Effect of pairing fluctuations on the spin resonance in Fe-based superconductors

Alberto Hinojosa,[1] Andrey V. Chubukov,[1] and Peter Wölfle[2]

[1]*Department of Physics, University of Wisconsin, Madison, Wisconsin 53706, USA*

[2]*Institute for Condensed Matter Theory and Institute for Nanotechnology, Karlsruhe Institute of Technology, D-76128 Karlsruhe, Germany*

The spin resonance observed in the inelastic neutron scattering data on Fe-based superconductors has played a prominent role in the quest for determining the symmetry of the order parameter in these compounds. Most theoretical studies of the resonance employ an RPA-type approach in the particle-hole channel and associate the resonance in the spin susceptibility $\chi_S(\mathbf{q},\omega)$ at momentum $\mathbf{Q} = (\pi,\pi)$ with the spin-exciton of an s^{+-} superconductor, pulled below 2Δ by residual attraction associated with the sign change of the gap between Fermi points connected by $\mathbf{Q}$. Here we explore the effect of fluctuations in the particle-particle channel on the spin resonance. Particle-particle and particle-hole channels are coupled in a superconductor and to what extent the spin resonance can be viewed as a particle-hole exciton needs to be addressed. In the case of purely repulsive interactions, we find that the particle-particle channel at total momentum $\mathbf{Q}$ (the π channel) contributes little to the resonance. However, if the interband density-density interaction is attractive and the π resonance is possible on its own, along with spin-exciton, we find a much stronger shift of the resonance frequency from the position of the would-be spin-exciton resonance. We also show that the expected double-peak structure in this situation does not appear because of the strong coupling between particle-hole and particle-particle channels, and $\mathrm{Im}\chi_S(\mathbf{Q},\omega)$ displays only a single peak.

I. INTRODUCTION

The spin resonance, observed by inelastic neutron scattering (INS) experiments first in the cuprates [1] and then in heavy-fermion [2] and Fe-based superconductors (FeSCs) [3], has been the subject of intense theoretical and experimental studies over the past decade using both metallic [4–7] and near-localized strong-coupling scenarios [8] (see Ref. [9] for a review). The theoretical interpretations of the resonance can be broadly split into two classes. The first class of theories assumes that the spin resonance is a magnon, overdamped in the normal state due to the strong decay into low-energy particle-hole pairs, but emerging prominently in the superconducting state due to reduction of scattering at low energies [7,10]. In this line of reasoning, the resonance energy Ω_{res} is the magnon energy and as such it is uncorrelated with the superconducting gap Δ. However, the decay of magnons into particle-hole pairs is only suppressed at energies below 2Δ, hence the magnons become sharp in a superconductor only if their energy is below 2Δ. The symmetry of the superconducting state does not play a crucial role here. It is only relevant that the superconducting gap is finite at the Fermi surface (FS) points connected by the gap momentum $\mathbf{Q}$.

Theories from the second class assume that the resonance does not exist in the normal state and emerges in the superconducting state as a feedback effect from superconductivity, like, e.g., the Anderson-Bogolyubov mode in the case of a charge neutral single condensate component, a Leggett mode in the case of several gap components, a wavelike excitation of a spin-triplet order parameter, or a pair vibration mode in the case of a gap parameter possessing internal structure [11]. These "feedback" theories can be further split into three subclasses. In the first, the resonance is viewed as a spin-exciton, i.e., the pole in the dynamical spin susceptibility $\chi(\mathbf{q},\Omega)$ dressed by multiple particle-hole bubbles [4–6]. Such $\chi(\mathbf{q},\Omega)$ can be obtained by using a computational scheme based on the random-phase approximation (RPA). It was argued that, if the superconducting gap changes sign between FS points

connected by $\mathbf{Q}$, the residual attraction pulls the resonance frequency to $\Omega_{\mathrm{res}} < 2\Delta$, where the decay into particle-hole pairs is reduced below T_c and vanishes at $T = 0$. As a result, at $T = 0$, $\chi''(\mathbf{q},\Omega)$ has a δ-functional peak at Ω_{res}. In this respect, if the resonance is an exciton, its existence necessary implies that the superconducting gap changes sign either between patches of the FS connected by $\mathbf{Q}$ or between different Fermi pockets again connected by $\mathbf{Q}$. The role of the resonance in allowing to determine the structure of the gap in a number of different superconductors has been highlighted in Ref. [12]. Theories of the second subclass explore the fact that in a superconductor the particle-hole and particle-particle channels are mixed and argue that the strongest resonance is in the particle-particle channel and the measurements of the spin susceptibility just reflect the "leakage" of this resonance into the particle-hole channel. The corresponding resonance has been labeled as the π exciton [13], where the π boson is a particle-particle excitation with total momentum $\mathbf{Q}$ (a "pair density-wave" in modern nomenclature [14–16]). Finally, theories of the third class explore the possibility that the resonance emerges due to coupling between fluctuations in particle-hole and particle-particle channels. Within RPA, such resonance is due to nondiagonal terms in the generalized RPA, which includes both particle-hole and particle-particle bubbles. It was called a plasmon [17] to stress the analogy with collective excitations in an electronic liquid.

