Pseudospin Symmetry and New Collective Modes of the Hubbard Model

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The Hubbard model possesses an SU(2) pseudospin symmetry, which contains the U(1) phase symmetry as a subgroup. The existence of such symmetry leads to interesting experimental consequences if the U(1) phase symmetry is spontaneously broken, i.e., if the ground state is superconducting. In this case, there must exist a pair of *massive* collective modes which together with the usual Goldstone mode form a triplet representation of the pseudospin group. These collective modes are collisionless and couple directly to external charge disturbances with the wave number π and can therefore be detected experimentally as sharp resonances.

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Ordinarily, when a theoretical model is proposed to explain a given experimental phenomenon, its validity can be easily accepted or rejected by comparing the theoretical consequences of the model with experimental data. However, three years have passed since the discovery of high-T_c superconductivity,[1] and no verdict has yet been reached on the question of whether the one-band Hubbard model gives a proper description of the phenomenon. The problem certainly lies in the difficulty of extracting unique and reliable consequences of a model which strongly correlates many degrees of freedom. In this Letter, we exploit the consequences of a special symmetry property of the Hubbard model. These consequences are unique to the Hubbard model, mathematically rigorous, and predict new resonances which could be detected experimentally.

Condensed-matter systems usually involve interactions of many degrees of freedom and various modes are strongly coupled to each other. A single mode typically decays with microscopic lifetime and cannot be easily identified in a macroscopic measurement. However, there exist well-defined collective modes in many-body systems whose decay is prevented by selection rules associated with symmetry principles. For example, charge conservation gives rise to the collective sound-wave modes in quantum Bose liquids, rotational invariance leads to spin waves in both ferromagnets and antiferromagnets, and the translational invariance is responsible for the collective cyclotron mode of electrons in a magnetic field. Since these modes have long lifetimes, they can be detected experimentally as sharp resonances and the systematic investigations of their properties yield a great deal of valuable information.

The one-band Hubbard model indeed possesses a very special symmetry, an SU(2) global symmetry which we call the pseudospin symmetry. It contains the usual U(1) phase symmetry as a subgroup. Interesting consequences follow if the U(1) phase symmetry is spontaneously broken, i.e., if one is in the superconducting phase. In this case, according to Goldstone's theorem, there must exist a massless collective mode which is well defined (collisionless) in the long-wavelength limit. In the Hubbard model, however, since the U(1) phase symmetry is a subgroup of a larger SU(2) symmetry group, we prove that there must exist two other *massive* modes, which can be viewed as the symmetry partner of the Goldstone mode. The lifetime of these modes becomes infinite as the crystal momentum approaches π [in the following π denotes the corner of the Brillouin zone, in two dimensions, it is the point $(\pi/a,\pi/a)$] and the energy disperses quadratically away from this point. They couple directly to the longitudinal density fluctuation with wave number π and can therefore be detected experimentally as sharp resonances, say, in the electron-energy-loss spectrum. Since the pseudospin symmetry is unique to the Hubbard model, the observation of these resonances in copper oxides could uniquely test the validity of the model. The position of the resonance determines the parameters in the Hubbard Hamiltonian, the quadratic curvature in the dispersion relation yields information about the form factor of the Cooper pair, the total intensity of the peak is proportional to the square of the superconducting order parameter, and the width of the peak is a measure of the departure of the Hubbard model from reality.

The one-band Hubbard model is defined by the Hamiltonian

$$H=-t\sum_{\langle r,r'\rangle,\sigma} c^\dagger_{r\sigma}c_{r'\sigma}+\text{H.c.}+U\sum_r n_{r\uparrow}n_{r\downarrow}-\mu\sum_{r\sigma}n_{r\sigma}\,. \quad (1)$$

We denote by $N=\sum_{r\sigma}n_{r\sigma}$ the total number of electrons and M the total number of lattice sites. μ is the chemical potential that fixes the density of the system. The lattice constant is taken to be unity. The following discussions are independent of the space dimensions, the filling fraction, and the sign of U.

In this model, the operators

$$J_-=\sum_r(-1)^r c_{r\uparrow}c_{r\downarrow},\quad J_+=J_-^\dagger,\quad J_0=\tfrac{1}{2}(N-M) \quad (2)$$

obey the commutation relations $[J_0,J_\pm]=J_\pm$, $[J_+,$

$J_-]=2J_0$ and therefore form an SU(2) algebra. In the following, we shall call it the pseudospin algebra. They are eigenoperators of the Hamiltonian[2] in the sense that

$$[H,J_\pm]=\pm(U-2\mu)J_\pm, \quad [H,J_0]=0. \tag{3}$$

Thus both J_0 and $J^2=\frac{1}{2}(J_+J_-+J_-J_+)+J_0^2$ commute with the Hamiltonian and are conserved quantities.[3] In recent work,[4] the representation of this symmetry on the Hilbert space is constructed explicitly. In order to extract direct experimental consequences, we now consider irreducible representations of this symmetry in terms of the *operators* rather than the *states* of the model.

