1}{2}[1 + (-)^l] \frac{1}{2^l} \binom{l}{l/2}. \qquad (16)$$

For α real, a sum rule (cf. Appendix C) can be used to reduce the double sum in Eq. (15) to a single one, giving for the local density profile

$$\rho(x) = \frac{(\rho_0/g)^{1/3}(1 + \alpha \cos qx)^{2n}}{\sum_{i=0}^{n} \binom{2n}{2i} I_{2i} \alpha^{2i}}. \qquad (17)$$

We form determinants Eq. (2), having a simple cubic lattice local density, by occupying states, dimension by dimension. For g-tuple occupancy this means that $(N/g)^{1/3}$ is an integer; furthermore, particle conservation requires that

$$(N/g)^{1/3} = \int_{-L/2}^{L/2} dx\, \rho(x) \qquad (18)$$

which, in view of the periodicity of $\rho(x)$, reduces to, for $m = \pm 1$ (cf. below)

$$1 = \left(\frac{g}{\rho_0}\right)^{1/3} \int_{-1}^{1} du\, \rho([g/\rho_0]^{1/3} u/2) \equiv \int_{-1}^{1} du\, g_n(\alpha; u),$$
$$\alpha \geq 0, \quad n = 0, 1, 2, \ldots, \qquad (19)$$

the point $u = 0$ corresponding to the lattice "site" while $u = \pm 1$ to the two associated "intersites." The *family* of functions $g_n(\alpha; u)$, for the orbitals Eqs. (12) and(15), respectively, are

$$g_n^{\mathrm{DW}}(\alpha; u) = \frac{(1 + \alpha^2 + 2\alpha \cos \pi u)^n}{\sum_{i=0}^{n} \binom{n}{i}^2 \alpha^{2i}} \quad (\text{DW-}n), \qquad (20a)$$

$$g_n^{\mathrm{DSW}}(\alpha; u) = \frac{(1 + \alpha \cos \pi u)^{2n}}{\sum_{i=0}^{n} \binom{2n}{2i} \alpha^{2i}} \quad (\text{DSW-}n). \qquad (20b)$$

Figures 1 and 2 show graphs of these functions for three values of α^2 and several values of n. The tendency towards a "static classical lattice" as n grows is appreciated. In fact, one can prove this for at least one value of $\alpha(=1)$, as then, for $u = 0$,

$$g_n^{\mathrm{DW}}(1; 0) = 2^{2n} \Big/ \sum_{i=0}^{n} \binom{n}{i}^2 = 2^{2n}/\binom{2n}{n}$$
$$= I_{2n}^{-1} \underset{n \gg 1}{\longrightarrow} \sqrt{2n\pi}, \qquad (21)$$

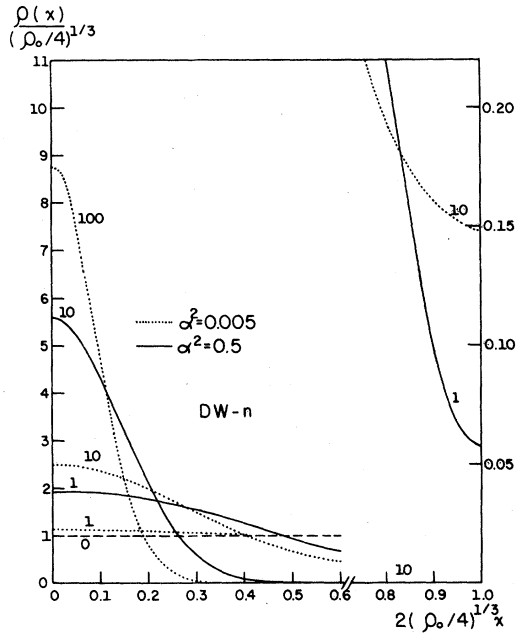

FIG. 1. Density profile for HF "density-wave" (DW) orbitals, about a given "site," for $g=4$, as given by Eq. (14) for two values of parameter α and several values of integer n. The case $n=0$ (dashed) corresponds to the (trivial) PW orbital. The profile near the "intersites," $2(\rho_0/4)^{1/3}x=1$, is on the expanded scale indicated at the right. The tendency towards a "static classical lattice" as n grows is appreciated.

