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Roothaan approach in the thermodynamic limit

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A systematic method for the solution of the Hartree-Fock equations in the thermodynamic limit is presented. The approach is seen to be a natural extension of the one usually employed in the finite-fermion case, i.e., that developed by Roothaan. The new techniques developed here are applied, as an example, to neutron matter, employing the so-called V_1 Bethe "homework" potential. The results obtained are, by far, superior to those that the ordinary plane-wave Hartree-Fock theory yields.

[NUCLEAR STRUCTURE Hartree-Fock approach; nuclear and neutron matter.]

I. INTRODUCTION

The exact solution, analytically or numerically, of an N-fermion ($N >> 1$) problem with realistic interparticle interactions will not be available in the immediate future. As for approximate treatments, two general microscopic approaches have been at our disposal for some years now: (1) variational,[1] of the Jastrow type, Fermi-hypernetted-chain approximation method, etc., and (2) perturbation theory,[2] based mainly on diagrammatic methods of the "ladder," "ring,"[2] or other infinite partial summations. More recently, the so-called "exp$S$" method has been shown to present us with a viable alternative.[3]

All these general approaches begin with an assumed one-particle, "zeroth-order" state, about which one then perturbs in one manner or another. This unperturbed ground vacuum state (u.g.s.) can be selected in several ways, that is, a conjecture must be made in this respect, and usually such a state is taken to be a single Slater determinant of plane-wave (PW) one-particle "orbitals," with occupied "k vectors" spanning a spherical Fermi sea in (momentum) k space [the "Fermi sphere" of radius k_F (the Fermi vector), which is related to the particle density ρ]. However, most authors would agree in considering that the best unperturbed, one particle Hamiltonian is that leading to the Hartree-Fock (HF) problem. This is nonlinear, thus giving rise to not one, but *several* solutions which may display quite different qualitative properties. The PW orbitals constitute *just one* of the possible HF solutions,[4] and the investigation of the properties associated with *other* such solutions is thus a task that may bear interesting results.

Much work has been devoted in recent years to this particular aspect of the many-body problem, and several non-PW HF solutions have been constructed and applied to different problems in the thermodynamic limit.[5–12] It has been found that orbitals giving rise to a spatially ordered, "crystal-like" structure yield, in many instances, a more tightly bound ground state (gs) than the spatially homogeneous ("fluid") PW one[5–12] at the HF stage.

The HF solutions studied in Refs. 5–12 have been found in a *heuristic* fashion, i.e., no systematic procedure was available that would allow one to derive them. They constitute *a posteriori* solutions to the HF equations, *and only for occupied states,* a fact that has caused some concern related to their stability against one-particle–one-hole excitations. Clearly, it would be of interest to have at our disposal a systematic way of generating non-PW HF solutions in the thermodynamic limit, and, moreover, to obtain orbitals of that kind that would be solutions both for occupied and for empty states. An attempt in this direction has recently been made, in the one dimensional case,[13] and applied to the attractive delta gas[14] problem.

The purpose of this work is to present a general treatment of the type prescribed in the previous paragraph, for any number of dimensions. The approach will be illustrated with reference to a semi-realistic problem: neutron matter, in the so-called

Bethe "homework" framework.

II. FORMALISM

In utilizing non-PW solutions to the HF equations (sometimes referred to as "nontrivial" ones) in the thermodynamic limit, as is done, for example, in Refs. 5–12, one is making a definite, heuristic conjecture as to what the nonperturbed ground vacuum state is. It has been suggested in Ref. 13 that in order to look for nontrivial HF states in a systematic fashion, one should employ the HF equations themselves:

$$\langle \phi_{k'} \mid \hat{T} \mid \phi_k \rangle + \sum_{l(\text{occ})} \langle \phi_{k'}\phi_l \mid \hat{V} \mid \phi_k\phi_l - \phi_l\phi_k \rangle = \epsilon_k \delta_{kk'} , \tag{1}$$

as a guide ($\hat{H} = \sum_i \hat{T}_i + \frac{1}{2}\sum_{i\neq j} \hat{V}_{ij}$ is the many-body Hamiltonian). A study of the HF problem in one dimension along these lines resulted in a definite prescription for obtaining nontrivial HF states.[13] We shall consider here the three-dimensional problem (and it will be seen that extension to any dimensionality is straightforward), but from a different perspective, somewhat less mathematical and more physical, than that of Ref. 13.

