Unconventional dynamics and spectroscopy in superconductors

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State of the art and objectives

The $U(1)$ symmetry breaking in superconducting (SC) systems comes along with the emergence of two types of collective modes (or excitations) as fluctuations of the macroscopic (complex) order parameter: the amplitude fluctuations, which are energetically costly, represent the analogous of the Higgs field in particle physics; whereas the phase fluctuations, which are massless at long wavelengths, represent the Goldstone mode, that can be gauged away to make the electromagnetic field massive giving rise to the Meissner effect.

The most direct way to find experimental evidences of the collective modes is to excite them via spectroscopic probing. Indeed the amplitude, which is a scalar, couples to the charge, probed by means of Raman spectroscopy. On the other hand the phase gradient couples to the current, which is probed by means of optics spectroscopy. Nevertheless, in conventional superconductors both the Higgs and Goldstone modes are usually very elusive for several concomitant reasons. Firstly, the amplitude fluctuations identify a weak square-root singularity at twice the SC gap $\Delta_0[1, 2]$, that is strongly over damped by the quasi-particle excitations. The resulting spectral function generally displays only a broad feature peaked at the edge $2\Delta_0$ where also the single-particle excitations start to develop. This is in contrast to what happens in Lorentz-invariant bosonic theories, where the Higgs appears as a sharp power-law resonance, whose signature has been observed in cold atoms experiments[3]. Moreover, in the weak coupling BCS limit the Higgs mode is expected to weakly couple to typical spectroscopic observables. Thus its resonance remains hidden unless one performs pumb-probe experiments[4, 5], in which the system is strongly perturbed out of equilibrium, or studies some particular ma-
terials like NbSe$_2$[6, 7], where the Higgs becomes visible via its coupling to the charge-density-wave (CDW) phonon[8, 9]. Furthermore, I have shown[10] that in the coexisting SC+CDW state the presence of the additional CDW gap modifies the nature itself of the SC amplitude fluctuations, which become undamped, acquiring a relativistic-like dynamics. About the phase mode, in a clean system it couples to a longitudinal vector potential but not to a transverse one: so it does not contribute to the (physical) response observed in optics measurements. Therefore the Goldstone mode remains optically inactive unless one breaks translational invariance by introducing disorder, which lets the phase gradient couple also to a transverse vector potential[11]. Such a coupling then leads to the emergence of an additional sub-gap optical absorption[12], in agreement with recent experimental observations in disordered SC thin films[13, 14]. At strong disorder these features acquire great importance in the context of the superconductor to insulator transition (SIT), a field which has drawn lots of attention in the last years[15, 16, 17].

The aim of my Phd project is to investigate the unconventional nature of the collective modes in some kinds of 2-d superconductors, questioning whether the amplitude and/or phase fluctuations can become visible via spectroscopic measurements.

As a prototype model for describing a conventional single band s-wave superconductor on the square lattice I adopt the well known attractive Hubbard Hamiltonian:

$$H_{U} = -t \sum_{\langle i,j \rangle \sigma} \left( c_{i\sigma}^{\dagger} c_{j\sigma} + \text{h.c.} \right) - \mu \sum_{i\sigma} c_{i\sigma}^{\dagger} c_{i\sigma} - U \sum_{i} c_{i\uparrow}^{\dagger} c_{i\downarrow}^{\dagger} c_{i\downarrow} c_{i\uparrow},$$  

(1)

where $c_{i\sigma}^{(\dagger)}$ is the annihilation (creation) operator for a fermion with spin $\sigma$ on the site $i$, $t > 0$ is the hopping amplitude, the sum over $\langle i, j \rangle$ is extended to all the distinct pairs of nearest-neighbor sites, $\mu$ is the chemical potential and $U > 0$ is the onsite interaction strength leading to the formation of the Cooper pairs below $T_c$.

