

Title: Two Studies in Incommensurate Charge Order

Date: Oct 25, 2016 03:30 PM

URL: <http://pirsa.org/16100064>

Abstract:

Incommensurate charge order is a phenomenon in which the electrons in a crystal attempt to order with a period irrationally-related to that of

the lattice spacing. In the first half of this talk I will present recent work [1] in which we demonstrate that incommensurately charge-ordered systems can lower their free energy by forming quasicrystals: slices through higher-dimensional crystals with properties lying between periodicity and disorder. The result potentially greatly increases the number of known, naturally-occurring quasicrystals from the two present examples, both of which were found in the same Siberian meteorite. In the second half I will present work from an ongoing experimental collaboration in which atomically-resolved scanning tunneling microscopy and atomic force microscopy on semiconducting monolayers of molybdenum diselenide (MoSe₂) see conducting edge states along one-dimensional mirror twin boundaries. Remarkably, these edge states then develop their own energy gap via charge ordering [2]. We see a number of features suggestive of incommensurate order. By employing a simple analytical model we demonstrate that the effect is in fact a result of fine-tuning between charge ordering and quantum well physics coming from the small system size (on the order of thirty atoms).

[1] F. Flicker and Jasper van Wezel, Physical Review Letters 115, 236401

(2015), Natural 1D Quasicrystals from Incommensurate Charge Order

[2] S. Barja et al., Nature Physics 12, 751-757 (2016), Charge density

wave order in 1D mirror twin boundaries of single-layer MoSe₂

Two Studies in Incommensurate Charge Order

Felix Flicker



The English-Speaking Union



Part I: Natural Quasicrystals from Incommensurate Charge Order

Part II: Incommensurate Charge Order in MoSe₂ Mirror Twin Boundaries

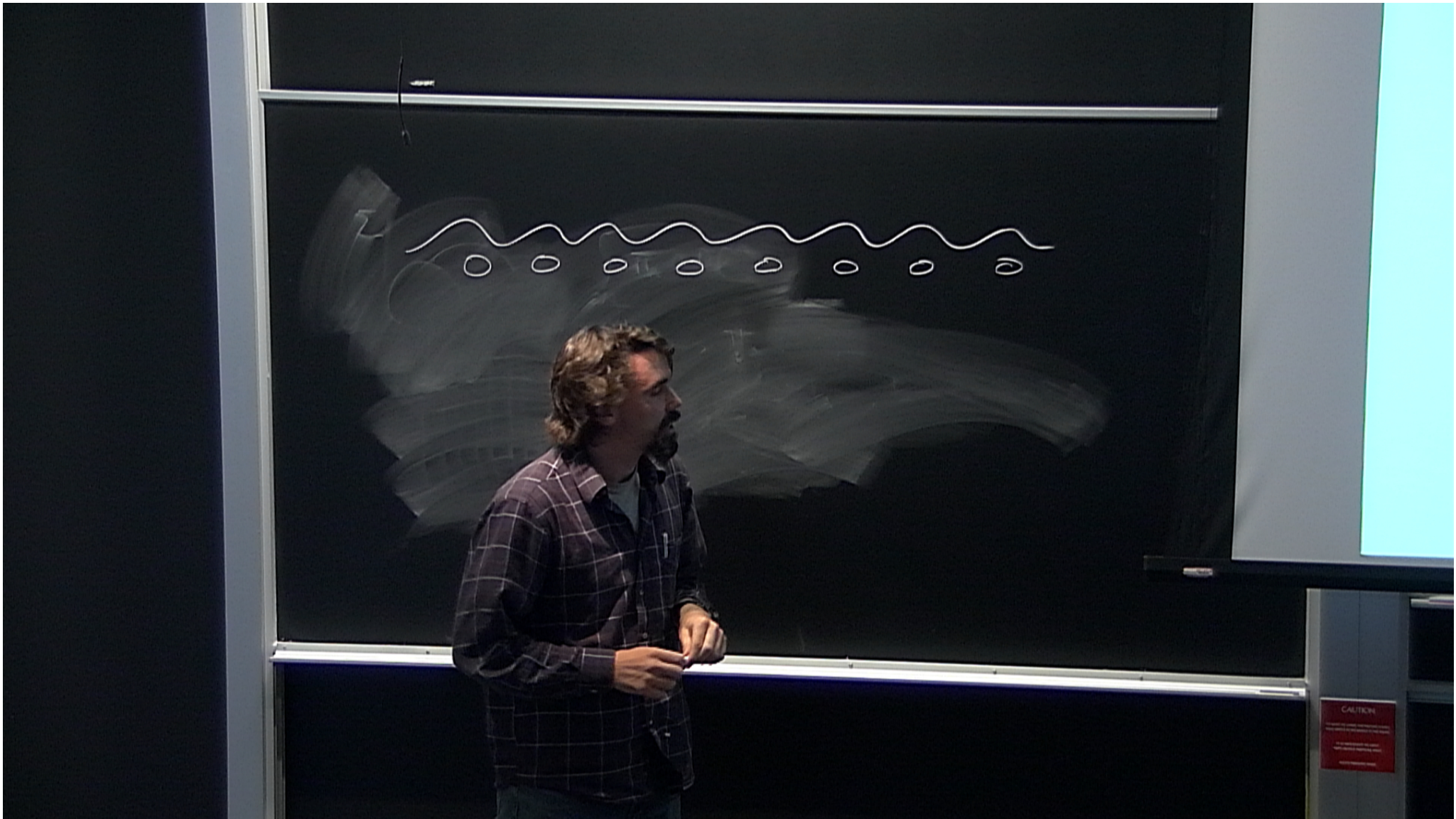
Part I: Natural Quasicrystals from Incommensurate Charge Order

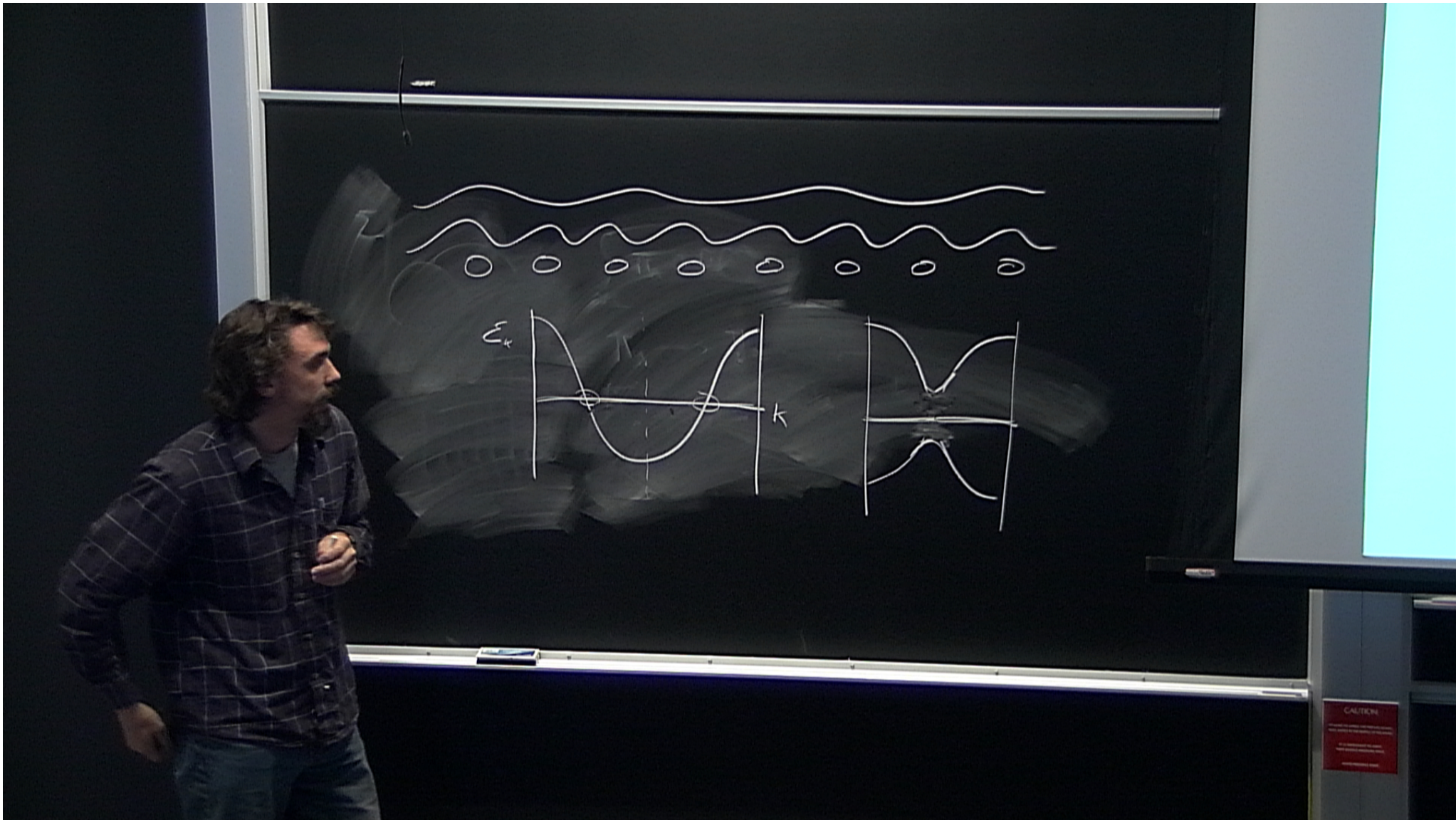
Part I: Natural Quasicrystals from Incommensurate Charge Order

