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1996 J. Phys.: Condens. Matter 8 4805

(http://iopscience.iop.org/0953-8984/8/26/012)

J. Phys.: Condens. Matter **8** (1996) 4805–4812. Printed in the UK

Pseudospin SU(2)-symmetry breaking, charge-density waves and superconductivity in the Hubbard model

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Received 10 October 1995, in final form 22 March 1996

Abstract. In this paper, we discuss the physical consequences of pseudospin SU(2)-symmetry breaking in a negative-U Hubbard model at half-filling. If pseudospin symmetry is spontaneously broken while its unique subgroup U(1) remains invariant, this will lead to a charge-density-wave (CDW) ground state. Furthermore, if the U(1) symmetry is also broken, the ground state will have off-diagonal long-range order, signalling a superconductor. In this case, CDW and superconductivity coexist and form a supersolid. Finally, we show that CDW suppress, but do not destroy superconductivity.

Spontaneous symmetry breaking in condensed-matter systems may produce some physically observable consequences [1]. For example, superfluidity and superconductivity come from the U(1)-symmetry breaking, and ferromagnetism and antiferromagnetism in an isotropic spin system come from the spontaneous spin SU(2)-symmetry breaking. Pseudospin SU(2) symmetry, discovered in the Kondo lattice model [2] and one-band Hubbard model [3, 4, 5], is a novel kind of rotational invariance in the particle–hole space, and has a dual relationship with the usual spin symmetry [6, 7]. It has generated a lot of interest among theoretical physicists and many studies have been carried out in this direction. Using pseudospin operators, Yang [3] has proposed the so-called 'η-pairing' mechanism of superconductivity, and his idea was later realized in the ground state of the negative-U Hubbard model [6, 8]. Zhang has discussed the physical consequences of pseudospin SU(2)-symmetry breaking in the 'η-pairing' superconductor [5]. Another important outcome of pseudospin SU(2) symmetry is the coexistence of charge-density waves (CDW) and superconductivity—i.e. a supersolid. By using the partial particle–hole transformation [9], the positive-U Hubbard model is mapped into a negative-U Hubbard model. It is believed that the ground state with positive U (at least in the large-U case) at half-filling is antiferromagnetic. The antiferromagnetic long-range order in the transverse direction for the positive-U model corresponds to the off-diagonal long-range order (ODLRO) in the negative-U model through the mapping, while the longitudinal antiferromagnetic order corresponds to the CDW long-range order. Therefore, in the negative-U Hubbard model there is possible a coexistence of superconductivity characterized by the ODLRO and CDW characterized by the diagonal long-range order (DLRO) [10]. Usually, ODLRO is characteristic of superconductivity, but in a supersolid with both ODLRO and DLRO whether this is still true is an open question. In [11] it was concluded that the critical magnetic field for a supersolid with pseudospin symmetry must be zero, since the superconducting state can freely rotate to the CDW state

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0953-8984/96/264805+08$19.50

because of the SU(2) symmetry and degeneracy. This leads to the question of how to explain the superconducting properties of a supersolid.

In this paper, we discuss some physical consequences of pseudospin SU(2) symmetry in the negative-U Hubbard model [12]. First, we show that if pseudospin symmetry is spontaneously broken while its unique subgroup U(1) remains invariant, this will lead to a CDW ground state, and the appearance of two massless collective modes according to the Goldstone theorem [14]. Second, if the U(1) symmetry is also broken, the ground state will have the ODLRO, signalling a superconductor. In this case, the ODLRO and CDW coexist and a supersolid is formed. U(1)-symmetry breaking will also give rise to a third branch of massless mode. Finally, we discuss the superconducting properties of a supersolid. We show that CDW suppress, but do not destroy superconductivity, and supersolids exhibit both the Meissner effect and zero resistance. We also calculate the penetration depth in terms of the order parameters for superconductors and CDW. We should point out that the traditional view is to consider CDW as being produced by breaking of the translational symmetry which is a discrete symmetry in the Hubbard model case. The significance of our work is that we find additional continuous symmetry for CDW which has important physical consequences (like Goldstone bosons). Our finding of the relationship between CDW and pseudospins may not be restricted to the Hubbard model. For example, pseudospin symmetry also exists in the Su–Schrieffer–Heeger Hamiltonian (see [15]) describing one-dimensional polymers.

