Some properties of the eigenstates in the many-electron problem

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A general hamiltonian $H$ of electrons in finite concentration, interacting via any two-body coupling inside a crystal of arbitrary dimension, is considered. For simplicity and without loss of generality, a one-band model is used to account for the electron-crystal interaction. The electron motion is described in the Hilbert space $S_\phi$, spanned by a basis of Slater determinants of one-electron Bloch wave-functions. Electron pairs of total momentum $K$ and projected spin $\zeta$, $\pm 1$ are considered in this work. The hamiltonian then reads $H = H_D + \sum_{K,\zeta} H_{K,\zeta}$, where $H_D$ consists of the diagonal part of $H$ in the Slater determinant basis. $H_{K,\zeta}$ describes the off-diagonal part of the two-electron scattering process which conserves $K$ and $\zeta$. This hamiltonian operates in a subspace of $S_\phi$, where the Slater determinants consist of pairs characterised by the same $K$ and $\zeta$. It is shown that the whole set of eigensolutions $\psi, \epsilon$ of the time-independent Schrödinger equation $(H - \epsilon)\psi = 0$ divides in two classes, $\psi_1, \epsilon_1$ and $\psi_2, \epsilon_2$. The eigensolutions of class 1 are characterized by the property that for each solution $\psi_1, \epsilon_1$ there is a single $K$ and $\zeta$ such that $(H_D + H_{K,\zeta} - \epsilon_1)\psi_{K,\zeta} = 0$ whereas each solution $\psi_2, \epsilon_2$ of class 2 fulfills $(H_D - \epsilon_2)\psi_2 = 0$. We prove also that the eigenvectors of class 1 have off-diagonal long-range order whereas those of class 2 do not. Finally our result shows that off-diagonal long-range order is not a sufficient condition for superconductivity.

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I. INTRODUCTION

There has been a long-standing interest for the study of electron correlations in condensed matter and particularly in the metallic state, because these are regarded as playing a paramount role in cooperative phenomena such as magnetism and superconductivity. Although electron correlation is essentially determined by the Coulomb repulsion effect, three different classes of models are currently used.

The first is based on the wide efficiency of the one-electron picture in metals and alloys, fostered by the success of the Fermi liquid theory. The electrons behave like a Fermi gas of independent quasi-particles defined by renormalised parameters and finite lifetimes.

The second concerns the magnetic case. It is the realm of the repulsive Hubbard model and its variations, notably the t-J model. As exact results are available only in one dimension and for small clusters in two dimensions, the groundstate has been approximated by different mean-field and variational procedures, such as Hartree-Fock, Gutzwiller, RVB, slave boson state, perturbation, and other calculations. These approximations are based on different assumptions, and the electron gas is supposed to be either a Fermi liquid of the Landau- or Luttinger types, or a gas giving rise to ferromagnetic and antiferromagnetic effects and there is no reliable argument to favor either model.

The last concerns the phenomenon of superconductivity. This is usually explained within the BCS picture where the electrons condense in a variational state characterized by off-diagonal long-range order. The BCS hamiltonian is obtained by truncating an attractive Hubbard hamiltonian in reciprocal space. Consequently the BCS hamiltonian, once Fourier-transformed back to real space, turns out to display four site, interelectron coupling terms which are not present in the Hubbard hamiltonian, used to describe electron interactions in the normal state.

Although the three above classes employ different hamiltonians, the Hilbert space is in all cases taken to be based on Slater determinants and is designated here as $S_\phi$.

Our work investigates the properties of the eigenstates of a general many-body hamiltonian $H$. We present a mathematical proof that the set of eigenstates of $H$ in $S_\phi$, including in particular the groundstate, divides in two classes $\psi_1$ and $\psi_2$ which differ by their off-diagonal long-range order properties. These results are valid for any electron concentration and arbitrary crystal dimension, and for any interelectron coupling provided it is of a two-body nature. The proof exploits specifically the property of the conservation of the pair momentum in every two-electron scattering event. An approximation, consisting of dealing with such pairs as if they were independent quasi-particles, has already provided the groundstate energy of the one-dimensional Hubbard model in excellent agreement with the exact results. In the general case of arbitrary dimension and general hamiltonian investigated in this work, it is necessary to introduce an auxiliary Hilbert space $S_\phi$ in order to derive the $\psi_1$ or $\psi_2$ like properties of the eigenstates. $S_\phi$ is built over a set of pairs characterised by their total momentum $K$ and projected spin $\zeta$. Other authors have also used such sets, nevertheless they remained within the framework of $S_\phi$.

The outline is as follows: in section 2 the many-body
Hamiltonian $H$ is presented and the problem to be solved is set out; section 3 provides the definition of the auxiliary space $S_\phi$, as well as its algebraic properties; sections 4 and 5 detail the proofs of two Theorems establishing the either $\psi_1$ like and $\psi_2$ like properties of the eigenstates of $H$ in the usual space of Slater determinants $S_\phi$ (a partial account of section 4 has been published elsewhere\(^{16}\)); the physical consequences of these results are summarised in the concluding section 6.

