Raman Scattering and Anomalous Current Algebra: Observation of Chiral Bound State in Mott Insulators

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Abstract

Recent experiments on inelastic light scattering in a number of insulating cuprates [1] revealed a new excitation appearing in the case of crossed polarizations just below the optical absorption threshold. This observation suggests that there exists a local exciton-like state with an odd parity with respect to a spatial reflection. We present the theory of high energy large shift Raman scattering in Mott insulators and interpret the experiment [1] as an evidence of a chiral bound state of a hole and a doubly occupied site with a topological magnetic excitation. A formation of these composites is a crucial feature of various topological mechanisms of superconductivity. We show that inelastic light scattering provides an instrument for direct measurements of a local chirality and anomalous terms in the electronic current algebra.

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1. Introduction

Recent Raman studies of a number of insulating cuprates revealed a resonant feature just below the optical absorption peak [1]. Remarkably, the most robust and prominent feature has been observed in crossed polarizations, i.e., in a scattering geometry corresponding to a pseudovector symmetry (so-called $A_2$ geometry). The present comment is motivated by these observations which suggest that

(i) within the Mott-Hubbard gap there is an exciton-like bound state,

(ii) this bound state has an odd symmetry under reflection of a two-dimensional square lattice.

Namely, we argue that the results of the experiments [1] can be interpreted as an evidence of a chiral character of charged excitations in cuprates.

Raman data have already yielded an important information about magnetic and phonon properties of insulating cuprates [2-5]. Furthermore, new experiments on high energy, large shift Raman scattering [1] provide a powerful tool for a study of charge excitations in Mott insulators. These data might also give the most valuable information for mechanisms of superconductivity in doped materials. In this paper we show that this technique presents a direct way to investigate the electronic current algebra and a chirality of excitations which are crucial features of various topological mechanisms of superconductivity [6,7].

2. Raman scattering cross section

A process of inelastic Raman scattering is an absorption of an incident photon with a frequency $\omega_i$, a wave vector $\vec{k}_i$, and a polarization $\vec{e}_i$ and a simultaneous emission of a scattered photon $(\omega_f, \vec{k}_f, \vec{e}_f)$. In the case of insulator the Raman scattering cross section is given by the Kramers-Heisenberg formula [8]:

$$R(\Omega) = \frac{\omega_f^3 \omega_i}{2 \pi \hbar^2 c^4} \sum_{i,f} e^{-\beta E_i} |M_{if}|^2 \delta(E_f - E_i + \hbar \Omega)$$ (0.1)

where

$$M_{if} = \sum_n \frac{i\langle j_i | n \rangle \langle n | j_f | f \rangle}{E_n - E_i - \omega_i} + \frac{\langle i | j_i | n \rangle \langle n | j_f | f \rangle}{E_n - E_i - \omega_f}$$ (0.2)
is the scattering tensor. Here the sum goes over all intermediate states \( |n> \) with energies \( E_n \) and \( j_{i,f} = \vec{j}(k_{i,f})\vec{e}_{i,f} \) is an electromagnetic current operator in the direction of a polarization of incident (scattered) photon. As a function of energy \( (\Omega = \omega_i - \omega_f) \) and momentum \( (\vec{q} = \vec{k}_f - \vec{k}_i) \) transfer the scattering rate can be written as a correlation function of a time dependent scattering tensor

\[
M = e_i^\mu e_f^\nu M_{\mu\nu}(\vec{r},\tau),
\]

\[
M_{\mu\nu}(\vec{r},\tau) = \int e^{-i\Omega\tau - i\vec{q}\vec{r}}M^{\mu\nu}(\vec{q},\Omega)d\vec{q}d\Omega =
\]

\[
i \int d\vec{r} \int_0^\infty d\tau' e^{-i\omega_i\tau' + i\vec{k}_i\vec{r}} [j_{\mu}(\vec{r} + \vec{r'},\tau + \tau'), j_{\nu}(\vec{r},\tau)]
\]  

(0.3)

Omitting the prefactor in the Eq.(0.1) we obtain at zero temperature

\[
R(\vec{q},\Omega) \sim Im < i|M^{\dagger}(\vec{q},\Omega)M(\vec{q},\Omega)|i >
\]  

(0.4)

Since photon wavelengths are always much larger than an interatomic separation one may neglect a spatial dispersion of the scattering tensor putting \( \vec{q} = 0 \) in Eqs.(3,4).

