The family of layered 2H dichalcogenides represents an interesting system in which charge-density wave (CDW) order co-exists with the superconductivity (SC) \[1, 2\]. The fact that the CDW transition temperature decreases, while the superconducting critical temperature \(T_C\) increases from TaSe\(_2\) through TaS\(_2\) and NbSe\(_2\) to NbS\(_2\), suggests that these two order parameters represent competing ground states. Indeed, it has been found that in TaS\(_2\) and NbSe\(_2\), \(T_C\) increases under pressure while \(T_{CDW}\) decreases \[3, 4\]. After CDW order disappears, \(T_C\) remains approximately constant. In NbS\(_2\), the system without CDW order, \(T_C\) is insensitive to pressure. Although various anomalies, including an apparent anisotropy of the Fermi energy \[11\], the Fermi surface of the 2H dichalcogenides is of conventional BCS character, mediated by strong electron-phonon coupling \[7\]. However, consensus on the exact mechanism that drives the system into the CDW state has still not been reached. Some authors \[1, 2, 9, 10\] argue, in analogy with a Pierls transition in one-dimensional systems, that the CDW transition is driven by a FS instability (nesting), where some portions of the FS are spanned by a CDW vector \(q_{CDW}\). In another scenario, the CDW instability is induced by the nesting of van Hove singularities (saddle points in the band structure with high density of states) if they are within a few \(k_BT_{CDW}\) of the Fermi energy \[11\]. The Fermi surface of the 2H dichalcogenides is rather complicated, being dominated by several open (2D-like) sheets and with one small 3D S(Se)-derived pancake-like FS \[7\]. In such a situation, one may anticipate anisotropic properties and in particular, an anisotropic electron-phonon coupling. The resistivity anisotropy, of the order of 10-50, is much smaller than in layered oxides, indicating a substantial inter-layer hopping \[12\]. Transport properties show relatively small anomalies at \(T_{CDW}\), suggesting that only a small portion of the FS becomes gapped in the CDW state. In addition, the 2H dichalcogenides become better conducting in the CDW state, indicating a higher degree of coherence.

We have previously studied the quasi-particle (QP) self-energy for the first member of the series, TaSe\(_2\), and found that it was strongly influenced by the CDW transition \[13\]. Sharp structure in both the dispersion ("kink") and the scattering rate at \(\sim 70\) meV in the CDW state weakened and shifted to \(\sim 35\) meV upon transition into the normal state. Similar "kinks", have been previously identified in conventional metals and attributed to electron-phonon coupling \[14\]. As the energy scale of the "kink" in the CDW state of TaSe\(_2\) was too large for phonons, we suggested that the excitation was electronic in origin: a fluctuation of the CDW order parameter. In this letter, we show that the self-energy of NbSe\(_2\) \((T_{CDW} \approx 35\) K and \(T_C = 7.2\) K) is less sensitive to the CDW transition and that it is dominated by electron-phonon coupling. Measured directly for the first time, the coupling is very anisotropic \((k\)-dependent) and much stronger than in TaSe\(_2\).
strumental energy resolution was set to ~4 meV for low temperature studies (T < 15K) and to ~6 meV elsewhere. The angular resolution was better than ±0.1° translating into a momentum resolution of ±0.0025Å⁻¹ at the 15.2 eV photon energy used in the present study. Samples, grown by the standard iodine vapor transport method, were mounted on a liquid He cryostat and cleaved in-situ in the UHV chamber with base pressure 3 × 10⁻⁹ Pa. The temperature was measured using a calibrated silicon sensor mounted near the sample.

