Resonant neutron scattering on the high Tc cuprates and π and η excitation of the t-J and Hubbard models

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We review the explanation for resonant neutron scattering experiments in $YBa_2Cu_3O_{6+\delta}$ and $Bi_2Sr_2Ca_2O_{8+\delta}$ materials from the point of view of triplet excitation in the particle-particle channel, the π excitation. Relation of these resonances to the superconducting condensation energy and their role in stabilizing the superconducting state is discussed. Due to the superconducting fluctuations, the π resonance may appear as a broad peak above Tc. Analogue problem to the π excitation for the case of s-wave pairing, the η excitation, is considered in the strong coupling limit with an emphasis on the resonance precursors in a state with no long range order.

Inelastic neutron scattering (INS) on optimally doped $YBa_2Cu_3O_7$ revealed a striking resonance at the commensurate wavevector $Q = (\pi/a, \pi/a)$ and energy 41 meV [1]. This resonance appears in the spin-flip channel only, therefore it is of magnetic origin and not due to scattering by phonons. The most remarkable feature of this resonance is that it appears only below Tc and therefore tells us about enhanced antiferromagnetic fluctuations in the superconducting state of this material. Similar resonances have later been found for the underdoped $YBa_2Cu_3O_{6+\delta}$ at smaller energies but the same wavevector of commensurate antiferromagnetic fluctuations $(\pi/a, \pi/a)$ [2]. A new feature of the resonances in underdoped materials is that they no longer disappear above Tc but have precursors appearing at some temperature above the superconducting transition temperature. Recently, resonant peaks below Tc have also been observed in INS experiments on $Bi_2Sr_2Ca_2O_{8+\delta}$ materials [3].

Several theories have been suggested to explain the observed resonances [4]. One of the proposals [5] was to identify them with a π-excitation, a triplet excitation at momentum $(\pi/a, \pi/a)$ in the particle-particle channel : $\pi^\dagger = \sum_p (cosp_x - cosp_y) c^\dagger_{p+Q\uparrow} c^\dagger_{-p\uparrow}$. This excitation is a well-defined collective mode for a wide range of lattice Hamiltonians, including the Hubbard Hamiltonian [6] and the t-J model [5,7,8]. A simple way to visualize the π-excitation is to think of a spin-triplet pair of electrons sitting on the nearest sites, having the center of mass momentum $(\pi/a, \pi/a)$ and the same relative wavefunction as a d-wave Cooper pair. When the system acquires a long-range superconducting order the d-wave Cooper pairs may be resonantly scattered into the π pairs and this gives rise to the sharp resonance seen in neutron scattering. Motivated by a recent proposal of Scalapino and White [9], we showed that last argument may be enhanced and we argued that it may be energetically favorable for the system to become superconducting, so that the π channel may contribute to the spin fluctuations and the system can lower its antiferromagnetic exchange energy [10]. In this way, the π excitation may be "promoted" from being a consequence of the d-wave superconductivity to being its primary cause. This argument is similar to the argument for the stabilization of the A phase of superfluid helium-3, where spin fluctuations are enhanced in the A phase relative to the B-phase [11]. So the effect of the spin fluctuation feedback may lead to stabilization of the A phase relative to the B base, which would always be favored in weak coupling BCS analysis. The hypothesis of the π excitation being the major driving force of the superconducting transition is supported by comparison of the superconducting condensation energy and the change in the antiferromagnetic exchange energy due to the appearance of the resonance. For optimally doped $YBa_2Cu_3O_7$ the resonance lowers the exchange energy by 18 K per unit cell [10], whereas the condensation energy for this material is 12 K per unit cell [12]. So the resonance by itself is sufficient to account for the superconducting condensation energy. At finite temperature there also seems to be a connection between the resonance intensity and the electronic specific heat, giving another indication of the important role played by the resonance in the thermodynamics of superconducting transition (see H. Mook's article in these proceedings). Another important aspect of the π excitation is that it allows to unify the spin $SU(2)$ and charge $U(1)$ symmetries into a larger $SO(5)$ symmetry and suggests a new effective low energy Lagrangian for the description of the high T_c cuprates [13]. From the point of view of $SO(5)$ symmetry π operator is one of the generators of the symmetry and resonances observed in neutron scattering are pseudo-Goldstone bosons of broken symmetry.

