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Signatures of pairing and spin-orbit coupling in correlation functions of Fermi gases

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We derive expressions for density-density and spin-spin correlation functions in the (greatly enhanced) pseudogap phase of spin-orbit coupled Fermi gases. Density-density correlation functions are found to be relatively insensitive to the presence of these Rashba spin-orbit effects. To arrive at spin-spin correlation functions we derive new f -sum rules, valid even in the absence of a spin conservation law. Our spin-spin correlation functions are shown to be fully consistent with these f -sum rules. Importantly, they provide a clear signature of the Rashba band-structure and separately help to establish the presence of a pseudogap.

Introduction.— Spin-orbit coupling (SOC) in superconductors and superfluids is a topic of much current interest [1–3]. This is in large part because there is some hope that (particularly in the presence of a magnetic field) they may relate to the much sought after spinless $p_x + ip_y$ superfluid [4]. Two communities have united around these issues: those working on cold Fermi superfluids with intrinsic Rashba SOC [5, 6] and those studying superconductivity that is proximity induced in a spin-orbit coupled material [7]. To achieve this ultimate goal it is important to establish that a given candidate for the $p_x + ip_y$ superfluid simultaneously exhibits signatures of *both* pairing and spin-orbit coupling. This would provide minimal evidence for a properly engineered ultracold atomic gas. One therefore needs experimental signatures of these simultaneous effects and this provides a central goal for the present paper.

Here we address the signatures of this anomalous spin-orbit coupled superfluid as reflected in spin-spin and density-density correlation functions. Our work builds on the observation [8–13] that in the presence of Rashba SOC, pairing (in the form of pseudogap effects [14, 15]) is significantly enhanced. For this reason (and because the correlation functions are free of the complications of collective mode effects) we focus here on the anomalous normal phase. We show how even without condensation, the frequency dependent spin response exhibits features which relate to the Rashba ring band-structure, as well as to the presence of a pairing gap. In contrast, the density response is relatively unaffected by SOC. Previous work has focused on identifying SOC without [16, 17] or with pairing [18] via the one body spectral function. As compared with Ref. [18], we find less subtle features in the two particle response. At the very least the spin-spin correlation functions provide complementary and accessible (via neutrons or two photon Bragg scattering [19]) information.

Validating any theory of correlation functions requires satisfying important constraints [20]. Indeed, the absence of conservation laws complicates all spin transport in spin-orbit coupled materials. Thus, it is extremely important to find underlying principles for establishing self consistency. To address this issue, here we use the

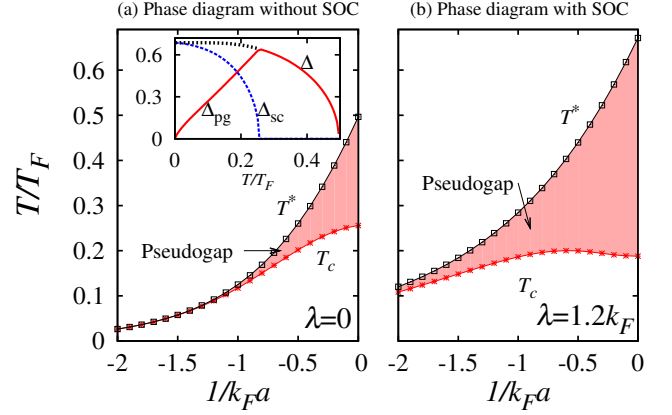


FIG. 1. Phase diagrams for a degenerate fermi gas without (a) and with (b) SOC. Plotted is T^* as a function of inverse scattering length, $1/k_F a$, indicating where pairing first sets in, while T_c marks the onset of condensation to the superfluid phase. The plot shows the weakly interacting regime with $1/k_F a < 0$. As spin-orbit coupling is turned on, pairing is enhanced leading to a larger pseudogap region. The inset in (a) indicates the temperature dependences of the component gap parameters (defined in the text) at unitarity, $1/k_F a = 0$.