The interplay between the "damped spin-wave" scenarios, the spin-exciton π resonance, and the plasmon scenarios for 2D high-T_c cuprates has been studied in detail in the past decade. The outcome is that near and above optimal doping the resonance is best described as a spin-exciton, with relatively weak corrections from coupling to the particle-particle channel [5,18,19], while in the underdoped regime, where superconductivity emerges from a pre-existing pseudogap phase, both spin-exciton and spin-wave scenarios have been argued to account for the neutron resonance [9]. The situation is more complicated in 3D heavy-fermion systems [10,20]

because there the excitonic resonance has a finite width even at $T = 0$ if the locus of FS points separated by **Q** intersects a line of gap nodes.

In this work, we discuss the interplay between spin-exciton, π resonance, and plasmon scenarios in FeSCs. Previous studies of the resonance in FeSCs [6] focused only on the response in the particle-hole (spin-exciton) channel and neglected the coupling between particle-hole and particle-particle channels. Our goal is to analyze the effect of such coupling.

As we said, the resonance peak has been observed below T_c in several families of FeSCs [3]. The spin response above T_c in FeSCs is rather featureless away from small doping, which implies that the magnetic excitations in the normal state are highly overdamped and don't behave as damped spin waves. The full analysis of the spin resonance in FeSCs is rather involved as these systems are multiband materials with four or five FSs, on which the superconducting gap has different amplitudes and phases. Still, the basic conditions for spin-excitonic resonance are the same as in the cuprates and heavy-fermion materials: namely, the resonance emerges at momentum **Q** if the superconducting gap changes sign between FS points connected by **Q**. This condition holds if the superconducting gap has s^{+-} symmetry, as most researchers believe, and changes sign between at least some hole and electron pockets. An alternative scenario [21], which we will not discuss in this paper is that the superconducting state has a conventional, sign-preserving s^{++} symmetry, and the observed neutron peak is not a resonance but rather a hump at frequencies slightly above 2Δ.

In FeSCs that contain both hole and electron pockets, the resonance has been observed at momenta around **Q** $= (\pi, \pi)$, which is roughly the distance between hole and electron pockets in the actual (folded) Brillouin zone. To account for the resonance and, at the same time, avoid unnecessary complications, we consider a minimal three-band model (one hole pocket and two electron pockets), and neglect the angular dependence of the interactions along the FSs. Including this dependence and additional hole pockets will complicate the analysis but we do not expect it to lead to any qualitative changes to our results.

We find that for repulsive density-density and pair-hopping interactions, the resonance peak is, to a good accuracy, a spin-exciton. The π resonance does not develop on its own, and the coupling between the resonant spin-exciton channel and the nonresonant π channel only slightly shifts the energy of the excitonic resonance. We also considered the case (less justified microscopically) when the interaction in the π channel is attractive, such that both spin-exciton and π resonance develop on their own at frequencies below 2Δ. One could expect in this situation that the full dynamical spin susceptibility has two peaks. We found, however, that this happens only if we make the coupling between particle-hole and particle-particle channels artificially small. When we restored the original coupling, we found, in general, only one peak below 2Δ. The peak is a mixture of a spin-exciton and π resonance and at least in some range of system parameters its energy is smaller than that of a spin-exciton and a π resonance. This implies that, when both channels are attractive, the coupling between the two plays a substantial role in determining the position of the true resonance which can, at least partly, be

viewed as a plasmon. A somewhat similar result has been obtained earlier for the cuprates [5,17,19]. For some system parameters, we did find two peaks in $\text{Im}\chi_S(\mathbf{Q}, \omega)$, but for one of them $\text{Im}\chi_S$ has wrong sign. We verified that this indicates that for such parameters the system is unstable either against condensation of π excitations (i.e., against superconductivity at momentum **Q**), or against the development of SDW order in co-existence with superconductivity.

The paper is organized as follows. In the next section, we consider the model. In Sec. III, we obtain the dynamical spin susceptibility within the generalized RPA scheme, which includes the coupling between particle-hole and particle-particle channels. In Sec. IV, we analyze the profile of $\chi_S(\mathbf{Q}, \omega)$ first for purely repulsive density-density and pair-hopping interactions, and then for the case when we allow the density-density interaction to become attractive. We summarize our conclusions in Sec. V.

II. THE MODEL

The FeSCs are multiband metals with two or three hole FS pockets centered around the Γ point $(0,0)$ and two elliptical electron pockets centered at (π, π) in the folded BZ with two iron atoms per unit cell. The electron pockets are elliptical and related by symmetry, while the hole pockets are C_4-symmetric, but generally differ in size. Since we are only interested in studying the role of the particle-particle channel in the spin response function, for which the nonequivalence between hole pockets is not essential, we consider the case of two hole pockets and assume that they are circular and identical, and also neglect the ellipticity of electron pockets. Under these assumptions our model reduces effectively to only one hole pocket (c fermions) and one electron pocket (f fermions). The fact that there are actually two hole and two electron pockets only adds up combinatoric factors.

