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# Quantum phase transition from triangular to stripe charge order in NbSe<sub>2</sub>

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The competition between proximate electronic phases produces a complex phenomenology in strongly correlated systems. In particular, fluctuations associated with periodic charge or spin modulations, known as density waves, may lead to exotic superconductivity in several correlated materials. However, density waves have been difficult to isolate in the presence of chemical disorder, and the suspected causal link between competing density wave orders and high-temperature superconductivity is not understood. Here we used scanning tunneling microscopy to image a previously unknown unidirectional (stripe) charge-density wave (CDW) smoothly interfacing with the familiar tridirectional (triangular) CDW on the surface of the stoichiometric superconductor NbSe<sub>2</sub>. Our low-temperature measurements rule out thermal fluctuations and point to local strain as the tuning parameter for this quantum phase transition. We use this quantum interface to resolve two longstanding debates about the anomalous spectroscopic gap and the role of Fermi surface nesting in the CDW phase of NbSe<sub>2</sub>. Our results highlight the importance of local strain in governing phase transitions and competing phenomena, and suggest a promising direction of inquiry for resolving similarly longstanding debates in cuprate superconductors and other strongly correlated materials.

competing order | scanning tunneling spectroscopy | transition metal dichalcogenides

Whereas a classical phase transition separates two states of matter at different temperatures, two ordered ground states of a material at zero temperature are separated by a quantum critical point (QCP). The competition between proximate ordered phases near the QCP can dramatically influence a large region of the phase diagram (1). Whereas the fluctuations from competing quantum states lead to exotic physics even at higher temperatures, low-temperature studies of these states may lead to a better understanding of the root of the competition. Density waves—charge- or spin-ordered states of collective origin driven by instabilities of the Fermi surface (FS)—exist in close proximity to superconductivity (SC) in several classes of correlated materials (2–4), and various proposals emerged recently to study their interplay in the presence of strong inhomogeneity in these systems (5). In this light, it is surprising that charge-density waves (CDWs) are not fully understood, even in the weakly correlated and stoichiometric transition metal dichalcogenides (TMDCs). Whereas a classic CDW arises from strong FS nesting, resulting in a sharply peaked susceptibility and a Kohn anomaly at the CDW wavevector, the quasi-2D TMDCs are known to deviate from this picture (6, 7).

NbSe<sub>2</sub> is a layered TMDC that has generated much recent interest (8–10) as a model system for understanding the interplay of the CDW and SC phases with onset at  $T_{\text{CDW}} \sim 33$  K and  $T_{\text{SC}} \sim 7$  K respectively (11, 12). Despite extensive study (9, 13–16), several key facts about its familiar tridirectional (3Q) CDW remain unresolved, including the role of FS nesting in determining its wavevector  $\vec{q}_{3Q}$  and the magnitude of the spectral gap and its

role in the energetics of the transition. First, angle-resolved photoemission (ARPES) studies have been unable to uniquely identify  $\vec{q}_{3Q}$ -nested FS regions in NbSe<sub>2</sub> (9, 13, 16–20). Meanwhile, recent studies indicate a broadly peaked susceptibility and a soft phonon over a range of wavevectors around  $\vec{q}_{3Q}$  (6, 15, 16), suggesting instead that the  $q$ -dependence of the electron–phonon coupling might play an important role in driving the transition. Second, kinks in tunneling spectra at  $\pm 35$  mV ( $\pm \varepsilon_K$ ), historically identified as gap edges, correspond to an anomalously large energy scale for the corresponding  $T_{\text{CDW}}$  ( $2\varepsilon_K/3.5k_B T_{\text{CDW}} \sim 7.05$ ) (21), whereas recent ARPES studies indicate a much smaller gap,  $\sim 3$ –5 mV (13, 16).

Our discovery, by low-temperature scanning tunneling microscopy (STM), of a unidirectional (1Q) CDW with distinct wavelength and tunneling spectra from the 3Q CDW, in conjunction with band structure calculations, allows us to resolve both longstanding questions of the wavevector and the gap. First, the distinct wavelengths demonstrate that FS nesting plays a negligible role in setting their magnitude. Second, the distinct tunneling spectra of the 1Q CDW region help us disentangle the 3Q CDW spectra to expose a particle-hole asymmetric gap, riding on top of a strong inelastic background.