The one-band Hubbard model on a bipartite lattice Λ made up of sublattices A and B is defined by the Hamiltonian

$$H = -t \sum_{\langle ij\rangle,\sigma} c^\dagger_{i\sigma} c_{j\sigma} + \frac{2}{3} U \sum_{i\in\Lambda} \tilde{\boldsymbol{S}}_i \cdot \tilde{\boldsymbol{S}}_i + 2\mu \sum_{i\in\Lambda} \tilde{S}^z_i \tag{1}$$

where $c^\dagger_{i\sigma}$ and $c_{i\sigma}$ are the creation and annihilation operators for an electron with spin σ at site i, respectively. The summation of $\langle ij\rangle$ runs over all possible nearest-neighbour pairs. μ is the chemical potential and is determined by the electron density. $\tilde{\boldsymbol{S}}_i$ is a pseudospin operator and is defined by

$$\begin{cases} \tilde{\boldsymbol{S}}^+_i = \epsilon(i) c_{i\uparrow} c_{i\downarrow} \\ \tilde{\boldsymbol{S}}^-_i = \epsilon(i) c^\dagger_{i\downarrow} c^\dagger_{i\uparrow} \\ \tilde{\boldsymbol{S}}^z_i = \frac{1}{2}(1 - n_{i\uparrow} - n_{i\downarrow}) \end{cases} \tag{2}$$

where $\epsilon(i) = +1$ for $i \in$ A, and -1 for $i \in$ B. They obey the same commutation relation as the regular spin operators. The total pseudospin operator is $\tilde{\boldsymbol{S}} = \sum_i \tilde{\boldsymbol{S}}_i$, and its three components can be used as the generators to construct a SU(2) group. The Hamiltonian in equation (1) obeys the commutation relations

$$[H, \tilde{\boldsymbol{S}}^\pm] = \mp 2\mu \tilde{\boldsymbol{S}}^\pm \qquad [H, \tilde{\boldsymbol{S}}^z] = 0. \tag{3}$$

Therefore, when $\mu = 0$, H has pseudospin SU(2) symmetry, and when $\mu \neq 0$, the symmetry is explicitly broken by the term containing the chemical potential. The latter is very similar to the case of the isotropic spin Heisenberg model in the presence of an external magnetic field. On the other hand, $\tilde{\boldsymbol{S}}^z$ always commutes with the Hamiltonian. Thus, the total number of electrons is conserved, and the Hamiltonian always possesses U(1) symmetry, where U(1) is the unique subgroup of SU(2). In this paper, we are interested in the physical consequences of spontaneous pseudospin SU(2)-symmetry breaking and for our purposes we will only discuss the case with $\mu = 0$ and $U < 0$. In this case, if the ground state does not possesses pseudospin SU(2) symmetry, as the Hamiltonian does, then the spontaneous symmetry breaking occurs.

From the structure of the SU(2) group, there are two possibilities for the pseudospin symmetry being spontaneously broken: (i) the SU(2) symmetry is broken while its subgroup U(1) remains invariant; and (ii) the U(1) symmetry is also broken. We show that case (i) will produce the CDW ground state. Its pseudospin-z-component operator is related to the charge density, and its corresponding long-range order is that of CDW. The CDW state at half-filling with the order parameter

$$\frac{1}{\sqrt{N_\Lambda}}\tilde{S}^z_Q = \frac{1}{N_\Lambda}\sum_i \epsilon(i)\langle\tilde{\boldsymbol{S}}^z_i\rangle = -\frac{1}{2N_\Lambda}\sum_{\boldsymbol{k},\sigma}\langle c^\dagger_{\boldsymbol{k},\sigma}c_{\boldsymbol{k}+\boldsymbol{\pi},\sigma} + c^\dagger_{\boldsymbol{k}+\pi,\sigma}c_{\boldsymbol{k},\sigma}\rangle$$

can be expressed as

$$|\mathrm{CDW}\rangle = \prod_{\boldsymbol{k},\sigma}(u_k c^\dagger_{\boldsymbol{k},\sigma} + v_k c^\dagger_{\boldsymbol{k}+\boldsymbol{\pi},\sigma})|0\rangle \tag{4}$$

with

$$\frac{1}{N_\Lambda}\sum_{\boldsymbol{k}} u_{\boldsymbol{k}} v_{\boldsymbol{k}} \neq 0$$

