A model for the neutron resonance in HgBa$_2$CuO$_{4+\delta}$

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We study the spin dynamics of the Resonant Excitonic State (RES) proposed, within the theory of an emergent SU(2) symmetry, to explain some properties of the pseudo-gap phase of cuprate superconductors. The RES can be described as a proliferation of particle-hole patches with an internal modulated structure. We model the RES modes as a charge order with multiple $2p_{||}$ ordering vectors, where $2p_{||}$ connects two opposite side of the Fermi surface. This simple modelization enables us to propose a comprehensive study of the collective mode observed at the antiferromagnetic (AF) wave vector $Q = (\pi, \pi)$ by Inelastic Neutron Scattering (INS) in both superconducting state (SC), but also in the Pseudo-Gap regime. In this regime, we show that the dynamic spin susceptibility accues a loss of coherence terms except at special wave vectors commensurate with the lattice. We argue that this phenomenon could explain the change of the spin response shape around $Q$. We demonstrate that the hole dependence of the RES spin dynamics is in agreement with the experimental data in HgBa$_2$CuO$_{4+\delta}$.

I. INTRODUCTION

Inelastic Neutron Scattering (INS) and Electronic Raman spectroscopy (ERS) are experimental probes based on two particles processes which allow the observation of coherence effects, like the superconducting (SC) coherence peak whose energy is proportional to the transition temperature $T_c$, or the emergence of collective modes, which act a signature of the symmetries of the system. The study of collective modes could be a key to reveal the physical mechanisms at the origin of high critical temperature SC of cuprate compounds. A long standing mystery of such compounds is the pseudo-gap (PG) critical temperature SC of cuprate compounds. A long stand

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1) The resonance stands below the $2\Delta^0_{SC}$, threshold of particle-hole continuum ($\Delta^0_{SC}$ is the maximum of the $d$-wave superconducting (SC) gap) and the frequency resonance $\omega_{res}$ decreases with underdoping. Moreover, a precursor of this resonance exists in the PG above $T_c$, the SC critical temperature$^{21}$ where the resonance is observed at the same frequency $\omega_{res}$ than in the SC state with a lower intensity. The latter has also been observed in other cuprate compounds$^{12-15,22-24}$.

2) The energy fluctuation spectrum around $Q$ has a peculiar behavior and distribution in phase space in the underdoped regime$^{21}$. The low and high energy parts of the fluctuation spectrum behave differently with temperature. The high energy part (for $\omega \gtrsim \omega_{res}$) of the energy fluctuation spectrum does not change across $T_c$ or $T^*$, the pseudo-gap (PG) critical temperature. This behavior most probably corresponds to the response of localized spins which originate the proximity of the AF phase. On the other hand, the low energy part (for $\omega \lesssim \omega_{res}$) of the energy fluctuation spectrum changes across $T_c$. Below, $T_c$, a gap opens around $Q$ and the intensity of the resonance increases from $T_c$ and $T = 0$. Moreover, two branches appear from either side of the momentum $Q$ and meet in $Q$ at $\omega = \omega_{res}$ forming the so-called X-shape- also called “hourglass”-shape. Above $T_c$, the gap at $Q$ closes and the two energy branches disappear, forming the so called Y-shape- while the intensity of the resonance decreases until $T^*$. This feature has been observed in other cuprate compounds$^{24-28}$.

3) A very specific doping dependence of the spin fluctuations is reported in monolayer Hg-based cuprate compound Hg-1201$^{21}$. In the underdoped regime, at hole doping below 0.12 ($p < 0.12$), a Y-shape has been observed close to the vector $Q$ in both the PG and the SC phase without any change at $T_c$. For higher doping, $p \geq 0.12$, the X-shape is recovered in the SC phase. A summary of the different features is presented in Fig.1.

Several models have been proposed to explain this collective mode$^{29-40}$. An exhaustive review of all these approaches is presented in Ref.$^{41}$. Among various scenarii to account for the spin excitation spectrum in the SC state, the INS resonance was ascribed to SO(5) emergent symmetry as a $\pi$-collective mode$^{32,42}$ relating SC to AF order. However, it has been shown that the $\pi$-mode has...
an anti-bounding with the optical mode which pushes it at a higher energy than experimentally observed\textsuperscript{34}. The most commonly accepted explanation within the framework of itinerant magnetism, is that the INS resonance is a particle-hole bound state below the spin gap (a spin-triplet exciton) which is stabilized by repulsive interaction left within the $d$-wave SC state.\textsuperscript{34–36,38–40,43,44} This scenario well reproduces the structure of the spin excitation in the SC state in the optimally and overdoped regime. In the underdoped regime, the observation of the INS resonance in the PG state above $T_c$ leads to a more complex situation. The shape of the resonance changes from “X” to “Y” with the presence of some additional spectral weight in the vicinity of $Q$, whereas, in Hg-1201, the energy of the collective mode remains unchanged compared to the SC phase (see Fig. 1). This observation is very difficult to account for theoretically. Recently, an incommensurate spiral spin order stabilized by quantum fluctuations upon doping the AF Mott insulator has been proposed to explain the evolution of the energy fluctuation spectrum around $Q$ with doping in YBCO\textsuperscript{45}. The main difficulties lies on a correct modelization of the PG phase which, if we believe the excitonic explanation in the SC phase, has to retain a certain amount of coherence if the collective mode is to be observed at all in this regime.

In parallel, ERS measurements in Hg-1201 provides very interesting and complementary information for the study of collective modes in the underdoped regime. A noticeable change of behavior is observed in Raman data around 0.12 hole doping. Raman scattering is a dynamical response, which probes the charge channel at $q = 0$. Moreover, specific structure factors enable to scan the Brillouin zone with respect to respective symmetries: the $A_{1g}$ response is isotropic, the $B_{1g}$ symmetry scans the anti-nodal (AN) regions $(0, \pm \pi)$ and $(\pm \pi, 0)$, while the $B_{2g}$ symmetry selects the nodal (N) region $(\pm \pi/2, \pm \pi/2)$\textsuperscript{36}. For doping $p < 0.12$, the Raman data exhibits a large SC coherence peak in the $B_{2g}$ symmetry, while its intensity is very low in the $B_{1g}$ symmetry. For higher doping, $p \geq 0.12$, the SC coherent peak has a huge intensity in the $B_{1g}$ symmetry and decreases in the $B_{2g}$ symmetry\textsuperscript{47,48}. This change of behavior around the same doping in both Raman and INS probes suggests that the coherence effect that are getting lost around $T_c$ are a key in the explanation of the feature 3). To the best of our knowledge, the feature 3) has only been observed in Hg-1201 compound.

