

Self-consistent pseudopotentials in the thermodynamic limit.

I. The correlation field

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The repulsive hard core of a pair-wise interaction acting between fermions is simulated by a constraint to be included in the variational principle. The Euler-Lagrange equations are usual Hartree-Fock equations with a self-consistent one-body pseudopotential. It can be seen that the imposed constraint generates a correlation field in addition to the regular portion of the two-body interaction. The origin of density waves in coordinate space is discussed in terms of the hard-core correlations.

[NUCLEAR STRUCTURE hard-core potentials, constrained Hartree-Fock, correlation field, pseudopotential; localized single-particle orbitals in nuclear matter.]

I. INTRODUCTION

It is usually believed that correlations induced by two-body interactions characterized by the presence of a hard core cannot be handled within the framework of the Hartree-Fock (HF) formalism. This assumed failure of the HF theory has led to the development of powerful methods that are able to deal with the strong short-range repulsion of the nuclear force (see Refs. 1-3 and references cited therein).

However, de Llano and Ramirez⁴ have shown that in the limit of infinitely repulsive potentials between pairs of particles, there exists for both fermions and bosons a periodic density HF solution. Although they did not give an explicit form for such solution, they showed that a Slater determinant of spatially localized, nonoverlapping, single-particle (sp) functions yields a noncollapsing ground state. More recently, Giraud and Orland⁵ have demonstrated that nonoverlapping orbitals make HF calculations possible in the presence of hard-core interactions. New HF solutions thus arise that break translational invariance and favor close packing. Crystalline or glass structures are then to be expected, an idea pioneered by Overhauser,⁶ which has received considerable attention.⁷⁻¹¹

A different approach to the hard-core problem is that of the pseudopotential method, which has proved to be an important tool to investigate the thermodynamic behavior of gases.¹²⁻¹⁶ In particular, this technique has been applied to the hard-sphere dilute gases¹⁷⁻²⁰ with special success in the case of the bosonic hard-sphere gas with

attractive interactions (see Ref. 21 for a survey).

The essence of the pseudopotential method resides in the replacement of the hard-core interaction by a figured potential that guarantees cancellation of the wave function at the hard-core radius. The idea is similar to that underlying the image method in electrostatic potential theories.

It may be of interest to relate the method of construction of a pseudopotential to the variational principle, in order to attempt a connection with the HF theory, and thus shed light on particular aspects of those HF orbitals that arise in the presence of a hard-core potential. In the present work, we show that the effect of the strong repulsion in the actual two-body force can be included as a constraint into the variational principle. This constraint forces the wave function to vanish at the hard-core radius. We derive the Euler-Lagrange equations for a one-dimensional system and show that they are of the Hartree-Fock type, but with a modified one-body field, the pseudopotential. The extra term in this field, which originates in the constraint, provides complementary correlations in momentum and coordinate space, and allows us to suggest a possible explanation for the origin of those density waves whose existence has been conjectured in nuclear matter.⁶⁻¹¹

In Secs. II to VI we present the theory and discuss the equations and their solutions. The conclusions are summarized in Sec. VII.

II. THE MODEL

We consider a system of N fermions enclosed in a (one-dimensional) container of volume L in

the thermodynamic limit, i.e., $N \rightarrow \infty$, $L \rightarrow \infty$,

$$\lim_{\substack{N \rightarrow \infty \\ L \rightarrow \infty}} N/L = \rho_0 = \text{finite.}$$

This system is acted upon by a hard-core pair-wise potential; let b , c be its range and hard-core radius, respectively. We shall find it useful to introduce the correlation function of the system²² as

$$G(1,2) = \frac{1}{\rho_0^2} \sum_{\lambda, \mu=1}^{N=\infty} |\psi_{\lambda\mu}(1,2)|^2, \quad (1)$$

where $\psi_{\lambda\mu}(1,2)$ is the antisymmetrized two-particle wave function. Hereafter, we shall consider $\psi_{\lambda\mu}$ to be purely spatial, in order to bypass cumbersome algebra which does not enlighten the main points to be discussed. The symmetrical spin functions contribute a degeneracy factor ρ_0 . Accordingly,

$$\psi_{\lambda\mu}(1,2) = \frac{1}{\sqrt{2}} [\psi_{\lambda}(1)\psi_{\mu}(2) - \psi_{\lambda}(2)\psi_{\mu}(1)]. \quad (2)$$