The free part of the Hamiltonian is

$$H_0 = \sum_{\mathbf{k},\sigma} \left(\xi_{\mathbf{k}}^c c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + \xi_{\mathbf{k}+\mathbf{Q}}^f f_{\mathbf{k}+\mathbf{Q}\sigma}^\dagger f_{\mathbf{k}+\mathbf{Q}\sigma} \right), \quad (1)$$

where

$$\xi_{\mathbf{k}}^c = \mu_c - \frac{k_x^2 + k_y^2}{2m_c}, \quad (2)$$

$$\xi_{\mathbf{k}+\mathbf{Q}}^f = -\mu_f + \frac{k_x^2 + k_y^2}{2m_f}. \quad (3)$$

We do not study here how superconductivity develops from interactions, as that work has been done elsewhere [22]. Instead, we simply assume that the system reaches a superconducting state with s^{+-} symmetry before it becomes unstable towards magnetism and take the superconducting gaps as inputs. In this state, the free part of the Hamiltonian is

$$H_0^{SC} = \sum_{\mathbf{k},\sigma} \left(E_{\mathbf{k}}^c c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + E_{\mathbf{k}+\mathbf{Q}}^f f_{\mathbf{k}+\mathbf{Q}\sigma}^\dagger f_{\mathbf{k}+\mathbf{Q}\sigma} \right), \quad (4)$$

where the dispersions are $E_{\mathbf{k}}^c = \sqrt{(\xi_{\mathbf{k}}^c)^2 + (\Delta^c)^2}$, $E_{\mathbf{k}+\mathbf{Q}}^f = \sqrt{(\xi_{\mathbf{k}+\mathbf{Q}}^f)^2 + (\Delta^f)^2}$, and $\Delta^c = -\Delta^f \equiv \Delta$.

Now we consider interactions that contribute to the spin susceptibility. They consist of a density-density interband interaction u_1 and a correlated interband hopping u_3. Intraband repulsion only affects the chemical potentials but does not otherwise contribute to the spin susceptibility. Interband exchange, in principle, contributes in the π channel but in renormalization group analysis it flows to small values [23]. In general, u_1 and u_3 depend on the angle in momentum space via coherence factors associated with the transformation from the orbital to the band basis [24]. However, this complication is not essential for our purposes and we take both interactions to be momentum independent. The interaction Hamiltonian is

$$
\begin{aligned}
H_{\text{int}} = u_1 & \sum_{[1234],\sigma \neq \sigma'} c^{\dagger}_{\mathbf{p}_1\sigma} f^{\dagger}_{\mathbf{p}_2\sigma'} f_{\mathbf{p}_3\sigma'} c_{\mathbf{p}_4\sigma} \\
& + u_3 \sum_{[1234],\sigma \neq \sigma'} \left(c^{\dagger}_{\mathbf{p}_1\sigma} c^{\dagger}_{\mathbf{p}_2\sigma'} f_{\mathbf{p}_3\sigma'} f_{\mathbf{p}_4\sigma} + \text{H.c.} \right),
\end{aligned}
\tag{5}
$$

where the sum over momenta obeys momentum conservation as usual ($\mathbf{p}_1 + \mathbf{p}_2 = \mathbf{p}_3 + \mathbf{p}_4$).

Because the interactions in the band basis are linear combinations of Hubbard and Hund interactions in the orbital basis, weighted with orbital coherence factors, the sign of u_1 and u_3 depends on the interplay between intraorbital and interorbital interactions [21,25]. The interaction u_3 contributes to the superconducting channel, and for an s^{+-} gap structure must be repulsive. The sign of u_1 is *a priori* unknown. In most microscopic studies, it comes out positive (repulsive), but in principle it can also be negative (attractive). We do not assume a particular sign of u_1 and consider first a case where u_1 is positive and then when it is negative. For the first case, we show that a resonance can only originate from the particle-hole channel. For negative u_1, the π channel can produce collective modes as well, and we show that in general the resonant mode is a mix between spin exciton and a π resonance.

III. SUSCEPTIBILITIES AND RPA

We focus on susceptibilities at antiferromagnetic momentum $\mathbf{Q}$, which separates the centers of hole and electron pockets. Following similar work done on the cuprates [5], we define spin and π operators as

$$
S^z(\mathbf{Q}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} \left[c^{\dagger}_{\mathbf{k}\alpha} \sigma^z_{\alpha\beta} f_{\mathbf{k}+\mathbf{Q}\beta} + f^{\dagger}_{\mathbf{k}+\mathbf{Q}\alpha} \sigma^z_{\alpha\beta} c_{\mathbf{k}\beta} \right], \tag{6}
$$

$$
\pi(\mathbf{Q}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} \left[c_{\mathbf{k}\alpha} \sigma^x_{\alpha\beta} f_{\mathbf{Q}-\mathbf{k}\beta} \right]. \tag{7}
$$

To make a closer connection to Ref. [5], the operator π can be equivalently defined as $\pi = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} [g_{\mathbf{k}} a_{\mathbf{k}\alpha} \sigma^x_{\alpha\beta} a_{\mathbf{Q}-\mathbf{k}\beta}]$, with $|g_{\mathbf{k}}| = 1/2$ and the sign of $g_{\mathbf{k}}$ is chosen so that it is positive near the hole FS and negative near the electron FS ($g_{\mathbf{k}} = -g_{\mathbf{Q}-\mathbf{k}}$).

