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_ϕ, spanned by a basis of Slater determinants of one-electron Bloch wave functions. Electron pairs of total momentum K and projected spin $\zeta=0,\pm1$ are considered in this work. The Hamiltonian then reads $H=H_D+\Sigma_{K,\zeta}H_{K,\zeta}$, 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 ζ. This Hamiltonian operates in a subspace of S_ϕ, where the Slater determinants consist of pairs characterized by the same K and ζ. It is shown that the whole set of eigensolutions ψ,ϵ of the time-independent Schrödinger equation $(H-\epsilon)\psi=0$ divides into two classes, ψ_1,ϵ_1 and ψ_2,ϵ_2. The eigensolutions of class 1 are characterized by the property that for each solution ψ_1,ϵ_1 there is a single K and ζ such that $(H_D+H_{K,\zeta}-\epsilon_1)\psi_{K,\zeta}=0$ where, in general, $\psi_1\neq\psi_{K,\zeta}$, whereas each solution ψ_2,ϵ_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. [S0163-1829(96)00743-6]

I. INTRODUCTION

There has been a long-standing interest in 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.[1] The electrons behave like a Fermi gas of independent quasiparticles defined by renormalized parameters and finite lifetimes.

The second concerns the magnetic case. It is the realm of the repulsive Hubbard model[2] and its variations, notably the t-J model.[3] As exact results are available only in one dimension[4–6] and for small clusters in two dimensions,[7] the ground state has been approximated by different mean-field and variational procedures, such as Hartree-Fock, Gutzwiller, RVB, slave boson state, perturbation,[2,8,9] 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,[1,10] 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,[11] where the electrons condense in a variational state characterized by off-diagonal long-range order.[12] 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_ϕ. 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_ϕ, including, in particular, the ground state, divides in two classes ψ_1 and ψ_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 quasiparticles,[13] has already provided the ground-state energy of the one-dimensional Hubbard model in excellent agreement with the exact result.[5] In the general case of arbitrary dimension and general Hamiltonian investigated in this work, it is necessary to introduce an auxiliary Hilbert space $S_{\otimes\phi}$ in order to derive the ψ_1 or ψ_2 like properties of the eigenstates. $S_{\otimes\phi}$ is built over a set of pairs characterized by their total momentum K and projected spin ζ. Other authors[11,14,15] have also used such sets, nevertheless they remained within the framework of S_ϕ.

The outline is as follows: in Sec. II, the many-body Hamiltonian H is presented and the problem to be solved is

set out; Sec. III provides the definition of the auxiliary space $S_{\otimes\phi}$ as well as its algebraic properties; Secs. IV and V detail the proofs of two theorems establishing the either ψ_1 like and ψ_2 like properties of the eigenstates of H in the usual space of Slater determinants S_ϕ (a partial account of Sec. IV has been published elsewhere[16]); the physical consequences of these results are summarized in the concluding Sec. VI.

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 $n\leqslant N$. Let the electrons be coupled via a spin independent pair potential V. The total system Hamiltonian H can be written in reciprocal space as

$$H=\sum_{k,\sigma} E(k)c^{\dagger}_{k,\sigma}c_{k,\sigma} + \sum_{K,k,k',\sigma_{i=1,\ldots,4}} V(K,k,k')c^{\dagger}_{k,\sigma_1}c^{\dagger}_{K-k,\sigma_2}c_{K-k',\sigma_3}c_{k',\sigma_4}, \tag{1}$$

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 $c^{\dagger}_{k,\sigma}$ and $c_{k,\sigma}$ are one-electron creation and annihilation operators on the Bloch state k,σ. 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 on $(k-k')$. 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 $E(k)=\cos(\Sigma k_i)$, 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_ϕ of dimension $d_\phi=\binom{2N}{2n}$. Each basis vector ϕ_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 $b_\zeta(k,k')$, $b_\zeta(k,k')$:

$$b^{\dagger}_{\pm 1}(k,k')=c^{\dagger}_{k,\pm}c^{\dagger}_{k',\pm}, \quad b_{\pm 1}(k,k')=c_{k',\pm}c_{k,\pm}$$
$$b^{\dagger}_{0}(k,k')=c^{\dagger}_{k,+}c^{\dagger}_{k',-}, \quad b_{0}(k,k')=c_{k',-}c_{k,+}. \tag{2}$$