In view of the experience gained by previous workers on the field,[5–12] we shall look for periodic HF orbitals $\mid \phi_k \rangle$ that are able to give rise to a "lattice" structure with vectors $\vec{a}_1$, $\vec{a}_2$, and $\vec{a}_3$. This lattice should be invariant under translations

$$\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3 , \tag{2}$$

so that the unitary translation operator $\hat{T}_{\vec{R}}$, which commutes both with $\hat{H}$ and with the HF Hamiltonian $\mathscr{H}$, will give

$$\hat{T}_{\vec{R}} \mid \phi_k \rangle = e^{i\vec{k}\cdot\vec{R}} \mid \phi_k \rangle . \tag{3}$$

Moreover, $\hat{T}_{\vec{R}}$ should not affect whatever particular occupation (among the available orbitals) one may choose in building up the Slater determinant

$$\Phi_0 = (N!)^{-1/2} \det[\phi_{k_i}(\vec{x}_i)] \tag{4}$$

that is going to represent the HF ground state.

Consequently, the solutions of (1) that are also eigenstates of $\hat{T}_{\vec{R}}$ should be Bloch functions:

$$\phi_{\vec{k}}(\vec{x}) = e^{i\vec{k}\cdot\vec{x}} u_{\vec{k}}(\vec{x}) , \tag{5}$$

with $u_{\vec{k}}(\vec{x}+\vec{R}) = u_{\vec{k}}(\vec{x})$, i.e., u has the same periodicity as the lattice (notice that for the sake of a lighter notation we are omitting spin and isospin subindexes). Now, in order to find the self-consistent Bloch orbitals u that we are looking for, we expand ϕ in plane waves:

$$\mid \phi_{\vec{k},n} \rangle = \sum_{\vec{G}} c_{n,\vec{G}}(\vec{k}) \mid \vec{k}+\vec{G} \rangle , \tag{6}$$

with

$$\mid \vec{k}+\vec{G} \rangle = e^{i(\vec{k}+\vec{G})\cdot\vec{x}} , \tag{7}$$

where $\vec{G}$ is a vector of the reciprocal lattice and $\vec{k}$ belongs to the first Brillouin zone. The index n in (6) labels the rows of the unitary matrix which performs the transformation implied by this equation. The problem of finding nontrivial HF orbitals reduces itself to that of finding the coefficients $c_{n,\vec{G}}$ of (6).

The idea is now to introduce the transformation (6) into the HF equation (1), which leads to an eigenvalue problem for the desired coefficients c:

$$\sum_{\vec{G}'} \langle \vec{k}+\vec{G} \mid \mathscr{H} \mid \vec{k}+\vec{G}' \rangle c_{n,\vec{G}'}(\vec{k}) = \epsilon_n(\vec{k}) c_{n,\vec{G}}(\vec{k}) . \tag{8}$$

In Sec. III we give the explicit form of the matrix elements of $\mathscr{H}$ for the case that we discuss as an example in the present work.

Our prescription for obtaining HF states in the thermodynamic limit would then read: (i) choose as a starting point the PW orthonormal set (a trivial HF set[4]), (ii) consider now the following set of orbitals: (a) $e^{i\vec{k}\cdot\vec{x}}$, with $\vec{k}$ belonging to the first Brillouin zone and (b) $(M-1)$ vectors of the reciprocal lattice, (iii) subject the members of this set to the unitary transformation (6) and obtain a new set $\mid \phi_{\vec{k},n} \rangle$, which is to be completed by adding plane waves to it *beyond the Mth Brillouin zone,* and (iv) select the relevant unitary transformation [that yields the coefficients $c_{n,\vec{G}}(\vec{k})$ in (6) in such a way that, within the subspace reached by the transformation, the $\mid \phi_{\vec{k},n} \rangle$ constitute a HF set].