Discussion of the π excitation in the state with long range superconducting order has been given within gauge invariant RPA formalism in [7] and from the point of view of $SO(5)$ symmetry in [13]. However thorough understanding of precursors of this excitation in the normal state of underdoped materials is still lacking. In reference [14] it was pointed out that the most likely origin of these precursors is the existence of strong superconducting fluctuations in the pseudogap regime of underdoped cuprates [15], an assumption phenomenologically supported by correlations between the temperature at which the resonance precursors appear and broadening of the singularity in the electronic specific heat above T_c. In weak coupling precursor of the π resonance have been identified with a process in which a π-pair and a preformed Cooper pair propagate in opposite directions [14] (see Figure 1), however quantitative analysis of such process is very difficult.

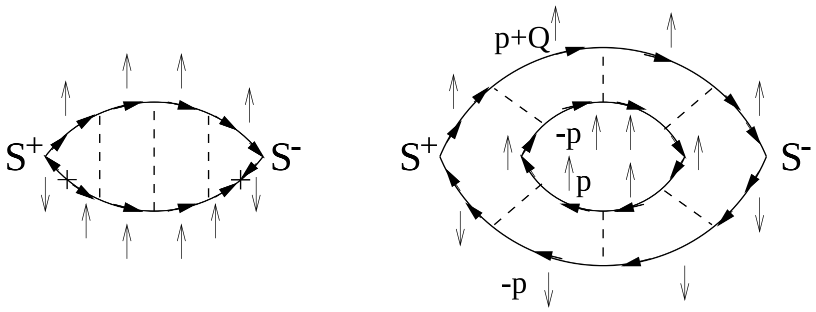

FIG. 1. Feynmann diagram for the π resonance below T_c contrasted with the diagram above T_c.

In this article we would like to point out that there is an analogue problem to the π-excitation, η excitation of the negative U Hubbard model [18,20], which allows a detailed study in the strong coupling limit, including the analysis of resonance precursors in a state without long range order. So in the remaining part of this article we will review the η excitation, pseudospin $SU(2)$ symmetry that it gives rise to [17] and discuss the strong coupling limit of the negative U Hubbard model.

As originally suggested by Yang and Zhang [17] the negative U Hubbard model (we consider $d=3$ case)

$$\mathcal{H} = -t \sum_{\langle ij \rangle \sigma} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i (n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2}) - \mu \sum_{i\sigma} c^\dagger_{i\sigma} c_{i\sigma} \tag{1}$$

at half filling has $SO(4)$ symmetry where in addition to the usual spin $SU(2)$ symmetry the system possesses pseudospin $SU(2)$ symmetry, generated by operators $\eta^\dagger = \sum_p c^\dagger_{p+Q\uparrow} c^\dagger_{-p\downarrow}$, $\eta_0 = \frac{1}{2}(N_e - N)$, and $\eta = \left(\eta^\dagger\right)^\dagger$, where N_e is the total number of electrons and N is the total number of sites. The η operator that was introduced is similar to the π operator that we discussed earlier in that it acts in the particle-particle channel and has momentum $Q = (\pi/a, \pi/a)$, however it is spin singlet operator and creates pairs of electrons where electrons sitting on the same site. While the $SO(5)$ symmetry of the t-J model is related to the competition between the antiferromagnetic and d-wave superconducting orders in this system, the pseudospin $SU(2)$ symmetry relates CDW and s-wave superconductivity in the negative U Hubbard model. At half filling when $\mu = 0$ the symmetry is exact and there is a degeneracy between the CDW state and state with superconducting order. Away from half-filling the symmetry is explicitly broken and superconducting state is energetically more favorable than the CDW state. The η operator no longer commutes with the Hamiltonian but satisfies $\left[\mathcal{H}, \eta^\dagger\right] = -2\mu\eta^\dagger$. Therefore, when it acts on the ground state it creates an exact excited state at the energy of -2μ. In the normal state such η excitation does not contribute to the density fluctuation spectrum, since it is charge 2 operator, however when the system becomes superconducting and there is a finite probability of converting particles into holes the η resonance shows as a resonance in the density fluctuation spectrum (one can also think of this as resonant scattering of s-wave Cooper pairs into η pairs). Another way to see how the η channel gets coupled to the density channel below T_c is to notice that there is an exact commutation relation $\left[\eta^\dagger, \rho_Q\right] = \Delta$ where $\rho_Q = \sum_{p\sigma} c_{p+Q\sigma} c_{p\sigma}$ is density operator at momentum Q and Δ is a superconducting s-wave order parameter. In the superconducting state the right hand side of this relation acquires an expectation value, so ρ_Q and Δ become conjugate variables and resonant peak in one of them shows up as a resonance in the other

[18].

