Extended $s_{\pm}$ scenario for the nuclear spin-lattice relaxation rate in superconducting pnictides

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Recently, several measurements of the nuclear spin-lattice relaxation rate T_1^{-1} in the superconducting Fe pnictides have been reported. These measurements generally show no coherence peak below T_c and indicate a low-temperature power-law behavior, the characteristics commonly taken as evidence of unconventional superconductivity with lines of nodes crossing the Fermi surface. In this work we show that (i) the lack of a coherence peak is fully consistent with the previously proposed nodeless extended $s_{\pm}$-wave symmetry of the order parameter (whether in the clean or dirty limit) and (ii) the low-temperature power-law behavior can be also explained in the framework of the same model but requires going beyond the Born limit.

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The recently synthesized[1] high-T_c superconducting ferropnictides may be the most enigmatic superconductors discovered so far. One of the biggest mysteries associated with these materials is that now, with improved sample quality and single-crystal availability, some experiments unambiguously see a fully gapped superconducting state[2–10] and an s-wave pairing[11] while others unequivocally point toward line nodes in the gap.[12–15] Particularly disturbing is that on both sides data of high quality were reported by highly reputable groups so experimental errors seem unlikely. It is possible that full reconciliation will require a highly advanced theory that will treat both superconducting and spin-density wave order parameters on equal footing, and include the interaction between the two. Nevertheless, it is interesting and important to investigate more conventional options first.

Evidence for fully gapped superconductivity comes from three different sources: Andreev reflection,[2–4] exponential temperature dependence of the penetration depths,[8–10] and angle-resolved photoemission spectroscopy (ARPES).[5–7] That three so different probes yield qualitatively the same result is very convincing. Yet the nuclear-magnetic-resonance (NMR) spin-lattice relaxation rate, $1/T_1$, does not show two classical fingerprints of conventional fully gapped superconductors: the Hebel-Slichter coherence peak and the exponential decay at low temperature, but rather a powerlike law,[12–15] usually referred to as T^3 but in reality somewhere between T^3 and $T^{2.5}$. Such behavior is usually taken to be evidence for a d wave or similar superconducting state with lines of nodes. However, it was pointed out[16] that, in dirty d-wave samples at low temperatures, the behavior changes from T^3 to T (as node lines are washed out into node spots by impurities) and this was not observed in ferropnictides.

So far the evidence in favor of nodeless superconductivity seems stronger. Therefore, it is interesting to check whether it may be possible to explain the results of the NMR experiments without involving an order parameter with node lines.

In this paper we calculate $1/T_1T$ for a model superconductor consisting of two relatively small semimetallic Fermi surfaces, separated by a finite wave vector $\mathbf{Q}$ (Fig. 1). This is an approximation to the Fermi surface of ferropnictides. We intentionally drop quantitative details that may differ from compound to compound, and consider the simplest possible case with the same densities of states on each surface.[17] We further assume that each surface features the same gap[17] but the relative phase between the two order parameters is π. This is the so-called $s_{\pm}$ model, proposed in Ref. 18 and discussed in Refs. 19–21, and a number of more recent publications by various groups. In the spirit of this model and of model calculations,[19–21] we will assume that the total (renormalized) spin susceptibility is strongly peaked at and around $\mathbf{Q}$.

We will show here that in this model the Hebel-Slichter peak is strongly suppressed already in the clean limit and can be entirely eliminated even by a very weak impurity scattering. On the contrary, the low-temperature behavior remains exponential even in the strong-coupling limit. Introducing impurities does create strong deviations from the exponential behavior. But in the Born approximation the effect is stronger just below superconducting temperature T_c and weaker at $T \to 0$ so that the observed power-law behavior (down to at least $0.1T_c$) is very difficult to reproduce. This behavior, however, can be reproduced if one goes beyond the Born limit of impurity scattering.

