Hartree-Fock Theory with Hard Cores

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Nonoverlapping orbitals make Hartree-Fock calculations possible in the presence of hard-core interactions. Such orbitals tend to be unfavorable to rotational invariance and to α clustering. They define a new type of collective motion, correlation vibration.

It is usually believed that Slater determinants cannot incorporate the correlations induced by the short-range repulsion which seems to occur in the bare nuclear interaction. This belief leads to an assumed failure of the Hartree-Fock (HF) theory and its replacement by the Brueckner, Levinson, and Mahmoud[1] or Jastrow[2] theories, or the regularization[3] theory, or the introduction of softer effective[4] interactions. It is shown here, however, that certain determinants are compatible with singular short-range repulsions.

For the sake of simplicity we assume the interaction $V(|\vec{r}_i-\vec{r}_j|)$, where $\vec{r}_i$ is the position of nucleon i, to be local, infinitely repulsive when $|\vec{r}_i-\vec{r}_j|<r_c$, and finite (and basically attractive) beyond that radius r_c, the hard-core radius. We now give a trivial example of a Slater determinant which generates a finite potential energy for that hard-core potential. We demand that each orbital φ_λ be confined with a domain $\mathfrak{D}_\lambda$ and the distance between any point of $\mathfrak{D}_\lambda$ and any point of $\mathfrak{D}_{\lambda'}$ $(\lambda\neq\lambda')$ be at least equal to r_c (see Fig. 1). Short-range exclusion is trivially satisfied by the determinant Φ made of such orbitals. Of course, ϕ_λ should have derivatives inside $\mathfrak{D}_\lambda$ and vanish at the boundary.

More specifically, the one-body density matrix corresponding to Φ is, as usual,

$$\rho(\vec{r},\vec{r}')\equiv\langle\Phi|\Psi^\dagger(\vec{r}')\Psi(\vec{r})|\Phi\rangle=\sum_{\lambda=1}^{N}\phi_\lambda(\vec{r})\phi_\lambda^*(\vec{r}'), \tag{1}$$

where Ψ, $\Psi^\dagger$ are the fermion field operators. The kinetic energy generated by the orbitals ϕ_λ is obviously finite. The potential energy is

$$\langle V\rangle=\tfrac{1}{2}\int d^3r\,d^3r'\,V(|\vec{r}-\vec{r}'|)[\rho(\vec{r},\vec{r})\rho(\vec{r}',\vec{r}')-|\rho(\vec{r},\vec{r}')|^2], \tag{2}$$

and it must be shown that the integrand vanishes when $|\vec{r}-\vec{r}'|<r_c$. From Eq. (1) and the confinement of ϕ_λ one finds that the only nonvanishing contributions to $\langle V\rangle$ occur when $\vec{r}$ is in a domain $\mathfrak{D}_\mu$ and $\vec{r}'$ is also in a domain $\mathfrak{D}_\nu$. [Indeed, if either $\vec{r}$ or $\vec{r}'$ (or both) were in one of the exclusion regions, we find from Eq. (1) that $\rho(\vec{r},\vec{r}')$ vanishes and that either $\rho(\vec{r},\vec{r})$ or $\rho(\vec{r}',\vec{r}')$ (or both) also vanishes.] It has been pointed out, furthermore, that the situation $|\vec{r}-\vec{r}'|<r_c$ can then occur only if $\mu=\nu$ (namely if $\mathfrak{D}_\mu$ and $\mathfrak{D}_\nu$ are the same). Then $\rho(\vec{r},\vec{r}')$ reduces to $\varphi_\mu(\vec{r})\phi_\mu^*(\vec{r}')$ in the domain $\mathfrak{D}_\mu$ and the two-body density matrix element which occurs in the right-hand side of Eq. (2) vanishes identically.

This kind of argument leads to the following generalization.

