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Quantum critical point and superconducting dome in the pressure phase diagram of $\alpha$-TaS$_3$

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We measure the electrical resistance of $\alpha$-TaS$_3$ between 1 and 300 K under pressures up to 20 GPa. We observe a gradual decrease of the charge density wave transition temperature $T_{\text{CDW}}$ with increasing pressure $P$ following a mean field quantum fluctuation power law $T_{\text{CDW}} = 215\,\text{K}[(P_c - P)/P_c]^{\gamma}$ with a quantum critical point at a pressure $P_c = 11.5\,\text{GPa}$ and $\gamma \approx 0.5$. Around the quantum critical point (QCP) we observe a superconducting dome with a maximum superconducting transition temperature $T_c = 3.1\,\text{K}$. Such dome is similar to superconducting domes around other types of order suggesting that the QCP is directly responsible for the enhancement of superconductivity through a universal mechanism still not well understood.

Linear transition-metal chalcogenides have been thoroughly studied due to their one-dimensional (1D) character. When metallic, the electronic bands yield almost flat Fermi surfaces (FS) that are prone to produce divergences in the Lindhard susceptibility at a wave vector $Q$.

When metallic, the electronic bands yield almost flat Fermi surfaces (FS) that are prone to produce divergences in the Lindhard susceptibility at a wave vector $Q$.

$T_c(0)$ = 3.34 $\pm$ 0.16 K. Such dome is universal in nature and is not the result of the enhancement of superconductivity through a universal mechanism still not well understood.

The structure of orthorhombic $\alpha$-TaS$_3$ is still unknown. The lattice parameters are very large in the directions perpendicular to the chain direction $c$ axis, namely, $a = 36.804\,\text{Å}$, $b = 15.173\,\text{Å}$, and $c = 3.34\,\text{Å}$, and may indicate that it comprises 6 $\times$ 4 chains parallel to the $c$ axis. A single CDW transition develops at $T_{\text{CDW}} = 215\,\text{K}$ with a CDW vector that is $Q = 2k_F$.

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above \( \sim 8 \) GPa the sample shows superconductivity, whose onset increases up to a maximum of \( \sim 3.3 \) K at the pressure where the CDW disappears altogether (Fig. 2).

We have measured the critical magnetic field of the superconducting state at different temperatures. The critical magnetic field at zero temperature \( H_c(0,P) \) can then be calculated at each pressure by fitting the expression:

\[
H_c(T,P) = H_c(0,P) \left[ 1 - \left( \frac{T}{T_c(P)} \right)^2 \right].
\] (1)

The pressure dependence of the correlation length can be obtained from the Ginzburg-Landau expression:

\[
\xi(P) = \left( \frac{\phi_0}{2\pi H_c(0,P)} \right)^{1/2},
\] (2)

where \( \phi_0 \) is the magnetic flux quantum. No significant variation is observed on the correlation length as a function of pressure (inset in Fig. 2 right panel).

The transition temperature to the CDW state \( T_{CDW} \) can be determined by the logarithmic derivative \( d \log R/dT \). However, we have observed that the same derivative but with respect to the inverse temperature \( d \log (R)/(1/T) \) is a more sensitive method that allows one to follow \( T_{CDW} \) down to stronger pressures, while coinciding with the other definition at lower pressures. We have thus adopted this method (Fig. 3).

In Fig. 4 we show the measured pressure phase diagram of \( \alpha\)-TaS\(_3\). We compare our results to older measurements with a good agreement between them. However, we are now able to
determine precisely the pressure dependence of $T_{\text{CDW}}$. Astonishingly, in all the pressure range, it follows a mean field quantum fluctuation power law $T_{\text{CDW}} \propto (P_c - P)/P_c$ with a critical pressure $P_c = 11.5$ GPa and $\gamma = 0.5$. This is unexpected, as for NbSe$_3$, a compound of the same 1D transition-metal trichalcogenide family but with a simpler structure, according to the reported results, pressure yields first an exponential decrease that, only when $T_{\text{CDW}}$ becomes small enough, changes towards a $\gamma = 0.5$ power law. The exponential decrease is expected due to the BCS dependence of $T_{\text{CDW}} = 5.43 T_F \exp[-\omega_q/g^2 N(E_F)]$, where $T_F$ is the Fermi energy, $\omega_q$ is the frequency of the phonon that stabilizes the CDW, $g$ is the coupling parameter, and $N(E_F)$ is the density of states at the Fermi level. The most important variation will be given by the exponential, where $\omega_q$ will obviously increase with pressure, while $N(E_F)$ is expected to decrease at the same time as should $g$. Supposing a linear variation of these parameters, we would expect an exponential decrease with pressure of $T_{\text{CDW}}$ until we are sufficiently near to the QCP, where fluctuations take over in the form of a power law $T_{\text{CDW}} \propto [(P_c - P)/P_c]^{0.5}$. This is the type of behavior observed in NbSe$_3$ and that has also been studied in detail in Cr metal, whose known itinerant antiferromagnetism is due to a BCS type of spin density wave. According to common belief the expectation for the dependence of $T_{\text{CDW}}$ with pressure is an exponential decrease with pressure characteristic of a weak coupling BCS state, followed at sufficiently low transition temperatures by a power law decrease due to quantum fluctuations. $\alpha$-TaS$_3$ thus seems to be anomalous, without regime of exponential pressure dependence, in spite of a high CDW transition temperature. Apparently quantum fluctuations control in the same unexpected way the variation with pressure of $T_{\text{CDW}}$ far away from the QCP.

Another important point of our measurements is the superconducting dome that we observe around the QCP within our error bars. In the field of heavy fermions, much discussion has been developed around the question if superconductivity is natural to expect the appearance of superconductivity as the CDW disappears, as given by the Bilbro-McMillan formula $T_{\text{CDW}}^{\alpha} = T_{\text{c}}$, where $n$ is the superconducting fraction of the Fermi surface and $T_{\text{c}}$ is the superconducting transition temperature without CDW. However, this formula, which does not predict a superconducting dome, is obtained considering that BCS controls the evolution of both transition temperatures. We have seen that for $\alpha$-TaS$_3$, in the entire phase diagram, and for NbSe$_3$ near the QCP, fluctuations control $T_{\text{CDW}}$. Thus it is clear that new theoretical ideas which could lead to a superconducting dome are most welcome as well as further theoretical and experimental studies which could assert their applicability to CDW systems.

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