Nonanalytic Spin Susceptibility of a Fermi Liquid: The Case of Fe-Based Pnictides

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We propose an explanation of the peculiar linear temperature dependence of the uniform spin susceptibility $\chi(T)$ in ferropnictides. We argue that the linear in T term appears to be due to the nonanalytic temperature dependence of $\chi(T)$ in a two-dimensional Fermi liquid. We show that the prefactor of the T term is expressed via the square of the spin-density-wave (SDW) amplitude connecting nested hole and electron pockets. Because of an incipient SDW instability, this amplitude is large, which, along with a small value of the Fermi energy, makes the T dependence of $\chi(T)$ strong. We demonstrate that this mechanism is in quantitative agreement with the experiment.

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Introduction.—The key hypothesis of the Fermi-liquid (FL) theory is that a system of strongly interacting fermions can be considered effectively as a gas of weakly interacting quasiparticles. In the absence of residual interaction between quasiparticles, the static uniform spin susceptibility, $\chi(T)$, and the specific heat coefficient, $\gamma(T)$, are finite at $T = 0$ and obey quadratic dependencies on T at low temperatures. The effect of residual interactions on $\chi(T)$ and $\gamma(T)$ has been studied intensively in recent years [1], with the key result that in two dimensions (2D) both $\gamma(T)$ and $\chi(T)$ are linear rather than quadratic in T [2–4].

Theory predicts that the behavior of $\gamma(T)$ is universal in a sense that the (negative) slope is given by the square of the backscattering amplitude [5]. This linear decrease has been observed in monolayers of ^{3}He [6]. On the contrary, a linear in T term in the spin susceptibility is not universal and can be of either sign [3,7], causing uncertainty in the interpretation of the experiments on semiconductor heterostructures [8].

Recently, a pronounced linear temperature dependence of the uniform susceptibility has been observed in high-T_c superconductors with iron-based layered structure [9–12]. It extends from temperatures above either the spin-density-wave (SDW) or superconducting transitions up to 500–700 K with an almost doping-independent slope. The T dependence is quite strong: $\chi(T)$ increases roughly by a factor of 2 between 200 K and 700 K. An explanation of this behavior based on the J_1-J_2 model of localized spins has been proposed in Ref. [13]; however, given that the linear T dependence persists up to large dopings, where local probes, such as nuclear magnetic resonance (NMR) and μSR, do not see localized moments [14,15], this explanation is questionable.

The itinerant character of Fe pnictides is suggested by the agreement between the band structure obtained in *ab initio* calculations [16] and observed in de Haas-van Alphen and angle-resolved photoemission spectroscopy (ARPES) experiments [17–21]. It is firmly established by now that the Fermi surface (FS) of Fe pnictides consists of two small hole pockets near (0, 0) and two electron pockets near (π, π) points of the folded Brillouin zone. In such a system, an obvious origin of the SDW order is a logarithmic divergence of a particle-hole vertex involving states on nested parts of the FS [16,22–26].

In this Letter, we propose an explanation of the experimental T dependence of spin susceptibility based on the itinerant picture. We argue that the origin of the linear increase of $\chi(T)$ with temperature in ferropnictides is the same as in a 2D FL. Furthermore, we show that this behavior is universal for FLs with strong (π, π) SDW fluctuations, namely, the slope of the linear in T dependence is determined by the square of the SDW amplitude with nesting momentum $\mathbf{Q} = (\pi, \pi)$. This amplitude is large which, along with a small value of the Fermi energy ε_F, amplifies the T dependence of $\chi(T)$. Choosing the SDW coupling to reproduce the observed SDW transition temperature T_N at zero doping, we find a good agreement between calculated and measured slopes of $\chi(T)$. The doping dependence of the slope also agrees with the data. We view this agreement as a strong indication that the linear temperature dependence of $\chi(T)$ in pnictides [9–12] is in fact the first unambiguous observation of a nonanalytic behavior of the 2D spin susceptibility. Besides being fundamentally important on its own right, this observation also strengthens the case for the itinerant scenario for Fe pnictides.

