$\omega / T$ scaling and magnetic quantum criticality in BaFe$_2$(As$_{0.7}P_{0.3}$)$_2$

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We used transport and inelastic neutron scattering to study the optimally phosphorus-doped BaFe$_2$(As$_{0.7}P_{0.3}$)$_2$ superconductor ($T_c = 30$ K). In the normal state, we find that the previously reported linear temperature dependence of the resistivity below room temperature extends to $\sim$ 500 K. Our analysis of the temperature and energy ($E = \hbar \omega$) dependence of spin dynamical susceptibility at the antiferromagnetic (AF) ordering wave vector $\chi'^\prime\prime(Q_{AF}, \omega)$ reveal an $\omega / T$ scaling within 1.1 < $E / k_BT < 110$. These results suggest that the linear temperature dependence of the resistivity is due to the presence of a magnetic quantum critical point in the cleanest iron pnictides near optimal superconductivity. Moreover, the results reconcile the strange-metal temperature dependences with the weakly first-order nature of the quantum transition out of the AF and nematic orders.

One of the hallmarks of unconventional superconductivity in copper oxide superconductors is the linear temperature dependence of the resistivity in the normal state below about 1000 K [1]. First discovered in La$_{2-x}$Sr$_x$CuO$_4$ and YBa$_2$Cu$_3$O$_7$ nearly optimal superconductivity [2-7], the linear temperature dependence of the resistivity is incompatible with Landau’s Fermi-liquid theory of metals, where temperature dependence of the resistivity is expected to be quadratic ($T^2$) [8], and suggests the presence of a quantum critical point (QCP) responsible for the breakdown of Fermi-liquid behavior and development of strange-metal properties [9,11].

In the case of iron pnictide superconductors [12-14], a linear temperature dependence of the resistivity has been found in different families of materials near optimal superconductivity, suggesting the presence of a QCP [15-20]. In particular, experimental evidence for a QCP in phosphorus-doped BaFe$_2$(As$_{1-x}P_x$)$_2$, envisioned in early theoretical studies [21], has been mounting [22,23]. This includes the linear temperature dependence of the resistivity [24], a peak in the effective electron mass [25], magnetic penetration depth [26], heat capacity [27] and nuclear magnetic resonance (NMR) [28]. The phosphorus doping does not involve the Fe-sites. As a result, this series is especially clean, as demonstrated by the relatively small residual resistivity and the observation of quantum oscillations [25]. Because the minimal disorder will allow for a clear understanding of the implications of the inelastic neutron scattering measurements (see below), here we focus on BaFe$_2$(As$_{1-x}P_x$)$_2$ near its optimal superconductivity.

In the undoped state, BaFe$_2$As$_2$ exhibits a tetragonal-to-orthorhombic structural transition at $T_s$, where a nematic phase with in-plane electronic anisotropy is established [21,29,31], followed by a collinear antiferromagnetic (AF) order below $T_N \approx 140$ K ($\leq T_c$) at $Q_{AF} \approx (0.5,0.5)$ [Figs. 1(a), 1(b)] [12,13]. When phosphorus is doped into BaFe$_2$As$_2$ to form BaFe$_2$(As$_{1-x}P_x$)$_2$ [22], a QCP is found in BaFe$_2$(As$_{0.7}P_{0.3}$)$_2$ near optimal superconductivity with suppressed orthorhombic lattice distortion and static AF order [Fig. 1(c)]. Increasing P-doping in BaFe$_2$(As$_{1-x}P_x$)$_2$ suppresses both $T_s$ and $T_N$, which are associated nematic and AF phase transitions, respectively. If both magnetic and nematic QCPs occur, one would expect to find gradually suppressed second order structural and magnetic phase transitions with increasing P-doping in BaFe$_2$(As$_{1-x}P_x$)$_2$. However, systematic neutron diffraction and NMR experiments on powder and single crystal samples of BaFe$_2$(As$_{1-x}P_x$)$_2$ reveal that the structural and AF phase transitions are coupled at all $x$, and AF phase transition around $x \approx 0.3$ become weakly first order near optimal superconductivity, thus suggesting an avoided magnetic QCP [32,34].

