LA-UR-16-22284

Title:	Numerical Studies of Nano-Film, Wire and Dot Transitions with Emergent Nano Properties
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Intended for:	UNM Comprehensive Exam Proposal Presentation
Issued:	2016-04-05

THE UNIVERSITY *of* NEW MEXICO

Numerical Studies of Nano-Film, Wire and Dot Transitions with Emergent Nano Properties[1]

Comprehensive Exam Proposal Presentation

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April 8, 2016

NanoScience and MicroSystems Engineering

UNM

[1]Numerical Studies of Approximate Zero Modes in Nano-

Outline

- Tour of Topological Insulators (TIs)
- Getting into the technical details
- What is proposed?
- How will it be done?
- What good is it?

Topological Insulator

- What is it?
- How is different from “normal” materials?
- Why nano-size?
- How do we “see” it?
- What good is this information?

What is a Topological Insulator?

- A homogeneous material that behaves differently at the edge than in the bulk.
  - What kind(s) of behavior?
  - What is the “edge”?
  - What is the bulk?

What is the Behavior of a TI?

- It is topological - it has a surface and an interior
- It is an Insulator or Conductor of Electrical Current by topological region

What is the Edge of a TI?

- The part of the material that conducts electrons.
- It is usually at the surface of the material.

What is the Bulk of a TI?

- The part of the material that is insulating.
- It is usually interior to the material (not on the surface).

What is Meso-Region of a TI?

- The region of the material that is
  - Between the edge and the bulk

  and/or
  - Unstable in its edge/bulk properties

How is it different?

It is both an insulator and conductor.

Conduction may scale to a lower power than expected for the material size increase.

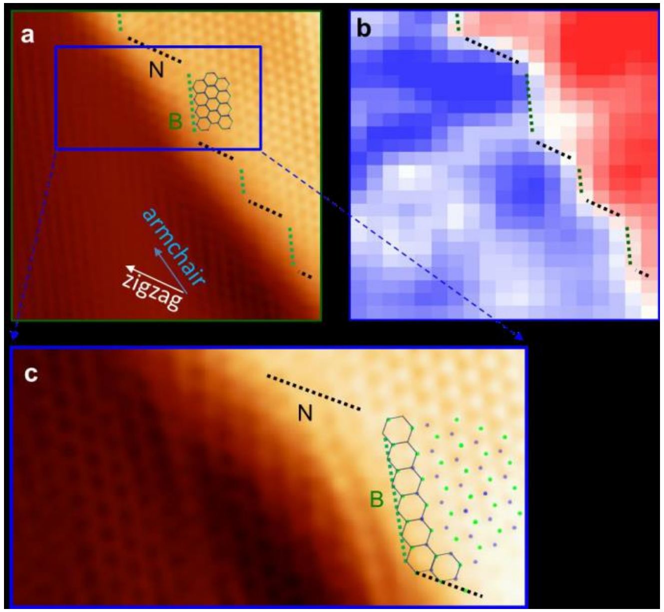
It may have spin currents with zero net current.

Why is it nano-size?

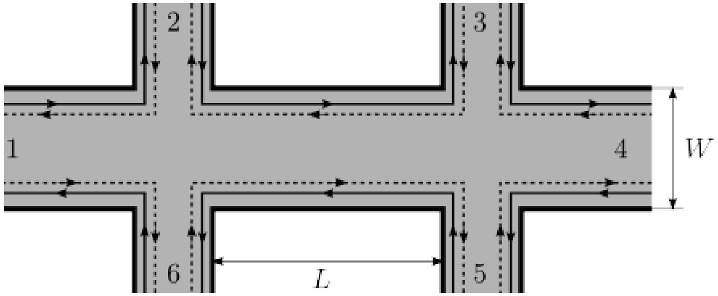
- The Hamiltonian is about atomic or molecular structure and the material is composed of at most on the order of about 10,000 atoms or molecules.

How can we "see" a TI?

