Asymmetry of the energy dependence the charge density wave modulation of 2*H*-$NbSe_2$ by STM/STS

Christian Lupien

Behnaz Behmand

Université de Sherbrooke, Qc, Canada

UNIVERSITÉ DE SHERBROOKE

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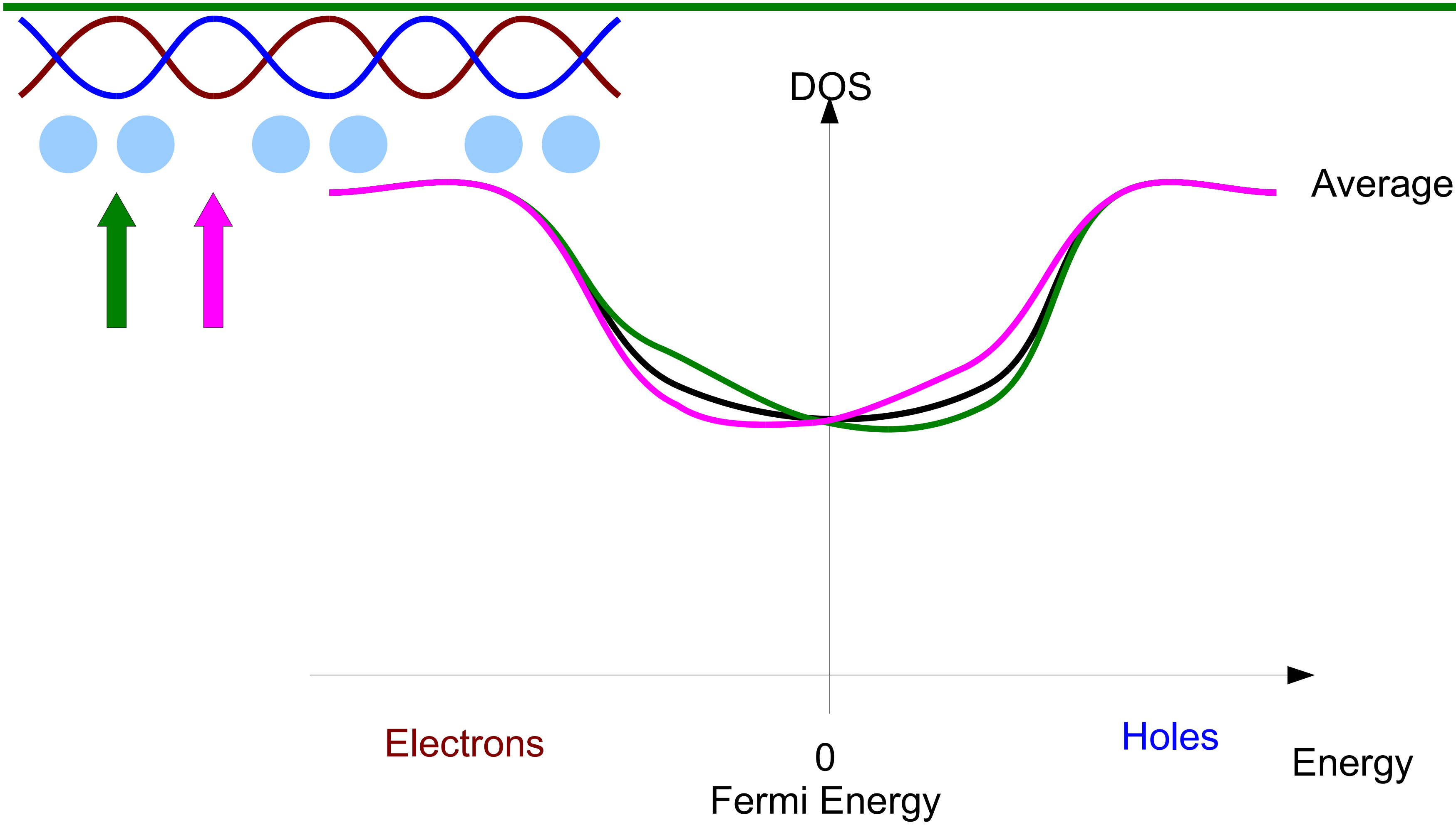
What kind of density modulation?

- Interest in the high-T_c superconductors (cuprates) but:
  - Complicated systems; complex phase diagrams
    - STM/STS measurements show many structures
  - Are some of them conventional CDW? Or are they pair-density waves (PDW), or ...

Charge modulation symmetry

- How to separate conventional CDW from a PDW for example
- Expect different symmetry for the modulation vs energy :
- For conventional 1D CDW: $n(E,\vec{q}) = -n(-E,\vec{q})$
- For a PDW: $n(E,\vec{q}) = n(-E,\vec{q})$

Model of conventional 1D CDW



How to identify symmetry in practice?

- STM/STS: conductance (*g*) is *proportional* to the LDOS (*n*)
- Therefore the STS conductance map should be able to identify the presence of a pure CDW.
- But constant current conditions on topo/maps:

$$g(V,\mathbf{r}) = I_0 \frac{n(eV,\mathbf{r})}{\int_0^{V_0} n(eV,\mathbf{r})dV}$$

Both terms vary in space!