Figure 1 shows the photoemission intensity, recorded at T =10 K, as a function of binding energy and momentum along three different momentum lines in the Brillouin zone. Nine Fermi crossings are included: three pairs on the double-layer split Fermi sheets centered around Γ and three crossings on the split sheets centered at the K point. A characteristic change in the QP velocity (“kink”) can be easily identified in all crossings. The kinks are also accompanied by a sharp change in the QP widths at the “kink” energy. These observations are indicative of (bosonic) excitations interacting with the QPs. It is obvious from Fig. 2(a) that not only is the magnitude of ReΣ different for different states, but also the peaks are at different energies, ranging from ~13 meV to ~35 meV. Various experimental and theoretical studies have shown that the phonon spectrum is fully consistent with these energies, with acoustical phonon branches laying below ω ~12 meV, and optical branches spanning the region 15 < ω < 40 meV [15]. Shifts of the ReΣ maxima would further suggest that some electronic states are coupled predominantly to acoustic modes while others couple more strongly to the optical modes, even though the states are sometimes very close in momentum (compare points 4 and 5, for example). A strong k-dependence of Σ would complicate the MDC line-shape in the energy region where the k-dependence exists. Although we have detected some deviation from Lorentzian lineshapes, we were not able to precisely determine the MDC’s line-shape due to the overlap of bi-layer split states. It is interesting that in spite of these differences in Σ, the resulting coupling constant does not vary much, λ ~ 0.85±0.15, within the experimental uncertainty. The only exception is the inner K-centered sheet (point 6), where λ ~ 1.9±0.2. We have completed several measurements on different samples, always with similar results for λ at, or close to that Fermi

FIG. 1: The photoemission intensities in the CDW state at T=10K for several momentum lines indicated in the schematic view of the Brillouin zone (lower left panel) by the dark-gray lines. The light-gray lines represent Nb-derived Fermi sheets.

The nine Fermi points are numbered. The MDC derived dispersions are represented by full circles. The high-energy part of the dispersions is fitted with a second-order polynomial (dashed lines) and the low energy part is fitted with straight lines.
FIG. 2: (a) Real parts of self-energies ReΣ extracted from measured dispersions from Fig. 4 for several Fermi points. (b) Temperature dependence of ReΣ for NbSe$_2$ for point 1 from Fig. 4 and (c) for TaSe$_2$ (taken from ref. [13]) near the same region on the Γ-centered FS.

point. This seemingly too large coupling constant is actually in a good agreement with the large measured value of linear specific heat coefficient, $\gamma \approx 18.5$ mJ mol$^{-1}$K$^{-2}$ [5, 16], which is proportional to the renormalized density of states (DOS) at the Fermi level, $N(0)(1 + \lambda)$, through $\gamma = (1/3)\pi^2k_B^2N(0)(1 + \lambda)$. Band structure calculations give the "bare" DOS $N(0) \approx 2.8$ states eV$^{-1}$ unit cell$^{-1}$ [7], suggesting $\lambda \approx 1.8$. However even this might be an underestimate for our state as $\gamma$ measures an average over the FS, weighted by each state’s DOS. A similar value for $\lambda$ is obtained from $c$-axis optical conductivity [17] suggesting that the $c$-axis transport is probably dominated by the K-H centered cylinders with largest warping.

It is instructive that in TaSe$_2$ the CDW gap opens up in the same region of the FS [15], while the Γ-A centered Fermi cylinders remain ungapped, and gain coherence in the CDW state [13]. Therefore, it seems plausible that both the superconductivity and the CDW state originate from the inner K sheet and are driven by strong electron-phonon coupling. This seems to be in line with the original suggestion of Wilson [4] that the self-nesting of the inner K sheet drives the CDW in 2H dichalcogenides. A lack of CDW gap on the Γ centered sheets in all of 2H dichalcogenides studied in ARPES suggests that these sheets support neither the self-nesting nor the nesting which would mix them with the K-centered sheets. In particular, the f-wave symmetry of the CDW gap [2] may be ruled out. The relative strength of the CDW and superconducting ordering is determined by the nesting properties of the inner K cylinder, while the upper limit for $T_C$ (when the CDW is destroyed by applying pressure, for example) is given by $\lambda$. Nesting weakens with increasing 3D character (increased warping with $k_Z$) under pressure and on moving from TaSe$_2$ to NbSe$_2$. $\lambda$ increases from TaSe$_2$ to NbSe$_2$ [14] and is essentially pressure independent. In agreement with previous ARPES studies [8, 20, 21], we do not see a CDW gap in NbSe$_2$, suggesting that the nested portion of the FS is very small and was not sampled in any study. As there is a non-trivial $k_Z$-dispersion (warping), it is possible that the in-plane $k_F$ might be tuned into the nesting and that the gap opens only near certain $k_Z$. Note that the energy splitting between the double walled sheets is larger for K-centered sheets. A similar $k$-dependence is also expected for the interlayer hopping, $t_{\perp}$, that produces the warping. Additionally, as Fermi velocities are larger for Γ-centered sheets, it is reasonable to expect that the in-plane $k_F$ varies with $k_Z$ much less on the Γ-cylinders than on the K-cylinders (the change in the in-plane Fermi momentum is approximately given by $\Delta k_F \propto t_{\perp}/v_F$). The measured FSs centered at Γ are too large at the sampled $k_Z$, and we do not expect them to ever reach the self-nesting condition $2k_F = q_{CDW}$. On the other hand, the inner K-centered sheet seems to be very close to producing the required nesting. A more detailed mapping is needed to explore the nesting properties and eventual CDW gap opening in this region. According to STM studies [22], the CDW gap is large ($\Delta_{CDW} \sim 35$ meV) and should be easily measurable in ARPES. The overall electronic properties in NbSe$_2$ are much less sensitive to the CDW transition than in TaSe$_2$. Even the CDW induced structure in the self-energy that existed in TaSe$_2$ is absent in NbSe$_2$. Both the ”kink” and the scattering rate are remarkably insensitive to the CDW (See Fig. 2b).