Theory.—We consider a two-band model of interacting fermions occupying the electron and hole FSs:

$$H = \sum_{\mathbf{k},\sigma} [\varepsilon^c_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \varepsilon^f_{\mathbf{k}} f^\dagger_{\mathbf{k}\sigma} f_{\mathbf{k}\sigma}] + \sum_{\mathbf{p}_i,\sigma,\sigma'} H_{\text{int}},$$

$$\begin{aligned} H_{\text{int}} = {} & u_1 c^\dagger_{\mathbf{p}_3\sigma} f^\dagger_{\mathbf{p}_4\sigma'} f_{\mathbf{p}_2\sigma'} c_{\mathbf{p}_1\sigma} + u_2 f^\dagger_{\mathbf{p}_3\sigma} c^\dagger_{\mathbf{p}_4\sigma'} f_{\mathbf{p}_2\sigma'} c_{\mathbf{p}_1\sigma} \\ & + \frac{u_3}{2}[f^\dagger_{\mathbf{p}_3\sigma} f^\dagger_{\mathbf{p}_4\sigma'} c_{\mathbf{p}_2\sigma'} c_{\mathbf{p}_1\sigma} + \text{H.c}] \\ & + \frac{u_4}{2} f^\dagger_{\mathbf{p}_3\sigma} f^\dagger_{\mathbf{p}_4\sigma'} f_{\mathbf{p}_2\sigma'} f_{\mathbf{p}_1\sigma} + \frac{u_5}{2} c^\dagger_{\mathbf{p}_3\sigma} c^\dagger_{\mathbf{p}_4\sigma'} c_{\mathbf{p}_2\sigma'} c_{\mathbf{p}_1\sigma}. \end{aligned} \qquad (1)$$

Here, $c_{\mathbf{k}\sigma}$ ($f_{\mathbf{k}\sigma}$) is the annihilation operator for a hole (electron) with momentum $\mathbf{k}$ and spin σ [for an electron, $\mathbf{k}$ is measured from the (π, π) point], $\varepsilon^c_{\mathbf{k}}$ and $\varepsilon^f_{\mathbf{k}} = -\varepsilon^c_{\mathbf{k}} + 2\mu$ represent single-particle dispersions, and μ measures a deviation from perfect nesting. Models of this type were considered in the past in the context of an "excitonic insulator" [27].

We assume that each of the electron and hole FSs is doubly degenerate. The terms with u_4 and u_5 are intraband interactions, the terms with u_1 and u_2 are interband interactions with momentum transfer 0 and $\mathbf{Q}$, respectively, and the term with u_3 is the interband pair hopping. All couplings flow from their initial values at energies of order of the bandwidth to renormalized values at ε_F [24,25]. We assume that this renormalization is already included into Eq. (1) and analyze the behavior of the system at energies below ε_F.

We first obtain the linear-in-T contribution to the spin susceptibility, $\delta\chi(T)$, to the second order in the interaction and then show that the prefactor of the T term in $\delta\chi(T)$ is expressed via the SDW vertex to all orders in the interaction.

Figure 1 depicts all topologically inequivalent second-order diagrams for the thermodynamic potential, $\Phi(T, H)$, describing both intra- and inter-band processes. Each of the diagrams contains the object

$$\varphi(T, H) = T^3 \sum_{\Omega} \int \frac{d^2\mathbf{q}}{(2\pi)^2} \sum_{\sigma,\sigma'} \sum_{\omega,\omega'} \int \frac{d^2\mathbf{k}\, d^2\mathbf{p}}{(2\pi)^4} \times G^\sigma_{\mathbf{k},\omega} G^\sigma_{\mathbf{p},\omega'} G^{\sigma'}_{\mathbf{p}+\mathbf{q},\omega'+\Omega} G^{\sigma'}_{\mathbf{k}+\mathbf{q},\omega+\Omega}, \qquad (2)$$