Theorem 1.—The operators

$$\Delta_-=\frac{1}{\sqrt{2}}\sum_r c_{r\uparrow}c_{r\downarrow}, \quad \Delta_+=-\Delta_-^\dagger, \qquad \Delta_0=\tfrac{1}{2}\sum_{r\sigma}(-1)^r n_{r\sigma} \tag{4}$$

form an irreducible tensor of rank $l=1$ under the SU(2) algebra defined by (2).

Proof: It can be easily checked that

$$[J_0,\Delta_m]=m\Delta_m, \qquad [J_\pm,\Delta_m]=\sqrt{l(l+1)-m(m\pm1)}\,\Delta_{m\pm1}, \tag{5}$$

where $l=1$ and $m=-1$, 0, and $+1$, respectively.

Physically, $\Delta_\pm$ are the on-site *s*-wave pairing operators while Δ_0 is the charge-density-wave operator. Equation (5) states the fact that they can be "rotated" into each other by the pseudospin generators. This crucial fact allows one to relate correlation functions of these different operators in a way that measurable consequences become manifest. Similar irreducible tensors can be easily constructed which include the extended *s*-wave or the *d*-wave pairing operators as part of the multiplet. All the following results apply to these multiplets also. However, for the sake of concreteness, we do not discuss them separately.

Information about collective modes are contained in the analytic properties of correlation functions. We consider the following response function:

$$D_+(t,t')=-\frac{i}{M}\theta(t-t')\langle[J_+(t),\Delta_0(t')]\rangle. \tag{6}$$

Since J_+ is an eigenoperator of the Hamiltonian, from (3), its time dependence in the Heisenberg representation can be determined explicitly, in particular, $J_+(t)=e^{i(U-2\mu)(t-t')}J_+(t')$. The equal-time commutator of J_+ and Δ_0 is given by Eq. (5); therefore, (6) can be calculated exactly. We thus obtain

$$D_+(\omega)=\frac{\sqrt{2}\rho}{\omega+(U-2\mu)+i\delta}, \tag{7}$$

where $\rho=\langle\Delta_+\rangle/M$, δ is a positive infinitesimal, and $D_+(\omega)=\int dt\,e^{i\omega(t-t')}D_+(t-t')$ is the Fourier transform of (6). Similarly, we have

$$D_0(t,t')=-\frac{i}{M}\theta(t-t')\langle[J_0(t),\Delta_+(t')]\rangle, \qquad D_0(\omega)=\frac{\rho}{\omega+i\delta}, \tag{8}$$

and

$$D_-(t,t')=-\frac{i}{M}\theta(t-t')\langle[J_-(t),\Delta_0(t')]\rangle, \qquad D_-(\omega)=\frac{-\sqrt{2}\rho^*}{\omega-(U-2\mu)+i\delta}. \tag{9}$$

We summarize the above results by the following theorem:

Theorem 2.—If $\rho\neq0$ in the ground state of the Hubbard model, then there is necessarily a triplet of collective modes, defined by the pole singularities in (7), (8), and (9) with energies $-(U-2\mu)$, 0, and $U-2\mu$, respectively.

Theorem 2 states a *consequence* of the spontaneous U(1) symmetry breaking, i.e., of superconductivity. It does not explain, nor does it depend on, the possible origin of this symmetry breaking. We note that (8) is nothing but the standard argument leading to the existence of the massless Goldstone boson.[5] Therefore, Theorem 2 can be viewed as a generalization of the Goldstone theorem to the case where the U(1) phase symmetry is a subgroup of a larger, in this case an SU(2), symmetry group. Note that $\mu=U/2$ fixes the density at half filling. In this case, the modes in (7) and (9) are *massless*. This is a manifestation of the fact that charge-density-wave order can coexist with superconductivity at half filling.[6] Away from half filling, the two new collective modes are *massive*.

