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SO_4 SYMMETRY IN A HUBBARD MODEL

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For a simple Hubbard model, using a particle-particle pairing operator η and a particle-hole pairing operator ζ, it is shown that one can write down two commuting sets of angular momenta operators **J** and **J**′, both of which commute with the Hamiltonian. These considerations allow the introduction of quantum numbers j and j', and lead to the fact that the system has $SO_4 = (SU_2 \times SU_2)/Z_2$ symmetry. j is related to the existence of superconductivity for a state and j' to its magnetic properties.

In a recent paper[1] it was found that a pairing operator η is useful for considering the Hamiltonian in a simple Hubbard model on an $L \times L \times L$ lattice, where $L = \text{even}$. We shall extend such considerations in the present paper. All notations are the same as in Ref. 1. We introduce here a Hamiltonian H' and a momentum operator $\mathbf{P}'$ which are trivially different from the H and $\mathbf{P}$ of Ref. 1, in order to bring out more *symmetries* of the system:

$$H' = T' + V' , \tag{1}$$

$$T' = -2\varepsilon \sum_{\mathbf{k}} (\cos k_x + \cos k_y + \cos k_z)(a_{\mathbf{k}}^+ a_{\mathbf{k}} + b_{\mathbf{k}}^+ b_{\mathbf{k}}) , \tag{2}$$

$$V' = 2W \sum_{\mathbf{r}} \left(a_{\mathbf{r}}^+ a_{\mathbf{r}} - \frac{1}{2}\right)\left(b_{\mathbf{r}}^+ b_{\mathbf{r}} - \frac{1}{2}\right) . \tag{3}$$

$$\mathbf{P}' = \Sigma\left(\mathbf{k} - \frac{1}{2}\boldsymbol{\pi}\right)(a_{\mathbf{k}}^+ a_{\mathbf{k}} + b_{\mathbf{k}}^+ b_{\mathbf{k}})\,(\mathbf{mod.2\pi}) . \tag{4}$$

(1) *The operators J_x, J_y, and J_z* — It is easy to verify that $\eta^+\eta - \eta\eta^+ = \Sigma(a^+a + b^+b) - M$, where $M = L^3$. Calculating the commutator of this commutator with η we obtain

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Theorem 1. Defining

$$\eta^+ = J_x + iJ_y\,, \quad \eta = J_x - iJ_y\,, \quad J_z = \frac{1}{2}\Sigma(a^+a + b^+b) - \frac{1}{2}M\,, \tag{5}$$

one finds that J_x, J_y, J_z commute with each other like the components of an angular momentum. Hence the eigenvalue of $\mathbf{J}^2$ is $j(j+1)$ where $2j$ = integer $\geqq 0$. Furthermore (as can be easily checked),

$$[T',\mathbf{J}]_- = [V',\mathbf{J}]_- = [H',\mathbf{J}]_- = [\mathbf{P}'\mathbf{J}]_- = 0\,. \tag{6}$$

(2) *The operators J'_x, J'_y and J'_z* — We now define a particle-hole pairing operator,

$$\zeta = \Sigma\, a_{\mathbf{k}} b_{\mathbf{k}}^+ = \Sigma\, a_{\mathbf{r}} b_{\mathbf{r}}^+\,. \tag{7}$$

Then

$$\zeta\zeta^+ - \zeta^+\zeta = -\Sigma\, a^+a + \Sigma\, b^+b\,.$$

Theorem 2. Defining

$$\zeta^+ = J'_x + iJ'_y\,, \quad \zeta = J'_x - iJ'_y\,, \quad J'_z = \frac{1}{2}\Sigma\, a^+a - \frac{1}{2}\Sigma\, b^+b\,, \tag{8}$$

one finds that J'_x, J'_y, J'_z commute with each other like the components of an angular momentum. Hence the eigenvalue of $\mathbf{J}'^2$ is $j'(j'+1)$ where $2j'$ = integer $\geqq 0$. Furthermore all 3 components of $\mathbf{J}$ commute with all 3 components of $\mathbf{J}'$, and

$$[T',\mathbf{J}']_- = [V',\mathbf{J}']_- = [H',\mathbf{J}']_- = [\mathbf{P}'\mathbf{J}']_- = 0\,. \tag{9}$$

ζ is the usual spin lowering operator and $\mathbf{J}'$ is the usual "spin" operator.