Heisenberg equations of motion to derive f -sum rules for the spin-spin correlation functions, which also provides important constraints on our numerical calculations. In order to avoid technical complexity, we ignore the complication of a magnetic field (which is necessary for arriving at topological order). Our formalism leading to the phase diagram and response functions can be extended to include arbitrary SOC and Zeeman fields. However, we expect the Rashba case to be representative of a large class of spin-orbit coupled Hamiltonians. We note there is a substantial literature investigating correlation functions in the superfluid phase (without pseudogap effects) which we cite here [21–24].

In this Rapid Communication we present two main results. The first is a consistent derivation of spin-spin correlation functions in spin-orbit coupled Fermi gases. The second establishes qualitative experimental signatures reflecting separately the presence of a pairing gap and of SOC. Readers interested in the experimental sig-

natures need only a cursory exploration of the mathematical derivation that precedes it.

Background Theory.— We consider a gas of fermions whose single particle Hamiltonian is $H^0(\mathbf{k}) = k^2/2m - \mu + \lambda \boldsymbol{\sigma} \cdot \mathbf{k}_\perp/m$ for a particle of mass m , spin-orbit coupling momentum λ , momentum $\mathbf{k} = (k_x, k_y, k_z)$, in-plane momentum $\mathbf{k}_\perp = (k_x, k_y, 0)$, and vector of Pauli matrices $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$. Throughout this paper we set $\hbar = k_B = 1$. To describe our spin-orbit coupled Fermi gas with pairing, we use a 4×4 inverse Nambu Green's function

$$\mathcal{G}^{-1}(K) = \begin{pmatrix} G_0^{-1}(K) & \Delta \\ \Delta & \tilde{G}_0^{-1}(K) \end{pmatrix}, \quad (1)$$

that acts on the spinor $\Psi_{\mathbf{k}}^T = (c_{\mathbf{k}\uparrow}, c_{\mathbf{k}\downarrow}, -c_{-\mathbf{k}\downarrow}^\dagger, c_{-\mathbf{k}\uparrow}^\dagger)$ for a fermion annihilation (creation) operator $c_{\mathbf{k}s}$ ($c_{\mathbf{k}s}^\dagger$) of spin $s = \uparrow, \downarrow$ and momentum \mathbf{k} . In the Green's function Δ is a pairing gap, the 4-vector $K = (i\omega, \mathbf{k})$ with Matsubara frequency $i\omega$, and the non-interacting inverse particle Green's function is $G_0^{-1}(K) = i\omega - H^0(\mathbf{k})$ and hole Green's function is $\tilde{G}_0^{-1}(K) = i\sigma_y [G_0^{-1}(-K)]^T i\sigma_y = i\omega + H^0(\mathbf{k})$.

This superfluid can be studied at the mean field level [8–13], where one has the usual gap equation:

$$1 = \frac{g}{2} \sum_K \text{Tr} [G(K) \tilde{G}_0(K)], \quad (2)$$

where $\sum_K = T \sum_{i\omega} \sum_{\mathbf{k}}$ is a sum over momentum and Matsubara frequencies at temperature T , and where the many-body Green's function $G(K)$ is found from the inverse of Eq. (1)

$$G^{-1}(K) - G_0^{-1}(K) = -\Sigma(K) = -\Delta^2 \tilde{G}_0(K). \quad (3)$$

Except for the matrix structure in the above equations, these are the usual definitions of the fermionic Green's functions and self energy associated with BCS theory; the gap equation also appears in the literature [8–13]. As in the cold atoms literature, we will regularize the gap equation by replacing the interaction strength g with the scattering length a through $1/g = m/4\pi a - 1/V \sum_{\mathbf{k}} m/\mathbf{k}^2$.