Here, we calculate the two-particle responses in both charge and spin sectors and compare them with experimental observations reported by ERS and INS in the underdoped regime, within a new theoretical explanation for the of the PG phase: the Resonant Excitonic State (RES) which can be described as preformed excitonic (particle-hole) pairs\textsuperscript{49,50}. Although different theoretical approaches have been developed to explain the PG phase, as stated above, the issue of the change of shape of the INS resonance across $T_c$ has never been addressed before and a comprehensive study of the relations between neutron and Raman susceptibilities in this region are given here for the first time. There have been many proposals for the PG phase of the cuprates, based on AF fluctuations\textsuperscript{51–53}, strong correlations\textsuperscript{54–56}, loop current\textsuperscript{57,58} or emergent symmetry models\textsuperscript{42,59}. A recent study proposes explain the PG phase with a SU(2) emergent symmetry model where the SU(2) symmetry relates the SC state to the charge sector\textsuperscript{60,61}. The PG
phase is then described by a composite $d$-wave SC and charge order parameter and the SU(2) symmetry is restored by thermal fluctuations.\textsuperscript{60,61} Recent investigations demonstrated that SU(2) symmetry could emerge from short-range AF interactions.\textsuperscript{49,50} Proceeding by integrating out the SU(2) pairing fluctuations, we describe the PG state as a new type of charge order called Resonant Excitonic State (RES).\textsuperscript{49,50} The RES can be described as excitonic (particle-hole pair) patches with an internal checkerboard charge modulation. In this scenario, the PG originates SU(2) pairing fluctuations and the whole physics in the underdoped regime is governed by SU(2) symmetry. Such a scenario naturally associates the physics in the underdoped regime is governed by SU(2) pairing fluctuations, we describe the PG state as a new type of charge order called Resonant Excitonic State (RES). The RES is...
the translational symmetry. We use a tight-binding description of the electronic spectrum of Hg-1201 with \( \xi_k = -2t_1(\cos(k_x a) + \cos(k_y a)) + 2t_2 \cos(k_x a) \cos(k_y a) + t_3(\cos(2k_x a) + \cos(2k_y a)) + t_4(\cos(2k_x a) \cos(k_y a) + \cos(k_x a) \cos(2k_y a)) - \mu \) where \( t_i \) are the \( i \)th neighbor hopping parameters. We have \( t_1 = -0.408 \, eV, \ t_2 = 0.093 \, eV, \ t_3 = 0.071 \, eV \) and \( t_4 = 0.036 \, eV \) (deduced from ab-initio calculations) which gives a bandwidth of 1.5 eV. \( a \) is the elementary cell parameter set to unity and \( \mu \) is the chemical potential adjusted to determine the hole doping. The Fermi surfaces of the spectrum \( \xi_k \) and \( \xi_{k+2p_{F}(k)} \) are presented on the figure 2. Note that the bandwidth of the spectrum \( \xi_k \) is larger than the bandwidth of the spectrum \( \xi_{k+2p_{F}(k)} \). We determined the Green’s functions of the model by inverting the matrix (3).

As highlighted in previous studies, the interplay of the SC and the RES order parameters is not trivial. For intermediate temperature \( T_c < T < T^* \), only RES remains in the system. The RES leads to the opening of a gap in the AN zone of the first BZ, and the formation of Fermi arcs observed by Angle Resolved Photo-Emission Spectroscopy (ARPES). Below \( T_c \) (\( T < T_c \)), we define a \( d \)-wave gap envelope \( C_k \) which will take into account the coexistence between the SC state and the RES. The definition of the RES order parameter is the same than above \( T_c \) (see relation 4). In the following we assume that the gap envelope is related to the SC and the RES order parameters by the relation:

\[
C_k = \sqrt{\Delta_{SC,k}^2 + \Delta_{RES,k}^2},
\]

Here \( \sigma_{x(y)} \) is the width of the Gaussian function in the \( k_x(k_y) \) direction (see Fig. 2). This parametrization has been used to explain the opening of the PG and the formation of Fermi arcs observed by Angle Resolved Photo-Emission Spectroscopy (ARPES). Below \( T_c \) (\( T < T_c \)), we define a \( d \)-wave gap envelope \( C_k \) which will take into account the coexistence between the SC state and the RES. The definition of the RES order parameter is the same than above \( T_c \) (see relation 4). In the following we assume that the gap envelope is related to the SC and the RES order parameters by the relation:

\[
\Delta_{RES,k} = \frac{\Delta_{RES}^{0}}{2} \gamma_k \exp\left(-\frac{(k_x^2a^2 + k_y^2a^2)}{2\sigma_k^2}\right),
\]

Here \( \sigma_k \) is the width of the Gaussian function in the \( k_x(k_y) \) direction (see Fig. 2). This parametrization has been used to explain the opening of the PG and the formation of Fermi arcs observed by Angle Resolved Photo-Emission Spectroscopy (ARPES). Below \( T_c \) (\( T < T_c \)), we define a \( d \)-wave gap envelope \( C_k \) which will take into account the coexistence between the SC state and the RES. The definition of the RES order parameter is the same than above \( T_c \) (see relation 4). In the following we assume that the gap envelope is related to the SC and the RES order parameters by the relation:

\[
C_k = \sqrt{\Delta_{SC,k}^2 + \Delta_{RES,k}^2},
\]

where \( C_k \) has a \( d \)-wave symmetry and a magnitude \( C^0_0 \). Considering, the relation (5), we can deduce the form of the SC order parameter, \( \Delta_{SC,k} = \sqrt{C_k^2 - \Delta_{RES,k}^2} \). The variation of the SC and RES order
parameters in the SC phase along the Fermi surface is presented in the Figs. 4 and 5. The RES develops solely in the nodal and anti-nodal zones. This momentum dependence of the SC and the RES order parameters in the first BZ is supported by electronic Raman Scattering experiments in Hg-1201 or Bi-2212 compounds as well as ARPES experiments. The resolution of the self-consistency equation derived from the minimal model is left for a forthcoming publication. In the following, we determine the value of the gap magnitude that reproduce the experimental data.