II. THE MANY-BODY HAMILTONIAN

In the following model we consider a crystal containing $N$ sites and $2n$ itinerant electrons where $N >> 1$ and $n >> 1$. The crystal can have arbitrary dimension. These electrons populate a single band where the one-electron energy reads $E(k)$ and $k$ is a vector of the Brillouin zone. To simplify the discussion and without loss of generality, we consider that $E(k)$ is independent of the electron spin $\sigma = \pm 1/2$. The Pauli principle requires that $n \leq N$. Let the electrons be coupled via a spin independent pair potential $V$. The total system hamiltonian $H$ can be written in reciprocal space as:

$$H = \sum_{k,\sigma} E(k)c_{k,\sigma}^\dagger c_{k,\sigma} + \sum_{K,k,k',\sigma_1=1,...,4} V(K,k,k')c_{K,k,\sigma_1}^\dagger c_{K-k,k',\sigma_2}^\dagger c_{K,k',\sigma_2} c_{K-k,k,\sigma_1}$$

(1)

where the first term denotes the one-electron contribution and the second denotes the most general expression to describe two-body interactions in a periodic crystal. The operators $c_{k,\sigma}$ and $c_{k,\sigma}^\dagger$ are one-electron creation and annihilation operators on the Bloch state $k, \sigma$. They obey the usual Fermi commutation rules. The real coefficients $V(K,k,k')$ are the matrix elements of the two-electron scattering process, conserving the momentum $K$ of each scattered pair. For usual pair potentials involving only two-site terms in real space, $V(K,k,k')$ is $K$-independent and depends only of $(k-k')$. The summations in eq 1 are carried out over all possible values of $K,k,k'$ in the Brillouin zone under the constraint of spin conservation $\sigma_1 + \sigma_2 = \sigma_3 + \sigma_4$ ($\sigma_i=1,...,4 = \pm 1/2$). A special case of eq 1 is the Hubbard hamiltonian\(^{17}\) which is recovered by setting $E(k) = \cos(\sum_{i} k_i)$ where the components of $k$ are identified by $k_i$, $\sigma_1 + \sigma_2 = 0$ and $V(K,k,k')$ is a constant $U/N$ for all scattering events. The hamiltonian $H$ describes the electron motion in the Hilbert space $S_\phi$ of dimension $d_\phi = \left( \frac{2N}{2n} \right)$. Each basis vector $\phi_i$ with $i = 1,...,d_\phi$ is a Slater determinant involving $2n$ one-electron Bloch states.

Since this discussion resorts repeatedly to electron pairs, it is convenient to introduce the following pair creation and annihilation operators $b_{\pm 1}^i(k,k')$, $b_i(k,k')$:

$$b_{\pm 1}^i(k,k') = c_{k,\pm}^i c_{k',\pm}^\dagger \quad , \quad b_{\pm 1}^i(k,k') = c_{k,\pm}^i c_{k',\pm}^\dagger$$

$$b_0^i(k,k') = c_{k,\pm}^i c_{k',\pm}^\dagger \quad , \quad b_0^i(k,k') = c_{k,\pm} c_{k',\pm}$$

(2)

The subscripts $+\ or -$ in the one-electron $c_{k,\pm}^i$ operators refer to the two possible directions of the electron spin. The subscript $\zeta = 0, \pm 1$ stands for the projection of the total spin of the pair where $\zeta = \pm 1$ indicates the same spin and $\zeta = 0$ indicates opposite spins on both electrons, before and after scattering. The commutation rules of such pairs are neither Fermi- nor Bose-like. It is useful to recast the hamiltonian $H$ of eq 1 in terms of the subsidiary hamiltonians $H_D$, $H_{K,\zeta}$ as follows:

$$H = H_D + \sum_{K,\zeta = 0,\pm 1} H_{K,\zeta}$$

(3)

where $H_D$ and $H_{K,\zeta}$ may be written as:

$$H_D = \sum_{k,\sigma} E(k)c_{k,\sigma}^\dagger c_{k,\sigma} + \sum_{k,k'} V(k+k',k,k')c_{k,\sigma}^\dagger c_{k',\sigma} + c_{k,\sigma} c_{k',\sigma}$$

$$+ \sum_{k,k',\sigma_1 \neq k,\sigma} V(k+k',k,k')c_{k,\sigma_1}^\dagger c_{k',\sigma_2} c_{k',\sigma_2} c_{k,\sigma_1}$$

$$H_{K,\zeta} = \sum_{k,k',\sigma_1 \neq k,\zeta} V(k,k')b_0^{\pm 1}(k,k')b_0^{\pm 1}(k,k')$$

(4)

The diagonal matrix elements of $H$ in the Slater determinant basis are regrouped in the hamiltonian $H_D$. Inversely the off-diagonal matrix elements of $H$ are regrouped in the hamiltonians $H_{K,\zeta}$. In the Hubbard hamiltonian, $H_D$ takes the form $\sum_{k,\sigma} E(k)c_{k,\sigma}^\dagger c_{k,\sigma}$ $+ \sum_{k,k'} V(k,k')b_0^{\pm 1}(k,k')b_0^{\pm 1}(k,k')$ and $H_{K,\zeta} = 0$ for every $K$. Note also that the BCS hamiltonian reads as $H_D + H_{K,\zeta} = 0$ where $H_D$ and $H_{K,\zeta} = 0$ are given by their particular expressions in the Hubbard hamiltonian.