We now want to include pair fluctuations, or pseudogap (pg) effects, in a fashion fully consistent with both the ground state and the mean field equations that have been extensively studied in previous work [8–13]. The approach we outline below was introduced in the context of high temperature superconductors [14, 25], but it has also been applied to spin-orbit coupled superfluids [26].

Pair fluctuations lower the phase transition temperature T_c relative to its mean field value denoted by T^* . The latter is the temperature at which the pairing gap, determined by Eq. (2), first becomes non zero. (Note that T^* does not reflect a broken symmetry state and is not a true phase transition). As a result, a central component

of the present theory is that the usual Thouless condition (on the t -matrix) for the instability of the normal phase [27] must be modified to include a well developed excitation gap.

Imposing consistency with mean field theory for the pairing gap $\Delta(T)$, obtained from Eq. (2), leads to a modified Thouless condition for the instability temperature:

$$t_{\text{pg}}(Q) \equiv \frac{g}{1 + g\chi(Q)} \rightarrow \infty, \text{ as } Q \rightarrow 0, \quad (4)$$

where $\chi(Q) \equiv -\frac{1}{2} \sum_K \text{Tr} [G(K) \tilde{G}_0(K - Q)]$. This ensures that T_c lies on the mean field Δ vs T curve. Establishing the specific value of T_c , however, requires that we find an additional constraint associated with the existence of a condensate. As reviewed in the Supplement and discussed in detail elsewhere [14], precisely at T_c we have the equation $\Delta^2 = -\sum_{Q \neq 0} t_{\text{pg}}(Q)$. The transition temperature T_c is, then, determined as the temperature at which this function constraining $\Delta(T)$ intersects with the mean field gap equation value.

Away from the point $T = T_c$, as discussed in the Supplement, the excitation gap contains the sum of condensed (sc) and non-condensed (pg) contributions: $\Delta^2 = \Delta_{\text{sc}}^2 + \Delta_{\text{pg}}^2$, where we have proved that below T_c $\Delta_{\text{pg}}^2 = -\sum_{Q \neq 0} t_{\text{pg}}(Q)$. Importantly we can interpret this last equation as suggesting that t_{pg} is a propagator for a thermal gas of composite (non-condensed) bosons. Above T_c we take Δ_{pg}^2 to be the mean field value, although this assumption is not necessary [28]. In the inset of Fig. 1(a), we plot the temperature dependence for both Δ_{sc} and Δ_{pg} , as well as the total excitation gap Δ .

We emphasize that a central distinguishing feature of the present approach is that T_c is determined in the presence of a well developed gap at T_c . This contrasts with the scheme of Nozieres and Schmitt-Rink [29]. In this scheme the pair susceptibility $\chi(Q)$ is given by two bare Green's functions which do not connect to the mean field gap equation, Eq. (2). This approach is similarly different from path integral-collective mode schemes [30]. The latter introduce Goldstone bosons, but importantly these do not renormalize the mean field transition temperature which remains at T^* .

Figure 1 shows the calculated phase diagram, plotting T_c and T^* , in the absence (a) and presence (b) of Rashba SOC. The latter is in reasonable agreement with the results of Ref. [26]. We restrict these plots to the weak pairing side of resonance. Here we observe a greatly enhanced pseudogap regime denoted by an enhancement of T^* without significant enhancement of T_c . The behavior of T^* has been attributed to the enhancement of the pairing attraction [8–13], due to an increased density of states near the minimum of the Rashba ring. Since T_c is obtained in the presence of a gap at T_c , stronger pairing (reflected in T^*) is offset by an increasingly gapped density of states. This leads to a relatively constant T_c as a function of interaction strength.

