Self-consistent long-range order in a deformable-jellium model

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A system of N fermions in a box interacting via repulsive delta forces and submersed in a deformable jellium background is analyzed in terms of several non-plane-wave Hartree-Fock states which are more stable than the classic Overhauser ones for charge-density waves, and which also show long-range order.

I. INTRODUCTION

Non-plane-wave Hartree-Fock (HF) orbitals which give rise to long-range order have been studied extensively for the metallic state. Many of these studies[1] have simulated the repulsive electron-electron interaction with a repulsive delta interaction acting between point particles. We have reexamined the problem by (i) including a "deformable-jellium" background in which the (point) particles are submersed and (ii) considering three classes of HF orbitals, different from the standard Overhauser charge-density waves, which give considerably lower energy for wide regions of the coupling and/or density in the model system, and wish to comment on the results obtained.

The Hamiltonian for a system of N fermions of spin-$\frac{1}{2}$ is given by

$$H = T + v_{bb} + v_{bp} + v_{pp} \approx T + v_{pp}^{\mathrm{exch}}\,, \qquad (1)$$

where T is the kinetic-energy operator, v_{bb} is the background-background, v_{bp} is the background-particle, and v_{pp} the particle-particle interaction. The last equation *defines* the "deformable-jellium" model, i.e., such that the background terms cancel against the direct part of the particle-particle potential term, when a Slater determinant is taken for the ground state. For the particle-particle interaction we suppose

$$v_{pp} = \sum_{i<j} v_{ij} = v_0 \sum_{i<j} \delta(\vec{r}_{ij})\,, \quad v_0 > 0\,. \qquad (2)$$

The ground state of the system is assumed describable by a single Slater determinant

$$\Phi_0 = (N!)^{-1/2} \det[\varphi_{\vec{k}_i}(\mathbf{r}_j)\chi_{\sigma_{3i}}(\sigma_{zj})]\,;$$

$$\varphi_{\vec{k}}(\vec{r}) \equiv \prod_{\nu=1}^{3} \varphi_{k_\nu}(x_\nu)\,, \qquad (3)$$

and, if the orbitals satisfy the usual HF equations, the HF energy is just

$$E_{\mathrm{HF}} = \langle \Phi_0 | H | \Phi_0 \rangle\,. \qquad (4)$$

Although one can show that the (exact) ground state of Eqs. (1) and (2) is a collapsed state of infinite density and binding, just from the Rayleigh-Ritz variational principle, the model may still be useful in observing the *relative* behavior of the different HF orbitals to be considered below, as a preliminary guide for the study of more realistic Hamiltonian systems.

II. HF ORBITALS

We consider the *orthonormal* Bloch-like orbitals (subject to periodic boundary conditions in a box of length L)

$$\phi_k(x) = L^{-1/2} e^{ikx} U_k(x)\,, \quad -k_0 < k < k_0\,,$$

where the function $U_k(x)$ is given in the five cases to be studied by

$$U_k(x) = \begin{cases} 1\,, & (5a) \\ u_k + v_k e^{-iqx}\,, \ \mathrm{sgn}k = \mathrm{sgn}q\,, & (5b) \\ A_n(\alpha)(1+\alpha e^{-iqx})^n\,, & (5c) \\ B_n(\alpha)(1+\alpha\cos qx)^n\,, & (5d) \\ C(\alpha)e^{\alpha\cos qx}\,, & (5e) \end{cases}$$

where (5a) is for plane wave (PW), (5b) for Overhauser, (5c) for density-wave-n (DW-n), (5d) for density-standing-wave-n (DSW-n), and (5e) for exponential (EXP), respectively, orbitals. Also, in Eqs. (5) we have

u_k, v_k real; $u_k^2+v_k^2=1$; $|q| \geq 2k_0$,

α real ≥ 0; $n=1,2,3,\ldots$;

$$A_n(\alpha) \equiv \left[\sum_{i=0}^{n} \binom{n}{i}^2 \alpha^{2i}\right]^{-1/2};$$

$$B_n(\alpha) \equiv \left[\sum_{i=0}^{n} \binom{2n}{2i} K_{2i}\,\alpha^{2i}\right]^{-1/2};$$

$$C(\alpha) \equiv [I_0(2\alpha)]^{-1/2}; \tag{6}$$

$$K_l \equiv \pi^{-1}\int_0^{\pi} dx \cos^l x = \tfrac{1}{2}[1-(-)^l]2^{-l}\binom{l}{\tfrac{1}{2}l};$$