This is a definite prescription which is easily seen to yield HF solutions *both for occupied and empty orbitals.* Equation (8) presents us with a nonlinear problem entirely similar to the one posed by Roothan's scheme,[15] usually employed for solving the HF equations in the finite fermion problem. The solution is to be obtained here as in

Roothan's case, namely by an iterative diagonalization of the HF Hamiltonian $\mathscr{H}$ (an $M\times M$ problem). Enlarging the single-particle basis in the finite case has in our case its counterpart in taking a larger number M of Brillouin zones into account. The fact that we are working in the thermodynamic limit has as a consequence, in practical calculations, the necessity of "discretizing" the first Brillouin zone, selecting a sample of m points from it. Our iterative process involves, then, m simultaneous $M\times M$ diagonalizations at each step. It is easily seen that the orbitals (6) constructed with the eigenvectors arising from these m diagonalizations are orthogonal among themselves, because of the orthogonality of the PW set.

III. A SIMPLE APPLICATION TO NEUTRON MATTER

A. Introductory remarks

The plausibility of non-plane-wave HF orbitals in a nuclear context has been studied, for example, in Refs. 7–10. Effective two body interactions of the Skyrme type were employed to that end in Refs. 7–9 and shown to lead to such nuclear effects as alpha-particle clustering at subnuclear densities. It would be of interest now to ask whether nontrivial HF orbitals are relevant when used with realistic (i.e., bare) two body forces, in view of the decisive role that the repulsive cores in the nucleon-nucleon force play for the establishment of long-range order in the form of crystallization. The importance of these repulsions (hard or soft) is well accepted both classically[16] and quantally,[17] and a step in the direction outlined here is that of Ref. 10, where some heuristic nontrivial HF states are studied in connection with the so-called homework potentials.[18]

Our present purpose is twofold: On the one hand, we wish to explore the consequences of using nontrivial HF orbitals in conjunction with two-body forces containing a repulsive core, and, on the other hand, it is our goal to provide a simple illustration of the formalism presented in the preceding section. With these objectives in mind we shall apply our techniques to neutron matter, employing the so-called V_1 homework potential,[18] defined by an interaction of the form

$$\sum_{\lambda} a_{\lambda}\frac{e^{-\lambda x}}{x}\ , \tag{9}$$

where $x=\mu r$, $\mu=0.7$ fm^{-1}, and $\lambda=1$, 4, and 7. The values of the coefficients a_{λ} are found, e.g., in Ref. 18.

B. Specialization of the theory to CSSDW orbitals

We shall deal in this section with orbitals of the type employed in Ref. 10, under the name of "corrugated-sheet-spin-density waves" (CSSDW). However, we shall treat them self-consistently according to the theory of Sec. II.

In the present situation the direct lattice is characterized by a single vector $\vec{a}_3$ of modulus P, P denoting the interval (period) between two successive spin-up particles along the Z axis. In the reciprocal lattice we have just one vector, $\vec{a}_3{}^*=\vec{q}$, of modulus $|\vec{q}|=q=2\pi/P$. The vectors $\vec{G}$ of Sec. II are given here by

$$\vec{G}=m\vec{q},\quad m \text{ integer}\ . \tag{10}$$

The CSSDW orbitals are characterized by an antiferromagnetic symmetry along the Z axis, together with the following point-symmetries:

(a) $R(\phi)$; a rotation, according to the angle ϕ, around the Z axis.

(b) σ_v; reflection with respect to planes containing the Z axis.

(c) σ_h; reflection with respect to a plane perpendicular to the Z axis (an atom of the lattice lies in this plane).

(d) inversion $I=R(\pi)\sigma_h$.