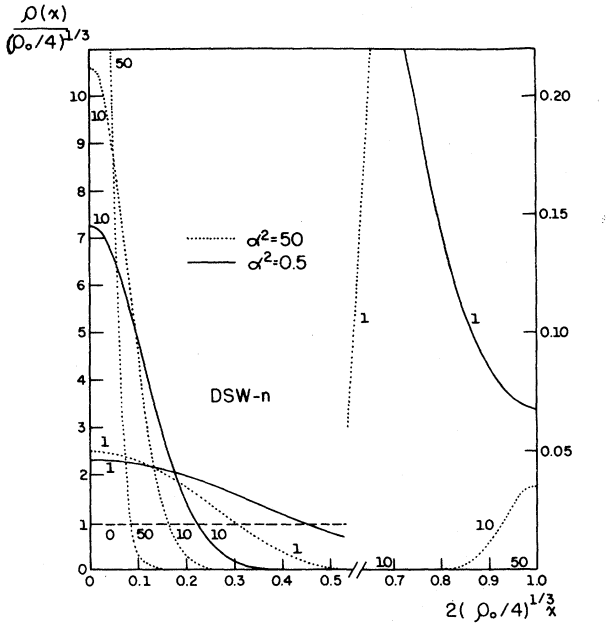

FIG. 2. Density profile for HF "density-standing-wave" (DSW) orbitals, about a given "site," for $g=4$, as given by Eq. (17) for two values of parameter α and several values of integer n. The case $n=0$ (dashed) corresponds to the (trivial) PW orbitals. The profile near the "intersites," $2(\rho_0/4)^{1/3}x=1$, is on the expanded scale indicated at the right. A "build-up" tendency at the "intersites" is appreciated for this family of orbitals, which however tends to disappear as n increases—compare, e.g., $n=1$, 10 and 50 for $\alpha^2=50$ (dotted). The tendency towards a "static classical lattice" as n grows is also appreciated.

where the Stirling approximation

$$\ln m! \underset{m\gg 1}{\longrightarrow} m\ln m - m + \ln\sqrt{2m\pi}, \tag{22}$$

with the uncommon third term, was used in the last step of Eq. (21). We have also that

$$g_n^{\mathrm{DSW}}(1;0) = 2^{2n}\Big/\sum_{i=0}^{n}\binom{2n}{2i} I_{2i} > g_n^{\mathrm{DW}}(1;0), \tag{23}$$

since, from Eq. (16),

$$\binom{2n}{2i} I_{2i} = \binom{2n}{2i}\binom{2i}{i}\Big/ 2^{2i} < \binom{n}{i}^2, \tag{24}$$

for all i non-negative integer, the last inequality following on application of the duplication formula[8] for factorials. Thus, $g_n^{\mathrm{DSW}}(1;0)$ also diverges as $n\to\infty$, but faster than $\sqrt{2n\pi}$. Furthermore, at the "intersites" $u=\pm 1$, one has

$$g_n^{\mathrm{DW}}(\alpha;\pm 1) = (1-\alpha)^{2n}\Big/\sum_{i=0}^{n}\binom{n}{i}^2\alpha^{2i} \underset{n\gg 1}{\longrightarrow} 0 \quad \text{if } \alpha \leq 1, \tag{25}$$

$$g_n^{\mathrm{DSW}}(\alpha;\pm 1) = (1-\alpha)^{2n}\Big/\sum_{i=0}^{n}\binom{2n}{2i} I_{2i}\alpha^{2i} \underset{n\gg 1}{\longrightarrow} 0 \quad \text{if } \alpha \leq 1, \tag{26}$$

and, using Eq. (24),

$$g_n^{\mathrm{DSW}}(\alpha;\pm 1) \geq g_n^{\mathrm{DW}}(\alpha;\pm 1) \tag{27}$$

for any real, non-negative α (equality if $\alpha=0$). In fact, a stronger version of Eqs. (21) and (25) can be proved, namely, from Eq. (20a) and (21),

$$g_n^{\mathrm{DW}}(1;u) = [\tfrac{1}{2}(1+\cos\pi u)]^n / I_{2n} \underset{n\gg 1}{\longrightarrow} [\tfrac{1}{2}(1+\cos\pi u)]^n\sqrt{2n\pi}$$
$$\to \sqrt{2n\pi} \quad \text{if } u=0$$
$$\to 0 \quad \text{if } 0<|u|\leq 1. \tag{28}$$

The above properties together with the normalization Eq. (19), which is independent of n, leads to the *theorem*[9]:

$$\lim_{n\to\infty} g_n(1;u) = \delta(u) \tag{29}$$

for both families DW-n and DSW-n. This limit then gives a density profile about each site characteristic of a "static classical lattice."