$$I_l(y) \equiv \sum_{s=0}^{\infty} [s!(s+l)!]^{-1}(\tfrac{1}{2}y)^{2s+l} = (-)^l I_l(-y)$$

$$\underset{y\to 0}{\sim} (n!)^{-1}(\tfrac{1}{2}y)^n$$

$$\underset{y\to\infty}{\sim} (2\pi y)^{-1/2}e^y ,$$

where the function $I_n(y)$ is the modified Bessel function.[2] We note that only in case (5b) does $U_k(x)$ depend on k. Also, in cases (5c)–(5e), α is an additional variational parameter, as well as the integer n for (5d) and (5e); and for (5b)–(5e) so is the wave number $|q| \geq 2k_0$, where $2k_0$ is the length of the Fermi cube being filled in all cases. The orbitals(5a)–(5e) explicitly satisfy the HF equations for the occupied states.[3]

The resulting single-particle (local) density is then

$$\rho(\vec{r}) = \prod_{\nu=1}^{3} \rho(x_\nu); \tag{7}$$

$$\rho(x) = 2^{1/3}\sum_{k(\text{occ})} |\phi_k(x)|^2 = 2^{1/3}L^{-1}\sum_{k(\text{occ})} |U_k(x)|^2$$

$$= \rho_0^{1/3} \equiv N^{1/3}/L = 2^{1/3}(k_0/\pi) \tag{8a}$$

$$= \rho_0^{1/3}(1+\Delta\cos qx); \quad \Delta \equiv 2\left(\frac{2}{N}\right)^{1/3}\sum_{k(\text{occ})} u_k v_k \tag{8b}$$

$$= \rho_0^{1/3}A_n^2(\alpha)(1+\alpha^2+2\alpha\cos qx)^n \tag{8c}$$

$$= \rho_0^{1/3}B_n^2(\alpha)(1+\alpha\cos qx)^{2n} \tag{8d}$$

$$= \rho_0^{1/3}I_0^{-1}(2\alpha)e^{2\alpha\cos qx}, \tag{8e}$$

and clearly corresponds to nonhomogeneous density with long-range order centered on a simple cubic lattice, which "dissolves" into the spatially homogeneous case (8a) when the "order parameters" Δ or α vanish. Furthermore, for (8c) and (8d), as $n\to\infty$ or, $\alpha\to\infty$ in (8e), one can see[3] that one approaches Δ functions centered on the lattice, where associated with each lattice site is a pair of spin-up and spin-down particles.

III. HF ENERGIES

For the purpose of comparing the relative stability of the different HF states given above, let

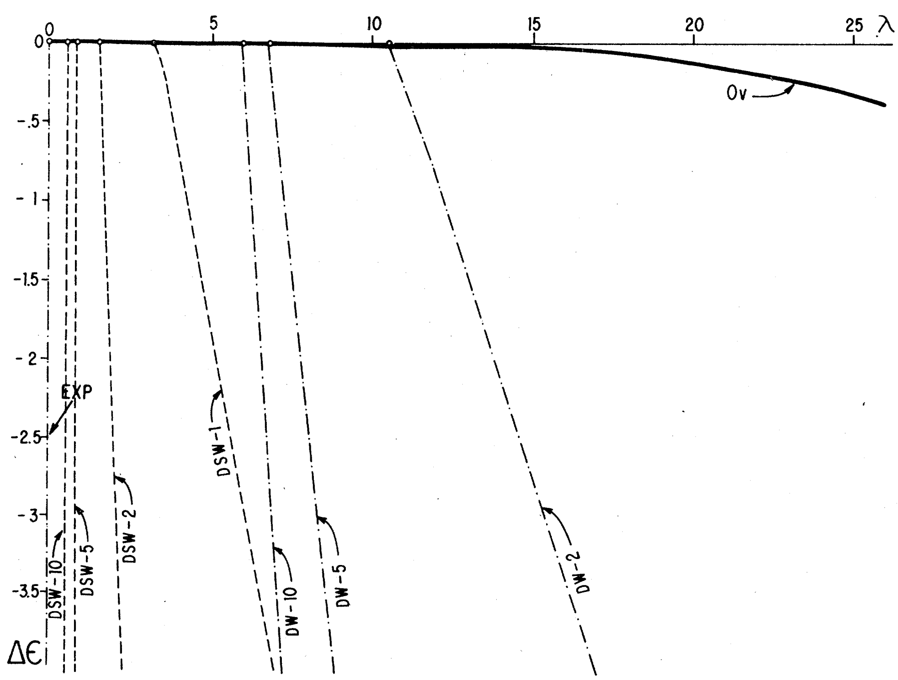

FIG. 1. Energy difference, in dimensionless units [Eq. (9)], between the various non-PW HF states discussed herein and the PW HF paramagnetic state, as function of dimensionless coupling λ [Eq. (10)], which resulted from minimizing, analytically in cases (5b) (Ov) and (5e) (EXP), and numerically in cases (5c) (DW-n) and (5d) (DSW-n), the HF energy for each value of λ. The state DW-1 is higher than the state Ov for all λ, as expected, and, beyond its critical λ, is indistinguishable in the present scale from the λ axis.