## Results

Fig. 1A shows a topographic image of a locally commensurate ( $3a_0$ ) CDW on 2H-NbSe<sub>2</sub>. Its microscopic 3Q nature is confirmed by the existence of a secondary CDW peak in the Fourier transform (FT) in Fig. 1B, in contrast to bulk measurements (10). Phase slips result in an overall periodicity of  $\lambda_{3Q} \simeq 3.05 a_0$ , corresponding to  $\vec{q}_{3Q} \simeq 0.328 \vec{Q}_0$ , where  $\vec{Q}_0$  is the Bragg vector (10, 11, 22). Our primary experimental discovery is shown in Fig. 2A, where regions of unidirectional (1Q) CDW with unique wavevector  $\vec{q}_{1Q}$  along a single 3Q direction form an atomically smooth interface with the 3Q CDW. The absence of atomic lattice discontinuities rules out the possibility of an NbSe<sub>2</sub> polytype interface (23). Although other TMDCs are known to exhibit a thermally induced triclinic CDW state that varies with doping near  $T_{\text{CDW}}$  (22, 24), no such anisotropy has been reported in 2H-NbSe<sub>2</sub>. Moreover, our observations are at temperatures  $T \ll T_{\text{CDW}}$ , where thermal fluctuations are

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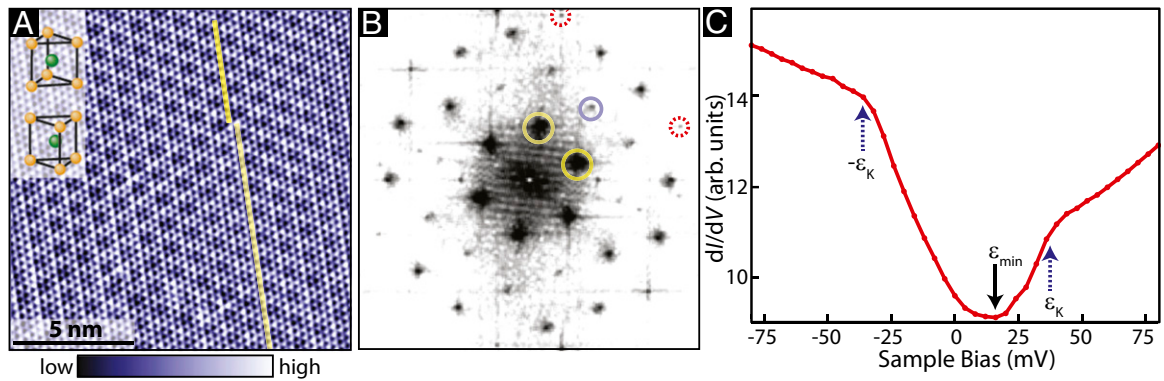
The authors declare no conflict of interest.

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**Fig. 1.** STM of the 3Q CDW. (A) Atomic resolution topograph showing the  $\sim 3 a_0$  periodic CDW. Yellow lines are overlaid on a one-atom shift of the CDW maximum (phase slip). (Inset) Crystal structure of  $2H\text{-NbSe}_2$ , with layers of Nb (green) atoms sandwiched between layers of Se (orange) atoms. (B) FT of a larger ( $\sim 45$  nm) topograph, displaying a 3Q CDW. Primary CDW wavevectors,  $\vec{q}_1$  and  $\vec{q}_2$  (yellow circles); a secondary CDW wavevector,  $\vec{q}_1 + \vec{q}_2$  (blue circle); and Bragg vectors (dashed red circles) are indicated. (C) Average  $dI/dV$  spectrum acquired from the area in A, showing kinks at  $\sim \pm 35$  mV ( $\pm \varepsilon_K$ ), the minimum  $\varepsilon_{\min}$  offset from  $\varepsilon_F$  ( $V_{\text{bias}} = 0$ ) by  $\sim 17$  mV, and marked asymmetry about  $\varepsilon_F$ . Setpoint parameters: sample bias,  $V_{\text{sample}} = -50$  mV (A),  $-60$  mV (B) and  $-80$  mV (C); junction resistance,  $R_j = 2.5$  G $\Omega$  (A),  $0.1$  G $\Omega$  (B), and  $0.4$  G $\Omega$  (C); and root mean square (RMS) lock-in excitation,  $V_{\text{rms}} = 3.5$  mV (C).