- Scanning Tunneling Electron Microscopy
- Functionally with a Quantum Hall Bar

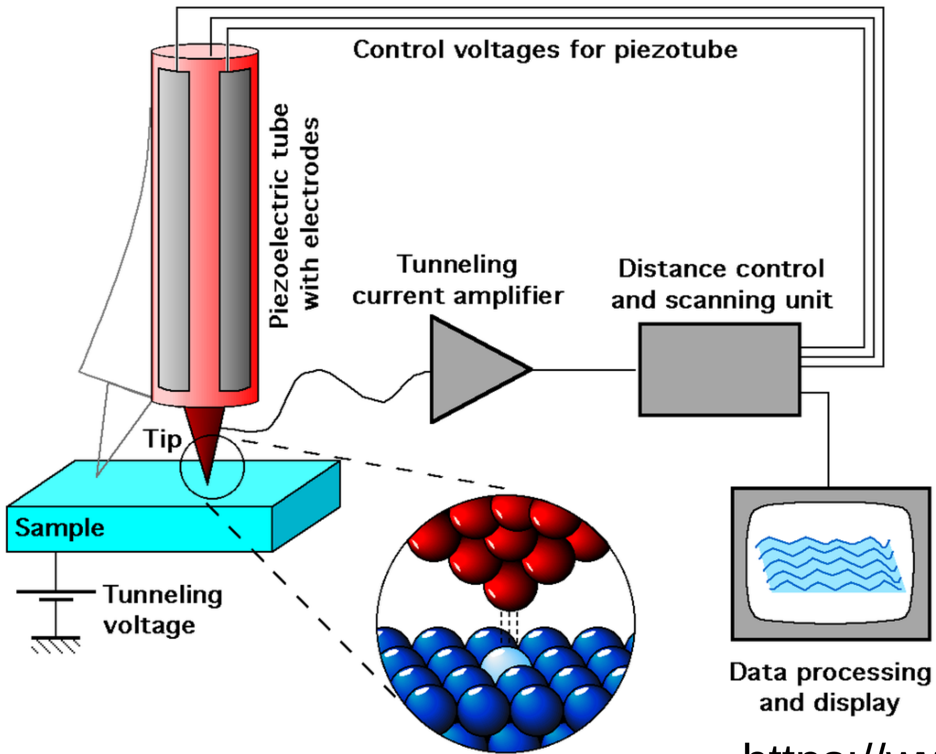


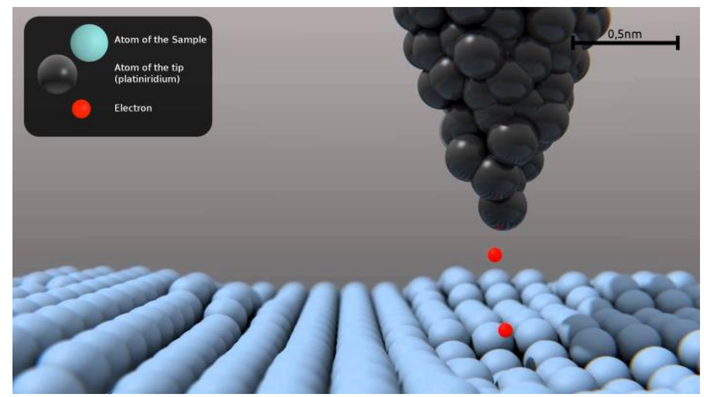
"Spatially resolved one-dimensional boundary states in graphene hexagonal boron nitride planar heterostructures," [26].



"A short course on topological insulators: Band-structure topology and edge states in one and two dimensions," [16].

Scanning Tunneling Electron Microscopy to “see” a TI.



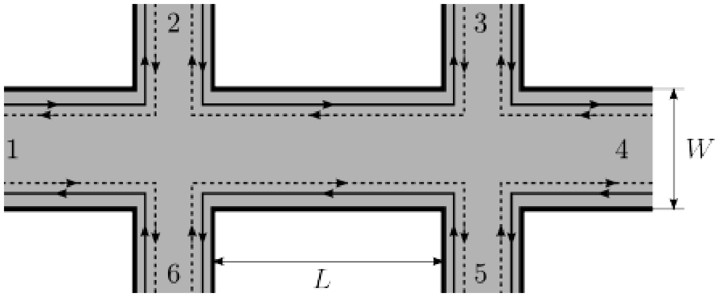


https://www.youtube.com/watch?v=EXcQxuWR1pI

https://en.wikipedia.org/wiki/Scanning_tunneling_microscope

Functionally "see" a TI?

- A Quantum Hall Bar



"A short course on topological insulators: Band-structure topology and edge states in one and two dimensions," [16].

What good is a TI?

