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OFF-DIAGONAL LONG-RANGE ORDER IN MANY-ELECTRON PROBLEM

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The interacting electron Hamiltonian $H = H_{\mathrm{D}} + \sum_{K,\zeta} H_{K,\zeta}$ is considered in the Hilbert space spanned by Slater determinants of Bloch wave functions. H_{D} consists of the diagonal part of H in this basis. K and $\zeta = 0, \pm 1$ stand for the total momentum and projected spin of electron pairs and $H_{K,\zeta}$ is the off-diagonal part of H describing the most general two-electron scattering process conserving K and ζ. It is shown that the eigenspectrum of H includes all eigenvalues of $H_{\mathrm{D}}+H_{K,\zeta}$ for every K and ζ value. The associated eigenvectors of H are shown to have off-diagonal long-range order.

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1. Introduction

The interest for the study of electron correlations in metals has kept growing because of their significance in magnetism and superconductivity [1, 2]. This work presents a mathematical proof that H, a general many-body Hamiltonian, operating in S_ϕ, the Hilbert space spanned by Slater determinants, has numerous eigenstates characterised by having off-diagonal long-range order [3] which was introduced as a fingerprint of the BCS state [2]. To work out the proof, it is necessary to introduce an auxiliary Hilbert space $S_{\otimes\phi}$ which is built over a set of pairs characterised by their total momentum K and projected spin ζ.

2. The many-body Hamiltonian

A crystal of arbitrary dimension, containing N sites and $2n$ electrons where $N \gg 1$ and $n \gg 1$ is considered hereafter. These electrons populate a single band of dispersion $E(k)$ where k is a vector of the Brillouin zone. $E(k)$ is assumed to be independent of the electron spin $\sigma = \pm 1/2$. The Pauli principle requires that $n \leq N$. The total system Hamiltonian H can be written in reciprocal space as

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

The Fermi operators $c^{+}_{k,\sigma}$ and $c_{k,\sigma}$ account for electron creation and annihilation on the Bloch state k, σ. The real coefficients $V(K,k,k')$ are the matrix elements of the two-electron scattering process. 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 $\sigma_1+\sigma_2=\sigma_3+\sigma_4$. The Hamiltonian H describes the electron motion in the Hilbert space S_ϕ of dimension d_ϕ. Each basis vector ϕ_i with $i=1\dots d_\phi$ is a Slater determinant involving $2n$ one-electron Bloch states.

It is convenient to introduce the pair creation and annihilation operators $b^+_{\pm1}(k,k')=c^+_{k,\pm\sigma}c^+_{k',\pm\sigma}$, $b_{\pm1}(k,k')=c_{k',\pm\sigma}c_{k,\pm\sigma}$, $b^+_0(k,k')=c^+_{k,\sigma}c^+_{k',-\sigma}$, $b_0(k,k')=c_{k',-\sigma}c_{k,\sigma}$. The subscript $\zeta=0,\pm1$ stands for the projection of the total spin of the pair. It is useful to recast the Hamiltonian H of Eq. (1) in terms of the subsidiary Hamiltonians $H_{\rm D}$, $H_{K,\zeta}$ as $H=H_{\rm D}+\sum_{K,\zeta=0,\pm1}H_{K,\zeta}$ where $H_{\rm D}$ and $H_{K,\zeta}$ read as

$$
\begin{aligned}
H_{\rm D} &= \sum_{k,\sigma}E(k)c^+_{k,\sigma}c_{k,\sigma}+\sum_{k,k'}V(k+k',k,k)c^+_{k,\sigma}c_{k,\sigma}c^+_{k',-\sigma}c_{k',-\sigma} \\
&\quad+\sum_{k,k',\sigma}\left[V(k+k',k,k)-V(k+k',k,k')\right]c^+_{k,\sigma}c_{k,\sigma}c^+_{k',\sigma}c_{k',\sigma}, \\
H_{K,0} &= \sum_{k,k'\neq k}V(K,k,k')b^+_0(k,K-k)b_0(k',K-k'), \\
H_{K,\pm1} &= \sum_{k,k'\neq(k,K-k)}V(K,k,k')b^+_{\pm1}(k,K-k)b_{\pm1}(k',K-k').
\end{aligned}
\tag{2}
$$

The purpose of this article is to demonstrate the following theorem characterising a class of eigensolutions ψ,ϵ of the Schrödinger equation $(H-\epsilon)\psi=0$ where H is given by Eq. (1) and ψ belongs to the Hilbert space S_ϕ:

3. Theorem

To each eigensolution $\psi_{K,\zeta},\epsilon$ where $(H_{\rm D}+H_{K,\zeta}-\epsilon)\psi_{K,\zeta}=0$, there corresponds an eigensolution ψ,ϵ of H such that $(H-\epsilon)\psi=0$.

Furthermore it will be shown that ψ has off-diagonal long-range order. Although it is easy to prove [4] this theorem in S_ϕ for a single pair ($n=1$), it becomes necessary to treat the problem in an auxiliary Hilbert space [5, 6] $S_{\otimes\phi}$ for $n>1$.