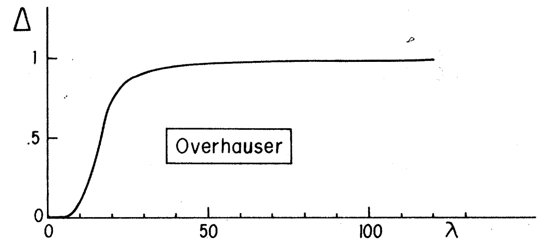

FIG. 2. Overhauser order parameter Δ defined by Eq. (8b) and given finally by Eq. (13), as a function of dimensionless coupling λ. The appearance of long-range order here is "gradual" and thus characteristic of a second-order transition.

us introduce a dimensionless energy per particle

$$\epsilon \equiv 2mE_{\rm HF}/N\hbar^2\pi^2\rho_0^{2/3} \tag{9}$$

and dimensionless coupling

$$\lambda \equiv mv_0\rho_0^{1/3}/\pi^2\hbar^2\,, \quad v_0>0\,. \tag{10}$$

Moreover, we define the HF energy difference with respect to the plane-wave (paramagnetic) HF energy $\epsilon_{\rm PW}$ as

$$\Delta\epsilon \equiv \epsilon - \epsilon_{\rm PW}\,. \tag{11}$$

For the Hamiltonian equation (1) and (2) HF energy ϵ for cases (5b)–(5e) can be minimized in q by inspection, giving $|q| = 2k_0$ and thus leaving one remaining variational (order) parameter Δ for (5b) and α for (5c)–(5e) as well, of course, as the integer n for (5c) and (5d).

The ensuing energy difference (11) is straightforwardly evaluated for cases (5b)–(5e) and we merely quote the results. We have

$$\Delta\epsilon_{\rm Ov} = 3\times 2^{-2/3}\{1-\coth[2^{-4/3}\lambda(1+\tfrac{1}{2}\Delta^2)^2]^{-1} + 2^{-4/3}\lambda(1+\tfrac{1}{2}\Delta^2)^2\Delta^2\} - 2^{-1}\lambda[(1+\tfrac{1}{2}\Delta)^3-1]\,, \tag{12}$$

where the order parameter Δ, defined in Eq. (8b), is

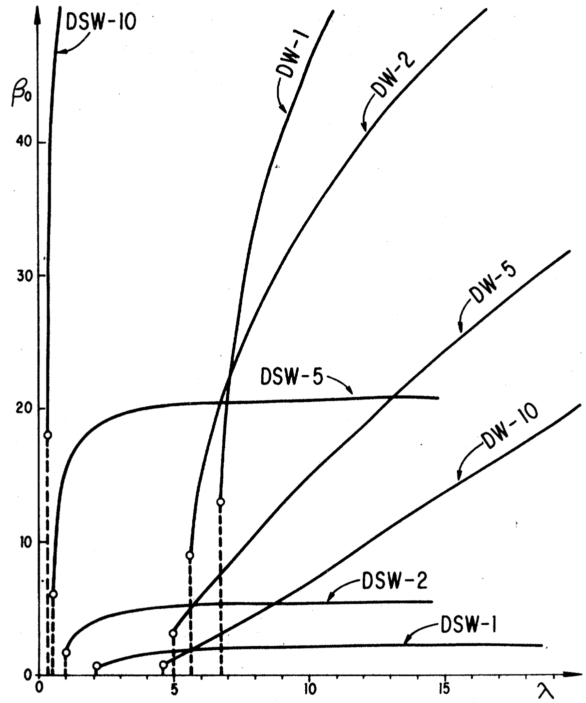

FIG. 3. Order parameter β_0, defined in Eq. (5c) for (DW-n) and Eq. (5d) for (DSW-n) as α_0^2, which minimizes the HF energy [Eqs. (14) or (15)] for each value of λ. Dashed vertical portions dropping from the open circles correspond to the "sudden" appearance of long-range order characteristic of 1st order phase transitions, as coupling and/or density are increased. (Note: the β_0 scale for the DW-n family is 10^{-2} times that shown.)