- The topological effect of a quantum Hall Bar is used to define the Ohm.
- Spintronics
- Nano Size Electrical Components

Technical Details

- Dimension and “Symmetries” matter
- Film is 2d, Wire is 1-d and Dot is 0-d
- Symmetries are determined by the material and the physics they are reflected in the Hamiltonian and the Matrix formulation

The 10-Fold way

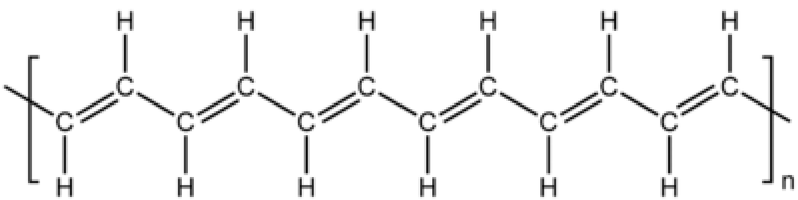
Cartan label	T	C	S	Hamiltonian	G/H (ferm. NLσM)
A (unitary)	0	0	0	$\mathrm{U}(N)$	$\mathrm{U}(2n)/\mathrm{U}(n)\times\mathrm{U}(n)$
AI (orthogonal)	+1	0	0	$\mathrm{U}(N)/\mathrm{O}(N)$	$\mathrm{Sp}(2n)/\mathrm{Sp}(n)\times\mathrm{Sp}(n)$
AII (symplectic)	−1	0	0	$\mathrm{U}(2N)/\mathrm{Sp}(2N)$	$\mathrm{O}(2n)/\mathrm{O}(n)\times\mathrm{O}(n)$
AIII (ch. unit.)	0	0	1	$\mathrm{U}(N+M)/\mathrm{U}(N)\times\mathrm{U}(M)$	$\mathrm{U}(n)$
BDI (ch. orth.)	+1	+1	1	$\mathrm{O}(N+M)/\mathrm{O}(N)\times\mathrm{O}(M)$	$\mathrm{U}(2n)/\mathrm{Sp}(2n)$
CII (ch. sympl.)	−1	−1	1	$\mathrm{Sp}(N+M)/\mathrm{Sp}(N)\times\mathrm{Sp}(M)$	$\mathrm{U}(2n)/\mathrm{O}(2n)$
D (BdG)	0	+1	0	$\mathrm{SO}(2N)$	$\mathrm{O}(2n)/\mathrm{U}(n)$
C (BdG)	0	−1	0	$\mathrm{Sp}(2N)$	$\mathrm{Sp}(2n)/\mathrm{U}(n)$
DIII (BdG)	−1	+1	1	$\mathrm{SO}(2N)/\mathrm{U}(N)$	$\mathrm{O}(2n)$
CI (BdG)	+1	−1	1	$\mathrm{Sp}(2N)/\mathrm{U}(N)$	$\mathrm{Sp}(2n)$

Table 1. Listed are the ten generic symmetry classes of single-particle Hamiltonians $\mathcal{H}$, classified according to their behavior under time-reversal symmetry ($\mathcal{T}$), charge-conjugation (or: particle-hole) symmetry ($\mathcal{C}$), as well as "sublattice" (or: "chiral") symmetry ($\mathcal{S}$). The labels T, C and S, represent the presence/absence of time-reversal, particle-hole, and chiral symmetries, respectively, as well as the types of these symmetries. The column entitled "Hamiltonian" lists, for each of the ten symmetry classes, the symmetric space of which the quantum mechanical time-evolution operator $\exp(it\mathcal{H})$ is an element. The column "Cartan label" is the name given to the corresponding symmetric space listed in the column "Hamiltonian" in Élie Cartan's classification scheme (dating back to the year 1926). The last column entitled "G/H (ferm. NLσM)" lists the (compact sectors of the) target space of the NLσM describing Anderson localization physics at long wavelength in this given symmetry class.

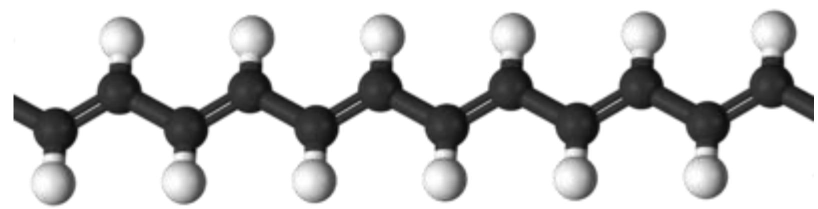
"Topological insulators and superconductors: tenfold way and dimensional hierarchy," [37].