I mainly focus on two scenarios: i) I study the behavior of both the amplitude and phase modes in the strong coupling regime $U/t \gg 1$, thus investigating the bosonic side of the (BCS-BEC) crossover from the weak coupling BCS regime to a state where the Cooper pairs make up a system of condensed composite bosons. ii) I introduce into (1) a disorder term: $H = H_{U} - \sum_{i\sigma} \xi_{i} c_{i\sigma}^{\dagger} c_{i\sigma}$, where the $\xi_i$ are random distributed variables. In such a disordered scenario I study the physics of the phase fluctuations by mapping the Hamiltonian into an effective pseudo-spin model[18]:

$$H_{PS} = -2 \sum_{i} \xi_{i} S_{i}^{z} - 2J \sum_{\langle i,j \rangle} \left( S_{i}^{+} S_{j}^{-} + \text{h.c.} \right),$$

which naturally allows to describe the SC phase mode as the spin wave of an XY ferromagnet. I first compute the phase contribution to the sub-gap optical conductiv-
ity, then I turn the attention to the possible effects of the electron-electron Coulomb repulsion on the optics behavior.

**First results**

**Behavior of the collective modes in the strong coupling regime**

As I have already mentioned, the dynamics of the Higgs mode in SC systems drastically differs from that occurring in a relativistic $O(2)$ theory. Indeed, while in the latter case the long wavelength amplitude fluctuations $\Delta$ identify a simple pole at the mass $m$ of the Higgs:

$$\langle |\Delta(q)|^2 \rangle = \frac{1}{\omega^2 - m^2 - c^2 q^2},$$

in a BCS (weak coupling) superconductor they are strongly over damped by the quasi-particle excitations, since the Higgs mass ($2\Delta_0$) and the optical gap ($2E_{\text{gap}}$) coincide. However, the equivalence between the two energy scales, $\Delta_0$ and $E_{\text{gap}}$, breaks down in the strong coupling limit, where $E_{\text{gap}}$ becomes larger than $\Delta_0$. One may then question what happens to the physics of the Higgs in this regime and particularly whether it becomes undamped (as happens in coexisting SC+CDW systems[10]), resembling a relativistic-like behavior and acquiring a finite spectral weight below $2E_{\text{gap}}$.

To address this issue I perform an RPA analysis, investigating the physics of both the amplitude and phase ($\theta$) SC collective modes from weak to strong coupling [19]. At weak coupling I recover the expected result: amplitude and phase fluctuations are decoupled (at gaussian level) due to the intrinsic particle-hole symmetry of the BCS solution and the action for the collective modes can be written as:

$$S[\Delta, \theta] \simeq \frac{1}{2} \sum_q (\Delta(-q) \theta(-q)) \hat{M} \left( \Delta(q) \theta(q) \right), \quad \hat{M} \equiv \begin{pmatrix} (4\Delta_0^2 - \omega^2)F(\omega) & 0 \\ 0 & -\frac{\omega^2}{4} \tilde{\kappa} + \frac{D_s}{4} q^2 \end{pmatrix},$$

where: $F(\omega) \simeq N_F \int \frac{d\xi}{E(\xi)|4E(\xi)^2 - \omega^2|}$, $E(\xi) = \sqrt{\xi^2 + \Delta_0^2}$, $N_F$ is the density of states evaluated at the Fermi level, $\tilde{\kappa} = N_F/(1 - UN_F/2)$ is the compressibility dressed with the RPA corrections in the density channel and $D_s$ the superfluid stiffness. The equivalence of $E_{\text{gap}}$ and $\Delta_0$ is encoded in the diverging behavior of the function $F$ as $\omega \to 2\Delta_0$: $F(\omega) \simeq \frac{1}{\sqrt{4\Delta_0^2 - \omega^2}}$, resulting in the weak square root singularity:

$$\langle |\Delta(\omega, q = 0)|^2 \rangle \simeq \frac{1}{\sqrt{\omega^2 - 4\Delta_0^2}}.$$
As a consequence, the Higgs spectral function acquires only a broad feature around \( \omega = 2\Delta_0 \).

