Doping induced spinless collective excitations of charge $2e$ in doped Mott insulators

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Based on the Hubbard model description of the doped Mott insulator, we prove that there must exist a spinless collective excitation of charge $2e$ and of energy $U - 2\mu$ peaked at momentum $(\pi/a, \pi/a)$ in the non-superconducting state due to doping. Such a collective excitation arises from the electron pair correlation. Its existence is related to the breakdown of an approximate SU(2) particle-hole symmetry, from which an effective field theory of the new excitations is constructed.

It has become clear that the normal state of the high-$T_c$ cuprate superconductors shows many highly unusual properties. These properties are related to the fact that the high-$T_c$ cuprate superconductors are doped antiferromagnetic (AF) Mott insulators. It is then not surprising that the unusual behaviors are even more striking in the underdoped region, when the concentration of doped holes is small. A number of theoretical scenarios have emerged to understand the dynamics of the doped Mott insulators. Anderson [1] introduced the notion of “spin-emergent” to understand the dynamics of the doped Mott insulators. Anderson [1] introduced the notion of “spin-emergent” to understand the dynamics of the doped Mott insulators. Anderson [1] introduced the notion of “spin-emergent” to understand the dynamics of the doped Mott insulators. Anderson [1] introduced the notion of “spin-emergent” to understand the dynamics of the doped Mott insulators. Anderson [1] introduced the notion of “spin-emergent” to understand the dynamics of the doped Mott insulators.

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Consider the extended Hubbard model in a 2D square lattice with spacing $a$, which we believe contains the essential physics of the doped Mott insulators. The Hamiltonian is

$$H = -t \sum_{(xx')} \langle x\sigma \rangle \langle x' \sigma' \rangle + h.c. + J \sum_{(xx')} \langle x \sigma \rangle \cdots \langle x' \sigma' \rangle + U \sum_x n_{\uparrow}(x)n_{\downarrow}(x) - \mu \sum_x n(x),$$

where $n_{\sigma}(x) = c_{\sigma}^\dagger(x)c_{\sigma}(x)$ with spin $\sigma (= \uparrow, \downarrow)$, $n(x) = n_{\uparrow}(x) + n_{\downarrow}(x)$, and $\mu$ is the chemical potential that fixes the density of the system.

The Hamiltonian is invariant under the transformation, $c_\sigma \to U_{\sigma} c_\sigma$. This is the usual SU(2) spin symmetry. Furthermore, near half-filling the model has another (approximate) SU(2) particle-hole symmetry, sometimes called pseudospin group $\mathbb{Z}_2\mathbb{Z}_2\mathbb{Z}_2$. To see the symmetry, let us introduce two pseudospin doublets

$$\psi_1(x) = \left(\begin{array}{c} c_\uparrow(x) \\ (-)^{x} c_\downarrow(x) \end{array}\right), \quad \psi_2(x) = \left(\begin{array}{c} c_\downarrow(x) \\ (-)^{x} c_\uparrow(x) \end{array}\right),$$

where $(-)^{x} \equiv e^{iQx}$ with $Q \equiv (\pi/a, \pi/a)$. In terms of the doublets $\psi_{\alpha}$, the Hamiltonian becomes

$$H = -\sum_{(xx')} \psi_1(x)\psi_{\alpha}(x') + J \sum_{(xx')} \langle x \sigma \rangle \cdots \langle x' \sigma' \rangle + 2U \sum_x \bar{\phi} \cdot \bar{\phi} + (U - 2\mu) \sum_x \phi_3,$$

where

$$\bar{S} = \frac{1}{4} \psi_{\alpha l}^\dagger x_{\alpha l} \psi_{\beta l},$$

and

$$\bar{\phi} \equiv \frac{1}{4} \psi_{\alpha l}^\dagger \bar{S}_{lm} \psi_{\alpha m}.$$

The $\bar{\phi}$ is a vector of the usual Pauli matrices. (Note: Indices $\alpha, \beta, \cdots$ label two pseudospin doublets; $l, m, \cdots$ label the rows of each.) Explicitly, $\phi_3 = \frac{1}{2}(n - 1)$, and $(\phi_1, \phi_2) = \frac{1}{\sqrt{2}} (\Delta_+ + \Delta_-, i\Delta_- - i\Delta_+)$ where $\Delta_\pm (x) \equiv c_\uparrow(x)c_\uparrow(x)$ and $\Delta_\pm \equiv \Delta_\pm^\dagger$ are the pairing fields. The theory is thus obviously invariant at half filling ($\mu = U/2$) under a global SU(2) pseudospin transformation: $\psi_{\alpha l} \to U_{lm} \psi_{\alpha m}$. Clearly, $\phi$ transforms as a pseudospin vector. The operators