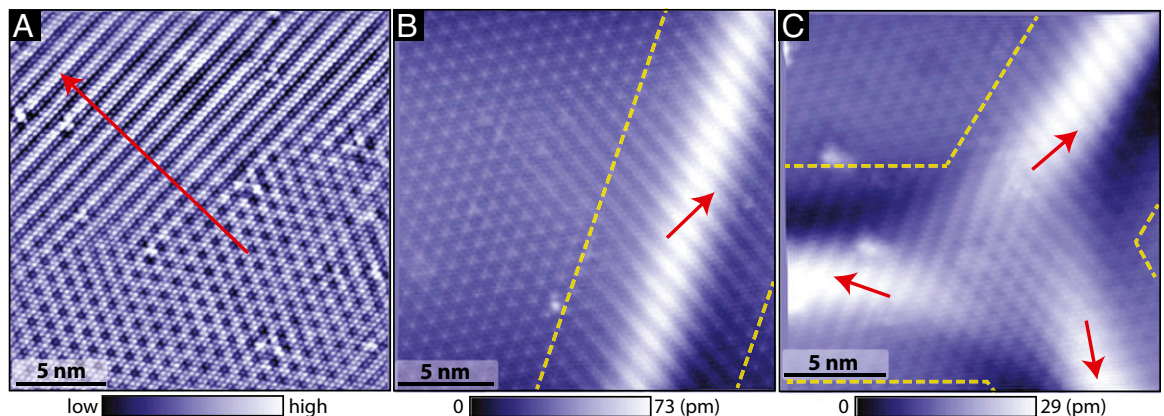
insignificant, implying that the 1Q CDW is a distinct quantum phase.

The 1Q CDW regions take the form of elevated topographic ribbons, exemplified in Fig. 2 B and C, suggesting a strain-induced phase (SI Text II). The observation of Y-junctions between ribbons with differently oriented  $\vec{q}_{1Q}$  rules out extrinsic uniaxial strain and suggests instead locally varying strain, perhaps because of underlying defects causing nanoscale buckling of the top few atomic layers. From a survey of several ribbons, we place upper bounds of 3% on the vertical strain and 0.06% on the lateral strain (SI Text II).

Fig. 3 A and B show the dominant Fourier peak for the 1Q modulation,  $\vec{q}_{1Q} \simeq (2/7)\vec{Q}_0$ , corresponding to a wavelength,  $\lambda_{1Q} \simeq 3.5 a_0$ . No similar periodicity or rich harmonic structure has been reported thus far in any TMDC system (12). We develop a phenomenological understanding of the 1Q harmonic structure following McMillan's Landau theory (22, 25). Rather than a uniform  $3.5 a_0$  charge modulation, the system could lower its energy by locking the charge modulation to the lattice with  $3 a_0$  periodicity. This would require compensation by a one-atom phase slip every two oscillations, corresponding to a  $2\pi/3$  discommensuration, as shown in Fig. 3C (22). The resulting har-

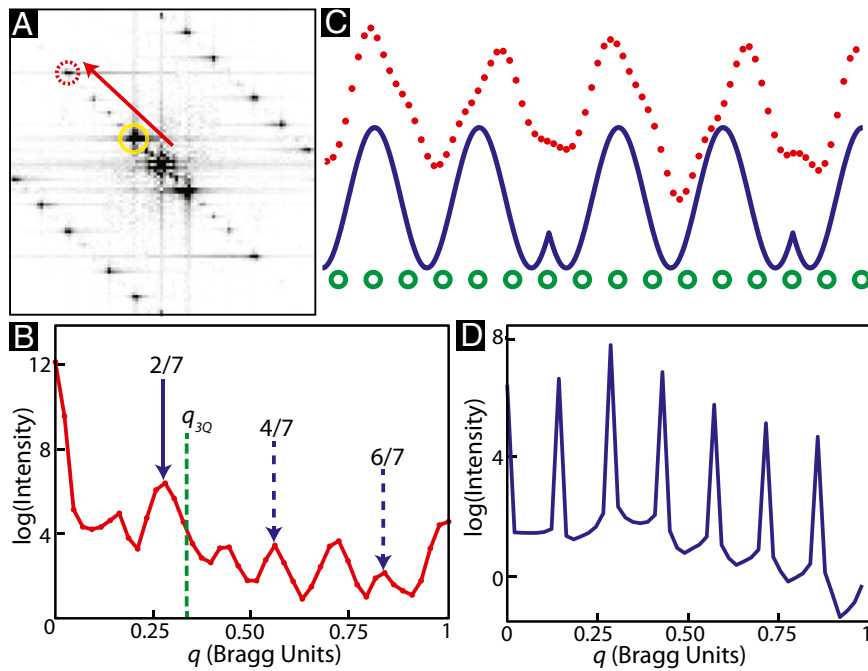
monic structure shown in Fig. 3D reproduces all observed peak positions. Moreover, the rich harmonic content we observe is another indication of the strong coupling of the electronic modulation to the lattice. An even better agreement with relative peak heights might be obtained by considering spatial variations in the order parameter amplitude (22).

