η Pairing and Off-Diagonal Long-Range Order in a Hubbard Model

Chen Ning Yang
State University of New York, Stony Brook, New York 11794-3840
and Chinese University of Hong Kong, Hong Kong
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It is shown in a simple Hubbard model that through a mechanism called η pairing one can construct many eigenstates of the Hamiltonian possessing off-diagonal long-range order. The intrapair distance is small. It is shown that these eigenstates are metastable and possess an energy gap.

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Since the discovery of high-temperature superconductivity[1,2] in 1986–1987 there have been many proposals for the theoretical mechanism for such phenomena. None has been generally accepted. Most proposals concern some kind of Hubbard model, which unfortunately is difficult to solve except in one dimension.

In this paper we show that for the simplest Hubbard model in three dimensions (also in one or two dimensions), many eigenfunctions of the Hamiltonian can be explicitly written down. Of particular interest is the fact that these eigenfunctions possess off-diagonal long-range order (ODLRO), the property of a dynamical system that is essential[3] for the phenomena of superconductivity and superfluidity. This is a rather subtle long-range order, especially for fermions, and no previous models of fermions in dimensions higher than one has been *proven* to have eigenstates with ODLRO. The usual BCS wave function[4] does have ODLRO via the mechanism of Cooper pairs,[5] but it is not an eigenstate of a Hamiltonian system with a local potential energy.

The mechanism essential for the eigenfunctions of the present paper is a η-pairing mechanism which seems to be peculiar to lattice models, and is absent in any continuum model.

For the attractive case these eigenfunctions are shown to be metastable at low temperatures. They possess ODLRO, and thus are superconducting.

(1) η pairing.— Consider a three-dimensional Hubbard model on a periodic $L\times L\times L$ lattice where L is even ($\epsilon>0$):

$$H=T+V, \tag{1}$$

$$T=\epsilon\sum_{\mathbf{k}}(6-2\cos k_x-2\cos k_y-2\cos k_z)\times(a_{\mathbf{k}}^\dagger a_{\mathbf{k}}+b_{\mathbf{k}}^\dagger b_{\mathbf{k}}), \tag{2}$$

$$V=2W\sum_{\mathbf{r}}a_{\mathbf{r}}^\dagger a_{\mathbf{r}}b_{\mathbf{r}}^\dagger b_{\mathbf{r}}, \tag{3}$$

where $a_{\mathbf{r}}$ and $b_{\mathbf{r}}$ are coordinate-space annihilation operators for spin-up and spin-down electrons, respectively, and $\mathbf{r}$ is a three-dimensional integral coordinate variable that designates the $L\times L\times L$ lattices sites. The annihilation operators $a_{\mathbf{k}}$ and $b_{\mathbf{k}}$ are momentum-space operators given by

$$a_{\mathbf{k}}=(L)^{-3/2}\sum_{\mathbf{r}}a_{\mathbf{r}}\exp(-i\mathbf{k}\cdot\mathbf{r}), \tag{4}$$

where

$$\mathbf{k}=2\pi/L\ \text{(three-dimensional integer)}\ (\text{mod}\,2\pi). \tag{5}$$

We choose the fermion operators so that

$$[a_{\mathbf{k}},a_{\mathbf{k}'}^\dagger]_+=\delta(\mathbf{k}-\mathbf{k}'),\ \text{etc.},$$

but

$$[a_{\mathbf{k}},b_{\mathbf{k}'}]_-=[a_{\mathbf{k}},b_{\mathbf{k}'}^\dagger]_-=0. \tag{6}$$

The kinetic energy T of Eq. (2) is trivially different from the kinetic energy in the usual Hubbard model in the appearance of the term 6, which is inserted here to make T a positive operator. This insertion makes it possible to compare with such concepts in the continuum problem as particles, collisions, bound states, etc. No physical conclusion is altered by this insertion.