If we express $\psi_{\lambda\mu}(1,2)$ and $G(1,2)$ in the center-of-mass system of particles 1 and 2, and integrate over the center-of-mass coordinate X_{12} , we obtain a one-body correlation function, namely

$$g(x_{12}) = \int_{-\infty}^{\infty} dX_{12} G(1,2). \quad (3)$$

The presence of the hard core in the potential causes $g(x_{12})$ to vanish at $x_{12} = c$. Our proposal is to include the boundary condition

$$g(c) = 0 \quad (4)$$

as a constraint in the variational principle through a Lagrange multiplier, α .²³ The two-body force in the Hamiltonian will be taken as the analytical continuation of the original one for $x \leq c$. For instance, if the two-body interaction were a square well hard-core potential,

$$V(x) = \begin{cases} 0, & |x| > b \\ -V_0, & c < |x| < b \\ \infty, & |x| < c \end{cases} \quad (5)$$

we should consider the analytical continuation

$$V(x) = \begin{cases} 0, & |x| > b \\ -V_0, & |x| < b \end{cases} \quad (6)$$

i.e., a regular square well. Let us show how it works and derive the modified Euler-Lagrange equation for the system.

III. THE EULER-LAGRANGE EQUATIONS

We assume that we can perform a Fourier analysis of the sp wave functions $\psi_{\lambda}(x)$,

$$\psi_{\lambda}(x) = \frac{1}{\sqrt{2\pi}} \int dk C_{\lambda}(k) e^{ikx}, \quad (7)$$

and that the correlated ground state $|\phi_c\rangle$ is a normalized Slater determinant of these orbitals. The constrained variational principle then reads

$$\delta \left(\langle \phi_c | H_0 | \phi_c \rangle - \alpha g(c) - \sum_{\lambda\mu} \epsilon_{\lambda\mu} \langle \lambda | \mu \rangle \right) = \delta f(C_{\lambda}) = 0. \quad (8)$$

The third term within the parentheses enforces orthonormality of the sp states.²³ The general form of the Hamiltonian in momentum representation is

$$H_0 = \int dk t(k) a_k^{\dagger} a_k + \frac{1}{4} \int \int \int \int dk_1 dk_2 dk_3 dk_4 V(k_1, k_2, k_3, k_4) \times a_{k_1}^{\dagger} a_{k_2}^{\dagger} a_{k_3} a_{k_4}, \quad (9)$$

where a_k^{\dagger} creates a plane wave state on the sp vacuum,

$$a_k^{\dagger} |0\rangle = |k\rangle, \quad \langle x | k \rangle = \frac{1}{\sqrt{2\pi}} e^{ikx}. \quad (10)$$

We introduce the one-body density matrix

$$\rho(k_2, k_1) = \langle \phi_c | a_{k_1}^{\dagger} a_{k_2} | \phi_c \rangle \quad (11)$$

through which Eq. (8) can be written as

$$\delta f(C_{\eta}) = \delta \left(\text{Tr} \rho \left(t + \frac{1}{2} \Gamma_1 \right) - \alpha g(c) - \sum_{\lambda} \epsilon_{\lambda} \int dk |C_{\eta}(k)|^2 \right) = 0 \quad (12)$$

with the self-consistent one-body potential

$$\Gamma_1(k_1, k_2) = \int \int dk_3 dk_4 V(k_1, k_3, k_2, k_4) \rho(k_4, k_3). \quad (13)$$

The detailed form of ρ is

$$\rho(k_2, k_1) = \sum_{\lambda \leq F} C_{\lambda}^*(k_1) C_{\lambda}(k_2), \quad (14)$$

where F is the self-consistent Fermi label, i.e., it denotes the last occupied sp level in the Fermi sea.