For notational convenience, we split S^z into two operators such that $S^z = S_c + S_f$, where

$$
S_c(\mathbf{Q}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\alpha} \sigma^z_{\alpha\beta} f_{\mathbf{k}+\mathbf{Q}\beta}, \tag{8}
$$

$$
S_f(\mathbf{Q}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} f^{\dagger}_{\mathbf{k}+\mathbf{Q}\alpha} \sigma^z_{\alpha\beta} c_{\mathbf{k}\beta}. \tag{9}
$$

TABLE I. Coefficients of bare susceptibilities. Note: $\mathbf{k}' = \mathbf{k} + \mathbf{Q}$.

a	b	$A_{ab}(\mathbf{k})$	$B_{ab}(\mathbf{k})$
1	1	$(v^c_{\mathbf{k}} u^f_{\mathbf{k}'})^2$	$(u^c_{\mathbf{k}} v^f_{\mathbf{k}'})^2$
1	2	$-u^c_{\mathbf{k}} v^c_{\mathbf{k}} u^f_{\mathbf{k}'} v^f_{\mathbf{k}'}$	$-u^c_{\mathbf{k}} v^c_{\mathbf{k}} u^f_{\mathbf{k}'} v^f_{\mathbf{k}'}$
1	3	$u^c_{\mathbf{k}} v^c_{\mathbf{k}} (u^f_{\mathbf{k}'})^2$	$-u^c_{\mathbf{k}} v^c_{\mathbf{k}} (v^f_{\mathbf{k}'})^2$
1	4	$(v^c_{\mathbf{k}})^2 u^f_{\mathbf{k}'} v^f_{\mathbf{k}'}$	$-(u^c_{\mathbf{k}})^2 u^f_{\mathbf{k}'} v^f_{\mathbf{k}'}$
2	2	$(u^c_{\mathbf{k}} v^f_{\mathbf{k}'})^2$	$(v^c_{\mathbf{k}} u^f_{\mathbf{k}'})^2$
2	3	$-(u^c_{\mathbf{k}})^2 u^f_{\mathbf{k}'} v^f_{\mathbf{k}'}$	$(v^c_{\mathbf{k}})^2 u^f_{\mathbf{k}'} v^f_{\mathbf{k}'}$
2	4	$-u^c_{\mathbf{k}} v^c_{\mathbf{k}} (v^f_{\mathbf{k}'})^2$	$u^c_{\mathbf{k}} v^c_{\mathbf{k}} (u^f_{\mathbf{k}'})^2$
3	3	$(u^c_{\mathbf{k}} u^f_{\mathbf{k}'})^2$	$(v^c_{\mathbf{k}} v^f_{\mathbf{k}'})^2$
3	4	$u^c_{\mathbf{k}} v^c_{\mathbf{k}} u^f_{\mathbf{k}'} v^f_{\mathbf{k}'}$	$u^c_{\mathbf{k}} v^c_{\mathbf{k}} u^f_{\mathbf{k}'} v^f_{\mathbf{k}'}$
4	4	$(v^c_{\mathbf{k}} v^f_{\mathbf{k}'})^2$	$(u^c_{\mathbf{k}} u^f_{\mathbf{k}'})^2$

We now define the susceptibilities $\chi_{ab}(\Omega_m)$ in terms of Matsubara frequencies as

$$
\chi_{ab}(\Omega_m) = \int_0^{1/T} d\tau' e^{i\Omega_m\tau'} \langle T_\tau A_a(\tau') A^{\dagger}_b(0) \rangle, \tag{10}
$$

where $A_a = (S_c, S_f, \pi, \pi^{\dagger})_a$. The actual spin susceptibility is given by $\chi_S = \chi_{11} + \chi_{12} + \chi_{21} + \chi_{22}$.

The bare susceptibilities χ^0_{ab} can be calculated in the usual way in terms of Green's functions and are given by bubbles made out of c and f fermions, with different Pauli matrices in the vertices. At $T = 0$ and after performing analytic continuation to real frequency space, the (retarded) susceptibilities have the following form:

$$
\begin{aligned}
\chi^0_{ab}(\omega) = \frac{2}{N} \sum_{\mathbf{k}} & \left[-\frac{A_{ab}(\mathbf{k})}{\omega - E^c_{\mathbf{k}} - E^f_{\mathbf{k}+\mathbf{Q}} + i\gamma} \right. \\
& \left. + \frac{B_{ab}(\mathbf{k})}{\omega + E^c_{\mathbf{k}} + E^f_{\mathbf{k}+\mathbf{Q}} + i\gamma} \right],
\end{aligned}
\tag{11}
$$

where χ^0_{ab}, A_{ab}, and B_{ab} are symmetric matrices. The expressions for A_{ab} and B_{ab} are presented in Table I in terms of coherence factors, which are given by

$$
u^c_{\mathbf{k}} = \sqrt{\frac{1}{2} \left(1 + \frac{\xi^c_{\mathbf{k}}}{E^c_{\mathbf{k}}} \right)}, \tag{12}
$$

$$
v^c_{\mathbf{k}} = \sqrt{\frac{1}{2} \left(1 - \frac{\xi^c_{\mathbf{k}}}{E^c_{\mathbf{k}}} \right)} \operatorname{sgn} \Delta^c, \tag{13}
$$

and similar expressions for $u^f_{\mathbf{k}'}$ and $v^f_{\mathbf{k}'}$.