where $G^\sigma_{\mathbf{k},\omega}$ is a Matsubara Green's function of either c or f fermion with momentum $\mathbf{k}$ and spin σ in a magnetic field H. As in an ordinary FL, the nonanalytic H^2T term in $\varphi(T, H)$ comes from a dynamic Kohn anomaly, i.e., from diagrams with momentum $2k_F$ carried by the interaction lines [3,4]. It is, however, more convenient to re-express the result via the polarization bubbles with small rather than $2k_F$ momenta. The Green functions in Eq. (2) can be combined in two different ways: either as $\Pi^{\sigma\sigma}_{\mathbf{q},\Omega}\Pi^{\sigma'\sigma'}_{\mathbf{q},\Omega}$, or as $\Pi^{\sigma\sigma'}_{\mathbf{q},\Omega}\Pi^{\sigma\sigma'}_{\mathbf{q},\Omega}$, where $\Pi^{\sigma\sigma'}_{\mathbf{q},\Omega} = T\sum_\omega \int \frac{d^2\mathbf{k}}{(2\pi)^2} G^\sigma_{\mathbf{k},\omega} G^{\sigma'}_{\mathbf{k}+\mathbf{q},\omega+\Omega}$ is a polarization bubble of the cc, ff, or cf type with small momenta $q \ll k_F$. A bubble depends on the magnetic field if the Zeeman energies of two fermions add up. One can readily show that the cc and ff bubbles depend on the field via $\Pi^{\uparrow\downarrow}_{\mathbf{q},\Omega}$, while the field enters the cf bubble through $\Pi^{\uparrow\uparrow}_{\mathbf{q},\Omega}$ and $\Pi^{\downarrow\downarrow}_{\mathbf{q},\Omega}$ terms. Evaluating individual diagrams, we find that each of them can be expressed as a product of two dynamic spin up/down bubbles:

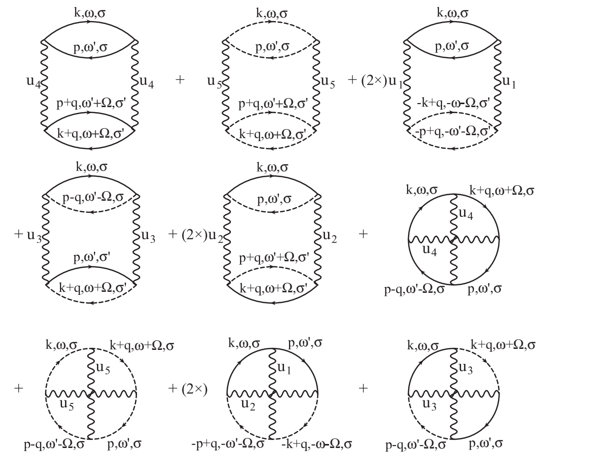

FIG. 1. Second-order diagrams for the thermodynamic potential. Solid and dashed lines correspond to f fermions (electrons) and to c fermions (holes), respectively.

$$\Pi_{\mathbf{q},\Omega} = \frac{m}{2\pi} \frac{|\Omega|}{\sqrt{(\Omega - 2i\mu_B H - 2i\mu^*)^2 + (v_F q)^2}}, \qquad (3)$$

where $\mu^* = 0$ for intraband scattering and $\mu^* = \mu$ for interband scattering. The rest of the calculations proceed in the same way as for an ordinary FL [3,4]. In short, one integrates $\Pi^2_{\mathbf{q},\Omega}$ over $\mathbf{q}$ first, replaces the Matsubara sum by a contour integral, differentiates the result twice with respect to H, sets $H = 0$, and obtains the $O(T)$ terms in χ. The first two diagrams in Fig. 1 describe intraband processes and give the same results for $\chi(T)$ as in Refs. [3,4]: $\delta\chi_{1,2}(T) = \lambda u^2_{4,5} T$, where $\lambda = 4\chi_0 N^2_F/(2\varepsilon_F)$, $\varepsilon_F = v_F k_F/2$, $\chi_0 = 2\mu^2_B N_F$ is the Pauli susceptibility per one sheet of the FS, and $N_F = m/2\pi$ is the density of states. A factor of 4 in λ results from the double degeneracy of electron and hole bands. The third through fifth diagrams involve interband scattering and yield $\delta\chi_3(T) = 2\lambda u^2_1 T\eta(\mu/T)$, $\delta\chi_4(T) = \lambda u^2_3 T\eta(\mu/T)$, and $\delta\chi_5(T) = 2\lambda u^2_2 T\eta(\mu/T)$, respectively. Here, $\eta(x) = 2x\coth x - x^2/\sinh^2 x - 2x$. The third and forth diagrams give finite contributions if $\sigma = \sigma'$, while the fifth diagram contributes if $\sigma = -\sigma'$. The sixth and seventh diagrams do not contribute to $\delta\chi(T)$, and the remaining two give $\delta\chi_8(T) = -2\lambda u_1 u_2 T\eta(\mu/T)$ and $\delta\chi_9(T) = -\lambda u^2_3 T\eta(\mu/T)$.