The real space picture is that the RES is formed of particle hole pairs, the proliferation occurs above a certain temperature $T_{\text{prolif}} \simeq \text{EP}$, which is the energy scale associated with the local object is always won-dered in the underdoped region, below which $E_{\text{CP}} < E_{\text{EP}}$. On the other hand, when $E_{\text{CP}} < E_{\text{EP}}$, then the proliferation of exciton droplets starts at very low temperature, which leads to $T_{\text{prolif}} \simeq 0$. For a simple discussion, we identify $E_{\text{CP}} \simeq T_c$ while $E_{\text{EP}} \simeq T_{\text{SU(2)}}$, which is the energy scale associated to the SU(2) fluctuations in our theory. As depicted in Fig.1, there is a critical doping $p_c$, situated in the underdoped region, below which $T_{\text{prolif}} \simeq 0$, whereas for $p > p_c$, $T_{\text{prolif}} \neq 0$. The critical doping $p_c$ is a crucial ingredient of our theory to explain the experimental data in Hg-1201.

B. The spin susceptibility

We turn to the evaluation of the spin susceptibility in the SC state and the RES. In the SC phase, we expect the spin-exciton process that explains the spin dynamics in the overdoped part of the cuprate phase diagram to be strongly affected by the emergence of RES in the underdoped part of the phase diagram. The spin operator writes $S_\mathbf{q} = \frac{1}{\sqrt{N}} \sum_\mathbf{k} \xi_\mathbf{k} \hat{c}_{\mathbf{k} - \mathbf{q}, \sigma}^\dagger \hat{c}_{\mathbf{k}, \sigma}$ which destroy a bosonic excitations at momentum $\mathbf{q}$ with a charge 0 and spin 1. Rewriting the Hamiltonian Eq. (2) with the spin operator, we get $\mathcal{H}_{\text{start}} = \sum_\mathbf{k,\sigma} \xi_\mathbf{k} \hat{c}_{\mathbf{k}, \sigma}^\dagger \hat{c}_{\mathbf{k}, \sigma} + \frac{1}{2} \sum_\mathbf{q} J_\mathbf{q} S_\mathbf{q}^\dagger S_\mathbf{q}$. The spin susceptibility is derived from the linear response of the spin operator and reads $\chi_S = -i\theta (t) \langle S_\mathbf{q}^\dagger (t) S_\mathbf{q} (0) \rangle$. Within the Random Phase Approximation (RPA), the full spin susceptibility writes:

$$\chi_S (\omega, \mathbf{q}) = \frac{\chi^0_S (\omega, \mathbf{q})}{1 + J (\mathbf{q}) \chi^0_S (\omega, \mathbf{q})}$$ (6)

with $J (\mathbf{q}) = 2 J_0 (\cos (q_x a) + \cos (q_y a))$ due to exchange between near-neighbor copper sites. In the equation (6), $\chi^0_S$ is the bare polarization bubble constructed from the Green’s function and $J (\mathbf{q})$ is super-exchange interaction from Eqn.(1). Note that full diagrammatic contributions to the bare susceptibility is discussed in Appendix A. The bare polarization can be evaluated by the formula:

$$\chi^0_S (\omega, \mathbf{q}) = -\frac{T}{2} \sum_\mathbf{\epsilon, k} \text{Tr} \left[ \hat{G} (\omega + \epsilon, \mathbf{k} + \mathbf{q}) \hat{G} (\epsilon, \mathbf{k}) \right]$$ (7)

where $\epsilon (\omega)$ is the fermionic (bosonic) Matsubara frequency, $\mathbf{k}, \mathbf{q}$ are the impulsions, $T$ the temperature and $\text{Tr}$ means Trace of the Green function matrix $\hat{G}$ deduced from Eq. (3). Using the relation (7) we describe the spin dynamics in pure RES, pure SC phase and coexisting SC-RES phases.

1. The bare spin susceptibility in the SC phase

In the pure $d$-wave SC state, the bare susceptibility writes the spectrum and $n_F$ is the Fermi-Dirac statistic. The $d$-
wave form factor of the SC-order parameter implies that the coherence factor is maximal on the Fermi surface. The imaginary part of the bubble exhibits a discontinuity at certain threshold, and coincidently the real part shows a logarithmic divergence. This observation alone enables us to explain in a self consistent way the formation of the triplet collective mode. Indeed, below this energy threshold, the divergence in the real part of the spin polarization cannot be screened by the imaginary part (which vanishes below the threshold), hence leading to the emergence of the collective mode. The value of the threshold is expected to be $2|\Delta_{SC}(k_{HS})|$- the factor 2 coming from the Green’s functions in the bubble, where $k_{HS}$ is the momentum of the hotspots. The latter divergence guarantees the emergence of a collective mode below threshold. In order to explain the emergence of a collective mode at $Q$, the coherent factors have to be non zero at the Fermi surface while the FS is gapped. This condition can be fulfilled if we consider a $d$-wave SC state$^{33}$. This description well reproduces the imaginary part of the dynamic spin susceptibility inside the SC state in the overdoped case$^{33,41}$, with in particular, the “X-shape” form of the dispersion of the modes around $(\pi, \pi)$ correctly given in shape and energy within this simple model. Further we consider that this model gives a good description of the phenomenon and focus on its generalization to the PG state.