Now we obtain a set of Euler-Lagrange equations for our system performing the derivatives $\partial f(C_{\eta}) / \partial C_{\eta}^*(k_1)$. It is easy to find the overall appearance of the result,

$$\int dk_1 [t(k_1, q) \delta(k_1 - k_2) + \Gamma_1(k_1, k_2)] C_{\eta}(k_1) - \frac{\alpha \partial g(c)}{\partial C_{\eta}^*(k_2)} = \epsilon_{\eta} C_{\eta}(k_2). \quad (15)$$

IV. THE PSEUDOPOTENTIAL

We shall show that the extra term in Eq. (15) generates a one-body potential $\Gamma_2(k_1, k_2)$. Inclusion of this potential under the integral sign leaves us with the well-known set of integral equations, known as Hartree-Fock equations²³⁻²⁵

$$\int dk_1 [t(k_1, k_2)\delta(k_1 - k_2) + \Gamma(k_1, k_2)]C_\eta(k_1) = \epsilon_\eta C_\eta(k_2), \quad (16)$$

where

$$\Gamma(k_1, k_2) = \Gamma_1(k_1, k_2) + \Gamma_2(k_1, k_2) \quad (17)$$

will be referred to as the (self-consistent) pseudopotential. We can think of the new one-body field Γ_2 as one created by a set of "image sources," following an electrostatic analogy,¹⁶ as needed to guarantee vanishing of the correlated wave func-

tion on the hard-core edge.

Notice that we are actually replacing the "true" hard-core condition

$$g(c) = 0 \text{ if } |x| \leq c \quad (18)$$

by the much looser statement (4) in which we force the relative wave function to exhibit a node at the given position. In a real calculation, we could obtain the correlation function g out of the solutions of (16) and simply drop that portion that lies inside the hard core. The outer portion will still be a reliable representation of the problem, since it is provided by the variational principle. The most important point to be stressed here is that interesting properties of the pseudopotential and the sp density can be discussed, which we can expect not to be substantially altered by substitution of (18) instead of (4).

V. EVALUATION OF THE PSEUDOPOTENTIAL

This is straightforward. We use Eqs. (2), (5), and (7) and integrate away the center-of-mass coordinate x , obtaining

$$|\psi_{\lambda\mu}(c)|^2 = \int \int \int \int dk_1 dk_2 dk_3 dk_4 C_\lambda(k_1) C_\lambda^*(k_2) C_\mu(k_3) C_\mu^*(k_4) \delta(k_1 + k_3 - k_2 - k_4) 2 \sin\left(\frac{k_1 - k_3}{2}\right) c \sin\left(\frac{k_2 - k_4}{2}\right) c. \quad (19)$$

Then

$$g(c) = \int \int \int \int dk_1 dk_2 dk_3 dk_4 \rho(k_2, k_1) \chi'(k_1, k_2, k_3, k_4) \rho(k_4, k_3), \quad (20)$$

where

$$\chi'(k_1, k_2, k_3, k_4) = \frac{2}{\rho_0^2} \delta(k_1 + k_2 - k_3 - k_4) \sin\left(\frac{k_1 - k_3}{2}\right) c \sin\left(\frac{k_2 - k_4}{2}\right) c. \quad (21)$$

It can be seen by inspection that χ' possesses the following symmetries:

$$\begin{aligned} \chi'(k_1, k_2, k_3, k_4) &= -\chi'(k_3, k_2, k_1, k_4) \\ &= -\chi'(k_1, k_4, k_3, k_2) \\ &= \chi'(k_3, k_4, k_1, k_2) \\ &= \chi'(k_2, k_1, k_4, k_3). \end{aligned} \quad (22)$$

Now if we define a one-body entity Γ_2 ,

$$\begin{aligned} \Gamma_2(k_1, k_2) &= -2\alpha \int \int dk_3 dk_4 \chi'(k_1, k_2, k_3, k_4) \\ &\quad \times \rho(k_4, k_3), \end{aligned} \quad (23)$$

and use Eq. (20) we can see that the boundary condition reads

$$\text{Tr}(\Gamma_2 \rho) = 0, \quad (24)$$

i.e.,

$$\langle \Gamma_2 \rangle_c = 0, \quad (25)$$

where the expectation value is taken with respect to the correlated g.s. $|\phi_c\rangle$. In addition, we see that the corrected Hamiltonian, $\langle H_0 \rangle - \alpha g(c)$, now reads

$$\langle H \rangle = \text{Tr} \rho (t + \frac{1}{2} \Gamma_1 + \frac{1}{2} \Gamma_2). \quad (26)$$

Γ_2 represents then the one-body potential that reflects the existence of the hard core in the real system; its fictitious nature is expressed in the fact that it vanishes in the average, as displayed by Eq. (23). (It means it does not contribute to the macroscopic or internal energy of the system, or to its equation of state.)