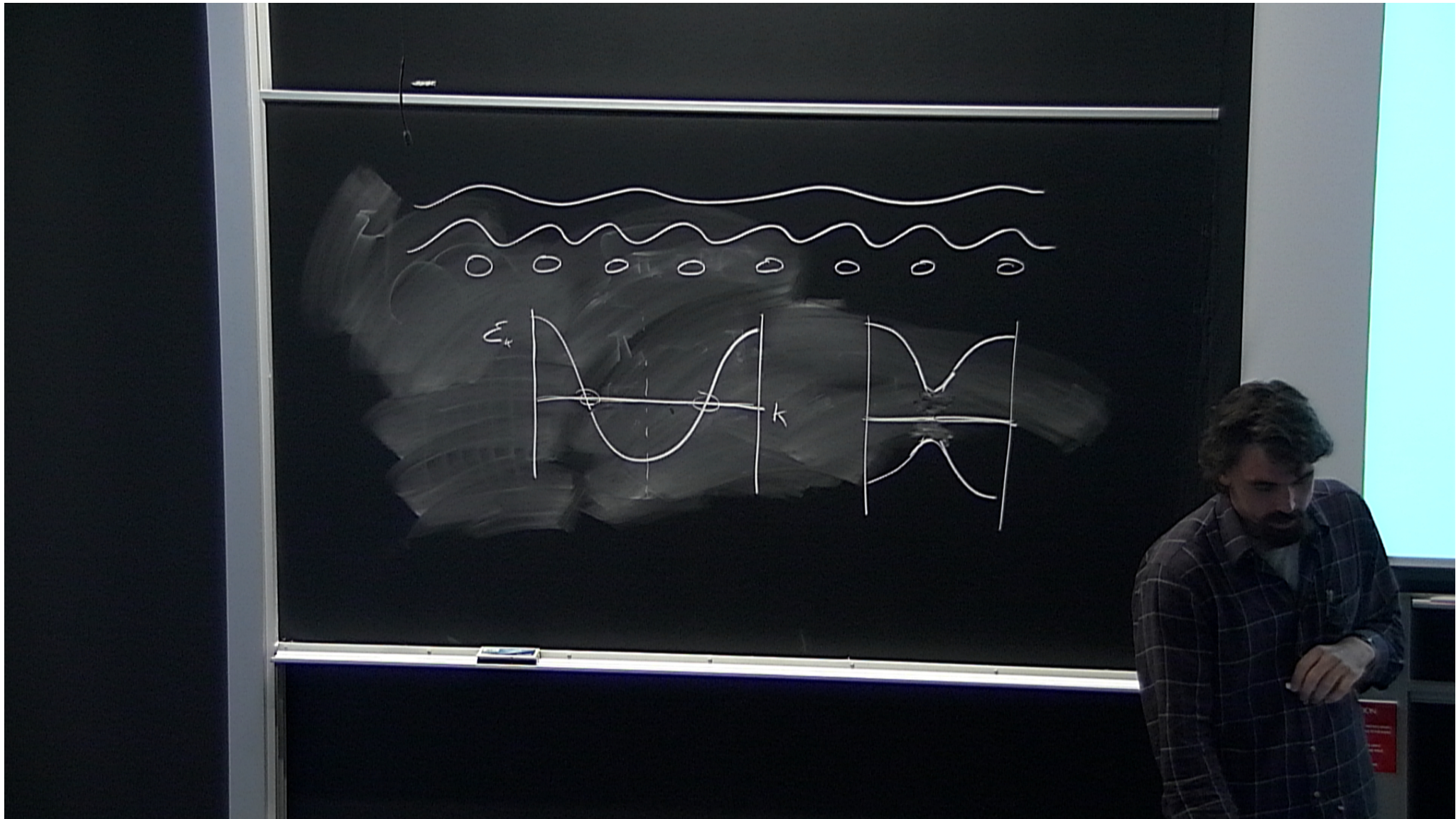


Jasper van Wezel

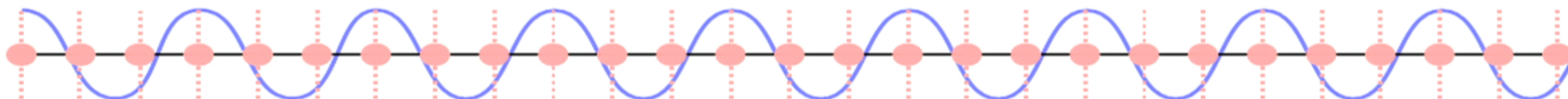
Part I: Natural Quasicrystals from Incommensurate Charge Order



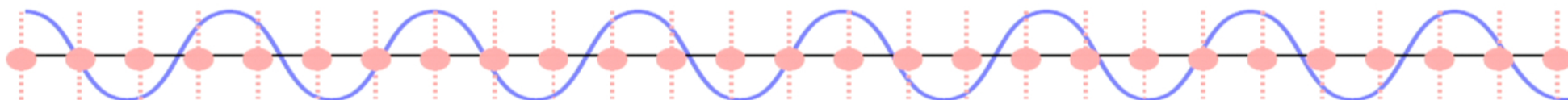




Commensurate



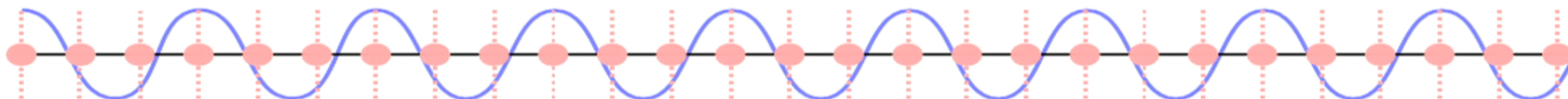
Incommensurate



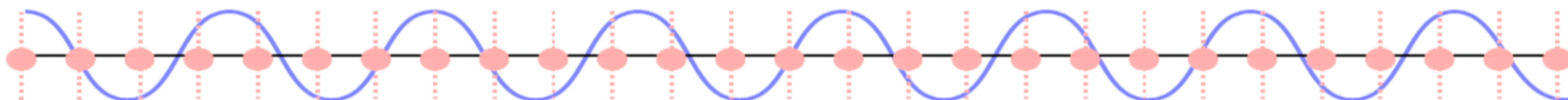
Discommensurations



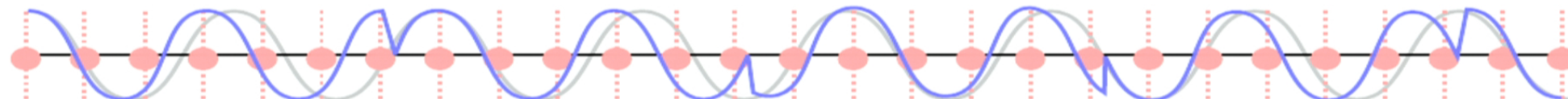
Commensurate



Incommensurate

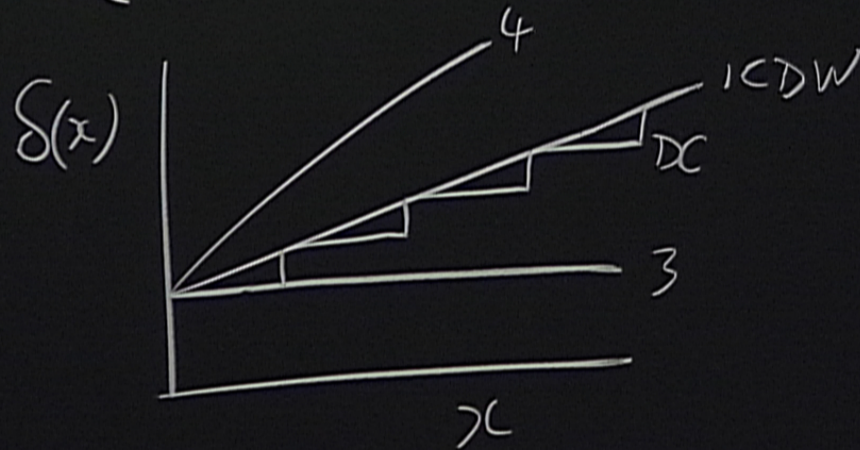


Discommensurations

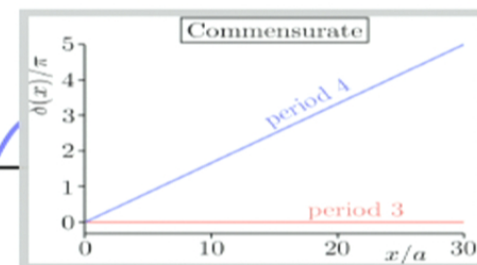
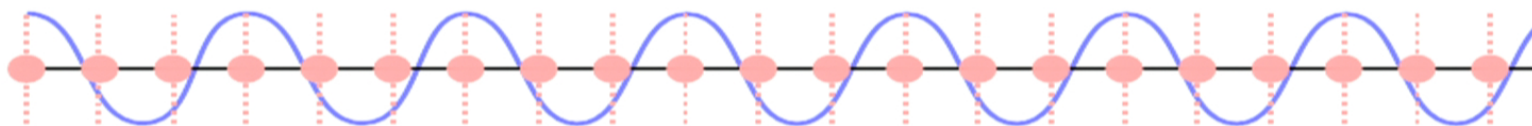


$$k = \frac{2\pi}{3a}$$

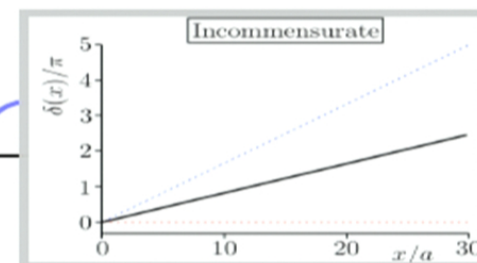
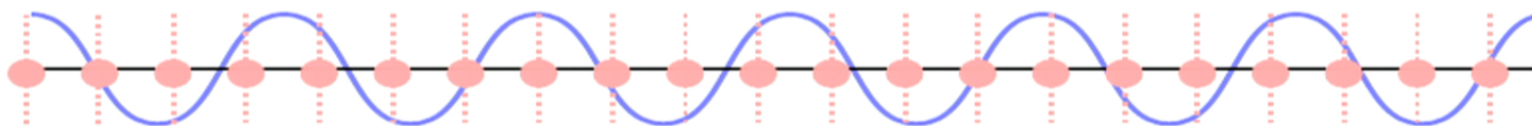
$$\rho(x) = \psi \cos(kx - \delta(x))$$



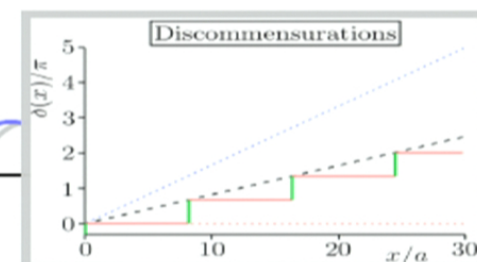
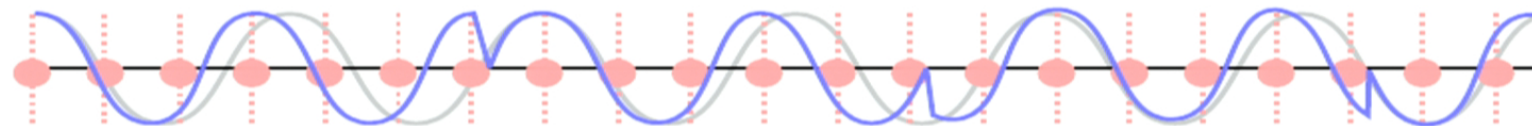
Commensurate



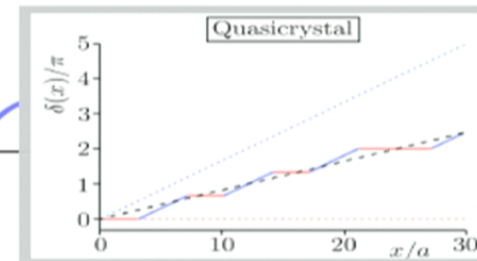
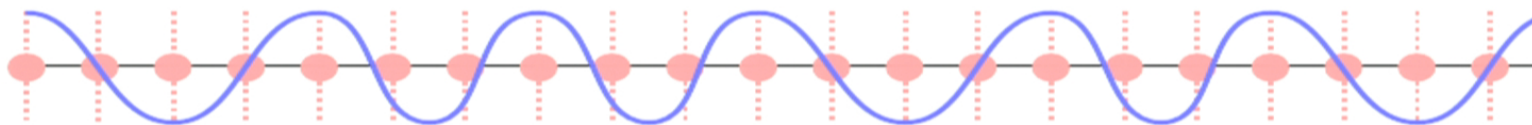
Incommensurate