At strong coupling and out of half-filling the violation of the particle hole symmetry does no longer allow to neglect the amplitude-phase mixing, so that non vanishing off-diagonal elements appear in the matrix \( \hat{M} \). As a consequence I find that, even though \( E_{gap} > \Delta_0 \), the coupling to the phase completely removes any signature of the Higgs at \( 2\Delta_0 \). Then, in the bosonic limit \( U/t = 0 \) only the zero-frequency (Bogolubov) sound mode is left: \( \det\hat{M} \approx \omega^2/U^2 \), with finite projection at \( q = 0 \) only in the phase sector. By retaining the leading orders in the small coupling \( \alpha \equiv 2t/U \) I show that the Higgs mode still preserves some small spectral weight above \( 2E_{gap} \), that is however strongly suppressed with respect to the weak coupling case. In addition, the tendency towards the “bosonic” limit is signaled by the suppression of the sound velocity, that is given by \( v_s = (4t^2/U)\sqrt{8n(2-n)} \) (a result already obtained in [20]), with \( n \) the electronic density. These findings on the strong coupling behavior of the collective modes are fully confirmed by the numerical solution of the lattice model (1), whose results are schematically shown in figure 1.

In conclusion, I show that the unavoidable presence of single-particle excitations leads to a non-trivial dynamics of the amplitude fluctuations in fermionic superconductors, that can never be described by the outcomes of the relativistic \( O(2) \) model, as it has been sometimes suggested [14, 21, 22].

**Phase mode contribution to the sub-gap optical absorption in disordered systems**

In a recent work[12] I already started to show that in a disordered system the breaking of translational invariance lets the phase mode acquire a finite dipole moment, which is responsible for an additional absorption below \( 2\Delta_0 \) in the optical conductivity. While in that work I didn’t consider the effects of the Coulomb repulsion between the electrons, now I include them by introducing in the Hamiltonian a long range interaction term. As one obviously expects the Coulomb repulsion moves the phase mode from the sound to the plasma frequency. As a consequence, the ratio \( \mathcal{J}/E_{ext} \) between the average current and the applied external electric field is featureless at low frequencies and exhibits an absorptive threshold around the plasma one. Nevertheless I show that in the optical conductivity computed as the ratio \( \sigma \equiv \mathcal{J}/E \) between the average current and the average electric field (which also displays a plasmonic behavior), the absorptive threshold is moved from the plasma in favor to the sound, so that the sub-gap optical absorption is preserved.
Figure 1: Intensity map of the spectral function of the amplitude and phase modes at $U = 8t$ for $n = 0.1$. The solid red lines mark the value of $2\Delta_0$ and the dashed black lines the value of $2E_{\text{gap}}$. Even though the bosonic limit $E_{\text{gap}} > \Delta_0$ is reached, the amplitude mode is strongly mixed with the phase, which dominates any sub-gap structure.
Future perspectives

Beyond the topics described until now, there are many other open questions I would like to better understand and scrutinize: for example nobody has yet developed analytical models to study the effects of CDW on the collective modes in multi-bands superconductors or to account for the spin-density-wave in the mixed SC+CDW state. Another issue to address concerning the coexistence of SC and CDW is to understand what is the fate of the Higgs mode when varying the pressure, as in a recent experiment on NbSe$_2$[23]. I think that this effect could be reproduced theoretically by varying the chemical potential of the system: in principle, the further the system is pushed out of half-filling, the more the SC order is favored compare to the CDW one, so one could expect an enhancement of spectral weight of the Higgs mode at the expense of the CDW phonon.

I would also plan to study the physics of the quantum Heisenberg XY model beyond the gaussian level, where the anharmonic processes, like multi-phonon ones, could have non-trivial consequences on the physical observables. In particular, I’m interested in the case of the optical conductivity, whose low-frequency power-law behavior observed in Quantum-Monte-Carlo simulations[24] could originate from a three-phasons process. One could question what are the processes dominating the high-frequency conductivity and how much the amplitude fluctuations influence them. Obviously, it would be interesting to highlight the connections to the realistic SC systems, especially the disordered ones.

Another promising field of interest is that of granular SC materials, whose low frequency optical behavior could be described by a quantum XY model with random couplings: indeed, it seems that the phase-induced sub gap feature of the conductivity I obtained numerically well reproduce some experimental data on granular aluminium[25].

References


[23] M. A. Méasson at al., to be published.