Constant current setpoint effect

- Setpoint parameters: I_0 and V_0
- Easy to show that

$$\int_0^{eV_0} g(E,k)\,dE = 0$$

- $\rightarrow$ g(E,k) needs to change sign at least once between 0 and eV_0 because of setpoint
- Also

$$g_0 = \frac{I_0}{N_0} n_0(E)$$

$$g_{k1} = \frac{I_0}{N_0}\left(n_{k1}(E) - n_0(E)\frac{N_{k1}}{N_0} \right)$$

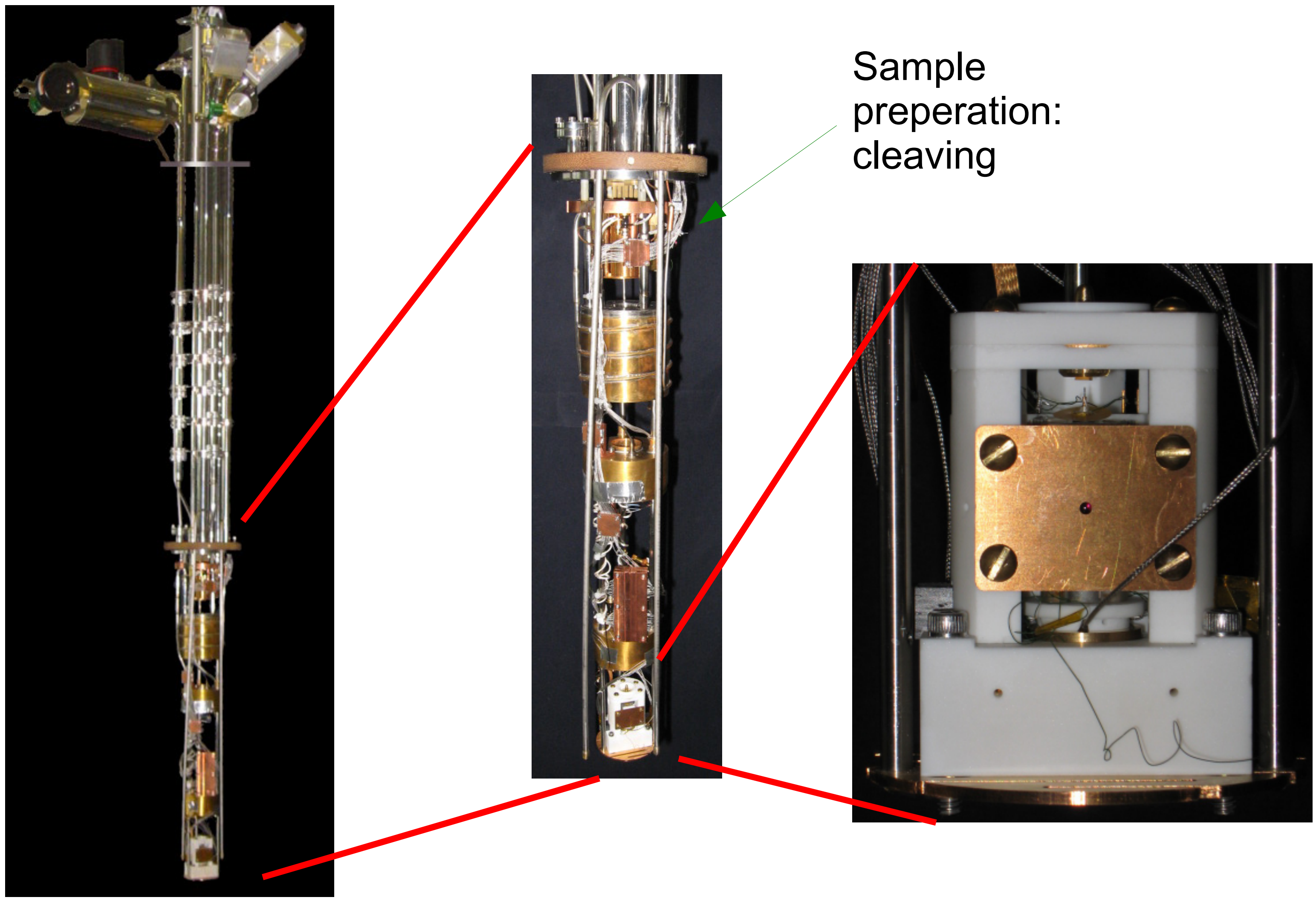
Expected terms

Effect of setpoint

$NbSe_2$

- Since cuprates are complicated systems
  - Want to check ideas/analysis on something simpler
- Choose $NbSe_2$
  - A well known CDW material (T_{CDW} ~ 33K)
  - Also a superconductor (T_C ~ 7K)
  - Surface prepares easily
  - Not fully understand (but better than cuprates) and very well characterized