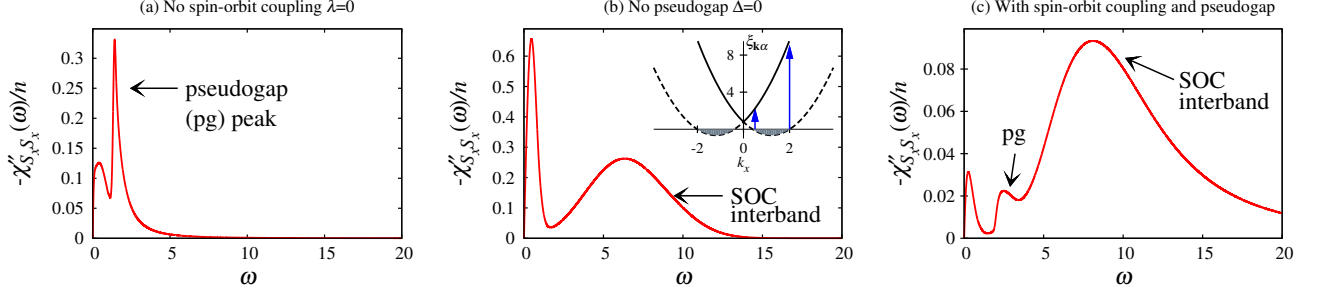


FIG. 2. The spin-spin response function as a function of frequency. Figure 2(a) corresponds to a pseudogap phase without SOC. The peak at lower ω reflects thermally excited fermions while the second peak is at ω comparable to the pseudogap energy scale, where pairs are now broken. Since $\lambda = 0$, the spin-spin and density-density correlation functions are the same. In Fig. 2(b) the pseudogap is set to zero with fixed $\lambda = 1.2k_F$. The lower energy intra-helicity band peak is enhanced and one sees an SOC-related peak. As shown in the inset, the low-energy threshold reflects the onset of inter-helicity band transitions, while the high-energy endpoint occurs when these transitions are no longer possible. In Fig. 2(c), in the presence of both a pseudogap and SOC, one sees a combination of the effects in the previous two panels. Spectral weight is transferred to yield a larger SOC peak, reflecting the gapping of the low energy contributions. All quantities are measured relative to the Fermi energy, E_F , or Fermi momentum k_F .

Density/current response and f -sum rules.— To characterize the anomalous normal, and superfluid phases in more detail, we investigate both the density/current-density/current and spin-spin correlation functions, considering the former first. For systems with a $U(1)$ symmetry, the Ward-Takahashi identity (WTI) provides an important constraint on the full vertex $\Gamma^\mu(\tilde{K}, K)$ which enters into the correlation functions. Given a mean field self energy, it is possible to analytically solve the WTI, and obtain the full vertex function along with the full correlation function [20, 31].

We define the generalized correlation function

$$P^{\mu\nu}(Q) = \sum_K \text{Tr} \left[G(\tilde{K}) \Gamma^\mu(\tilde{K}, K) G(K) \gamma^\nu(K, \tilde{K}) \right], \quad (5)$$

where $\tilde{K} \equiv K + Q$ and $\gamma^\mu(\tilde{K}, K)$ is a bare vertex. From this we have the density-density $\chi_{\rho\rho}(Q) \equiv P^{00}(Q)$ and current-current correlation functions $\tilde{\chi}_{JJ}(Q) \equiv P^{ij}(Q), i, j \in \{1, 2, 3\}$. The bare and full vertices satisfy respectively

$$q_\mu \gamma^\mu(\tilde{K}, K) = G_0^{-1}(\tilde{K}) - G_0^{-1}(K), \quad (6)$$

$$q_\mu \Gamma^\mu(\tilde{K}, K) = G^{-1}(\tilde{K}) - G^{-1}(K), \quad (7)$$

with the latter a consequence of the WTI. We now specialize to systems with the self energy as in Eq. (3). Using the WTI above T_c we have

$$\Gamma^\mu(\tilde{K}, K) = \gamma^\mu(\tilde{K}, K) + \Delta^2 \tilde{G}_0(\tilde{K}) \tilde{\gamma}^\mu(\tilde{K}, K) \tilde{G}_0(K), \quad (8)$$

where $\tilde{\gamma}^\mu(\tilde{K}, K) = \sigma_y \gamma^\mu(-\tilde{K}, -K)^T \sigma_y$ is a time-reversed vertex. Inserting the full vertex into Eq. (5) then gives the correlation functions above T_c .