In general, scattering rates appear to be strongly dependent on photon polarizations. The scattering tensor (3) can be decomposed into four one dimensional irreducible representations of the square lattice point group \( D_{4h} \) [4]:

\[
M_{A_1} = M_{xx} + M_{yy},
\]

\[
M_{B_1} = M_{xx} - M_{yy},
\]

\[
M_{A_2} = M_{xy} - M_{yx},
\]

\[
M_{B_2} = M_{xy} + M_{yx}
\]  

(0.5)

Below we shall draw the main attention to the \( A_2 \) scattering amplitude which is odd under reflection on the square lattice and gives the strongest signal in the experiments [1].

3. High energy Raman scattering and the current algebra

In experiments [1] the frequency of the incident light was \( \omega_i = 3.4 - 3.8\text{ev} \) and the \( A_2 \) resonance was found at Raman shift \( \Omega \approx 1.5\text{ev} \) - which is about \( 0.15 - 0.20\text{ev} \) below the optical absorption peak. To elucidate the mechanism of the \( A_2 \) scattering we exaggerate
the conditions of the experiment, assuming that energies of incident and scattered light are much larger than the widths of relevant electronic bands, so one can neglect the dispersion of $E_n$ in denominators of the Eq.(2).

In this limit the time separation between current operators in the Eq.(3) is very small and in the leading approximation the scattering tensor is given by an equal-time current-current commutator. Apparently, a nontrivial scattering occurs only in the $A_2$ geometry:

$$M \approx M_{A_2} = \frac{1}{\omega_i} [j_x(\tau), j_y(\tau)]$$

(0.6)

where $\vec{j}(\tau) = \int d\vec{r} \vec{j}(\vec{r}, \tau)$ is the spatial average of the current operator.

Thus, we conclude that at large laser energy the Raman scattering in the insulator is only due to a nonzero value of the equal time current-current commutator

$$R(\Omega) \approx R_{A_2}(\Omega) = \frac{\omega_i^3}{\omega_i^2 2\pi \hbar^2 c^4} \int d\tau e^{i\Omega \tau} < 0|[j_x(\tau), j_y(\tau)][j_x(0), j_y(0)]|0>$$

(0.7)

Scattering rates in even geometries $A_1$ and $B_2$ appear in the second order in $\omega_i^{-1}$ while the amplitude of the $B_1$ scattering is even smaller:

$$M_{A_1} = \frac{1}{i\omega_i^2} \left( \frac{d}{d\tau} [j_x(\tau), j_x(\tau)] + \frac{d}{d\tau} [j_y(\tau), j_y(\tau)] \right),$$

$$M_{B_2} = \frac{1}{i\omega_i^2} \left( \frac{d}{d\tau} [j_x(\tau), j_y(\tau)] + \frac{d}{d\tau} [j_y(\tau), j_x(\tau)] \right),$$

$$M_{B_1} = \frac{1}{\omega_i^3} \left( \frac{d^2}{d\tau^2} [j_x(\tau), j_x(\tau)] - \frac{d^2}{d\tau^2} [j_y(\tau), j_y(\tau)] \right)$$

(0.8)

Below we shall ignore any intraatomic structures and apply the simplest two band Hubbard Hamiltonian as a model of the Mott insulator. Then $\frac{d}{d\tau} \vec{j} = -i[H, \vec{j}]$ can be easily calculated. Introducing one fermion translation operators $T_\mu(\vec{r}) = \sum_{\sigma=\uparrow, \downarrow} c_\sigma^+(\vec{r} + \mu) c_\sigma(\vec{r})$ we express the current as $j_\mu(\vec{r}) = \frac{\alpha \tau}{2\hbar c}(T_\mu(\vec{r}) - T_{-\mu}(\vec{r}))$. Then keeping terms up to the third order in $\omega_i^{-1}$ we obtain

$$M_{A_2} = \frac{1}{\omega_i} [j_x(\tau), j_y(\tau)] (1 + \frac{U^2}{\omega_i^2}) + \frac{t^2}{\omega_i^3} (j_x(\tau)(\sum_{\vec{r},\mu} T_\mu(\vec{r})^2 j_y(\tau) - j_y(\tau)(\sum_{\vec{r},\mu} T_\mu(\vec{r})^2 j_x(\tau))),$$

$$M_{A_1} = -\frac{2U}{\omega_i^2} (j_x^2(\tau) + j_y^2(\tau)),$$

$$M_{B_2} = -\frac{2U}{\omega_i^2} \{j_x(\tau), j_y(\tau)\}$$

(0.9)
where $U$ is the energy of the onsite Coulomb repulsion and $t$ is the hopping amplitude (We kept the last term in the formula for $M_{A_2}$ because it is the only one which contributes to the rate of the $A_2$ quasielastic scattering ($\Omega \to 0$). The latter has been considered by Shraiman and Shastry [4] under assumption $|U - \omega_i| << \min (U, \omega_i)$).