(3) *Explicit eigenfunctions of H'* — We can find many eigenstates of H' with Theorems 1 and 2 as follows. We diagonize $\mathbf{J}^2$, $\mathbf{J}'^2$, J_z, J'_z, H' and $\mathbf{P}'$ simultaneously. These states can be sorted out into multiplets $\{j, j'\}$, each comprising of $(2j+1)(2j'+1)$ states, as illustrated in Fig. 1, where N_a and N_b are eigenvalues of Σa^+a and Σb^+b,

$$j_z = \frac{1}{2}(N_a + N_b - M)\,, \quad j_z = \frac{1}{2}(N_a - N_b)\,. \tag{10}$$

As explained in Fig. 1, $j + j'$ = integer, i.e., not all representations of $SU_2 \times SU_2$ are present. This means that the true symmetry of the problem is $(SU_2 \times SU_2)/Z_2 = SO_4$.

Consider now the states in one spot on the bottom row of Fig. 1. For these states, $N_a = 0$. The operators H' and $\mathbf{P}'$ for such states are easily diagonizable since for such states, there are no a-particle — b-particle interac-

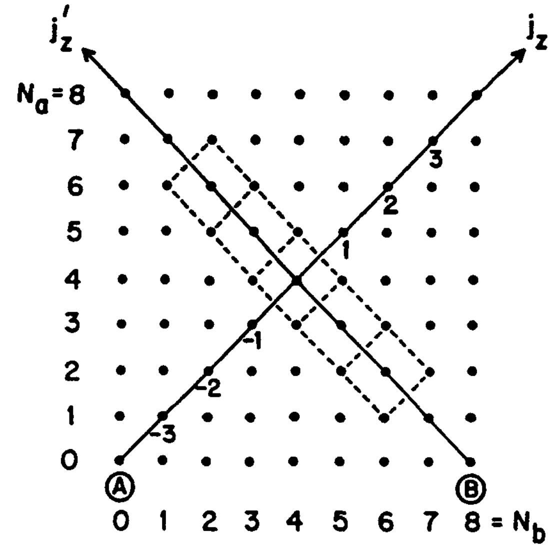

Fig. 1. (N_a, N_b) diagram for $M = 8$. The relationship between (j_z, j_z') with (N_a, N_b) is given by Eq. (10). Each multiplet $\{j, j'\}$ is represented by a rectangular set of states centered at $j_z = j_z' = 0$ in this diagram. The number of states in the multiplet is $(2j+1)\,(2j'+1)$. Illustrated is the multiplet $\left\{\frac{1}{2}, \frac{5}{2}\right\}$. All states of a multiplet share the same eigenvalue of H' and $\mathbf{P}'$. The lowest corner in the multiplet is where $j_z = -j$, $j_z' = -j'$. One can generate all states of a multiplet by starting from its lowest corner and repeatedly operate on it with $\eta^+ = J_x + iJ_y$ (which increases j_z) and with $\zeta^+ = J_x' + iJ_y'$ (which increases j_z'). Obviously $j + j'$ = integer. Notice that for fixed j and j', there are in general a large number of multiplets $\{j, j'\}$, except for $\{M/2, 0\}$ and $\{0, M/2\}$, each of which occurs only once. For the former, the lowest corner is the point A where $N_a = N_b = 0$ which is a single state. For the latter, the lowest corner is B where $N_a = 0$, $N_b = M$ which is also a single state.

tions, so that the problem reduces to that of N_b noninteracting fermions. One can thus trivially write down the eigenstates of H' and $\mathbf{P}'$ in momentum space. There are $\binom{M}{N_b}$ such states. Operating with η^+ and ζ^+ on these states generates $\binom{M}{N_b}$ multiplets $\{j, j'\}$. Now obviously

$$j = \frac{1}{2}(M - N_b)\ , \quad j' = \frac{1}{2}N_b\ .$$

Thus we can easily write down explicitly the eigenfunctions for H' and $\mathbf{P}'$ for $\binom{M}{N_b}$ multiplets $\left\{\frac{1}{2}(M - N_b), \frac{1}{2}N_b\right\}$. The total number of such states is $\Sigma\binom{M}{N_b}(M - N_b + 1)(N_b + 1)$, where the summation extends from $N_b = 0$ to M. The summation is equal to $2^{M-2}(M^2 + 3M + 4)$. This is an enormous number of eigenstates, but still very small compared to the total number of eigenstates which is 4^M. We remark here that the eigenstates ψ_N of Ref. 1 are special cases of the states discussed in this section.