One can incorporate superconducting (or equivalently superfluid) terms within this formalism building on

Eq. (8) and, for example, address the superfluid density [25, 32, 33], as outlined in the supplement. One considers the transverse response $P_T^{\mu\nu}(Q)$ which contains no collective modes:

$$P_T^{\mu\nu}(Q) = \sum_K \text{Tr} \left\{ \left[G(\tilde{K}) \gamma^\mu(\tilde{K}, K) G(K) + F_{\text{pg}}(\tilde{K}) \tilde{\gamma}^\mu(\tilde{K}, K) \tilde{F}_{\text{pg}}(K) - F_{\text{sc}}(\tilde{K}) \tilde{\gamma}^\mu(\tilde{K}, K) \tilde{F}_{\text{sc}}(K) \right] \gamma^\nu(K, \tilde{K}) \right\}, \quad (9)$$

where $F_\kappa(K) = \Delta_\kappa \tilde{G}_0(K) G(K) = \tilde{F}_\kappa(K)$ for $\kappa \in \{\text{sc}, \text{pg}\}$. Note that F_{pg} does not represent an anomalous Green's function, but rather reflects a vertex correction to the correlation functions [20].

As shown in the supplementary material, when one integrates over the entire frequency range, a consequence of the WTI is that the f -sum rule is satisfied:

$$\int \frac{d\omega}{\pi} (-\omega \chi''_{\rho\rho}(\omega, \mathbf{q})) = \frac{nq^2}{m}, \quad (10)$$

where $\chi''_{\rho\rho}$ is the imaginary part of the density response function. This f -sum rule depends on the total particle number n and the bare mass m . Since λ does not enter, the presence of spin-orbit coupling does not modify the weight of the f -sum rule.

Spin response and f -sum rules.— In the spin channel, there is no $U(1)$ symmetry to justify the use of the WTI. Nevertheless, we are able to provide an *a posteriori* check on any proposed correlation function via a sum rule which we now derive. We define $\chi_{S_i S_j}(i\omega, \mathbf{q}) \equiv \int d\tau e^{i\omega\tau} \langle T_\tau S_{\mathbf{q}i}(\tau) S_{-\mathbf{q}j}(0) \rangle$ where T_τ is the time ordering operator and $S_{\mathbf{q}i} = \sum_{\mathbf{k} s s'} c_{\mathbf{k} s}^\dagger(\sigma_i)_{ss'} c_{\mathbf{k}+\mathbf{q} s'}$ is the many-body spin density operator. Using the Heisenberg equations of motion and the properties of Fourier transforms, the sum rule for the spin-spin correlation function

$\chi''_{S_i S_j}$ can be shown [34] to be

$$\int \frac{d\omega}{\pi} \left(-\omega \chi''_{S_i S_j}(\omega, \mathbf{q}) \right) = \langle [\mathcal{H}_0, S_{\mathbf{q}i}], S_{-\mathbf{q}j} \rangle, \quad (11)$$

where $\mathcal{H}_0 = \sum_{ss'} c_{\mathbf{k}s}^\dagger H_{ss'}^0(\mathbf{k}) c_{\mathbf{k}s'}$ and $\chi''_{S_i S_j}$ is the singular part of $\chi_{S_i S_j}$ [35], found by analytically continuing $i\omega \rightarrow \omega + i\delta$ and then taking the $\delta \rightarrow 0$ limit. A similar analysis relating sum rules to the equation of motion was presented for Bose gases in Ref. [36].