Theorem.—Let V be a two-body, local interaction, which contains a hard core. Let Φ be a N-particle Slater determinant compatible with a finite expectation value $\langle V\rangle$ and ρ the corresponding density matrix. Then the domain $\mathfrak{D}$ in which $\rho(\vec{r},\vec{r})$ differs from zero is disconnected and made of N distinct domains $\mathfrak{D}_\lambda$. The distance between two points in two different domains is at least equal to the hard-core radius. Exchange terms disappear from $\langle V\rangle$.

Proof.—Because of the hard core, it is necessary that

$$\rho(\vec{r},\vec{r})\rho(\vec{r}',\vec{r}')-|\rho(\vec{r},\vec{r}')|^2=0 \text{ if } |\vec{r}-\vec{r}'|<r_c, \tag{3}$$

in order to keep $\langle V\rangle$ finite, Eq. (2). From the very definition of ρ in terms of field operators, Eq. (1), an alternative form of Eq. (3) is

$$|\langle\Phi|\Psi^\dagger(\vec{r}')\Psi(\vec{r})|\Phi\rangle|=\|\Psi(\vec{r})|\Phi\rangle\|\,\|\Psi(\vec{r}')|\Phi\rangle\| \text{ if } |r-r'|<r_c, \tag{4}$$

where $\|\Psi(r)|\Phi\rangle\|$ is the length of the corresponding vector in Hilbert space. One recognizes a scalar product in the left-hand side of Eq. (4) and can take advantage of Schwartz inequality to deduce that, whenever $|\vec{r}-\vec{r}'|<r_c$, the two vectors $\Psi(\vec{r})|\Phi\rangle$ and $\Psi(\vec{r}')|\Phi\rangle$ are proportional. Let us choose $\vec{r}$ as a fixed point inside $\mathfrak{D}$, where by definition $\rho(\vec{r},\vec{r})$ is strictly positive, and define the normalized vector

$$|u(\vec{r})\rangle=[\rho(\vec{r},\vec{r})]^{-1/2}\Psi(\vec{r})|\Phi\rangle. \tag{5}$$

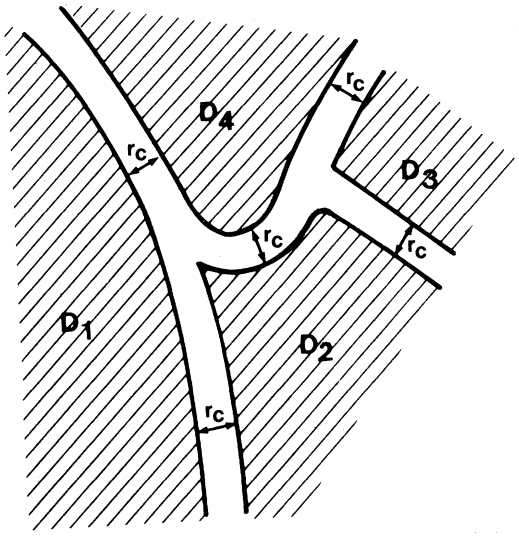

FIG. 1. A most general configuration of available domains. The picture is schematic and two dimensional, for the sake of simplicity. Notice that each domain is here not only connected but also simply connected. Because of nuclear attraction beyond the hard core, the self-consistent orbitals for these domains will likely be concentrated near the sharper borders. This configuration induces therefore a certain amount of compactness.

If $\mathfrak{D}$ is connected, any point $\vec{r}'$ inside $\mathfrak{D}$ can be reached by a certain number of steps (starting from $\vec{r}$) of length smaller than r_c and remaining inside $\mathfrak{D}$. There exists therefore a function $\sigma(\vec{r}')$ such that

$$\Psi(r')|\Phi\rangle = \sigma(\vec{r}')|u(\vec{r})\rangle . \tag{6}$$

This function vanishes nowhere inside $\mathfrak{D}$. One may ask whether its phase may depend on the path generated by the steps. But the modulus $|\sigma(\vec{r}')|$ is well defined, for

$$\rho(\vec{r}', \vec{r}') = |\sigma(\vec{r}')|^2 . \tag{7}$$

From Eq. (7) one then derives

$$\rho(\vec{r}', \vec{r}'') = \sigma(\vec{r}')\sigma^*(\vec{r}'') , \tag{8}$$

a kernel of rank 1. Whenever $N>1$, we know from Eq. (1) that ρ is of rank N, which gives a contradiction. Therefore $\mathfrak{D}$ cannot be connected.