The subscripts $+$ or $-$ in the one-electron $c^{(\dagger)}$ 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:

$$H=H_D+\sum_{K,\zeta=0,\pm 1} H_{K,\zeta}, \tag{3}$$

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

$$H_D=\sum_{k,\sigma} E(k)c^{\dagger}_{k,\sigma}c_{k,\sigma}+\sum_{k,k'} V(k+k',k,k) \times c^{\dagger}_{k,+}c_{k,+}c^{\dagger}_{k',-}c_{k',-}+\sum_{k,k',\sigma}[V(k+k',k,k) - V(k+k',k,k')]c^{\dagger}_{k,\sigma}c_{k,\sigma}c^{\dagger}_{k',\sigma}c_{k',\sigma},$$

$$H_{K,0}=\sum_{k,k'\neq k} V(K,k,k')b^{\dagger}_0(k,K-k)b_0(k',K-k'),$$

$$H_{K,\pm 1}=\sum_{k,k'\neq (k,K-k)} V(K,k,k')b^{\dagger}_{\pm 1}(k,K-k)b_{\pm 1} \times (k',K-k'). \tag{4}$$

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 $\Sigma_{k,\sigma}E(k)c^{\dagger}_{k,\sigma}c_{k,\sigma}+(U/N)\Sigma_{k,k'}c^{\dagger}_{k,+}c_{k,+}c^{\dagger}_{k',-}c_{k',-}$ and $h_{K,\pm 1}=0$ for every K. Note also that the BCS Hamiltonian reads as $H_D+H_{K=0,\zeta=0}$, where H_D and $H_{K=0,\zeta=0}$ are given by their particular expressions in the Hubbard Hamiltonian.

The main purpose of this paper is to present and demonstrate two theorems which characterize the two classes of eigensolutions ψ,ϵ of the time-independent Schrödinger equation $(H-\epsilon)\psi=0$, where H is given by Eq. (1) and ψ belongs to the Hibert space S_ϕ. These classes are designated, respectively, as ψ_1,ϵ_1 and ψ_2,ϵ_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* ψ_1,ϵ_1 *of* H *such that* $(H-\epsilon_1)\psi_1=0$.

The characteristic property of each ψ_1 is that its linear expansion over the basis vectors of S_ϕ contains at least one Slater determinant ϕ which can be written as

$$\phi=\prod_{j=1}^{n} b^{\dagger}_{\zeta}(k_j,K-k_j)|0\rangle, \tag{5}$$

where $|0\rangle$ designates the no-electron state. Note that $\psi_{K,\zeta}$, in general, is not an eigenvector of H although ϵ_1 is indeed an eigenvalue of H.

Theorem 2: *For every* ψ_2,ϵ_2, *the equation* $(H-\epsilon_2)\psi_2=0$ *implies that* $(H_D-\epsilon_2)\psi_2=0$.

Each ψ_2 is characterized by the property that its linear expansion over the basis vectors of S_ϕ contains no Slater determinant such as ϕ in Eq. (5) for every K and ζ.

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 $N_{K,\zeta}$:

$$N_{K,\zeta}=\sum_k b^\dagger_\zeta(k,K-k)b_\zeta(k,K-k). \tag{6}$$

Our aim hence is to generalize the result of reference[17] 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_ϕ of Slater determinants. It becomes then necessary to treat the problem in an auxiliary Hilbert space $S_{\otimes\phi}$, which is purposely constructed so that H and $N_{K,\zeta}$ commute in this space, keeping invariant their definitions as in Eq. (1) and Eq. (6).

As ψ_1 eigenstates will be shown in addition to have off-diagonal long-range order whereas ψ_2 eigenstates do not have off-diagonal long-range order, it is necessary to recall the definition of the two-body correlation function attached to this particular kind of long-range order characterizing the BCS state:

$$f_{\text{odlro}}(|\tau|)=\sum_{i,j,l,m,\sigma_{h=1,\ldots,4}}\langle\phi|c^\dagger_{i,\sigma_1}c^\dagger_{j,\sigma_2}c_{l,\sigma_3}c_{m,\sigma_4}|\phi\rangle, \tag{7}$$

where the Wannier operator $c^{(\dagger)}_{i,\sigma_h}$ destroys (creates) an electron with spin σ_h at site i labeled by the lattice vector r_i and the sum is done with $(r_j-r_i)=(r_m-r_l)=\rho$, $(r_i-r_l)=\tau$, and $\sigma_1+\sigma_2=\sigma_3+\sigma_4$. Equation (7) extends to the $\rho\neq0$ case the usual definition of off-diagonal long-range order[12] 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 ρ 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 characterized by the following two-body correlation function:

$$f_{\text{rslro}}(|\tau|)=\sum_{i,j,\sigma_{h=1,..4}}(\langle\phi|c^\dagger_{i,\sigma_1}c_{i,\sigma_2}c^\dagger_{j,\sigma_3}c_{j,\sigma_4}|\phi\rangle - \langle\phi|c^\dagger_{i,\sigma_1}c_{i,\sigma_2}|\phi\rangle\langle\phi|c^\dagger_{j,\sigma_3}c_{j,\sigma_4}|\phi\rangle), \tag{8}$$

where the sum is done with $(r_i-r_j)=\tau$ 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 $f_{\text{rslro}}(|\tau|)$ oscillates versus $|\tau|$ without decaying to zero for $|\tau|\to\infty$. By comparing the definition in Eq. (7) with that in Eq. (8), it is realized that $f_{\text{odlro}}(|\tau|)\neq f_{\text{rslro}}(|\tau|)$ even if $\rho=0$. Besides from the experimental point of view, real space long-range order gives rise to Bragg difffraction in a neutron or x-ray scattering experiment while off-diagonal long-range order does not.

III. PROPERTIES OF THE AUXILIARY HILBERT SPACE $S_{\otimes\phi}$

Any Slater determinant ϕ_e of S_ϕ can be written as

$$\phi_e=\prod_{K,\zeta}\left(\prod_{j=1}^{n_{K,\zeta}}b^\dagger_\zeta(k_j,K-k_j)\right)|0\rangle, \tag{9}$$

where all pairs $b^\dagger_\zeta(k_j,K-k_j)|0\rangle$ having the same K and ζ 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 $n_{K,\zeta}\geq0$ designates the total number of pairs characterized by K,ζ in ϕ_e, and the $n_{K,\zeta}$'s satisfy $\Sigma_{K,\zeta}n_{K,\zeta}=n$. The basis vector $\Phi_{e,\alpha}$ of $S_{\otimes\phi}$ is defined from ϕ_e as

$$\Phi_{e,\alpha}=\otimes_{K,\zeta}\phi_{K,\zeta},\quad \phi_{K,\zeta}=\prod_{j=1}^{n_{K,\zeta}}b^\dagger_\zeta(k_j,K-k_j)|0\rangle, \tag{10}$$

where the tensor product replaces the simple product $\Pi_{K,\zeta}$ of Eq. (9) and each $\phi_{K,\zeta}$ is a Slater determinant containing $n_{K,\zeta}$ of pairs K,ζ. The sequence of integers $\{n_{K,\zeta}\}$ in Eqs. (9), (10) defines uniquely the pair configuration α of ϕ_e. Therefore $n_{K,\zeta}$ will be denoted $n_{K,\zeta,\alpha}$ in the following. The set of pair configurations of ϕ_e can be obtained by selecting m permutations of $2n$ one-electron Bloch states defining ϕ_e. The number of pair configurations $m=(2n)!/(2^n(n!))$ is smaller than that of permutations $(2n)!$ because many different permutations correspond to the same pair configuration. The basis vectors $\Phi_{e,\alpha}$ of $S_{\otimes\phi}$ are generated by letting the subscripts $e=1,..d_\phi$ and $\alpha=1,..m$ run over all possible values, which implies that the dimension of $S_{\otimes\phi}$ is equal to md_ϕ. The pair number operator $N_{K,\zeta}$ is taken to act on $\Phi_{e,\alpha}$ as follows:

$$N_{K,\zeta}\Phi_{e,\alpha}=n_{K,\zeta,\alpha}\Phi_{e,\alpha}. \tag{11}$$

As the $\Phi_{e,\alpha}$'s are chosen to be orthonormal, Eq. (11) entails that $n_{K,\zeta,\alpha}=\langle\Phi_{e,\alpha}|N_{K,\zeta}|\Phi_{e,\alpha}\rangle$.