The NMR relaxation rate, assuming a Fermi contact hyperfine interaction,[22] is given by the standard formula: $(1/T_1T) \propto \lim_{\omega\to 0} \Sigma_{\mathbf{q}} \mathrm{Im}\chi_{\pm}(\mathbf{q},\omega)/\omega$, where $\chi_{\pm}(\mathbf{q},\omega)$ is the analytic continuation of the Fourier transform of the correlation function $\chi_{\pm}(\mathbf{r},\tau) = -\langle\langle T_\tau S_+(\mathbf{r},-\mathrm{i}\tau) S_-(\mathbf{0},0)\rangle\rangle_{\mathrm{imp}}$, averaged (if needed) over the impurity ensemble. Here, $S_{\pm}(\mathbf{r},-\mathrm{i}\tau) = \exp(H\tau) S_{\pm}(\mathbf{r}) \exp(-H\tau)$, where H is the electronic Hamiltonian, τ denotes imaginary time, and $S_{\pm}$ is expressed via the electron operators as $S_+(\mathbf{r}) = \psi_\uparrow^\dagger(\mathbf{r})\psi_\downarrow(\mathbf{r})$ and $S_-(\mathbf{r}) = \psi_\downarrow^\dagger(\mathbf{r})\psi_\uparrow(\mathbf{r})$. Adopting the above-described model, we can keep only the interband contribution to χ, in which case this formula simplifies to

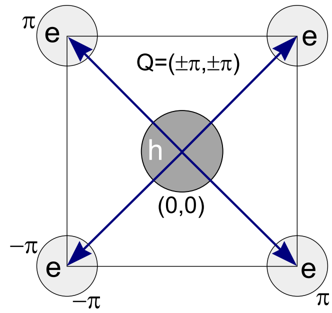

FIG. 1. (Color online) A depiction of the Fermi-surface geometry for the Fe-based oxypnictides. Hole and electron Fermi-surface pockets are indicated, and an antiferromagnetic wave vector **Q** is also shown.

$$1/T_1T \propto \lim_{\omega\to 0} \mathrm{Im}\ \chi_{12}(\omega)/\omega, \tag{1}$$

where $\chi_{12}(\omega)$ is obtained by integrating over all **q**'s connecting the two Fermi surfaces (obviously, only $\mathbf{q}\sim\mathbf{Q}$ contribute). In the case of a weakly coupled clean superconductor below T_c, we have

$$\frac{1}{T_1T} \propto \sum_{\mathbf{kk}'}\left(1+\frac{\Delta_1\Delta_2}{E_{\mathbf{k}}E_{\mathbf{k}'}}\right)\left[-\frac{\partial f(E_{\mathbf{k}})}{\partial E_{\mathbf{k}}}\right]\delta(E_{\mathbf{k}}-E_{\mathbf{k}'}), \tag{2}$$

where **k** and **k**′ lie on the hole and the electron Fermi surfaces, respectively, $E_{\mathbf{k}}$ is the quasiparticle energy in the superconducting state, Δ_1 and Δ_2 are the superconducting gaps on hole and electron Fermi surfaces, and $f(E)$ is the Fermi distribution function. This is a straightforward generalization of the textbook expression.[23] Following the usual BCS prescription, $\Sigma_k \to \int_\Delta^\infty EdE/\sqrt{E^2-\Delta^2}$, the **k**-space sum can be converted to an energy integral, and for a conventional s-wave superconductor with $\Delta_1=\Delta_2=\Delta$, one finds

$$\frac{1}{T_1} \propto \int_{\Delta(T)}^{\infty} dE\frac{E^2+\Delta^2}{E^2-\Delta^2}\mathrm{sech}^2\left(\frac{E}{2T}\right). \tag{3}$$

The denominator gives rise to a peak just below T_c, the famous Hebel-Slichter peak. As pointed out in Ref. 18, it is suppressed for the $s_\pm$ state. Indeed, if $\Delta_1=-\Delta_2=\Delta$,

$$\frac{1}{T_1} \propto \int_{\Delta(T)}^{\infty} dE\frac{E^2-\Delta^2}{E^2-\Delta^2}\mathrm{sech}^2\left(\frac{E}{2T}\right) = \int_{\Delta(T)}^{\infty} dE\ \mathrm{sech}^2\left(\frac{E}{2T}\right).$$

As T decreases from T_c, the integral decreases monotonically.