If $\mathfrak{D}$ splits into two separate domains $\mathfrak{D}_1$ and $\mathfrak{D}_2$, the same argument based on Eq. (4) and Schwartz inequality yields

$$\Psi(\vec{r}')|\Phi\rangle = \sigma_1(\vec{r}')|u(\vec{r}_1)\rangle \text{ if } \vec{r}' \in \mathfrak{D}_1 , \tag{9a}$$

$$\Psi(\vec{r}')|\Phi\rangle = \sigma_2(\vec{r}')|u(\vec{r}_2)\rangle \text{ if } \vec{r}' \in \mathfrak{D}_2 , \tag{9b}$$

where $\vec{r}_1$ and $\vec{r}_2$ are two fixed points inside $\mathfrak{D}_1$ and $\mathfrak{D}_2$, respectively. There must be no way to go from $\mathfrak{D}_1$ to $\mathfrak{D}_2$ by a step of length smaller than r_c if $|u(\vec{r}_1)\rangle$ and $|u(\vec{r}_2)\rangle$ are required to be independent vectors. Under that condition of independence, it is possible to define $\sigma_1(\vec{r}')$ as a vanishing function out of $\mathfrak{D}_1$, to extend σ_2 out of $\mathfrak{D}_2$ in the same way, and to obtain finally

$$\rho(\vec{r}', \vec{r}'') = \sigma_1(\vec{r}')\sigma_1^*(\vec{r}'') + \sigma_2(\vec{r}')\sigma_2^*(\vec{r}'') , \tag{10}$$

the rank of which is compatible with $N=2$. The generalization to $N>2$ is obvious. It is then trivial to identify $\sigma_\lambda(\vec{r}')$ with an orbital $\phi_\lambda(\vec{r}')$. This orbital can be normalized, and it is strictly confined inside the domain $\mathfrak{D}_\lambda$. Linear independence of orbtials is guaranteed by the fact that the domains must be separated from each other by at least r_c. Finally, since exchange terms involve products $\phi_\lambda(\vec{r})\phi_\mu(\vec{r})$ with $\lambda \neq \mu$, they identically vanish. It follows that the Hartree-Fock theory reduces here to the Hartree theory.

One then obtains a doubly variational procedure, namely (i) given a set of domains $\mathfrak{D}_\lambda$, find the orbitals ϕ_λ which generate the lowest energy for Φ, and (ii) find the domains $\mathfrak{D}_\lambda$ which minimize that lowest energy. This variational procedure can be carried in the following way:

(i) For fixed domains $\mathfrak{D}_\lambda$, the variational procedure gives the Hartree equations

$$-\frac{\hbar^2}{2m}\nabla^2\phi_\lambda(\vec{r}) + U_\lambda(\vec{r})\phi_\lambda(\vec{r}) = e_\lambda\phi_\lambda(\vec{r}) , \tag{11}$$

where

$$U_\lambda(\vec{r}) = \sum_{\mu\neq\lambda}\int d^3r' v(\vec{r}-\vec{r}')|\phi_\mu(\vec{r}')|^2 . \tag{12}$$

The distance between two domains being greater than r_c guarantees that the potential $U_\lambda(\vec{r})$ is finite in $\mathfrak{D}_\lambda$.

Furthermore, for self-consistency, it is needed that at each point outside the domain $\mathfrak{D}_\lambda$, where indeed the wave function ϕ_λ vanishes, the potential $U_\lambda(\vec{r})$ be infinite positive. This constraint is easily achieved by choosing the domains $\mathfrak{D}_\lambda$ in such a way that each point of the surface S_λ of $\mathfrak{D}_\lambda$ is at a distance r_c from the surface S_μ of another domain $\mathfrak{D}_\mu$ (see Fig. 1).