The question that we want to address is what happens if we do not have long range order but only strong superconducting fluctuations. Can they lead to precursors of the η resonance in the density-density correlation function and what is the form of such precursors. The limit that we want to consider is strong coupling limit when $U >> t$. We perform a particle-hole transformation on a bipartite lattice

$$c_{i\uparrow} \rightarrow c_{i\uparrow} \qquad c_{i\downarrow} \rightarrow \left\{ \begin{array}{l} c_{i\downarrow}^{\dagger}, i \in A, \\ -c_{i\downarrow}^{\dagger}, i \in B \end{array} \right\} \tag{2}$$

where A and B denote two sublattices. This transformation maps the negative U Hubbard model at finite doping (i.e. finite μ) into positive U Hubbard model at half-filling but in the presence of magnetic field along z-axis. Pseudospin $SU(2)$ symmetry goes into the spin $SU(2)$ symmetry and η resonance becomes a Larmor resonance in the transverse spin channel. Particle-hole transformation maps superconducting order parameter into antiferromagnetic order parameter in the x-y plane and a CDW order parameter into antiferromagnetic order parameter in z direction. The advantage of doing such particle-hole transformation is that strong coupling limit of the positive U Hubbard model at half filling is well known. It is the Heisenberg model with the nearest neighbor exchange interaction $J = 4t^2/U$ [19]. So the effective Hamiltonian in strong coupling is

$$\mathcal{H} = J \sum_{\langle ij \rangle} \mathbf{S}_i \mathbf{S}_j + H_z \sum_i S_i^z \tag{3}$$

with $H_z = 2\mu$. At $T = 0$ Heisenberg model in external field will develop a long range antiferromagnetic order in the plane perpendicular to the direction of the applied field (xy plane in our case, which corresponds to the superconducting order in the original negative U model). When this happens, $N_{\pm}$ get expectation values and we can use the commutation relation $[S_{\pm}, N_z] = \pm N_{\pm}$ to show that Larmor resonance, which was originally present in $S_{\pm}$ channels only, will appear in the N_z-N_z correlation function as well. However we are interested in the regime when we have only finite range antiferromagnetic correlations (although strong) and we want to find possible precursors of the Larmor resonance in the N_z channel.

This effect is conveniently studied by using Schwinger boson representation of the Heisenberg model [19]. On a bipartite lattice one represents spin operators as $S_i^+ = a_i^\dagger b_i$ and $S_i^z = 1/2\ (a_i^\dagger a_i - b_i^\dagger b_i)$ on sublattice A, and $S_i^+ = -b_i^\dagger a_i$ and $S_i^z = 1/2\ (b_i^\dagger b_i - a_i^\dagger a_i)$ on sublattice B. Provided that constraint $a_i^\dagger a_i + b_i^\dagger b_i = 1$ is satisfied at each site and a and b obey the usual bosonic commutation relation we easily recover the proper commutation relations for spin $SU(2)$ algebra at each site. In terms of a and b operators Hamiltonian (3) can be written as

$$\mathcal{H} = -\frac{J}{2}\sum_{\langle ij\rangle} A_{ij}^\dagger A_{ij} + \frac{H_z}{2}\sum_i (-)^i (a_i^\dagger a_i - b_i^\dagger b_i) + \sum_i \lambda_i (a_i^\dagger a_i + b_i^\dagger b_i - 1) \tag{4}$$

where $A_{ij} = a_i a_j + b_i b_j$ and the last terms enforces the constraint at each site. In the mean field approximation the last Hamiltonian may be diagonalized by quasiparticles $\alpha_{a\mu,k}$ ($a = 1,2$, $\mu = \pm$, and momentum k runs in the magnetic zone only) with dispersion $\omega_{a\pm,k} = \omega_k \pm H_z/2$, where $\omega_k = \sqrt{\lambda^2 - 4Q^2\gamma_k^2}$ and $\gamma_k = cosk_x + cosk_y$. Mean-field parameters λ and Q have to be found from minimizing the free energy

$$F = \frac{2}{\beta}\sum_k ln\left\{sinh[\frac{\beta}{2}(\omega_k + \frac{B_z}{2})]\right\} + \frac{2}{\beta}\sum_k ln\left\{sinh[\frac{\beta}{2}(\omega_k - \frac{B_z}{2})]\right\} - 2\lambda N + \frac{4Q^2}{J}N \tag{5}$$

