

## Relation between pseudospin-rotation invariance and a supersolid

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In this paper, we discuss the physical meaning of pseudospin symmetry, which is actually a kind of particle-hole rotation invariance. In an isotropic state with the total pseudospin  $\tilde{S} = 0$ , by using the invariance of the pseudospin rotation in space, we shall establish a relation between off-diagonal long-range order (ODLRO) and charge-density waves (CDW). This result indicates that ODLRO and CDW must coexist in such an isotropic state, which is usually called a *supersolid*. Finally, we present two examples to show that a supersolid exists.

Pseudospin symmetry was first found in the Kondo lattice model by Jones *et al.*<sup>1</sup> in 1988 and then in the Hubbard model by Yang and Zhang<sup>2</sup> in 1990. Before their works, many relevant properties had been found in the study of the negative- $U$  Hubbard model. For example, in the large  $|U|(\gg t)$  case, the Hubbard model is approximately equivalent to an effective Hamiltonian in terms of the pseudospin operators.<sup>3</sup> In 1989, Yang<sup>4</sup> found that the pseudospin is possibly related to superconductivity and proposed a so-called “ $\eta$ -pairing” mechanism for the Hubbard model. For an eigenstate, if its total pseudospin and its  $z$  component have  $\tilde{S}^2 - \tilde{S}_z^2 = O(N_\wedge^2)$  ( $N_\wedge$  is the total number of the lattice sites), then the state possesses off-diagonal long-range order (ODLRO), which is characteristic of superconductivity as Yang argued. Yang's idea was realized in some theoretical models.<sup>5,6</sup> One of us<sup>7</sup> and his collaborator showed that for a finite negative- $U$  Hubbard model on a bipartite lattice with  $N_A > N_B$ , when  $2N_A > N_e > 2N_B$ , its ground state has the total pseudospin  $\tilde{S} = (N_A - N_B)/2$  and possesses ODLRO, which provides a novel direction to look for such a novel type of superconducting materials.

The origin of pseudospin symmetry is now a challenging problem. Yang<sup>4</sup> and Zhang<sup>8</sup> thought that, in the Hubbard model, it is an intricate combination of both forms of the kinetic and the potential energies, which gives rise to a coherent propagation of the  $\eta$  pairs. In this case, the pair has a zero kinetic energy, and cannot be scattered by the third electron on the same site due to the Pauli principle. However, pseudospin symmetry has a deeper physical background. Just like the spin symmetry corresponding to the invariance of the spin rotation in space, pseudospin symmetry also corresponds to a particle-hole rotation invariance.

In this paper, we first discuss the rotation transformation for the pseudospin and present a physical interpretation. For an isotropic state with  $\tilde{S} = 0$ , we establish a relation for two correlation functions characterizing ODLRO and the charge-density wave (CDW), respectively. The result indicates that ODLRO and the

CDW must coexist in this state. (Usually, the coexistence of ODLRO and the CDW is called a supersolid.<sup>9</sup>) Finally, we present two examples: One is the pseudospin Heisenberg model and another is the negative- $U$  Hubbard model on a hypercubic lattice at half filling, which have the SU(2) pseudospin symmetry and their ground states have the total pseudospin  $\tilde{S} = 0$ , and are a supersolid.

The total pseudospins are defined on a bipartite lattice  $\wedge$  by

$$\begin{cases} \tilde{\mathbf{S}}^+ = \sum_{i \in \wedge} \tilde{\mathbf{S}}_i^+ = \sum_{i \in \wedge} \epsilon(i) c_{i\uparrow} c_{i\downarrow}, \\ \tilde{\mathbf{S}}^- = \sum_{i \in \wedge} \tilde{\mathbf{S}}_i^- = \sum_{i \in \wedge} \epsilon(i)^\dagger c_{i\downarrow}^\dagger c_{i\uparrow}^\dagger, \\ \tilde{\mathbf{S}}^z = \sum_{i \in \wedge} = \frac{1}{2} \sum_{i \in \wedge} (1 - n_{i\uparrow} - n_{i\downarrow}), \end{cases} \quad (1)$$

where  $\epsilon(i)$  is a phase factor of modulus 1.<sup>10</sup> The  $z$  component is just one-half of the difference between the number of the lattice sites and that of the electrons. These operators obey the commutation relations of the angular momentum,

$$[\tilde{\mathbf{S}}^z, \tilde{\mathbf{S}}^\pm] = \pm \tilde{\mathbf{S}}^\pm \quad \text{and} \quad [\tilde{\mathbf{S}}^+, \tilde{\mathbf{S}}^-] = 2\tilde{\mathbf{S}}^z. \quad (2)$$