Although the AF phase transition in BaFe$_2$(As$_{1-x}P_x$)$_2$ is weakly first order near optimal superconductivity [32,34], the small ordered moment and low ordering temperature do not exclude the possibility of an extended temperature and energy range where quantum criticality underlies the linear resistivity. This is consistent with the fact that when superconductivity in BaFe$_2$(As$_{0.7}P_{0.3}$)$_2$ is suppressed by a magnetic field, the temperature dependence of the resistivity is quadratic below the zero field $T_c = 30$ K, deviating from the linear temperature dependence above 30 K [see inset of Fig. 1(d)] [35]. Figure 1(d) shows our measurement of the resistivity for BaFe$_2$(As$_{0.7}P_{0.3}$)$_2$ from 2 K to 790 K. In addition to...
confirming the linear temperature dependence of the resistivity from 30 K to 300 K [24], the data reveal that it extends all the way up to ∼ 500 K, above which a clear deviation from the linear behavior is seen; this exemplifies the extended temperature range for the strange-metal behavior. The nematic QCP [19] alone is unlikely to be responsible for the observed linear temperature dependent resistivity [24], given that fluctuations at small wavevectors are inefficient in degrading an electrical current. If linear temperature dependence of the resistivity in BaFe$_2$(As$_{0.7}$P$_{0.3}$)$_2$ in Fig. 1(d) is associated with a magnetic quantum critical fluctuations, one would expect that spin dynamics at $\mathbf{Q}_{AF}$ to follow $\omega/T$ scaling within a finite energy ($E = \hbar \omega$, where $\omega$ is frequency) and temperature range [36,39].

To test this hypothesis, we use inelastic neutron scattering to study BaFe$_2$(As$_{0.7}$P$_{0.3}$)$_2$ ($T_c$ ≈ 30 K), focusing...
on temperature and energy dependence of spin fluctuations near $Q_{AF}$. In previous inelastic neutron scattering experiments on \( \text{BaFe}_2(\text{As}_{0.3}\text{P}_{0.7})_2 \) \[40\] \[12\], a $c$-axis dispersive neutron spin resonance coupled to superconductivity has been identified. By using neutron triple-axis and time-of-flight spectroscopy, we find that energy and temperature dependence of the imaginary part of dynamic susceptibility at $Q_{AF} \chi''(Q_{AF}, \omega)$, which is related to magnetic scattering \( S(Q_{AF}, \omega) \) via \( \chi''(Q_{AF}, \omega) \propto (1 - e^{\omega/k_B T}) S(Q_{AF}, \omega) \), follows the $\omega/T$ scaling for $9 < \omega < 61$ meV and $5 < T < 200$ K. For energies less than about $E = 10$ meV, the $\omega/T$ scaling fails to describe the data. These results suggest that the observed linear temperature dependence of the resistivity in Fig. 1(d) may arise from magnetic quantum critical fluctuations important for controlling the transport and nematic properties of \( \text{BaFe}_2(\text{As}_{0.3}\text{P}_{0.7})_2 \).

We used the standard four-probe method to measure the resistivity of \( \text{BaFe}_2(\text{As}_{0.3}\text{P}_{0.7})_2 \) from 10 K to 790 K in a Janis 4 K closed cycle refrigerator with high temperature capability. As we can see from Fig. 1(d), the remarkable linear temperature dependence of the resistivity extends up to 500 K. Combined with previous transport measurements below 30 K when superconductivity is suppressed by a high magnetic field [see inset of Fig 1(d)] \[35\], we find that the temperature range for linear resistivity is from 30 K to 500 K.

Our inelastic neutron scattering experiments were carried out on the Wide Angular-Range Chopper Spectrometer (ARCS) at the Spallation Neutron Source and HB-3 triple axis spectrometer at the High-Flux Isotope Reactor, both at Oak Ridge National Laboratory. For the time-of-flight measurement on ARCS, we used $E_t = 80$ meV with $k_t$ parallel to the $c$ axis. Total mass 17 g high-quality \( \text{BaFe}_2(\text{As}_{0.3}\text{P}_{0.7})_2 \) single crystals were co-aligned in the $[H, H, L]$ scattering plane with an in-plane mosaic $< 5.5^\circ$ \[12\]. We define $Q = (H, K, L) = \frac{2\pi}{a} H \hat{i} + \frac{2\pi}{a} K \hat{j} + \frac{2\pi}{c} L \hat{k}$, where the tetragonal lattice constants are $a = b \approx 3.96 \AA$ and $c \approx 12.87 \AA$.