2. The bare spin susceptibility in the RES

In our theory for the PG state, we evaluate the spin susceptibility in the RES. The bare spin susceptibility in the RES writes$^{69}$:

$$
\chi_{S,RES}^{0}(\omega, q) = \sum_{k} \left[ \frac{1}{4} \left( \frac{1}{(W_{+,-}k - W_{-,-}k)(W_{+,+}k - W_{-,+}k)} \right) \left( \frac{n_F(W_{+,-}k) - n_F(W_{-,+}k) + n_F(W_{+,+}k) - n_F(W_{-,-}k)}{\omega + i\eta + W_{-,+}k - W_{+,+}k} \right) + \frac{1}{4} \left( \frac{1}{(W_{+,-}k - W_{-,-}k)(W_{+,+}k - W_{-,+}k)} \right) \left( \frac{n_F(W_{-,+}k) - n_F(W_{+,+}k) + n_F(W_{+,+}k) - n_F(W_{-,+}k)}{\omega + i\eta + W_{-,+}k - W_{+,+}k} \right) \right] \left( \frac{(\xi_{k} - \xi_{k+2p_{F}}(k))(\xi_{k+q} - \xi_{k+q+2p_{F}}(k+q)) + 4\Delta_{RES,k}^{2}\Delta_{RES,k+q}f(q)}{(W_{+,-}k - W_{-,+}k)(W_{+,+}k - W_{-,+}k)} \right)
$$

(9)

where $W_{\pm,k} = \frac{1}{2} (\xi_{k} + \xi_{k+2p_{F}}(k)) \pm \sqrt{(\xi_{k} - \xi_{k+2p_{F}}(k))^{2} + 4\Delta_{RES,k}^{2}}$ is the RES excitations spectrum and $f(q)$ a function of momentum $q$ that takes into account the coherence conditions of the RES, as detailed further in the text and in Appendix A.

The contribution to the bare spin susceptibility in the RES (equation (9)) can be divided in two parts : the intraband contribution (upper terms in relation (9)) and the interband contribution (lower terms in the relation (9)). Close to $q = Q$, the intraband contribution can be neglected and the whole signal is produced by interband processes. As the FS formed by the hybridized bands cannot be connected by the vector $Q$, the bare spin susceptibility is gapped up to the energy $2|\Delta_{RES}(k_{HS})|$. Far from $q = Q$, the intraband processes become non negligible.

Deeper investigation on the SU(2) symmetry have shown that the SU(2) pairing fluctuations emerging from non-linear $\sigma$ model only exist in a restricted area $S_k$ in the AN part of the first BZ (see Ref.$^{49}$ for the detailed demonstration and particularly the figure 9 where $S_k$ is represented). In the following, one important element is that we assume a symmetrization of this restricted area between two adjacent AN area (in $k$ and $k + Q$ with $Q = (\pi, \pi)$) such that $S_k = S_{k+Q}$.

The coherence terms are described by the Feynman diagram shown in Fig. 3 a) and we observe that the outgoing vector of the Feynman diagram does not equal the incoming vector $q$ up to the difference $\delta_{2p_{F}} = 2p_{F}(k + q) - 2p_{F}(k)$. The difference $\delta_{2p_{F}}$ vanishes ($\delta_{2p_{F}} = 0$) only if $q$ is commensurate and differs from zero ($\delta_{2p_{F}} \neq 0$) for incommensurate $q$ vectors (see Fig. 3). Consequently the coherence terms exist only close $q = 0, Q$ and cannot exist far from commensurate vectors. In the following, we modelize the RES coherence terms in Eq. (9) by the the terms $\Delta_{RES,k}\Delta_{RES,k+q}f(q)$ where $f(q)$ vanishes for incommensurate $q$ vectors. More precisely, the function $f(q)$ equals one around $q = 0$ and $q = Q$ and vanishes for other vectors. A full description of the function $f(q)$ on the spin susceptibility is studied in appendix B.

In contrast to the preformed Cooper pair scenario$^{33}$ we observe a resurgence of the coherence terms around incoming wave vectors commensurate with the lattice, like $q = Q$. In the RES scenario, the coherence terms only exist close to commensurate $q$ vectors. This peculiar behavior is different from the scenario of preformed Cooper
pairs where the coherence terms vanish for all $\mathbf{q}$ vectors.

Close to the FS, we can linearize the shifted spectrum $\xi_{\mathbf{k} - 2\mathbf{p}(\mathbf{k})}$. This linearization leads to the relation $\xi_{\mathbf{k} - 2\mathbf{p}(\mathbf{k})} \approx -\xi_{\mathbf{k}}$ only valid close to the FS. In this approximation, the relation (9) is equal to the relation (8). We can deduce that the low energy spectrum in the RES and the SC state are nearly the same.

The Raman Response

A detailed study of the whole Feynman diagram that contributes to the bare susceptibility is presented in Appendix A. The main contribution of the SC and the RES states does not qualitatively change regarding the pure state study. The threshold in the bare susceptibility occurs at an energy $2\sqrt{\Delta_{\text{RES}}(\mathbf{k}_{HS}) \Delta_{\text{SC}}(\mathbf{k}_{HS})}$ and depends on both SC and RES states. In addition to the RES coherent terms, note that a mixed SC+RES exists and also contributes only close to commensurate $\mathbf{q}$ vectors (see Appendix A).

C. Raman response function

The Raman Response $\chi_\lambda$ is the response function of a modified density operator $\rho^\lambda = \sum_{\mathbf{k}} \chi^\lambda_{\mathbf{k} \mathbf{k}^\prime} \mathbf{k}^\prime$ where $\chi^\lambda$ is the Raman vertex in the symmetry $\lambda^{46,70}$. The Raman susceptibility strongly depends on the symmetry of the system. We can take into account these symmetries by considering vertices in the phonon-matter interaction different from unity. In cuprates compounds, we typically study three symmetries which are written within the effective mass approximation:

\[
\gamma^{B_{1g}} = \frac{1}{2} \left[ \frac{\partial^2 \xi_{\mathbf{k}}}{\partial k_x^2} - \frac{\partial^2 \xi_{\mathbf{k}}}{\partial k_y^2} \right],
\gamma^{B_{2g}} = \frac{1}{2} \left[ \frac{\partial^2 \xi_{\mathbf{k}}}{\partial k_x \partial k_y} + \frac{\partial^2 \xi_{\mathbf{k}}}{\partial k_y \partial k_x} \right],
\gamma^{A_{1g}} = \frac{1}{2} \left[ \frac{\partial^2 \xi_{\mathbf{k}}}{\partial k_x^2} + \frac{\partial^2 \xi_{\mathbf{k}}}{\partial k_y^2} \right]
\]