III. HARTREE-FOCK ENERGY AND DIRECT VARIATION

For a Hamiltonian Eq. (1) with a δ interaction,

$$v_{ij} = v_0\delta(\vec{r}_{ij}), \quad v_0 \text{ constant}, \tag{30}$$

the energy with HF determinants Φ_0,

$$E = \langle \Phi_0 | H | \Phi_0 \rangle, \tag{31}$$

will contain potential energy

$$\langle \Phi_0 | v_0 \sum_{i<j}^{N} \delta(\vec{r}_{ij}) | \Phi_0 \rangle \propto v_0 \left(\int_{-L/2}^{L/2} \rho^2(x)\, dx \right)^3. \tag{32}$$

In terms of dimensionless energy per particle ϵ and coupling constant λ defined as

$$\epsilon \equiv 2ME/\hbar^2 k_0^2 N, \quad \lambda \equiv 3Mv_0 k_0/\pi^3\hbar^2, \tag{33}$$

the plane-wave (PW) HF energy, i.e., Eq. (31) with a determinant made of PW orbitals Eq. (6), is just, for $g=4$,

$$\epsilon_{\mathrm{PW}}(\lambda) = 1 + \lambda. \tag{34}$$

On the other hand, the corresponding evaluation of Eq. (31), with HF orbitals Eqs. (12) and (15), is somewhat tedious but straightforward. We thus simply state the results.

For the "density-wave" (DW-n) orbitals one has, putting $\beta \equiv |\alpha|^2$, for $g=4$,

$$\epsilon_{\mathrm{DW}-n}(|m|, \beta; \lambda) = 1 + 12m^2 \frac{\sum_{i=0}^{n} \binom{n}{i}^2 i^2 \beta^i}{\sum_{i=0}^{n} \binom{n}{i}^2 \beta^i} + \lambda \left\{ \frac{\sum_{i=0}^{2n} \binom{2n}{i}^2 \beta^i}{\left(\sum_{i=0}^{n} \binom{n}{i}^2 \beta^i\right)^2} \right\}^3 \geq \epsilon_{\mathrm{DW}-n}(1, \beta; \lambda), \tag{35}$$

the energy depending only on $|\alpha|^2$, we henceforth take $\alpha^* = \alpha$ for this family. The last inequality signifies that the energy is minimized in the parameter m is non-negative) for the lowest value of $|m|$ permitted by Eq. (12), namely, $|m| = 1$.

For the "density-standing-wave" (DSW-n) orbitals, *assuming* $\alpha^* = \alpha$ (cf. below), which allows reducing double to single sums by using the sum rule (Appendix C), one gets with $\beta \equiv \alpha^2$, for $g=4$,

$$\epsilon_{\mathrm{DSW}-n}(|m|, \beta; \lambda) = 1 + 12m^2 n^2 \beta \frac{\sum_{i=0}^{n-1} \binom{2n-2}{2i} I_{2i} \beta^i/(2i+2)}{\sum_{i=0}^{n} \binom{2n}{2i} I_{2i} \beta^i} + \lambda \left\{ \frac{\sum_{i=0}^{2n} \binom{4n}{2i} I_{2i} \beta^i}{\left(\sum_{i=0}^{n} \binom{2n}{2i} I_{2i} \beta^i\right)} \right\}^3 \geq \epsilon_{\mathrm{DSW}-n}(1, \beta; \lambda), \tag{36}$$

where, again, minimization in m gives $|m| = 1$, by inspection. The assumption of α real is suggested by the result, easily proved, that

$$\epsilon_{\mathrm{DSW}-1}(|m|, \alpha, \alpha^*; \lambda) \geq \epsilon_{\mathrm{DSW}-1}(|m|, \alpha^* = \alpha; \lambda), \tag{37}$$

if $\lambda < 0$, namely that the energy is *not* lowered (at least for $n=1$) by taking α complex, for an attractive δ interaction. Both Eqs. (35) and (36) reduce to the PW case Eq. (34) as $\beta \to 0$, as of course they should.