To obtain the full susceptibilities χ_{ab}, we used the generalized RPA approach. Within this approach

$$
\chi_{ab} = (1 - \chi^0 V)^{-1}_{ac} \chi^0_{cb}, \tag{14}
$$

where the sum over repeated indices is implied and V is given by

$$
V = \frac{1}{2} \begin{pmatrix} u_1 & u_3 & 0 & 0 \\ u_3 & u_1 & 0 & 0 \\ 0 & 0 & -u_1 & 0 \\ 0 & 0 & 0 & -u_1 \end{pmatrix}. \tag{15}
$$

The solution for the full spin susceptibility can be written in a simpler form once we note that the matrix χ^0_{ab} has additional symmetry. Indeed, the functions $A_{ab}(\mathbf{k})$ and $B_{ab}(\mathbf{k})$ can be separated into parts that are even or odd with respect to $\xi^c_{\mathbf{k}}$ and $\xi^f_{\mathbf{k}}$. If the momentum sums are evaluated only near the FSs, where the integration region can be chosen to be symmetric with respect to positive and negative values of $\xi^c_{\mathbf{k}}$ and $\xi^f_{\mathbf{k}}$, then the odd parts cancel out and χ^0_{ab} acquires the following form:

$$\chi^0 = \begin{pmatrix} a & b & c & -d \\ b & a & d & -c \\ c & d & e & f \\ -d & -c & f & e \end{pmatrix}. \tag{16}$$

If we rotate the basis of operators from $(S_c, S_f, \pi, \pi^\dagger)$ to $(S_c + S_f, \pi - \pi^\dagger, S_c - S_f, \pi + \pi^\dagger)$ we find that both V and χ^0 become block diagonal, so the first 2×2 system decouples from the second one. In this case, the solution for the subset $(S_c + S_f, \pi - \pi^\dagger)$ takes the simple form

$$\chi_S = \frac{\chi^0_S + \delta\chi^0_S}{1 - u_S(\chi^0_S + \delta\chi^0_S)}, \tag{17}$$

$$\chi_\pi = \frac{\chi^0_\pi + \delta\chi^0_\pi}{1 - u_\pi(\chi^0_\pi + \delta\chi^0_\pi)}, \tag{18}$$

where

$$\delta\chi^0_S = \frac{u_\pi}{1 - u_\pi\chi^0_\pi}(\chi^0_{S\pi})^2, \tag{19}$$

$$\delta\chi^0_\pi = \frac{u_S}{1 - u_S\chi^0_S}(\chi^0_{S\pi})^2. \tag{20}$$

and $u_S = (u_1 + u_3)/4$ and $u_\pi = -u_1/4$. The bare susceptibilities in this basis are given by

$$\chi^0_S = \chi^0_{11} + \chi^0_{12} + \chi^0_{21} + \chi^0_{22} = 2(\chi^0_{11} + \chi^0_{12}), \tag{21}$$

$$\chi^0_\pi = \chi^0_{33} - \chi^0_{34} - \chi^0_{43} + \chi^0_{44} = 2(\chi^0_{33} - \chi^0_{34}), \tag{22}$$

$$\chi^0_{S\pi} = \chi^0_{13} - \chi^0_{14} + \chi^0_{23} - \chi^0_{24} = 2(\chi^0_{13} - \chi^0_{14}). \tag{23}$$

The first two bare susceptibilities contain contributions of products of two normal Green's functions and of two anomalous Green's functions, while $\chi^0_{S\pi}$ is composed of one normal and one anomalous Green's function (see Fig. 1 for some contributions of $\chi^0_{S\pi}$ to the spin response function).

We obtained expressions for the real parts of the bare susceptibilities by replacing the momentum sums by integrals and evaluating them within an energy range from $-\Lambda$ to Λ
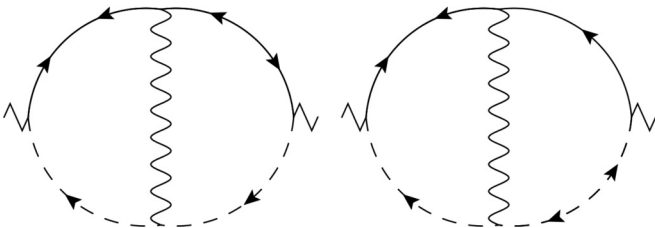

FIG. 1. Some mixed-channel contributions to the spin susceptibility and Raman scattering. The solid lines represent f fermions and the dashed lines c fermions, corresponding to quasiparticles from the electron and hole pockets, respectively.
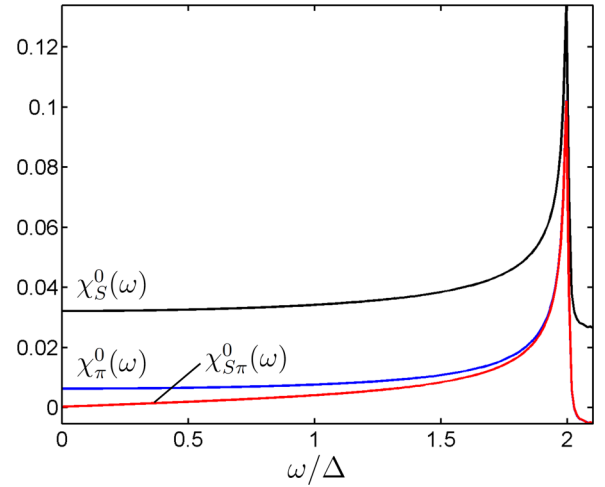