were the $B_{1g}$ symmetry that probes the AN zone of the first BZ, the $B_{2g}$ symmetry probes the N zone of the first BZ And the $A_{1g}$ symmetry probes the whole Brillouin zone. Here, we do not consider the $A_{2g}$ symmetry, $\gamma^{A_{2g}} = 0$. In the following, we only focuses on the $B_{1g}$ and $B_{2g}$ symmetries. The specific case of $A_{1g}$ symmetry has already been studied in the framework of a charge order and superconducting coexisting state$^{71}$. In both the $B_{1g}$ and the $B_{2g}$ symmetries, the Coulomb screening can be neglected$^{70}$. In the $B_{1g}$ and $B_{2g}$ symmetries, the bare Raman susceptibility write$^{46,70}$:

\[
\chi_\lambda (\omega, \mathbf{q} = 0) = -\frac{T}{2} \sum_{\epsilon, \mathbf{k}} \text{Tr} \left[ \bar{\chi}^\lambda (\mathbf{k}) \bar{G} (\omega + \epsilon, \mathbf{k}) \bar{\chi}^\lambda (\mathbf{k}) \bar{G} (\epsilon, \mathbf{k}) \right],
\]

where $\bar{\chi}^\lambda (\mathbf{k}) = \chi^\lambda (\mathbf{k}) \tau_3$ with $\tau_3$ is the Pauli matrix evolving in the particle-hole space in the $\lambda$ symmetry (with $\lambda = B_{1g}$ or $B_{2g}$).

III. RESULTS

We perform a study at optimal doping $p = 0.16$ and in the underdoped regime $p = 0.1$ in Hg-1201. At both $p = 0.1$ and $p = 0.16$, the SC critical temperature $T_c$ is lower than the $T^*$, $T_c < T^*$. We consider that in the SC state $T < T_c$, the SC and RES coexist while above $T_c$ ($T_c < T < T^*$) only the RES remains. The RES disappears at $T^*$.

At $p = 0.1$, we choose $\Delta_{\text{RES}}^0 = 0.09eV$ and $\Delta_{\text{SC}}^0 = 0eV$ in the RES state while $\Delta_{\text{RES}}^0 = 0.06eV$ and $C_0 = 0.06eV$ in the SC state. The order magnitude of the RES and SC order parameter on the Fermi surface is presented in Fig. 4 a) and b). The SC order parameter develops in the N region and decreases in the AN zone while the RES order parameter vanishes in the N region and increases in the AN region. At the zone edges, the SC gap represents 30% of the whole gap magnitude while the RES is at 70%.

At optimal doping ($p = 0.16$), we choose $\Delta_{\text{RES}}^0 = 0.065eV$ and $\Delta_{\text{SC}}^0 = 0eV$ in the RES state while $\Delta_{\text{RES}}^0 =$...
0.01\,eV and $C^0 = 0.042\,eV$ in the SC state as presented on Fig. 5. The SC order parameter develops on the whole Fermi surface while the RES order parameter only exists in the AN zone. At the zone edges, the SC gap represents 95% of the whole gap magnitude while the RES is at 5%. The SC order parameter exhibits a $d$-wave aspect at optimal doping while this aspect is weaken in the underdoped regime. The RES gap dependence is different than a pure $d$-wave dependence as observed by ARPES in Bi-2212\cite{46,47} and Hg-1201\cite{48}.

From a technical point of view, the calculation of the bare polarization bubbles is done as follow. The summation over the internal impulsion is done in a 400x400 grid in the first BZ after doing the analytical integration over the internal Matsubara frequencies at $T = 0K$. Note that we neglected the temperature dependence of the order parameters. We have done the analytical continuation on the external Matsubara frequency replacing $\omega$ by $\omega + i\eta$ where $\eta$ is a small damping parameter taken here to $\eta = 3\,meV$. This small parameter can be understood as residual scattering caused by the impurities. The susceptibilities are in the unit of states per eV per CuO$_2$ formula unit and should be multiplied $2\mu_B^2$ to compare to neutron-scattering data ($\mu_B$ is the Bohr magneton).

A. The density of states.

The electronic density of states (DOS), $\rho(\omega) = \frac{2}{\pi} \sum_{\mathbf{k}} \text{Im} \left[ \lim_{\eta \to 0} G^{11}(\omega + i\eta, \mathbf{k}) \right]$ in the normal metal, RES and SC phases are plotted in Fig. 4 for hole doping $p = 0.1$ and Fig. 5 for $p = 0.16$. Both SC and RES open a symmetric gap at the Fermi level ($\omega = 0$). At $p = 0.1$, the magnitude of the gap is $39\,meV$ in the SC phase and $75\,meV$ in the RES phase. At $p = 0.16$, the magnitude of the gap is $54\,meV$ in the SC phase and $59\,meV$ in the RES phase. The amplitude of the gap in the RES and the SC state are in good agreement with experimental gaps deduced from Raman scattering\cite{27,28}. The low energy behavior of the DOS differs a little between the RES and the SC state. The coherent peak seen in the SC state is weakened in the RES state as observed in cuprate compounds\cite{72}. Note that the Van Hove singularity is well defined by a peak at negative energy. The from of the DOS at low energy (close to $\omega = 0\,eV$) is typical of the $d$-wave momentum dependence of the SC gap\cite{72} but does not give more information about the nature of the order parameter. In order to observe specific signature of both RES and SC state, we need probes that are sensible to the coherence between the quasiparticles such as Raman scattering and INS.

B. The Raman susceptibility

We calculate the Raman response in the $B_{1g}$ and the $B_{2g}$ symmetry in the SC state at $p = 0.1$ and $p = 0.16$ (see Fig. 6)\cite{46,70}. Our approximation is able to reproduce the decreasing of the frequency resonance in the $B_{1g}$ symmetry with hole doping, (see Fig. 6) from $\omega_{zc} = 101\,meV$ at $p = 0.1$ until $\omega_{zc} = 77\,meV$ at $p = 0.16$. Moreover, the intensity of the $B_{1g}$ Raman resonance is lower at low doping ($p=0.1$) than close to optimal doping ($p=0.16$). Both features are in good agreement with experimental Raman scattering in Hg-1201 compound\cite{47,48}.