where the $\boldsymbol{k}$ is within half of the Brillouin zone, although we have $\langle\mathrm{CDW}|\tilde{\boldsymbol{S}}^\pm|\mathrm{CDW}\rangle = \langle\mathrm{CDW}|\tilde{\boldsymbol{S}}^z|\mathrm{CDW}\rangle = 0$, but only $\tilde{\boldsymbol{S}}^z|\mathrm{CDW}\rangle = 0$ and $\tilde{\boldsymbol{S}}^\pm|\mathrm{CDW}\rangle \neq 0$. The SU(2) symmetry in a state has been broken unless all eigenvalues for the operator $\tilde{\boldsymbol{S}}$ are zero. Therefore, $|\mathrm{CDW}\rangle$ preserves the conservation of the particle number (or U(1) symmetry), but destroys the SU(2) symmetry.

One of the strong pieces of evidence to support CDW as products of pseudospin symmetry breaking is the existence of massless modes, i.e., Goldstone bosons. According to the Goldstone theorem [14], when a continuous symmetry is spontaneously broken, there must exist some massless modes. The appearance of CDW will produce two massless modes. To see this, we first consider the following correlation functions:

$$F_+(t,t') = -\mathrm{i}\theta(t-t')\left\langle\left[\tilde{\boldsymbol{S}}^+(t), \sum_i \epsilon(i)\tilde{\boldsymbol{S}}^-_i(t')\right]\right\rangle \tag{5}$$

$$F_-(t,t') = -\mathrm{i}\theta(t-t')\left\langle\left[\tilde{\boldsymbol{S}}^-(t), \sum_i \epsilon(i)\tilde{\boldsymbol{S}}^+_i(t')\right]\right\rangle \tag{6}$$

where $\langle\cdots\rangle$ indicates the thermodynamic average. By using the commutation relation between pseudospin operators and the Hamiltonian, we have

$$F_\pm(\omega) = 2\left\langle\sum_i \epsilon(i)\tilde{\boldsymbol{S}}^z_i\right\rangle\Big/(\omega \mp 2\mu + \mathrm{i}\delta). \tag{7}$$

If the CDW order parameter

$$\left\langle\sum_i \epsilon(i)\tilde{\boldsymbol{S}}^z_i\right\rangle\Big/N_\Lambda \neq 0$$

then there are two collective modes $\omega_0 = \pm 2|\mu|$. It should be noticed that if the chemical potential μ is not equal to zero, i.e., the symmetry is explicitly broken, the two collective modes are massive. If the CDW state arises in the half-filling case, which is our interest in this paper, then $\mu = 0$ and there appear two massless modes according to equation (7), which illustrates that it is the symmetry-breaking CDW ground state which produces the two massless modes. We should point out that only one branch is directly observable because the other one is of negative energy.

Case (ii) will lead to the coexistence of CDW and superconductivity. As is well known, the U(1)-symmetry breaking gives rise to a superconductor. The BCS superconducting state with an order parameter $\langle c^\dagger_{\boldsymbol{k},\uparrow} c^\dagger_{-\boldsymbol{k},\downarrow}\rangle$ can be written as [16]

$$|\mathrm{BCS}\rangle = \prod_{\boldsymbol{k}} (u_{\boldsymbol{k}} + v_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k},\uparrow} c^\dagger_{-\boldsymbol{k},\downarrow})|0\rangle. \tag{8}$$

Here $\boldsymbol{k}$ is within the Brillouin zone. Clearly, $|\mathrm{BCS}\rangle$ breaks the conservation of the particle number since $|\mathrm{BCS}\rangle$ is not an eigenstate of $\tilde{\boldsymbol{S}}^z$. Superconductivity in a system with pseudospin symmetry can be understood as follows. Pseudospin operators, like the usual spin-1/2 operators, can be regarded as operators for hard-core bosons. The raising and lowering operators consist of the local singlet pairs of electrons. Obviously, no two pairs can occupy one site by the Pauli principle. If the hard-core bosons condense macroscopically at a low temperature, this gives rise to superconductivity (the boson here has charge $2e$). If the condensation happens at the momentum value $\boldsymbol{q} = \boldsymbol{\pi}$, the order parameter can be written as