He3 cryostat + Microscope



330 mK for 50 hours

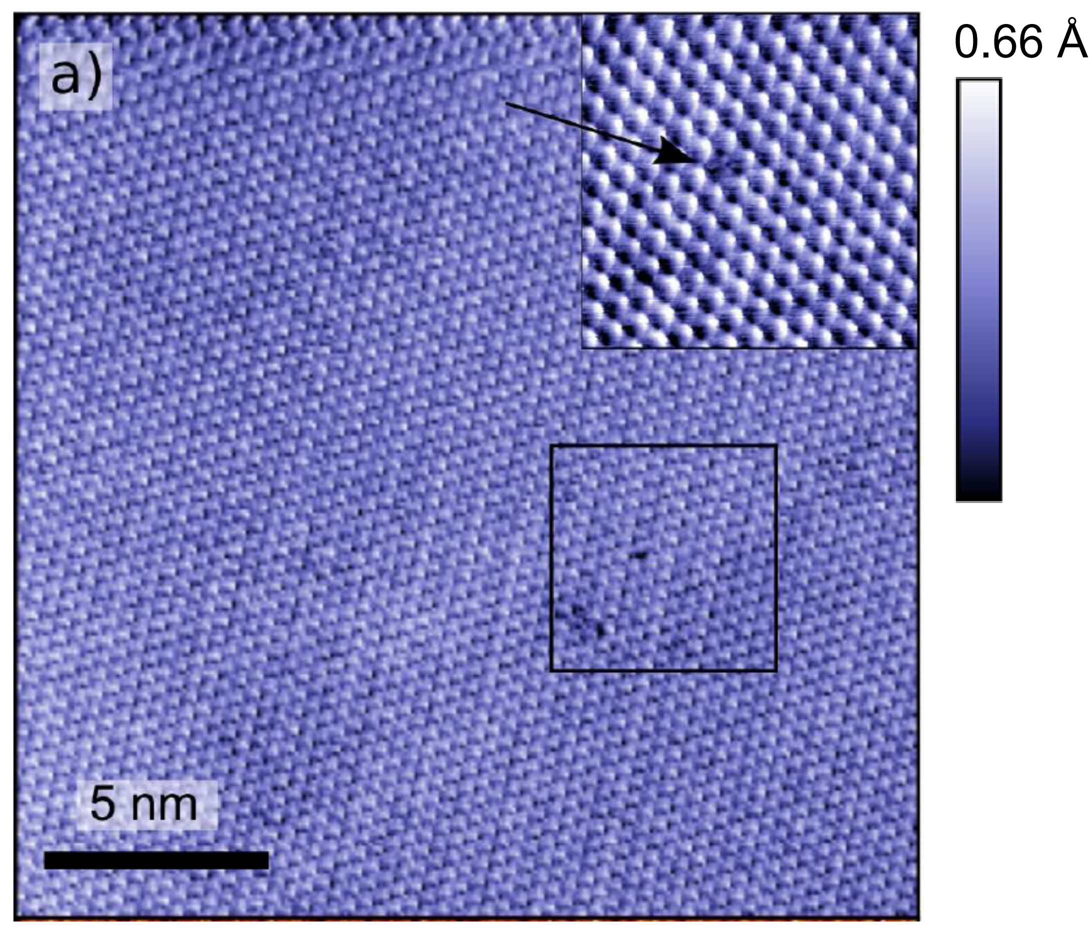
$NbSe_2$ Topography

Samples from T.T.M Palstra (Groningen)

Conditions:

- Temperature = ~450 mK
- V_{sample} = -100 mV
- I_{tunnel} = 100 pA
- Image size: 20x20 nm

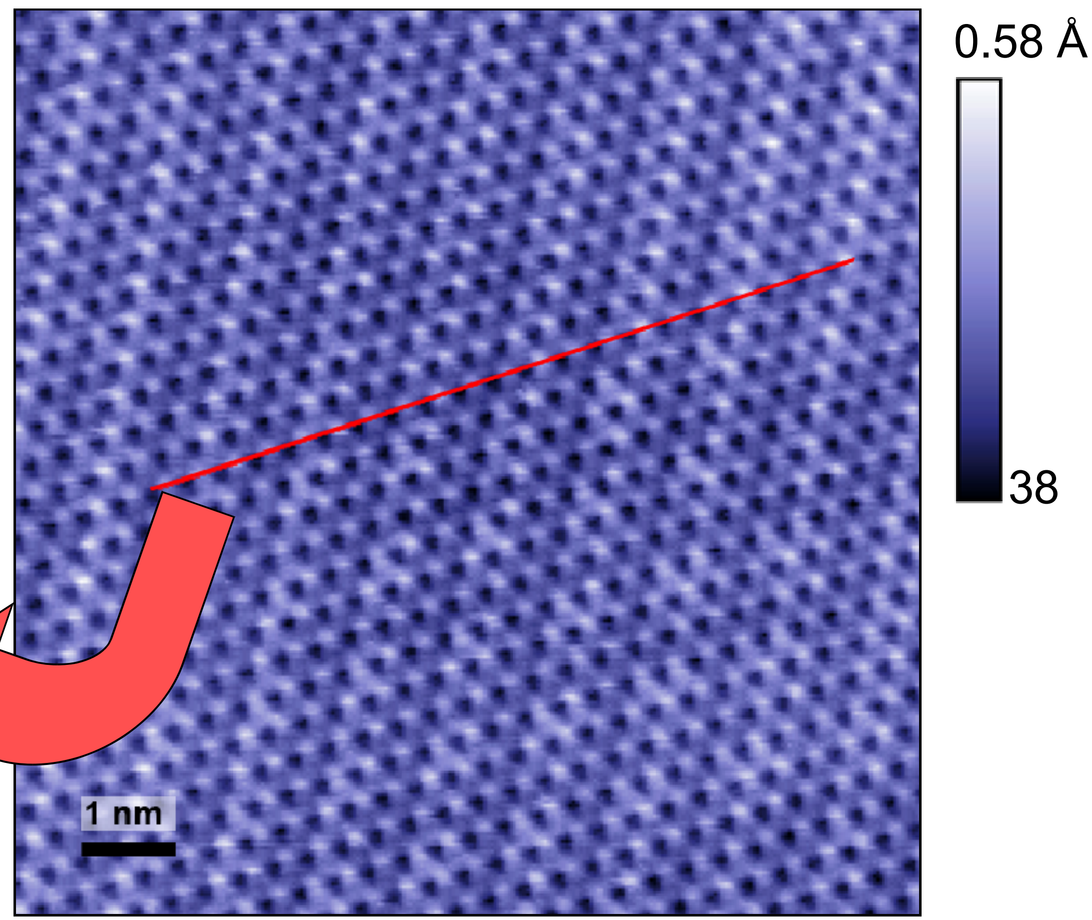
A defect on the surface is present (good resolution)