A direct variation of Eqs. (35) and (36), in the remaining parameter β, was carried out numerically for each value of the coupling λ. The value $\bar{\beta}$ satisfying both

$$\epsilon'(\bar{\beta}) = 0 \text{ and } \epsilon''(\bar{\beta}) > 0 \tag{38}$$

was substituted into Eqs. (35) and (36) and the resulting non-positive energy differences

$$\Delta\epsilon(\lambda) \equiv \epsilon(1, \bar{\beta}; \lambda) - \epsilon_{\mathrm{PW}}(\lambda) \leq 0 \tag{39}$$

are plotted in Fig. 3 vs $-\lambda$, as only for attraction is $\Delta\epsilon$ ever non-positive.

Bifurcation points in the energy [equality in Eq. (39)] occur for a well-defined critical value of $\bar{\beta} = \beta_c$, for each family member. The "transition" to the new (nontrivial) state can be characterized according to the way in which the long-range order (LRO) appears in the density profile: *smoothly* or *abruptly*; and we have (i) first order (*abrupt* appearance of LRO) if $\beta_c > 0$, (ii) second order (*smooth* appearance of LRO) if $\beta_c = 0$. We further note that all but the first member ($n=1$) of the DSW-n family is stabler than the PW state for coupling λ *weaker* than the critical value sufficient for unstabilizing the PW state, under attractive δ interaction, which can be found from Eq. (B12) to be (for PW-Fermi cube)

$$\lambda \leq -\tfrac{5}{9} = -0.5555\ldots \quad \text{(instability)} \tag{40}$$

and is marked on Fig. 3. [The corresponding value

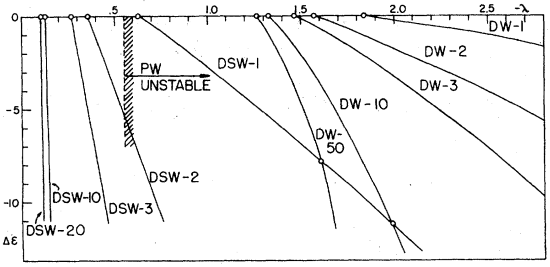

FIG. 3. HF energy gain $\Delta\epsilon$, (Eq. 39), vs coupling parameter λ for the delta interaction, in dimensionless units defined in Eq. (33), for both orbital families and several values of n, corresponding to the "order parameter" value $\bar{\beta}$ which minimizes the respective energies Eqs. (35) and (36) at each (negative) value of λ. Open circles denote bifurcation points. Shaded "edge" denotes the critical value of $\lambda = -\frac{5}{9} = -0.555\ldots$, below which the HF PW state with Fermi cube filling can rigorously be established to become unstable (cf. Appendix B) to the appearance of a lower-energy HF state with inhomogeneous local density $\rho(\vec{r})$. All but the first ($n=1$) member of the "density-standing-wave" (DSW) family are seen to appear, with greater stability than the PW, at *weaker* coupling. (The case DW-1 was discussed in I.)

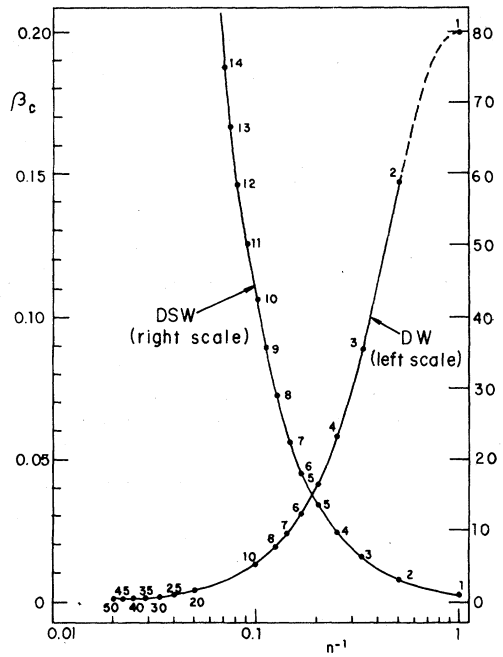

FIG. 4. Critical β values, i.e., at which the new HF energies begin to be stabler than the PW HF energy, for both orbital families, for several values of n (indicated on dots), plotted against n^{-1}. A tendency to achieve a zero (second-order transition) or very small value, as n grows indefinitely, is appreciated for the "density wave" (DW) family, while it grows without limit (first-order transition) for the "density-standing-wave" family, as n grows.

