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Short Communication

Pair wave functions for strongly correlated fermions and their determinantal representation

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Résumé.— Nous montrons que l'amplitude de toute fonction BCS à nombre de particules fixé est un déterminant. Ceci à une importance numérique considérable et permet une approche variationnelle de ces fonctions, appliquée à l'hélium-3 liquide ou au modèle de Hubbard. Nous proposons d'autre part un nouveau type de fonction d'onde, décrivant un état *mixte* composé de fermions appariés et célibataires. Les propriétés physiques de cet état sont suggérées.

Abstract.— We show that a (Jastrow projected or not) BCS wave function with any fixed number of fermions can be represented as a determinant. This is important for their numerical investigation, with applications to liquid He³ and Hubbard's model. We also propose a new type of wave function, describing a *mixed* state composed of paired and unpaired fermions. The physical properties of such a state are tentatively discussed.

1. Introduction.

Most approaches to N -fermion systems are based on an antisymmetrical wave function (w-f) made of *individual orbitals* arranged in a Slater determinant : this is the case of e.g. the shell model in atomic and nuclear physics, the Gutzwiller w-f for Hubbard's model, the Jastrow-Slater function for He³, etc. Usually, one further assumes *weak coupling* or Landau's

adiabaticity ansatz for Fermi liquids and chooses as individual orbitals the three fermion orbitals (or some distorted versions of them to improve variational calculations). However, a notorious counter-example of *non-Slater* fermionic w-f is given by the B.C.S. theory of superconductivity which takes as basic entities *pair wave functions* and build with them a correctly antisymmetrized state. Those pair correlations handle

the *attractive interaction* between fermions more efficiently.

Until recently, one only considered B.C.S. wave functions which differed only *weakly* from plane-wave Slater determinants : all the action usually takes place within a thin energy shell ($\sim T_c/E_f$) around the Fermi-surface.

However, for *strongly* interacting fermionic systems, one should *a priori* exploit the full variational character of the B.C.S. wave functions and let the momentum distribution $N(k)$ adopt its optimal shape, which may be quite far from the usual Heavyside step and in fact may not satisfy perturbative requirements such as the Migdal-Luttinger theorem imposing a discontinuity of $N(k)$ at $k_F^0 = (3\pi^2\rho)^{1/3}$.

This possibility has recently been independently suggested for high T_c superconductors [2] and for liquid He³ [3], leading to a *new* description of the normal state as a non superfluid, strongly paired liquid, for which the superfluid transition and the pairing correlations are characterized by two very different energy scales : it is quite possible to have strong pair correlations while off-diagonal long range order or phase rigidity cannot establish due e.g. to

the importance of hard cores heavily suppressing density fluctuations [2]. In order to test this idea, numerical approaches (such as variational calculations) are vital, and some encouraging results have been obtained on the singlet RVB pair w-f (for Hubbard's model) [4, 5] and on the triplet Jastrow-BCS w-f for liquid He³ [3]. Those numerical approaches are nevertheless *a priori* difficult, because of the $N!$ terms present in these antisymmetrized pairs w-f. The aim of this note is to show that all BCS type w-f (including RVB or Jastrow-projected BCS) can be given a determinantal representation. This allows numerical calculations as easily as for Slater-type w-f and could also help to make some analytical progress on e.g. Nagaoka-Brinkmann-Rice bandwidth calculations [6, 7, 8].

In a second part, which is more speculative, we propose to generalize the B.C.S. w-f to describe a *mixed-state* where some fermions are paired and the remaining fraction left in individual orbitals, while preserving *global antisymmetry*. This w-f can be given a determinantal representation as well. We briefly speculate on the physics of such a state, which perhaps gives some variational content to the *Heavy-Boson* model proposed by Ranninger *et al.* [9] to describe heavy fermions and He³.

2. The fixed number of particles B.C.S. function.

One usually write the B.C.S. w-f in a grand canonical ensemble representation, for which the number of particles is not kept fixed. For the usual singlet states, one has (see e.g. [10])

$$\Psi_{\text{BCS}} = \prod_k (u_k + v_k a_{k\uparrow}^+ a_{-k\downarrow}^+) |O\rangle = e^{\sum_k \varphi_k a_{k\uparrow}^+ a_{-k\downarrow}^+} |O\rangle \quad (2.1)$$

with $\varphi_k = \frac{v_k}{u_k}$

Projecting on the state with exactly N particles yields ($P = N/2$ being the number of pairs)
(¹):

$$\Psi_{\text{BCS}}^N = \left(\sum_k \varphi_k a_{k\uparrow}^+ a_{-k\downarrow}^+ \right)^P |O\rangle = \sum_{k_1 \dots k_p} \varphi_{k_1} \dots \varphi_{k_p} a_{k_1\uparrow}^+ \dots a_{k_p\downarrow}^+ a_{-k_{11}\downarrow}^+ \dots a_{-k_{p1}\downarrow}^+ |O\rangle \quad (2.2)$$

The free gas Slater-determinant is simply obtained by setting $\varphi_k = 1$ if $k < k_f$ and $\varphi_k = 0$ otherwise.