The eigenstates of H' constructed above obviously do not depend on W and are simultaneous eigenstates of T' and V'. We believe they are the only W-independent eigenstates of H', but we do not know how to prove this statement except in special cases.

(4) *ODLRO* — We shall show

Theorem 3. For any state ψ for which $j^2 - j_z^2 = O(M^2)$, there is ODLRO.

The 2-particle reduced density matrix ρ_2 has matrix element

$$\langle b_{\mathbf{s}}\, a_{\mathbf{s}} | \rho_2 | b_{\mathbf{r}}\, a_{\mathbf{r}} \rangle = \psi^+ a_{\mathbf{r}}^+ b_{\mathbf{r}}^+ a_{\mathbf{s}}\, b_{\mathbf{s}} \psi \ .$$

Thus

$$\begin{aligned}\Sigma\, e^{i\pi\cdot(\mathbf{r}-\mathbf{s})} \langle b_{\mathbf{s}}\, a_{\mathbf{s}} | \rho_2 | b_{\mathbf{r}}\, a_{\mathbf{r}} \rangle &= \psi^+ \eta^+ \eta \psi = \psi^+ (J_x + iJ_y)(J_x - iJ_y)\psi \\ &= j^2 - j_z^2 + j + j_z \ .\end{aligned}$$

Using

$$\langle b_{\mathbf{r}'} a_{\mathbf{r}} | \phi \rangle = M^{-1/2} e^{i\pi\cdot\mathbf{r}} \delta(\mathbf{r} - \mathbf{r}')$$

as a trial wave function for ρ_2, we find the expectation value of ρ_2 to be

$$\langle \rho_2 \rangle = \frac{1}{M}(j^2 - j_z^2) + O(1) = O(M) \geqq 0.$$

Thus the largest eigenvalue of ρ_2 is $O(M)$ and the state has ODLRO.[2]

In Ref. 1 we had showed that the states ψ_N have ODLRO. That fact is a special case of the above theorem, because for ψ_N, $j = M/2$, and $j_z = -M/2 + N$.

In the above discussions, the pairs are particle-particle pairs. If the particle is charged e, then the state exhibits[2] flux quantization in units of $ch/2e$. If $j'^2 - j_z'^2 = O(M^2)$, the system exhibits particle-hole ODLRO. There is no superconductivity for such a system.[2,3] Thus *j is related to superconductivity and j' to magnetic properties.*

(5) *Unitary Operators U_b and X* — We define these two operators as follows:

$$U_b a_{\mathbf{r}} U_b^{-1} = a_{\mathbf{r}} \ , \quad U_b b_{\mathbf{r}} U_b^{-1} = e^{i\pi\cdot\mathbf{r}} b_{\mathbf{r}}^+ \ , \quad U_b^2 = 1 \ , \tag{11}$$

and

$$X a_{\mathbf{r}} X^{-1} = e^{i\pi\cdot\mathbf{r}} a_{\mathbf{r}} \ , \quad X b_{\mathbf{r}} X^{-1} = e^{i\pi\cdot\mathbf{r}} b_{\mathbf{r}} \ , \quad X^2 = 1 \ . \tag{12}$$

Operator X is well known and operator U_b has been discussed in the literature.[4] We observe that

$$U_b b_{\mathbf{k}} U_b^{-1} = b_{\pi-\mathbf{k}}^+ \ , \tag{13}$$

and

$$\zeta = U_b \eta U_b^{-1} . \tag{14}$$

Theorem 4. Writing $H'(W)$ for H', we have

$$U_b H'(W) U_b^{-1} = H'(-W) , \tag{15}$$

$$U_b (\Sigma b^+ b) U_b^{-1} = M - \Sigma b^+ b , \quad U_b (\Sigma a^+ a) U_b^{-1} = \Sigma a^+ a . \tag{16}$$

Theorem 5.