An interesting question is whether the anisotropic electron-phonon coupling constant $\lambda$ would be projected into the magnitude of the superconducting gap. A recent photoemission study [8] has shown that the superconducting gap is indeed anisotropic, being quite uniform, $\Delta \sim 1$ meV, on the Nb-derived Fermi cylinders, but reduced beyond the experimental sensitivity ($\Delta \approx 0$) on the 3D pancake-like FS. No data for the inner K-H cylinder has been reported. In Fig. 3 we show the spectral intensity at two Fermi points, 6 and 7 for several temperatures. The coupling constant differs by a factor of $\sim 2$ at these two points and yet, the superconducting gap, that clearly opens up below $T_C$ at both Fermi points, is the same within the experimental error. This is in contrast to MgB$_2$, where the ”hot” regions are gapped by correspondingly larger gaps [23]. The equalizing of the superconducting gap for states with different coupling strengths but similar symmetries represents a $k$-space analogous of the proximity effect [24].

NbSe$_2$ has several properties in common with other layered materials. One of the most obvious peculiarities is the fact that the transport becomes more metallic in the CDW state even though a portion of the FS is ”destroyed” (gapped). We suggest that this is a manifestation of anisotropic Fermi surfaces where strongly coupled portions, or ”hot spots”, generally play a negative role in normal state conductivities, acting as scattering ”sinks” for the remaining, less renormalized regions. These ”hot
spots” drive the system into an ordered state, but it is the "cold spots" that usually dominate the conductivities. This duality has recently been detected in MgB$_2$ where the normal state transport shows an extremely weak coupling, while the superconducting properties are dictated by strongly coupled portions on the FS [23]. A Similar situation also exists in the cuprates where the in-plane nodal regions reduce the in-plane conductivities, while the opening of the pseudogap improves them.

Another similarity with the cuprates exists in that the pseudogap ($T^*$) and $T_C$ lines in the $T - x$ phase diagram of cuprates show similar behavior to the $T_{CDW}$ and $T_C$ lines in the $T - pressure$ phase diagram of dichalcogenides. As $T^*(T_{CDW})$ goes down, $T_C$ increases with doping (pressure). This analogy suggests that the cuprate phase diagram might be shaped by similar competing orders. However, the analogy is no longer valid in the overdoped regime where $T_C$ turns back down, even when the pseudogap no longer exists, suggesting that some other, more exotic coupling mechanism might be acting in the cuprates. Here, we would like to point out that the high energy of the "kinks" observed in TaSe$_2$ [13] and recently in NbSe$_2$ [24] rules out the phonon scenario and represents an unambiguous evidence that the "kinks" may indeed be caused by other mechanisms. Consequently, the "kinks" observed in the cuprates do not necessarily reflect the electron-phonon coupling.

In conclusion, we have detected a strong anisotropy of the self-energy in a layered dichalcogenide, 2H-NbSe$_2$, with the electron-phonon coupling constant $\lambda$ ranging from 0.8 to 1.9 on Nb-derived sheets. The strongest coupling has been found on the inner K-H cylinder, which plays a central role in both CDW and SC transitions in 2H-dichalcogenides. The anisotropy in coupling strength does not induce the anisotropy in the SC gap.

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**FIG. 3:** Temperature dependence of the EDCs taken at Fermi points of the inner (a) and the outer (b) Fermi sheets centered at K. The superconducting gap, measured as the shift of the inflection point of the leading edge, is the same even though the measured $\lambda$ differs by a factor of 2.

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