In a more general case, when $\Delta_1\Delta_2<0$ and $|\Delta_1|\neq|\Delta_2|$,

$$\frac{1}{T_1T} \propto \int_{\max\{|\Delta_1|,|\Delta_2|\}}^{\infty} d\varepsilon\left(-\frac{\partial f(\varepsilon)}{\partial\varepsilon}\right)\frac{\varepsilon^2-|\Delta_1\Delta_2|}{\sqrt{\varepsilon^2-\Delta_1^2}\sqrt{\varepsilon^2-\Delta_2^2}}. \tag{4}$$

Following Fibich,[24,25] we assume $[-\partial f(\varepsilon)/\partial\varepsilon]$ to be a slow varying function and obtain (for $\Delta_1>|\Delta_2|$)

$$1/T_1T \propto f(\Delta_1) + 2I(\Delta_1,\Delta_2)f(\Delta_1)[1-f(\Delta_1)]/T,$$

$$I(\Delta_1,\Delta_2) = \mathbf{K}(\Delta_1/\Delta_2)(\Delta_1+\Delta_2) - \mathbf{E}(\Delta_1/\Delta_2)\Delta_1,$$

where $\mathbf{K}(x)$ and $\mathbf{E}(x)$ are the complete elliptic integrals of the first and second kind, respectively. When $\Delta_1=\Delta_2$, I is reduced to the standard BCS formula, and when $\Delta_1=-\Delta_2$, it vanishes identically.

Let us now include impurity scattering and move to the strong-coupling limit. Following Samokhin and Mitrović,[26,27] we can write down the following formula:

$$\frac{1}{T_1T} \propto \int_0^\infty d\omega\left(-\frac{\partial f(\omega)}{\partial\omega}\right)\{[\mathrm{Re}g_1^Z(\omega)+\mathrm{Re}g_2^Z(\omega)]^2 + [\mathrm{Re}g_1^\Delta(\omega)+\mathrm{Re}g_2^\Delta(\omega)]^2\}.$$

For our model $g_i^Z(\omega)=n_i(\omega)Z_i(\omega)\omega/D_i(\omega)$ and $g_i^\Delta(\omega)=n_i(\omega)\phi_i(\omega)/D_i(\omega)$, where $D_i(\omega)=\sqrt{[Z_i(\omega)\omega]^2-\phi_i^2(\omega)}$, $Z_i(\omega)$ is the mass renormalization, $\phi_i(\omega)=Z_i(\omega)\Delta_i(\omega)$, and $n_i(\omega)$ is a partial density of states.

The renormalization function $Z_i(\omega)$ and complex order parameter $\phi_i(\omega)$ have to be obtained by a numerical solution of the Eliashberg equations. On the real frequency axis they have the form (we neglect all instant contributions and consider a uniform impurity scattering with the impurity potential $v_{ij}=v$)

$$\phi_i(\omega) = \sum_j\int_{-\infty}^{\infty} dzK_{ij}^\Delta(z,\omega)\mathrm{Re}\ g_j^\Delta(z) + \mathrm{i}\gamma\frac{g_1^\Delta(\omega)-g_2^\Delta(\omega)}{2\mathcal{D}},$$

$$[Z_i(\omega)-1]\omega = \sum_j\int_{-\infty}^{\infty} dzK_{ij}^Z(z,\omega)\mathrm{Re}\ g_j^Z(z) + \mathrm{i}\gamma\frac{g_1^Z(\omega)+g_2^Z(\omega)}{2\mathcal{D}},$$

where $\mathcal{D}=1-\sigma+\sigma\{[g_1^Z(\omega)+g_2^Z(\omega)]^2-[g_1^\Delta(\omega)-g_2^\Delta(\omega)]^2\}$, $\gamma=2c\sigma/\pi N(0)$ is the normal-state scattering rate, $N(0)$ is the density of states at the Fermi level, c is the impurity concentration, and $\sigma=\frac{[\pi N(0)v]^2}{1+[\pi N(0)v]^2}$ is the impurity strength ($\sigma\to 0$ corresponds to the Born limit while $\sigma=1$ to the unitary one). Kernels $K_{ij}(z,\omega)$ are

$$K_{ij}^{\Delta,Z}(z,\omega) = \int_0^\infty d\Omega\frac{\tilde{B}_{ij}(\Omega)}{2}\left[\frac{\tanh\frac{z}{2T}+\coth\frac{\Omega}{2T}}{z+\Omega-\omega-\mathrm{i}\delta} - \{\Omega\to-\Omega\}\right],$$

where $\tilde{B}_{ij}(\Omega)$ is equal to $B_{ij}(\Omega)$ in the equation for Δ and to $|B_{ij}(\Omega)|$ in the equation for Z. Note that all retarded interactions enter the equations for the renormalization factor Z with a positive sign.