The stark contrast between our observation of two CDW wavevectors  $\vec{q}_{1Q}$  and  $\vec{q}_{3Q}$  of the same orientation but with 13% difference in magnitude, and the recent X-ray measurements reported by Feng et al. (10), provides strong evidence against FS nesting at one particular wavevector as a driving force for either CDW. Although our 13% wavevector difference arose from moderate anisotropic strain (up to 0.06% in-plane), Feng et al. applied hydrostatic pressure sufficient to induce in-plane lattice distortions up to 1.6%, yet observed no measurable deviation of the CDW wavevector from  $q_{3Q}$  (10). The observed insensitivity of  $q_{3Q}$  to hydrostatic pressure would clearly indicate that the FS does not qualitatively change in the presence of even relatively large lattice distortions, and thus would rule out a change in the FS as the source of our observed 13% wavevector difference. Furthermore, consistent with our experiment and with previous calculations (6, 15, 16), we find no sharp peak in the susceptibility



**Fig. 2.** The 1Q–3Q interface. (A) Topograph showing an atomically smooth interface between the 3Q (Bottom) and 1Q (Top) CDWs. (B) Topograph showing formation of 1Q CDW along a “ribbon.” Ribbons are typically 10–20 nm in width and elevated by 20–40 pm. Dashed yellow lines indicate the approximate extent of the ribbon; the red arrow points along the 1Q CDW direction ( $\vec{q}_{1Q}$ ). (C) Topograph showing a Y-junction among three such 1Q ribbons, each with a different 1Q CDW direction. The topograph in A has been leveled by removing a polynomial background to show the CDW interface clearly. Setpoint parameters:  $V_{\text{sample}} = -50$  mV,  $R_j = 1$  G $\Omega$  (A and C), and  $5$  G $\Omega$  (B).

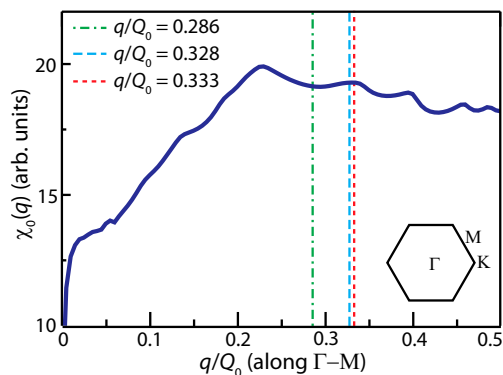




**Fig. 3.** The 1Q CDW. (A) FT of the out-of-feedback current at +50 mV over a 1Q region (upper left quadrant of Fig. 2A). The dominant CDW wavevector (yellow circle) and Bragg vector (dashed red circle) are indicated. (B) Linecut of the FT intensity parallel to the red line in A from the center to the Bragg peak, in units of the Bragg vector  $Q_0$ . The dominant peak,  $q_{1Q} \approx (2/7)Q_0$  (solid blue arrow), and its harmonics (dashed blue arrows) are identified and are distinct from the 3Q wavevector  $q_{3Q}$  (dashed green line). The remaining peaks are Bragg reflections of these three peaks. Setpoint parameters:  $V_{\text{sample}} = -50$  mV and  $R_j = 0.2$  G $\Omega$ . (C) Phenomenological model of the observed 1Q CDW wavelength,  $\lambda_{1Q} \approx 3.5 a_0$  (details in text). The atomic periodicity is indicated by green circles, and the phase of the CDW order parameter from the model is shown in blue (22). A topographic linecut (red dots) is extracted from Fig. 2A along the red arrow ( $\vec{q}_{1Q}$ ), filtered to remove atomic corrugations and overlaid for comparison. (D) Simulated FT intensity from the cartoon CDW modulation in C, for comparison with experimental peak positions in B.