In what follows we shall omit the absolute scale of the scattering rates given by the factor

$$\frac{\omega^3}{2\pi \omega_i \hbar^2 e^4 (\frac{e}{2\hbar c})^4}$$

and set $\frac{e}{2\hbar c} = 1$.

4. Chirality operator

A charge excitation in the Mott insulator involves a distortion of the magnetic state. As a result, a phase of the excitation wavefunction depends not only on its current location but also on a path, which the hole passed to arrive at the site. Therefore a hole inserted to the Mott insulator may acquire a phase while moving along the closed path. This property is the quantum holonomy which is determined by a nonzero spin chirality of the insulating magnetic state [9,10]. We define it quantitatively as a measure of noncommutativity of one electron translation operators $T_\mu$ as applied to the insulating ground state

$$T_x T_y = e^{i\hat{\Phi}} T_y T_x = e^{i\hat{\Phi}} T_{x+y}$$

The chiral operator $\exp i\hat{\Phi}$ is defined as a product of translation operators over a closed lattice contour $C$. On the other hand it can be expressed in terms of spin operators by means of the relation

$$\prod_C T_\mu(\vec{r}) = tr \prod_C (1 + 2\sigma \vec{S}(\vec{r}))$$

(0.10)

We show that high energy Raman scattering is an instrument to measure matrix elements of the chirality operator.

5. Integrated intensity and elastic scattering

Some information about spin chiralities can be already obtained from the integrated Raman intensity $R^\text{int} = \int_0^\infty d\Omega R(\Omega)$ and from the elastic scattering rate $R^\text{el}(\Omega) = R(\Omega \to 0)$. In the leading order of $\omega_i^{-1}$ the integrated intensity is given by the formula

$$R^\text{int} \approx R^\text{int}_{A_2} \sim <0|[j_x, j_y]|2|0>$$

(0.11)
Since in (11) all four current operators appear at the same moment of time they have to be located in adjacent points on a plaquette to form a four step closed contour. Then it is easy to see that the integrated intensity measures fluctuations of a local chirality. After a simple algebra we obtain

$$R^{\text{int}} \sim < 0 | (\sin \frac{1}{2} \Phi)^2 | 0 >$$

(0.12)

It can be also expressed in terms of spin operators

$$R^{\text{int}} \sim 4 \sum_P < 0 | 1 - 3/2(\vec{S}_a \vec{S}_{a'}) + 2(\vec{S}_a \vec{S}_b)(\vec{S}_a \vec{S}_{b'}) - (\vec{S}_a \vec{S}_{a'})(\vec{S}_b \vec{S}_{b'}) | 0 >$$

(0.13)

where $a, a'$ and $b, b'$ are the nearest neighbouring sites on $A$ and $B$ sublattices. The integrated intensity in other scattering geometries is smaller and does not contain any information about chirality: $R^{\text{int}}_{A_1} \sim R^{\text{int}}_{B_2} \sim (U/\omega_i)^2$.

The amplitude of an elastic scattering is a more informative object. In the leading order in $\omega_i^{-1}$ it measures an averaged difference between holonomies associated with two oppositely oriented elementary closed contours which is equal to the average chirality of the ground state. From the Eq.(9) we obtain

$$R^{\text{el}}(\Omega) \sim | < 0 | M_{A_2} | 0 > |^2 \delta(\Omega) \approx \left( \frac{t}{\omega_i} \right)^4 \sum_P < 0 | T_x T_y T_{-x} T_{-y} - T_{-x} T_y T_x T_{-y} | 0 > |^2 \delta(\Omega)$$

(0.14)

where the sum goes over all plaquettes. The matrix element staying in the Eq.(14) yields the total solid angle formed by all spins in the ground state

$$R^{\text{el}}(\Omega) \sim \left( \frac{t}{\omega_i} \right)^4 \sum_P < 0 | (\vec{S}_1 \times \vec{S}_2) \cdot \vec{S}_3 | 0 > |^2 \delta(\Omega)$$

(0.15)

where the triple $1, 2, 3$ denotes any three nearest neighbouring sites on the plaquette $P$.