$$\left\langle \frac{1}{N_\Lambda} \sum_i \exp\,(\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{\pi}) \tilde{\boldsymbol{S}}^+_i \right\rangle = \frac{1}{N_\Lambda} \sum_{\boldsymbol{k}} \langle c_{\boldsymbol{k}\uparrow} c_{-\boldsymbol{k}\downarrow}\rangle$$

which is that of the usual BCS superconductor. If the condensation happens at $\boldsymbol{q} = \boldsymbol{0}$, its order parameter is

$$\left\langle \frac{1}{N_\Lambda} \sum_i \tilde{\boldsymbol{S}}^+_i \right\rangle = \frac{1}{N_\Lambda} \sum_{\boldsymbol{k}} \langle c_{\boldsymbol{k}+\boldsymbol{\pi}\uparrow} c_{-\boldsymbol{k}\downarrow}\rangle.$$

In this case, the pseudospin obeys the relationship $\tilde{S}^2 - \tilde{S}_z^2 = \mathrm{O}(N_e^2)$, which is the criterion for the η-pairing superconductor, as Yang proposed [3]. Such a phenomenon only happens in the ground state of the negative-U case with $2N_A > N_e > 2N_B$ (N_A and N_B are two sublattice site numbers), and there it is found that

$$\left|\left\langle \frac{1}{N_\Lambda} \sum_i \epsilon(i) \tilde{S}^\pm_i \right\rangle\right| > \left|\left\langle \frac{1}{N_\Lambda} \sum_i \tilde{\boldsymbol{S}}^\pm_i \right\rangle\right| \neq 0$$

in the thermodynamic limit [17]. Thus, the two kinds of ODLRO must coexist in the η-pairing superconductor. When the condensation occurs, adding or removing a boson in the condensate does not change the total energy. Thus the chemical potential μ is equal to zero. Furthermore, the condensation also breaks the U(1) symmetry in the thermodynamic limit. Therefore, *the local pairing superconductivity is product of both pseudospin symmetries SU(2) and U(1) spontaneously breaking*. The breaking of U(1) should give rise to another massless mode [19]. The correlation function is defined as [5]

$$F_0(t, t') = -\mathrm{i}\theta(t - t')\left\langle\left[\tilde{\boldsymbol{S}}^z(t), \sum_i \epsilon(i)\tilde{\boldsymbol{S}}_-(t')\right]\right\rangle \tag{9}$$

and

$$F_0(\omega) = -\left\langle \sum_i \epsilon(i) \tilde{\boldsymbol{S}}_- \right\rangle \Big/ (\omega + \mathrm{i}\delta). \tag{10}$$

Together with the two massless modes produced by CDW, there are three massless modes when U(1) symmetry is also broken: two for CDW and one for superconductivity, as we list in equations (7) and (10), which coincides with the Goldstone theorem [14]. Therefore, in this case, the CDW and superconductivity must coexist. *The SU(2) and U(1) symmetry spontaneously breaking gives rise to a supersolid*.

Although we are not restricted to low-dimensional systems, we would like to mention that spontaneous pseudospin symmetry breaking even occurs in some low-dimensional systems. Quantum fluctuation in low-dimensional systems is usually very strong, which tends to kill long-range order. However, there are some counter-examples. For instance, [6] provides a rigorous example of quasi-one-dimensional system where the ground state possesses ODLRO. In this case it appears that the geometric structure of system plays a central role for the long-range correlations of electrons. It is able to suppress quantum fluctuation, and ODLRO and CDW LRO survive in the ground state. In a positive-U case at half-filling, the same geometric structure is also able to suppress the quantum fluctuation and to preserve the antiferromagnetic LRO in the ground state [18, 20]. However, the possibility of spontaneous pseudospin symmetry breaking was ruled out by Kubo and Kishi for three and fewer dimensions [13].