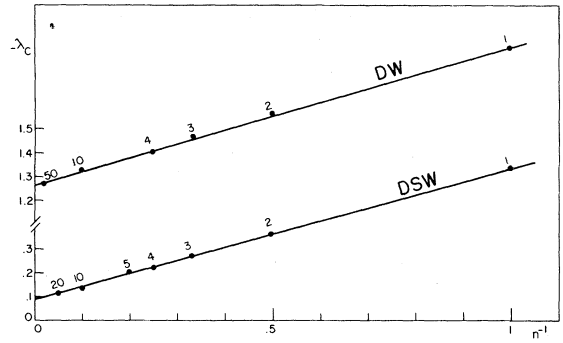

FIG. 5. Critical value of λ, i.e., at which the new HF energies begin to be stabler than the PW HF energy, for both orbital families, for several values of n (indicated on dots), plotted against n^{-1}. Extrapolation to $n \to \infty$ suggest $\lambda_c \simeq -0.08$ for the "density-standing-wave" (DW) family.

for PW Fermi *sphere* instability is $-(4/3\pi^2)^{1/3} = -0.5131$.]

Figure 4 shows the critical β_c values for different members of both families, plotted vs n^{-1}. Extrapolation to $n \to \infty$, if possible, appears to suggest that β_c either tends to zero (second order) or, at least, to a very small value ("almost" second order) for the DW family, while β_c grows without limit (first order) for the DSW family. Figure 5 shows the critical λ_c values (which mark the bifurcation points in Fig. 3) vs n^{-1}. Again, extrapolation to $n \to \infty$ indicates the limiting critical coupling values of ~ -1.26 (DW) and ~ -0.08 (DSW).

IV. DISCUSSION

The results presented, though here limited to δ-potential interacting particles, can be applied to the study, in a self-consistent HF picture, of possible long-range order in the ground state of such N-body systems like (1) nuclear matter, particularly α-clustering effects[3] at subnuclear densities (i.e., at the nuclear surface); (2) neutron matter, particularly crystallization,[4] probably at supranuclear densities; (3) He^3 and He^4 systems; and, (4) the electron (or Wigner) lattice problem,[5] for which, as the interparticle forces are repulsive, spin-ordering can be introduced in the generalized orbitals, as in I, to yield (considerably) stabler states for repulsive δ interactions. These applications are in progress.

APPENDIX A: HF SELF-CONSISTENCY

A brief sketch is given here of the proof that the generalized orbitals Eq. (8), which include as special cases those studied in this paper, Eqs. (12) and (15), explicitly satisfy the HF equations (4) and (5) for occupied states. The proof is done in one dimension, the extension to three being direct. Equation (8) can be rewritten

$$\phi_k(x) = Ce^{ikx} \sum_{l_1 l_3} \binom{n_3}{l_3} \binom{n_1 + l_3}{l_1} \frac{\alpha^{l_3}}{2^{n_1 + l_3}} \times \exp[i(n_1 + n_2 l_3 + l_3 - 2l_1)qx] \quad \text{(A1)}$$

where for simplicity we take $\alpha = \alpha^*$, and the sums are over all non-negative integers allowed by the binomial coefficients present. The kinetic energy term in Eq. (4) is then

$$\frac{\hbar^2 C^2}{2M} \sum_{l_1 l_1' l_3 l_3'} \binom{n_3}{l_3} \binom{n_3}{l_3'} \binom{n_1 + l_3}{l_1} \binom{n_1 + l_3'}{l_1'} \frac{\alpha^{l_3 + l_3'}}{2^{2n_1 + l_3 + l_3'}} [k + (n_1 + n_2 l_3 + l_3 - 2l_1)q]^2 \times \int_{-L/2}^{L/2} dx \exp\{i[k - k' + (n_2 l_3 + l_3 - 2l_1 - n_2 l_3' - l_3' + 2l_1')q]x\} \quad \text{(A2)}$$

which, since in the limit $L \to \infty$ the integral gives $L\delta_{k,k'-lq}$ where l is an integer, reduces, given the conditions on occupied k_x and on q given in Eq. (8), to a constant times $\delta_{k,k'}$. The proof is complete if the potential energy part of Eq. (4) gives a similar result. We have, using Eqs. (5) and (A1), and letting the variable $x_1 \equiv x_1 + x_2$,