The real space representation of this paired w-f is obtained -by a Fourier transform of (2.2) as :

$$\Psi_{\text{BCS}}^N (\mathbf{r}_1 \dots \mathbf{r}_N) = \mathcal{A} [\tilde{\varphi}(12)\tilde{\varphi}(34)\tilde{\varphi}(56)\dots] \quad (2.3)$$

where \mathcal{A} stands for the total antissymmetrizer and $\tilde{\varphi}$ is an odd spin-orbital w-f, which reads, in the singlet state :

(¹) In all that follows, we deliberately omit overall phase factors and normalizations, which are of no interest for our purpose.

$$\tilde{\varphi}(12) = \frac{1}{\sqrt{2}} \varphi(\mathbf{r}_1 - \mathbf{r}_2) | 1\uparrow 2\downarrow -1\downarrow 2\uparrow \rangle \quad (2.4)$$

in which $\varphi(\mathbf{r})$ is the even orbital function, simply related to φ_k by a Fourier transform.

The triplet states can also be represented by (2.3), with :

– for $M_S = 0$

$$\begin{aligned} \tilde{\varphi}(12) &= \frac{1}{\sqrt{2}} \varphi(\mathbf{r}_1 - \mathbf{r}_2) | 1\uparrow 2\downarrow +1\downarrow 2\uparrow \rangle \\ &\varphi(\mathbf{r}) \text{ odd} \end{aligned} \quad (2.5)$$

– and for $M_S = \pm 1$

$$\begin{aligned} \tilde{\varphi}(12) &= \varphi(\mathbf{r}_1 - \mathbf{r}_2) | 1\uparrow 2\uparrow \rangle \text{ (or } | 1\downarrow 2\downarrow \rangle) \\ &\varphi(\mathbf{r}) \text{ odd} \end{aligned} \quad (2.6)$$

For example, for 4 particles, (2.3), reads :

$$\Psi^4 = [\tilde{\varphi}(12)\tilde{\varphi}(34) - \tilde{\varphi}(13)\tilde{\varphi}(24) + \tilde{\varphi}(14)\tilde{\varphi}(23)]$$

In order to carry variational calculation, one needs to calculate average values $\langle \Psi | O | \Psi \rangle = \bar{O}$ of operators (Hamiltonian, spin correlations, identity (norm)).

The standard Monte-Carlo method takes as a complete basis for the Hilbert space, the set of positions of the fermions, say $\{R_i^\uparrow\}_{i=1\dots P}$ for the up spins and $\{R_j^\downarrow\}_{j=1\dots P}$ for the down spins.

\bar{O} is then obtained in the form :

$$\bar{O} = \sum_{\substack{\{R_i^\uparrow\} \{R_j^\downarrow\} \\ \{\bar{R}_i^\uparrow\} \{\bar{R}_j^\downarrow\}}} \langle \Psi | \{R_i^\uparrow\} \{R_j^\downarrow\} \rangle \langle \{R_i^\uparrow\} \{R_j^\downarrow\} | 0 | \{\bar{R}_i^\uparrow\} \{\bar{R}_j^\downarrow\} \rangle \langle \{\bar{R}_i^\uparrow\} \{\bar{R}_j^\downarrow\} | \Psi \rangle \quad (2.7)$$

One thus needs to compute, for each generated configuration, the *amplitude* $\langle \{R_i^\uparrow\} \{R_j^\downarrow\} | \Psi \rangle$ for the chosen w-f. We shall now show that this amplitude is not as hard to calculate as (2.3) might suggest, since it can be written as a $p \times p$ *determinant*, thus computable in p^3 steps. Note that if one chooses a Jastrow (or Gutzwiller) projected BCS w-f (such as an RVB state), the amplitude is simply *multiplied* by some configuration dependent reduction factor, which in no way spoils the usefulness of this determinantal representation.