VI. PROPERTIES OF THE CORRELATION FIELD

We can learn more about the correlation potential Γ_2 by studying Eq. (21). If we let

$$\chi = -2\alpha\chi' \quad (27)$$

we get

$$\Gamma_2(k_1, k_2) = \int \int dk_3 dk_4 \chi(k_1, k_2, k_3, k_4) \rho(k_4, k_3). \quad (28)$$

Comparing this structure with that of Γ_1 given in Eq. (13), we see that Γ_2 looks like a typical correlation field similar to the pairing field in superconductivity.²⁶ In this case, the two-particle force originating this field is the one whose matrix elements in momentum space are $\chi(k_1, k_2, k_3, k_4)$, which in turn are entirely induced by the boundary condition.

Another way of looking at $\Gamma_2(k_1, k_2)$ may be depicted as follows. We can write Eq. (28) as

$$\begin{aligned} \Gamma_2(k_1, k_2) &= \text{Tr}[\chi_{\text{op}}(k_1, k_2)\rho] \\ &= \langle \chi_{\text{op}}(k_1, k_2) \rangle_c \end{aligned} \quad (29)$$

where $\chi_{\text{op}}(k_1, k_2)$ is an operator in sp momentum space, parametrized by the values of k_1, k_2 . In fact, the form of this operator is

$$\begin{aligned} \chi_{\text{op}}(k_1, k_2) &= -\frac{4}{\rho_0^2} \delta(k_1 + \vec{k} - k_2 - \vec{k}) \\ &\quad \times \sin\left(\frac{k_1 - \vec{k}}{2}\right)_c \sin\left(\frac{k_2 - \vec{k}}{2}\right)_c, \end{aligned} \quad (30)$$

the arrows pointing at the direction in which the momentum operator acts. It can be easily checked that

$$\langle k_3 | \chi_{\text{op}}(k_1, k_2) | k_4 \rangle = \chi(k_1, k_2, k_3, k_4). \quad (31)$$

Notice that $\chi_{\text{op}}(k_1, k_2)$ is non-Hermitian, in agreement with our previous knowledge of pseudopotentials.¹⁶⁻²¹ It satisfies the symmetry relation in the parameters

$$\chi_{\text{op}}^\dagger(k_1, k_2) = \chi(k_2, k_1), \quad (32)$$

which ensures symmetry in Γ_2 ,

$$\Gamma_2(k_1, k_2) = \Gamma_2(k_2, k_1). \quad (33)$$

Expression (30) displays the nature of the correlation field and its role in the many-body system. We can see that $\chi_{\text{op}}(k_1, k_2)$ creates correlations in momentum space. On the other hand, it can be verified that the most familiar set of Hartree-Fock solutions, namely the plane waves, do not satisfy the modified Euler-Lagrange Eq. (16). In fact, they are not even zero-order approximations, since $\Gamma_2(k_1, k_2)$ will diverge if attempted to be evaluated with a plane wave density. Now a characteristic of plane waves is its localization in momentum space. The oscillating inhomogeneities created by the momentum operators in $\chi_{\text{op}}(k_1, k_2)$ will destroy that localization, giving rise to sub-

sequent confinement in configuration space. (Actually, the correlations are provided by the sin operators. The δ operator is only in charge of securing a selection rule, i.e., conservation of total momentum.) We could thus argue that this may be interpreted as a justification for the widespread use of Overhauser-type orbitals in nuclear matter calculations.⁴⁻¹¹ Furthermore, we may suggest an explanation of the origin of the so-called "density waves" in Fermi systems in the thermodynamic limit. The present investigation shows that waves in the local density are associated with the way in which the correlation function has to bend in order to reach a node at a relative distance equal to the hard-core radius.