$$X H'(W) X^{-1} = -H'(-W) , \tag{17}$$

$$X(\Sigma a^+ a) X^{-1} = \Sigma a^+ a , \quad X(\Sigma b^+ b) X^{-1} = \Sigma b^+ b . \tag{18}$$

It follows that

$$\begin{aligned}
(XU_b)(H'(W))(XU_b)^{-1} &= -H'(W) , \\
(XU_b)(\Sigma a^+ a)(XU_b)^{-1} &= \Sigma a^+ a , \\
(XU_b)(\Sigma b^+ b)(XU_b)^{-1} &= M - \Sigma b^+ b .
\end{aligned} \tag{19}$$

Denoting by Spm (W, N_a, N_b) the spectrum of $H'(W)$ for given N_a and N_b, we have, by Theorem 4,

Theorem 6.

$$\begin{aligned}
\mathrm{Spm}\,(W, N_a, N_b) &= \mathrm{Spm}\,(-W, N_a, M - N_b) \\
&= \mathrm{Spm}\,(-W, M - N_a, N_b) \\
&= \mathrm{Spm}\,(W, M - N_a, M - N_b) .
\end{aligned} \tag{20}$$

By Theorem 5, we have

Theorem 7.

$$\mathrm{Spm}\,(W, N_a, N_b) = -\mathrm{Spm}(-W, N_a, N_b) . \tag{21}$$

Combining these two results we obtain

$$\begin{aligned}
\mathrm{Spm}\,(W, N_a, N_b) &= -\mathrm{Spm}\,(W, N_a, M - N_b) \\
&= -\mathrm{Spm}\,(W, M - N_a, N_b) \\
&= \mathrm{Spm}\,(W, M - N_a, M - N_b) .
\end{aligned} \tag{22}$$

(6) *Limit* $M \to \infty$ — We shall now put $\varepsilon = 1$ in (2). Diagonalizing $\mathbf{J}^2$, $\mathbf{J}'^2$, J_z, J'_z, H', $\mathbf{P}'$, we have also diagonalized N_a and N_b because of (10). Let the lowest eigenvalue of H' at a fixed N_a, N_b be denoted by $E_0(W, N_a, N_b)$. Now keeping fixed the values of

$$N_a/M = \rho_a \ , \quad N_b/M = \rho_b$$

we approach the limit $M \to \infty$. It can be proved, by a method used in Ref. 5, that $M^{-1}E_0$ approaches a limit which we shall denote by $f(W, \rho_a, \rho_b)$. f is the lowest eigenvalue of H' per site at fixed densities ρ_a and ρ_b.

The function f has many symmetries. Because of Theorems 1 and 2,

$$f(W, \rho_a, \rho_b) = f(W, \rho_b, \rho_a) = f(W, 1 - \rho_a, 1 - \rho_b) = f(W, 1 - \rho_b, 1 - \rho_a) \ . \tag{23}$$

Because of (20),

$$f(W, \rho_a, \rho_b) = f(-W, \rho_a, 1 - \rho_b) = f(-W, 1 - \rho_a, \rho_b) \ . \tag{24}$$

These symmetries are illustrated in Fig. 2.

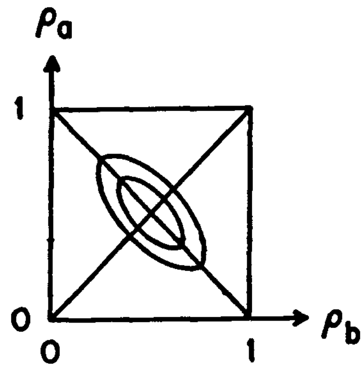

Fig. 2. Equi-f contours in ρ_a, ρ_b plane (schematic). Because of (23), these contours are reflection symmetrical with respect to the $\rho_a = \rho_b$ axis and the $\rho_a + \rho_b = 1$ axis. Because of Theorem 8, these contours are convex. One can obtain the $(-W)$ contours from the (W) contours by a rotation through 90° around the center of the square.

Theorem 8. $f(W, \rho_a, \rho_b)$ as a function of ρ_a and ρ_b is continuous and concaves upwards.

Theorem 9. $f(W, \rho_a, \rho_b)$ as a function of W concaves downwards.

These two theorems can be proved using the methods of Ref. 5.