$$J_{\pm} = \sum_x (\phi_1 \pm i\phi_2) = \sum_x (-)^x \Delta_\pm, \quad J_3 = \sum_x \phi_3,$$

generate the (approximate) SU(2) pseudospin symmetry, in the sense that

$$[H, J_{\pm}] = \pm (U - 2\mu) J_{\pm}, \quad [H, J_3] = 0.$$}

The symmetry becomes exact at half filling with $\mu = U/2$. Note that $J$’s commute with the ordinary spin operators $\bar{S}$.
Consider the non-superconducting, underdoped regime of the phase diagram. Hole doping breaks the $SU(2)$ pseudospin symmetry down to the ordinary charge $U(1)$ subgroup in two ways. At first, it breaks the symmetry explicitly at the Hamiltonian level. This is obvious from Eq. (5). Secondly, doping forces the ground state to ‘line’ up in the 3-direction (or $z$) in the pseudospin space while leaving the usual spin symmetry intact. This point is manifested by noticing that doping induces a ground state such that $\langle \phi_3 \rangle_0 = -\frac{\mu}{U} \neq 0$ where $\delta_h \equiv 1 - (n_i)_0$ is the concentration of doped holes. The second way of breaking the symmetry is reminiscent of the notion of spontaneous symmetry breaking. One would immediately conclude from the Goldstone theorem that the Goldstone modes must appear at low energy. However, the present case substantially differs from the case of spontaneously broken symmetries in that upon withdrawal of doping the ground state recovers the full $SU(2)$ pseudospin invariance. The usual Goldstone theorem does not apply in the present case. We need to carefully examine the breakdown of the pseudospin symmetry.

Collective excitations, if any, can be identified by examining the analytical properties of correlation functions. Consider the Fourier transform of the following (retarded) electron-pair correlation function

$$D^{R+}(x-x',t-t') = -i\theta(t-t')\langle [\Delta_-(x,t),\Delta_+(x',t')]_0 \rangle.$$  

At momentum $k = Q$,

$$D^{R+}(Q,t-t') = -i\theta(t-t')\langle [j_-(t),(-)^x\Delta_+(x',t')]_0 \rangle,$$

where we have used the identity $j_-(t) = \sum x e^{-iQ\cdot x} \Delta_-(x)$. From (5), the time dependence of $j_-$ can be determined via the equation of motion:

$$j_-(t) = e^{-i(U-2\mu)(t-t')}j_-(t').$$

Also, we have the equal-time commutator $[j_-(t),(-)^x\Delta_+(x')] = -2\phi_3(x')$. Therefore, we obtain exactly

$$D^{R+}(Q,\omega) = -\frac{2\langle \phi_3 \rangle_0}{\omega - (U-2\mu) + i\eta}.$$  

The spectral function, defined in the Lehmann representation as

$$A(k,\omega) = \frac{(2\pi)^2}{a} \sum_N \langle 0|\Delta_-(0)|N\rangle^2 \delta^2(k-k_N)\delta(\omega-\omega_N),$$

can be determined exactly at momentum $Q$ from (5):

$$A(k = Q,\omega) = -2\text{Im}D^{R+}(Q,\omega) = -4\langle \phi_3 \rangle_0 \pi \delta(\omega - (U-2\mu)).$$

Thus as long as the symmetry is broken by doping with $\langle \phi_3 \rangle_0 = -\frac{\mu}{U} \neq 0$, $A(Q,\omega)$ cannot vanish, but rather consists entirely of a term proportional to $\delta(\omega - (U-2\mu))$. Such a term can obviously only arise in a theory that has particles of spectrum $\omega = U-2\mu$ at $k = Q$. Furthermore, a delta function $\delta(\omega - (U-2\mu))$ can only arise from single particle states; multi-particle states would contribute a continuum. The operator $\Delta_-$ is bosonic, so $\langle 0|\Delta_-|N\rangle$ vanishes for any fermion state $N$. The state $\Delta_-^\dagger |0\rangle$ is rotationally invariant in spin space, so $\langle 0|\Delta_-|N\rangle$ must vanish for any state $N$ of non-zero spin. (We assumed a ground state of no long-range spin order; an AF order will change our conclusion.) Also $\langle 0|\Delta_-|N\rangle$ vanishes for any state $N$ that has different (unbroken) internal quantum numbers from $\Delta_-$. A similar analysis beginning with the correlation function $D^{R+}$ in place of $D^{R+}$ shall lead to another collective mode of energy $-(U-2\mu)$ at $k = Q$.

We then conclude that there must exist two (spinless) bosonic collective excitations of energy $\pm(U-2\mu)$ at momentum $Q$ and of the same (unbroken) internal quantum numbers as $\Delta_-$. And $\Delta_+$, respectively.