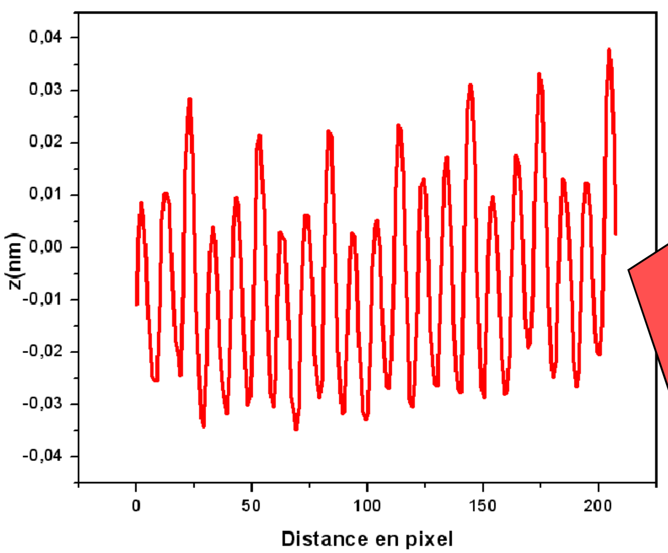


$NbSe_2$ CDW modulation

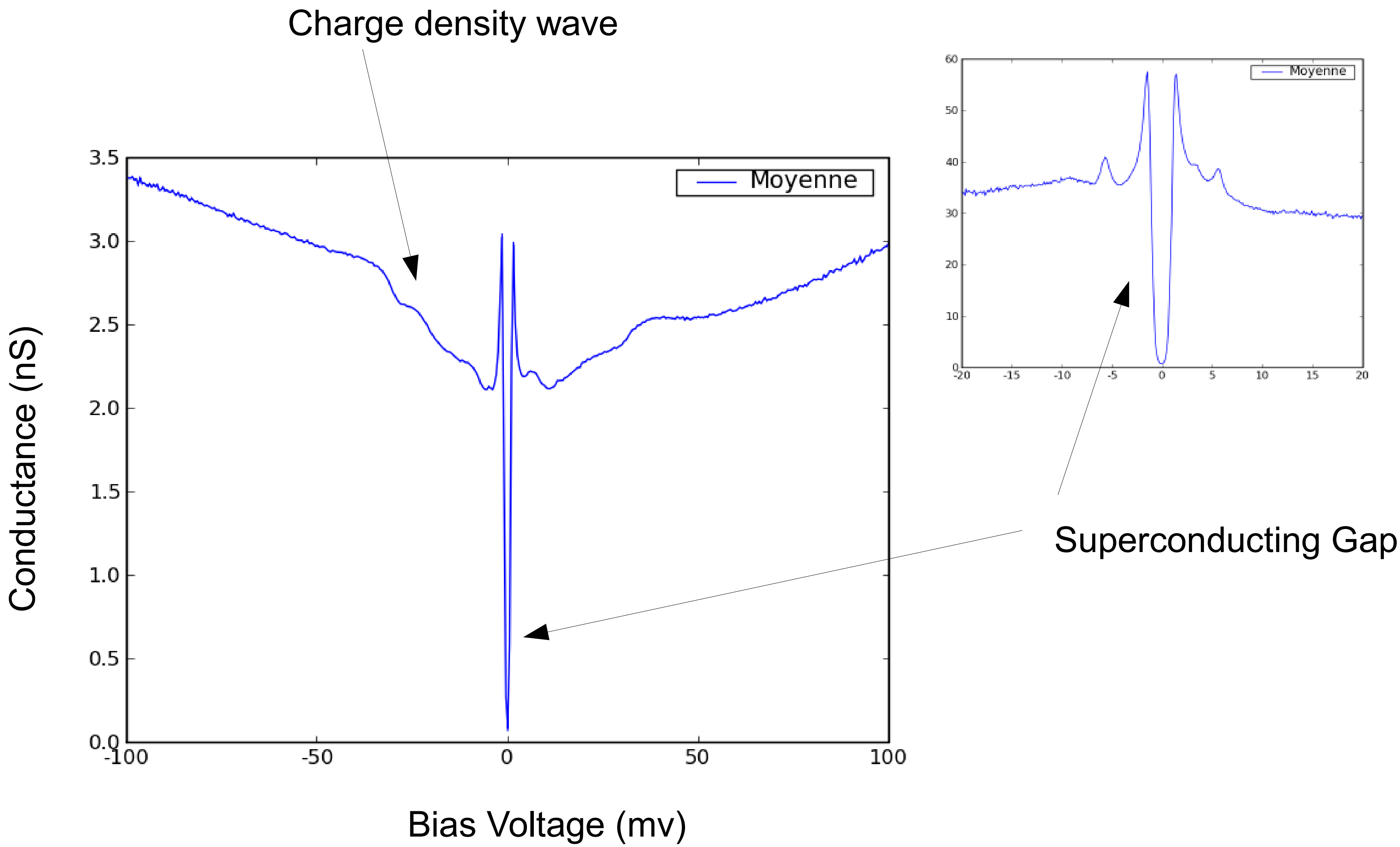
Temperature = ~450 mK

- V_{sample} = -100 mK
- I_{tunnel} = 100 pA
- Image size: 10x10 nm