These operators and the usual spin operators are related to each other due to a duality transformation  $\mathbf{T}$ :<sup>7</sup>

$$\mathbf{T} \cdot \mathbf{S} \cdot \mathbf{T}^{-1} = \tilde{\mathbf{S}}. \quad (3)$$

The transformation operator  $\mathbf{T}$  can be written in terms of the creation and annihilation operators of electrons with spin up,

$$\mathbf{T} = \prod_{i \in \wedge} [c_{i\uparrow} - \epsilon(i) c_{i\uparrow}^\dagger], \quad (4)$$

which is not very different from the so-called partial particle-hole transformation.<sup>11</sup>

For a system with pseudospin SU(2) symmetry, its Hamiltonian  $H$  should commute with the total pseudospin operator  $\tilde{\mathbf{S}}$ , i.e.,  $[H, \tilde{\mathbf{S}}] = 0$ . In other words, we can define a unitary transformation  $\exp(i\delta \mathbf{n} \cdot \tilde{\mathbf{S}})$  in which  $\mathbf{n} = (n_x, n_y, n_z)$  is a unit axis vector, and the Hamilto-

nian is invariant under this transformation,

$$e^{i\delta\mathbf{n}\cdot\tilde{\mathbf{S}}} H e^{-i\delta\mathbf{n}\cdot\tilde{\mathbf{S}}} = H. \quad (5)$$

As for the pseudospin, we have

$$e^{i\delta\mathbf{n}\cdot\tilde{\mathbf{S}}} \tilde{\mathbf{S}} e^{-i\delta\mathbf{n}\cdot\tilde{\mathbf{S}}} = \mathbf{n} \cdot (\mathbf{n} \cdot \tilde{\mathbf{S}}) + [\mathbf{n} \times (\mathbf{n} \times \tilde{\mathbf{S}})] \cos \delta + (\mathbf{n} \times \tilde{\mathbf{S}}) \sin \delta. \quad (6)$$

Both  $\tilde{\mathbf{S}}_i^2$  and  $\tilde{\mathbf{S}}^2$  are invariant under this transformation. Therefore, it does not change the magnitude of the pseudospin, and just changes its direction.

Let us consider a pair of the transformed operators of electrons,  $c_{i\uparrow}$  and  $c_{i\downarrow}^\dagger$ ; we have

$$e^{i\delta\mathbf{n}\cdot\tilde{\mathbf{S}}} \begin{pmatrix} c_{i\uparrow} \\ c_{i\downarrow}^\dagger \end{pmatrix} e^{-i\delta\mathbf{n}\cdot\tilde{\mathbf{S}}} = \cos \frac{\delta}{2} + i \sin \frac{\delta}{2} \tau_i \cdot \mathbf{n} \begin{pmatrix} c_{i\uparrow} \\ c_{i\downarrow}^\dagger \end{pmatrix}, \quad (7)$$

where

$$\tau_{xi} = \begin{pmatrix} 0 & \epsilon(i) \\ \epsilon^\dagger(i) & 0 \end{pmatrix}, \quad \tau_{yi} = \begin{pmatrix} 0 & i\epsilon(i) \\ -i\epsilon^\dagger(i) & 0 \end{pmatrix}, \\ \tau_{zi} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (8)$$