Figures 2(a)-(d) show images of spin excitations $S(Q, \omega)$ at $E = 12 \pm 3, 22 \pm 3, 42 \pm 3, 52 \pm 3$ meV, respectively, at $T = 120$ K. Consistent with earlier work \[31\], spin excitations form transversely elongated ellipses centered around $Q_{AF}$ that disperse outward with increasing energy. We convert $S(Q, \omega)$ to $\chi''(Q, \omega)$ and fit the in-plane dynamical susceptibility with two-dimensional Gaussian function to get the absolute intensity of $\chi''(Q, \omega)$ at $Q = Q_{AF} = (0.5, 0.5)$. Figures 2(e) and 2(f) show energy dependence of $\chi''(Q_{AF}, \omega)$ at $T = 32$ and 120 K, respectively. The solid lines in the figures are fits to the data with typical paramagnetic relaxation form $\chi''(Q_{AF}, \omega) = I \frac{1 - e^{\omega/\Gamma}}{1 + e^{\omega/\Gamma}}$, where $\Gamma$ is related to full width at half maximum of the excitations, corresponding to the relaxation lifetime of the excitations, and $I$ is the peak intensity of the excitations. Figures 2(g) and 2(h) show temperature dependence of $\Gamma$ and $I$, respectively. While $\Gamma$ increases approximately linearly with increasing temperature, $I$ decreases with increasing temperature.

To test if the measured imaginary part of the dynamic susceptibility at $Q_{AF}$ follows the $\omega/T$ scaling expected for magnetic quantum critical fluctuations, we consider $\chi''(Q_{AF}, \omega) T^\alpha = F(Q_{AF}, \omega/T)$, where the scaling exponent $\alpha$ and the scaling function $F(Q_{AF}, \omega/T)$ are determined through the best-observed collapse of the data onto one universal curve \[38\]. We exclude the data under
We have shown that the energy and temperature dependent of $\chi''(Q_{AF}, \omega)$ in BaFe$_2$(As$_{1-x}$P$_x$)$_2$ follows $\omega/T$ scaling within an extended temperature and energy range. To appreciate the importance of this material being clean, we recall that, in the case of doped heavy-Fermion materials such as UCu$_5$-Pd$_x$, the observed $\omega/T$ and associated non-Fermi liquid behavior such as linear temperature dependence of the resistivity have been attributed to either quantum criticality of the ground state or long-range magnetic order. The spin fluctuations in these energies are not obeyed. Gray points are the data from 20 to 100 meV collected on MAPS at 10 K with $E_i = 250$ meV. Plots (c) and (d) are data from HB-3.

By fitting the data with this function, we find $\chi''(Q_{AF}, \omega)$ due to the appearance of the neutron spin resonance in superconducting state [40, 41]. By fitting the data with this function, we find $\alpha = 0.605$ independent of the functional form of $F(Q_{AF}, \omega/T)$ [Fig. 4(a), (b)]. For $E/T$ from 1.1 to about 110, the data collapse into a single curve. From neutron time-of-flight measurements on BaFe$_2$(As$_{1-x}$P$_x$)$_2$, we know that spin excitations disperse transversely away from Q$_{AF}$ for energies above 100 meV. Figures 4(a) and 4(b) suggest that spin excitations up to 100 meV follow $\omega/T$ scaling. However, low-energy spin excitations ($E/T < 1.1$) seem to deviate from the scaling curve, consistent with transport measurements where resistivity deviates from linear temperature dependence below 30 K.

To further explore if the low-energy spin fluctuations follow $\omega/T$ scaling, we carried out inelastic neutron scattering measurements using HB-3 triple axis spectrometer. Figure 3 shows $\chi''(Q, \omega)$ for $E = 4, 6, 10$ meV at various temperatures. The spin fluctuations in these energies are fitted to a Gaussian function and give the dynamical susceptibility at Q$_{AF}$. The spin fluctuations at $E = 4, 6, 10$ meV are dramatically suppressed with increasing temperature, but still present even at 300 K [Figs. 3(a)-(c)]. By combining results from constant-energy and constant-Q scans, we deduce the data using the same parameters as in Figs. 4(a) and 4(b) and the outcome is shown in Figs. 4(c) and 4(d) with $\alpha = 0.605$. Clearly, the $\omega/T$ scaling fails for low-energy spin fluctuations with energy approximately below 10 meV.

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follows from a large-\(N\) saddle-point calculation \cite{50}.

In summary, we have systematically measured the temperature and energy evolution of spin fluctuations in the optimal doped \(\text{BaFe}_2(\text{As}_{0.7}\text{P}_{0.3})_2\). We find evidence for the \(\omega/T\) scaling in spin fluctuations over extended temperature and energy range, consistent with linear temperature dependence of the resistivity. These results provided strong evidence that the linear temperature dependence of resistivity arises \(\text{BaFe}_2(\text{As}_{0.7}\text{P}_{0.3})_2\), which is located near optimal superconductivity, from magnetic quantum criticality. Therefore, the presence of a magnetic QCP may ultimately be responsible for the anomalous transport and magnetic properties of the iron pnictides and strongly influence their superconductivity.

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