Su-Schreifer and Heeger Model

A segment of *trans*-polyacetylene



Structural diagram



Ball-and-stick model

Chemical Compound: Polyacetylene usually refers to an organic polymer with the repeating unit (C_2H_2). The name refers to its conceptual construction from polymerization of acetylene to give a chain with repeating olefin groups. Wikipedia Formula: $[C_2H_2]_n$

Wikipedea and [16].

Su-Schreifer and Heeger Model

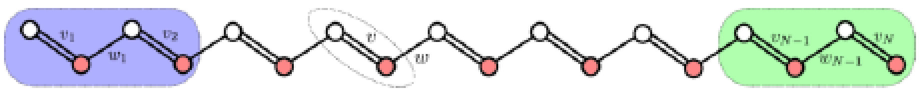


Figure 1.1: Geometry of the SSH model. A 1D chain with two atoms in the unit cell (circled by dashed line). The hopping amplitudes are staggered: w (double line) and v (single line). The long chain consists of the left edge (blue shaded background), the translationally invariant bulk (no background) and the right edge (green shaded background). The hopping amplitudes at the edges are subject to disorder, in the bulk, however, are fixed. .

Polyacetylene chain

$$\hat{H} = \sum_{n=1}^{N} \left(v_n \hat{c}^{\dagger}_{2n-1} \hat{c}_{2n} + w_n \hat{c}^{\dagger}_{2n} \hat{c}_{2n+1} + h.c. \right)$$

$$\hat{H} = v \sum_{m=1}^{N} |m\rangle \langle m| \otimes \hat{\sigma}_x \ + w \sum_{m=1}^{N-1} \left(|m+1\rangle \langle m| \otimes \frac{\hat{\sigma}_x + i\hat{\sigma}_y}{2} + h.c. \right)$$

$$\hat{\sigma}_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \qquad \hat{\sigma}_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

- The winding number is a topological index
- Bulk-boundary correspondence to net number of edge states: $\mathrm{N_A} - \mathrm{N_B}$
- Simple robust predictions about the low energy physics at the edge or of the edge state

fizipedia.bme.hu/images/1/14/Topological_insulators.pdf and [16].

Rice-Mele Model

- Adiabatic Charge Pumping
- Time Dependent
- Number of Pumped Particles is the Chern Number

$$\begin{aligned}\hat{H}(t) = &\ v(t)\sum_{m=1}^{N}\left(|m,B\rangle\langle m,A| + h.c.\right)\\ &+ w(t)\sum_{m=1}^{N-1}\left(|m+1,A\rangle\langle m,B| + h.c.\right)\\ &+ u(t)\sum_{m=1}^{N}\left(|m,A\rangle\langle m,A| - |m,B\rangle\langle m,B|\right)\end{aligned}$$

[16]

Qi-Wu-Zhang Model

- Two dimensional
- Chern Number is the topological invariant
- Half BHZ model (Next slide)

$$\hat{H} = \sum_{m_x=1}^{N_x-1} \sum_{m_y=1}^{N_y} \left(|m_x+1, m_y\rangle \langle m_x, m_y| \otimes \frac{\hat{\sigma}_z + i\hat{\sigma}_x}{2} + h.c. \right) + \sum_{m_x=1}^{N_x} \sum_{m_y=1}^{N_y-1} \left(|m_x, m_y+1\rangle \langle m_x, m_y| \otimes \frac{\hat{\sigma}_z + i\hat{\sigma}_y}{2} + h.c. \right) + u \sum_{m_x=1}^{N_x} \sum_{m_y=1}^{N_y} |m_x, m_y\rangle \langle m_x, m_y| \otimes \hat{\sigma}_z$$

$$\hat{\sigma}_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \qquad \hat{\sigma}_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \qquad \hat{\sigma}_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

[16]

Bernevig-Hughes-Zhang Model

- $\hat{C}$ = Hermitian Coupling Operator acting on Internal degrees of freedom
- $\hat{C} = 0$ for the 4 band model of HgTe

$$\hat{H}_{\mathrm{BHZ}}(\mathbf{k}) = \hat{s}_0 \otimes [(u + \cos k_x + \cos k_y)\hat{\sigma}_z + \sin k_y \hat{\sigma}_y] + \hat{s}_z \otimes \sin k_x \hat{\sigma}_x + \hat{s}_x \otimes \hat{C}$$