Theorem 8 and Eq. (23) show that the minimum of $f(W, \rho_a, \rho_b)$ for fixed W is $f(W, 1/2, 1/2)$. This minimum value may be shared by f at other values of (ρ_a, ρ_b) than (1/2, 1/2). Let the region of (ρ_a, ρ_b) where this is true be denoted by R, and call the states that have this minimum value of f *lowest states.* (23) shows that R is reflection symmetrical with respect to the axis: $\rho_a = \rho_b$, and with respect to the axis: $\rho_a + \rho_b = 1$. Using Theorem 8 we can show

Theorem 10. The region R in (ρ_a, ρ_b) where $f(W, \rho_a, \rho_b) = f(W, 1/2, 1/2)$ is convex. Possible schematic shapes of R are illustrated in Fig. 3.

Each of the *lowest state* belongs to a multiplet $\{j, j'\}$. Within that multiplet the leading state (i.e. where $j_z = j, j'_z = j$,) is also a *lowest state*. Hence it must be in the $j_z \geqq 0, j'_z \geqq 0$ quadrant of R. Thus

Theorem 11. All the *lowest states* on the boundary of R have $j = |j_z|, j' = |j'_z|$. Finally we remark that for the points $\rho_a = 0$ (or $\rho_b = 0$,) the system is devoid of a (or b) particles. Hence the value of $f(W, 0, \rho_b)$ and $f(W, \rho_a, 0)$ can be easily evaluated. (23) then allows one to write down $f(W, 1, \rho_b)$ and $f(W, \rho_a, 1)$. Thus the value of f on the boundary of the square in Fig. 2 is known.

We now define $g(W, \rho_a, \rho_b)$ to be highest eigenvalue of H' per site. Equation (22) then shows that

$$g(W, \rho_a, \rho_b) = -f(W, \rho_a, 1 - \rho_b) = -f(W, 1 - \rho_a, \rho_b) . \tag{25}$$

More generally we define the free energy per site by

$$F(\beta, W, \rho_a, \rho_b) = \lim (-M\beta)^{-1} \ln (\text{p.f.}) \tag{26}$$

where

$$(\text{p.f.}) = \text{trace of block of } \exp(-\beta H') \text{ belonging to given } \rho_a, \rho_b , \tag{27}$$

and the limit is for $M \to \infty$. Then

$$F(\infty, W, \rho_a, \rho_b) = f(W, \rho_a, \rho_b) ,$$
$$F(-\infty, W, \rho_a, \rho_b) = g(W, \rho_a, \rho_b) . \tag{28}$$

The function F has many symmetries. Theorems 1 and 2 show that

$$\begin{aligned} F(\beta, W, \rho_a, \rho_b) &= F(\beta, W, \rho_b, \rho_a) \\ &= F(\beta, W, 1 - \rho_a, 1 - \rho_b) \\ &= F(\beta, W, 1 - \rho_b, 1 - \rho_a) . \end{aligned} \tag{29}$$

Equation (20) shows that

$$F(\beta, W, \rho_a, \rho_b) = F(\beta, -W, \rho_a, 1 - \rho_b) = F(\beta, -W, 1 - \rho_a, \rho_b) . \tag{30}$$

Equation (21) shows that

$$F(\beta, W, \rho_a, \rho_b) = -F(-\beta, -W, \rho_a, \rho_b) . \tag{31}$$

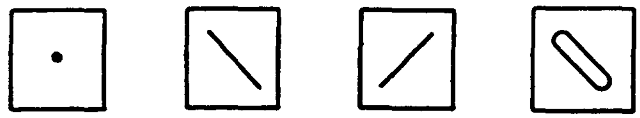

Fig. 3. Possible shapes for R. R is convex and is reflection symmetrical with respect to the $\rho_a = \rho_b$, and the $\rho_a + \rho_b = 1$ axes. For case c there is particle-particle ODLRO at low temperatures in the open line segment. For case d there is particle-particle ODLRO at low temperatures *inside* of the region R. These cases exhibit superconductivity.

These two last equations together show that

$$F\left(0, W, \rho_a, \frac{1}{2}\right) = F\left(0, W, \frac{1}{2}, \rho_b\right) = 0 \ . \tag{32}$$

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