FIG. 2. (Color online) Real part of the bare spin susceptibilities ($T = 0$, units of Δ^{-1}) in the case of perfectly nested circular pockets ($m \equiv m_c = m_f = \frac{1}{100\Delta}$). In all numerical calculations, $\mu = 10\Delta$ and we include a finite broadening $\gamma = \Delta/200$ when evaluating momentum integrals.

about the FSs. They are valid in the range $0 < \omega < 2\Delta$ in the limit when the broadening $\gamma \to 0$:

$$\mathrm{Re}\,\chi^0_S(\omega) = L + \frac{\omega^2}{4\Delta^2}\mathrm{Re}\,\chi^0_\pi(\omega), \tag{24}$$

$$\mathrm{Re}\,\chi^0_\pi(\omega) = \frac{m}{\pi}\frac{4\Delta^2}{\omega\sqrt{4\Delta^2 - \omega^2}}\arctan\left(\frac{\omega}{\sqrt{4\Delta^2 - \omega^2}}\right), \tag{25}$$

$$\mathrm{Re}\,\chi^0_{S\pi}(\omega) = \frac{\omega}{2\Delta}\mathrm{Re}\,\chi^0_\pi(\omega), \tag{26}$$

where $L = \frac{m}{\pi}\ln(2\Lambda/\Delta)$ and we have neglected terms of order $(\Delta/\Lambda)^2$.

In Fig. 2, we present the results of numerical calculations of the bare susceptibilities in the case of perfectly nested FSs ($\mu_c = \mu_f \equiv \mu$). The susceptibility χ^0_S would diverge at $\omega = 0$ in the absence of superconductivity, but becomes finite at a finite Δ. Conversely, χ^0_π at $\omega = 0$ would be zero in the absence of superconductivity, but becomes nonzero because of Δ. Note that all three susceptibilities monotonically increase with frequency in the domain $0 \leqslant \omega \leqslant 2\Delta$ and diverge at $\omega = 2\Delta$. The imaginary parts of the three bare susceptibilities (not shown in the plot) are infinitesimally small and undergo a discontinuous jump at $\omega = 2\Delta$. If we make the electron pocket elliptical, the divergence in the real part is replaced by a local maximum.

We see that $\chi^0_S(\omega)$ and $\chi^0_\pi(\omega)$ have finite value at $\omega = 0$. We recall that, in the absence of superconductivity, $\chi_S(0)$ would diverge and $\chi_\pi(0)$ would vanish at perfect nesting. At $\omega = 2\Delta$, both bare susceptibilities diverge. The cross-susceptibility $\chi^0_{S\pi}(\omega)$ vanishes at $\omega = 0$ simply because it is composed from one normal and one anomalous Green's function but rapidly increases with ω and becomes comparable to $\chi_S(\omega)$ and $\chi_\pi(\omega)$ at $\omega \leqslant 2\Delta$.

The cross-susceptibility between particle-hole and particle-particle channels has been recently analyzed for an s^{+-} superconductor in the context of Raman scattering [26]. There, it was

computed in the charge channel and was found to be very small due to near-cancellation between contributions from Fermi surfaces with plus and minus values of the superconducting gap. In our case, we found that the contributions from hole and electron FSs add up rather than cancel. The difference is that in Raman scattering the side vertices in the susceptibility bubble have the spin structure given by $\delta_{\alpha,\beta}$, while in our case the spin structure is, say, $\sigma^z_{\alpha,\beta}$. For an s^{+-} gap, Raman bubbles from hole and electron pocket have the same vertex structure but differ in the sign of the anomalous Green's function, hence the two contributions to cross-susceptibility have opposite signs, resulting in a cancellation that is complete in the case of perfect nesting and near-complete in the case of one circular and one elliptical pocket. This cancellation does not occur in our case because the σ^z structure of the side vertices additionally flips the sign of one of the two diagrams, and the contributions to $\chi^0_{S\pi}(\omega)$ from hole and electron FSs add constructively.

We next note that the terms $\delta\chi^0_S$ and $\delta\chi^0_\pi$ are precisely what is neglected when the particle-particle channel is not included in the calculation of the spin susceptibility. Setting these terms to zero reduces the expressions for the full χ_S and χ_π to the usual RPA results:

$$\chi_S = \frac{\chi^0_S}{1 - u_S\chi^0_S}, \quad \chi_\pi = \frac{\chi^0_\pi}{1 - u_\pi\chi^0_\pi}. \quad (27)$$

The effect of coupling the two channels can be seen more clearly by substituting (19) into (17), which yields

$$\chi_S = \frac{\chi^0_S(1 - u_\pi\chi^0_\pi) + u_\pi(\chi^0_{S\pi})^2}{(1 - u_S\chi^0_S)(1 - u_\pi\chi^0_\pi) - u_S u_\pi(\chi^0_{S\pi})^2}$$
$$= \frac{1}{u_S}\left[-1 + \frac{1 - u_\pi\chi^0_\pi}{(1 - u_S\chi^0_S)(1 - u_\pi\chi^0_\pi) - u_S u_\pi(\chi^0_{S\pi})^2}\right]. \quad (28)$$

The positions of resonance peaks are given by the zeros of the denominator in this equation and we can see that the particle-hole and particle-particle channels are coupled through the mixed-channel susceptibility $\chi^0_{S\pi}(\omega)$.