Combining all diagrams, we obtain

$$\delta\chi(T) = \lambda T[u^2_4 + u^2_5 + 2(u^2_1 + u^2_2 - u_1 u_2)\eta(\mu/T)]. \qquad (4)$$

The first two terms are the contributions from intraband processes—they are the same as in an ordinary FL. The rest of the terms correspond to interband processes, specific to the electronic structure of ferropnictides. For $T \gg \mu$ (perfect nesting), $\eta(\mu/T) \approx 1$ and both intra- and inter-band processes contribute to the linear term in the spin susceptibility. In the opposite limit of $T \ll \mu$ (poor nesting), $\eta(\mu/T) \sim \exp(-2\mu/T)$ and the interband contribution to $\chi(T)$ is suppressed exponentially. In the intermediate regime $T \sim \mu$, $\eta(\mu/T)$ is nonmonotonic. Note that the pair-hopping term u_3, which gives rise to an attraction in the extended s-wave pairing channel, does not contribute to the T term in $\chi(T)$.

The coupling constants in Eq. (4) are interactions at the scale of the Fermi energy. These couplings are already renormalized from their bare values at the scale of the bandwidth [24] by the parquet renormalization group, in such a way that u_4, u_5, and u_1 flow to the same value, while u_2 flows to a smaller value. The renormalized couplings at the scale of ε_F depend only weakly on the incoming and transferred momenta. Further renormalization *below* ε_F differentiates between u_i with different transferred and incoming momentum. Such renormalization is particularly relevant for our system as the coupling u_1, which corresponds to the scattering process, $u_1(\mathbf{k}, \mathbf{p}+\mathbf{q}; \mathbf{p}, \mathbf{k}+\mathbf{q}) c^\dagger_{\mathbf{p}} f^\dagger_{\mathbf{k}+\mathbf{q}} f_{\mathbf{p}+\mathbf{q}} c_{\mathbf{k}}$, diverges at the onset of the SDW instability for $\mathbf{q} = \mathbf{0}$ (we recall that momenta for f fermions are measured from $\mathbf{Q}$, so that the momentum transfer between c and f fermions is actually $\mathbf{q} = \mathbf{Q}$). The singular vertex is $u_1(\mathbf{k}, \mathbf{p}; \mathbf{p}, \mathbf{k})$, which means that electrons and holes swap their respective momenta. Note that the divergence occurs for any angle between $\mathbf{k}$ and $\mathbf{p}$. At weak coupling, the enhancement of u_1 is confined to $q \ll k_F$, while for a generic $q \sim k_F$ the coupling u_1 retains its bare value.

We now show that the u_1^2 term in $\chi(T) \propto T$ is the same coupling that diverges at the SDW instability. To see this, we first note that the fermionic momenta in diagrams for $\Phi(T, H)$ are constrained by two requirements: (i) the momentum transfers are near $2k_F$ and (ii) all four momenta are near the FS. For the third diagram in Fig. 1, this implies that $\mathbf{p} \approx -\mathbf{k}$, $|\mathbf{k}| \approx k_F$, while q is small ($\sim T/v_F$). Therefore, the vertex in this diagram is $u_1(\mathbf{k}, -\mathbf{k}; -\mathbf{k}, \mathbf{k})$. This is an analog of the backscattering amplitude in a 2D FL. The vertex $u_1(\mathbf{k}, -\mathbf{k}; -\mathbf{k}, \mathbf{k})$ is a special case of the SDW vertex $u_1(\mathbf{k}, \mathbf{p}; \mathbf{p}, \mathbf{k})$ for $\mathbf{p} = -\mathbf{k}$.