These are symmetries of the total Hamiltonian H. They will also be symmetries of the HF Hamiltonian if we choose our occupied states in a convenient fashion. This entails occupying states with both rotation and reflection symmetry with respect to a plane perpendicular to the Z axis. As a matter of fact, it suffices to find those HF solutions lying on the surface of the volume generated as a (in principle arbitrary) figure, drawn on the x-z plane, rotates around the Z axis (only the positive semiaxis is needed). The remaining states can afterwards be obtained with the help of the relationship[19]

$$\hat{R}\phi_{\vec{k}}(\vec{x})=\phi_{\vec{k}}(\hat{R}^{-1}\vec{x})=\phi_{\hat{R}\vec{k}}(\vec{x})\ . \tag{11}$$

The spin degree of freedom must be dealt with explicitly here, on account of the antiferromagnetic symmetry (see Ref. 10). This entails adding to our previous list of symmetries the following:

(e) $\hat{K}\hat{T}_{P/2}$; a half-period translation ($\hat{T}_{P/2}$) and

time-reversal ($\hat{K}$), which produces "spin flip."

We have[19]

$$\phi_{-\vec{k},-1/2}(\vec{x})=e^{i\alpha}\hat{K}\hat{T}_{P/2}\phi_{\vec{k},1/2}(\vec{x}) , \tag{12}$$

where the phase factor is to be selected so as to simplify our calculations.

It should be clear now that we need to look just for those solutions corresponding to the k_xk_z plane with $k_x,k_z\geq 0$, and $\sigma_3=\frac{1}{2}$, i.e. [see Eqs. (6) and (10)],

$$\phi_{\vec{k},n,\sigma_3}(\vec{x})=\sum_m c_{n,m}(\vec{k},\sigma_3)e^{i(\vec{k}+m\vec{q})\cdot\vec{x}}\chi_{\sigma,\sigma_3} , \tag{13}$$

where χ_{σ,σ_3} denotes a spin wave function, for $\vec{k}=(k_x,0,k_z)$ with $k_x,k_z\geq 0$, and $\sigma_3=\frac{1}{2}$. Thus,

$$\begin{aligned}(\vec{k}+m\vec{q})\cdot\vec{x}&=k_xx+k_zz+mqz\\&=k_x\rho\cos\phi'+(k_z+mq)z .\end{aligned} \tag{14}$$

We use now the relationship (11)

$$\phi_{\hat{R}(\phi)\vec{k}}(\vec{x})=\phi_{\vec{k}}[\hat{R}(-\phi)\vec{x}] , \tag{15}$$

which is tantamount to replacing in (14) the angle ϕ by the angle $\phi'-\phi$. Moreover, since k_x is the projection of $\vec{k}$ onto the x-y plane, it can be identified with that projection corresponding to the cylindrical coordinate ρ, i.e., with k_ρ, which allows one to write, instead of (14),

$$(\vec{k}+m\vec{q})\cdot\vec{x}=k_\rho\rho\cos(\phi'-\phi)+(k_z+mq)z , \tag{16}$$

and, consequently,

$$\phi_{\vec{k},n,1/2}(\vec{x})=\sum_m c_{n,m}(k_\rho,k_z,\tfrac{1}{2})e^{i(\vec{k}+m\vec{q})\cdot\vec{x}}\chi_{\sigma,1/2} \tag{17}$$

for $k_z\geq 0$. The inversion symmetry gives

$$\phi_{-\vec{k},1/2}(\vec{x})=\phi_{\vec{k},1/2}(-\vec{x}) , \tag{18}$$

which implies

$$c_{n,m}(-\vec{k},\tfrac{1}{2})=c_{n,-m}(\vec{k},\tfrac{1}{2}) . \tag{19}$$

If we now employ the result (12), we can write

$$\begin{aligned}\phi_{-\vec{k},-1/2}(\vec{x})&=e^{i\alpha}(-i\sigma_y\hat{K}_0\hat{T}_{P/2})\phi_{\vec{k},1/2}(\vec{x})\\&=e^{i\alpha}(-i\sigma_y)\phi^*_{\vec{k},1/2}\left[\vec{x}+\frac{\vec{P}}{2}\right] ,\end{aligned} \tag{20}$$

and, remembering that $i\sigma_y\chi_{\sigma,1/2}=\chi_{\sigma,-1/2}$, we obtain, with the choice $\alpha=\pi+\vec{k}\cdot\vec{P}/2$,

$$c_{n,m}(\vec{k},-\tfrac{1}{2})=(-1)^m c^*_{n,-m}(-\vec{k},\tfrac{1}{2}) , \tag{21}$$

or, according to (19),

$$c_{n,m}(\vec{k},-\tfrac{1}{2})=(-1)^m c^*_{n,m}(\vec{k},\tfrac{1}{2}) . \tag{22}$$