The main purpose of this article is to present and demonstrate two Theorems which characterise the two classes of eigensolutions $\psi, \epsilon$ of the time-independent Schrödinger equation $(H - \epsilon)\psi = 0$ where $H$ is given by eq 1 and $\psi$ belongs to the Hilbert space $S_\phi$. These classes are designated respectively as $\psi_1, \epsilon_1$ and $\psi_2, \epsilon_2$.

**Theorem 1**: To each eigensolution $\psi_{K,\zeta}, \epsilon_1$ where $(H_D + H_{K,\zeta} - \epsilon_1)\psi_{K,\zeta} = 0$, there corresponds an eigensolution $\psi_1, \epsilon_1$ of $H$ such that $(H - \epsilon_1)\psi_1 = 0$.

The fingerprint of each $\psi_1$ is that its linear expansion over the basis vectors of $S_\phi$ involves at least one Slater determinant $\phi$ which can be written as:

$$\phi = \prod_{j=1}^n \delta_\zeta^i (k_j, K-k_j)|0\rangle$$

(5)

where $|0\rangle$ designates the no-electron state. Note that $\psi_{K,\zeta}$ in general is not an eigenvector of $H$ although $\epsilon_1$ is indeed an eigenvalue of $H$.

**Theorem 2**: For every $\psi_2, \epsilon_2$, the equation $(H - \epsilon_2)\psi_2 = 0$ implies that $(H_D - \epsilon_2)\psi_2 = 0$.

Each $\psi_2$ is characterised by its linear expansion over the basis vectors of $S_\phi$ containing no Slater determinant such as $\phi$ in eq 5 for every $K$ and $\zeta$.

In the simple case of a two-electron system, that is a single pair $(n = 1)$, Theorem 1 has been demonstrated previously\(^{17}\). This result follows since $H$ and $H_{K,\zeta}$ commute with each other and with the pair number operator.
\[ N_{K, \zeta} = \sum_k b_\zeta^\dagger (k, K-k) b_\zeta (k, K-k) \quad (6) \]

Our aim hence is to generalise the result of reference\textsuperscript{5} to the \( n > 1 \) case. While it is easy to show that \( H_{K, \zeta} \) and \( N_{K, \zeta} \) still commute for any \( n \), the operators \( H \) and \( N_{K, \zeta} \) however no longer commute in this general case. Therefore the \( n > 1 \) case cannot be dealt with in the Hilbert space \( S_\phi \) of Slater determinants. It becomes then necessary to treat the problem in an auxiliary Hilbert space \( S_{\phi_0} \) which is purposely constructed so that \( H \) and \( N_{K, \zeta} \) commute in this space, keeping invariant their definitions as in eq\textsuperscript{4} and eq\textsuperscript{6}.

As \( \psi_1 \) eigenstates will be shown in addition to have off-diagonal long range order whereas \( \psi_2 \) eigenstates do not have, it is in order to recall the definition of the two-body correlation function attached to this particular kind of long range order characterising the BCS state:

\[ f_{\text{odlro}}(|\tau|) = \sum_{i,j,l,m,\sigma_n=1,4} \langle \phi | c_\sigma_n^\dagger c_\sigma_1^\dagger c_\sigma_2 c_\sigma_3 | \phi \rangle , \quad (7) \]

where the Wannier operator \( c_{\sigma_n}^\dagger \) destroys (creates) an electron with spin \( \sigma_n \) at site \( i \) labeled by the lattice vector \( r_i \) and the sum is done with \( (r_j - r_i) = (r_m - r_i) = \rho \), \( (r_1 - r_2) = \tau \) and \( \sigma_1 + \sigma_2 = \sigma_3 + \sigma_4 \). Eq\textsuperscript{7} extends to the \( \rho \neq 0 \) case the usual definition of off-diagonal long-range order\textsuperscript{2} given in the Hubbard model for \( \rho = 0 \) and \( \sigma_1 = -\sigma_2 \). A many-electron state \( \phi \in S_\phi \) is said to have off-diagonal long range order if \( f_{\text{odlro}}(|\tau|) \), calculated at \( \rho \) kept fixed, oscillates versus \( |\tau| \) without decaying to zero for \( |\tau| \to \infty \). It must be noticed that off-diagonal long range order differs from real space long range order, typical of crystalline matter, magnetic materials, spin- and charge-density waves. This latter type of long range order is characterised by the following two-body correlation function:

\[ f_{\text{strlo}}(|\tau|) = \sum_{i,j,\sigma_n=1,4} \left( \langle \phi | c_\sigma_n^\dagger c_{\sigma_1} c_{\sigma_2}^\dagger c_{\sigma_3} c_{\sigma_4} | \phi \rangle - \langle \phi | c_\sigma_n^\dagger c_{\sigma_1} c_{\sigma_2} c_{\sigma_3}^\dagger c_{\sigma_4} | \phi \rangle \langle \phi | c_{\sigma_n}^\dagger c_{\sigma_3} c_{\sigma_2} c_{\sigma_1} | \phi \rangle \right) , \quad (8) \]

where the sum is done with \( (r_1 - r_j) = \tau \) and \( \sigma_1 + \sigma_3 = \sigma_2 + \sigma_4 \). Charge and spin fluctuations correspond respectively to \( \sigma_1 = \sigma_2 \) and \( \sigma_1 = -\sigma_2 \). A state \( \phi \in S_\phi \) is said to have real space long range order if \( f_{\text{strlo}}(|\tau|) \) oscillates versus \( |\tau| \) without decaying to zero for \( |\tau| \to \infty \). By comparing the definition in eq\textsuperscript{7} with that in eq\textsuperscript{8} it is realized that \( f_{\text{odlro}}(|\tau|) \neq f_{\text{strlo}}(|\tau|) \) even if \( \rho = 0 \). Besides from the experimental point of view, real space long range order gives rise to Bragg diffraction in a neutron or X-ray scattering experiment while off-diagonal long range order does not.