It is well known that pair-breaking impurity scattering dramatically increases the subgap density of states just below T_c, and even weak magnetic scattering can eliminate the Hebel-Slichter peak in conventional superconductors. In our model, the same effect is present due to the nonmagnetic interband scattering (the magnetic scattering, on the contrary, is not pair breaking in the Born limit).[28] Since the Hebel-Slichter peak is not present in this scenario even in a clean sample, the pair-breaking effect is more subtle: it changes exponential behavior below T_c to a more power-law-like one (the actual power and extent of the temperature range with a power-law behavior depend on the scattering strength). Note that in the Born approximation the exponential behavior is always restored at low enough temperature unless the impurity concentration is so strong that T_c is suppressed by at least a factor of two.[28]

Another well-known pair-breaking effect is scattering by thermally excited phonons (or other bosons). This is, of course, a strong-coupling effect. For instance, strong coupling can nearly entirely eliminate the Hebel-Slichter peak in a conventional superconductor.[29,30] However, this effect is even more attached to a temperature range just below T_c since at low temperature boson excitations are exponentially suppressed.

Currently, most experimental data for ferropnictides go down in temperature to $\sim 0.2-0.3T_c$ but some results are available at temperatures as low as $0.1T_c$. So far exponential behavior has not been observed, which casts doubt that Born impurity scattering may be responsible for such behavior.

Unitary scattering, on the other hand, has rather different low-temperature behavior. As discussed, for instance, by Preosti and Muzikar,[31] unitary scattering in the case of the $s_\pm$ superconducting gap (our choice of $|\Delta_1|=|\Delta_2|$ corresponds to their parameter r set to zero), the subgap density of states is controlled by the unitarity parameter σ while the suppression of T_c is controlled by a *different* parameter: namely, by the net scattering rate γ. The unitary limit corresponds to $\sigma \to 1$ but γ may be rather small at low concentrations. The physical meaning is that here the diluted unitary limit corresponds to the so-called "Swiss cheese" model: each impurity creates a bound state that contributes to the subgap density of states but hardly to the T_c suppression. Indeed, Preosti and Muzikar have shown (see Fig. 1 in Ref. 31) that in this limit nonzero density of states at the Fermi level appears already at zero temperature at arbitrary low impurity concentration. That is to say, the bound state has zero energy. This is a qualitatively different effect compared to the Born limit: In a dilute unitary regime ($\gamma \ll \Delta$), the NMR relaxation at $T\approx 0$ is mainly due to the bound states at $E=0$; upon heating $1/T_1T$ initially remains constant or may even slightly decrease because of depopulating of the bound state. When the temperature increases further, at some crossover temperature the relaxation becomes dominated by thermal excitations across the gap and $1/T_1T$ starts growing exponentially. When the gap is suppressed by the temperature as to become comparable with γ, yet another effect kicks in: broadening of the coherence peak near T_c (less important for our $s_\pm$ state). Thus, unitary scattering makes the $1/T_1T$ temperature dependence rather complex although the strongly unitary regime with low impurity concentration is rather far from a power-law behavior (even though being strongly nonexponential, see Fig. 3).

These qualitative arguments suggest that neither purely Born nor purely unitary limits are well suited for explaining the observed $1/T_1$ behavior: the former leads to an exponential behavior at low temperatures while the latter to Korringa behavior. On the other hand, an *intermediate* regime seems to be rather promising in this aspect. Indeed, the energy of the above-mentioned bound state is related to σ as $E_b = |\Delta|\sqrt{1-\sigma}$. Thus, by shifting σ toward an intermediate scattering $\sigma \sim 0.5$ (which is probably more realistic than either