(Fig. 4) computed from our modeled band structure (SI Text III). Therefore, our observations and calculations both indicate that the FS can play only a minor role in determining CDW wavevectors in NbSe<sub>2</sub>. This highlights the key role the  $q$ -dependence of alternative mechanisms, such as electron–phonon coupling, may play in driving the transition, and particularly the manner in which these mechanisms may be influenced by local strain.

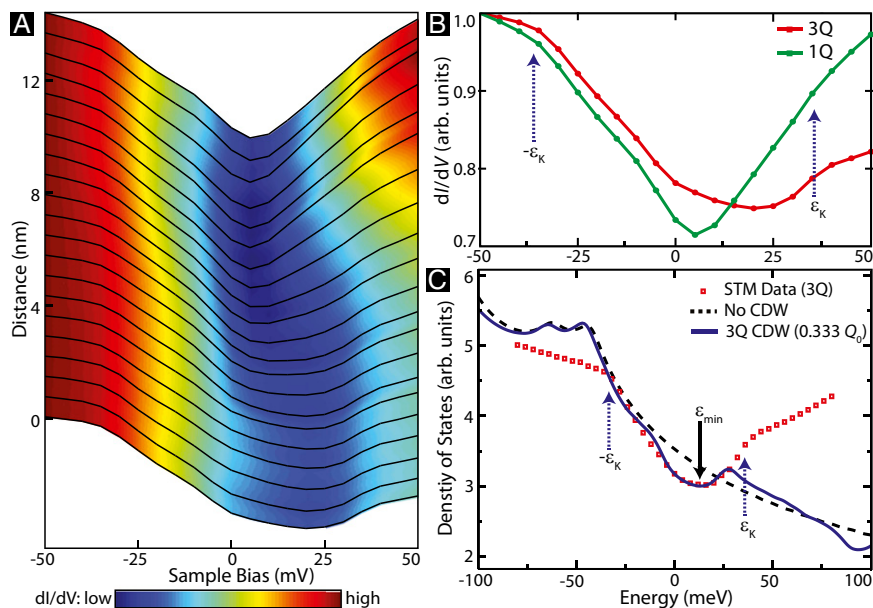
The two CDW regions display quite different tunneling spectra, as shown in Fig. 5 A and B. We use a fit to the NbSe<sub>2</sub> band



**Fig. 4.** Susceptibility. The noninteracting susceptibility  $\chi_0(q, \omega=0)$  calculated from a fit to the NbSe<sub>2</sub> band structure (SI Text III) along the  $\Gamma$ –M direction of the reciprocal lattice, displaying a broad maximum over a range of wavevectors:  $\vec{q} \sim (0.25 - 0.4)Q_0$  (6, 15, 16). The CDW wavevectors  $q_{1Q}$ ,  $q_{3Q}$ , and  $Q_0/3$  are overlaid for comparison. (Inset) Brillouin zone (BZ) of the hexagonal NbSe<sub>2</sub> lattice.

structure (SI Text III) and impose a CDW wavevector  $\vec{q}$ , gap  $\tilde{\Delta}$ , and broadening parameter  $\tilde{\Gamma}$  to calculate the density of states (DOS) in Fig. 5C (SI Text IV). For the 3Q CDW state, the measured  $dI/dV$  spectrum, proportional to the DOS, is reproduced best using  $\vec{q} = (0.333 \pm 0.004)Q_0$  (the observed local CDW periodicity),  $\tilde{\Delta} = (12 \pm 2)$  mV (which previously was not apparent from direct observations by spectroscopic techniques), and  $\tilde{\Gamma} = 5$  mV. The calculations capture the overall shape, width, and center  $\varepsilon_{\text{min}}$  of the gap structure within 30 mV of  $\varepsilon_F$  (SI Text IV). The fact that  $\varepsilon_{\text{min}}$  is offset from  $\varepsilon_F$  should be unsurprising for a quasi-2D system (26), but had not been understood or observed in NbSe<sub>2</sub> until now because of the limitations of spectroscopic techniques, which are sensitive to filled states only (13).