In the $B_{1g}$, the superconducting coherence peak occurs at the energy $2\sqrt{\Delta_{\text{RES}}^2(k_{ZE}) + \Delta_{\text{SC}}^2(k_{ZE})}$ where k$_{ZE}$ is the point of the FS localized at the zone edge (see Fig. 2). The frequency of the superconducting coherent peak depends on the magnitude of both the SC and RES order parameters at the zone edge. Consequently, this frequency is larger than twice the magnitude of the SC.
order parameter and does not scale with $T_c$. However, the intensity of the SC coherent peak only depends on the magnitude of the SC order parameter at the zone edge. In step with the SC gap dependence discussed in section II A and shown in Figs. 4 and 5, the intensity of the SC coherent peak in the $B_{1g}$ symmetry increases with the hole doping.

In the $B_{2g}$ channel, we see the emergence of a peak at low frequency$^{47,48}$. The $d$-wave symmetry of the gap implies a small intensity of the SC coherent peak.

C. The bare spin susceptibility

The real and imaginary parts of the bare polarization bubble at $Q = (\pi, \pi)$ for a) $p = 0.1$ in the RES state, b) $p = 0.16$ in the RES state c) $p = 0.1$ in the SC state, d) $p = 0.16$ in the SC state. The amplitude of the order parameters are the same as in Figs. 4 and 5. We observe a gap opening in both SC state and RES.

The real and imaginary parts of the bare polarization bubble in the RES and SC phases at hole doping $p = 0.1$ and $p = 0.16$ are presented in Fig. 7 as a function of $\omega$ at $Q = (\pi, \pi)$. In the RES, (Figs. 7 a) and b)), a gap opens in the imaginary part of $\chi^R_S$ very similarly than the quasiparticle gap opening in the SC state (Figs. 7 c) and d)). In the RES, the threshold in the Imaginary part the logarithmic divergence in the real part occur at energies close to $2\Delta_{RES}(k_{HS})$. The energy of the threshold move from $94 \text{meV}$ at $p = 0.1$ until $64 \text{meV}$ at $p = 0.16$ in the RES. On the other hand, the threshold is defined at the energy $2\sqrt{\Delta_{RES}(k_{HS}) + \Delta_{SC}(k_{HS})}$. 

FIG. 5. Dependence of the RES (solid line), SU(2) envelop (dotted line) and SC gap (dashed line) on the FS as a function of energy of states in the Normal metal factor at $p = 0.1$. The SC order parameter as $d$-wave behavior in the whole Brillouin zone. Bottom panel) Density of states in the Normal metal $\rho^N(\omega)$ (dotted lines), the RES $\rho^{RES}(\omega)$ (solid lines) and the SC state $\rho^{SC}(\omega)$ (dashed line) as a function of energy $\omega$ for $p = 0.16$. The SC and RES order parameters open a symmetric gap centered around the Fermi level $\omega = 0 \text{eV}$. The $d$-wave symmetry leads to the typical form of the density of state at low energy. The Van-Hove singularity arises in the metallic spectrum at $\omega = -292 \text{meV}$ for $p = 0.16$. The magnitude of the gap is $39 \text{meV}$ in the SC phase and $59 \text{meV}$ in the RES phase. Note that the amplitudes of the gaps are qualitatively in accordance with the experimental data.

FIG. 6. The Raman susceptibility in the $B_{1g}$ and the $B_{2g}$ symmetry at a) $p=0.1$ in the RES state, b) and b) $p=0.16$. The calculated responses are in promising agreement with the experimental data. In the $B_{2g}$ channel, the intensity does not vary with doping but the frequency resonance increases at low doping. In the $B_{1g}$ channel, the frequency resonance increases at low doping but the intensity fall down as observed experimentally.

FIG. 7. The real and imaginary parts of the bare polarization bubble at $Q = (\pi, \pi)$ for a) $p = 0.1$ in the RES state, b) $p = 0.16$ in the RES state c) $p = 0.1$ in the SC state, d) $p = 0.16$ in the SC state. The amplitude of the order parameters are the same as in Figs. 4 and 5. We observe a gap opening in both SC state and RES.
in the SC phase. The energy of the threshold moves from 129 meV at \( p = 0.1 \) down to 66 meV at \( p = 0.16 \) in the SC. The bare spin susceptibilities in the SC and RES states are very similar because the gap mechanism is nearly the same close to the FS. This feature is emphasized by the fact that close to the FS, we can apply the identity \( \xi_{k-2pF(k)} = -\xi_k \) and the bare spin susceptibility in the RES becomes the same than the SC one.

D. The RPA spin susceptibility

The amplitude of the imaginary part of the RPA susceptibility for the RES and SC phases are presented in Figs. 8 and 9 for \( p = 0.1 \) and \( p = 0.16 \) respectively, as a function of \( \omega \) in the diagonal direction \( q_y = q_x \) from \(-\pi/2a\) to \(3\pi/2a\) (with \( a \) that the unit cell parameter set to unity).

At \( p = 0.16 \), the magnitude of the super-exchange interaction \( J_0 = 151 \text{ meV} \) is adjusted to set the resonance at \( Q \) at 60 meV while at \( p = 0.1 \), we put \( J_0 = 169 \text{ meV} \) to ensure a resonance at 50 meV. In both RES and SC state, we observe a resonance at \( Q \). The intensity as well as the form of the resonance does not vary a lot between the two states at both doping (Figs. 8 c) and 9 c).

At \( p = 0.1 \), the RES order parameter is dominant in both SC and RES state resulting on a Y-shape in both cases. At optimal doping, the SC order parameter dominates in the SC states leading to the X-shape. The loss of coherent terms in the RES erases the X-shape observed in the SC state.

IV. DISCUSSION

We discuss below the three main findings of our theory, compared to other approaches proposed so far.