The transformed operators are a mixture of  $c_{i\uparrow}$  and  $c_{i\downarrow}^\dagger$ . If we regard  $c_{i\downarrow}^\dagger$  as creating a particle with spin down, and  $c_{i\uparrow}$  as creating a hole also with spin down, this transformation just rotates the pseudospin in particle-hole space. For instance, let  $\mathbf{n} = (0, 1, 0)$  and  $\delta = \pi$ ; then we have

$$c_{i\uparrow} \rightarrow -\epsilon(i)c_{i\downarrow}^\dagger, \\ c_{i\downarrow}^\dagger \rightarrow \epsilon(i)c_{i\uparrow}. \quad (9)$$

In this case, the total number changes  $N_e \rightarrow 2N_\Lambda - N_e$ , which is also a kind of a particle-hole transformation. From this example, we see that the usual particle-hole transformation in the Hubbard model<sup>2</sup> is not an additional symmetry, but just a combination of the spin and pseudospin rotations in a special case. In summary, pseudospin symmetry is a particle-hole rotation symmetry.

In the following, we make use of the rotation invariance of the pseudospin in space to prove a theorem on superconductivity and the CDW in an isotropic pseudospin state. According to the definitions of  $\tilde{\mathbf{S}}^\pm$  and  $\tilde{\mathbf{S}}^z$ , they are related to two sorts of long-range orders, respectively: The former is ODLRO and the later is a CDW. Following Yang,<sup>12</sup> for a state  $|\Psi\rangle$ , we can define a two-particle correlation matrix

$$\hat{M}^{+-} = \{M_{ij}^{+-}\} = \{\langle \Psi | \tilde{\mathbf{S}}_i^+ \tilde{\mathbf{S}}_j^- | \Psi \rangle\}. \quad (10)$$

Suppose the system is periodic and homogeneous; the  $M_{ij}$  should be a function in terms of  $i - j$ , i.e.,  $M_{ij} = m(\mathbf{r}_i - \mathbf{r}_j)$ . By using of the technique of Fourier transformation, it is easy to obtain that the  $N_\Lambda$  eigenvalue of  $\hat{M}^{+-}$  is<sup>13</sup>

$$m^{+-}(\mathbf{q}) = \langle \Psi | \tilde{\mathbf{S}}_{\mathbf{q}}^+ \tilde{\mathbf{S}}_{-\mathbf{q}}^- | \Psi \rangle, \quad (11)$$

where  $\tilde{\mathbf{S}}_{\mathbf{q}}^\pm$  is the Fourier transform of  $\tilde{\mathbf{S}}_i^\pm$ ,

$$\tilde{\mathbf{S}}_{\mathbf{q}}^\pm = \frac{1}{\sqrt{N_\Lambda}} \sum_{i \in \Lambda} e^{\mp i\mathbf{q}\cdot\mathbf{r}_i} \tilde{\mathbf{S}}_i^\pm. \quad (12)$$

If for a certain momentum  $\mathbf{q}_0$ ,  $m^{+-}(\mathbf{q}_0)$  has of order  $N_\Lambda$ , according to Yang's definition<sup>12</sup>, the state  $|\Psi\rangle$  possesses ODLRO, which characterizes the superconductivity. Similarly, let us consider a correlation function for the z components,

$$m^{zz}(\mathbf{q}) = \langle \Psi | \tilde{\mathbf{S}}_{\mathbf{q}}^z \tilde{\mathbf{S}}_{-\mathbf{q}}^z | \Psi \rangle. \quad (13)$$

Substituting the definition of  $\tilde{\mathbf{S}}^z$  into Eq. (13), we have

$$m^{zz}(\mathbf{q}) = \frac{1}{4} \langle \Psi | n_{\mathbf{q}} n_{-\mathbf{q}} | \Psi \rangle + \frac{N_\Lambda}{4} \left( 1 - 2 \frac{N_e}{N_\Lambda} \right) \delta_{\mathbf{q},0}, \quad (14)$$

which is just a density-density correlation function except for the point  $\mathbf{q} = 0$  [ $n_{\mathbf{q}} = \frac{1}{N_\Lambda} \sum_i e^{i\mathbf{q}\cdot\mathbf{r}_i} (n_{i\uparrow} + n_{i\downarrow})$ ]. If  $m^{zz}(\mathbf{q})$  also is of order  $N_\Lambda$ , it characterizes the charge density wave. These two correlation functions are related to each other in an isotropic pseudospin state. Our result can be summarized in the following theorem:

*Theorem:* For a state  $|\Psi\rangle$  with pseudospin  $\tilde{S} = 0$ , we have

$$m^{+-}(\mathbf{q}) = m^{+-}(-\mathbf{q}) = 2m^{zz}(\mathbf{q}). \quad (15)$$

*Proof:* For a state  $|\Psi\rangle$  with pseudospin  $\tilde{S} = 0$ , we have

$$\tilde{\mathbf{S}}^\pm |\Psi\rangle = \tilde{\mathbf{S}}^z |\Psi\rangle = 0. \quad (16)$$

Thus this state is invariant under the unitary transformation  $e^{i\delta\mathbf{n}\cdot\tilde{\mathbf{S}}}$ , where  $\delta$  and  $\mathbf{n}$  are arbitrary, i.e.,

$$e^{i\delta\mathbf{n}\cdot\tilde{\mathbf{S}}} |\Psi\rangle = |\Psi\rangle. \quad (17)$$

From Eqs. (6) and (17), we can obtain

$$\langle \Psi | \tilde{\mathbf{S}}_i^x \cdot \tilde{\mathbf{S}}_j^x | \Psi \rangle = \langle \Psi | \tilde{\mathbf{S}}_i^y \cdot \tilde{\mathbf{S}}_j^y | \Psi \rangle = \langle \Psi | \tilde{\mathbf{S}}_i^z \cdot \tilde{\mathbf{S}}_j^z | \Psi \rangle \quad (18)$$

and

$$\langle \Psi | \tilde{\mathbf{S}}_i^x \cdot \tilde{\mathbf{S}}_j^y | \Psi \rangle = \langle \Psi | \tilde{\mathbf{S}}_i^y \cdot \tilde{\mathbf{S}}_j^z | \Psi \rangle = \langle \Psi | \tilde{\mathbf{S}}_i^z \cdot \tilde{\mathbf{S}}_j^x | \Psi \rangle = 0. \quad (19)$$

For example, choose  $\mathbf{n} = (0, 1, 0)$  and  $\delta = (n + 1/2)\pi$ ; then

$$e^{i(n+1/2)\pi\tilde{\mathbf{S}}^y} \tilde{\mathbf{S}}_i e^{-i(n+1/2)\pi\tilde{\mathbf{S}}^y} = ((-1)^n \tilde{\mathbf{S}}_i^z, \tilde{\mathbf{S}}_i^y, (-1)^{n+1} \tilde{\mathbf{S}}_i^x) \quad (20)$$

and we have

$$\langle \Psi | \tilde{\mathbf{S}}_i^x \cdot \tilde{\mathbf{S}}_j^x | \Psi \rangle = \langle \Psi | e^{i(n+1/2)\pi\tilde{\mathbf{S}}^y} \tilde{\mathbf{S}}_i^x \cdot \tilde{\mathbf{S}}_j^x e^{-i(n+1/2)\pi\tilde{\mathbf{S}}^y} | \Psi \rangle \\ = \langle \Psi | \tilde{\mathbf{S}}_i^z \cdot \tilde{\mathbf{S}}_j^z | \Psi \rangle \quad (21)$$

and

$$\langle \Psi | \tilde{\mathbf{S}}_i^x \cdot \tilde{\mathbf{S}}_j^y | \Psi \rangle = \langle \Psi | e^{i(n+1/2)\pi\tilde{\mathbf{S}}^y} \tilde{\mathbf{S}}_i^x \cdot \tilde{\mathbf{S}}_j^y e^{-i(n+1/2)\pi\tilde{\mathbf{S}}^y} | \Psi \rangle \\ = (-1)^n \langle \Psi | \tilde{\mathbf{S}}_i^z \cdot \tilde{\mathbf{S}}_j^x | \Psi \rangle = 0. \quad (22)$$