We shall show that many eigenstates of the Hamiltonian H can be explicitly written down with the aid of an operator η defined as

$$\eta=\sum_{\mathbf{k}}a_{\mathbf{k}}b_{\boldsymbol{\pi}-\mathbf{k}},\quad \boldsymbol{\pi}=(\pi,\pi,\pi). \tag{7}$$

Notice that this definition is only meaningful when L is even, because otherwise $\mathbf{k}$ and $\boldsymbol{\pi}-\mathbf{k}$ would not be simultaneously possible $\mathbf{k}$ values. Using (4), we also have

$$\eta=\sum_{\mathbf{r}}e^{-i\boldsymbol{\pi}\cdot\mathbf{r}}a_{\mathbf{r}}b_{\mathbf{r}}. \tag{8}$$

It is easy to prove

$$\eta^\dagger T-T\eta^\dagger=-12\epsilon\eta^\dagger, \tag{9}$$

by going into the representation where all $a_{\mathbf{k}}^\dagger a_{\mathbf{k}}$ and all $b_{\mathbf{k}}^\dagger b_{\mathbf{k}}$ are simultaneously diagonal. The basic kets in this representation will be denoted by $|n\rangle$. Now take $\langle n'|\ |n\rangle$ of both sides of (9). Since T is diagonal in this representation, (9) becomes

$$\langle n'|\eta^\dagger|n\rangle[\langle n|T|n\rangle-\langle n'|T|n'\rangle]=-12\epsilon\langle n'|\eta^\dagger|n\rangle. \tag{9'}$$

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Now (7) shows that $\langle n'|\eta^\dagger|n\rangle$ is nonvanishing if and only if $|n'\rangle$ is obtainable from $|n\rangle$ by creating, onto the state $|n\rangle$, a pair of a and b's with momenta $\mathbf{k}$ and $\boldsymbol{\pi}-\mathbf{k}$. If it is so obtainable, then

$$\langle n|T|n\rangle-\langle n'|T|n'\rangle=-12\epsilon .$$

Thus we have proved (9′). Hence also (9). Similarly we can prove

$$\eta^\dagger V-V\eta^\dagger=-2W\eta^\dagger \tag{10}$$

by going into the representation where all $a_\mathbf{r}^\dagger a_\mathbf{r}$ and all $b_\mathbf{r}^\dagger b_\mathbf{r}$ are simultaneously diagonal. Adding (9) and (10) we obtain

$$\eta^\dagger H-H\eta^\dagger=-(12\epsilon+2W)\eta^\dagger . \tag{11}$$

The total momenta operator $\mathbf{P}$ is

$$\mathbf{P}=\sum_\mathbf{k}(a_\mathbf{k}^\dagger a_\mathbf{k}+b_\mathbf{k}^\dagger b_\mathbf{k}) . \tag{12}$$

Both $\mathbf{P}$ and $\mathbf{k}$ are defined (mod2π). It is easy to prove, in the same way we proved (9), that

$$\eta^\dagger\mathbf{P}-\mathbf{P}\eta^\dagger=-\boldsymbol{\pi}\eta^\dagger . \tag{13}$$

Using (11) and (13) we can prove the following theorem:

Theorem 1.— If ϕ is a simultaneous eigenstate of H and of $\mathbf{P}$,

$$H\phi=E_\phi\phi,\quad \mathbf{P}\phi=\mathbf{P}_\phi\phi , \tag{14}$$

then a new simultaneous eigenstate ϕ' of H and of $\mathbf{P}$,

$$H\phi'=(E_\phi+12\epsilon+2W)\phi',\quad \mathbf{P}\phi'=(\mathbf{P}_\phi+\boldsymbol{\pi})\phi' , \tag{15}$$

is generated by $\phi'=\eta^\dagger\phi$, provided $\eta^\dagger\phi\neq 0$. Notice that ϕ' has one more a particle and one more b particle than ϕ.