Next we discuss the diamagnetism and resistance in a supersolid that result from spontaneous pseudospin symmetry breaking on the basis of the mean-field theory. CDW have diagonal long-range order and this might suppress superconductivity characterized by ODLRO. However, whether it could destroy superconductivity completely is an interesting and open question. As an example, here we discuss the case of a three-dimensional cubic lattice. It is believed that the ground state is a supersolid. The mean-field approach is useful only if the ground state possesses corresponding long-range correlations. In the mean-field theory, the Hamiltonian for the coexistence of CDW and superconductivity is reduced to

$$H = \sum_{\boldsymbol{k},\sigma} \gamma_{\boldsymbol{k}} c^{\dagger}_{\boldsymbol{k},\sigma} c_{\boldsymbol{k},\sigma} + \sum_{\boldsymbol{k}} (\Delta^{*} c_{-\boldsymbol{k},\downarrow} c_{\boldsymbol{k},\uparrow} + \Delta c^{\dagger}_{\boldsymbol{k},\uparrow} c^{\dagger}_{-\boldsymbol{k},\downarrow}) - \rho \sum_{\boldsymbol{k}} c^{\dagger}_{\boldsymbol{k},\sigma} c_{\boldsymbol{k}+\boldsymbol{\pi},\sigma} + N_{\Lambda} \frac{3}{2|U|} (\Delta^2 + \rho^2) \tag{11}$$

where

$$\Delta = \frac{2}{3} \frac{1}{N_{\Lambda}} U \sum_{i} \mathrm{e}^{\mathrm{i}\boldsymbol{\pi}\cdot\boldsymbol{r}_i} \langle \tilde{\boldsymbol{S}}^{+}_{i} \rangle \qquad \text{and} \qquad \rho = \frac{2}{3} \frac{1}{N_{\Lambda}} U \sum_{i} \mathrm{e}^{\mathrm{i}\boldsymbol{\pi}\cdot\boldsymbol{r}_i} \langle \tilde{\boldsymbol{S}}^{z}_{i} \rangle.$$

The kinetic energy is $\gamma_{\boldsymbol{k}} = -2t(\cos k_x + \cos k_y + \cos k_z)$. In this approximation, one finds that the ground-state energy, the kinetic energy and the equation for the order parameters depend only on the parameter $R = \sqrt{\Delta^2 + \rho^2}$, and the states with pure CDW and pure superconductivity are degenerate. However, we should point out that the supersolid has a unique non-degenerate ground state, as shown beyond the mean-field theory [7, 20].

Generally speaking, the Meissner effect and zero resistance are two hallmarks of a superconductor. In this model, the current operator is

$$\boldsymbol{j}_0 = \mathrm{i}et \sum_{i,\boldsymbol{\delta},\sigma} \boldsymbol{\delta} c^{\dagger}_{i+\boldsymbol{\delta},\sigma} c_{i,\sigma} \tag{12}$$

where $\boldsymbol{\delta}$ is the lattice vector for the nearest-neighbour sites. When the system is in the presence of a weak magnetic field, the linear response theory [19, 21] tells us that the response current can be expressed by

$$j_{\mu} = -te^2 \sum_{i,\sigma} \langle g | c^{\dagger}_{i+e_{\mu},\sigma} c_{i,\sigma} + c^{\dagger}_{i,\sigma} c_{i+e_{\mu},\sigma} | g \rangle A_{\mu}(\boldsymbol{r}_i, t) + \mathrm{i} \sum_{i,i',\nu} \int \mathrm{d}t' \, \langle g | [j_{0,\mu}(\boldsymbol{r}_i, t), j_{0,\nu}(\boldsymbol{r}'_i, t')] | g \rangle \theta(t - t') A_{\nu}(\boldsymbol{r}'_i, t'). \tag{13}$$

$\boldsymbol{e}_{\mu}$ is a unit vector along the direction $\mu = (x, y, z)$ and $|g\rangle$ is the ground state in the absence of the field. The first term in equation (13) is diamagnetic and the second term is paramagnetic. Furthermore,

$$j_i(\boldsymbol{q},\omega) = -e^2[\langle -K_i\rangle\delta_{ij} - R_{ij}(\boldsymbol{q},\omega)]A_j(\boldsymbol{q},\omega) \tag{14}$$

where

$$\langle K_i\rangle = -\frac{2}{3}\frac{1}{N_\Lambda}\sum_{\boldsymbol{k}}\frac{\gamma_{\boldsymbol{k}}^2}{\omega_{\boldsymbol{k}}} \tag{15}$$

and

$$R_{ij}(\boldsymbol{k},\omega) = -\mathrm{i}\int_{-\infty}^{\infty}\frac{\mathrm{d}t}{2\pi}\,\mathrm{e}^{\mathrm{i}\omega t}\langle g|[j_i(\boldsymbol{q},t),\,j_j(-\boldsymbol{q},0)]|g\rangle\theta(t). \tag{16}$$