First, as shown in Figs. 8 and 9 the model gives a good agreement for the frequency resonance and the intensity of the resonance observed at \( Q \) in Hg-1201. The frequency resonance is determined by the values of the RES and SC order parameters as well as the value of the super-exchange \( J_0 \). The values of the RES and SC order parameter have been determined to reproduce the Raman coherent peak in the \( B_{1g} \) and \( B_{2g} \) symmetry. The value of \( J_0 \) is in the right range of values for cuprate compounds. Moreover, the decrease of the magnitude with doping is consistent with the decrease of the two-magnon peak in Raman data.\(^{47,48}\) The frequency and intensity of the resonance is the same in both the SC and the RES in the underdoped regime and optimal doping.\(^{26-28}\) At

FIG. 8. Amplitude of the Imaginary part of the spin susceptibility \( \chi_S \) as a function of \( \omega \), for \( q_y = q_x \) and \( q_x \) from \(-\pi/2a\) to \(3\pi/2a\) at \( p = 0.1 \) for \( J_0 = 169 \text{ meV} \) and \( V = 100 \) in a) the SC state and b) the RES. The solid line is set at \( q = (\pi/a, \pi/a) \). c) Cut at \( Q = (\pi, \pi) \) of the imaginary part of \( \chi_S \) in the RES (dashed line) and SC (solid line) state.
FIG. 9. Amplitude of the Imaginary part of the spin susceptibility $\chi_S$ as a function of $\omega$, for $q_x = q_y$ and $q_z$ from $-\pi/2a$ to $3\pi/2a$ at $p = 0.16$ for $J_0 = 151$ meV and $V = 100$ in a) the SC state and b) the RES state. The solid line is set at $q = (\pi/a, \pi/a)$. c) Cut at $Q = (\pi, \pi)$ of the imaginary part of $\chi_S$ in the RES (dashed line) and SC (solid line) state.

optimal doping, the same intensity observed in both RES and SC state is in agreement with the absence of any signature on the intensity of the resonance at $T_c$.26–28 The same intensity in both the RES and SC state is a by-product of our model where we did not adjust the damping that could be higher in a non-homogeneous state as RES. Indeed, our model produces naturally intrinsic inhomogeneities due to the proliferation of local objects. This aspect will be studied in future publications.

Second, our model reproduces in a promising agreement the fluctuation spectrum around $Q$ in both the SC and RES states. The disappearance of the low energy fluctuation spectrum in the SC state when we pass to the RES (and then the transformation from the X-shape to the Y-shape) can be explained by the loss of the coherence terms in the RES away from the vector $Q$. The enhancement of the coherence close to the $Q$ vector leads to the increasing of the value of the spin susceptibility at $Q$ in the RES and the emergence of the Y shape in the energy fluctuation spectrum. In our model, we have modeled this loss of coherence by a function $f(q)$ which vanishes away from $Q$. The effect of the width of the function $f(q)$ on the spin susceptibility is studied in the Appendix B.

A simple explanation for the emergence of spectral weight at $Q$ in the pseudo gap phase can be given as follows. Since their origin lies in the SU(2) fluctuations, the RES patches are acting on a small part of the BZ, and are gapping out the anti-nodal region of the Fermi surface, close to the hot spots. Fluctuations associated with the SU(2) scenario are thus restricted to these regions. The typical wave vectors connecting these regions to one another are $q = Q$ and $q = 0$, but due to the presence of the $d$-wave phase factor, the positive sign necessary for forming bound state (as opposed to anti-bound) selects the wave vector $Q$. Hence the two main ingredients for the emergence of spectral weight at $Q$ and the presence of the factor $f(q)$ in Eqn.(9) are the localization of the RES around the hot spots (which selects the mode modulation vectors $q = 0$ and $q = Q$) in the anti-nodal region and retaining a certain coherence with $d$-wave form factor (which finally selects the modulation vector around $q = Q$). In order to test this idea, we show in Appendix C the same calculation for a SC state with the SC gap formation restricted to a small region around the hot spots. We see in Fig. 12 that it gives some additional spectral weight around $q = Q$ as desired. For a SC state, the form of the additional spectral weight is more like a spot rather than the “Y”-shape. The elongation of the tail of the “Y” at $Q$ is a consequence of the “nesting” feature $k \rightarrow k - 2p_F$ when the energy is lowered.

Lastly, the dependence in doping of the fluctuation spectrum can be explained by the nature of the RES. The proliferation of excitonic patches occurs at zero temperature at low doping while it occurs at much higher temperature close to optimal doping (see Fig. 1). This difference implies that RES order is strong at low doping and coexist with SC order parameter while it weakens at op-
timal doping consistently with Raman experiments\textsuperscript{47,48}. Consequently, the RES state drives the physics close to AF critical vector at low doping explaining the Y-shape of energy fluctuation spectrum in both SC and RES. At optimal doping, the RES weakens in the AN zone and the physics is dominated by SC order parameter which implies the appearance of the X-shape.

A possible extension of this work should be the calculation of the RES response in bilayered systems. In such systems, the interlayer coupling creates bonding and anti-bonding states and gives rise to even and odd spin susceptibilities. Leaving aside the stability of the RES in such bilayer compounds, we expect the even and odd susceptibilities to behave similarly than in the monolayer compound. However, the exact vector where the resonance occurs could change because of the mismatch between the bonding and anti-bonding Fermi surfaces. The effect of exotic structure like CuO chains in YBCO compounds on the spin dynamics is still unclear. The CuO chains could stabilize nematic order\textsuperscript{73} which could reciprocally affect of spin susceptibility and produce incommensurability. This nematic order could be strong in the SU(2) scenario\textsuperscript{49}. We let the detailed calculations for forthcoming publications.

V. CONCLUSION

We proposed a description of the energy spectrum of the dynamic spin susceptibility, observed by INS in recent experiments on the cuprate compounds Hg-1201, for both the SC and the PG states. This explanation is based on a new concept for the PG phase which shows the emergence of particle-hole pairs, forming excitonic droplets, or patches with multiple modulation wave vectors 2p\textsubscript{F}. The RES state behaves “almost” like a d-wave SC, but gaps out the anti-nodal region of the first BZ, leading to the formation of Fermi “arcs”\textsuperscript{64}. In the PG regime, this restriction provokes a loss of coherence terms except at some peculiar wave vectors commensurate with the lattice, like the AF vector Q. This description of the PG phase is able to reproduce the main features of the Raman scattering in Hg-1201, and is a promising candidate for PG state of superconducting cuprates.