Here we give the explicit result, for two example cases of interest and present further details in the supplementary material:

$$\int \frac{d\omega}{\pi} \left(-\omega \chi''_{S_i S_i}(\omega, \mathbf{q}) \right) = \frac{nq^2}{m} - \frac{4\lambda}{m} \sum_{\mathbf{k}\alpha} \alpha f_{ii} n_{\mathbf{k}\alpha}. \quad (12)$$

where $i \in \{x, z\}$, $f_{zz} = k_\perp$, $f_{xx} = k_x^2/k_\perp$ and $n_{\mathbf{k}\alpha} = T \sum_{i\omega} G_H^\alpha(K)$, with $G_H^\alpha(K)$ a helicity Green's functions to be defined in the next section.

Correlation functions in the helicity basis.— In the absence of a magnetic field, helicity is a good quantum number, and the correlation functions are most easily expressed in terms of the helicity Green's functions [26]:

$$G_H^\alpha(K) \equiv \frac{u_{\mathbf{k}\alpha}^2}{i\omega - E_{\mathbf{k}\alpha}} + \frac{v_{\mathbf{k}\alpha}^2}{i\omega + E_{\mathbf{k}\alpha}}, \quad (13)$$

$$F_H^\alpha(K) \equiv u_{\mathbf{k}\alpha} v_{\mathbf{k}\alpha} \left(\frac{1}{i\omega + E_{\mathbf{k}\alpha}} - \frac{1}{i\omega - E_{\mathbf{k}\alpha}} \right), \quad (14)$$

where $E_{\mathbf{k}\alpha} = \sqrt{\xi_{\mathbf{k}\alpha}^2 + \Delta^2}$, $\xi_{\mathbf{k}\alpha} = k^2/2m - \mu + \alpha\lambda k_\perp/m$ is an eigenvalue of $H^0(\mathbf{k})$, and $F_H^\alpha(K)$ represents the pseudogap, or equivalently vertex contribution. Here $\alpha = \pm$ denotes the helicity index and the coherence factors satisfy $u_{\mathbf{k}\alpha}^2 = \frac{1}{2}(1 + \xi_{\mathbf{k}\alpha}/E_{\mathbf{k}\alpha})$, $u_{\mathbf{k}\alpha}^2 + v_{\mathbf{k}\alpha}^2 = 1$.

It follows from the vertex function in Eq. (8) that the explicit form for the f -sum rule [20] consistent density-density correlation function is

$$\begin{aligned} \chi_{\rho\rho}(\omega, \mathbf{q}) &= \frac{1}{2} \sum_{K, \alpha, \alpha'} (1 + \alpha\alpha' \cos(\phi_{\mathbf{k}+\mathbf{q}} - \phi_{\mathbf{k}})) \\ &\times \left[G_H^\alpha(K) G_H^{\alpha'}(\tilde{K}) + F_H^\alpha(K) F_H^{\alpha'}(\tilde{K}) \right]. \end{aligned} \quad (15)$$

The angle $\exp(i\phi_{\mathbf{k}}) = (k_x + ik_y)/k_\perp$, so that $\exp(i\phi_{-\mathbf{k}}) = -\exp(i\phi_{\mathbf{k}})$.

The spin-spin correlation functions are constructed using their form below T_c (deduced using the path integral [21]) appropriately modified in the pseudogap state relative to the condensed phase. These modifications are essential for satisfying sum rules.

As can be shown, in the normal phase the following expression for the spin-spin correlation functions are fully compatible with the spin f -sum rules given in Eq. (12):

$$\begin{aligned} \chi_{S_i S_i}(\omega, \mathbf{q}) &= \frac{1}{2} \sum_{K, \alpha, \alpha'} (1 \pm \alpha\alpha' \cos(\phi_{\mathbf{k}+\mathbf{q}} \pm \phi_{\mathbf{k}})) \\ &\times \left[G_H^\alpha(K) G_H^{\alpha'}(\tilde{K}) + F_H^\alpha(K) F_H^{\alpha'}(\tilde{K}) \right], \end{aligned} \quad (16)$$

where the $+$, $-$ signs are for $\chi_{S_x S_x}, \chi_{S_z S_z}$ respectively.