### III. Properties of the Auxiliary Hilbert Space \( S_\phi \)

Any Slater determinant \( \phi_e \) of \( S_\phi \) can be written as:

\[ \phi_e = \prod_{K, \zeta} \left( \prod_{i=1}^{n_{K, \zeta}} b_\zeta^\dagger (k_j, K-k_j) \right) |0\rangle , \quad (9) \]

where all pairs \( b_\zeta^\dagger (k, K-k) |0\rangle \) having the same \( K \) and \( \zeta \) have been regrouped together. In the product with respect to the index \( j \), the \( e \) dependence of \( j \) has been dropped for simplicity. The integer \( n_{K, \zeta} \geq 0 \) designates the total number of pairs characterised by \( K, \zeta \) in \( \phi_e \), and the \( n_{K, \zeta} \)’s satisfy \( \sum_{K, \zeta} n_{K, \zeta} = n \). The basis vector \( \Phi_{e, \alpha} \) of \( S_\phi \) is defined from \( \phi_e \) as:

\[ \Phi_{e, \alpha} = \bigotimes_{K, \zeta} \phi_{K, \zeta} \quad , \quad \phi_{K, \zeta} = \prod_{j=1}^{n_{K, \zeta}} b_\zeta^\dagger (k_j, K-k_j) |0\rangle , \quad (10) \]

where the tensor product replaces the simple product \( \prod_{K, \zeta} \phi_{K, \zeta} \) and each \( \phi_{K, \zeta} \) is a Slater determinant containing \( n_{K, \zeta} \) pairs of \( K, \zeta \). The sequence of integers \( \{ n_{K, \zeta} \} \) in eq\textsuperscript{10} defines uniquely the pair configuration \( \alpha \) of \( \phi_e \). Therefore \( n_{K, \zeta} \) will be denoted \( n_{K, \zeta, \alpha} \) in the following. The set of pair configurations of \( \phi_e \) can be obtained by selecting \( m \) permutations of \( 2n \) one-electron Bloch states defining \( \phi_e \). The number of pair configurations \( m = (2n)!/(2^n (n!)^2) \) is smaller than that of permutations \( (2n)! \) because many different permutations correspond to the same pair configuration. The basis vectors \( \Phi_{e, \alpha} \) of \( S_\phi \) are generated by letting the subscripts \( e = 1, \ldots d_\phi \) and \( \alpha = 1, \ldots m \) run over all possible values, which implies that the dimension of \( S_\phi \) is equal to \( m d_\phi \). The pair number operator \( N_{K, \zeta} \) is taken to act on \( \Phi_{e, \alpha} \) as follows:

\[ N_{K, \zeta} \Phi_{e, \alpha} = n_{K, \zeta, \alpha} \Phi_{e, \alpha} \quad . \quad (11) \]

As the \( \Phi_{e, \alpha} \)’s are chosen to be orthonormal, eq\textsuperscript{11} entails that \( n_{K, \zeta, \alpha} \Phi_{e, \alpha} = \sum_{\alpha=1}^{m} \Phi_{e, \alpha} \). The subspace \( S_\phi \subset S_\phi \) is then introduced as spanned by the basis vectors \( \Phi_{e, \alpha} \) defined by:

\[ \Phi_{e, \alpha} = \sum_{\alpha=1}^{m} \Phi_{e, \alpha} \quad , \quad (12) \]

where the sum is carried over \( m \) pair configurations \( \alpha \) of \( \phi_e \). The one to one correspondence between \( \phi_e \in S_\phi \) and \( \Phi_{e} \in S_\phi \) ensures that the dimension of \( S_\phi \) is equal to \( d_\phi \). Although \( S_\phi \) and \( S_\phi \) obey the Pauli principle by construction, the vectors \( \Phi_e \in S_\phi \) and \( \Phi_{e, \alpha} \in S_\phi \) do not exhibit the antisymmetry property typical of Slater determinants with respect to interchanging two electrons. The question of redundancy, encountered here, since the dimension of \( S_\phi \) is larger than that of \( S_\phi \), arises as in other works\textsuperscript{11,12} dealing with electron pairs. However in our treatment this redundancy does not pose any particular problem. The significance of \( \Phi_e, \Phi_{e, \alpha}, n_{K, \zeta, \alpha} \) is
illustrated in detail in the appendix for the exemplifying case of a four electron system.