The superfluid density is determined by

$$\left(\frac{n_s}{m}\right)^* \equiv \langle -K_i\rangle - R_{ii}(q_i=0, q_{j\neq i}\to 0, \omega=0) = 8t^2\frac{1}{N_\Lambda}\sum_{\boldsymbol{k}}\sin^2 k_i\frac{\Delta^2}{\omega_{\boldsymbol{k}}^3}. \tag{17}$$

For a pure CDW state with $\rho = R$ and $\Delta = 0$,

$$\left(\frac{n_s}{m}\right)^*_{\rho=R,\Delta=0} = \frac{2}{3}\frac{1}{N_\Lambda}\sum_{\boldsymbol{k},\sigma}\frac{\gamma_{\boldsymbol{k}}^2}{\omega_{\boldsymbol{k}}} - 8t^2\frac{1}{N_\Lambda}\sum_{\boldsymbol{k}}\sin^2 k_x\frac{R^2}{\omega_{\boldsymbol{k}}^3} = 0 \tag{18}$$

[22]. Therefore, the superfluid density $(n_s/m)^*$ for the supersolid ground state with both CDW and superconductivity is proportional to Δ^2 and is always positive and non-zero as long as $\Delta \neq 0$. Furthermore, as the quasiparticle spectrum has a finite energy gap R, the Drude weight is equal to the superfluid weight [21]:

$$\frac{D}{\pi e^2} \equiv \left(\frac{n}{m}\right)^* \equiv \langle -K_x\rangle - \mathrm{Re}\{R_{ii}(q=0,\omega\to 0)\} = \left(\frac{n_s}{m}\right)^* \neq 0 \tag{19}$$

which implies zero resistance. The penetration depth for a supersolid is

$$\lambda_s = (4\pi n_s e^2/mc^2)^{-1/2}$$

and

$$\lambda_c = \left(\frac{4\pi e^2}{3c^2 N_\Lambda}\sum_{\boldsymbol{k}}\frac{\gamma_{\boldsymbol{k}}^2}{\omega_{\boldsymbol{k}}}\right)^{1/2}$$

is the penetration depth for a pure superconductor with $\rho = 0$ and $\Delta = R$. We have

$$\lambda_s = \left(1 + \frac{\rho^2}{\Delta^2}\right)^{1/2}\lambda_c \geqslant \lambda_c. \tag{20}$$

This expression indicates that the perfect diamagnetism arises as soon as ODLRO is present, i.e., $\Delta \neq 0$. When $\Delta \to 0$, λ_s approaches infinity, and the diamagnetism disappears. Hence, the order parameter Δ guarantees superconductivity with both the Meissner effect and zero resistance. λ_s will increase with the CDW order parameter ρ. Thus, in the supersolid the CDW suppresses the superconductivity, but does not destroy it completely. In the negative-U case on a cubic lattice, the SU(2) symmetry ensures that the ratio for ρ and Δ is fixed at $\rho/\Delta = 1/\sqrt{2}$ [7], which gives the value $\lambda_s = \sqrt{3/2}\lambda_c$. Therefore, we conclude that the supersolid is a true superconductor, not an insulator as was being claimed in previous studies [11, 23].

Before ending the paper, we would like to discuss some experimental implications of our results. The following discussions are only meaningful if the experimental samples can be approximately described by Hamiltonians which contain the pseudospin SU(2) symmetry. The coexistence of CDW and superconductivity has been observed in several materials

[24]. The collective modes are the products of the spontaneous symmetry breaking. There are two branches of massless modes accompanying the appearance of CDW, but only one is experimentally observable, due to the negative energy of the other branch for finite momentum. After U(1)-symmetry breaking, a new branch of massless mode should appear. The massless mode and massive mode correspond to the phase mode and amplitude mode of the order parameter; thus, they usually appear as a pair [25]. The massive modes have been observed experimentally [26]. The number of modes is one if the system is a CDW ground state and two if CDW coexist with superconductivity; these numbers agree with our findings.

In summary, the CDW in the Hubbard model is the product of spontaneous pseudospin SU(2)-symmetry breaking, and furthermore if its subgroup U(1) symmetry is also broken, there is coexistence of both CDW and superconductivity. The additional global and continuous symmetry breaking presents important and physically observable consequences, and provides a natural understanding of a supersolid.

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