We disentangle the CDW gap from other effects in the 3Q spectra through a comparison with the 1Q spectra in Fig. 5B. These V-shaped 1Q spectra resemble the linear tunneling conductance background historically attributed to the inelastic coupling of tunneling electrons to a flat bosonic spectrum (27). That this background is much stronger in the 1Q region, obscuring band structure effects, likely is a strain-induced phenomenon, which may be related to the buckling and associated decoupling of the topmost layers in the 1Q region. Meanwhile, present in both 1Q and 3Q spectra (thus, unlikely to be associated with these different CDWs), yet absent in calculations (thus, unlikely to be a band structure effect), are the  $\pm 35$  mV kinks, previously and mistakenly identified as the CDW gap (21). We universally observe the kinks even well above  $T_{\text{CDW}}$ , which further demonstrates their lack of bearing on the CDW phase (SI Text IV). ARPES studies observe a prominent band structure kink at a similar energy in the Se  $\Gamma$ -pocket (16, 19), attributed to coupling to an optical phonon (14). Therefore, we conclude that this self-energy effect is responsible for the  $\varepsilon_K$ -kinks in the tunneling spectra as well. The discrepancy between the data



**Fig. 5.** Spectroscopy across the 1Q–3Q interface. (A) Linecut of  $dI/dV$  spectra across the 1Q–3Q interface taken along the red arrow in Fig. 2A. (B) Representative spectra in the 3Q (red) and 1Q (green) regions of Fig. 2A are overlaid for comparison. The 1Q spectra have a minimum close to  $\epsilon_F$ , a deep V-shape with reduced asymmetry, and kinks at  $\pm\epsilon_K$ . The spectra are normalized at  $-50$  mV. Setpoint parameters:  $V_{\text{sample}} = -50$  mV,  $R_f = 0.2$  G $\Omega$ , and  $V_{\text{rms}} = 3.5$  mV. (C) Calculated DOS for NbSe<sub>2</sub> in the “normal” state (black) and in the presence of a 3Q CDW (blue) using  $\tilde{q} = 0.333Q_0$ ,  $\tilde{\Delta} = 12$  mV, compared with the 3Q STM spectrum (red) (details in *SI Text IV*). The calculations reproduce the observed asymmetry, offset  $\epsilon_{\text{min}}$ , and shape of the gap structure.

and band structure calculations above  $\sim 30$  mV in Fig. 5C thus may be attributed to the inelastic tunneling background and self-energy effects.

## Discussion

We therefore resolve a longstanding debate about the anomalous CDW gap magnitude reported by STM measurements (21), and caution that not all  $\epsilon_F$ -symmetric kinks in tunneling spectra are associated with order (e.g., density wave or superconducting gaps). On the contrary, we emphasize that the true CDW signature in NbSe<sub>2</sub> is offset from  $\epsilon_F$ , which has confused an active research community for two decades, and has been disentangled now only by a combination of spatially resolved filled- and empty-state spectroscopy of a proximate (1Q) phase and band structure calculations (26). This emphasizes the need for full experimental exploration of proximate phases in other pertinent materials, combined with quantitative modeling. We further suggest that controlled local strain, through epitaxy or intentional defects, may be a useful tuning parameter to access the necessary proximate phases for comparison.

Beyond providing unique insight into the nature of the 3Q CDW in NbSe<sub>2</sub>, our work motivates the utility of the 1Q–3Q interface in NbSe<sub>2</sub> as a platform to explore competing quantum phases in the weakly correlated limit, as a step toward understanding them in strongly correlated systems. In the Landau picture of CDWs (25), a quantum phase transition between 3Q and 1Q states may arise by tuning the coefficient of the interaction term among the three inequivalent CDW propagation directions (although in our case, the magnitude of  $q$  differs between the two states). In NbSe<sub>2</sub>, even at low temperatures  $T \ll T_{\text{CDW}}$ , where the amplitude of the order parameter is already large, moderate strain is seen to have a strong influence, indicating that the system is intrinsically close to the QCP separating these states. We note that a related phase transition between the observed 1Q CDW phase and a “hidden” 2Q phase has been suggested, but not directly visualized, in the rare-earth tritellurides (28, 29).