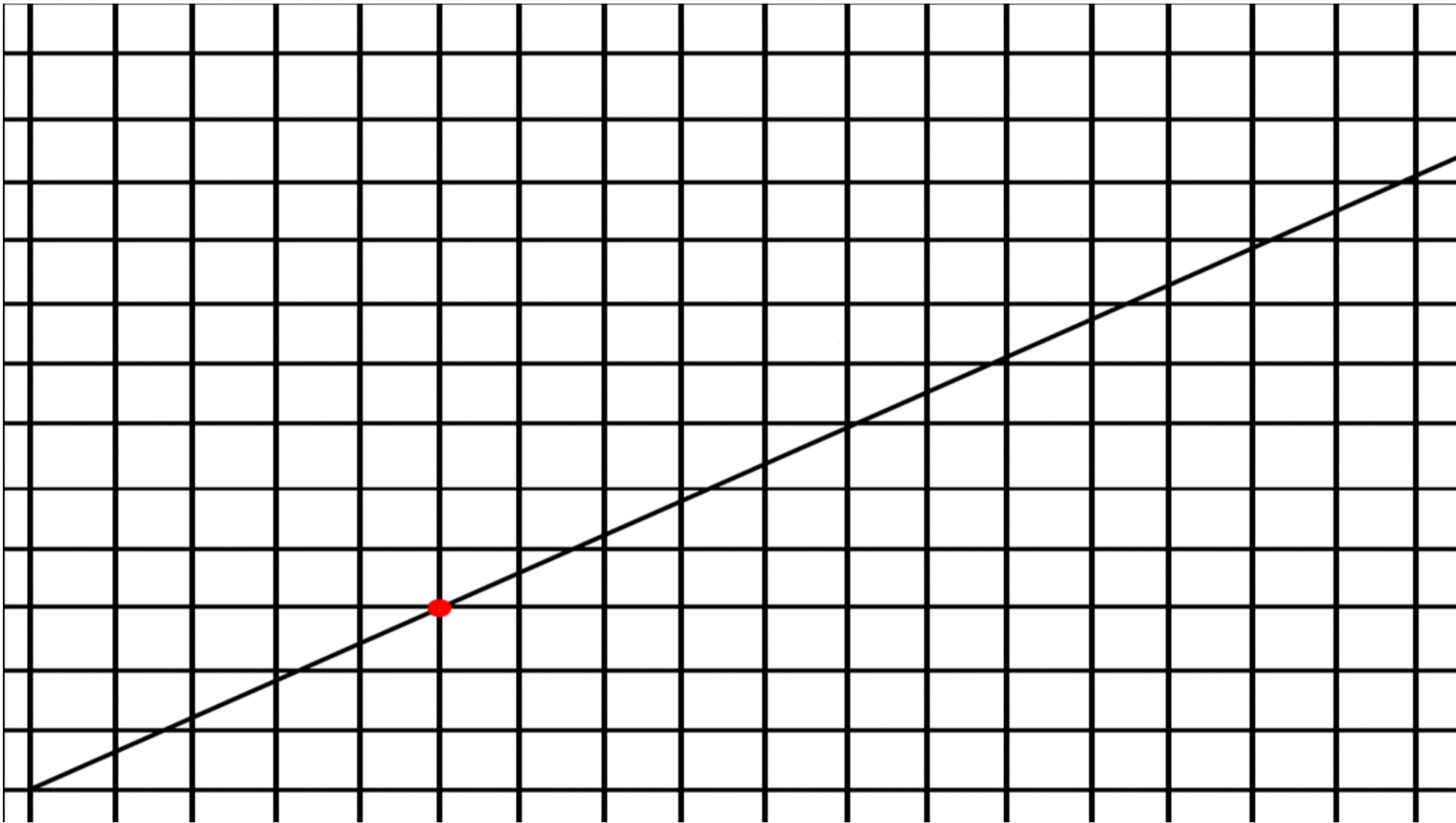


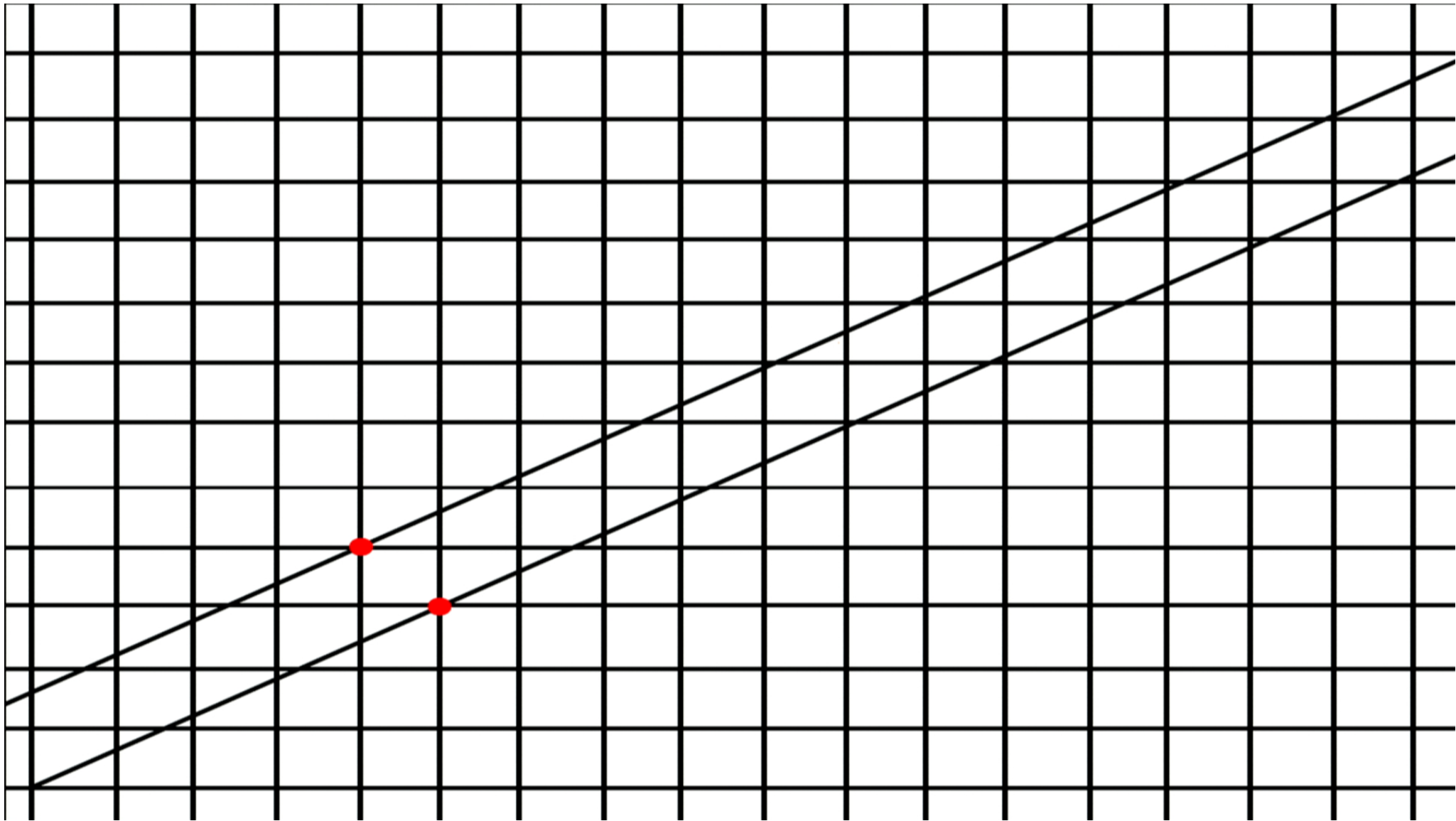
Discommensurations

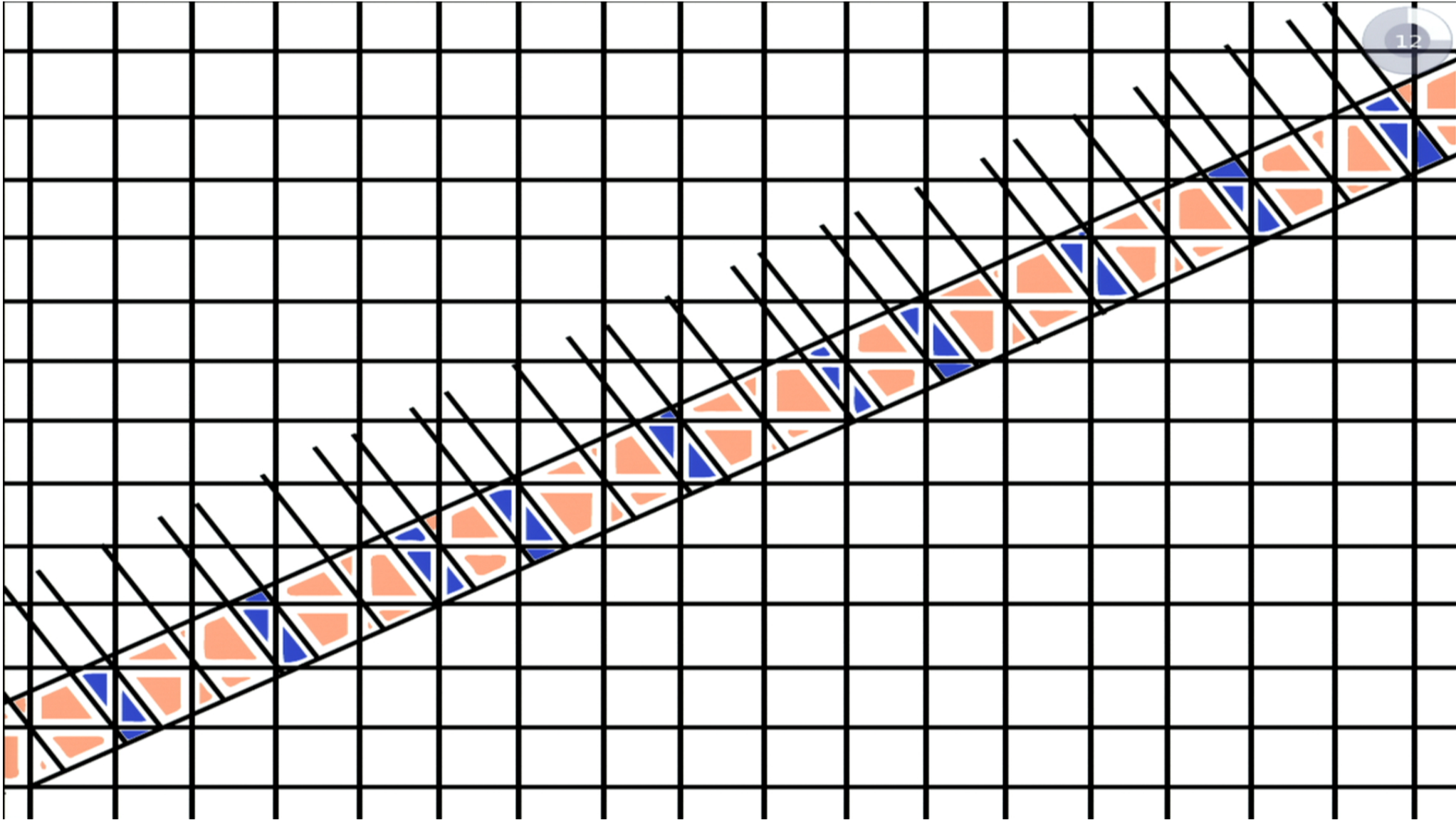


Quasicrystal

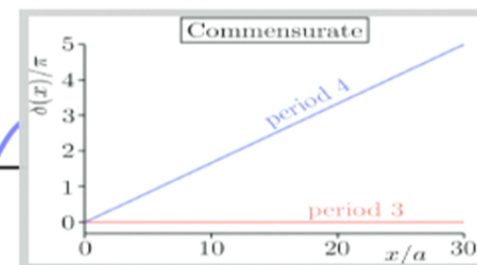
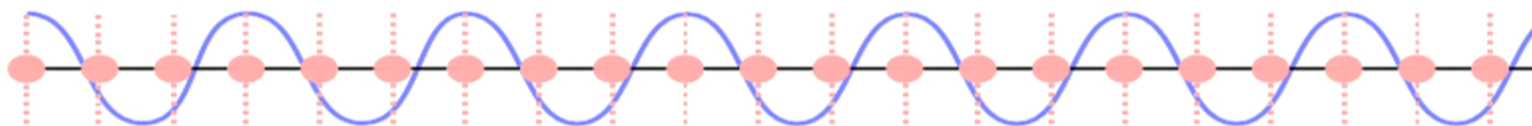




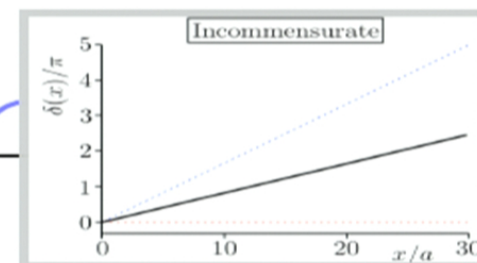
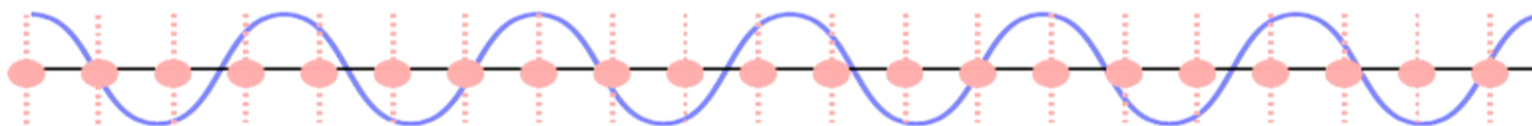