When such a choice of domains has been made, the Hartree equations can be solved, as usual, by iteration, and the diagonalization of the Hartree Hamiltonians provides a complete set of orthonormal wave functions in each domain $\mathfrak{D}_\lambda$. This leads to the possibility of particle-hole excitations, as in usual HF theory.

Although we have thus shown that a Hartree-Fock theory is still possible in the presence of hard cores, it is not obvious that it makes sense,

namely that one gets a bound state. The numerical example which follows gives such evidence.

(ii) This first problem having been solved in fixed domains $\mathfrak{D}_\lambda$, the Hartree wave functions φ_λ, as well as the single-particle energies e_λ, become functionals of all the domains $\mathfrak{D}_\lambda$. It should be possible, by a minimization of the total energy with respect to the shape of the domains, to obtain equations for the domains themselves.

Investigations are actually carried out in order to obtain such equations. Symmetry as well as hydrodynamical considerations may be crucial in order to solve this problem; in particular, the consideration of surface energies, which appear as a special feature of such confined single-particle wave functions, should be very important in order to minimize the total energy (like in the search of junctions between soap films).

A very simple example has been studied, in a very restrained class of wave functions. We have studied the case of four particles, in a two-dimensional space, interacting through a two-body potential $v(r_{ij})$:

$$v(r_{ij}) = \begin{cases} +\infty, & r_{ij} < r_c, \\ -V_0, & r_c < r_{ij} < r_0, \\ 0, & r_0 < r_{ij}, \end{cases}$$

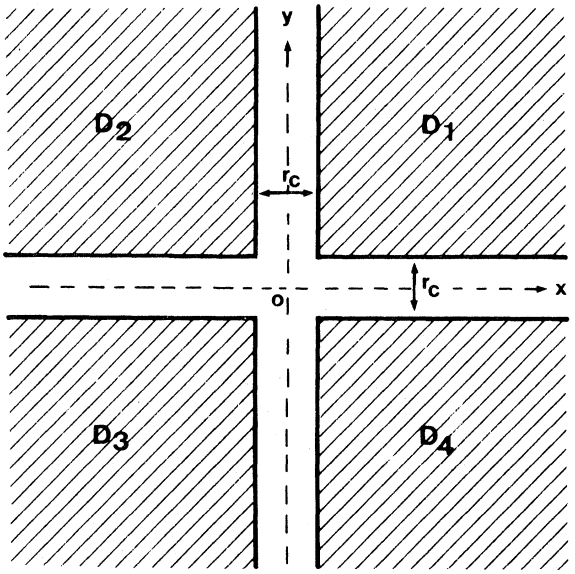

FIG. 2. The configuration retained for the numerial example, two-dimensional ^{4}He. Actually the trial orbitals used in that example depend only on two parameters, the shift and width of the Gaussian from which these trial orbials are generated.

where we have chosen the numerical values

$$V_0 = 40 \text{ MeV}, \quad r_c = 0.7 \text{ fm}, \quad r_0 = 1.7 \text{ fm}.$$

The trial wave functions are ($i = 1, 2, 3, 4$)

$$\phi_i(b, \sigma; x, y) = \left[\frac{1}{2\pi\sigma^2}\right]^{1/2} (x - \tfrac{1}{2}\epsilon_i r_c)(y - \tfrac{1}{2}\eta_i r_c) \times \exp\left[-\frac{(x - \epsilon_i b)^2 + (y - \eta_i b)^2}{4\sigma^2}\right],$$

where b and σ are two variational parameters. The parameters ϵ_i and η_i are

$$\epsilon_1 = \eta_1 = -\epsilon_2 = \eta_2 = -\epsilon_3 = -\eta_3 = \epsilon_4 = -\eta_4 = 1,$$

and the domains $\mathfrak{D}_1, \mathfrak{D}_2, \mathfrak{D}_3, \mathfrak{D}_4$ where the wave functions $\phi_1, \phi_2, \phi_3, \phi_4$ are nonvanishing are shown in Fig. 2.