$$\Delta^{-1} = 2^{-4/3}\lambda(1+\tfrac{1}{2}\Delta^2)^2\sinh[2^{-4/3}\lambda(1+\tfrac{1}{2}\Delta^2)^2]^{-1}\,, \tag{13}$$

and is obtained by minimizing (analytically) $\epsilon_{\rm Ov}$ with respect to either u_k or v_k. To obtain $\Delta\epsilon$ as a function of coupling λ only, one must use (13) to eliminate Δ from (12), and this was done numerically. Also, for cases (5c) and (5d) one gets, putting $\alpha^2 \equiv \beta$,

$$\Delta\epsilon_{{\rm DW}-n}(\beta) = 12\times 2^{-2/3}\left[\sum_{i=1}^{n}\binom{n}{i}^2\beta^i\right]^{-1}\sum_{j=1}^{n}\binom{n}{j}^2 j^2\beta^j - 2^{-1/3}\lambda\left\{\left[\sum_{i=0}^{n}\binom{n}{i}^2\beta^i\right]^{-6}\left[\sum_{j=0}^{2n}\binom{2n}{i}^2\beta^i\right]^3 - 1\right\}; \tag{14}$$

$$\Delta\epsilon_{{\rm DSW}-n}(\beta) = 12\times 2^{-2/3}\eta^2\beta\left[\sum_{i=0}^{n}\binom{2n}{2i}K_{2i}\beta^i\right]^{-1}\sum_{j=0}^{n-1}\binom{2n-2}{2j}K_{2j}(2j+2)^{-1}\beta^j - 2^{-1/3}\lambda\left\{\left[\sum_{i=0}^{n}\binom{2n}{2i}K_{2i}\beta^i\right]^{-6}\left[\sum_{j=0}^{2n}\binom{4n}{2j}K_{2j}\beta^j\right]^3 - 1\right\}, \tag{15}$$

which were minimized numerically in $\beta \geqslant 0$, for each λ. Finally, case (5e) gives

$$\Delta\epsilon_{\rm EXP}(\alpha) = 3\times 2^{1/3}\alpha I_0^{-1}(2\alpha)I_1(2\alpha) - 2^{-1/3}\lambda[I_0^{-6}(2\alpha)I_0^3(4\alpha)-1]\,. \tag{16}$$

This last case gives the *lowest* HF energy than that of the previously mentioned cases, for any finite λ. In fact, (16) does not have a minimum in α, for finite λ, but an "infimum" for $\alpha \to \infty$, since

$$\Delta\epsilon_{\mathrm{EXP}}(\alpha) \underset{\alpha \gg 1}{\sim} 3 \times 2^{1/3}\alpha - 2^{-1/3}\lambda[(2\pi\alpha)^{3/2} - 1] , \tag{13a}$$

where the modified Bessel function asymptotic values given in Eq. (6) were used. But Eq. (13a), valid for very large α, can be negative (and infinitely so) for any $\lambda > 0$ no matter how small. The corresponding state is a simple cubic lattice of "dimers" at *zero* density: the similarity with the Cooper pairs of BCS theory[4] and/or electron pairs in the Wigner lattice of Ref. 5 is at least suggestive.

IV. RESULTS

The results obtained are summarized in Figs. 1–3. The energy difference Eq. (11) between the various non-PW HF states and the (trivial) PW HF one are shown in Fig. 1 where, for each value of the coupling λ the value of the order parameter minimizing the energy was employed. The open circles represent bifurcation points of the new state relative to the PW HF paramagnetic one. For both cases (5c) and (5d), DW-n and DSW-n, respectively, the critical value of λ beyond which the new state is stabler tends, as $n \to \infty$, to a small but finite value which in cases (5b) and (5e), Overhauser and exponential, respectively, happens to be zero.

The order parameters which minimize the corresponding energy at each value of λ are plotted in Figs. 2 and 3 for cases (5b), (5c), and (5d) as function of coupling λ. For case (5e), of course, the order parameter α diverges for arbitrarily small λ, Eq. (13a). We note finally, that the onset of long-range order is "abrupt" for DW-n and DSW-n and "continuous" for both Overhauser and exponential orbitals, indicating, respectively, first- and second-order transitions.

The present work shows that long-range order is possible in a system of many fermions with repulsive interactions as has been hypothesized, e.g., for the Wigner lattice,[6] with new states which are stabler than the classic Overhauser charge-density waves.

ACKNOWLEDGMENT

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