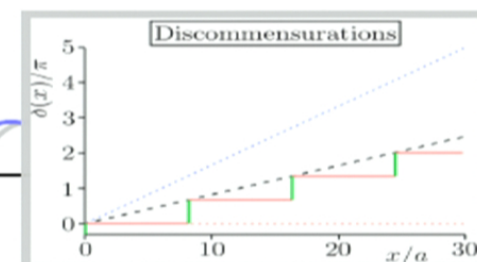
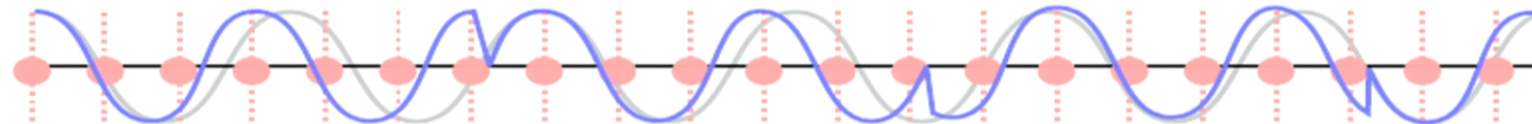
Commensurate



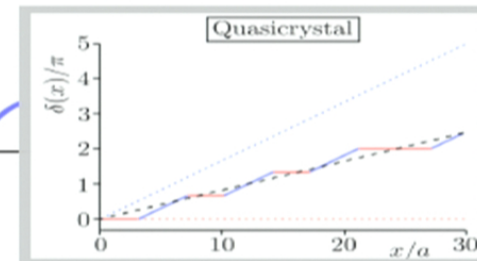
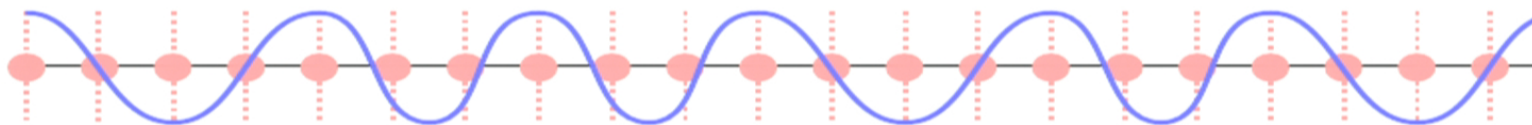
Incommensurate



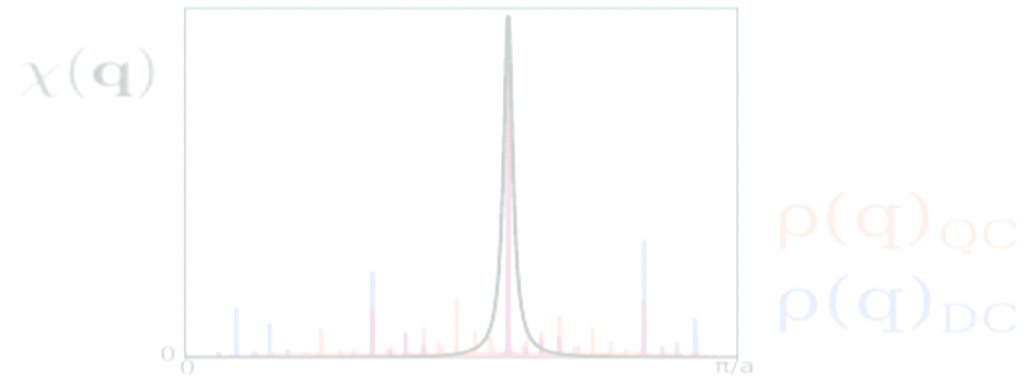
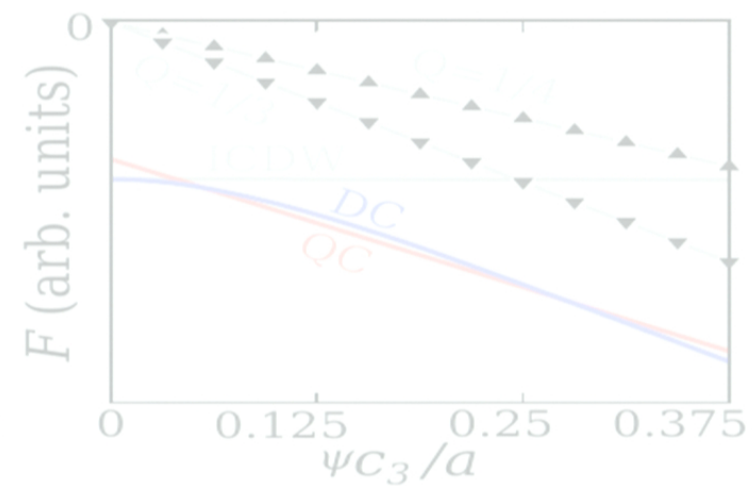
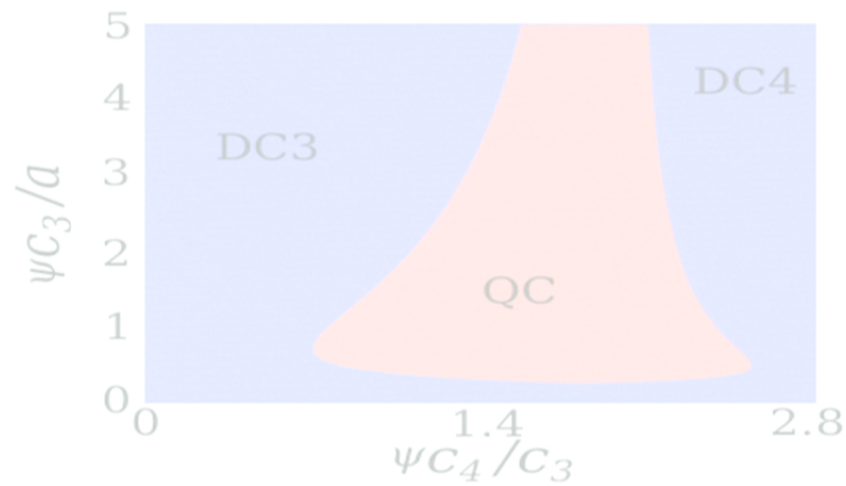
Discommensurations

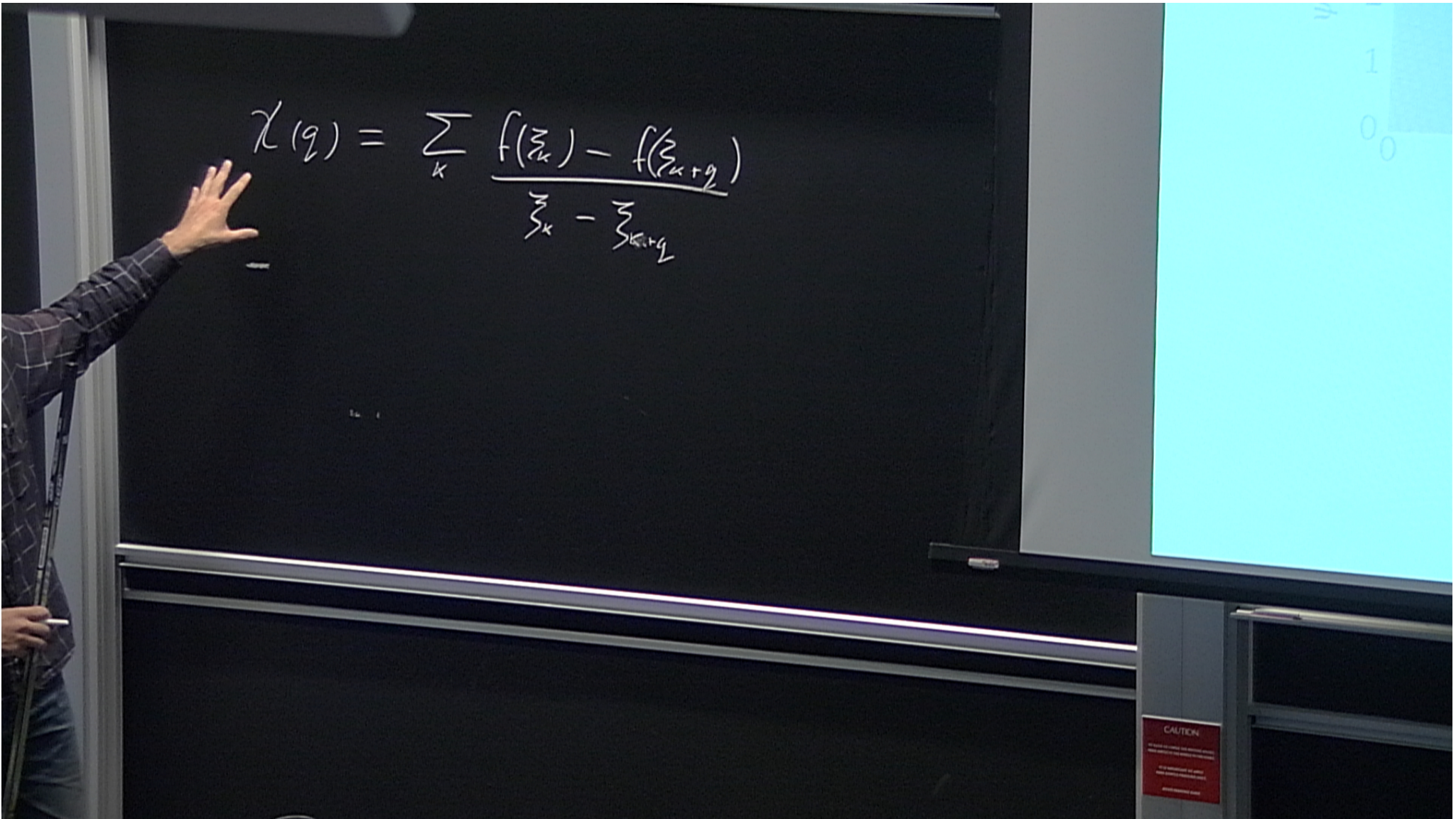


Quasicrystal

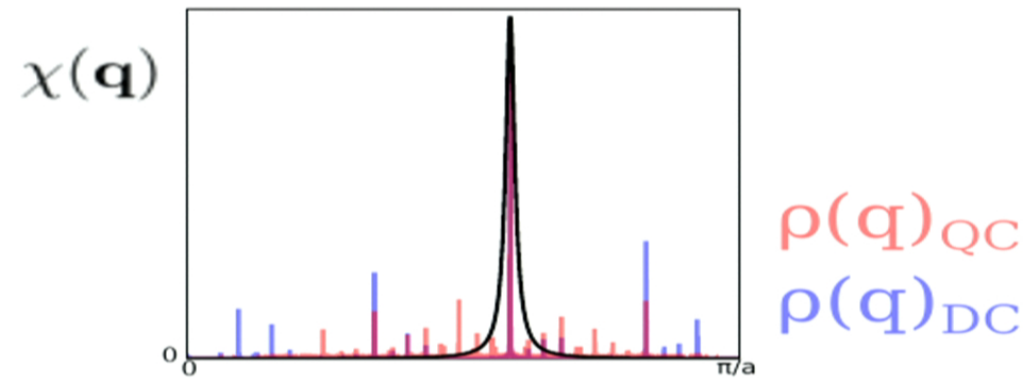
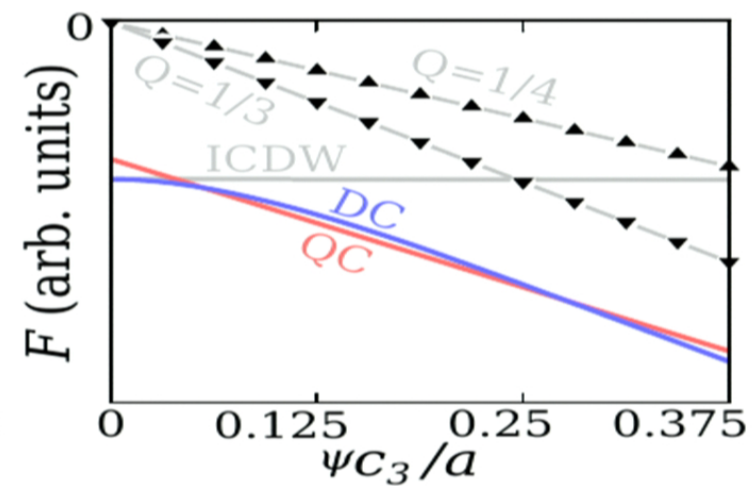
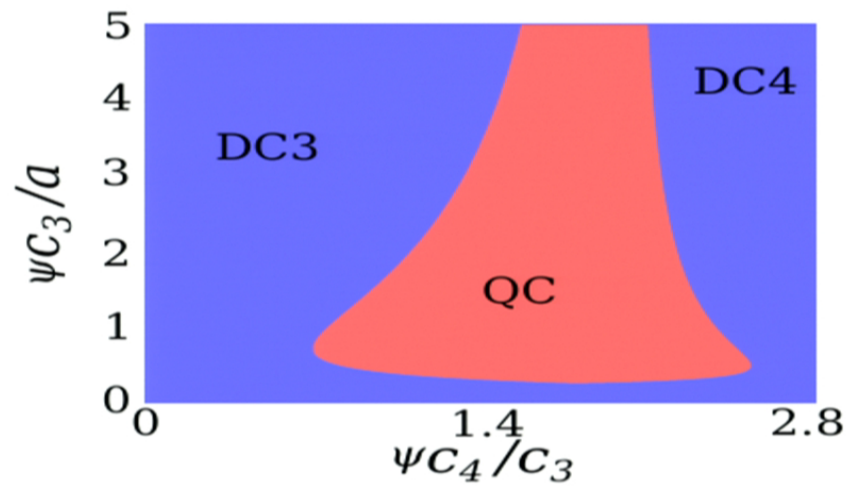