Like the Goldstone mode, the collective modes found in (7) and (9) are in fact smooth limits of dispersion branches in the momentum space. To see this, let us define

$$J_-(q)=\sum_k c_{k+q\uparrow}c_{-k\downarrow}, \quad J_+(q)=J_-(q)^\dagger, \qquad \Delta_0(q)=\tfrac{1}{2}\sum_{k\sigma}c_{k+q\sigma}^\dagger c_{k\sigma}, \tag{10}$$

and form the correlation function

$$D_+(q,t)=-\frac{i}{M}\theta(t)\langle[J_+(q,t),\Delta_0(-q,0)]\rangle. \tag{11}$$

For $q=\pi$, (11) reduces to (6). Since the correlation function contains a single pole for $q=\pi$, we expect that it is also dominated by the pole contributions in the vicinity of π. This is the well-known single-mode approximation, first introduced by Feynman in the context of quantum Bose liquid.[7] In this approximation, one makes the ansatz that

$$D_+(q,\omega) = \frac{f(q)}{\omega - \omega(q) + i\delta}\,. \tag{12}$$

The unknown functions $f(q)$ and $\omega(q)$ can be determined explicitly by the moment sum rules

$$f(q) = \frac{1}{M}\langle [J_+(q), \Delta_0(-q)]\rangle\,,$$
$$f(q)\omega(q) = -\frac{1}{M}\langle [[H, J_+(q)], \Delta_0(-q)]\rangle\,, \tag{13}$$

from which one finds that $f(q) = \sqrt{2}\rho$ and

$$\omega(q) = -(U-2\mu) + \frac{1}{2\sqrt{2}\rho}(\delta q)^2 \frac{1}{M}\sum_k (\partial^2 \epsilon_k)\langle c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}\rangle \tag{14}$$

for $\delta q = q - \pi \ll 1$, where $\epsilon_k = -2t(\cos k_x + \cdots)$. As we see, the energy of this collective mode disperses quadratically away from $q = \pi$ with a curvature determined by the form factor of the Cooper pair $\langle c^\dagger_{k\uparrow} c^\dagger_{k\downarrow}\rangle$. For large enough δq, this mode eventually merges into the single-particle continuum.

While Theorem 2 is an exact mathematical result, some intuition may be gained by understanding the physical origin of these modes through Feynman diagrams. Imagine that an external charge disturbance is applied to the system at time t', so that a particle-hole pair is created by the operator Δ_0. Equation (9) gives the probability amplitude that a particle-particle pair, with the quantum numbers specified by J_-, is observed at later time t (see Fig. 1). Such a process occurs only in the superconducting phase where a hole can be scattered by the superconducting condensate and emerge as a particle. The pseudospin symmetry of the Hubbard model [Eq. (3)] guarantees that such a particle-particle pair can propagate *coherently* with frequency $U-2\mu$ throughout the system without any scattering. This coherent propagation shows up in the amplitude (9) as a single pole.

In realistic systems, there are always interactions present which spoil the exact symmetry of the Hubbard model. To the extent that they can be treated as perturbative corrections to the Hubbard model, they give rise to broadening of the δ-function peaks in the absorptive parts of the correlation functions. The width of these peaks is therefore a measure of the departure of the Hubbard model from reality. In the case of the massless Goldstone mode, however, the long-range part of the Coulomb interaction not included in the Hubbard model has a drastic effect. It leads to a singular perturbation in the long-wavelength limit and pushes the Goldstone mode up to the plasma frequency.[8] A similar effect does not happen for the new collective modes, since they only couple to density fluctuations with short wavelength (near π) and cannot be affected by the long-range part of the Coulomb interaction.

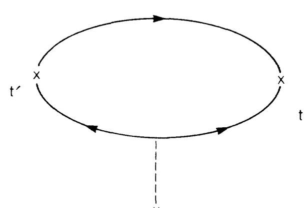

FIG. 1. External charge disturbance is applied to the system at time t', so that a particle-hole pair is created by Δ_0. The hole scatters with the superconducting condensate (denoted by the cross and the dotted line) and emerges as a particle. The particle-particle pair is observed at later time t.

From the above analysis we conclude that if the Hubbard model is a proper theoretical description of high-T_c superconductivity, it necessarily predicts a set of new collective modes in the superconducting phase, independent of detailed mechanisms through which superconductivity occurs. Since these modes couple directly to longitudinal density fluctuations through the operator Δ_0, the energy of an external charge disturbance can be absorbed into these modes, with power dissipation given by the δ-function peaks in the imaginary parts of the response functions (7), (9), and (12). An ideal measurement would be the electron-energy-loss experiment, in which external electrons scatter inelastically from the sample with a momentum transfer near $\Delta q = \pi$. Plotting the intensity as a function of the energy loss, one would find broad background distributions, due to single-particle scattering, above T_c and a sharp resonance peak below T_c, due to the scattering with the collective modes. Since the existence of such resonances are dictated by the symmetries of the Hubbard model, the outcome of such an experiment uniquely tests the validity of the Hubbard model as a description of high-T_c superconductivity.

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