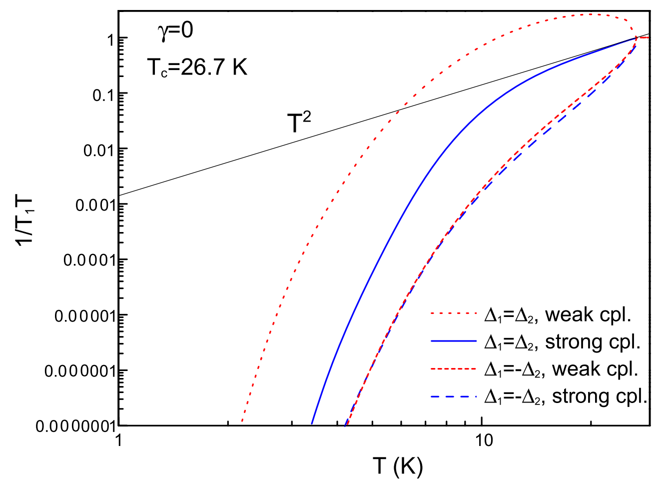

FIG. 2. (Color online) Temperature dependence of the spin-lattice relaxation rate $1/T_1T$ calculated in the clean limit ($\gamma=0$) for a conventional s-wave superconductor ($\Delta_1=\Delta_2$) and for a $s_\pm$ superconductor ($\Delta_1=-\Delta_2$). Results of both weak- and strong-coupling approximations are shown.

limit anyway) and increasing γ, we create a broad and monotonously increasing density of states much closer to what would be expected from the NMR data. It is worth noting that a *distribution* of σ's (presence of different impurities with different scattering strength), which we do not consider here, will also lead to broadening of the bound state and work as an effectively enhanced γ (therefore it is reasonable to try relatively large γ's, keeping in mind that this part is simulating).

We now illustrate the above discussion using specific numerical models. First, we present numerical solutions of the Eliashberg equations using a spin-fluctuation model for the spectral function of the intermediate boson: $B_{ij}(\omega) = \lambda_{ij}\pi\Omega_{sf}/(\Omega_{sf}^2+\omega^2)$, with the parameters $\Omega_{\rm sf}=25$ meV, $\lambda_{11} = \lambda_{22}=0.5$, and $\lambda_{12}=\lambda_{21}=-2$. This set gives a reasonable value for $T_c \simeq 26.7$ K. A similar model was used in Ref. 32 to describe optical properties of ferropnictides. The actual details of the function are in fact not important; our usage of this particular function does not constitute an endorsement or preference compared to other possibilities but is just used here for concreteness.

In Fig. 2 we compare the temperature dependence of the relaxation rate calculated as described above in the clean limit for a conventional s-wave superconductor ($\Delta_1=\Delta_2$) and for an $s_\pm$ superconductor ($\Delta_1=-\Delta_2$), both in the weak- and in the strong-coupling limits. We observe that, while in the conventional case strong coupling makes a big difference by suppressing the coherence peak, in the $s_\pm$ state where no coherence effects take place, strong coupling is not really important. In Fig. 3 we show the effect of impurities in the Born limit. We have found that for an impurity scattering of the order of $0.4T_{c0}$, where T_{c0} is the transition temperature in the absence of impurities, there is a moderate suppression of T_c (less than 20%). More importantly, the strong deviation from exponential behavior in $1/T_1T$ appeared. Above $\sim 0.2T_c$ the dependence can be well represented by a power law but with an exponent closer to 5.5 for clean and 4 for

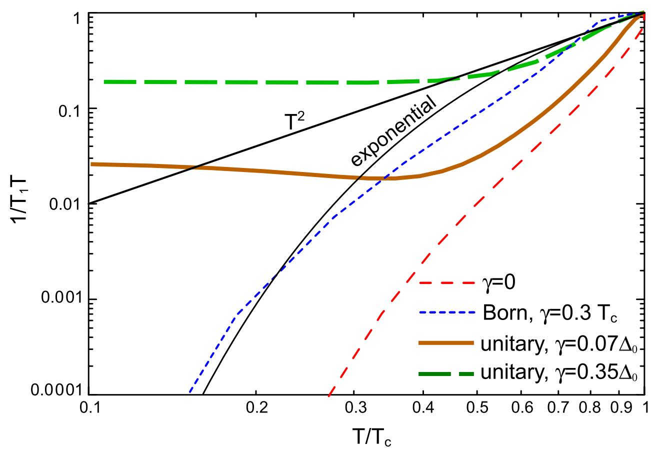

FIG. 3. (Color online) Calculated temperature dependence of the spin-lattice relaxation rate $1/T_1T$ for an $s_\pm$ superconductor in the strong-coupling approximation without impurities ($\gamma=0$), with impurities in the Born limit ($\gamma=0.3T_c$), and in the unitary limit for small ($\gamma=0.07\Delta_0$) and large ($\gamma=0.35\Delta_0$) impurity concentrations.