$$F = - \int d\mathbf{q} \chi(\mathbf{q}) \rho^2(\mathbf{q}) + \int d\mathbf{x} b \rho^4(\mathbf{x}) - \sum_{n, \mathbf{K}} c_n \cos(\mathbf{K} \cdot \mathbf{x}) \rho^n(\mathbf{x})$$





$$F = - \int d\mathbf{q} \chi(\mathbf{q}) \rho^2(\mathbf{q}) + \int d\mathbf{x} b \rho^4(\mathbf{x}) - \sum_{n, \mathbf{K}} c_n \cos(\mathbf{K} \cdot \mathbf{x}) \rho^n(\mathbf{x})$$



Conclusions

Part I: Natural Quasicrystals from Incommensurate Charge Order

- Quasicrystalline ground state expected for many incommensurate CDWs
- Potentially greatly extends number of known natural quasicrystals
- Applicable to other incommensurate systems

Conclusions

Part I: Natural Quasicrystals from Incommensurate Charge Order

- Quasicrystalline ground state expected for many incommensurate CDWs
- Potentially greatly extends number of known natural quasicrystals
- Applicable to other incommensurate systems

Conclusions

Part I: Natural Quasicrystals from Incommensurate Charge Order

- Quasicrystalline ground state expected for many incommensurate CDWs
- Potentially greatly extends number of known natural quasicrystals
- Applicable to other incommensurate systems

Part II: Incommensurate Charge Order in MoSe₂

Part II: Incommensurate Charge Order in MoSe_2



Sebastian Wickenburg



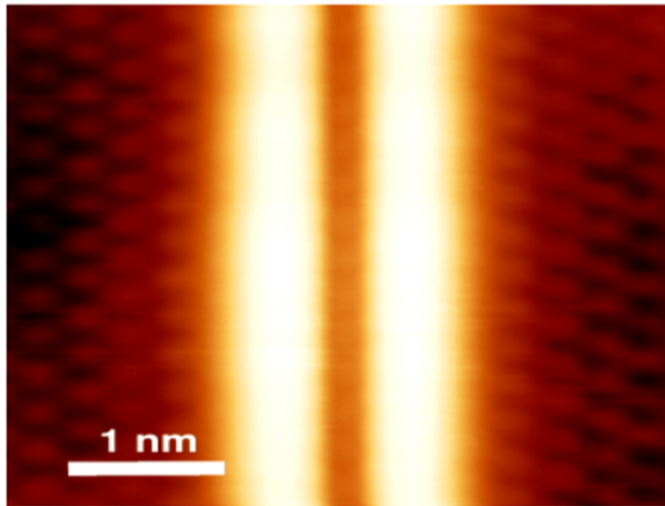
Sara Barja



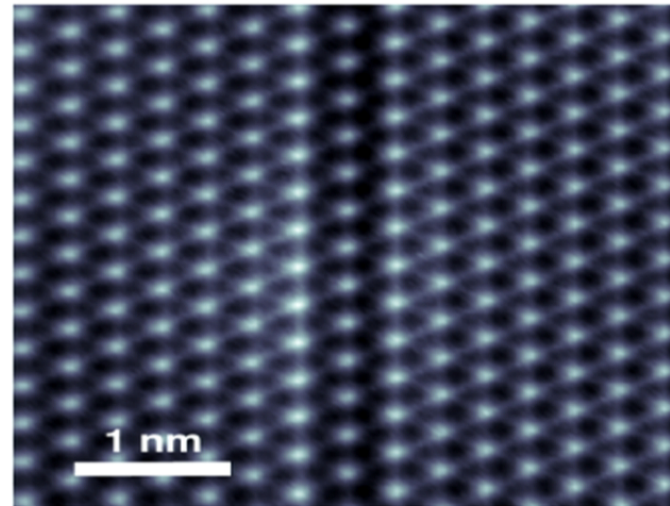
Alex Weber-Bargioni



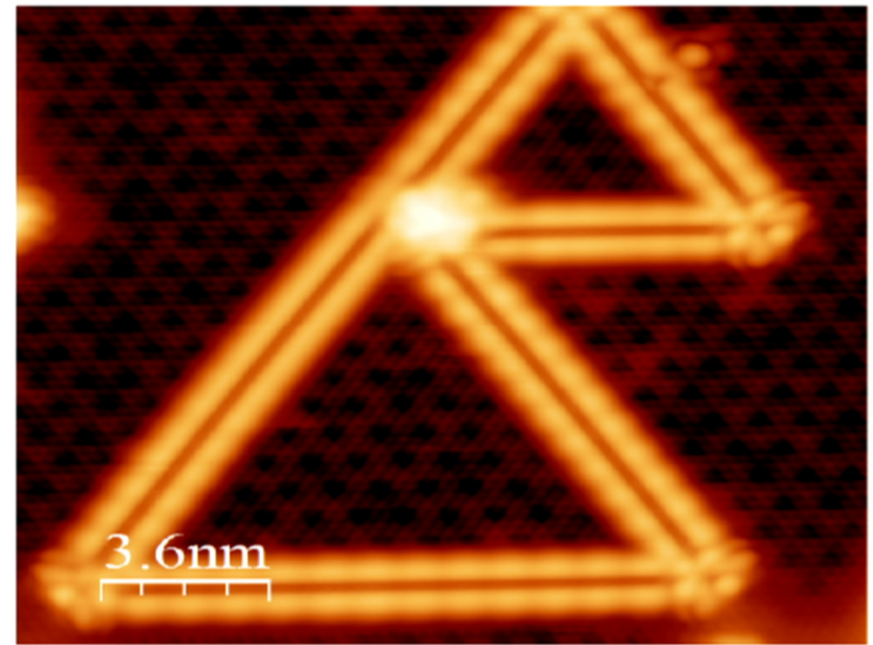
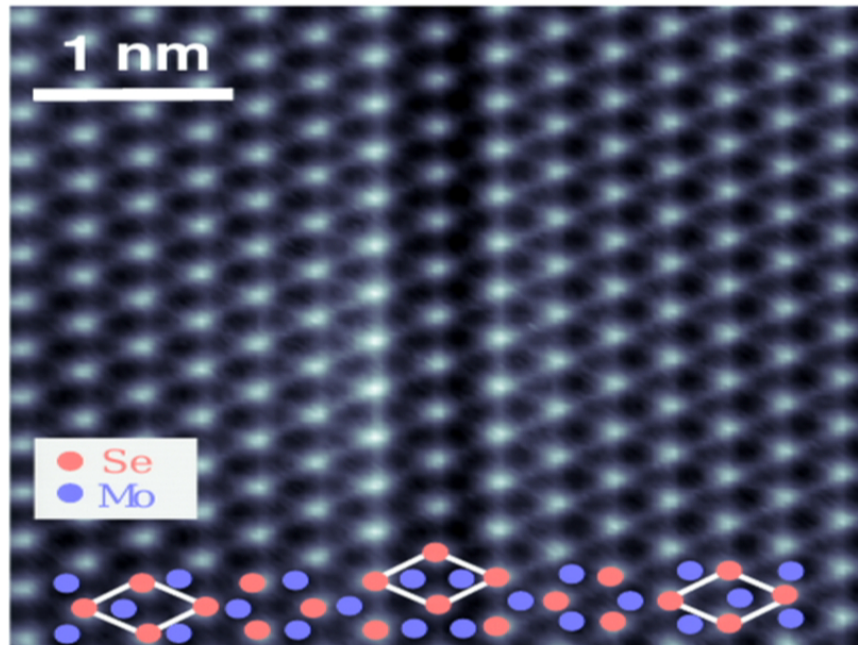
STM



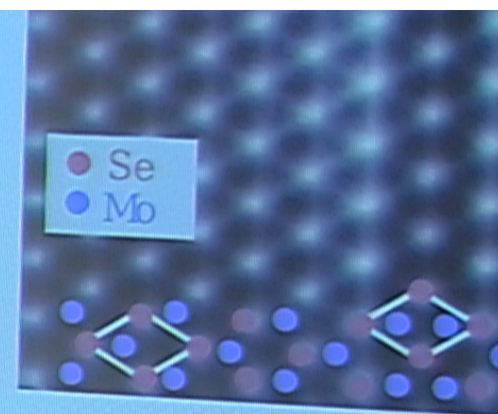
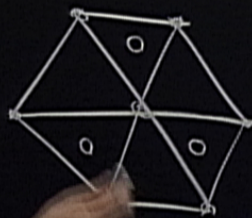
AFM



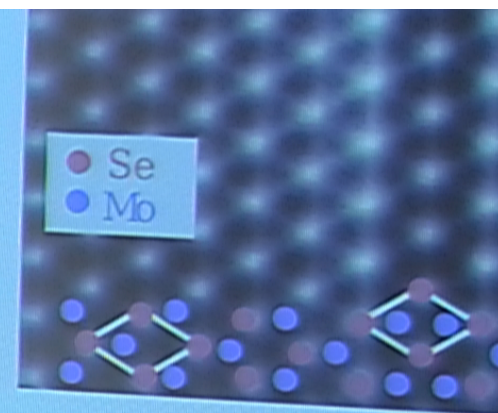
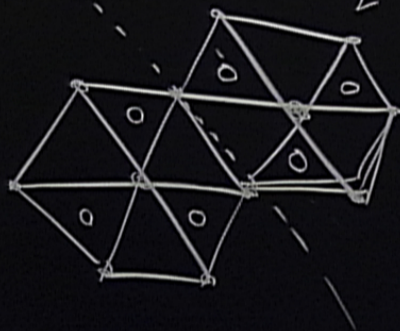
S. Barja *et al.* Nat. Phys. 12, 751-757 (2016)