Let us denote two collective modes by $W^-$ and $W^+$, respectively, and consider how they should transform under the unbroken $U(1)$ symmetry. The quantum charge operator, if represented in terms of electron operators, is $Q = -e\sum x n = -2e(J_3 + \frac{\mu}{U})$ where $M$ is the total number of sites of the lattice and the electron charge is $-e$ in our convention. Since $W^+ (W^-)$ must have the same $U(1)$ quantum number as $\Delta_+ (\Delta_-)$, the commutation relation of $Q$ and $\zeta_\pm$ has to be identical with that of $Q$ and $\Delta_\pm$. Therefore,

$$[Q, W^\pm] = \mp 2eW^\pm.$$  

Physically, this means that $W^-$ and $W^+$ create bosonic excitations of charges $2e$ and $-2e$, respectively. Obviously $W^+$ and $W^-$ are conjugate, so there exists in fact only one kind of such modes. (Hereafter, we shall simply use $W$ to denote the collective excitation.) We summarize these results into

**Theorem.** If the ground state of the Hubbard model is such that $\langle \phi_3 \rangle_0 = -\frac{\mu}{U} \neq 0$ but $\langle \Delta_\pm \rangle_0 = 0$, then there must exist a (spinless) collective excitation of charge $-2e$ and energy $|U-2\mu|$.

We note that the above collective excitation may be viewed as a ‘pseudo-Goldstone-like’ mode from the breakdown of the pseudospin symmetry. But we emphasize that the present case conceptually differs from that of the spontaneously broken symmetry, as discussed above (see also the note [12]). Since $\mu = U/2$ when half-filled, we expect that the energy of the collective excitation, $|U-2\mu|$, is low for small $\delta_h$. As we shall show below from the viewpoint of effective field theory, the energy of this collective mode disperses quadratically away from $k = Q$.

We would like to comment that the (spinless) collective excitation discussed in the present paper is related to the *triplet* of collective excitations of Zhang [11] and the $\pi$ excitations (though of spin quantum number 1) in
the unified SO(5) theory \cite{12}. However, the triplet was proven to exist in the superconducting state only, and Zhang \cite{10} argued that there is no direct way to couple to $J_3$ pair excitations experimentally unless the ground state is superconducting. By contrast, our collective excitation can physically show up in the non-superconducting state with $\delta_h$ acting as the role of order parameter. For instance, Eq. \cite{6} suggests that the collective excitation here should be experimentally observable in the electron pair response function at finite doping while the pairs need not to be condensed. This is the main result of the present paper.

It is quite tempting to find an expression of the state of the collective excitation $W$ in terms of electron states. The spectral function \cite{5} peaking at momentum $Q$ suggests that $\langle \Delta_-(0)|W(k)\rangle \neq 0$. So a naive way of looking for a state $|W(k)\rangle$ is perhaps out of the states $\Delta^\perp(x = 0)|0\rangle$, projecting out all states of momenta different than $k$. We can then write the state $|W(k)\rangle$ in a general form

$$|W(k)\rangle = \int_{BZ} d^2q f(q) c_\alpha^\dagger(k - q)c_\beta^\dagger(q)|0\rangle + \cdots. \tag{11}$$

$f(q)$ is some function of $q$ undetermined. The terms indicated by `$\cdots$' represent all other possible states of appropriate quantum numbers. So a simple $W$ boson may be viewed as a pair of electrons of opposite spins moving with a center-of-mass momentum $k$, and is not condensed in the normal state (i.e., $|W\rangle_0 = 0$). This is consistent with the picture of preformed pairs in the non-superconducting state \cite{3, 8}. The formation of bound states of holes has been seen numerically in a hole-doped antiferromagnet \cite{13}.

But one cannot simply identify the operator $W$ with $\Delta_-$. By a direct calculation,

$$\langle \Delta_-(x), \Delta^\perp(x') \rangle = -2\phi_3(x) \delta_{x,x'},$$

$$= [\delta_h - \hat{n}'(x)] \delta_{x,x'}, \tag{12}$$

where $\hat{n}' \equiv n - \langle n \rangle$. Therefore, $\Delta_-$ cannot describe a true Boson since it fails yielding the standard Bose-Einstein statistics, as required of $W$ as a collective excitation. Rather, Eq. \cite{12} implies that $W$ should describe the collective motion of electron pairs with the quantum fluctuation $\hat{n}'$ integrated out. This point shall become a little more manifest in the language of effective field theory.