Introduce now the subspaces $S_{K,\zeta} \subset S_\Phi$ and $S_2 \subset S_\Phi$, where $S_{K,\zeta}$ is defined for each $K, \zeta$ as spanned by the basis vectors $\Phi_{i=1...d_0}$, $d_0$ being the dimension of $S_{K,\zeta}$. By definition each $\Phi_i$ is associated with a Slater determinant $\phi_i$ of $13$, each $\Phi_{p,q}$ is defined in eq.13, and comprising $n$ pairs, all having the same $K$ and $\zeta$. The dimension $d_0$ of $S_{K,\zeta}$ is $d_0 = \binom{N}{n}$ or $d_{\pm 1} = \binom{N}{n}/2$ depending whether $\zeta = 0$ or $\zeta = \pm 1$, respectively. The characteristic property of each $\Phi_i$ is that its pair configuration expansion, as given in eq.14, involves a particular value $\gamma$ defined by:

$$
\Phi_i = \sum_{\alpha=1}^{m} \phi_{i,\alpha} , \ n_{K,\zeta},\gamma = |\Phi_{i,\gamma}|N_{K,\zeta}|\Phi_{i,\gamma} = n \Rightarrow n_{K',\zeta',\gamma},
$$

where $K'$ and $\zeta'$ take all possible values different from $K$ and $\zeta$ respectively. Each $\Phi_{i,\gamma}$ of $S_{\Phi}$ is then written in the same expression as $\phi_i \in S_\Phi$ of eq.13 associated with $\Phi_i \in S_{K,\zeta}$, because the tensor product yielding $\Phi_{i,\gamma}$ as in eq.10 reduces to a single Slater determinant of $n$ pairs $K, \zeta$. Inversely the subspace $S_2$ is spanned by the basis vectors $\Phi_{p=1...d_0}$, $d_0$ being the dimension of $S_2$ ($S_2$ is named so because it will be shown hereafter to include all $\psi_2$ like eigenvectors). Each $\Phi_p$ is characterised by:

$$
\Phi_p = \sum_{\beta=1}^{m} \phi_{p,\beta} , \ n_{K,\zeta},\beta = |\Phi_{p,\beta}|N_{K,\zeta}|\Phi_{p,\beta} |< n , \forall K, \zeta ,
$$

where the inequality holds for every $\beta$ value involved in the pair configuration expansion of $\Phi_p$. As the subspaces $S_2$ and $S_{K,\zeta}$ are disjoint, because their characteristic properties as expressed by eqs.13,14 exclude one another, they provide a basis for $S_\Phi$:

$$
S_\Phi = S_2 \bigoplus_{K,\zeta} S_{K,\zeta} , \quad d_\Phi = d_2 + N(d_0 + 2d_{\pm 1}) .
$$

Consider now the following expression for the hamiltonian $H'$ in $S_{\Phi}$:

$$
H' = \sum_{i,j} \langle \phi_i | H | \phi_j \rangle |\Phi_{i,\gamma}\rangle |\Phi_{j,\gamma}\rangle + \sum_{p,q,\beta} m_{pq} \langle \phi_p | H | \phi_q \rangle |\Phi_{p,\beta}\rangle |\Phi_{q,\beta}\rangle
$$

where the sum with respect to $i,j$ is performed on all Slater determinants $\phi_i$ and $\phi_j$ associated respectively with $\Phi_i \in S_{K,\zeta}$ and $\Phi_j \in S_{K,\zeta}$; the pair configuration $\gamma$ is defined in eq.13 and $K, \zeta$ take all possible values. The sum with respect to $p,q$ is carried over all $\Phi_p$ and $\Phi_q$ such that $\Phi_p$ or $\Phi_q$ belong to $S_2$. The matrix elements $\langle \phi_p | H | \phi_q \rangle$ and $\langle \phi_q | H | \phi_p \rangle$ are calculated with $H$ given by eq.1. As $\langle \phi_p | H | \phi_q \rangle \neq 0$ requires that the Slater determinants $\phi_p$ and $\phi_q$ differ by one pair only, and they read $\phi_p = b_{\zeta}^i (k, K - k) \phi_{pq|0}$ and $\phi_q = b_{\zeta'}^j (k', K - k') \phi_{pq|0}$ where $\phi_{pq}$ comprises the product of $(n - 1)$ pairs, the sum with respect to $\beta$ is made with $m_{pp} = 1/m$ and $m_{pq} = (2n - 1)/m$ over $m/(2n - 1)$ pair configurations common to $\Phi_p$ and $\Phi_q$. The definition of $H'$ ensures that the matrix elements $\langle \phi_p | H' | \phi_f \rangle$ and $\langle \phi_f | H' | \phi_f \rangle$ are equal for all $e, f$ values where $\phi_e, \phi_f$ are two Slater determinants of $S_\Phi$ and $\Phi_e, \Phi_f$ are the corresponding basis vectors of $S_\Phi$. It follows that the Schrödinger equations $(H - \epsilon) \psi = 0$ and $(H' - \epsilon) \Psi = 0$, where $\psi \in S_\Phi$ and $\Psi \in S_\Phi$, have the same spectrum of eigenvalues $\epsilon$ and there is a one to one correspondence between $\psi$ and $\Psi$.