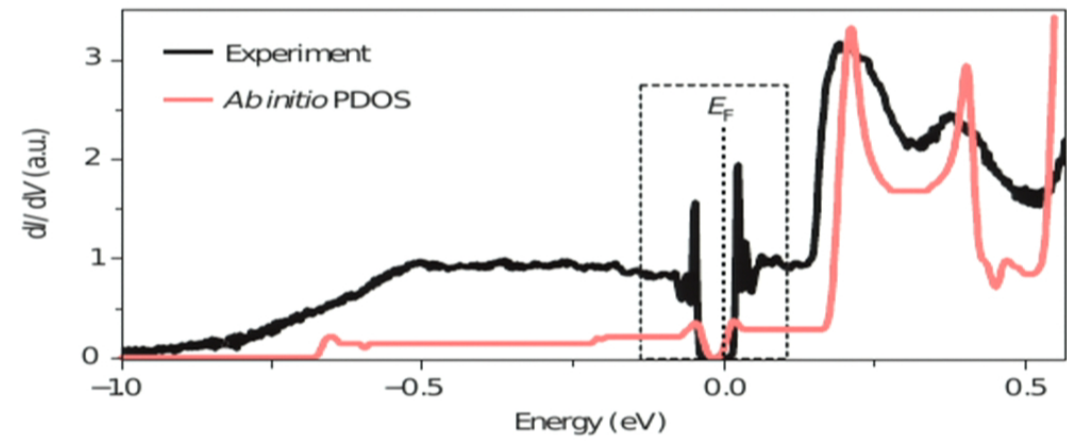
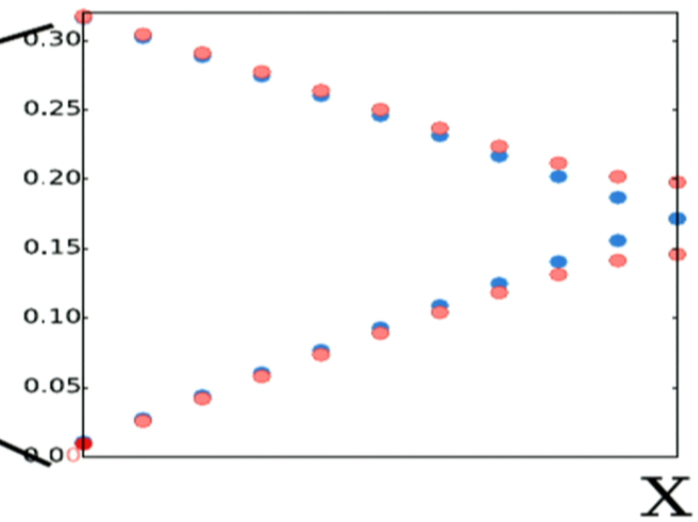
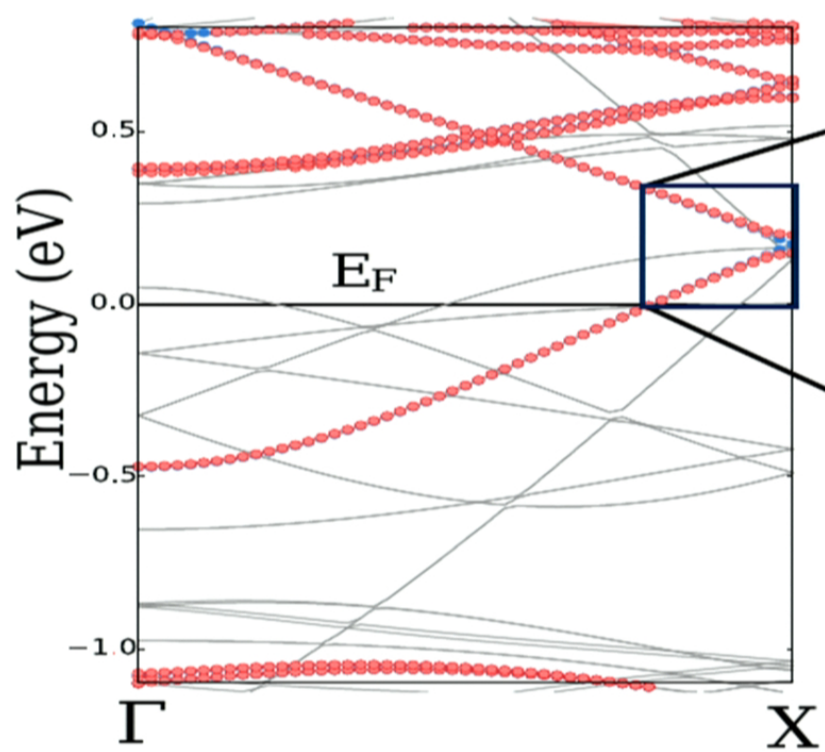


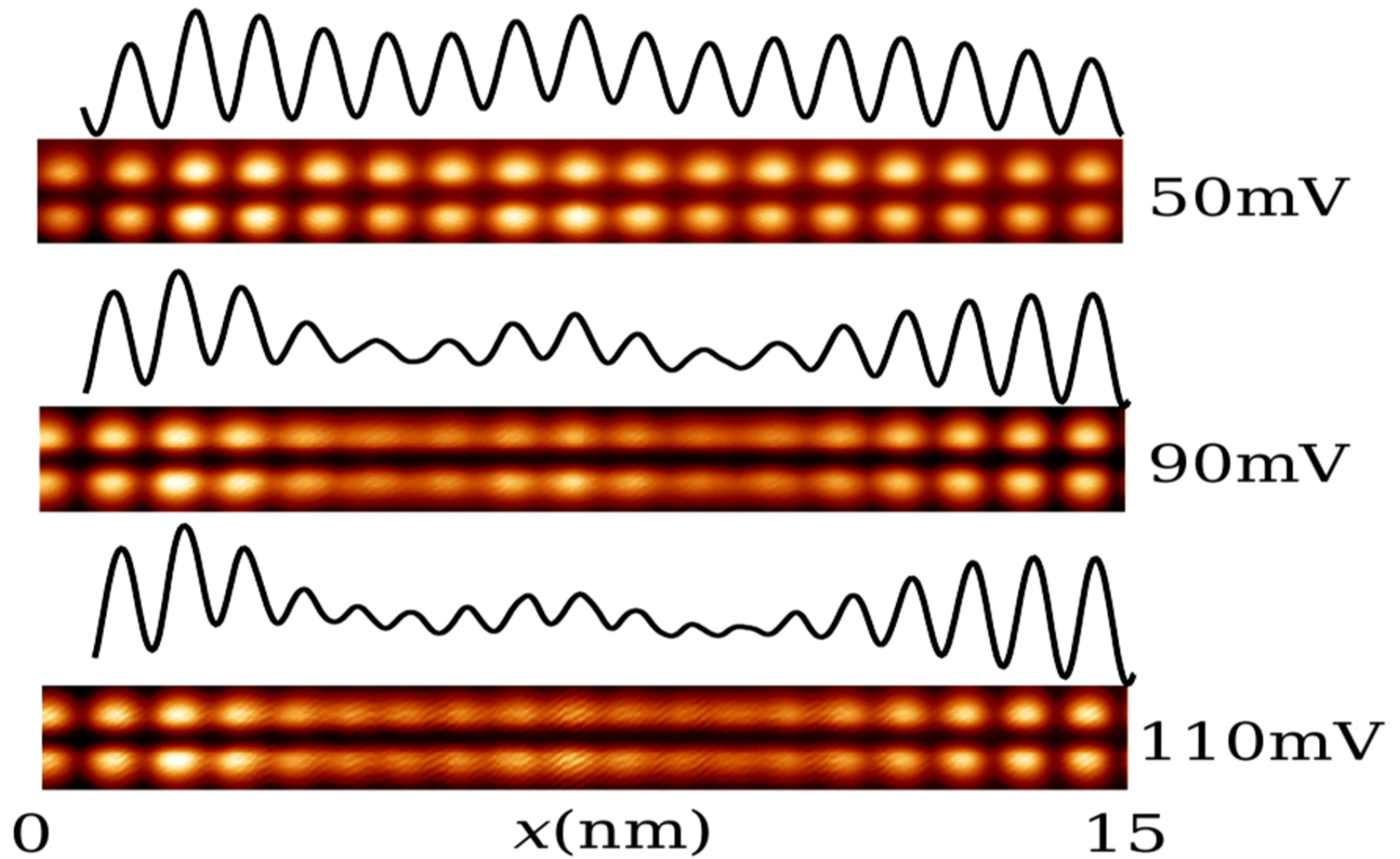
$$\chi(q) = \sum_k \frac{f(\vec{k}) - f(\vec{k} + q)}{\vec{k} - \vec{k} + q}$$

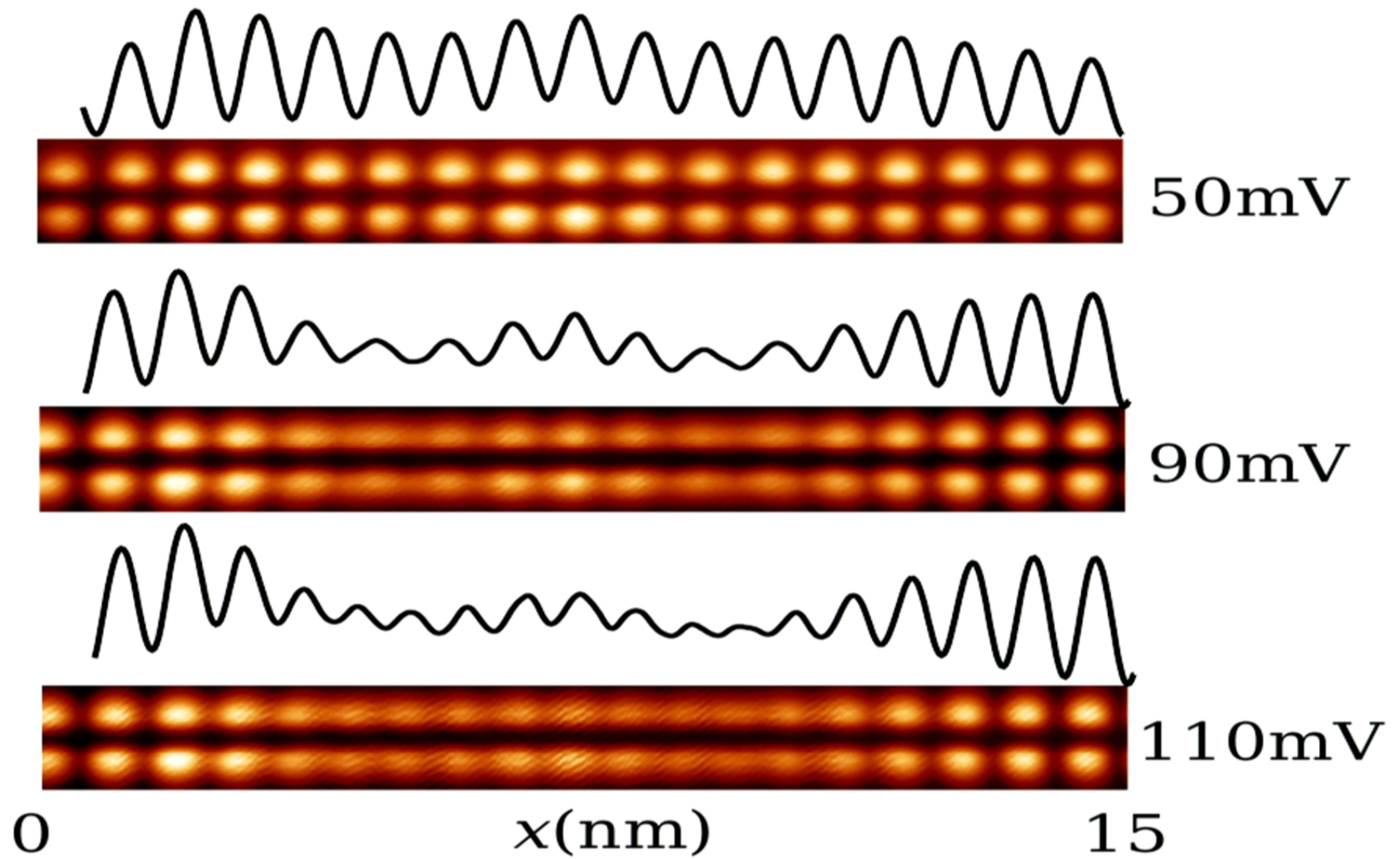


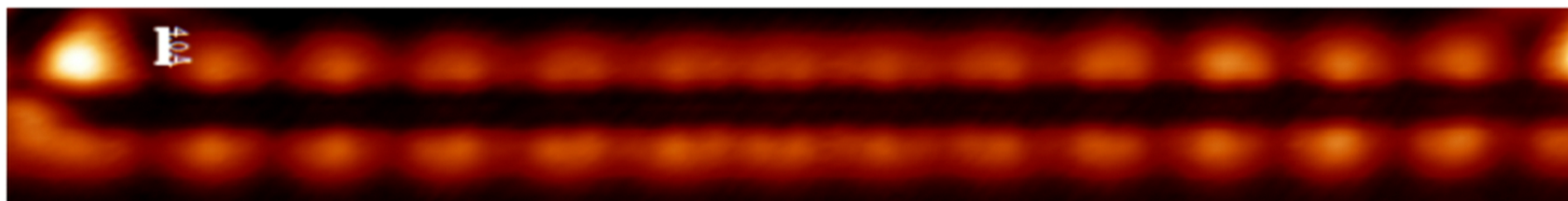
$$\chi(q) = \sum_k \frac{f(\vec{k}) - f(\vec{k} + q)}{\vec{k} - \vec{k} + q}$$