$$\langle \phi_k | U_1 | \phi_{k'} \rangle = C^4 \sum_{k\,\mathrm{occ}} \sum_{\mathrm{all}\ l's} \binom{n_3}{l_3'} \binom{n_1 + l_3'}{l_1'} \binom{n_3}{l_3} \binom{n_1 + \bar{l}_3}{\bar{l}_1} \binom{n_3}{l_3} \binom{n_1 + l_3}{l_1} \binom{n_3}{l_3''} \binom{n_1 + l_3''}{l_1''} \frac{\alpha^{l_3' + \bar{l}_3 + l_3 + l_3''}}{2^{4n_1 + l_3' + \bar{l}_3 + l_3 + l_3''}}$$

$$\times \int_{-L/2}^{L/2} dx_2 \int_{-L/2 - x_2}^{L/2} dx\, v(x) \exp\{-i[k' + (n_1 + n_2 l_3' + l_3' - 2l_1)q](x + x_2)\} \exp\{-i[k + (n_1 + n_2 \bar{l}_3 + \bar{l}_3 - 2\bar{l}_1)q]x_2\}$$

$$\times \big(\exp\{i[k + (n_1 + n_2 l_3 + l_3 - 2l_1)q](x + x_2)\} \exp\{i[k + (n_1 + n_2 l_3'' + l_3'' - 2l_1'')q]x_2\}$$

$$- \exp\{i[k + (n_1 + n_2 l_3 + l_3 - 2l_1)q]x_2\} \exp\{i[k + (n_1 + n_2 l_3'' + l_3'' - 2l_1'')q](x + x_2)\} \big)$$

provided only that the interaction is independent of the center of mass $\frac{1}{2}(x_1 + x_2)$ of the two particles. If $L \gg$ range of $v(x)$ the x_2 dependence in the integral over x can be neglected and the integration over x_2 carried out first. In analogy to the kinetic energy case above, the final result leaves a constant times $\delta_{k'k}$, Q.E.D.

APPENDIX B: HF PW INSTABILITY

A (sufficient) condition on the Fermi gas density and coupling strength, of any Fourier-analyzable two-body interaction, for plane-wave instability, in the HF equations, to occur has been discussed elsewhere.[10] Here we give a simpler proof, and in the main text apply the resulting criterion to the delta interaction used therein.

The *theorem* states that there exists a non-plane-wave HF state with lower HF energy E as well, therefore, as *lower vacuum state energy* W_0, whenever

$$\frac{\partial P}{\partial \rho_0} < 0 \text{ with } P \equiv \rho_0^2 \frac{\partial E/N}{\partial \rho_0}. \tag{B1}$$

Proof. Consider a Slater determinant with N orbitals such that the local density is *slightly* inhomogeneous, but the total volume L^3 and N are constant, i.e.,

$$\begin{aligned} &\rho(\vec{r}) = \rho_0 + \rho_1(\vec{r}), \\ &|\rho_1(\vec{r})/\rho_0| \ll 1, \\ &\int_{L^3} d^3 r\, \rho_1(\vec{r}) = 0. \end{aligned} \tag{B2}$$

The HF energy per unit volume, for the homogeneous case, is

$$e(\rho_0) \equiv E/L^3 = \rho_0 E/N, \tag{B3}$$

while for the inhomogeneous case it is, by Taylor-expanding,

$$\begin{aligned} e(\rho_0 + \rho_1) &\equiv \tilde{E}/L^3 \\ &= e(\rho_0) + e'(\rho_0)\rho_1(\vec{r}) + \tfrac{1}{2} e''(\rho_0)\rho_1^2(\vec{r}) + \cdots . \end{aligned} \tag{B4}$$

The HF energy difference is then

$$\begin{aligned} \Delta E \equiv \tilde{E} - E &= \int_{L^3} d^3 r\, [e(\rho_0 + \rho_1) - e(\rho_0)] \\ &= \tfrac{1}{2} e''(\rho_0) \int d^3 r\, \rho_1^2(\vec{r}) + \cdots \end{aligned} \tag{B5}$$

where the last of Eqs. (B2) was used. Since the last integral in Eq. (B5) is non-negative, we have that

$$\Delta E \gtrless 0 \Longleftrightarrow e''(\rho_0) \gtrless 0 \Longleftrightarrow \partial P/\partial \rho \gtrless 0. \tag{B6}$$