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Appendix A: Feynman Diagram in the spin susceptibility

We consider the spin susceptibility originating the t-J model\textsuperscript{31,62} which writes:

\begin{equation}
\chi_S(\omega, q) = \frac{\chi^0_S(\omega, q)}{1 + J(q)\chi^0_S(\omega, q)}
\end{equation}

with \(J(q) = J_0 (\cos(q_x a_0) + \cos(q_y a_0))\). In the equation (6), \(\chi^0_S\) is the bare polarization bubble constructed from the Green’s function and \(J(q)\) is super-exchange interaction. Note that momentum dependence of the super-exchange term \(J(q)\) originates the exchange between near neighbor Copper sites. The bare polarization can be evaluated by the formula\textsuperscript{33,69}:

\begin{equation}
\chi^0_S (\omega, q) = -\frac{T}{2} \sum_{\epsilon, k} \text{Tr} \left[ \hat{G}(\omega + \epsilon, k + q) \hat{G}(\epsilon, k) \right]
\end{equation}

where \(\epsilon(\omega)\) is the fermionic (bosonic) Matsubara frequency, \(k(q)\) is the impulsion, \(T\) the temperature and Tr means Trace of the Green function matrix \(\hat{G}\). The relation (A2) describes the whole polarization of the system that is the sum of the polarizations \(\Pi\):

\begin{equation}
\chi^0_S = \frac{1}{8} \left( \sum_{i,j} \Pi^{ij} \right)
\end{equation}

where \(\Pi^{ij}\) are the polarizations described by the diagrams of the Fig.10 with \(\Pi^{ij} = \Pi^{ii} = \Pi^{jj}\) for \(j \neq i\). \(\Pi^{11(44)}\) (diagram (a) and (d)) of Fig.10 is the response of the electrons (holes) with momentum \(k\) while \(\Pi^{22(33)}\) (diagram (b) and (c)) of Fig.10 is the response of the electrons (holes) with momentum \(k + 2p_F(k)\). The polarization \(\Pi^{41(32)}\) (diagram (e) and (f)) of Fig.10 is the response of the Cooper pairs while \(\Pi^{31(42)}\) (diagram (g) and (h)) of Fig.10 is the response of the particle-hole pairs. The polarization \(\Pi^{21(43)}\) (diagram (i) and (j)) of Fig.10 is the mixed SC-RES response.

Note that the superconducting coherent factors comes from the terms \(\Pi^{41(32)}\).

As shown in the diagram (g) to (j) of Fig.10, the outgoing external vector depends on the difference \(\delta_{2p_F} = 2p_F(k + q) - 2p_F(k)\). In order to these diagrams to contribute to the global polarization \(\Pi^{21(31,42,43)} \neq 0\), this difference must vanish, \(\delta_{2p_F} = 0\). Obviously, this difference vanishes for \(q = 0\). This difference also vanishes for \(q = Q\). The RES polarization contributes around \(q \approx 0\) and \(q \approx Q\) but will vanish if \(q\) is far from 0 or \(Q\). To take modelize this effect, we introduce a momentum dependent function in the relation (A3) which transforms itself as :

\begin{equation}
\chi^0_S = \frac{1}{8} \left( \Pi^{11} + \Pi^{22} + \Pi^{33} + \Pi^{44} + 2(\Pi^{32} + \Pi^{41}) + 2f(q)(\Pi^{21}_{RES} + \Pi^{31}_{RES} + \Pi^{42}_{RES} + \Pi^{53}_{RES}) \right)
\end{equation}
where \( f(\mathbf{q}) \) acts on the RES and SC-RES mixed polarizations. The function \( f(\mathbf{q}) \) has the form:

\[
  f(\mathbf{q}) = \frac{1}{1 + V(\sin^2(q_x a) + \sin^2(q_y a))}
\]

which is a Lorentzian centered in \( \mathbf{q} = (0, 0) \) and \( \mathbf{q} = \mathbf{Q} = (\pi, \pi) \) whose width can be tuned by the parameter \( V \). If \( V \) tends toward zero, the function \( f(\mathbf{q}) \) uniformly tends to unity. If \( V \) tends toward infinity, the function \( f(\mathbf{q}) \) is a dirac distribution centered in \((0,0)\) and \((\pi, \pi)\). The effect of the function \( f \) on the spin susceptibility is detailed in the Appendix B.

**Appendix B: Effect of the \( f \) function on the spin susceptibility \( \chi_S \) around \( \mathbf{Q} \)**

In this section, we present the effect of the width of the function \( f \) on the spin susceptibility \( \chi_S \). The function \( f \) is a Lorentzian whose width can be tuned by the value of the parameter \( V \) (see formula A5). If \( V \) vanishes then \( f \) is uniformly unity, \( f = 1 \). If \( V \) tends toward infinity then \( f \) becomes a Dirac function centered in \( \mathbf{Q} \). In the Fig. 11, we present the spin susceptibility \( \chi_S \) as a function of the parameter \( V \). We observe that for \( V = 0 \) (Fig. 11 c), the energy fluctuation in the RES looks like the one in the pure SC state with the two branches from either side of the momentum \( \mathbf{Q} \) but with a particle-hole continuum at \( \mathbf{Q} \). When the parameter \( V \) increases (Fig. 11 a) and b), the two branches are completely lowered and only the resonance at \( \mathbf{Q} \) remains.

**Appendix C: Effect of the SC order parameter momentum dependence on the spin susceptibility**

In this section, we present the effect of the momentum dependence of the SC order parameter on the form of the spin susceptibility. If we consider a SC gap centered only on the hot-spot (see Fig. 12 a)), the spin susceptibility is maximal around the vector \((\pi, \pi)\) only and the X shape disappears, as shown in Fig. 12.b).
FIG. 10. Polarizations $\Pi^V$ that contribute to the bare polarization $\chi_0$ (see equation (A3)). In a) to d) are the diagrammatic representation of the polarization with normal contribution. In e) and f) are presented the contribution of superconducting state. In g) and h) are presented the contribution of the RES. In i) and j) are shown the mixed SC-RES contribution. The contribution of the RES and SC-RES mixed polarization (diagrams from g) to j)) only exist for $q$ close to $(0,0)$ and $(\pi,\pi)$. In k) are presented the diagrammatic representation of the Green function.

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