(+145mV)

$$\hat{H} = -t \sum_{\langle i j \rangle} \left(\hat{c}_i^\dagger \hat{c}_j + \hat{c}_j^\dagger \hat{c}_i \right) + g \sum_{\langle i j \rangle} \hat{n}_i \hat{n}_j + \sum_i (U_i - \mu) \hat{n}_i$$

$$\begin{aligned} \Delta_i^{(site)} &\triangleq g \langle \hat{n}_i \rangle \\ \Delta_i^{(bond)} &\triangleq \frac{g}{2} \left\langle \hat{c}_i^\dagger \hat{c}_{i+1} + \hat{c}_{i+1}^\dagger \hat{c}_i \right\rangle \end{aligned}$$

LDOS:

$$\nu(x, E) = \frac{1}{N} \sum_n \delta(E - \epsilon_n) |\langle x | n \rangle|^2$$

~charge density:

$$\langle x | \hat{n} | x \rangle = \frac{1}{N} \sum_n f(\epsilon_n) |\langle x | n \rangle|^2$$

$$\hat{H} = -t \sum_{\langle i j \rangle} \left(\hat{c}_i^\dagger \hat{c}_j + \hat{c}_j^\dagger \hat{c}_i \right) + g \sum_{\langle i j \rangle} \hat{n}_i \hat{n}_j + \sum_i (U_i - \mu) \hat{n}_i$$

$$\begin{aligned} \Delta_i^{(site)} &\triangleq g \langle \hat{n}_i \rangle \\ \Delta_i^{(bond)} &\triangleq \frac{g}{2} \left\langle \hat{c}_i^\dagger \hat{c}_{i+1} + \hat{c}_{i+1}^\dagger \hat{c}_i \right\rangle \end{aligned}$$

LDOS: $\nu(x, E) = \frac{1}{N} \sum_n \delta(E - \epsilon_n) |\langle x | n \rangle|^2$

~charge density: $\langle x | \hat{n} | x \rangle = \frac{1}{N} \sum_n f(\epsilon_n) |\langle x | n \rangle|^2$

$$\hat{H} = -t \sum_{\langle i j \rangle} \left(\hat{c}_i^\dagger \hat{c}_j + \hat{c}_j^\dagger \hat{c}_i \right) + g \sum_{\langle i j \rangle} \hat{n}_i \hat{n}_j + \sum_i (U_i - \mu) \hat{n}_i$$

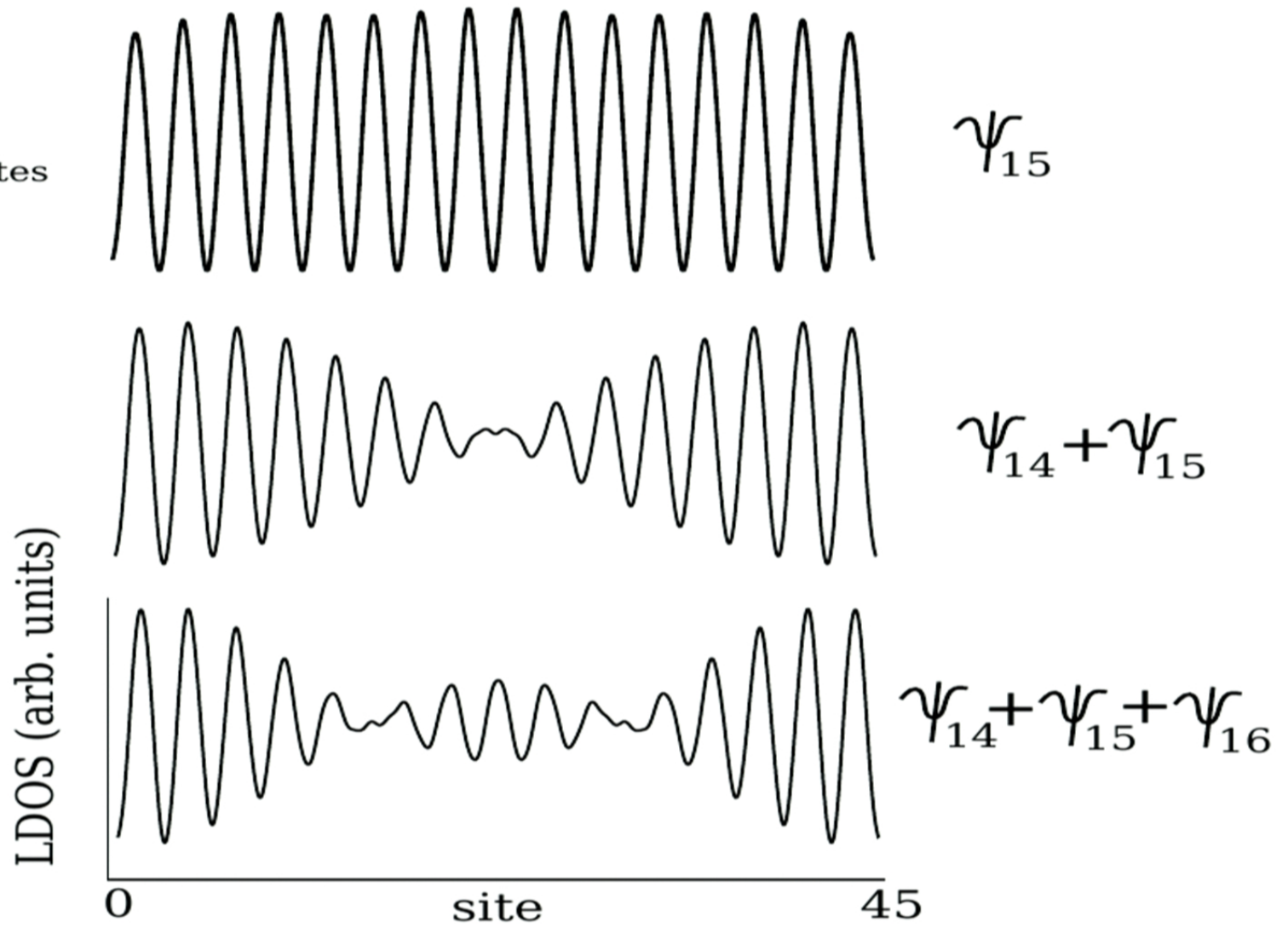
$$\begin{aligned} \Delta_i^{(site)} &\triangleq g \langle \hat{n}_i \rangle \\ \Delta_i^{(bond)} &\triangleq \frac{g}{2} \left\langle \hat{c}_i^\dagger \hat{c}_{i+1} + \hat{c}_{i+1}^\dagger \hat{c}_i \right\rangle \end{aligned}$$

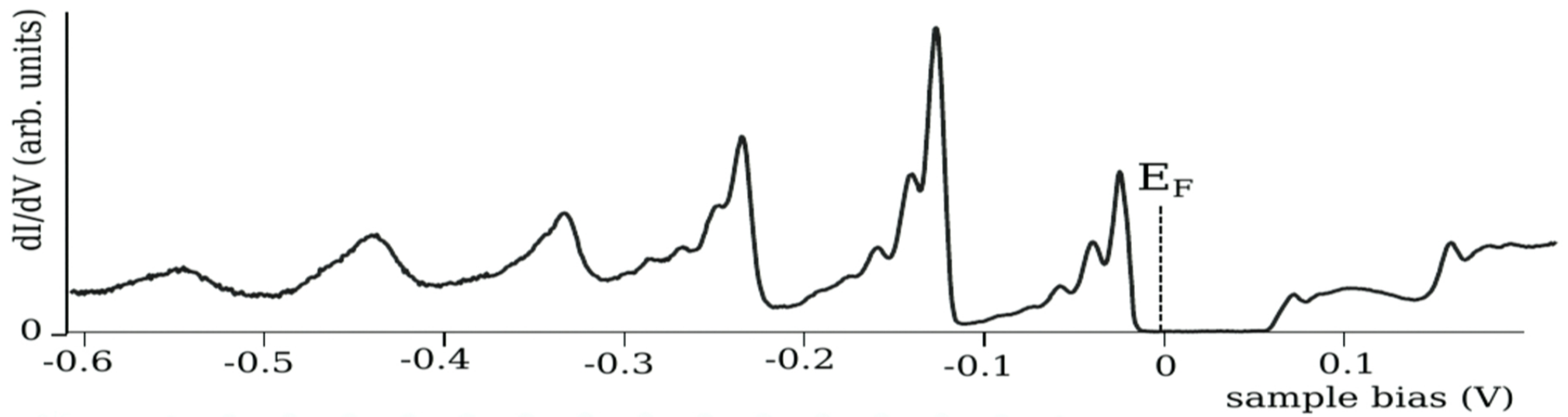
LDOS: $\nu(x, E) = \frac{1}{N} \sum_n \delta(E - \epsilon_n) |\langle x | n \rangle|^2$

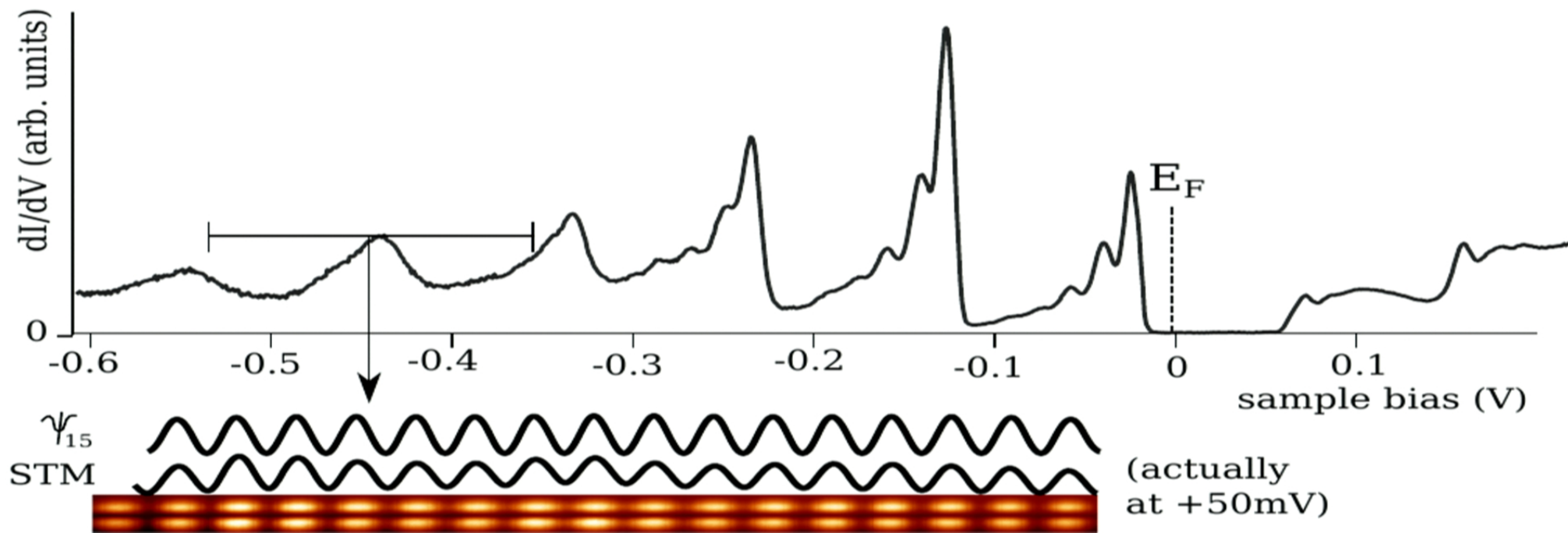
~charge density: $\langle x | \hat{n} | x \rangle = \frac{1}{N} \sum_n f(\epsilon_n) |\langle x | n \rangle|^2$