3. Amplitudes as determinants.

3.1 THE $M_s=0$ CASE (SINGLET OR TRIPLET).— For pair wave functions of the type (2.4, 5), we will now show the following results :

$$\langle \{R_i^\uparrow\}, \{R_j^\downarrow\} | \Psi \rangle = \text{Det } M_{ij} \quad (3.1)$$

$$\text{with } M_{ij} = \varphi(R_i^\uparrow - R_j^\downarrow)$$

The proof is quite straightforward using (2.2) as a starting point : indeed, one has :

$$\begin{aligned}
\langle \left\{ \mathbf{R}_i^\uparrow \right\}, \left\{ \mathbf{R}_j^\downarrow \right\} | \Psi \rangle &= \sum_{k_1 \dots k_p} \varphi_{k_1} \dots \varphi_{k_p} \langle \left\{ \mathbf{R}_i^\uparrow \right\} | a_{k_1}^+ \dots a_{k_p}^+ | O \rangle \langle \left\{ \mathbf{R}_j^\downarrow \right\} | a_{-k_1}^+ \dots a_{-k_p}^+ | O \rangle \\
&= \sum_{k_1 \dots k_p} \varphi_{k_1} \dots \varphi_{k_p} \frac{1}{\sqrt{p!}} \text{Det} \left[e^{ik_\alpha R_\beta^\downarrow} \right] \frac{1}{\sqrt{p!}} \text{Det} \left[e^{-ik_\alpha R_\beta^\downarrow} \right] \\
&= \sum_{k_1 \dots k_p} \varphi_{k_1} \dots \varphi_{k_p} \frac{1}{p!} \sum_{\sigma \sigma'} \epsilon_\sigma \epsilon_{\sigma'} \prod_\alpha e^{ik_\alpha [R_{\sigma(\alpha)}^\uparrow - R_{\sigma'(\alpha)}^\downarrow]}
\end{aligned}$$

(using the very definition of a determinant).

So

$$\langle \left\{ \mathbf{R}_i^\uparrow \right\}, \left\{ \mathbf{R}_j^\downarrow \right\} | \Psi \rangle = \frac{1}{p!} \sum_{\sigma \sigma'} \epsilon_{\sigma'} \epsilon_\sigma \prod_\alpha \varphi \left(\mathbf{R}_{\sigma(\alpha)}^\uparrow - \mathbf{R}_{\sigma'(\alpha)}^\downarrow \right)$$

Reindexing the sum with σ'' -replacing σ' such that $\sigma'(\alpha) = \sigma''(\sigma(\alpha))$, one has

$$\frac{1}{p!} \sum_{\sigma \sigma''} \epsilon_\sigma (\epsilon_{\sigma''} \epsilon_\sigma) \prod_\alpha \varphi \left(\mathbf{R}_{\sigma(\alpha)}^\uparrow - \mathbf{R}_{\sigma''(\sigma(\alpha))}^\downarrow \right) = \frac{1}{p!} \sum_\sigma \text{Det} \varphi \left(\mathbf{R}_{\sigma(\alpha)}^\uparrow - \mathbf{R}_{\sigma(\beta)}^\downarrow \right) = \text{Det} [M_{ij}],$$

hence the result (3.1) [5]. Note that the usual Slater determinants of plane waves can also be written in the form (3.1). Indeed, the free fermions ground state is given by (2.2) with $\varphi_k = 1$ if $k < k_f$ and zero otherwise. The same algebra thus immediately yields :

$$\left. \begin{aligned} \Psi_{\text{free}} &= \text{Det} [\varphi_0 (\mathbf{R}_i^\uparrow - \mathbf{R}_j^\downarrow)] \\ \text{with } \varphi_0 (\mathbf{R}) &= 4\Pi \int_0^{k_f} k^2 \frac{\sin kR}{kR} dk \end{aligned} \right\} \quad (3.2)$$

Thus some kind of pair correlations do exist in the free gas w-f, characterized by a slow oscillating decay with distance. When attraction is switched on, a bound state appears, and thus a length scale ξ governing the exponential decrease of φ for large R .

3.2 CALCULATION OF OPERATOR AVERAGES.— Using (3.1), one can easily express e.g. the norm $\langle \Psi | \Psi \rangle$ as a sum over configurations \mathcal{C} :

$$\langle \Psi | \Psi \rangle = \sum_{\mathcal{C}=\{R_i^\uparrow, R_j^\downarrow\}} \left[\det \varphi \left(R_i^\uparrow - R_j^\downarrow \right) \right]^2$$

Assume for definiteness that we deal with Hubbard's model. Then $\{R_i^\uparrow, R_j^\downarrow\}$ are restricted to take discrete values, and the kinetic energy reads $K = -t (\Sigma_{\langle ij \rangle} C_i^+ C_j^-)$ ($\langle ij \rangle$ means that the sum is restricted to nearest neighbours). In this case, one has :

$$\langle \Psi | K | \Psi \rangle = -t \sum_{\mathcal{C}} \sum_i \det \varphi(\mathcal{C}) \det \varphi(\mathcal{C}'_i)$$

where \mathcal{C}'_i is a configuration obtained from \mathcal{C} by moving atom i by one lattice spacing.