Since $H'$ in eq.16 does not display such terms as $|\Phi_{p,\alpha}|\langle \Phi_{p,\beta}| \Psi_\alpha, \Psi_\beta \rangle$ which would mix two different pair configurations $\alpha$ and $\beta$, the Schrödinger equation $(H' - \epsilon) \Psi = 0$, where $\Psi$ belongs to $S_\Phi$, splits into partial Schrödinger equations:

$$
\Psi_1 = \Psi_{K,\zeta} + \Psi'_1 , \quad \Psi_{K,\zeta} = \sum_{i=1}^{d_2} a_i \Phi_i , \quad \Psi'_1 = \sum_{p=1}^{d_0} a_p \Phi_p ,
$$

where the coefficients $a_i, a_p$ are real and the $\Phi_i$'s and $\Phi_p$'s are basis vectors of $S_{K,\zeta}$ and $S_2$, respectively. We now apply eq.17 to $\Psi_1$ for the particular pair configuration $\gamma$ defined in eq.13:

$$
(H' - \epsilon) \Psi_{1,\gamma} = 0 , \quad \Psi_{1,\gamma} = \Psi_{K,\zeta,\gamma} + \Psi'_{1,\gamma} .
$$

As the vector $\Psi'_1$ is inferred from the definition of $\Phi_p$ in eq.13 not to contribute to $\Psi_{1,\gamma}$, it ensues that $\Psi_{1,\gamma}$ reduces to $\Psi_{K,\zeta,\gamma}$. Because of $\langle \phi_i | H | \phi_j \rangle = \langle \phi_i | H_D + H_{K,\zeta} | \phi_j \rangle$ which holds for the hamiltonians $H_D$ and $H_{K,\zeta}$ in eq.1 and any two Slater determinants $\phi_i, \phi_j$ associated with the basis vectors $\Phi_i, \Phi_j$ of $S_{K,\zeta}$, it comes finally:

$$
(H' - \epsilon_1) \Psi_{1,\gamma} = 0 \Rightarrow (H_D + H_{K,\zeta} - \epsilon_1) \Psi_{K,\zeta,\gamma} = 0 \Rightarrow (H_D + H_{K,\zeta}) \Psi_{K,\zeta,\gamma} = 0 \Rightarrow (H_D + H_{K,\zeta}) \psi_{K,\zeta} = 0
$$

where $\psi_{K,\zeta} \in S_\Phi$ is in one to one correspondence with $\Psi_{K,\zeta} \in S_\Phi$. Eq.20 means that, if $\psi_{K,\zeta} + \psi'_1$ is an eigenvector and eigenvalue of $H$ in $S_\Phi$, the vector $\psi_{K,\zeta}$ and $\epsilon_1$ are eigenvector and eigenvalue of $(H_D + H_{K,\zeta})$ in $S_\Phi$ too. To complete the proof of Theorem 1 it must be shown in addition that every eigensolution $\psi_{K,\zeta}, \epsilon_1$ of $(H_D + H_{K,\zeta})$ gives rise to an eigensolution $\psi_1, \epsilon_1$ of $H$. The latter will be proved now by contradiction. Suppose that there is an eigensolution of some hamiltonian $(H_D + H_{K,\zeta})$ which is not an eigenvalue of $H$. Then the
corresponding \( S_{K,\zeta} \) will contribute only \((d_\zeta - 1)\) eigenvalues instead of \(d_\zeta\) to the spectrum of \(H\), which will result in an incomplete diagonal basis for \(H\) and is thus at odds with the property of \(H\) being hermitian. \textbf{Q.E.D.}

Both \(\psi_{K,\zeta}\) and the BCS variational states consist of a linear combination of Slater determinants of pairs having the same \(K,\zeta\). They differ, however, by the number of pairs in each determinant, which ranges from 0 up to \(N\) in the BCS state while it is always equal to \(n\) for \(\psi_{K,\zeta}\). As for the BCS state, off-diagonal long-range order, as defined in eq. (4) is a fingerprint of \(\psi_{K,\zeta}\):

\[
 f_{\text{odlro}}(|\tau|) = \cos(K,\tau)\Delta, \quad \Delta = \sum_{k,k'} e^{i(k-k',\rho)} \langle \psi_{K,\zeta} | b_\zeta^+ (k, -k') \rangle
\]

where \(\Delta\) is a two-body correlation parameter attached to \(\psi_{K,\zeta}\). Actually \(f_{\text{odlro}}(|\tau|)\) results from a sum over all \((K',\zeta')\) but the contributions with \((K',\zeta') \neq (K,\zeta)\) vanish identically. \(f_{\text{odlro}}(|\tau|)\) oscillates without decaying for \(|\tau| \to \infty\) provided \(\Delta \neq 0\). It will be shown in the following section that \(\psi_{K,\zeta}\) (see eq. (15) contributes nothing to \(f_{\text{odlro}}(|\tau|)\) for \(|\tau| \to \infty\) so that \(\psi_{K,\zeta}\) and \(\psi_1\) have the same off-diagonal long-range order parameter. In the Hubbard model, the validity of Theorem 1 has been confirmed24 for a large class of many-electron eigenstates \((K = (\pi, \pi, \pi), \zeta = 0)\), built with help of the \(\eta\)-pairing mechanism, for arbitrary interelectron coupling \(U\) and electron concentration.