Our discovery provides a unique perspective on the role of density wave order in complex systems. First, our resolution of

two longstanding debates about NbSe<sub>2</sub> puts this much-studied material on firmer footing as a well-understood model system for CDW studies and competing ground states in superconductors. We have disentangled the true CDW gap, and clarified that FS nesting plays a minor role in determining the CDW wavevectors in this material, thereby highlighting the role of other mechanisms in driving the transition. Second, our revelation of a particle-hole asymmetric CDW gap emphasizes the limitations of filled-state-only probes, e.g., ARPES, for investigating phases other than SC—which is unambiguously particle-hole symmetric. Full spectral probes such as STM, in combination with quantitative calculations, are necessary to understand the competition between SC and particle-hole asymmetric phases. Third, our observation of the local effect of even moderate strain in driving a quantum phase transition calls for a reinvestigation of possible phase inhomogeneity in other strongly correlated systems, in which larger strain may occur (30, 31).

In the cuprate superconductors, an analogous phase boundary between unidirectional (1Q) charge “stripes” and bidirectional (2Q) “checkerboard” has been predicted (32, 33). The introduction of quenched disorder results in discommensurations in the 2Q phase and disordered orientational order in the 1Q phase, making them hard to distinguish—especially in the cuprate superconductors, thought to be in proximity to the 1Q–2Q phase boundary (32, 33). Recent STM studies of the  $\sim 4a_0$  charge order in the cuprate Bi<sub>2</sub>Sr<sub>2</sub>Ca<sub>n-1</sub>Cu<sub>n</sub>O<sub>2n+4+x</sub> (BSCCO) have had conflicting interpretations, with independent suggestions of fluctuating 2Q and 1Q order (34, 35). However, the influence of strain, from the supermodulation lattice buckling or from randomly distributed dopants, is seldom accounted for. Previous studies have shown that both these strain phenomena correlate with nanoscale electronic inhomogeneity (30, 36). A possible explanation is local stabilization of the 1Q state, producing 1Q–2Q and 1Q–1Q interfaces with spectral differences, analogous to Figs. 2 and 5A and B. Although the presence of strong disorder [up to 12% strain variations on a nanometer length scale (30)] complicates the interpretations in BSCCO, we stress the importance of isolating and modeling strain effects for better

understanding and control of the phase transitions in cuprates. Finally, the microscopic visualization of the role of strain in stabilizing new order suggests a controlled route toward engineering novel quantum phases and interfaces and studying symmetry breaking in strongly correlated materials. In this regard, we suggest a connection to the emerging importance of strain as a route to high- $T_c$  superconductivity in novel iron-based materials (37, 38).

## Materials and Methods

**STM Experiments.** Measurements were performed using a home-built STM at temperatures between 2 K and 10 K. Magnetic fields of up to 6 T were used to suppress the superconducting state as needed. Single crystals of 2H-NbSe<sub>2</sub> were cleaved in situ in cryogenic ultrahigh vacuum and inserted into the STM. A mechanically cut Pt-Ir tip, cleaned by field emission and characterized on gold, was used for the measurements. Spectroscopy data were acquired using a lock-in technique at 1.115 kHz. The topographic and spectroscopic signatures of the 1Q ribbons have been verified with several tips.

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**Band Structure and DOS Calculations.** The band structure of 2H-NbSe<sub>2</sub> close to  $E_F$  consists of two Nb-4d-derived bands and one Se-4p “pancake”-shaped hole pocket (6). The Nb-4d bands are modeled using a tight-binding fit to the observed ARPES band structure (16), and the Se-4p pocket is approximated by a simple quadratic form to fit first principles calculations (6) (details in *SI Text III*). Using all three bands, the DOS in the presence of a CDW is calculated by imposing a constant coupling between electronic states connected by any one of the three  $q$ -vectors. The strength of the coupling  $\Delta$  is taken as a free parameter in the reproduction of the experimentally observed DOS, and the size of  $\tilde{q}$  is allowed to vary slightly around the observed value of 0.328  $Q_0$  (details in *SI Text IV*).

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