In other geometries an elastic scattering appears only in the next order in $\omega_i^{-1}$ and doesn’t contain holonomy. The intensity of the elastic $A_1$ scattering has the same order of magnitude as the corresponding integrated intensity $R^{\text{el}}_{A_1} \sim R^{\text{int}}_{A_1}$ while the $B_2$ elastic rate is much smaller than the integrated one $R^{\text{el}}_{B_2} \sim \frac{t}{U/\omega_i} R^{\text{int}}_{B_2}$. 
An observation of a separate peak in the $A_2$ elastic scattering would mean a spontaneous parity breaking in the ground state [9-11]. Despite of a small amplitude, a peak in the elastic scattering (if any), could be detected experimentally. However it has never been observed. Although an additional experimental study is desirable, it seems most likely that the ground state of the half-filled Mott insulator is parity even.

6. Resonant scattering

The most interesting information can be extracted from the resonant Raman features observed at energies close to the charge-transfer gap [1]. To interpret the results obtained in [1] we suppose that there exists an isolated bound state $|s>$ of a hole and a doubly occupied site (doublon) inside the Hubbard band. The energy of this state is by $E_b \sim J$ lower than the optical absorption threshold $\omega_T \approx U$ corresponding to the location of the upper Hubbard band. It follows from the Eq.(9) that at $\Omega \sim \omega_T - E_b$ the leading contribution to the resonant cross section comes from the $A_2$ scattering. Thus we obtain that the observable Raman intensity is determined by the matrix element of the current-current commutator taken between the ground state and the excited bound state

$$R_{A_2}(\Omega) \sim |\langle 0|[j_x, j_y]|s>|^2 \delta(\Omega - \omega_T + E_b) \quad (0.16)$$

Due to a semiclassical character of light scattering at large laser energy the locations of the currents $j(\vec{r})$ in the Eq.(16) have to belong to the same diagonal of a plaquette, otherwise in the leading order in $\omega_i^{-1}$ the matrix element vanishes.

We characterize the bound state by hole and doublon coordinates and by a spin configuration $\{|\sigma}\rangle$ which locally differs from the ground state: $|s> = \int d\vec{r} d\vec{r}' \Psi(\vec{r}, \vec{r}') c^\dagger(\vec{r}) c(\vec{r}') |\{\sigma\}\rangle$ where $\Psi(\vec{r}, \vec{r}')$ is the bound state wave function. Then the expectation value of the current commutator acquires the form

$$|\langle 0|[j_x, j_y]|s>|^2 \approx 4 |\int d\vec{r} <0|T_{-x}T_{-y}T_{x+y} - T_{-y}T_{-x}T_{x+y}|0 \Psi(\vec{r}, \vec{r} + \hat{x} + \hat{y})|^2 \quad (0.17)$$

The spin distorsion due to the presence of a localized bound state extends to very few plaquettes. Therefore we can neglect a difference between the ground and the excited spin
configurations when calculating an overlap factor $<0|\{\sigma\}|0>$. Similar to the case of an
elastic scattering (14,15), the expectation value of the holonomy operator is equal to the
solid angle subtended by three spins belonging to the same plaquette

$$R_{A_2}(\Omega) \sim \sum_P <0|\vec{S}_1 \times \vec{S}_2 \cdot \vec{S}_3|0>^2 \delta(\Omega - \omega_T + E_b)|\Psi(1,3)|^2$$

where (1,2,3) are three neighbouring sites on a plaquette such as 1 and 3 belong to the
same sublattice. An essential difference, however, is that a resonant scattering measures a
spin chirality locally- just in a position of a charged excitation while an elastic scattering
(Eq.(15)) gives the information about its spatial average.

Similarly, the other symmetries contribute in the next order in $\omega_i^{-1}$ and are independent
of chirality:

$$R_{A_1} \sim \left(\frac{U - \Omega}{\omega_i}\right)^2 \sum_{\mu=x,y} \int d\vec{r}|<0|T_{-\mu}T_{-\mu}\sigma|\Psi(\vec{r},\vec{r} + 2\vec{\mu})|^2,$$  \hspace{1cm} (0.19)

$$R_{B_2} \sim \left(\frac{U - \Omega}{\omega_i}\right)^2 \int d\vec{r}|<0|T_{-x}T_{-y}T_{x+y} + T_{-y}T_{-x}T_{x+y}|0 > |\Psi(\vec{r},\vec{r} + \vec{x} + \vec{y})|^2$$  \hspace{1cm} (0.20)

These can be also expressed in terms of spins according to the formula (10).