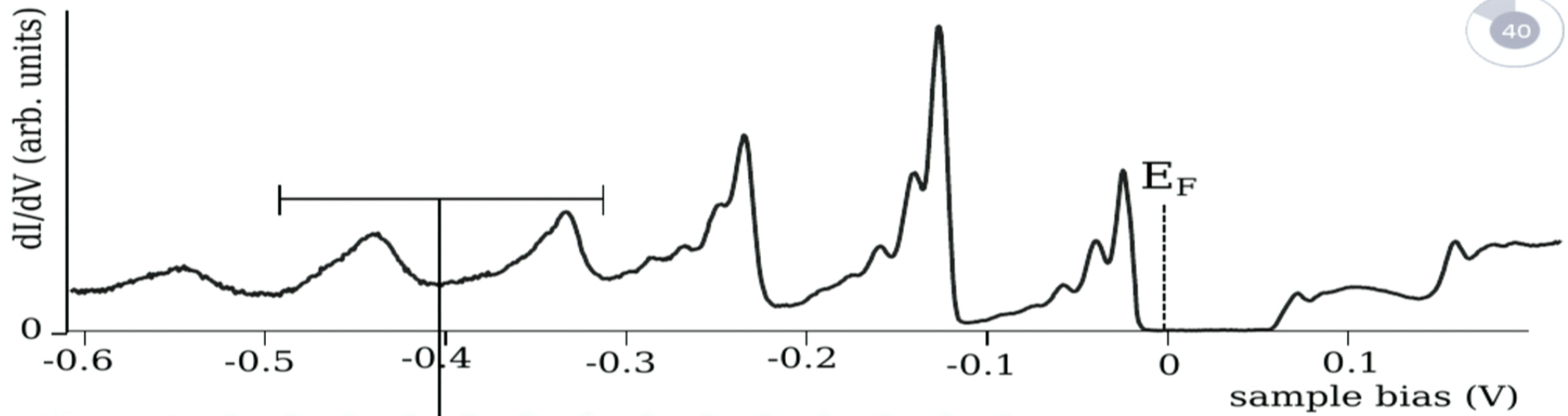
$$g/t=0.1$$

15 electrons in 45 sites



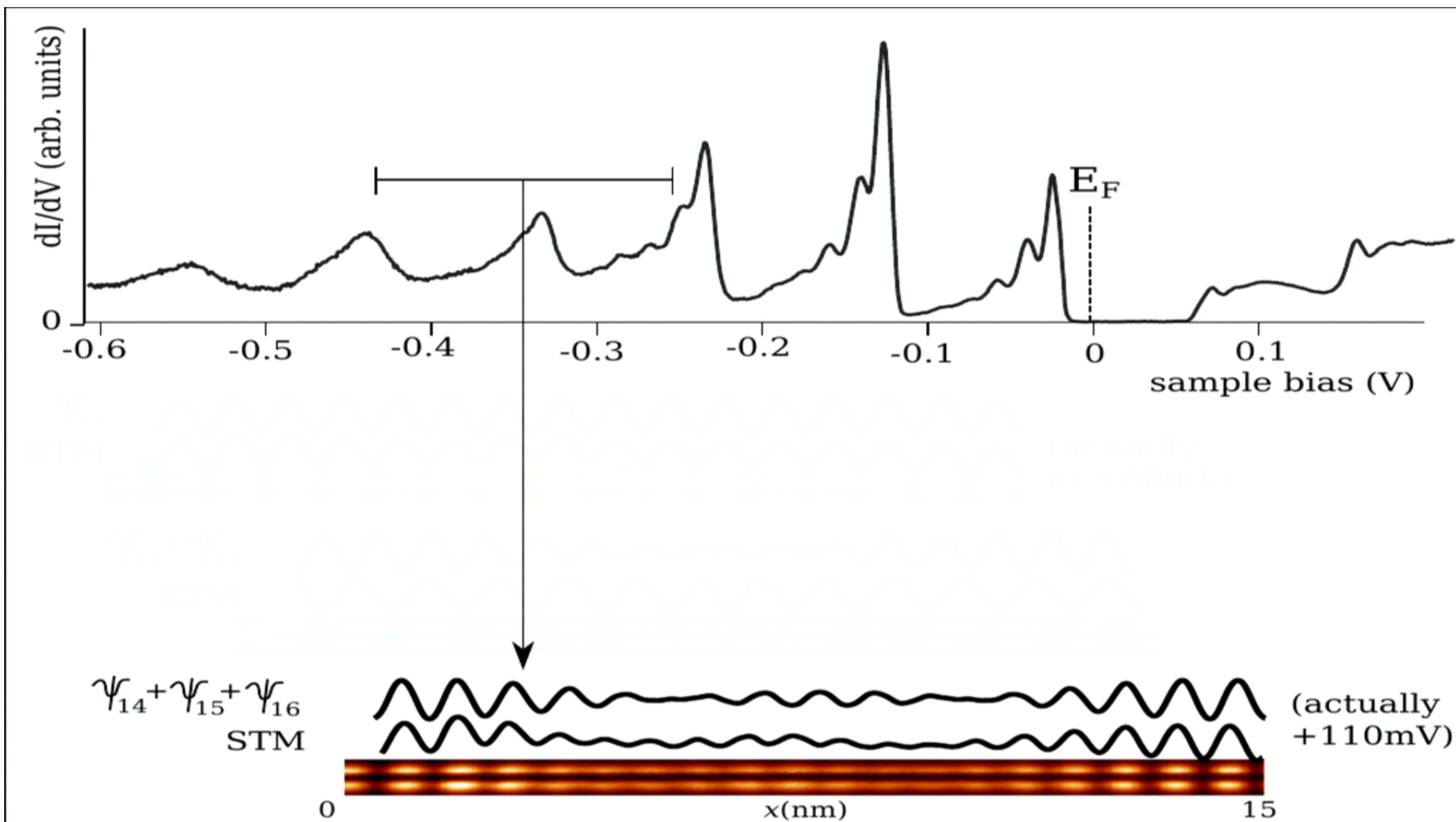


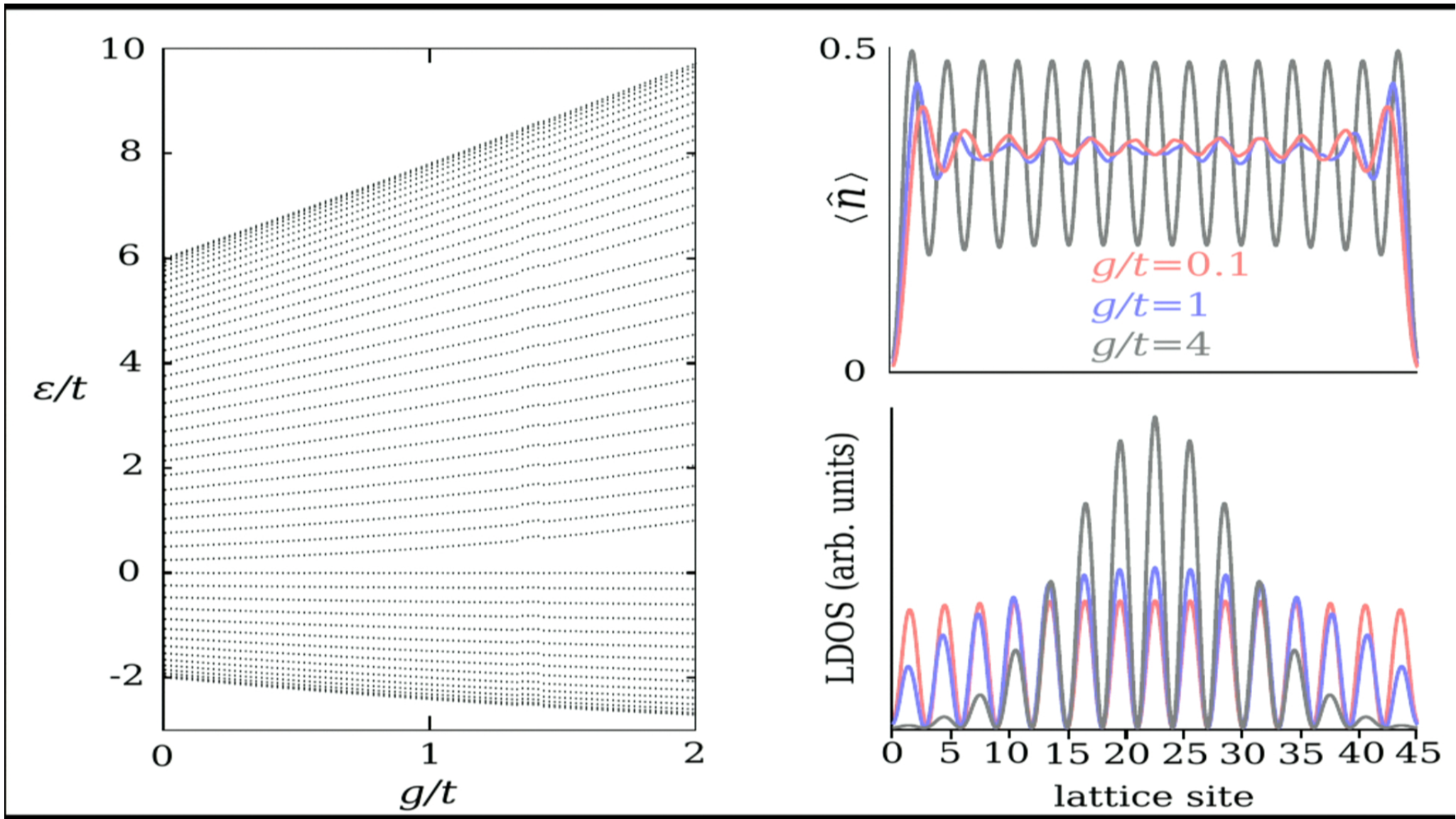




$\psi_{14} + \psi_{15}$
STM







Conclusions

Part I: Natural Quasicrystals from Incommensurate Charge Order

- Quasicrystalline ground state expected for many incommensurate CDWs
- Potentially greatly extends number of known natural quasicrystals
- Applicable to other incommensurate systems

Part II: Incommensurate Charge Order in MoSe_2

- MTBs form small enough systems that CDW/QW crossover important
- 'Solitons' are mostly due to LDOS seeing sums of QW states, $g/t < 1$; but...
- Gap demonstrates CDW also important, so $g/t \lesssim 1$

Conclusions

Part I: Natural Quasicrystals from Incommensurate Charge Order

- Quasicrystalline ground state expected for many incommensurate CDWs
- Potentially greatly extends number of known natural quasicrystals
- Applicable to other incommensurate systems

Part II: Incommensurate Charge Order in MoSe_2

- MTBs form small enough systems that CDW/QW crossover important
- 'Solitons' are mostly due to LDOS seeing sums of QW states. $g/t < 1$; but...
- Gap demonstrates CDW also important, so $g/t \lesssim 1$

Conclusions

Part I: Natural Quasicrystals from Incommensurate Charge Order

- Quasicrystalline ground state expected for many incommensurate CDWs
- Potentially greatly extends number of known natural quasicrystals
- Applicable to other incommensurate systems

Part II: Incommensurate Charge Order in MoSe_2

- MTBs form small enough systems that CDW/QW crossover important
- 'Solitons' are mostly due to LDOS seeing sums of QW states. $g/t < 1$; but...
- Gap demonstrates CDW also important, so $g/t \lesssim 1$

Thanks for listening

Part I:

F. Flicker and J. van Wezel, Physical Review Letters 115, 236401 (2015)

see also:

F. Flicker and J. van Wezel, Europhysics Letters 111, 37008 (2015)

Y. Feng *et al.*, Nature Physics 11, 865-873 (2015)

Part II:

S. Barja et al., Nature Physics 12, 751-758 (2016)