The aim of such a very simple calculation is to show that it is possible to find indeed a negative energy for the minimizing determinant. Table I shows the energy behavior as a function of b and σ. An approximate minimum is obtained for $\sigma = 2.2$ fm and $b = 0.09$ fm, and gives an energy $E_{\min} = -1.3$ MeV. This is not a large amount of binding, but of course the class of trial functions was quite small. What is nevertheless important is that we actually get binding.

We have shown that, in the case of a two-body interaction with a repulsive hard core, it is possible to construct Slater determinants giving rise to finite total energy. Such Slater determinants can be constructed by a doubly variational procedure, with respect to the wave functions and to the domains. The salient features of such determinants are the following.

(i) They break translational invariance and, in order to favor close packing, also tend to break rotational invariance. Such symmetries could, however, be restored by appropriate linear combinations of degenerate Slater determinants obtained under translation and rotation, and this procedure would therefore wash out the zero-density regions inherent in these Slater determinants.

TABLE I. Total binding energy (in MeV) as a function of b (in fm) and σ (in fm).

σ \ b	0.	0.08	0.09	0.1	0.2
2.0	8.26	3.02	2.44	2.27	−0.22
2.1	4.70	−0.65	−0.74	−0.83	−1.25
2.2	−1.13	−1.28	−1.30	−1.28	−1.17
2.3	−1.02	−1.11	−1.09	−1.07	−0.88

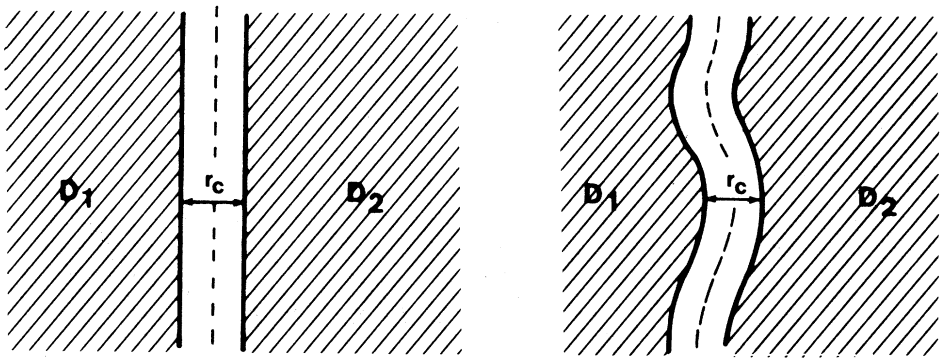

FIG. 3. Elementary deformation of two neighboring domains. If there exists coherence between similar deformation propagating through all domains, this coherence would define "correlation vibrations."

(2) Among possible configurations, crystalline or glass structure can be expected (the idea is not new), but we want to emphasize again that many other types of configurations are allowed, and that the minimizing configuration should be obtained by a variational procedure.

(3) Nonoverlapping orbitals are obviously unfavorable to space-symmetric α clustering, since there is only one orbital in each domain. Some clustering might be reinstated by configuration mixing under spin and isospin exchanges between domains and under angular momentum projection.

(4) The study of the system around the minimizing configuration should exhibit new modes of collective excitations, namely vibrations of the surfaces of the domains. These modes could be called correlation vibrations, because they propagate through the constraints imposed on the domains, which are to be at a distance exactly equal to r_c from each other (Fig. 3).

(5) Hard-core radii can be used as generator coordinates in this theory (i) to take into account defects of charge invariance or symmetries, (ii) to lower the energy, and (iii) to solve for singular repulsions softer than hard cores.

It is straightforward to generalize all these considerations to time-dependent Hartree-Fock theory.

While this work was being completed we have been informed that similar ideas have been developed by B. Grammaticos and D. Vautherin. It is a pleasure to thank them for sending results of their Hartree-Fock calculation of crystalline nuclear matter in presence of a hard core.

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