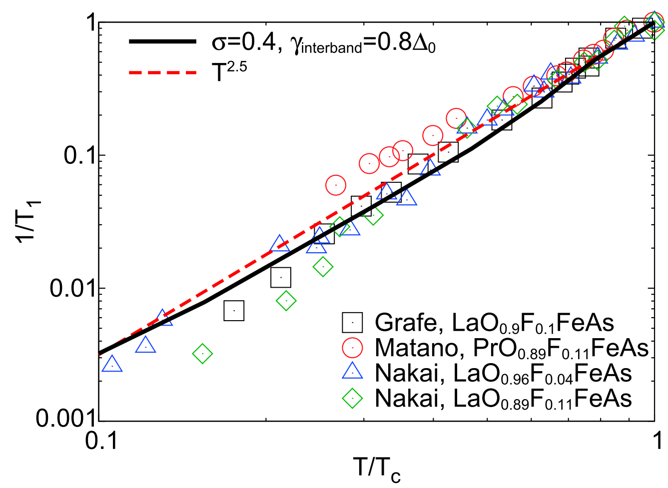

FIG. 4. (Color online) Calculated spin-lattice relaxation rate for the $s_\pm$ superconducting state together with experimental $1/T_1$ data from several groups, as indicated. $T^{2.5}$ trend is also shown.

dirty samples (as opposed to the experimentally observed 1.5–2). A further increase in the scattering rate leads to a too strong suppression of transition temperature and a too large relaxation rate right below T_c. Thus, impurity scattering in the Born limit cannot fully explain the NMR data.

As shown in Fig. 3, the unitary limit also does not reproduce the experimental data (represented by the approximate behavior $1/T_1T \propto T^2$) either for small or for large impurity concentrations and even predicts a slight nonmonotonicity for small $\gamma=0.07\Delta_0$. Here, Δ_0 is the low-temperature value of the energy gap without impurity scattering.

On the other hand, the experimental results can be reproduced very well if one assumes the intermediate regime of impurity scattering. Figure 4 shows various experimental data[12–14] together with our calculations for the $s_\pm$ gap with σ taken as 0.4 and interband γ taken as $0.8\Delta_0$. This γ corresponds to a relatively dirty superconductivity but the effect of interband scattering on T_c, for given γ, in this $s_\pm$ state is smaller than would be effected by intraband scattering of the same magnitude.[33,34] Besides, as mentioned above, a distribution of σ's will lead to a similar broadening of the DOS for smaller γ. We observe again that the $s_\pm$ state exhibits no coherence peak. As opposed to the Born and unitary limits, intermediate-σ scattering is capable of reproducing the experimental behavior, usually described as cubic but in fact probably closer to $T^{2.5}$ in $1/T_1$. Note that there is no universality after the 2.5 power of T; it is simply the result of a fitting.

We want to emphasize that this analysis does not *prove* that the origin of the power-law behavior is dirty-limit intermediate-σ scattering in an $s_\pm$ state. It is fairly possible that more complex physics, possibly related to coexistence of superconductivity and spin-density wave order, plays a role. But it clearly demonstrates that such a behavior does not prove existence of gap nodes on the Fermi surface.

To summarize, we have shown that the lack of a coherence peak is very naturally explained in the framework of the $s_\pm$ superconducting state even in the clean limit, and even more so in the presence of impurities. However, a *clean* $s_\pm$ superconductor would show an exponential decay of the relaxation rate $1/T_1$ below T_c, contrary to what has been observed in NMR experiments. Strong coupling effects and impurity scattering in Born approximation transform this exponential behavior into a power law-like for temperatures $T \gtrsim 0.2T_c$ but it is difficult to reproduce the actual experimental temperature dependence. On the other hand, an intermediate-limit scattering (neither Born nor unitary) can reproduce the experimental observations rather closely. While we did not address in this paper any effects that strong scattering may have on the other physical properties (this is left for future publications), we want to emphasize that there is an important difference between the scattering effect on the properties related to the $\mathbf{q}=0$ response (penetration depth, tunneling, specific heat) and $1/T_1$ that probes mainly the $\mathbf{q} \sim \mathbf{Q}$ response.

Note added. Recently we became aware of related work by Chubukov *et al.*,[35] who arrived at similar conclusions using a different approach. Also, Bang and Choi[36] reported similar but independent research, again reaching some of the same conclusions as ours.

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