7. Evidence of a new magnetic order

Equations (17) and (18) lead to the following conclusion: the Raman data [1] provide
an evidence that the ground state is characterized by long range correlations between triads
of adjacent spins. It is important to notice that this kind of order does not mean a parity
breaking. The simplest possibility to get a nonzero holonomy, while saving the ground state
invariance under the largest subgroup of the magnetic class including parity, is presented by
the so-called $\pi$-flux state. In this state $<0|\hat{\Phi}|0>=\pi$ on every plaquette and translation
operators anticommute

$$<0|T_xT_yT_{-x-y}|0> = - <0|T_{-y}T_xT_{-x+y}|0> = i\Delta,$$

$$(T_xT_y + T_yT_x)|0> = 0$$  \hspace{1cm} (0.21)

In this state the solid angle of three adjacent spins alternates from one plaquette to another,
so its spatial average staying in (15) vanishes
\[ < 0 | (\vec{S}_1 \times \vec{S}_2) \cdot \vec{S}_3 | 0 > = - < 0 | (\vec{S}_{1'} \times \vec{S}_{2'}) \cdot \vec{S}_{3'} | 0 > = \Delta, \]

\[ \sum_P < 0 | (\vec{S}_1 \times \vec{S}_2) \cdot \vec{S}_3 | 0 > = 0 \] (0.22)

Here \{1, 2, 3\} and \{1', 2', 3'\} label any three nearest sites on adjacent plaquettes with the same orientation. Let us note, that the three-spin order (22) does not contradict with the antiferromagnet long range order. Moreover it is conceivable that this kind of ordering is realized in a \( S = 1/2 \) Heisenberg model on a square lattice and can be revealed by means of the spin wave theory, although further analysis is necessary.

Note also that according to (20), it should be no scattering in the \( B_2 \) geometry if translations do anticommute (see (21)). Indeed no \( B_2 \) contribution to the resonant scattering at \( \Omega \approx U \) has been detected in [1].

Next we argue that the magnetic ground state with the three-spin order (22) which is symmetric under reflection: i) supports bound holon-doublon states ii) the bound state by itself is odd under spatial reflection as well as time inversion.

8. Zero mode

The observation of the Raman resonance in the \( A_2 \) geometry (16-17) leads to the conclusion: the equal time commutator \([j_x, j_y]\) has a nonzero matrix element between the ground state and an excited state \(|s>\). In turn, it means that the ground state and the excited state \(|s>\) have different parities. At the first glance it seems impossible because all eigenstates of the Hubbard Hamiltonian on a square lattice are doubly degenerate as a consequence of the reflection symmetry \( \hat{R} \). Namely, if there is an eigenstate \(|\Psi>\) with currents \( j_x|\Psi>\), \( <\Psi|j_y \, \), then there is also an eigenstate \( \hat{R}|\Psi>\) with currents \( j_y|\Psi>\), \( <\Psi|j_x \, \). Thus commutator \([j_x, j_y]\) vanishes

\[ [j_x, j_y] = \sum_{|\Psi>} \{ j_x|\Psi> <\Psi|j_y - j_y|\Psi> <\Psi|j_x \} = 0 \] (0.23)

An obvious way out this problem is to assume a spontaneous parity breaking in the ground state: \( \hat{R}|0 > \neq |0 > \). Once parity is broken a topological magnetic excitation \(|\sigma>\) restores parity locally and then it contributes to the \( A_2 \) scattering. This mechanism is supposed to
work in the case of the "chiral spin liquid" state proposed in [9-11]. Although this scenario seems to be unlikely, particularly, because it is incompatible with the symmetry of the square lattice, and also because of the lack of experimental evidence, we shall briefly discuss it to contrast with our mechanism.

The chiral spin liquid state is characterized by the uniform expectation value of the chirality operator on each plaquette

$$<0|T_y T_x T_{-x-y} |0> = <0| (\vec{S}(\vec{r}) \times \vec{S}(\vec{r} + \vec{x})) \cdot \vec{S}(\vec{r} + \vec{x} + \vec{y}) |0> = \Delta \exp(i \frac{\Phi_0}{2}),$$

(0.24)

where

$$|\Delta|^2 = |<0|1 + 4\vec{S}_1 \cdot \vec{S}_2 + 4\vec{S}_1 \cdot \vec{S}_3 + 4\vec{S}_3 \cdot \vec{S}_2 |0>|^2 + |8 <0|(\vec{S}_1 \times \vec{S}_2) \cdot \vec{S}_3 |0>|^2$$

(0.25)