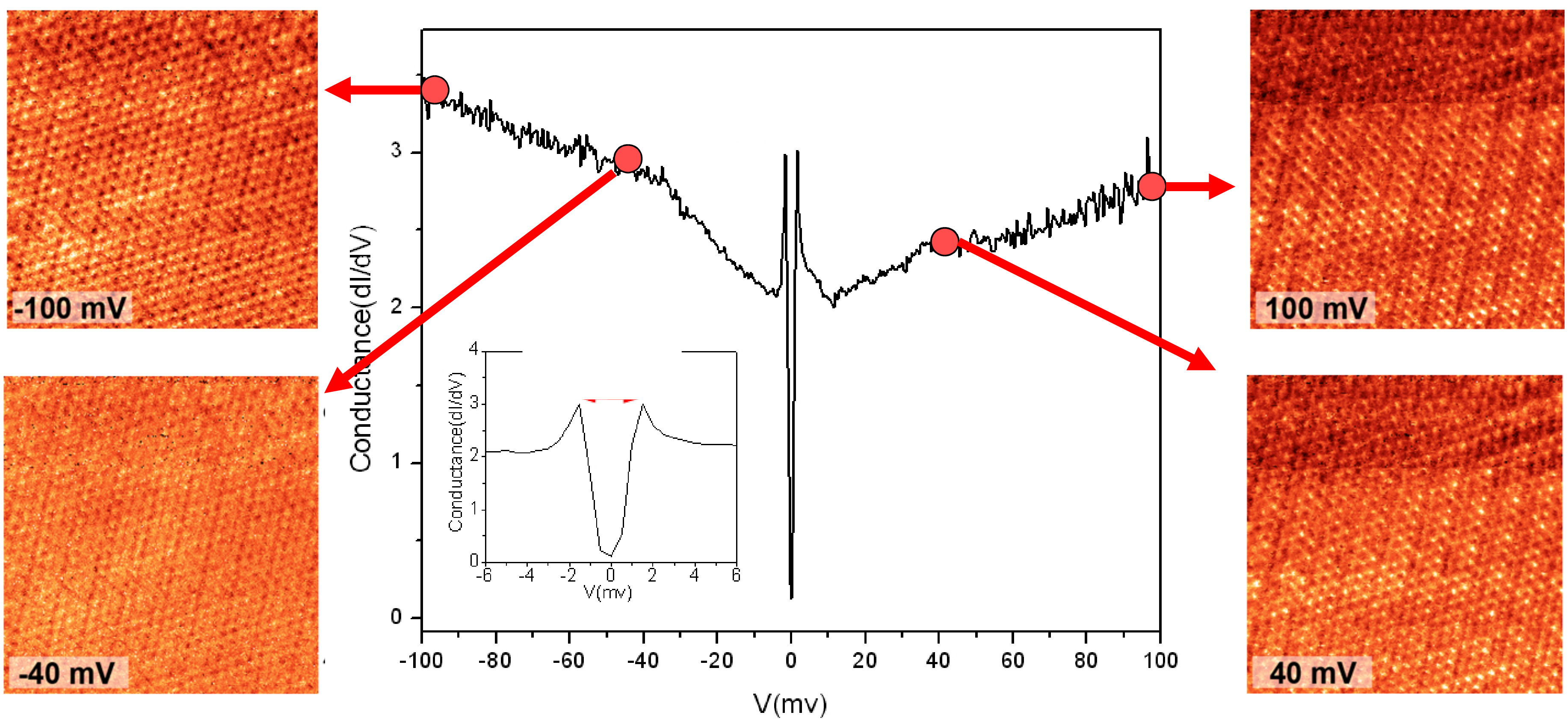




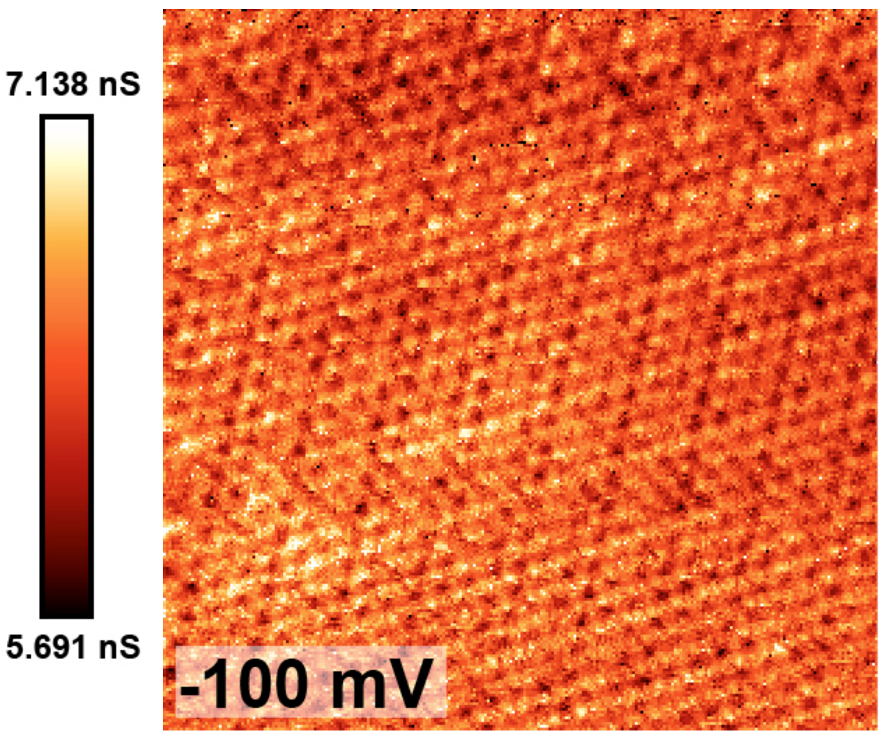
Average spectra @ 450 mK



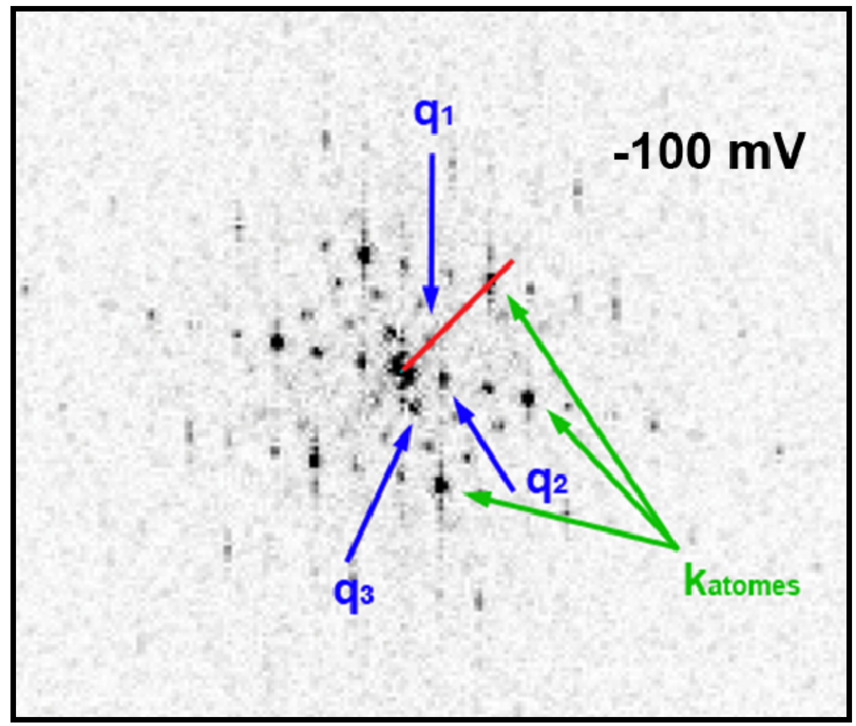
Conductance maps



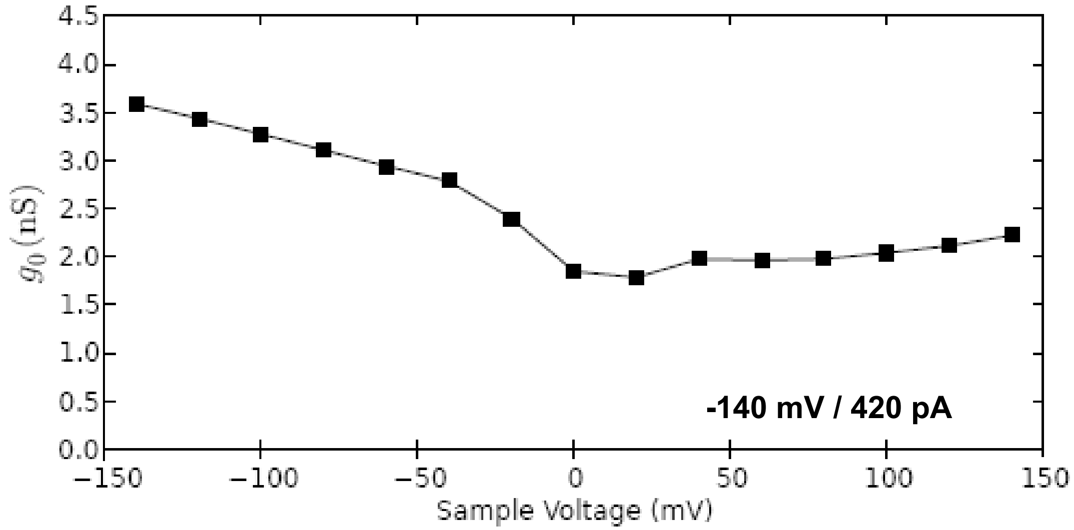
Fourier transform