The last result follows from Eqs. (B1) and (B3) which give

$$e''(\rho_0) = \frac{1}{\rho_0} \frac{\partial P}{\partial \rho_0}. \tag{B7}$$

This completes the proof regarding the HF energy. Furthermore, the HF vacuum state energy

$$W_0 = \langle T \rangle + \langle U \rangle, \tag{B8}$$

where U is the single-particle HF potential, defined self-consistently by

$$\langle U \rangle = 2\langle v \rangle, \quad v \equiv \sum_{i<j}^{N} v_{ij}, \tag{B9}$$

and all expectation values being between HF determinants. But, using Eqs. (B8) and (B9),

$$\begin{aligned} E = \langle H \rangle &= \langle T \rangle + \langle U \rangle + \langle v \rangle - \langle U \rangle = W_0 - \langle v \rangle \\ &= \tfrac{1}{2} W_0 + \tfrac{1}{2} \langle T \rangle. \end{aligned} \tag{B10}$$

Since the tilde above refers to the *inhomogeneous* state,

$$\Delta E \gtrless 0 \Leftrightarrow \tilde{W}_0 \gtrless W_0 + \langle T \rangle - \langle \tilde{T} \rangle \leq W_0, \tag{B11}$$

the last inequality following from the fact that the kinetic energy difference, by the Rayleigh-Ritz variational principle, is non-positive. Note, however, that *only* when Eq. (B7) is *negative* can one conclude anything definite[11] [as this involves combining the last two inequalities in Eq. (B11)] and one arrives at

$$\partial P/\partial \rho_0 \leq 0 \Rightarrow \tilde{W}_0 \leq W_0, \tag{B12}$$

namely the existence of a lower-energy HF vacuum state. In particular, *any* two-body interaction capable of *binding* in first-order with the plane-waves determinant satisfies[10] Eq. (B12).

We note finally, that the instability (sufficient) condition Eq. (B12) is *more general* than random phase approximation (RPA) instability theory, as this is generally[12] restricted to *long* wavelengths, whereas the inhomogeneity allowed in Eq. (B2) can be either (a) of long wavelength, (b) of finite wavelength (a periodic oscillation of finite "lattice" spacing), or (c) an aperiodic oscillation including, in particular, a solitary wave or "soliton"[13] (e.g., a single "droplet") solution characteristic of nonlinear equations[14] such as the HF equations.

APPENDIX C: A SUM RULE

We state and prove a sum rule over binomial coefficients $\binom{z_i}{k_i}$ and quantities $Q_{k_1+k_2+\cdots+k_n}$ symmetric in their integer indices k_i. The identity was used throughout the above to reduce double to simple sums. It is

$$\sum_{k_1,k_2,\ldots,k_n} \binom{z_1}{k_1}\binom{z_2}{k_2}\cdots\binom{z_n}{k_n} Q_{k_1+k_2+\cdots+k_n} = \sum_k \binom{z_1+z_2\cdots z_n}{k} Q_k \tag{C1}$$

where the summation indices take on *all* non-negative values allowed by the associated binomial coefficients.

Proof. For $n=1$ the theorem is obvious. Suppose it is true for some arbitrary positive integer value of n. For $n+1$ one then has, putting $j = k_n + k_{n+1}$,

$$\sum_{k_1,k_2,\ldots,k_{n+1}} \binom{z_1}{k_1}\binom{z_2}{k_2}\cdots\binom{z_{n+1}}{k_{n+1}} Q_{k_1+k_2+\cdots+k_{n+1}} = \sum_{k_1 k_2 \cdots k_n j} \binom{z_1}{k_1}\binom{z_2}{k_2}\cdots\binom{z_n}{k_n}\binom{z_{n+1}}{j-k_n} Q_{k_1+k_2+\cdots+k_{n-1}+j}. \tag{C2}$$

Since now the sum over k_n affects only the last two binomials, we have

$$\sum_{k_n} \binom{z_n}{k_n}\binom{z_{n+1}}{j-k_n} = \binom{z_n+z_{n+1}}{j} \tag{C3}$$

by the Vandermonde identity. The right side of (C2) then gives

$$\sum_k \binom{z_1+z_2+\cdots+z_n}{k} Q_k \tag{C4}$$

which completes the proof.

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