In terms of α operators the uniform and staggered spin operators can be written as

$$M_+ = \frac{1}{N}\sum_k \left(\alpha_{1+,k}^\dagger \alpha_{2-,k} - \alpha_{2+,k}^\dagger \alpha_{1-,k}\right) \qquad M_z = \frac{1}{N}\sum_{ak}\left(\alpha_{a+,k}^\dagger \alpha_{a+,k} - \alpha_{a-,k}^\dagger \alpha_{a-,k}\right) \tag{6}$$

$$N_z = \frac{1}{N}\sum_{a\mu k}(-)^a \left\{cosh(2\theta_k)\alpha_{a\mu,k}^\dagger \alpha_{a\mu,k} + \frac{1}{2}sinh(2\theta_k)[\ \alpha_{a\mu,k}^\dagger \alpha_{a\mu,-k}^\dagger + \alpha_{a\mu,k}\alpha_{a\mu,-k}\ ]\right\} \tag{7}$$

$$N_x = \frac{1}{N}\sum_{\mu k}\{\ cosh(2\theta_k)\ \alpha_{1\mu,k}^\dagger \alpha_{2\bar{\mu},k} + \frac{1}{2}sinh(2\theta_k)\ [\ \alpha_{1\mu,k}^\dagger \alpha_{2\bar{\mu},-k}^\dagger + \alpha_{1\mu,k}\alpha_{2\bar{\mu},-k}\ ]\ \} \tag{8}$$

where $tanh(2\theta_k) = -2Q\gamma_k/\lambda$. From equation (6) we notice that the M_+ operator has the exact energy of H_z due to the fact that the mean-field approximation on Schwinger bosons does not break spin symmetry. The correlation function for N_z is given by

$$D(\omega > 0) = Im\int dt e^{i\omega t}\theta(t)\langle N_z(t)N_z(0)\rangle = \frac{1}{N}\sum_k (1 + N(\omega_{+,k}) + N(\omega_{-,k}))\,\delta(\omega - \omega_{+,k} - \omega_{-,k}) \tag{9}$$

where $N(\omega) = 1/(e^{\beta\omega} - 1)$. At $T < T_c$, bosons $\alpha_{1-,k=0}$ and $\alpha_{2-,k=0}$ are condensed so there is a δ-function resonance in $D(\omega)$ at frequency $H_z = 2\mu$ with the weight $sinh^2(2\theta_{k=0}) = \langle N_x^2 \rangle / \langle M_z \rangle$ as dictated by the $SU(2)$ symmetry [17,18,20]. There is also an additional broad peak due to $\alpha_{a-,k\neq 0}$ that starts at energy 2μ and then extends in a frequency range of around T with an integrated weight proportional to $T^{3/2}$. Above the Neel ordering temperature the δ-peak in $D(\omega)$ is absent, however there is a broadened peak at the energy slightly larger than 2μ (the lower energy threshold is given by $\omega_{min} = \omega_{-,k=0} + \omega_{+,k=0} = 2\mu + 2\omega_{-,k=0}$, and $\omega_{-,k=0}$ is small since it vanishes at T_c). The width of this broad feature is T and the total spectral weight is proportional to $T^{3/2}e^{-\omega_{-,k=0}/T}$. As the temperature is lowered and the system approaches Bose condensation at T_c, the energy $\omega_{-,k=0}$ becomes smaller leading to a smooth increase of the integrated intensity of the peak. So the intensity of the resonance changes continuously across T_c but as may be shown by a detailed analysis there is a jump in the derivative. On Figure 2 we show a sketch of $D(\omega)$ for temperatures below and above T_c.

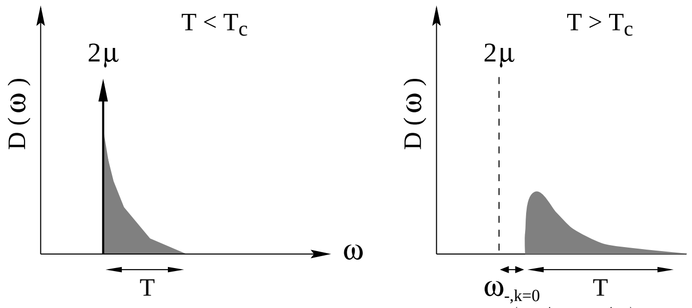

FIG. 2. Density response function at momentum $Q = (\pi/a, \pi/a)$ for the negative-U Hubbard model in the large U limit. For $T < T_c$ $D(\omega)$ has a δ-peak at $\omega = 2\mu$ (η resonance) and a broad feature starting at the same energy. For $T > T_c$ there is only a broad peak at the energy slightly higher then 2μ.

Before concluding we would like to remark that that many features of the precursors of the η excitations that we discussed here, such as temperature dependent shift to higher energies and considerable broadening are likely to be present for the π-excitation of the t-J model as well. INS on underdoped $YBa_2Cu_3O_{6+\delta}$ reveals considerable broadening of the resonance above T_c, however the current accuracy of experiments does not allow to see any changes in the energy of the resonance above the superconducting transition.

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