If we now restrict ourselves to working with real coefficients $c_{n,m}$, and, furthermore, only the first Brillouin zone ($n=1$) is occupied, filling a Fermi sphere of radius k_F such that

$$\rho_0=k_F{}^3/3\pi^2 , \tag{23}$$

the usual selection[7-10] $q=2k_F$ allows us to write the matrix elements of the HF Hamiltonian $\mathscr{H}$ of Eq. (8) in the form

$$\begin{aligned}\langle\vec{k}+\vec{G}'\,|\,\mathscr{H}\,|\,\vec{k}+\vec{G}\rangle&=\langle\vec{k}+r\vec{q}\,|\,\mathscr{H}\,|\,\vec{k}+s\vec{q}\rangle\\&=\frac{\hbar^2}{2m}k_F{}^2[z^2+4s(s+zu)]\delta_{rs}\\&\quad+\frac{k_F}{\mu\pi}\int_0^1x^2dx\int_0^1dy\sum_m a_m(x,y)a_{m+r-s}(x,y)\{\cdots\} ,\end{aligned} \tag{24}$$

$$\{\cdots\}=\sum_\lambda a_\lambda\left\{\frac{2[1+(-1)^{s-r}]}{(\lambda\mu/k_F)^2+4(s-r)^2}-[I(m-s,1)+I(-m-r,-1)]\right\} , \tag{25}$$

where

$$\begin{aligned}I(\alpha,\beta)=\{&[(\lambda\mu/k_F)^2+(2\alpha-zu+\beta xy)^2\\&+x^2(1-y^2)+z^2(1-u^2)]^2\\&-4x^2z^2(1-y^2)(1-u^2)\}^{-1/2}\end{aligned} \tag{26}$$

and

$$a_i(z,u)=c_{1,i}(k_z/k_F,\cos\theta,\tfrac{1}{2}) . \tag{27}$$

C. Results

The integrals in (26) were evaluated according to the Gaussian method, which entails the evaluation

of the a's [Eq. (27)] in those m points required by the integration method. The HF Hamiltonian matrix $\mathscr{H}_{rs}$ was then diagonalized iteratively, until reaching self-consistency. For this we choose the criterion that all a's involved in the problem should agree, when evaluated in two successive iterations to eight digits. Up to five Brillouin zones were used in order to define the HF transformation, i.e., our self-consistent HF orbitals were linear combinations of PW belonging to five different Brillouin zones. In order to sample the first Brillouin zone, as described in the previous section, several selections of the corresponding number of points m were made. It was found that the results are independent of m for $m \geq 7\times 7$, up to four significant digits. (Notice that one is dealing with a double integration problem.)

Our main results are displayed in Fig. 1. We show there the HF binding energy per neutron as a function of density, for $M=1$ (PW case), 2 (Overhauser-type[10–20]), 3, 4, and 5. The new results are those for $M \geq 3$, where saturation is attained. The energy gain obtained for $M \geq 3$, with respect to the cases $M=1$, 2, is enormous (more than 100%). Surprisingly enough, taking into account the strong repulsion that characterizes the