The subspace $S_\Phi\subset S_{\otimes\phi}$ is then introduced as spanned by the basis vectors Φ_e defined by

$$\Phi_e=\sum_{\alpha=1}^{m}\Phi_{e,\alpha}, \tag{12}$$

where the sum is carried over m pair configurations α of ϕ_e. Owing to the one to one correspondence between $\phi_e\in S_\phi$ and $\Phi_e\in S_\Phi$, the dimension of S_Φ is inferred to be equal to d_ϕ. Although S_Φ and $S_{\otimes\phi}$ obey the Pauli principle by construction, the vectors $\Phi_e\in S_\Phi$ and $\Phi_{e,\alpha}\in S_{\otimes\phi}$ 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 $S_{\otimes\phi}$ is larger than that of S_Φ, arises as in other works[14,15] 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.

We now introduce the subspaces $S_{K,\zeta}\subset S_\Phi$ and $S_2\subset S_\Phi$, where $S_{K,\zeta}$ is defined for each K,ζ as spanned by the basis vectors $\Phi_{i=1,..d_\zeta}$, d_ζ being the dimension of $S_{K,\zeta}$. By definition each Φ_i is associated with a Slater determinant ϕ_i of S_ϕ, such as in Eq. (5) and thus comprising n pairs, all having the same K and ζ. The dimension d_ζ of $S_{K,\zeta}$ is $d_0=\binom{N}{n}$ or $d_{\pm1}=\binom{N/2}{n}$ depending on whether $\zeta=0$ or $\zeta=\pm1$, respectively. The characteristic property of each

Φ_i is that its pair configuration expansion, as given in Eq. (12), involves a particular value γ defined by

$$\Phi_i=\sum_{\alpha=1}^{m}\Phi_{i,\alpha},\quad n_{K,\zeta,\gamma}=\langle\Phi_{i,\gamma}|N_{K,\zeta}|\Phi_{i,\gamma}\rangle=n\Rightarrow n_{K',\zeta',\gamma}=\langle\Phi_{i,\gamma}|N_{K',\zeta'}|\Phi_{i,\gamma}\rangle=0, \tag{13}$$

where K' and ζ' take all possible values different from K and ζ, respectively. Each $\Phi_{i,\gamma}$ of $S_{\otimes\phi}$ is then written in the same expression as the Slater determinant ϕ_i of S_ϕ of Eq. (5), associated with Φ_i of $S_{K,\zeta}$, because the tensor product yielding $\Phi_{i,\gamma}$ as in Eq. (10) reduces to a single Slater determinant of n pairs K,ζ. Inversely the subspace S_2 is spanned by the basis vectors $\Phi_{p=1,..d_2}$ of S_Φ, d_2 being the dimension of S_2 (S_2 is named so because it will be shown hereafter to include all ψ_2-like eigenvectors). Each Φ_p is characterized by

$$\Phi_p=\sum_{\beta=1}^{m}\Phi_{p,\beta},n_{K,\zeta,\beta}=\langle\Phi_{p,\beta}|N_{K,\zeta}|\Phi_{p,\beta}\rangle<n,\quad\forall K,\zeta, \tag{14}$$

where the inequality holds for every β value involved in the pair configuration expansion of Φ_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_Φ:

$$S_\Phi=S_2\oplus\underset{K,\zeta}{S_{K,\zeta}},\quad d_\phi=d_2+N(d_0+2d_{\pm1}). \tag{15}$$

Consider now the following expression for the Hamiltonian H' in $S_{\otimes\phi}$:

$$H'=\sum_{i,j}\langle\phi_i|H|\phi_j\rangle|\Phi_{i,\gamma}\rangle\langle\Phi_{j,\gamma}|+\sum_{p,q,\beta}m_{pq}\langle\phi_p|H|\phi_q\rangle|\Phi_{p,\beta}\rangle\langle\Phi_{q,\beta}|, \tag{16}$$