The magnetic excitation $|\sigma>$ locally reduces the value of the ground state chirality by canting spins at the location of the excitation. As a result, the sum in (23) doesn’t vanish which gives the $A_2$ Raman intensity

$$R_{A_2}(\Omega) \sim \sum_P \Delta^2 |<0| \sin \frac{\Phi_0}{2} |0> |^2 \delta(\Omega - U)$$

(0.26)

Fortunately, it is not necessary to break parity in the ground state. It may happen that there exists an excited state $|\Psi_0>$ annihilated by the reflection operator: $\hat{R}|\Psi_0> = 0$ which has no reflection partner. This kind of state is known as a zero mode [12]. Indeed a zero mode having no parity partner could be the only state contributing to the current commutator

$$[j_x, j_y] = j_x |\Psi_0> <\Psi_0 |j_y - j_y |\Psi_0> <\Psi_0 |j_x$$

(0.27)

Below we shall show that a zero mode is always a bound state (with the energy of order $U$) which appears inside the Hubbard gap.

In absence of an experimental evidence in favor of any other parity odd states we identify the $A_2$ final state $|s>$ as the zero mode with energy $E_b = \omega_T - U \sim J$. In fact it is a bound state of a hole and a doublon in presence of a topological spin soliton. As we have seen
the existence of the zero mode resulting to a nonvanishing commutator \([j_x, j_y]\) dictates unambiguously the main property of the magnetic ground state: holonomies (21) must be nontrivial. A more complicated analysis [7] shows that this is also sufficient for the described magnetic ground state to possess a zero mode.

Eventually, the zero mode contribution which appears to be the only one present in the case of the resonant \(A_2\) scattering (16-18) can be estimated as

\[
R_{A_2}(\Omega) \sim 4 \sum_{\vec{r}} \Delta^2 |\Psi_0(\vec{r})|^4 \delta(\Omega - U) \tag{0.28}
\]

where \(\Delta\) is given by (25).

9. Adiabatic approximation

In order to see that a zero mode is always a bound state (in fact the lowest bound state) let us consider a charged excitation in a slowly varying (adiabatic) spin background. Following the Ref. [13-14] we describe a charged excitation in the Mott insulator by a coherent state of a hole \(\psi(\vec{r})\) and a hard core boson \(z_\sigma(\vec{r})\) representing a local spin: \(<0|\vec{S}(\vec{r})|0>=\bar{z}_\sigma(\vec{r})\vec{S}_\sigma z_\sigma(\vec{r})\) with the constraint \(|z_1|^2 + |z_2|^2 = 1 - \psi^\dagger \psi\).

In terms of these variables the translation operator can be written as \(T_\mu(\vec{r}) = \bar{z}(\vec{r} + \hat{\mu}) z(\vec{r})\) and the \(t - J\) Hamiltonian now reads

\[
H = \sum_{\vec{a}, \vec{b}} t \Delta_{\vec{a}, \vec{b}} \psi^\dagger(\vec{a}) \psi(\vec{b}) + c.c. + H_J \tag{0.29}
\]

where

\[
H_J = \sum_{\vec{r}} U \psi^\dagger(\vec{r}) \psi(\vec{r}) + \sum_{\vec{a}, \vec{b}} J(1 - \psi^\dagger(\vec{r}) \psi(\vec{r})) \vec{S}_a \vec{S}_b
\]

are Coulomb and magnetic terms in the Hamiltonian, \(\Delta_{\vec{a}, \vec{b}} = \bar{z}_\sigma(\vec{a}) z_\sigma(\vec{b})\) and \(\vec{a}\) and \(\vec{b}\) denote nearest neighbouring sites on the \(A\) and \(B\) sublattices of the square lattice. Since in the ground state spins are approximately antiparallel the energy of a holon-doublon pair located on the nearest sites is by order of \(J\) higher than if they were put on the next nearest sites. If the hopping energy \(t\) is less than the exchange energy \(J\) a hole and a doublon appear on different sublattices only virtually. Therefore in the leading order in \(t/J\) one may consider only processes of two subsequent jumps described by the effective Hamiltonian.
\[
H = \sum_{\vec{a},\vec{b},\vec{a}',\vec{b}'} t' \{ \psi^\dagger(\vec{a}) \Delta_{\vec{a},\vec{b}} \Delta_{\vec{b}',\vec{a}'} \psi(\vec{a}') + \psi^\dagger(\vec{b}) \Delta_{\vec{b},\vec{a}} \Delta_{\vec{a}',\vec{b}'} \psi(\vec{b}') \} + H_J
\]  