(2) Eigenstate ψ_N.— Starting from the vacuum state $|\text{vac}\rangle$, by repeated use of the above theorem, we generate the state

$$\psi_N=\beta(\eta^\dagger)^N|\text{vac}\rangle , \tag{16}$$

which is a simultaneous eigenstate of H and P:

$$H\psi_N=N(12\epsilon+2W)\psi_N,\quad \mathbf{P}\psi_N=N\boldsymbol{\pi}\psi_N . \tag{17}$$

The constant β is a normalization factor, which is equal to

$$\beta=[N!(M-N)!/M!]^{1/2},\quad M=L^3 . \tag{18}$$

Is the state ψ_N the ground state for the system with N particles a and N particles b? The answer is no, because we can construct another state ψ_N' which has the same expectation value for H as ψ_N, but which is not an eigenstate. To construct ψ_N' we use the Cooper-pairing operator

$$\eta_C=\sum_\mathbf{k}a_\mathbf{k}b_{-\mathbf{k}}=\sum_\mathbf{r}a_\mathbf{r}b_\mathbf{r} \tag{19}$$

to define

$$\psi_N'=\beta'(\eta_C^\dagger)^N|\text{vac}\rangle . \tag{20}$$

It is easy to prove

$$\eta_C^\dagger V-V\eta_C^\dagger=-2W\eta_C^\dagger . \tag{21}$$

Thus

$$V\psi_N'=2NW\psi_N' . \tag{22}$$

It remains to prove $\langle\psi_N'|T|\psi_N'\rangle=12N\epsilon$. Using $\eta_C=\sum_\mathbf{k}a_\mathbf{k}b_{-\mathbf{k}}$ we find from (20) that ψ_N' is a sum of states, each of which is N Cooper pairs of a and b. For each such state ϕ_0 there is a corresponding state ϕ_1 in ψ_N' in which each Cooper pair's momenta is changed from $\mathbf{k}$ and $-\mathbf{k}$ to $\boldsymbol{\pi}-\mathbf{k}$ and $-(\boldsymbol{\pi}-\mathbf{k})$. Now ϕ_0 and ϕ_1 have equal weights in ψ_N'. Also ϕ_0 and ϕ_1 have kinetic energies whose arithmetic mean is $12N\epsilon$. Hence we have verified $\langle\psi_N'|T|\psi_N'\rangle=12N\epsilon$, and have thus proved that ψ_N is not the ground state.

It should be observed that the above does not *prove* that the true ground state has Cooper pairing.

The state ψ_1 is a bound pair (ab), bound in the sense that the average distance between a and b is zero, as is evident from (8). Its energy is $12\epsilon+2W$ which can be positive. The existence of such states is a peculiarity of the lattice model, which is absent in the many-particle problem in continuum models.

(3) ψ_N has ODLRO.— The eigenstate ψ_N defined by (16) is of a standard form for a state with ODLRO (cf. Appendix A of Ref. 3). The off-diagonal element of the reduced density matrix ρ_2 for this pure state ψ_N can be shown to be $\psi_N^\dagger a_\mathbf{s}^\dagger b_\mathbf{s}^\dagger b_\mathbf{r}a_\mathbf{r}\psi_N$, which is readily evaluated from (8) and (16):

$$\langle b_\mathbf{s}a_\mathbf{s}|\rho_2|b_\mathbf{r}a_\mathbf{r}\rangle=\frac{N(M-N)}{M(M-1)}e^{i\boldsymbol{\pi}\cdot(\mathbf{r}-\mathbf{s})}\quad(\mathbf{r}\neq\mathbf{s}) , \tag{23}$$

where

$$M=L^3=\text{number of states } a . \tag{24}$$

State ψ_N has ODLRO because the right-hand side of (23) does not approach zero as $\mathbf{r}-\mathbf{s}$ increases. It was shown in Ref. 3 that with such ODLRO the system should exhibit magnetic-flux quantization with flux unit $ch/2e$, the factor of 2 arising from the total charge of the pair (ab).

We observed that the size of the pair (ab) is zero lattice unit, much smaller than the usual Cooper pair.