Numerical Results.— We now look for qualitative new physics in the spin-spin response functions. We numerically calculate the response function $\chi''_{S_x S_x}(\mathbf{q}, \omega)$ at fixed $\mathbf{q} = (0.5, 0, 0)k_F$ as a function of ω [37], and for definiteness consider $T = 0.28T_F > T_c$ and unitary scattering, $1/k_F a = 0$. We plot the results in Fig. 2. In order to illustrate the physics, in Fig. 2(a) and Fig. 2(b), Rashba SOC or pseudogap effects were set to zero respectively, while Fig. 2(c) shows their combined effects. The f -sum rules derived above are important for constraining numerical results of the spin-spin and density-density correlation functions. Comparison between our numerical calculations and the exact f -sum rules agreed to within a few percent.

In Fig. 2(a) we set $\lambda = 0$. In this case, above T_c the spin and density correlations are equal ($\chi''_{S_x S_x} = \chi''_{\rho\rho}$) and this function is plotted in the figure. Two low energy peaks are observable, as found in our earlier work [38]. The lower frequency peak reflects contributions from thermally excited fermions, while the higher frequency peak is associated with the contribution from broken pairs which appears at a threshold associated with the pseudogap.

In Fig. 2(b) we set $\Delta_{\text{pg}} = 0$ and plot $\chi''_{S_x S_x}$ for a pure SOC system with $\lambda = 1.2k_F$. (We do not show $\chi''_{\rho\rho}$ since there is still no qualitative signature of $\lambda \neq 0$.) The response $\chi''_{S_x S_x}$ shows two peaks, but one is at a considerably higher energy compared to Fig. 2(a). The lower frequency peak reflects intra-helicity band contributions while the larger frequency peak is due to inter-helicity effects.

Importantly, this figure shows how the physics of the Rashba ring band-structure can be directly probed by the spin-spin response function. To illustrate this, in the inset we plot the dispersion relation of two helicity bands. The horizontal line denotes the self-consistently determined chemical potential, chosen so that occupied fermions mostly reside in the Rashba ring. The onset of the inter-helicity band transition energy is given by the energy difference between two bands positioned on the inner circle of the ring, while the endpoint frequency for this peak is determined by the outer circle. These energy differences roughly match the width observed in the high frequency peak in the main plot. (The smearing of the width is because we have a non-zero momentum \mathbf{q} and $T \neq 0$.)

Finally, in Fig. 2(c) we plot $\chi''_{S_x S_x}$ for the case where both pseudogap and Rashba SOC are present. Here we observe three distinct peaks. The first is associated with thermally excited fermions within the lowest helicity band, the second with the breaking of the preformed (pg) pairs and the third mainly with the inter-helicity transitions discussed in the previous panel. We also observe some inter-play between pairing and the high frequency SOC peak, as this inter-helicity band peak is pushed toward slightly higher energies.

As far as experimental observability, we note the overall small size of the pg-labelled pseudogap peak in Fig. 2(c). What is most important is not the small size of this specific feature but rather the reduction in the overall low frequency weight (for example, relative to Fig. 2(b)) associated with the presence of a pseudogap. Such a reduction then shows up as an enhancement of the response at higher frequencies.

Conclusion.— A major finding of this paper is that spin-spin correlations provide a clear signature of the simultaneous presence of Rashba modified band-structure and of a pairing gap. Signatures of both are a necessary (but clearly not sufficient) condition for ultimately obtaining a topological superfluid. This should complement observations which are based on the single particle response functions in different experiments either in cold gases [16–18] or in condensed matter. Our spin-spin correlation functions are consistent with f -sum rules, which we derive in this paper. These provide important constraints on the spin response, which is complicated by the fact that spin conservation laws are absent in spin-orbit coupled systems.

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