V. PROOF OF THEOREM 2

We turn now to the Schrödinger equation \((H' - \epsilon_2)\Psi_2 = 0\) where \(H'\) is given by eq. (16) and the eigenvector \(\Psi_2\) belongs to the subspace \(S_2\) of \(S_{K,\zeta}\):

\[
 \Psi_2 = \sum_{p=1}^{d_2} \Phi_p, \quad \Phi_p = \sum_{\beta=1}^{m} \Phi_{p,\beta}, \quad \Psi_{2,\beta} = \sum_{p=1}^{d_2} a_p \Phi_{p,\beta}, \quad \Psi_2
\]

where the \(a_p\)'s are real and the pair configuration expansion of \(\Phi_p\) is done with respect to \(\beta\). To demonstrate the validity of Theorem 2 it is sufficient to show that the matrix element \(\langle \Phi_p | H' | \Phi_q \rangle\) vanishes for all \(\Phi_p\) and \(\Phi_q\) in the linear expansion giving \(\Psi_2\) in eq. (22) if \(p \neq q\). The proof proceeds by contradiction. Suppose that \(\langle \Phi_p | H' | \Phi_q \rangle \neq 0\) for \(p = 1\) and \(q = 2\) whereas \(\langle \Phi_p | H' | \Phi_q \rangle = 0\) for \(p \neq 1, 2, q \neq 1, 2\) and \(p \neq q\). This implies for the Schrödinger equation \((H' - \epsilon_2)\Psi_2 = 0\):

\[
 (H' - \epsilon_2)(a_1 \Phi_1 + a_2 \Phi_2) + \sum_{q=1,2} \langle \Phi_q | H_D | \Phi_q \rangle = 0.
\]

As the basis vectors \(\Phi_q\) are linearly independent, eq. (23) implies that:

\[
 (H' - \epsilon_2)(a_1 \Phi_1 + a_2 \Phi_2) = 0, \quad \langle \Phi_q | H_D | \Phi_q \rangle = \epsilon_2, \quad \forall q \neq 1, 2.
\]

As seen in eq. (16) \(\langle \Phi_1 | H' | \Phi_2 \rangle \neq 0\) requires that \(\Phi_1\) and \(\Phi_2\) differ by one pair only so that they read \(\Phi_1 = b^+(k_1, k_2)|0\rangle \otimes \Phi_{12}\) and \(\Phi_2 = b^+(k_3, k_4)|0\rangle \otimes \Phi_{12}\) where the spin index \(\zeta\) is dropped for simplicity till the end of this proof, \(k_1 + k_2 = k_3 + k_4\) and \(\Phi_{12}\) includes \((n - 1)\) pairs. Moreover due to eq. (17) the expression \((H' - \epsilon_2)(a_1 \Phi_{1,\beta} + a_2 \Phi_{2,\beta}) = 0\) where the pair configuration index \(\beta\) runs over all values allowed by eq. (22). The particular case of \(\beta\), where the pair numbers \(n_{k_1 + k_2, \beta} = n_{k_1 + k_4, \beta} = 1\), is of interest, in order to work out the proof. Then eq. (16) entails that:

\[
 (H' - \epsilon_2)(a_1 b^+(k_1, k_2)|0\rangle + a_2 b^+(k_3, k_4)|0\rangle = 0
\]

Because of \(\Phi_{12} \neq 0\), eq. (26) implies that each eigenvalue \(\epsilon_2\) of \(H'\) is also an eigenvalue of \(H'\) in the subspace of Slater determinants made up of a single pair, the dimension \(d_s\) of which is equal to \(N\) or \(N/2\) according to \(\zeta = 0\) or \(\zeta = \pm 1\). It ensues that the dimension \(d_s\) of \(S_2\) is such that \(d_s \leq d_s\), which is in contradiction with the inequality \(d_s << d_2\) resulting from the fact that \(S_2\) is spanned by Slater determinants made up of \(n\) pairs with \(n >> 1\). In addition eq. (24) yields \(\langle \Phi_p | H_D | \Phi_p \rangle = \epsilon_2\) for every \(\Phi_p\) making up the linear expansion of \(\Psi_2\) in eq. (22).

\textbf{Q.E.D.}

As every off-diagonal term \(\langle \Phi_p | H'| \Phi_q \rangle\) vanishes for the \(\Phi_p, \Phi_q\) states coming up in the linear expansion of \(\Psi_2\) in eq. (22) the off-diagonal and real space long-range order parameters in eqs. (7) reduce both for \(\psi_2\) to a two-particle distribution function:

\[
 f_{\text{dolro}}(|\tau|) = \sum_{k,k',\sigma} d(k+k',\tau) - \cos(k+k',\tau) + (k-k',\rho) \langle \Psi_2 | \phi_{k,+,c_{k+,\sigma}}^+ \rangle
\]

As a consequence of Riemann-Lebesgue’s Theorem due to the oscillating character of \(\cos(k \pm k',\tau)\), \(f_{\text{dolro}}(|\tau|)\) and \(f_{\text{orf}}(|\tau|)\), calculated with \(\rho\) kept fixed, decay towards

\[
 = \sum_{\Phi} \Phi | \Phi \rangle \rightarrow \infty \text{ so that } \psi_2 \text{ has neither off-diagonal nor real space long-range order. Furthermore they may behave like power laws for large } |\tau|, \text{ in similarity with previous results worked out in one dimension}^{18}.