(4) State near ψ_N.— What are the eigenstates of H near ψ_N? We confine ourselves to those states ζ that have the same total momenta as ψ_N:

$$H\zeta=E_\zeta\zeta,\quad \mathbf{P}\zeta=N\boldsymbol{\pi}\zeta . \tag{25}$$

We can construct many such states ζ with the operators

$$\eta_\mathbf{a}=\sum_\mathbf{k}e^{i\mathbf{k}\cdot\mathbf{a}}a_\mathbf{k}b_{\boldsymbol{\pi}-\mathbf{k}}=\sum_\mathbf{r}e^{-i\boldsymbol{\pi}\cdot\mathbf{r}}a_{\mathbf{r}+\mathbf{a}}b_\mathbf{r} . \tag{26}$$

Notice

$$\eta_0 = \eta\,, \tag{27}$$

$$[\eta_\alpha, \eta_\gamma]_- = 0\,. \tag{28}$$

It is easy to show that

$$(T - 12\epsilon)\,|\,\eta_\alpha^\dagger\,|\text{vac}\rangle = 0 \quad (\text{all } \alpha)\,, \tag{29}$$

$$V\,|\,\eta_\alpha^\dagger\,|\text{vac}\rangle = 0 \quad \text{if} \quad \boldsymbol{\alpha} \neq 0\,. \tag{30}$$

Thus $\eta_\alpha^\dagger|\text{vac}\rangle$ is an eigenstate of H with eigenvalue 12ϵ, if $\boldsymbol{\alpha}\neq 0$. It is obviously also an eigenstate of $\mathbf{P}$ with eigenvalue $\boldsymbol{\pi}$. Using Theorem 1 we thus find a set of eigenstates ζ

$$\zeta = (\eta_0^\dagger)^{N-1}\eta_\alpha^\dagger|\text{vac}\rangle \quad (\boldsymbol{\alpha}\neq 0) \tag{31}$$

satisfying (25) with energy $E_\zeta = 12\epsilon N + 2W(N-1)$. These states are degenerate, and their energy is different from that of ψ_N by $-2W$.

From this point on we shall assume $W<0$. Now states (31) are of the form

$$\zeta = (\eta_0^\dagger)^{N-1}\xi_1^\dagger|\text{vac}\rangle\,, \tag{32}$$

where $\xi_1^\dagger|\text{vac}\rangle$ describes a state with one particle a and one particle b:

$$\xi_1^\dagger = \left[\sum c_{\mathbf{k}\mathbf{k}'}a_{\mathbf{k}}b_{\mathbf{k}'}\right]^\dagger. \tag{33}$$

We shall now prove that all states (32) that satisfy (25) are either ψ_N or a linear superposition of the degenerate states (31). ψ_N will be called the zero-pair state. A linear superposition of (31) will be called a one-pair state. Both are eigenstates of the Hamiltonian, with the energy of one-pair states *higher* than that of the zero-pair state by $-2W>0$.

To prove our statement we observe that for the state (32) to have total momentum $N\boldsymbol{\pi}$, as implied by (25), $\xi_1^\dagger|\text{vac}\rangle$ must have momentum $\boldsymbol{\pi}$. Thus in (33) the summation is over all $\mathbf{k}+\mathbf{k}'+\boldsymbol{\pi}$ only,

$$\xi_1^\dagger = \left[\sum_{\mathbf{k}} c_{\mathbf{k}}a_{\mathbf{k}}b_{\boldsymbol{\pi}-\mathbf{k}}\right]^\dagger.$$

Making a Fourier expansion of $c_{\mathbf{k}}$ shows that ξ_1 is a linear sum of the η_α's of (26). Thus

$$\zeta = (\eta_0^\dagger)^{N-1}\left[\sum_\alpha d_\alpha \eta_\alpha\right]^\dagger|\text{vac}\rangle\,. \tag{34}$$

The term on the right-hand side with $\boldsymbol{\alpha}=0$ is the zero-pair state. The other terms together are a one-pair state. Since these two have different energies, (34) must be *either* exclusively the former, *or* exclusively the latter, proving our statement.

We have so far found L^3-1 one-pair states (31) above the zero-pair state ψ_N, with an energy gap of $-2W$. It is natural to look for two-pair states in a generalization of (32):

$$\zeta = (\eta_0^\dagger)^{N-2}\xi_2^\dagger|\text{vac}\rangle\,, \tag{35}$$

where $\xi_2^+|\text{vac}\rangle$ describes a state with two particles a and two particles b. Because of Theorem 1, it is sufficient for (35) to satisfy (25) that $\xi_2^\dagger|\text{vac}\rangle$ is a simultaneous eigenstate of H and $\mathbf{P}$, with the eigenvalue of $\mathbf{P}$ equal to $\mathbf{0}(\text{mod}2\pi)$.