In the last step of Eq. (22), it is obvious that  $n$  can be taken to be even or odd. Furthermore, their corresponding Fourier components are

$$\langle \Psi | \tilde{\mathbf{S}}_{\mathbf{q}}^x \cdot \tilde{\mathbf{S}}_{-\mathbf{q}}^x | \Psi \rangle = \langle \Psi | \tilde{\mathbf{S}}_{\mathbf{q}}^y \cdot \tilde{\mathbf{S}}_{-\mathbf{q}}^y | \Psi \rangle = \langle \Psi | \tilde{\mathbf{S}}_{\mathbf{q}}^z \cdot \tilde{\mathbf{S}}_{-\mathbf{q}}^z | \Psi \rangle \quad (23)$$

and

$$\langle \Psi | \tilde{\mathbf{S}}_{\mathbf{q}}^x \cdot \tilde{\mathbf{S}}_{-\mathbf{q}}^y | \Psi \rangle = \langle \Psi | \tilde{\mathbf{S}}_{\mathbf{q}}^y \cdot \tilde{\mathbf{S}}_{-\mathbf{q}}^x | \Psi \rangle = \langle \Psi | \tilde{\mathbf{S}}_{\mathbf{q}}^z \cdot \tilde{\mathbf{S}}_{-\mathbf{q}}^z | \Psi \rangle = 0. \quad (24)$$

Substituting these Eqs. (23) and (24) into the definition of  $m^{+-}(\mathbf{q})$  [Eq. (11)], one obtains

$$\begin{aligned} m^{+-}(\mathbf{q}) &= \langle \Psi | (\tilde{\mathbf{S}}_{-\mathbf{q}}^x + i\tilde{\mathbf{S}}_{-\mathbf{q}}^y)(\tilde{\mathbf{S}}_{\mathbf{q}}^x - i\tilde{\mathbf{S}}_{\mathbf{q}}^y) | \Psi \rangle \\ &= \langle \Psi | \tilde{\mathbf{S}}_{\mathbf{q}}^x \cdot \tilde{\mathbf{S}}_{-\mathbf{q}}^x | \Psi \rangle + \langle \Psi | \tilde{\mathbf{S}}_{\mathbf{q}}^y \cdot \tilde{\mathbf{S}}_{-\mathbf{q}}^y | \Psi \rangle \\ &= 2\langle \Psi | \tilde{\mathbf{S}}_{\mathbf{q}}^z \cdot \tilde{\mathbf{S}}_{-\mathbf{q}}^z | \Psi \rangle. \end{aligned} \quad (25)$$

Q.E.D.

The physical meaning of this theorem is that, if superconductivity characterized by ODLRO via a local singlet pairing mechanism arises, then so does the charge density wave, and vice versa. In other words, a supersolid exists in this state if one of long-range order arises.

Finally, we present two examples as an application of this theorem. An exact example that the ground state is a supersolid is a Heisenberg model in terms of the pseudospin operators on a cubic lattice,

$$H_1 = J \sum_{ij} \tilde{\mathbf{S}}_i \cdot \tilde{\mathbf{S}}_j, \quad (26)$$

with the constraint of the condition of empty or double occupancy at every site, i.e.,  $n_{i\uparrow} = n_{i\downarrow} = 0$  or 1. For the antiferromagnetic Heisenberg model on a cubic lattice, it has been proved that its ground state possesses antiferromagnetic long-range order.<sup>14</sup> Following their derivation, it is easy to write down that

$$m^{+-}(\mathbf{Q}) = 2m^{zz}(\mathbf{Q}) = O(N_{\wedge}) \quad (27)$$

for the ground state of  $H_1$  when  $\tilde{S}_z = 0$  and  $S_z = 0$ . Alternatively, it can be also obtained by utilizing the partial particle-hole transformation.