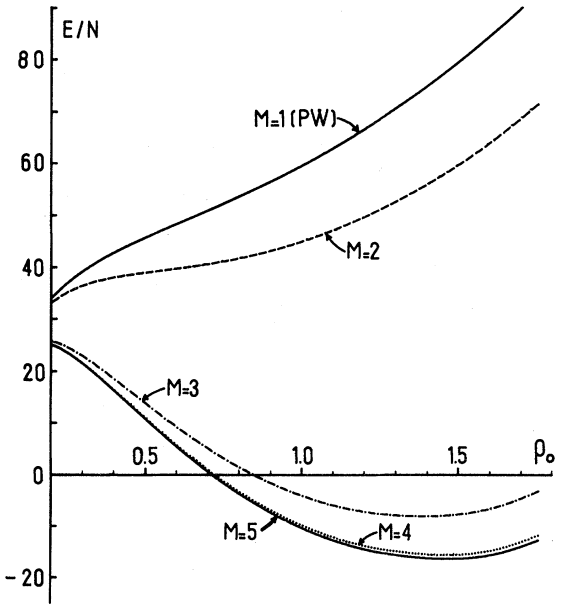

FIG. 1. Binding energy per particle (MeV) as a function of the total density (fm^{-3}) obtained with the V_1 Bethe homework potential for different HF solutions. M denotes the number of Brillouin zones taken into account in the calculations. $M=1$ corresponds to the trivial plane-wave HF solution.

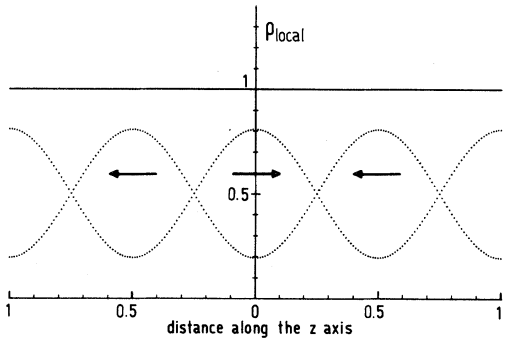

FIG. 2. Variation along the z axis of the spin-up spin-down (dotted lines) and total (solid line) spatial densities (fm^{-3}) for the (V_1 Bethe homework potential) HF solution corresponding to the case $M=2$ (Overhauser-type orbitals). The horizontal scale is normalized to $2\pi/q$. The total density (N/V) is 1.33 fm^{-3}.

V_1 potential, *the system is bound for* $M \geq 3$. The main qualitative difference between the cases $M<3$ and $M \geq 3$ lies in the fact that in the former, the spatial density is constant, while in the latter, definitely, inhomogeneities are observed. An example is shown in Fig. 2. Concerning the spin density along the z axis, we have an homogeneous distribution for $M=1$ and an antiferromagnetic structure for $M=2$, but with an homogeneous *net* spin density. For $M \geq 3$ we have still an antiferromagnetic structure with a nonvanishing *net* total density (see Fig. 3).

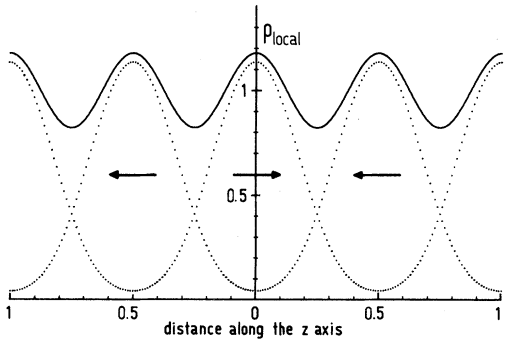

FIG. 3. Variation along the z axis of the spin-up, spin-down (dotted lines) and total (solid lines) spatial densities (fm^{-3}) for the (V_1 Bethe homework potential) HF solution corresponding to $M=3$. The horizontal scale is normalized to $2\pi/q$. The total density (N/V) is 1.33 fm^{-3}. Notice that there is an inhomogeneous total spatial density.

IV. CONCLUSIONS

In the finite-fermion problem, the method commonly employed in order to tackle the Hartree-Fock equations is that developed by Roothaan.[15] We have in the present paper presented a natural extension of Roothaan's approach to the thermodynamic limit. A *definite prescription* is thus obtained in order to generate nontrivial (non-plane-wave) solutions to the HF equations in that limit, which should replace the *heuristic* approach usually followed in this connection.[1-5] Moreover, the orbitals generated with the techniques introduced here are HF solutions both for occupied and for (some, but the most important ones) empty states, which is not the case for the heuristic orbitals.

The power of the new approach has been illustrated by an application to neutron matter, in which the v_1 Bethe homework potential is employed. The results are much better, energy-wise, than those one obtains with the trivial, plane-wave HF solution.

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