Now $\xi_2^\dagger|\text{vac}\rangle$ is a four-particle state. Unfortunately it is difficult to find explicit eigenstates for such four-particle problems. However, when the lattice is large, the energy spectrum of this four-particle state has a continuum starting at energy equal to $0+$, with possibly bound states below zero. Thus there are many states (35) with energy

$$E_\zeta = (N-2)(12\epsilon + 2W) + (0+)\,.$$

Thus

$$E_\zeta - (\text{energy of } \psi_N) = -24\epsilon - 4W\,, \tag{36}$$

showing that there are many two-particle states below the zero-particle state, if $24\epsilon > -4W$.

We digress here to ask the following: Since one-pair states are above the zero-pair state by $-2W$ in energy, why are the two-pair states not above the zero-pair state by $-4W$, but instead by $-24\epsilon - 4W < -4W$? The answer to this question lies in the facts already presented above, that $\xi_1^\dagger|\text{vac}\rangle$ has momenta $\mathbf{P}=\pi$ while $\xi_2^\dagger|\text{vac}\rangle$ has momenta $\mathbf{P}=\mathbf{0}(\text{mod}2\pi)$. These are peculiar to the lattice model and are not present for continuum models.

(5) Metastability of ψ_N.—While the zero-pair state ψ_N is not the ground state, we shall argue that it is metastable.

Starting from ψ_N, adiabatic heat input and output could lead to two-pair states that have lower energies than ψ_N, hence to instability. But to reach such instability the system has to tunnel through the one-pair states (31) which have an energy higher than that of ψ_N by the gap $-2W>0$.

The physical picture is as follows: Without disturbance the zero-pair state has ODLRO and is time independent. When adiabatic heat input and output are applied, a pair of excitations described by one-pair states may occur, requiring an energy of $-2W$. In each region of space the one-pair excitation is still an eigenstate and does not cause instability. But when two pairs of excitations collide, a two-pair state may be reached with energy lower than ψ_N causing instability. At low temperatures, much lower than $-2W$, the one-pair excitations are rare and collisions are infrequent. Thus ψ_N is metastable.

(6) Variations of the theme.—(a) It is clear that if the potential energy V is such that it is equal to $2W$ for two particles at a distance β, and zero otherwise,

$$V = 2W\sum_{\mathbf{r}} a_{\mathbf{r}+\beta}^\dagger a_{\mathbf{r}+\beta}b_{\mathbf{r}}^\dagger b_{\mathbf{r}}\,,$$

we can still obtain η pairing with η_β replacing the operator $\eta=\eta_0$ of the previous sections. (b) In the model defined in section (1), for $W<0$, the potential energy is attractive for a and b particles on the same site. But one can easily construct a model where strong repulsion prevents a and b to occupy the same site. For example, consider a simple cubic lattice of A atoms interlaced with a simple cubic lattice, of the same size, of B atoms such that each A atom has one and only one nearest-neighbor B atom. Assume that electrons a can only attach themselves to A atoms and electrons b only to B atoms. Assume that if nearest-neighbor A-B atoms have simultaneously an a electron attached to A and a b electron attached to B, then there is a contribution of $2W$ to the potential energy of the system. This model is mathematically the same as the model discussed in the present paper. (c) Writing the energy per particle with momentum $\mathbf{k}$ in (2) as $\epsilon(\mathbf{k})$, so that

$$T=\sum_{\mathbf{k}} \epsilon(\mathbf{k})(a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}+b_{\mathbf{k}}^{\dagger}b_{\mathbf{k}}),$$

we find that the essential property of $\epsilon(\mathbf{k})$ that makes possible η pairing is

$$\epsilon(\mathbf{k})+\epsilon(\boldsymbol{\pi}-\mathbf{k})=\text{independent of } \mathbf{k}. \tag{37}$$

This equation is satisfied for any $\epsilon(\mathbf{k})$ equal to a summation of $\cos(mk_x)$, $\cos(mk_y)$, and $\cos(mk_z)$, where $m=0$ or odd. If the lattice is not a simple cubic lattice, appropriate generalizations of (37) can be written down easily.

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