(0.30)

where \( t' = -t^2 / \sum \mu J < 0 |\vec{S}(\vec{r}) \cdot \vec{S}(\vec{r} + \hat{\mu})|0 > \). Now the effective two-step hopping processes within one sublattice only slightly change a spin configuration and therefore these can be treated adiabatically. Namely, we may consider the Schrödinger equation for a hole and a doublon in an equilibrium spin configuration. The Schrödinger operator in the Eq.(30) is a square of the elementary translation operator, so we may apply a standard argument about a zero mode [15]. Since the effective hopping operator (30) is a hermitian operator squared, the energy of any state is positive or zero. All states with nonzero energy are doubly degenerate. Let us write down the eigenstates in the sublattice basis. If \( |\Psi > = (\Psi(\vec{a}), \Psi(\vec{b})) \) is an eigenstate then its partner \( |\tilde{\Psi} > = (\sum_{\vec{b}} \Delta_{\vec{a},\vec{b}} \Psi(\vec{b}), -\sum_{\vec{a}} \Delta_{\vec{b},\vec{a}} \Psi(\vec{a})) \) which is obtained by the time reversal transformation is also an eigenstate with the same energy. Since in the half-filled case each of these states remains invariant under the charge conjugation we conclude that these can be transformed to each other by parity transformation (spatial reflection) and then their contributions to the current-current commutator (23) cancel out. The only nondegenerate state could be that one which has a zero energy and is annihilated by one of the operators \( \Delta_{\vec{a},\vec{b}} \) or \( \tilde{\Delta}_{\vec{b},\vec{a}} \). Since \( < 0 |(\vec{S}_1 \times \vec{S}_2) \cdot \vec{S}_3|0 > \neq 0 \) the operators \( \Delta_{\vec{a},\vec{b}} \) and \( \tilde{\Delta}_{\vec{b},\vec{a}} \) do not commute, so only one of them may have a zero mode for a given spin configuration. Thus there are two candidates: (i) a zero mode \( \Psi_0(\vec{b}) \) of the operator \( \Delta_{\vec{a},\vec{b}} \Psi_0(\vec{b}) = 0 \) and \( \Psi_0(\vec{a}) = 0 \) and (ii) a zero mode \( \tilde{\Psi}_0(\vec{a}) \) of the operator \( \tilde{\Delta}_{\vec{b},\vec{a}} \tilde{\Psi}_0(\vec{a}) = 0 \) and \( \tilde{\Psi}_0(\vec{b}) = 0 \). In each of the two cases the zero mode is nondegenerate and breaks the two dimensional parity. Note that charge excitations occupying the zero mode state stay on only one of the two sublattices.

All other states including possible bound states have higher energies. Therefore we conclude that (i) if a zero mode exists then it appears to be the midgap state, (ii) it exists only if translations in the ground state do not commute. Since the magnetic ground state is assumed to be parity even the translations must anticommute (21).

Many properties of zero modes are universal and depend only on the crystal symmetry of the lattice. They constitute the subject of the "index" theorem. In particular, the index
theorem states that the spin configuration which supports a zero mode must have a nontrivial topology.

This gives us to a simple geometrical interpretation of the spin configuration surrounding a bound state of a hole and a doublon. It is a magnetic hedgehog which carries one quantum of the flux on the top of the ground state. One quantum of the topological charge creates a zero mode which can accommodate one hole and one doublon. Moreover a local "holon" density of the occupied zero mode is given by the topological charge density of the magnetic hedgehog

\[ q(\vec{r}) = \frac{1}{2\pi} \left[ \frac{d}{dx} \vec{n}(\vec{r}) \times \frac{d}{dy} \vec{n}(\vec{r}) \right] \cdot \vec{n}(\vec{r}) \]  (0.31)

where \( \vec{n}(\vec{r}) \) describes a spin configuration on the sublattice which carries charge excitations. Finally, combining Eqs.(17) and (32) we obtain that the current-current commutator possesses the anomalous Schwinger term given by a topological density of the spin configuration

\[ [j_x(\vec{r}), j_y(\vec{r}')]|s> \sim iq(\vec{r}) \delta(\vec{r} - \vec{r}')|s> \]  (0.32)

which appears explicitly in the scattering rate (28).