where the sum with respect to i,j is performed on all Slater determinants ϕ_i and ϕ_j associated, respectively, with $\Phi_i\in S_{K,\zeta}$ and $\Phi_j\in S_{K,\zeta}$, the pair configuration γ is defined in Eq. (13) and K,ζ take all possible values. The sum with respect to p,q is carried over all Φ_p and Φ_q such that Φ_p or Φ_q belong to S_2. The matrix elements $\langle\phi_i|H|\phi_j\rangle$ and $\langle\phi_p|H|\phi_q\rangle$ are calculated with H given by Eq. (1). As $\langle\phi_p|H|\phi_q\rangle\neq0$ requires that the Slater determinants ϕ_p and ϕ_q differ by one pair only, and they read $\phi_p=b_\zeta^\dagger(k,K-k)\phi_{pq}|0\rangle$ and $\phi_q=b_\zeta^\dagger(k',K-k')\phi_{pq}|0\rangle$, where ϕ_{pq} comprises the product of $(n-1)$ pairs, the sum with respect to β is made with $m_{pp}=1/m$ and $m_{pq}=(2n-1)/m$ over $m/(2n-1)$ pair configurations common to Φ_p and Φ_q. The definition of H' in Eq. (16) ensures that the matrix elements $\langle\Phi_e|H'|\Phi_f\rangle$ and $\langle\phi_e|H|\phi_f\rangle$, are equal for all e,f values where ϕ_e,ϕ_f are two Slater determinants of S_ϕ and Φ_e,Φ_f are the corresponding basis vectors of S_Φ. 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 ϵ and there is a one to one correspondence between ψ and Ψ.

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

$$(H'-\epsilon)\Psi=0,\quad\Psi=\sum_{e=1}^{d_\phi}a_e\Phi_e,\quad\Phi_e=\sum_{\alpha=1}^{m}\Phi_{e,\alpha}\Rightarrow(H'-\epsilon)\Psi_\alpha=0,\quad\Psi_\alpha=\sum_{e=1}^{d_\phi}a_e\Phi_{e,\alpha},\quad\Psi=\sum_\alpha\Psi_\alpha, \tag{17}$$

where the coefficients a_e are real, the sum over α is the pair configuration expansion of Φ_e, and Ψ_α belongs to $S_{\otimes\phi}$.

IV. PROOF OF THEOREM 1

Consider the Schrödinger equation $(H'-\epsilon_1)\Psi_1=0$, where the eigenvector $\Psi_1\in S_\Phi$ is assumed to have a nonvanishing projection in $S_{K,\zeta}$ and thus reads

$$\Psi_1=\Psi_{K,\zeta}+\Psi_1',\quad\Psi_{K,\zeta}=\sum_{i=1}^{d_\zeta}a_i\Phi_i,\quad\Psi_1'=\sum_{p=1}^{d_2}a_p\Phi_p, \tag{18}$$

where the coefficients a_i,a_p are real and the Φ_i's and Φ_p's are basis vectors of $S_{K,\zeta}$ and S_2, respectively. We now apply Eq. (17) to Ψ_1 for the particular pair configuration γ defined in Eq. (13):

$$(H'-\epsilon)\Psi_{1,\gamma}=0,\quad\Psi_{1,\gamma}=\Psi_{K,\zeta,\gamma}+\Psi_{1,\gamma}'. \tag{19}$$

As the vector Ψ_1' is inferred from the definition of Φ_p in Eq. (14) 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. (4) and any two Slater determinants ϕ_i,ϕ_j associated with the basis vectors Φ_i,Φ_j of $S_{K,\zeta}$, it comes finally

$$(H'-\epsilon_1)\Psi_{1,\gamma}=0\Rightarrow(H_D+H_{K,\zeta}-\epsilon_1)\Psi_{K,\zeta,\gamma}=0\Leftrightarrow(H_D+H_{K,\zeta}-\epsilon_1)\psi_{K,\zeta}=0, \tag{20}$$

where $\psi_{K,\zeta}\in S_\phi$ is in one to one correspondence with $\Psi_{K,\zeta}\in S_\Phi$. Equation (20) means that, if $(\psi_{K,\zeta}+\psi_1')$ and ϵ_1 are eigenvector and eigenvalue of H in S_ϕ, the vector $\psi_{K,\zeta}$ and ϵ_1 are eigenvector and eigenvalue of $(H_D+H_{K,\zeta})$ in S_ϕ 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 ψ_1,ϵ_1 of H. The latter will be proved now by contradiction. Suppose that there is an eigenvalue 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_ζ to the spectrum of

H, which will result in an uncomplete diagonal basis for H and is thus at odds with the property of H being hermitian. Q.E.D.