An effective field theory of the $W$ collective excitation can be derived from the breakdown of the pseudospin symmetry: SU(2)→U(1)$_c$ with $\langle \phi_3 \rangle_0 \neq 0$. According to the effective field theory approach of broken symmetries \cite{14}, the (Goldstone-like) charge bosons may be identified (apart from normalization) with variables parameterizing the coset space SU(2)/U(1)$_c$. We can write $\psi_\alpha$ as an SU(2) transformation acting on $\psi_\alpha$:

$$\psi_\alpha(x, t) = U(x, t) \tilde{\psi}_\alpha(x, t), \tag{13}$$

where $\tilde{\psi}_\alpha$ is chosen such that

$$\tilde{\phi} = \frac{1}{4}\tilde{\phi}_\alpha^\dagger \tilde{\phi}_\alpha = (0, 0, \sigma).$$

Accordingly, the $\tilde{\phi}$ is expressed as $\phi_3(x, t) = R_{\alpha\beta}(x, t)\sigma(x, t)$ where $R_{\alpha\beta}(x, t)$ is a $3 \times 3$ orthogonal matrix determined by $U^{-1}\tau_3 U = R_{\alpha\beta}\tau_3$. Clearly, $\sigma(x, t) = \sqrt{\sum_\alpha \phi_\alpha(x, t)^2}$. In place of the field variables $\psi_\alpha$, our variables now are $\tilde{\psi}_\alpha$ and whatever other variables are needed to parameterize the transformation $U(x, t)$. We choose

$$U(x, t) = [1 - i \sum_{r = 1}^2 \tau_r (-)^x \tilde{\zeta}_r(x, t)]/\sqrt{1 + \tilde{\phi}(x, t)^2} \tag{14}$$

with

$$(-)^x \tilde{\zeta}_1 = -\phi_2/\phi_3 + \sigma, \tag{15}$$

$$(-)^x \tilde{\zeta}_2 = \phi_1/\phi_3 + \sigma. \tag{16}$$

The lattice factor $(-)^x$ is inherited from the definition of $\phi_i$ (see text following Eq. \cite{2}) and is factorized out to ensure not to double the period of the lattice. The field variables $\tilde{\zeta}_r$ can be combined into a complex scalar field

$$W = \tilde{\zeta}_1 + i\tilde{\zeta}_2,$$

which may be identified as the collective excitation whose properties have been described in the theorem.

As an example, consider a simple case in which holes are uniformly distributed: $\langle \sigma(x)\rangle_0 = \langle \phi_3(x)\rangle_0 = 0 \neq \frac{q_x}{2}$. Also, we would generally expect a non-vanishing expectation value of the valence bond field $\tilde{x}_{xy} \equiv t\langle c_\alpha^\dagger(x)c_\alpha(y)\rangle_0 \tag{15}$. Starting with the Lagrangian corresponding to \cite{2}, we replace the $\psi_\alpha$ fields at each spacetime point with Eq. \cite{13} and keep terms only relevant to the collective excitation field:

$$L_W = -2\sigma \sum_x \frac{W^\ast \delta_t \left(\frac{W}{\sqrt{1 + |W|^2}}\right)}{\sqrt{1 + |W|^2}^2}$$

$$+ \sum_{\langle xy\rangle} \left\{ \chi_{xy}^\ast [1 - W^\ast(x)W(y)] + c.c. \right\} \sqrt{|1 + |W(x)|^2||1 + |W(y)|^2|}$$

$$+ \sigma(U - 2\mu) \sum_x \frac{|W(x)|^2 - 1}{|W(x)|^2 + 1}. \tag{17}$$

This gives the effective theory of lower energy excitations about the ground state we assumed. Substituting all $\sigma$ and $\chi$ fields with their expectation values and expanding the Lagrangian in powers of $W$ and $W^\ast$, we have

$$L_{\text{eff}} = \delta_h \sum_x W^\ast[i\delta_t - (U - 2\mu)] W - \sum_{\langle xy\rangle} 2\Re \chi_{xy} W(x) W^\ast(y)$$

$$+ \sum_{\langle xy\rangle} [\chi_{xy} W^\ast(x) W(y) + c.c.] + \cdots. \tag{18}$$
The terms indicated by ‘⋯’ will contain high powers of the $W$ field. (A detailed justification of the above effective field theory will be given elsewhere.) Different mean-field values of $\chi$ have been obtained for different phases of the Heisenberg-Hubbard model [15]. For a real uniform $\bar{\chi}_{xy} = \chi$, the Lagrangian (18) yields the lowest order energy spectrum $E(k) = \frac{2\hbar}{\sqrt{2}} [2 + \cos(k_x a) + \cos(k_y a)] + (U - 2\mu)$. Other phases of $\chi$ would yield different forms of energy spectrum but all should have energy $U - 2\mu$ at $(\pi/a, \pi/a)$.

In conclusion, we predicted a spinless collective excitation of charge $-2e$ in the non-superconducting state of the underdoped high $T_c$ cuprates by analyzing the electron pair correlation. Identifying these new excitations thus offers an opportunity of testing the validity of the Hubbard model for the high $T_c$ cuprates. Our result is consistent with the proposals of spin-charge separation [1], and preformed pairs [3, 4], which are widely used to explain many important features of the normal state.

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