Further properties of the correlation field arise from the following observations. The self-consistent one-body potential Γ_1 can be expressed in a formal analogy with Γ_2 , as

$$\begin{aligned} \Gamma_1(k_1, k_2) &= \text{Tr}[V_{\text{op}}(k_1, k_2)\rho] \\ &= \langle V_{\text{op}}(k_1, k_2) \rangle_c \end{aligned} \quad (34)$$

with

$$\begin{aligned} V_{\text{op}}(k_1, k_2) &= \delta(k_1 + \vec{k} - k_2 - \vec{k}) \\ &\quad \times \left[v\left(\frac{k_1 - \vec{k} - k_2 + \vec{k}}{2}\right) - v\left(\frac{k_1 - \vec{k} + k_2 - \vec{k}}{2}\right) \right] \end{aligned} \quad (35)$$

$v(k)$ is the Fourier transform of the two-body force $V(x)$ with respect to the transferred momentum between the scattering sp states; the double term in (35) is due to antisymmetrization. We can rewrite χ_{op} in a similar fashion,

$$\begin{aligned} \chi_{\text{op}}(k_1, k_2) &= -\frac{2}{\rho_0^2} \delta(k_1 + \vec{k} - k_2 - \vec{k}) \\ &\quad \times \left[\cos\left(\frac{k_1 - \vec{k} - k_2 + \vec{k}}{2}\right)_c \right. \\ &\quad \left. - \cos\left(\frac{k_1 - \vec{k} + k_2 - \vec{k}}{2}\right)_c \right], \end{aligned} \quad (36)$$

and we can interpret the first and second terms in (36) as Fourier transforms of "direct" and "exchange" fields, respectively.

Now if we consider the two-body model potential given by (6), we find

$$v(\kappa) \sim \frac{\sin \kappa b}{\kappa}, \quad (37)$$

which, in addition to representing a damped oscillation, is out of phase with respect to the correlation field (36). The phase shift between $\Gamma_1(k_1, k_2)$ and $\Gamma_2(k_1, k_2)$ will cause the momentum space to deform itself into unlocalized one-body densities in order to fulfill the variational principle.

On the other hand, if we consider the "direct"

matrix element

$$\chi^D(k_1, k_2, k_3, k_4) \sim \cos kc \quad (38)$$

through Fourier antitransforming we obtain the spatial representation for the correlation potential

$$\chi(x) \sim \delta(x+c) + \delta(x-c), \quad (39)$$

whose functional dependence on the relative coordinate agrees with the one-dimensional version of former pseudopotentials.^{16,20,27} The whole procedure is then equivalent to that of substituting the original hard core by a pair of transparent, although infinite, walls at $x = \pm c$.

As a final remark, we point out that the separable nature of the correlation field (30) implies that the one-body density has to be nonlocal in momentum space, in the sense that it cannot depend only on the transferred momentum. In fact, if $\rho(k_4, k_3) = f(k_4 - k_3)$, we have

$$\begin{aligned} \Gamma(k_1, k_2) &\sim f(k_1 - k_2) \int dk_3 \sin\left(\frac{k_1 - k_3}{2}\right) c \\ &\quad \times \sin\left(\frac{k_1 + k_3}{2} - k_2\right) c \\ &\sim \int dk_3 [e^{i(k_1 - k_3)c/2} - e^{-i(k_1 - k_3)c/2}] \\ &\quad \times [e^{i(k_1 + k_3/2 - k_2)c} - e^{-i(k_1 + k_3/2 - k_2)c}]. \quad (40) \end{aligned}$$

The integral in (40) is divergent. It means that a finite Γ_2 is necessarily caused by a nonlocal ρ . We could thus say ρ is "unlocalized and nonlocal" in momentum space.

VII. SUMMARY AND CONCLUSIONS

We have shown that substitution of the hard-core part of the actual two-body interaction in a Fermi system, according to the pseudopotential model philosophy, leads to Hartree-Fock type of equations. The one-body field thus appearing is modified by an extra term which can be interpreted as provided in a self-consistent fashion by a two-particle correlation field. This field destroys translational invariance through the creation of momentum correlations. Accordingly, the solutions of the modified Hartree-Fock problem are expected to be localized in coordinate space. In this way, the real hard-core potential is represented by the correlation field; and causes "solid-like" sp orbitals to be expected as solutions of this problem.

We feel that the arguments presented in this work encourage further work on the subject. The general discussion applies equally well to one-dimensional boson systems and the extension to three dimensions is straightforward, although laborious. A numerical procedure to solve the integral equations is in progress and the results will be published elsewhere.

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