IV. THE RESULTS

A. Purely repulsive interaction, $u_1 > 0, u_3 > 0$

For repulsive interactions $u_S > |u_\pi| > 0$ and $u_\pi < 0$. In the absence of $\chi^0_{S\pi}$, the resonance in χ_S is present for any u_S because the bare susceptibility χ^0_S is positive and diverges at $\omega = 2\Delta$, hence the equation $1 - u_S\mathrm{Re}\chi^0_S(\omega) = 0$ has a solution for $0 < u_S < (\mathrm{Re}\chi^0_S(0))^{-1}$. In contrast, the fact that $\mathrm{Re}\chi^0_\pi > 0$ means that no resonance originates from this channel. When $\chi^0_{S\pi}$ is included, we found in our numerical calculations that the effect of the particle-particle channel is that the peak in the imaginary part of the full susceptibility is shifted to a higher frequency [since $\mathrm{Re}(u_S u_\pi(\chi^0_{S\pi})^2) < 0$]. We show representative behavior of real and imaginary parts of the full spin susceptibility in Fig. 3

This result is also obtained when we consider an elliptical electron pocket, except that there is a minimum value for u_S below which no resonance is observed. This is due to the fact
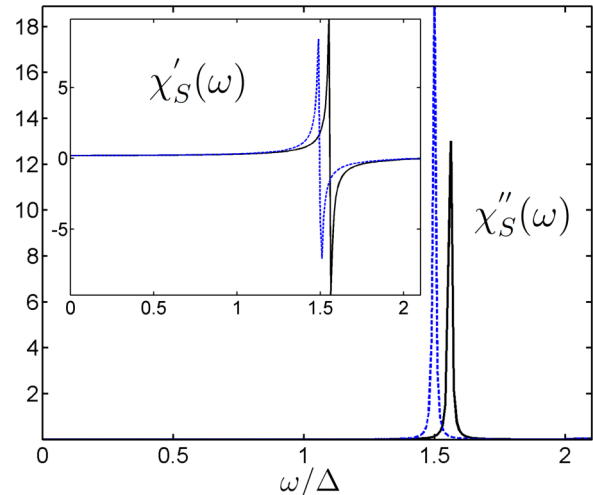

FIG. 3. (Color online) Imaginary part (main plot) and real part (insert) of the full spin susceptibility ($T = 0$, units of Δ^{-1}) in the case of repulsive interactions. In this plot, $u_S = 26\Delta$ and $u_\pi = -13\Delta$. The solid, black line indicates the full calculation. For comparison, the dashed, blue line indicates a calculation that neglects particle-particle contributions.

that the bare susceptibilities have a local maximum instead of a divergence at $\omega = 2\Delta$.

B. Partially attractive interaction, $u_1 < 0, u_3 > 0$

We now consider an alternative case where the density-density interaction $u_1 < 0$, hence $u_\pi = -u_1/4 > 0$. We still assume $u_3 > |u_1|$ such that $u_S > 0$. For positive u_π, the π channel can acquire a resonance on its own since the equation $1 - u_\pi\mathrm{Re}\chi^0_\pi(\omega) = 0$ necessarily has a solution at a frequency between 0 and 2Δ if $u_\pi < (\mathrm{Re}\chi^0_\pi(0))^{-1}$. We assume that this inequality holds together with $u_S < (\mathrm{Re}\chi^0_S(0))^{-1}$. If any of these two conditions are not satisfied, the system becomes unstable either towards π superconductivity with total momentum of a Cooper pair $\mathbf{Q}$ or towards magnetic order. In both cases, the analysis of the spin susceptibility has to be modified to include the new condensates. If the spin-exciton and π channels were not coupled [i.e., if $\chi^0_{S\pi}(\omega)$ was absent], we would find resonances in the spin and π channels at frequencies ω_S and ω_π, respectively, set by $1 - u_S\mathrm{Re}\chi^0_S(\omega_S) = 0$ and $1 - u_\pi\mathrm{Re}\chi^0_\pi(\omega_\pi) = 0$. This suggests the possibility that there may be two resonance peaks in the full spin susceptibility $\chi_S(Q,\omega)$ once we restore the coupling $\chi^0_{S\pi}(\omega)$.

However, we found that for all values of u_S and u_π for which the pure s^{+-} state is stable, there is only a single peak in the spin susceptibility at a frequency lower than both ω_S and ω_π. We show representative behavior in Fig. 4. The existence of a single peak is due to the fact that $\chi^0_{S\pi}$ is small at small frequencies, hence it does not prevent the increase of the real part of the spin susceptibility with increasing ω (see insert in Fig. 4) and only shifts the position of the lower pole (ω_S or ω_π) to a smaller value ω_{res}. At the same time, at higher frequencies, $\chi^0_{S\pi}$ is no longer small relative to the other bare susceptibilities χ^0_S and χ^0_π. As a result, the denominator in $\chi_S(\mathbf{Q},\omega)$ in (28) passes through zero at $\omega = \omega_{\mathrm{res}}$ and then remains negative all the way up to $\omega = 2\Delta$ and does not cross zero for the second time.
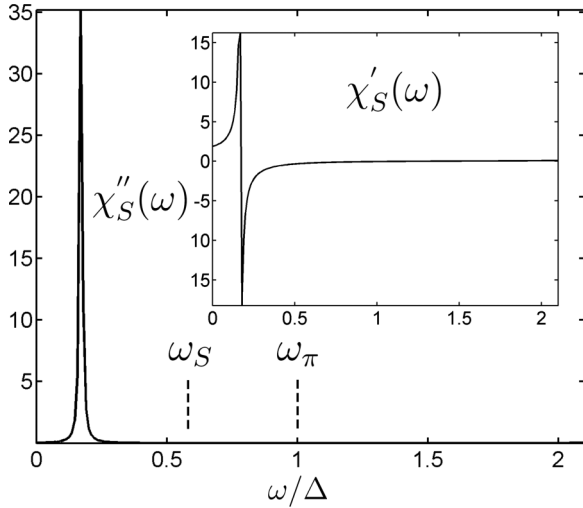
FIG. 4. Imaginary part (main plot) and real part (insert) of the full spin susceptibility ($T = 0$, units of Δ^{-1}) in the case of $u_S = 30.5\Delta$ and $u_\pi = 130\Delta$. In the absence of coupling we would observe resonance peaks in the spin and π channels at frequencies $\omega_S \approx 0.57\Delta$ and $\omega_\pi \approx 1.0\Delta$, respectively, indicated on the plot.