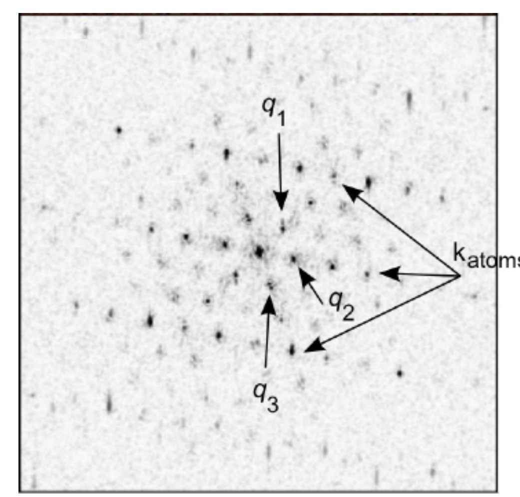
10 x 10 nm   -400 mV/120 pA

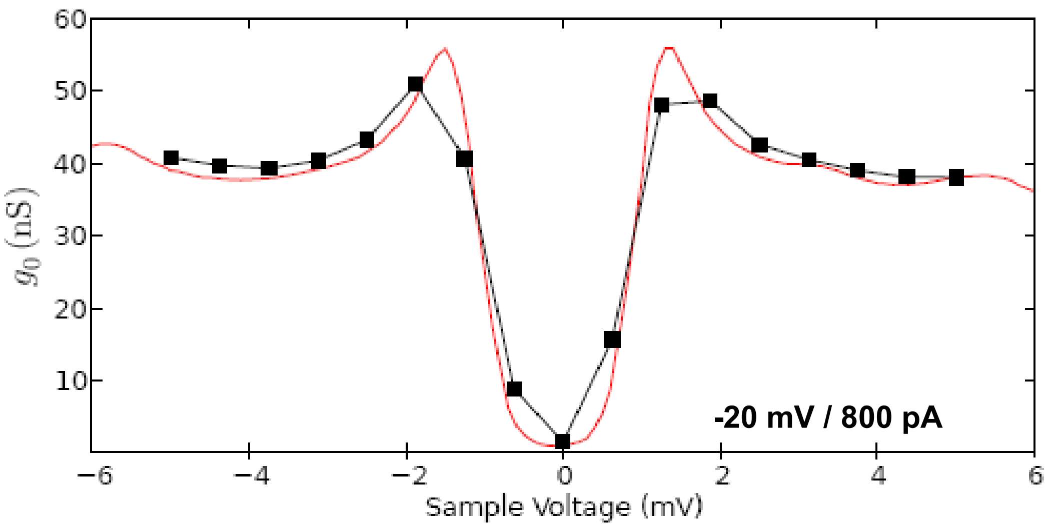


Average conductance signal: n(q=0,E)



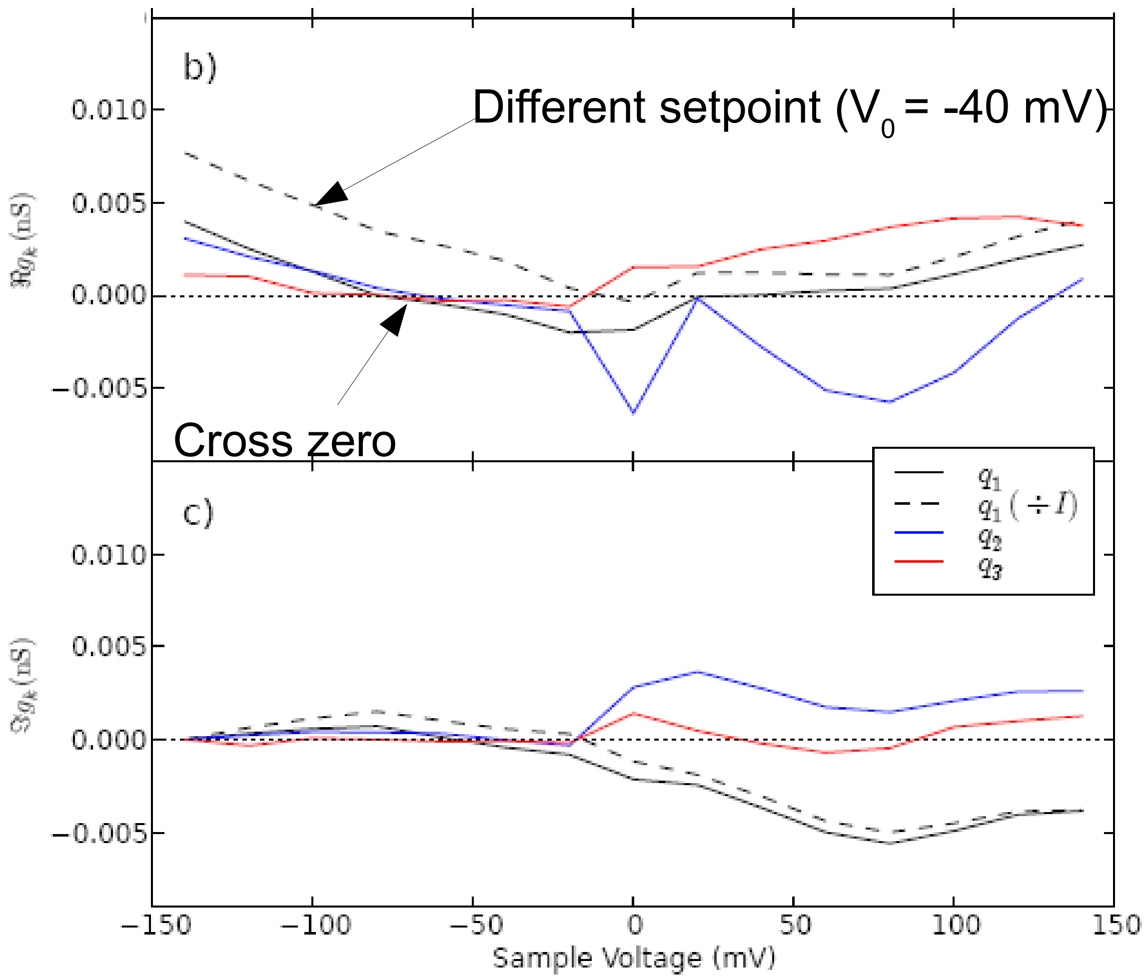
High energy
(some asymmetry)