Next, we consider higher-order diagrams. They can be separated into two classes. In diagrams of the first class, one obtains the nonanalyticity by keeping only two dynamic bubbles $\Pi_{\mathbf{q},\Omega}$ and lumping the rest of the diagram into renormalization of the static scattering amplitude. In particular, the backscattering amplitude $u_1(\mathbf{k}, -\mathbf{k}; -\mathbf{k}, \mathbf{k})$ is renormalized into an effective coupling $u_1^{\rm eff}$, which diverges at the SDW instability. Singular renormalizations of u_1 form a ladder series which is summed into

$$u_1^{\rm eff} = \frac{u_1}{1 - u_1 N_F \ln\frac{\varepsilon_F}{\max(T,\mu)}}. \qquad (5)$$

The second class of higher-order diagrams contain three and more dynamic bubbles. Terms of order of u_1^3 etc. are *not* expressed in terms of backscattering amplitude but rather contain u_1 with typical q of order k_F. In this range of momenta, u_1 is not enhanced by SDW fluctuations and remains small at weak coupling.

In addition, the diagrams of both classes also contain analytic, $(T/\varepsilon_F)^2$ terms. Such terms have been analyzed numerically in the study of a linear in T behavior of the Fermi velocity in a 2D FL [28] and found to be small even when $T \sim \varepsilon_F$. We assume that the same happens here and neglect regular terms below.

Neglecting u_2 and setting $u_1 = u_4 = u_5 \equiv u > 0$, we finally obtain

$$\delta\chi(T) \approx \frac{8(uN_F)^2\chi_0}{v_F k_F} T\left[1 + \frac{\eta(\mu/T)}{(1 - uN_F \ln\frac{\varepsilon_F}{\max(T,\mu)})^2}\right]. \qquad (6)$$

This full result for $\delta\chi(T)$ was obtained from the second-order expression by replacing $u_1 = u$ by the exact SDW amplitude $u_1^{\rm eff}$, given by Eq. (5). This is similar to the result for the specific heat [5], but differs from the result for $\delta\chi(T)$ in an ordinary 2D FL, where the full $\delta\chi(T)$ is not expressed via the backscattering amplitude [3,7]. This difference can be traced down to the symmetry between the particle-particle (Cooper) channel in an ordinary FL and the particle-hole channel in a nested FL. Indeed, the backscattering contribution to both $\gamma(T)$ and $\delta\chi(T)$ for the ordinary case undergoes logarithmic renormalization in the Cooper channel. However, the Cooper ladder for the ordinary case is identical to the particle-hole ladder for the nested case, except for that the sign of the interaction is reversed, i.e., the SDW instability for $u > 0$ for the nested case is related to the Cooper instability for $u < 0$ for the ordinary case. In both cases, there are also nonbackscattering contributions to $\delta\chi(T)$. For the ordinary case, the