Both $\psi_{K,\zeta}$ and the BCS variational state[11] consist of a linear combination of Slater determinants of pairs having the same K,ζ. 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,[12] off-diagonal long-range order, as defined in Eq. (7), is a fingerprint of $\psi_{K,\zeta}$:

$$f_{\mathrm{odlro}}(|\tau|)=\cos(K\tau)\Delta, \tag{21}$$

$$\Delta=\sum_{k,k'} e^{i[(k-k')\rho]}\langle\psi_{K,\zeta}|b_\zeta^\dagger(k,K-k)b_\zeta(k',K-k')|\psi_{K,\zeta}\rangle,$$

where Δ is a two-body correlation parameter attached to $\psi_{K,\zeta}$. Actually $f_{\mathrm{odlro}}(|\tau|)$ results from a sum over all K',ζ' but the contributions with $(K',\zeta')\neq(K,\zeta)$ vanish identically. $f_{\mathrm{odlro}}(|\tau|)$ oscillates without decaying for $|\tau|\to\infty$ provided $\Delta\neq 0$. It will be shown in the following section that ψ_1' [see Eq. (18)] contributes nothing to $f_{\mathrm{odlro}}(|\tau|)$ for $|\tau|\to\infty$, so that $\psi_{K,\zeta}$ and ψ_1 have the same off-diagonal long-range order parameter. In the Hubbard model, the validity of theorem 1 has been confirmed[12] for a large class of many-electron eigenstates $[K=(\pi,\pi,\pi),\zeta=0]$, built with help of the η- 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 Ψ_2 belongs to the subspace S_2 of S_Φ:

$$\Psi_2=\sum_{p=1}^{d_2} a_p\Phi_p,\quad \Phi_p=\sum_{\beta=1}^{m}\Phi_{p,\beta},$$

$$\Psi_{2,\beta}=\sum_{p=1}^{d_2} a_p\Phi_{p,\beta},$$

$$\Psi_2=\sum_\beta \Psi_{2,\beta}, \tag{22}$$

where the a_p's are real and the pair configuration expansion of Φ_p is done with respect to β. 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 Φ_p and Φ_q in the linear expansion giving Ψ_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 $(H'-\epsilon_2)\Psi_2=0$:

$$(H'-\epsilon_2)(a_1\Phi_1+a_2\Phi_2)+\sum_{q\neq 1,2}(\langle\Phi_q|H_D|\Phi_q\rangle-\epsilon_2)a_q\Phi_q=0. \tag{23}$$

As the basis vectors Φ_q are linearly independent, Eq. (23) implies that:

$$(H'-\epsilon_2)(a_1\Phi_1+a_2\Phi_2)=0,\quad \langle\Phi_q|H_D|\Phi_q\rangle=\epsilon_2,$$

$$\forall q\neq 1,2. \tag{24}$$

As seen in Eq. (16), $\langle\Phi_1|H'|\Phi_2\rangle\neq 0$ requires that Φ_1 and Φ_2 differ by one pair only so that they read $\Phi_1=b^\dagger(k_1,k_2)|0\rangle\otimes\Phi_{12}$ and $\Phi_2=b^\dagger(k_3,k_4)|0\rangle\otimes\Phi_{12}$, where the spin index ζ is dropped for simplicity until the end of this proof, $k_1+k_2=k_3+k_4$ and Φ_{12} includes $(n-1)$ pairs. Moreover, due to Eq. (17), the expression $(H'-\epsilon_2)(a_1\Phi_1+a_2\Phi_2)=0$ in Eq. (24) splits in $S_{\otimes\phi}$ into partial Schrödinger equations $(H'-\epsilon_2)(a_1\Phi_{1,\beta}+a_2\Phi_{2,\beta})=0$, where the pair configuration index β runs over all values allowed by Eq. (22). The particular case of β, where the pair numbers $n_{k_1+k_2,\beta}=n_{k_3+k_4,\beta}=1$, is of interest, in order to work out the proof. Then Eq. (16) entails that

$$(H'-\epsilon_2)(a_1\Phi_{1,\beta}+a_2\Phi_{2,\beta})=0\Leftrightarrow$$

$$\{(H'-\epsilon_2)[a_1b^+(k_1,k_2)|0\rangle+a_2b^+(k_3,k_4)|0\rangle]\}\otimes\Phi_{12}=0. \tag{25}$$

Because of $\Phi_{12}\neq 0$, Eq. (25) implies that each eigenvalue ϵ_2 of H' in S_2 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_2 of S_2 is such that $d_2\leqslant d_s$, 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 Φ_p making up the linear expansion of Ψ_2 in Eq. (22). Q.E.D.