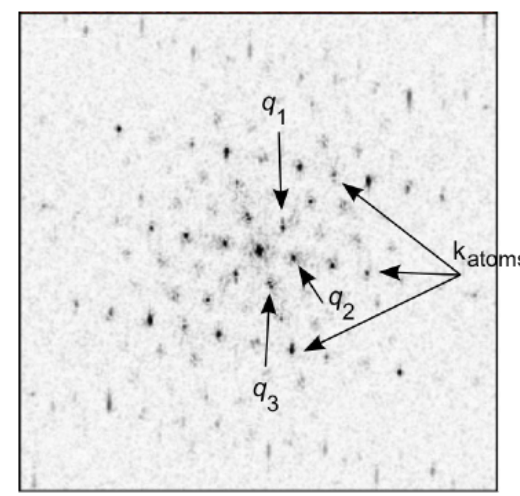
Low energy
(superconducting gap)

$n(q_{CDW},E)$ real and imaginary parts



-140 mV / 420 pA

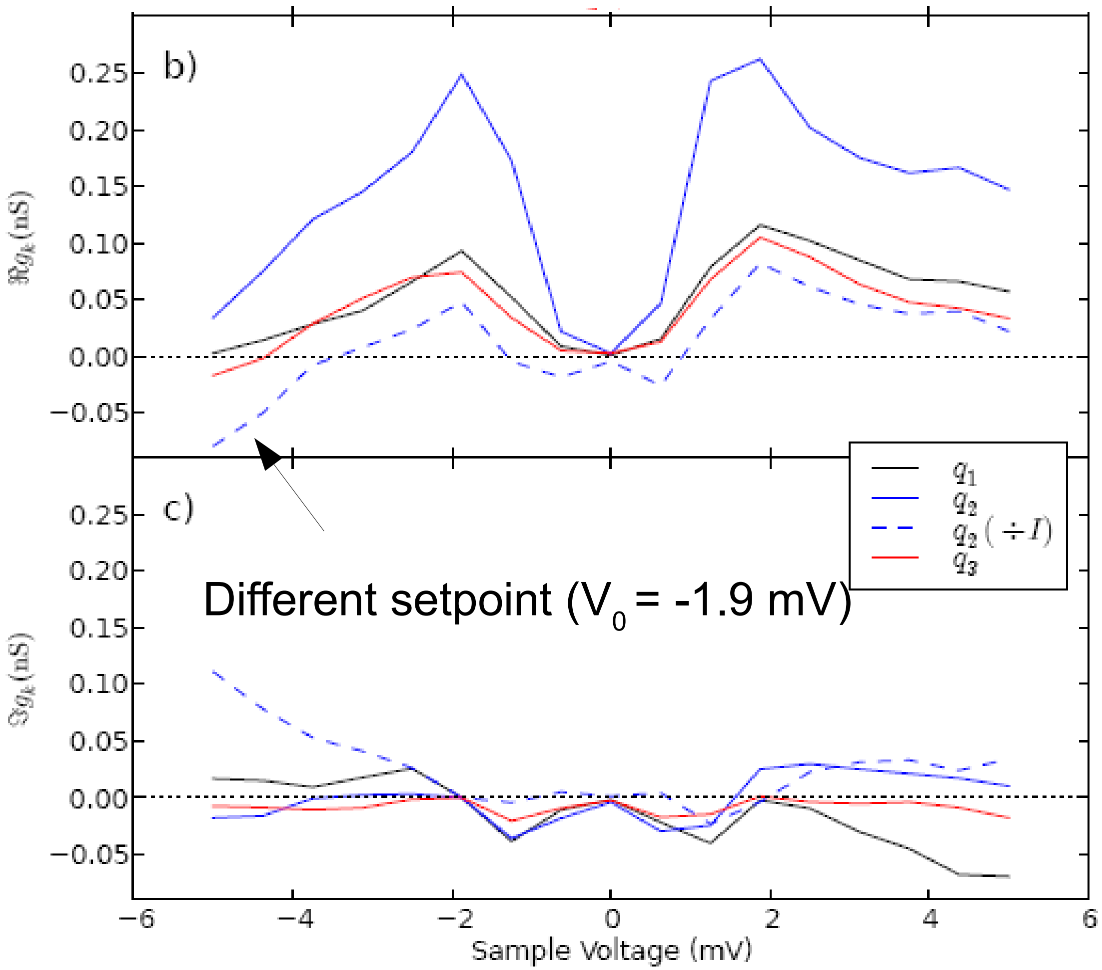
$$g_{k1} = \frac{I_0}{N_0}\left(n_{k1}(E) - n_0(E)\frac{N_{k1}}{N_0}\right)$$



$NbSe_2$ expects 120° instead of 180°

Sacks, Roditchev & Klein, PRB 57, 13118 (1998).