10. Zero mode and topological mechanism of superconductivity

A presence of zero modes in the insulating state implies remarkable properties of the doped state. Due to the particle-hole symmetry of the half filled band the spin configuration \( |s> \) in presence of two holes contains a spin soliton in the same way as in the case of a holon-doublon pair. Therefore at small doping which does not destroy the magnetic ground state two holes couple with each other inside the topological spin bag. A residual interaction between zero modes lifts their degeneracy and opens a narrow midgap band which is a cornerstone of the topological mechanism of superconductivity. Although the midgap band is completely filled it always remains compressible. To show this let us suppose that we insert two additional holes. To get accommodated to the midgap band these will create a topological soliton increasing a midgap band capacity by an extra zero mode state. The corresponding energy cost is proportional to doping and the midgap band remains completely filled.
The most significant feature of the topological superfluid state is its current algebra including the anomalous term similar to Eq.(32) which is now realized in the (doped) ground state

\[ <0| [j_x(\vec{r}), j_y(\vec{r}')] |0>_\sim <0| \rho(\vec{r}) \delta(\vec{r} - \vec{r}') |0>_\sim q(\vec{r}) \delta(\vec{r} - \vec{r}') \]

11. Elastic Raman scattering in the Quantum Hall effect

As another comment we also state that an anomalous current algebra gives rise to a nontrivial elastic light scattering in the Quantum Hall Effect. For simplicity we consider the case of the Integer Quantum Hall Effect of spin polarized fermions which allows us to ignore any intra-Landau level excitations as well as a magnetoroton mode. Then the spectrum contains only charge transfer inter-Landau level excitons with a gap equal to the cyclotron frequency \( \omega_c \). According to our previous discussion the light scattering should be observed at zero energy transfer, i.e. inside the gap where there are no real states. This happens due to the anomalous equal time current-current commutator in an external magnetic field

\[ [j_x, j_y] = i \frac{2\mu}{m} B \]

where \( \mu \) is the Bohr magneton, \( m \) is an electron mass and \( B \) is the magnetic field strength. Substituting this expression to the Eq.(7) we get

\[ R(\Omega) = \frac{\omega_s^3 \omega_i^2}{c^4} B^2 \delta(\Omega) \]

Thus a nontrivial elastic Raman scattering can be found even in an incompressible liquid provided its current algebra is anomalous. In fact, this phenomenon is quite similar to the dissipationless Hall current in an incompressible magnetized electron liquid.

12. Experiment

Below we discuss some features of the experiments [1] which motivated the proposed mechanism.

The Raman measurements were made on insulating cuprates \( Y(Pr)Ba_2Cu_3O_{6+x} \) and \( Gd(Nd)_{2}CuO_{4} \). A strong \( A_2 \) peak has been observed in all these materials about 0.2 ev below the optical absorption peak. This value which is of the order of the magnetic exchange
energy $J$ gives the distance between the zero mode energy level and a continuous part of the spectrum (upper Hubbard band). We consider it as a strong indication that the observed phenomenon has a magnetic origin and is due to the many-body effects. It should be contrasted to any mechanism based on local interatomic transitions between oxygen and copper orbitals.

Beyond the adiabatic approximation the $A_2$ peak broadens and acquires a width of the order of the inverse spin relaxation time which remains of the order of $J$ even at low temperatures. This does not contradict with the experiments [1] which show that the width of the peak remains of the same order and only slightly narrows as temperature decreases.

A weaker Raman feature was resolved in the $A_1$ geometry at approximately the same energy as the $A_2$ peak, while no $B_2$ feature was found. According to the eq.(19) the $A_1$ scattering rate is indeed less then the $A_2$ rate by the factor $(\frac{J}{\omega i})^2$. The vanishing of the $B_2$ rate (20) is another strong indication in favor of the anticommutativity of translations (see (21)).

As we saw the anomalous $A_2$ peak is quite universal. It primarily depends on the symmetry of the magnetic structure and does not depend on details of the Hubbard-type Hamiltonian. On the contrary, the $A_1$ scattering rate (19) does depend on details of the Hamiltonian. These features were also observed and especially stressed in the Ref.[1] - the $A_1$ intensity changes among different substances and, in particular, it was not observed in $YBa_2Cu_3O_{6.1}$.

13. Summary

In summary, we showed that inelastic light scattering in the Mott insulator at large energy transfers provides a direct way to measure the current algebra and the symmetry of charged excitations. The observation of Raman features in insulated cuprates below the optical absorption threshold in cross polarizations is a strong indication on the existence of an anomalous current algebra and midgap states (zero modes) formed by topological spin solitons bounded with two charged excitations (a hole and a doubly occupied site). This observation suggests that in the doped case electronic currents also obey the anomalous
algebra and two holes also bind together with a topological soliton.

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