More interesting is the mean value of the spin correlation function

$$\left\langle \Psi \left| \sum_{ij} \mathbf{S}_i \mathbf{S}_j \delta(R - R_{ij}) \right| \Psi \right\rangle = \rho_S(R)$$

Writing $2\mathbf{S}_i \mathbf{S}_j = P_{ij}^\chi - \frac{1}{2}$ where P_{ij}^χ permutes the spins of atoms i and j , one obtains :

$$\left\langle \Psi \left| \sum_{ij} P_{ij}^X \delta(R - R_{ij}) \right| \Psi \right\rangle = \sum_{C, (i,j)=} [\det \varphi(C)]^2 \delta(R - R_{ij}) - \sum_{C, (i,j)\neq} \det \varphi(C) \det \varphi(P_{ij}C) \delta(R - R_{ij})$$

where $\Sigma_{(i,j)=}$ denotes the sum over identical spins and $\Sigma_{(i,j)\neq}$ over reversed spins, and $P_{ij}C$ is the configuration obtained from C by permuting $R_i \uparrow$ and $R_j \downarrow$.

3.3 THE $|M_S|=1$ CASE (EQUAL SPIN PAIRING).— In this case we have obtained the slightly weaker result (which we have used in [3] for our numerical calculations) :

$$\begin{aligned} \left\langle \left\{ \mathbf{R}_i^\uparrow \right\}, \left\{ \mathbf{R}_j^\uparrow \right\} \mid \Psi \right\rangle^2 &= \text{Det } M_{\alpha\beta}^\uparrow \times \text{Det } M_{\alpha\beta}^\downarrow \\ \text{with } \left\{ \begin{array}{l} M_{\alpha\beta}^\uparrow = \varphi(\mathbf{R}_\alpha^\uparrow - \mathbf{R}_\beta^\uparrow) \\ M_{\alpha\beta}^\downarrow = \varphi(\mathbf{R}_\alpha^\downarrow - \mathbf{R}_\beta^\downarrow) \end{array} \right. & \end{aligned} \quad (3.3)$$

Note the uncertainty in the *sign* of the amplitude, which prevents from calculating, the off-diagonal elements of the 1-particle density matrix.

Working directly with (2.3), one notices that the *spin* part of the w-f completely factorizes, leaving to evaluate

$$\mathcal{A}[\varphi(12)\varphi(34)\dots\varphi(p-1, p)] \equiv \mathcal{A}\varphi$$

Now, this is equal to a Gaussian integral over Grassmann variables z_i [11]

$$\begin{aligned} ([z_i, z_j]_+ = 0, \int dz_i = 0, \int dz_i z_i = 1) : \\ \mathcal{A}\varphi \equiv \frac{1}{\left[\frac{p}{2}\right]!} \int dz_1 \dots dz_p e^{\sum_{ij} z_i \varphi_{ij} z_j} \end{aligned} \quad (3.4)$$

This can easily be seen by expanding the exponential in powers of φ . Only the terms of order $\varphi^{p/2}$ survive the integration over the z_i 's and the anticommutation rules. Those terms appear with the correct sign thanks to these anticommutation rules. It is a standard result of Grassmannian algebra that the integral (3.4) is a Gaussian representation of the square root of a determinant [11]:

$$\int dz_1 \dots dz_p e^{\sum_{ij} z_i \varphi_{ij} z_j} \propto \pm \sqrt{\text{Det } \varphi}$$

This leads, up to a normalization of Ψ , to the result (3.3).

4. A new variational wave function : “the fermion-boson mixed state”.

4.1 PRESENTATION.— it is quite tempting to think that, for a generic interaction potential, a w-f for which part of the atoms are paired and part of them left in individual states could be favoured as compared to the usual BCS state : indeed, the variational space is thereby considerably enlarged (the fraction of paired fermions is a new variational parameter) and improvement appears compulsory. New interesting physics seem to be contained in such a w-f, which we describe more formally before commenting on. Let $\tilde{\varphi}$ be the $M_S = 0$ pair w-f of paragraphe 3 and $\tilde{\theta}_\alpha$ some one particle w-f characterized by α (e.g. plane waves of wave vector k_α , or localized states around impurities, etc.). Then, the N -body w-f which describes our unpolarized *fermion-boson mixed state*⁽²⁾ reads :

⁽²⁾ As for the BCS w-f there are no true bosonic entities in this description : the fermionic symmetry of the basic entities is strictly built in.