To better understand this, we artificially add a factor ϵ to $\chi_{S\pi}^0$ and consider how the solutions evolve as we progressively increase ϵ between 0 and 1. At small ϵ, the two solutions obviously survive and just further split from each other—the peak that was at a higher frequency shifts to a higher frequency and the other peak shifts to to a lower frequency. As ϵ increases, the peak at a higher frequency rapidly moves towards 2Δ. If we keep Imχ_{ab}^0 strictly zero, this peak survives up to $\epsilon = 1$ with exponentially vanishing amplitude. If, however, we keep a small but finite fermionic damping in the computations of χ_{ab}^0, we find that the functions $\chi_{ab}^0(\omega)$ increase but do not diverge at 2Δ. In this situation, the higher frequency peak in $\chi_S(\mathbf{Q},\omega)$ vanishes already at some $\epsilon < 1$.

We also considered the evolution of the two-peak solution with ϵ in a different way: we postulated that the two peaks should be at $\omega_{\text{res},1}$ and $\omega_{\text{res},2}$, both below 2Δ and solved the set of equations for u_S and u_π which would correspond to such a solution. At small ϵ, we indeed found some real u_S and u_π which satisfy "boundary conditions" $u_S\chi_S^0 < 1$ and $u_\pi\chi_\pi^0 < 1$. However, this holds only up to some ϵ_{cr}. At higher ϵ, the solutions for u_s and u_π become complex, which implies that the two-peak solution is no longer possible. At even higher ϵ real solutions for u_s and u_π reappear, but they do not satisfy the boundary conditions. We searched for a range of $\omega_{\text{res},1}$ and $\omega_{\text{res},2}$ and for all values that we tested we found $\epsilon_{\text{cr}} < 1$, i.e., again there is only a single peak for the actual case of $\epsilon = 1$.

Another way to see that there is only one peak in the full χ_S is to substitute the expressions for the real parts of the susceptibilities, Eqs. (24)–(26), into the denominator of Eq. (28) and express the real part of the term $D =$

$(1 - u_S\chi_S^0)(1 - u_\pi\chi_\pi^0) - u_S u_\pi (\chi_{S\pi}^0)^2$ via $\chi_\pi^0 = \chi_\pi^0(\omega)$. We obtain

$$\text{Re} D = (1 - u_S L) - \left[u_S \frac{\omega^2}{4\Delta^2} + u_\pi(1 - u_S L) \right] \text{Re}\left[\chi_\pi^0(\omega)\right].$$
$$(29)$$

Because $(1 - u_S L)$ and $(1 - u_\pi\chi_\pi^0(0))$ are required to be positive for the stability of the paramagnetic state, at zero frequency, D is surely positive. At finite ω, the first term in (29) is positive, while the second one is negative and its magnitude monotonically increases with increasing ω. As a result, the denominator crosses zero only once, at some $\omega < 2\Delta$.

The single resonance peak is a mixture of a spin-exciton and π resonance and for the representative case shown in Fig. 4 its energy is smaller that that of spin-exciton and a π resonance. This implies that, when both channels are attractive, the coupling between the two plays substantial role in determining the position of the true resonance. From this perspective, the resonance at $u_1 < 0$ can, at least partly, be viewed as a plasmon. A somewhat similar result has been earlier obtained in the analysis of the resonance in the cuprates in the parameter range where π resonance is allowed [5,17,19].

V. CONCLUSIONS

We have studied the spin resonance at antiferromagnetic momentum (π,π) in an s^{+-} superconducting state of FeSCs by including contribution from the particle-particle channel, which in the superconducting state gets mixed with the particle-hole channel. We have shown that for purely repulsive interactions the inclusion of this channel does not qualitatively change the spin resonance, which remains predominantly spin-exciton and only slightly shifts to higher frequencies. For attractive density-density interaction, when both spin-exciton resonance in the particle-hole channel and π resonance in the particle-particle channel are allowed, we found that strong coupling between the two channels destroys the two-peak structure and only one peak survives, whose frequency is smaller than would be that of a spin-exciton and π resonance in the absence of the coupling. We argued that strong coupling between the particle-hole and particle-particle channels is peculiar to the spin susceptibility, while for the charge susceptibility, which, e.g., is relevant for Raman scattering, the coupling is much smaller.

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