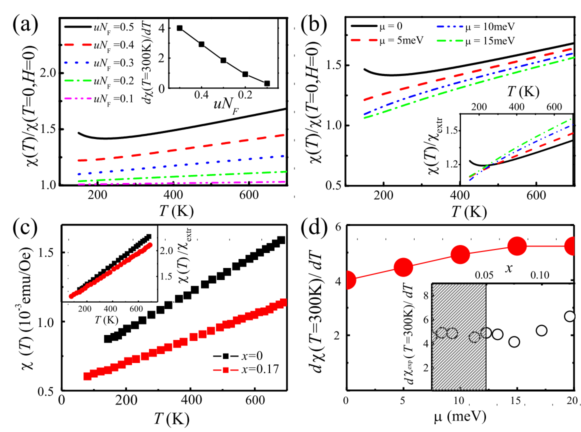

FIG. 2 (color online). (a) T dependence of the spin susceptibility $\chi(T)$, as given by Eq. (6), for perfect nesting ($\mu = 0$) and for a range of couplings uN_F, as indicated in the plot. In a calculation, $\max(T, \mu)$ in Eq. (6) is approximated by $\sqrt{T^2 + \mu^2}$. Inset: Calculated slope $d\chi(T)/dT$ as a function of uN_F at $T = 300$ K (chosen to match Ref. [11]). (b) Calculated $\chi(T)$ for $uN_F = 0.5$ for a range of μ, as shown in the plot. Inset: Same curves as in (a) normalized by $\chi_{\rm extr}$, obtained by extrapolating $\chi(T)$ down to $T = 0$. (c) $\chi(T)$ in $BaFe_{2-x}Co_xAs_2$ from Ref. [12]. Inset: Same data as in the main panel normalized by $\chi(0)$. (d) Calculated slope $d\chi(T = 300\ {\rm K})/dT$ as a function of μ. Inset: Measured slope as a function of doping (from Ref. [11]).

backscattering term is reduced by Cooper renormalization, and nonbackscattering contributions play the dominant role. For the nested case, SDW renormalization enhances the backscattering term, and other contributions can be ignored. On the other hand, the Cooper channel composed of electrons and holes for the nested case is equivalent to the particle-hole channel for an ordinary case and, therefore, is not logarithmically divergent.

Comparison with experiments.—We now apply Eq. (6) to ferropnictides. The experimental results for $\chi(T)$ in $BaFe_{2-x}Co_xAs_2$ [12] are shown in panel (c) of Fig. 2. From the data, we estimate the slope of the T dependence as $[\chi(700\ \mathrm{K})/\chi(0)]_{\mathrm{expt}} \approx 2$, where $\chi(0)$ is obtained by extrapolating $\chi(T)$ to $T = 0$ (theoretically, $\chi(0) \approx 4\chi_0$). Taking $v_F = 0.45\ \mathrm{eV}\cdot\mathrm{\AA}$ and $k_F \approx 0.16\ \mathrm{\AA}^{-1}$ from the ARPES data [21], we obtain $\varepsilon_F \sim 0.04$ eV [29]. The only unknown parameter of the theory—the dimensionless coupling constant uN_F—is fixed by requiring that the SDW vertex u_1^{eff} increases upon approaching T_N ($T_N =$ 140 K at zero doping). As Eq. (5) is an approximate one-loop formula, we set a criterion that u_{eff} increases by a factor of 2 at T_N. This yields $uN_F \approx 0.5$. We then find $[\chi(T = 700\ \mathrm{K})/\chi(0)]_{\mathrm{theor}} \approx 1.7$, which is quite close to the experimental value $[\chi(700\ \mathrm{K})/\chi(0)]_{\mathrm{expt}} \approx 2$. A more detailed comparison between the experiments and Eq. (6) is presented in Fig. 2, where we also show the dependencies of the slope on uN_F and μ. We find quite a good agreement with the experimental data.

We also make a simple prediction for future experiments. Within our theory, the slope of the linear in T term should increase in a magnetic field, as $\chi(T, H) = \chi(T, 0)[1 + (\mu_B H/T)^2]$ for $\mu_B H \ll T$ [4]. Near optimal doping, the linear in T dependence of $\chi(T)$ continues down to $T \sim T_c$, and experiments in fields of about 10 T should be able to observe this behavior.

Conclusion.—To summarize, we analyzed a nonanalytic, linear in T term in the spin susceptibility of a 2D Fermi-liquid with nearly nested electron and hole pockets of the Fermi surface. We found that the prefactor of the T term contains the same interband coupling u_1^{eff}, which is enhanced by SDW fluctuations. These results describe quantitatively a strong temperature dependence of the spin susceptibility in ferropnictides, observed in a number of recent experiments. An immediate consequence of the proposed mechanism is that χ should exhibit equally strong linear dependencies on the magnetic field and on the wave number [3]. We suggest to perform these measurements as a crucial test for the origin of the observed effect.

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[29] We assume that ε_F in pnictides is much smaller than $T^* \equiv \sqrt{N_F/N_F''}$, the energy scale separating the regimes of Fermi and Boltzmann statistics at which higher than linear terms in $\delta\chi(T)$ become important.