$$\Psi = \mathcal{A} \left[\tilde{\varphi}(12) \dots \tilde{\varphi}(M-1, M) \tilde{\theta}_1^\dagger(M+1) \dots \tilde{\theta}_{\frac{N-M}{2}}^\dagger(N) \right]$$

It is possible to show that the amplitude of Ψ is also a determinant (of dimension $N - M/2$), thus allowing numerical investigations of this new state :

$$\langle \{\mathbf{R}_i^\dagger\}, \{\mathbf{R}_j^\dagger\} | \Psi \rangle_\infty \underset{(p=\frac{N}{2})}{\propto} \begin{pmatrix} \varphi(11') & \varphi(21') & \dots & \varphi(P1') & \theta_1(1') & \dots & \theta_{\frac{N-M}{2}}(1') \\ \varphi(12') & \varphi(22') & \dots & & & & \\ \varphi(1P') & \dots & & \varphi(PP') & \theta_1(P') & & \theta_{\frac{N-M}{2}}(P') \\ \theta_1(1) & \theta_1(2) & & \theta_1(P) & 0 & & 0 \\ \theta_{\frac{N-M}{2}}(1) & \theta_{\frac{N-M}{2}}(2) & \underbrace{\theta_{\frac{N-M}{2}}(P)}_{p + \frac{N-M}{2}} & 0 & 0 & & \end{pmatrix}$$

where the unprimed numbers are associated with the R_i^\dagger and the primed ones with R_i^\dagger .

4.2 PHYSICAL CONTENT.— Suppose that the optimal momentum distribution is found to have the shape drawn in figure 1, meaning that θ 's are plane waves with wave vectors less than or equal to k^* . The ground state of the fermionic assembly would thus contain a mixture of pairs and of *normal* atoms. (In a sense, a certain number of spinons [2] are present in the ground state). Such a state would exhibit Fermi liquid like behaviour (linear specific heat, constant susceptibility, etc.) characterized by a Fermi momentum which is not dictated by the liquid density as it is the case in Landau's canonical theory. Such a ground state can be unstable against Cooper pairing of the solitary fermions, which undergo their own BCS transition at a temperature not *a priori* related to the energy scale of the pre-existing pairs⁽³⁾. This possibility is extremely interesting with regard to He³, since it allows us to reconcile our variational results [3] suggesting strong pair correlations, and the familiar Landau description of its low temperature properties⁽⁴⁾. We thus propose that the ground

state structure of liquid He³ has the exotic nature, realizing a true non-adiabatic, strong coupling Landau-Fermi liquid.

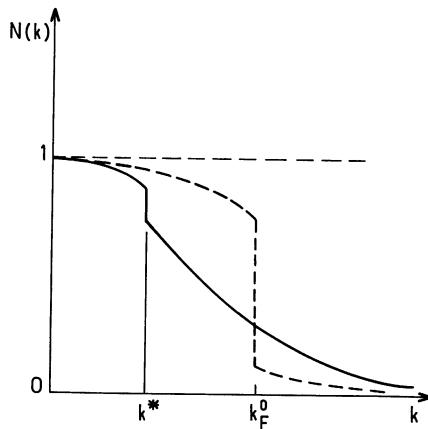


Fig. 1. - Momentum distribution of an interacting Fermi liquid : (a) dashed line : canonical Landau-Fermi liquid, with its Migdal-Luttinger discontinuity at k_F^0 ; (b) solid line : distribution expected for a mixed state, with a discontinuity at shifted k^* (corresponding to the density of unpaired fermions), around which quasiparticle excitations may develop.

⁽³⁾ The symmetry of the spinons pair w-f is also *a priori* different from that of the preexisting pairs.

⁽⁴⁾ We cannot of course exclude the existence of a weak discontinuity of $N(k)$ at the $k_F^0 = (3\pi^2\rho)^{1/3}$. What we really mean is that, in a strong coupling regime, the Pauli principle is ensured through proper pair antisymmetrization, and has no reason to impose anything special at k_F^0 .

5. Conclusion.

In this paper, we have shown that the absolute value of the amplitude of *any* fixed number of particles B.C.S. w-f (singlet or triplet) can be expressed as determinants. We feel that this result is of some importance for more analytical

and numerical work on those wave functions, especially in the strong coupling regime.

We have also proposed a new variational family of w-f which contains both the *BCS branch* and the standard Fermi liquid as limits

and which again can be calculated as determinants. These w-f allow us to consider an intriguing state for fermions *made* of paired atoms and unpaired entities. A crucial question is to know whether such a state exists, with liquid He³ as a good possible candidate.

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