VI. CONCLUSION

The general hamiltonian \(H\) of eq. (1) has been shown to have two types of eigenstates and eigenvalues \(\psi_1, \epsilon_1\) and \(\psi_2, \epsilon_2\) in the space of Slater determinants. The \(\psi_1\)’s are characterised by a non vanishing projection in the space \(S_{K,\zeta}\), denoted \(\psi_{K,\zeta}\). This latter is responsible for off-diagonal long-range order and fulfils \((H_D + H_{K,\zeta} - \epsilon_1)\psi_{K,\zeta} = 0\) whereas the \(\psi_2\)’s obey \((H_D - \epsilon_2)\psi_2 = 0\) and do not have off-diagonal long-range order. These results are valid for arbitrary crystal dimension, electron concentration and two-electron coupling provided it conserves \(K\) and \(\zeta\) in a scattering process.

To realize that off-diagonal long-range order and real space long-range order have different properties, it is il-
luminating to discuss the simple case of two electrons coupled by a one-dimensional Hubbard Hamiltonian\textsuperscript{15}. This system sustains a single band of bound eigenstates $\psi_{K,\zeta=0}$. As $\psi_{K,\zeta=0}$ is $\psi_1$-like, its off-diagonal long-range order parameter $f_{odiro}(|\tau|)$ oscillates like $\cos(K,\tau)$ while its real space long-range order parameter $f_{rsoro}(|\tau|)$ decays like $e^{-|\tau|}$ where $l$ represents the size of the bound electron pair. Each $\psi_{K,\zeta=0}$ is thus seen to have off-diagonal long-range order but no real space long-range order. Note also that Mermin-Wagner’s Theorem\textsuperscript{3} which rules out the possibility of real space long-range order in one and two dimensions is not relevant to Theorems 1 and 2 because this statement is based actually on a thermal average which fails to say anything upon the correlation properties of the many-body eigenstates. Thus if an eigenstate happens to have long-range order of any kind, Mermin-Wagner’s Theorem merely says that its statistical weight in the thermal average is too weak to give rise to long-range order at finite temperature in the whole electron system. Anyhow as the eigenstates of all interacting electron systems, thus including metals with long-range magnetic order but finite resistivity, have been shown to be either $\psi_1$- or $\psi_2$-like, Theorem 1 ensures that off-diagonal long-range order is not a sufficient criterion for superconductivity.

As far as $\psi_1$-like solutions are concerned, the results of this work enable one to diagonalise $H$ on a cluster of size considerably larger than currently reached, because the dimension of $S_{K,\zeta}$ is much smaller than that of $S_{\phi}$. At last they provide useful constraints on the variational states currently used in the many-body problem such as those quoted in section 1. Indeed any variational state within the frame of reference of this work which is recognised to be neither $\psi_1$- nor $\psi_2$-like is unphysical even though it may fortuitously approximate the ground-state energy. In particular as the groundstate energies of the one- and two-dimensional Hubbard Hamiltonians are smaller\textsuperscript{22} than the lowest eigenvalue of $H_D$, the respective groundstates are inferred to be $\psi_1$-like. Since the spectrum of eigenvalues of $H$ has been shown to include all eigenvalues of every $H_{K,\zeta}$ and the BCS Hamiltonian is equal to $H_{K=0,\zeta=0}$ in the particular case where the Hubbard Hamiltonian is equal to $H$, the Hubbard Hamiltonian, currently used to study the normal state, turns out to account for the properties of the superconducting state too. Finally this work provides a unified picture for the electron interaction in solids, valid for normal, magnetic and superconducting metals as well.

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**Appendix**

In the four electron case ($n = 2$), a Slater determinant reads $\phi = c_{k_1}^\dagger c_{k_2}^\dagger c_{k_3}^\dagger c_{k_4}^\dagger |0\rangle$ where $k_1$, $k_2$, $k_3$, $k_4$ are four vectors of the Brillouin zone and the spin indices $\sigma, \zeta$ are dropped for simplicity in this example. An application of eqs.\textsuperscript{10,12} yields $n = 3$ and $\Phi_{\alpha=1} = b^{\dagger}(k_1,k_2)|0\rangle \otimes b^{\dagger}(k_3,k_4)|0\rangle, \Phi_{\alpha=2} = b^{\dagger}(k_1,k_3)|0\rangle \otimes b^{\dagger}(k_2,k_4)|0\rangle$ and $\Phi = (\Phi_1 + \Phi_2 + \Phi_3)$, if it is assumed that $k_1 + k_2 \neq k_3 + k_4, k_1 + k_3 \neq k_4 + k_2, k_1 + k_4 = k_2 + k_3$. The pair configurations $\alpha = 1, 2, 3$ are characterised by the pair numbers $n_{k_1+k_2,\alpha=1} = n_{k_3+k_4,\alpha=1} = n_{k_1+k_3,\alpha=2} = n_{k_2+k_4,\alpha=2} = 1, n_{k_1+k_4,\alpha=3} = 2$. Notice that $\Phi_1, \Phi_2, \Phi_3$ are three linearly independent vectors of $S_{\phi,\alpha}$, all associated with the same vector $\Phi$ of $S_{\phi}$ or equivalently $\phi$ of $S_{\phi}$.

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