The second example is the Hubbard model on a bipartite lattice,

$$\begin{aligned} H_2 &= -t \sum_{(ij),\sigma} c_{i\sigma}^\dagger c_{j\sigma} - U \sum_{i \in \wedge} \left( n_{i\uparrow} - \frac{1}{2} \right) \left( n_{i\downarrow} - \frac{1}{2} \right) \\ &\quad + \mu \sum_{i\sigma} n_{i\sigma}, \end{aligned} \quad (28)$$

where the summation in the first term runs over all pairs of the nearest neighbor sites. When the system is exactly half filled, the chemical potential is  $\mu = 0$ . In this case, the Hamiltonian possesses pseudospin SU(2) symmetry rather than the usual spin SU(2) symmetry, as Yang and Zhang pointed out.<sup>2</sup> One can also check it by deriving the commutation relation  $[H, \tilde{\mathbf{S}}] = 0$ , and in this case the phase factor  $\epsilon(i)$  should be taken to be 1 for  $i \in A$  and  $-1$  for  $i \in B$ .<sup>15</sup> At large  $|U| \gg t$ , this model is approximately equivalent to model (26) in an expansion of order  $t^2/|U|$  in the subspace  $S_z = 0$ . When  $N_A = N_B$ , e.g., on a  $d$ -dimensional hypercubic lattice, the ground state has the pseudospin  $\tilde{S} = 0$  at half filling.<sup>7</sup> The result is independent of  $U$  (only required to be negative) and the lattice dimensionality. Due to the fact of an attractive potential arising between electrons on the same site, it leads to Cooper's instability<sup>16</sup> in the ground state ( $d \geq 2$ ). Mean field theory and enormous numerical calculations<sup>3</sup> indicate that in the ground state electrons form a local singlet pair with zero momentum [in our notation,  $\mathbf{q} = \mathbf{Q} = (\pi, \pi, \dots)$ ] and superconductivity arises. Simultaneously, when the system is exactly half filled, our theorem tells us that the CDW appears. This is the well-known phenomenon of the coexistence of superconductivity and the CDW in the negative Hubbard model.<sup>17</sup> This point is clearly manifested by Eq. (27), which comes from the invariance of the pseudospin rotation in the ground state. It should be stressed that the result holds only for a state  $\tilde{S} = 0$ , and when the system deviates from the half filling case, the corresponding ground state must have  $\tilde{S} > 0$ . In this case, we could not obtain the result by utilizing the invariance of the pseudospin in space.

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<sup>9</sup> The supersolid was considered by O. Penrose and L. Onsager, Phys. Rev. **104**, 576 (1956). Since then, this subject has been revisited by various authors. One can refer to A. F. Andreev and I. M. Lifshitz, Sov. Phys. JETP **29**, 1107

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<sup>10</sup> In Yang's paper (Ref. 4), he called these operators "η pairing." In an earlier paper by E. Lieb [*Phys. Rev. Lett.* **62**, 1201 (1989)], he called them "the pseudospin" operators, though he did not find pseudospin symmetry in the Hubbard model.

<sup>11</sup> The partial particle-hole transformation has been discussed extensively; see H. Shiba, *Prog. Theor. Phys.* **48**, 217 (1972); Y. Nagaoka, *ibid.* **52**, 1716 (1974), V. J. Emery, *Phys. Rev.* **B14**, 2989 (1972). The transformation defined in Eq. (4) is not very different from the usual definition. Under this transformation

$$\begin{aligned} \mathbf{T}c_{i\uparrow}\mathbf{T}^{-1} &= (-1)^{N\wedge\epsilon(i)}c_{i\uparrow}^\dagger, \\ \mathbf{T}c_{i\downarrow}\mathbf{T}^{-1} &= (-1)^{N\wedge}c_{i\downarrow}. \end{aligned}$$

For an even number of lattice sites, it is just the usual def-

inition; but for an odd number of lattice sites, it has an additional negative sign, which fortunately does not affect the physical results due to the fact that the third component is a good quantum number, i.e., the U(1) symmetry in the model.

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<sup>15</sup>  $\epsilon(i)$  can be taken in another form in the different models, for example, in a one-dimensional Hubbard model on a ring in the presence of a flux in the original point [see Gang Su, Bao-Heng Zhao, and Mo-Lin Ge, *Phys. Rev. B* **46**, 14 909 (1992)].

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