4. Properties of $S_{\otimes\phi}$

Any Slater determinant ϕ_i of S_ϕ can be written as

$$
\phi_i=\prod_{K,\zeta}\left(\prod_{j=1}^{n_{K,\zeta}}b^+_\zeta(k_j,K-k_j)\right)|0\rangle, \tag{3}
$$

where $|0\rangle$ designates the no-electron state and all pairs $b^+_\zeta(k_j,K-k_j)|0\rangle$ having the same K and ζ have been regrouped together. In the product with respect to the index j, the i dependence of j has been dropped for simplicity. The integer $n_{K,\zeta}\geq 0$ designates the total number of pairs characterised by K,ζ in ϕ_i, and the $n_{K,\zeta}$'s satisfy $\sum_{K,\zeta}n_{K,\zeta}=n$. The basis vector $\Phi_{i,\alpha}$ of $S_{\otimes\phi}$ is defined from ϕ_i as

$$
\Phi_{i,\alpha}=\bigotimes_{K,\zeta}\phi_{K,\zeta},\quad \phi_{K,\zeta}=\prod_{i=1}^{n_{K,\zeta}}b^+_\zeta(k_j,K-k_j)\,|0\rangle, \tag{4}
$$

where the tensor product replaces the simple product $\prod_{K,\zeta}$ of Eq. (3) 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. (3), (4) defines uniquely the pair configuration α of ϕ_i. As a large number of linearly independent vectors $\Phi_{i,\alpha} \in S_{\otimes\phi}$ are characterised by the same pair configuration α, $n_{K,\zeta}$ does not depend on the index i but conversely depends on the index α and will therefore be denoted $n_{K,\zeta,\alpha}$ in the following. The whole set of pair configurations of ϕ_i is obtained by selecting m permutations of $2n$ one-electron Bloch states defining ϕ_i. The basis vectors $\Phi_{i,\alpha}$ of $S_{\otimes\phi}$ are generated by allowing the subscripts $i = 1\dots d_\phi$ and $\alpha = 1\dots m$ to run over all possible values, which implies that the dimension of $S_{\otimes\phi}$ is equal to md_ϕ. The $\Phi_{i,\alpha}$'s are chosen to be orthonormal.

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

$$\Phi_i = \sum_{\alpha=1}^{m} \Phi_{i,\alpha}, \tag{5}$$

where the sum is carried over m pair configurations α of ϕ_i. Owing to the one to one correspondence between $\phi_i \in S_\phi$ and $\Phi_i \in S_\Phi$, the dimension of S_Φ is inferred to be equal to d_ϕ.

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,ζ as spanned by the basis vectors $\Phi_{i=1\dots d_\zeta}$, d_ζ being the dimension of $S_{K,\zeta}$. By definition each Φ_i is associated with a Slater determinant of S_ϕ, comprising n pairs, all having the same K and ζ. Hence the characteristic property of each Φ_i is that its pair configuration expansion, as given in Eq. (5), involves a particular value γ so that the tensor product yielding $\Phi_{i,\gamma}$ as in Eq. (4) reduces to a single Slater determinant $\phi_{K,\zeta}$ containing n of pairs K,ζ. Consequently every number of pairs K',ζ' in $\Phi_{i,\gamma}$ where K' and ζ' take all possible values different from K and ζ respectively, vanish for every $\Phi_{i,\gamma}$. Inversely the subspace S_2 is spanned by the basis vectors $\Phi_{p=1\dots d_2}$ of S_Φ, d_2 being the dimension of S_2. Each Φ_p is characterised by $n_{K,\zeta,\beta} < n$ for every K,ζ,β value where β is the pair configuration index of Φ_p and $n_{K,\zeta,\beta}$ stands for the number of pairs K,ζ in $\Phi_{p,\beta}$. As the subspaces S_2 and $S_{K,\zeta}$ are disjoint, they provide a basis for S_Φ.

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

$$H' = \sum_{i,j} \langle\phi_i|H|\phi_j\rangle|\Phi_{i,\gamma}\rangle\langle\Phi_{j,\gamma}| + \sum_{p,q,\beta} m_{pq}\langle\phi_p|H|\phi_q\rangle|\Phi_{p,\beta}\rangle\langle\Phi_{q,\beta}|, \tag{6}$$

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 $\Phi_j \in S_{K,\zeta}$ characterised by the pair configuration γ. 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 sum with respect to β is made with $m_{pp} = 1/m$ and $m_{pq} = (2n-1)/m$ over all pair configurations common to Φ_p and Φ_q. This definition of H' in Eq. (6) ensures that the matrix elements $\langle\Phi_e|H'|\Phi_f\rangle$, where H' is given by Eq. (6), and $\langle\phi_e|H|\phi_f\rangle$, where H is given by Eq. (1), are equal for all $e,f = 1\dots d_\phi$ 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. This ensures 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.