$n(q_{CDW},E)$ at low energy



-20 mV / 800 pA

Looks symmetric. PDW?

No!
Setpoint effect

Symmetry from Z ratio

$$Z(V,\mathbf{r}) = \frac{g(V,\mathbf{r})}{g(-V,\mathbf{r})}$$

⇒ **The ratio removes the setpoint effect**

$$Z_{k1} = \frac{g_0^+}{g_0^-}\left(\frac{g_{k1}^+}{g_0^+} - \frac{g_{k1}^-}{g_0^-}\right)$$

≠ 0 if asymmetric

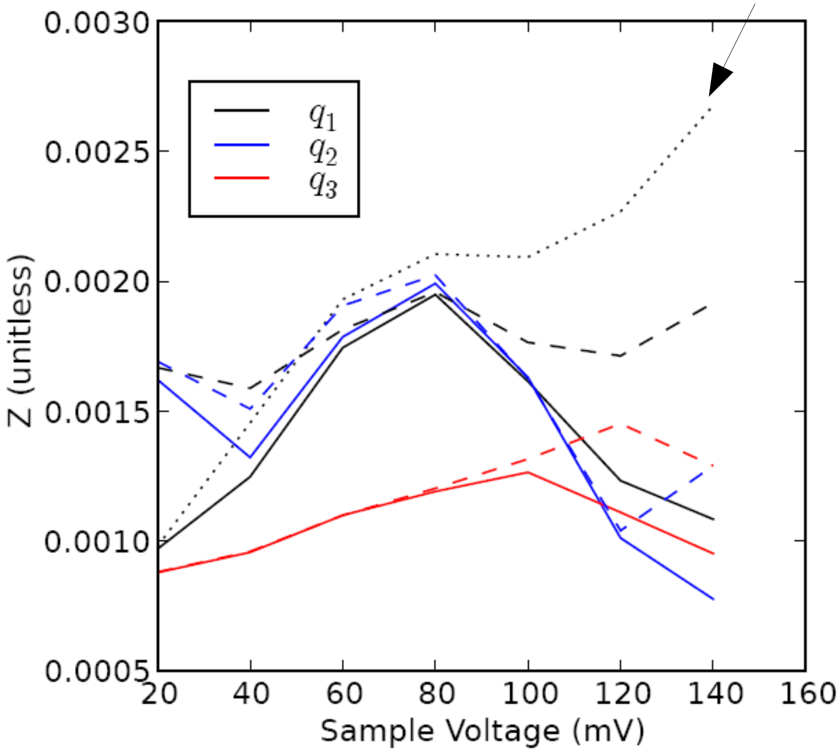
= 0 if symmetric or nothing

Forcing the asymmetry

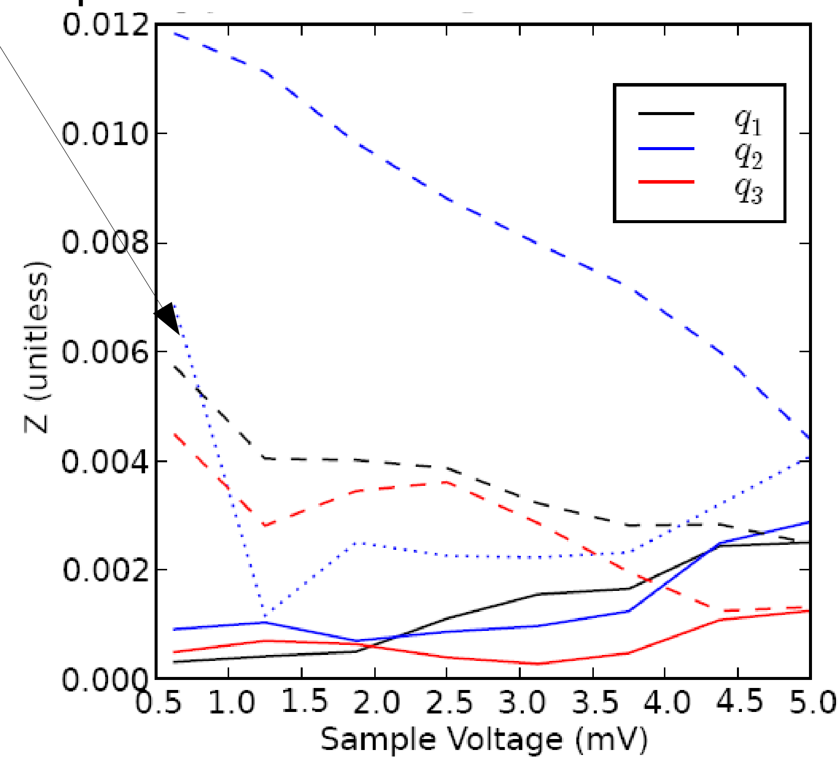
$$Z_{\max}(V,q) = \frac{g_0^+}{g_0^-}\sqrt{\left(\left|\frac{\Re_{g_q^+}}{g_0^+}\right| + \left|\frac{\Re_{g_q^-}}{g_0^+}\right|\right)^2 + \left(\left|\frac{\Im_{g_q^+}}{g_0^+}\right| + \left|\frac{\Im_{g_q^-}}{g_0^+}\right|\right)^2}$$

Zratio

Different setpoint



-140 mV / 420 pA



-20 mV / 800 pA

Signal similar to Z_{max}
Peaks ~ 80 mV

Signal small (PDW or nothing)
Very different from Z_{max}
Except for modified setpoint.

Conclusions

- Extracting energy symmetry at particular wavevector is hard even for the simpler $NbSe_2$
  - Effect of setpoint
- $NbSe_2$ is asymmetric as expected but modulations are present over a large energy range (peeking around 80 meV)