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Inelastic X ray scattering under pressure to probe the quantum phase transition in the transition metal dichalcogenides

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Transition metal dichalcogenides are systems in which the interplay of strong electron – electron and electron-phonon interactions give rise to a wide variety of electronic states at low temperature ranging from metal, Mott-insulator or an electronic spatial modulation : charge density wave. The temperature below which the charge density wave appears (T_{cdw}) can be tuned continuously down to 0K by applying an external parameter such as pressure. In the vicinity of this point a superconducting state appears.

One of the key ingredient of both the superconducting and charge density wave states is the phonon spectrum. Indeed, a charge density wave is associated to a periodic lattice distortion stabilised by a strong electron-phonon coupling, and, in most cases, phonons are responsible for the formation of Cooper pairs.

Recently, we performed inelastic X-ray scattering up to 16 GPa and down to very low temperature. Temperature and pressure dependences of the soft mode associated to the charge density wave have been measured in several transition metal dichalcogenides among them NbSe₂ and NbS₂. A strong anisotropy of the phonon dispersions along different crystallographic directions has been observed. In NbS₂ at ambient pressure, we observed a huge temperature dependence of the phonon softening. By comparing it with the temperature dependence of the phonon spectra of NbSe₂ under pressure, we show that NbS₂ is at the vicinity of a charge density wave instability. By explicitly taking into account anharmonic effects, we obtain an accurate, quantitative, description of the (P,T) dependence of the phonon spectrum, and accounts for the rapid destruction of the CDW under pressure by zero mode vibrations - or quantum fluctuations - of the lattice. At least, this pressure and temperature dependence could be general to other dichalcogenides for which electron-electron correlations are stronger.

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