Since H' in Eq. (6) 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 $(H'-\epsilon)\Psi = 0$ splits into partial Schrödinger equations

$$(H'-\epsilon)\Psi = 0, \quad \Psi = \sum_{e=1}^{d_\phi} a_e \Phi_e, \quad \Phi_e = \sum_{\alpha=1}^{m} \Phi_{e,\alpha} \Rightarrow (H'-\epsilon)\Psi_\alpha = 0,$$
$$\Psi_\alpha = \sum_{e=1}^{d_\phi} a_e \Phi_{e,\alpha}, \quad \Psi = \sum_\alpha \Psi_\alpha, \tag{7}$$

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

5. Proof of the theorem

Consider the Schrödinger equation $(H'-\epsilon)\Psi = 0$ where H' is given by Eq. (6) and the eigenvector $\Psi \in S_\Phi$ is assumed to have a non-vanishing projection in $S_{K,\zeta}$ and thus reads

$$\Psi = \Psi_{K,\zeta} + \Psi', \quad \Psi_{K,\zeta} = \sum_{i=1}^{d_\zeta} a_i \Phi_i, \quad \Psi' = \sum_{p=1}^{d_2} a_p \Phi_p, \tag{8}$$

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. (7) to Ψ for the particular pair configuration γ:

$$(H'-\epsilon)\Psi_\gamma = 0, \quad \Psi_\gamma = \Psi_{K,\zeta,\gamma} + \Psi'_\gamma. \tag{9}$$

As the vector Ψ' is inferred from its definition not to contribute to Ψ_γ, it ensues that Ψ_γ reduces to $\Psi_{K,\zeta,\gamma}$. Because of $\langle\phi_i|H|\phi_j\rangle = \langle\phi_i|H_\mathrm{D} + H_{K,\zeta}|\phi_j\rangle$ which holds for the Hamiltonians H_D and $H_{K,\zeta}$ in Eq. (2) 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

$$(H'-\epsilon)\Psi_\gamma = 0 \Rightarrow (H_\mathrm{D} + H_{K,\zeta} - \epsilon)\Psi_{K,\zeta,\gamma} = 0$$
$$\Leftrightarrow (H_\mathrm{D} + H_{K,\zeta} - \epsilon)\psi_{K,\zeta} = 0, \tag{10}$$

where $\psi_{K,\zeta} \in S_\phi$ is in one to one correspondence with $\Psi_{K,\zeta} \in S_\Phi$. Equation (10) means that if $(\psi_{K,\zeta} + \psi')$ and ϵ are eigenvector and eigenvalue of H in S_ϕ, the vector $\psi_{K,\zeta}$ and ϵ are eigenvector and eigenvalue of $(H_\mathrm{D} + H_{K,\zeta})$ in S_ϕ too. To complete the proof of theorem it must be shown in addition that every eigensolution $\psi_{K,\zeta}, \epsilon$ of $(H_\mathrm{D} + H_{K,\zeta})$ gives rise to an eigensolution ψ, ϵ of H. The latter will be proved now by contradiction. Suppose that there is an eigenvalue of some Hamiltonian $(H_\mathrm{D} + H_{K,\zeta})$ 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.

Because $\psi_{K,\zeta}$ and the BCS variational state [2] consist both of a linear combination of Slater determinants of pairs having the same K, ζ, they are characterised by off-diagonal long-range order [3]:

$$f_{odlro}(|\tau|) = \sum_{i,j,l,m,\eta} \langle\phi|c^+_{i,\sigma} c^+_{j,\eta\sigma} c_{m,\eta\sigma} c_{l,\sigma}|\phi\rangle, \tag{11}$$

where $\eta = \pm 1$, the Wannier operator $c_{i,\sigma}^{(+)}$ destroys (creates) an electron with spin σ at site i labeled by the lattice vector r_i, $(r_j - r_i) = (r_m - r_l) = \rho$, $(r_i - r_l) = \tau$. The two-body correlation function $f_{odlro}(|\tau|)$ is calculated at ρ kept fixed. The state $\phi \in S_\phi$ is said to have off-diagonal long-range order if $f_{odlro}(|\tau|)$ oscillates without decaying to zero for $|\tau| \to \infty$. Because for $\psi_{K,\zeta}$ and the BCS state it comes $f_{odlro}(|\tau|) = \cos(K\tau)\Delta$ where $\Delta = \sum_{k,k'} \cos[(k-k')\rho]\langle b_\zeta^+(k, K-k) b_\zeta(k', K-k')\rangle$, these both states are seen to have off-diagonal long-range order provided $\Delta \neq 0$.

6. Conclusion

The conclusion of the theorem is valid for arbitrary crystal dimension, electron concentration and two-electron coupling provided it conserves K and ζ. It enables one to find out all eigenstates of H having off-diagonal long-range order 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.

I dedicate this work to the memory of my parents Jochweta and Chaim and my niece Denise Lévy and I thank my wife Rachel and children Jérémie and Judith for providing encouragement.

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