As every off-diagonal term $\langle\Phi_p|H'|\Phi_q\rangle$ vanishes for the Φ_p,Φ_q states coming up in the linear expansion of Ψ_2 in Eq. (22), the off-diagonal and real space long-range order parameters in Eqs. (7), (8) reduce both for ψ_2 to a two-particle distribution function:

$$f_{\mathrm{odlro}}(|\tau|)=\sum_{k,k',\sigma}\{\cos[(k+k')\tau]-\cos[(k+k')\tau+(k-k')\rho]\}\langle\psi_2|c_{k,+}^\dagger c_{k,+}c_{k',\sigma}^\dagger c_{k',\sigma}|\psi_2\rangle$$

$$\times f_{\mathrm{rslro}}(|\tau|)=\sum_{k,k',\sigma}\cos[(k-k')\tau]\times\langle\psi_2|c_{k,+}^\dagger c_{k,+}c_{k',\sigma}^\dagger c_{k',\sigma}|\psi_2\rangle. \tag{26}$$

As a consequence of Riemann-Lebesgue's theorem due to the oscillating character of $\cos[(k\pm k')\tau]$, $f_{\mathrm{rslro}}(|\tau|)$ and $f_{\mathrm{odlro}}(|\tau|)$, calculated with ρ kept fixed, decay towards zero for $|\tau|\to\infty$ so that ψ_2 has neither off-diagonal nor real space long-range order. Furthermore they may behave like power laws for large $|\tau|$ 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 ψ_1, ϵ_1 and ψ_2, ϵ_2 in the space of Slater determinants. The ψ_1's are characterized by a nonvanishing projection in the space $S_{K,\zeta}$, denoted $\psi_{K,\zeta}$. This latter is responsible for off-diagonal long-range order and fulfills $(H_D + H_{K,\zeta} - \epsilon_1)\psi_{K,\zeta} = 0$, whereas the ψ_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 ζ in a scattering process.

To realize that off-diagonal long-range order and real space long-range order have different properties, it is illuminating to discuss the simple case of two electrons coupled by a one-dimensional Hubbard Hamiltonian.[17] This system sustains a single band of bound eigenstates $\psi_{K,\zeta=0}$. As $\psi_{K,\zeta=0}$ is ψ_1-like, its off-diagonal long-range order parameter $f_{\mathrm{odlro}}(|\tau|)$ oscillates like $\cos(K\tau)$, while its real space long-range order parameter $f_{\mathrm{rslro}}(|\tau|)$ decays like $e^{-|\tau|/l}$, 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 the theorem of Mermin-Wagner,[3] which rules out that 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, the theorem of Mermin-Wagner 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 ψ_1- or ψ_2-like, theorem 1 ensures that off-diagonal long-range order is not a sufficient criterion for superconductivity.

As far as ψ_1-like solutions are concerned, the results of this work enable one to diagonalize 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_ϕ. At last they provide useful constraints on the variational states currently used in the many-body problem such as those quoted in Sec. I. Indeed any variational state within the frame of reference of this work which is recognized to be neither ψ_1- nor ψ_2-like is unphysical even though it may fortuitously approximate the ground-state energy. In particular, as the ground-state energies of the one- and two-dimensional Hubbard Hamiltonians are smaller[5,7] than the lowest eigenvalue of H_D, the respective ground states are inferred to be ψ_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 $\phi = c^\dagger_{k_1} c^\dagger_{k_2} c^\dagger_{k_3} c^\dagger_{k_4} |0\rangle$ where k_1, k_2, k_3, k_4 are four vectors of the Brillouin zone and the spin indices σ, ζ are dropped for simplicity in this example. An application of Eqs. (10), (12) yields $m=3$ and $\Phi_{\alpha=1} = b^\dagger(k_1,k_2)|0\rangle \otimes b^\dagger(k_3,k_4)|0\rangle$, $\Phi_{\alpha=2} = b^\dagger(k_1,k_3)|0\rangle \otimes b^\dagger(k_4,k_2)|0\rangle$, $\Phi_{\alpha=3} = b^\dagger(k_1,k_4) b^\dagger(k_2,k_3)|0\rangle$, 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 characterized by the pair numbers $n_{k_1+k_2,\alpha=1} = n_{k_3+k_4,\alpha=1} = n_{k_1+k_3,\alpha=2} = n_{k_4+k_2,\alpha=2} = 1, n_{k_1+k_4,\alpha=3} = 2$. Notice that Φ_1, Φ_2, Φ_3 are three linearly independent vectors of $S_{\otimes\phi}$, all associated with the same vector Φ of S_Φ or equivalently ϕ of S_ϕ.

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