Mercury telluride is a binary chemical compound of mercury and tellurium. It is a semi-metal related to the II-VI group of semiconductor materials. Alternative names are mercuric telluride and mercury telluride. Wikipedia
Formula: HgTe
Molar mass: 329.18 g/mol
Density: 8.1 g/cm³

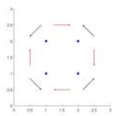
$$\hat{\sigma}_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \qquad \hat{\sigma}_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \qquad \hat{\sigma}_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

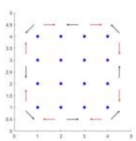
[16]

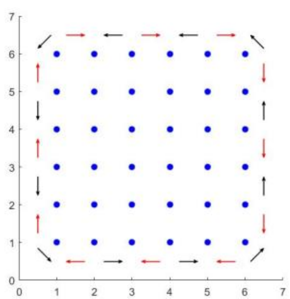
What is Proposed?

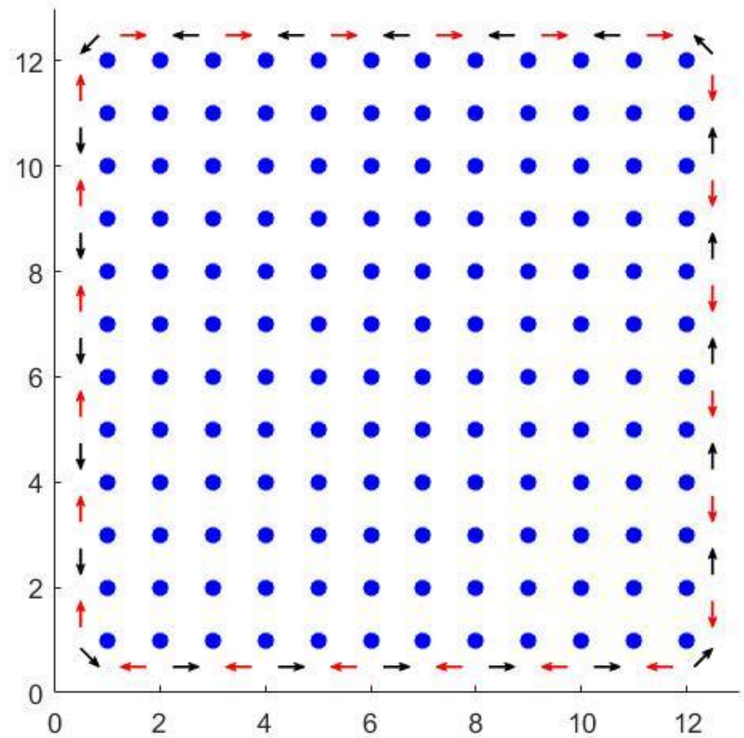
- Properties of TI Regions
  - Size
  - Shape
  - Disorder
  - Robustness
- Transition from Film to Wire
- Transition from Wire to Dot
- Numerical Experiments

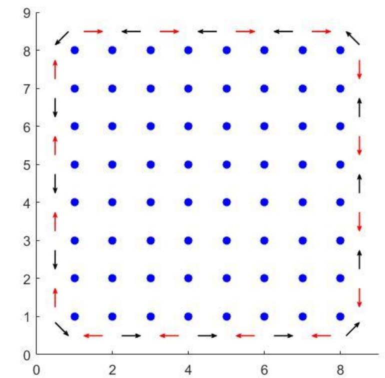
Size

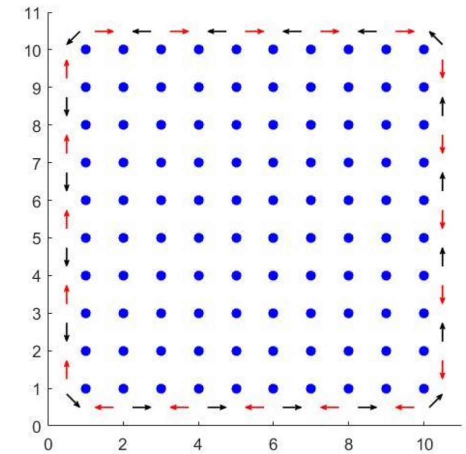




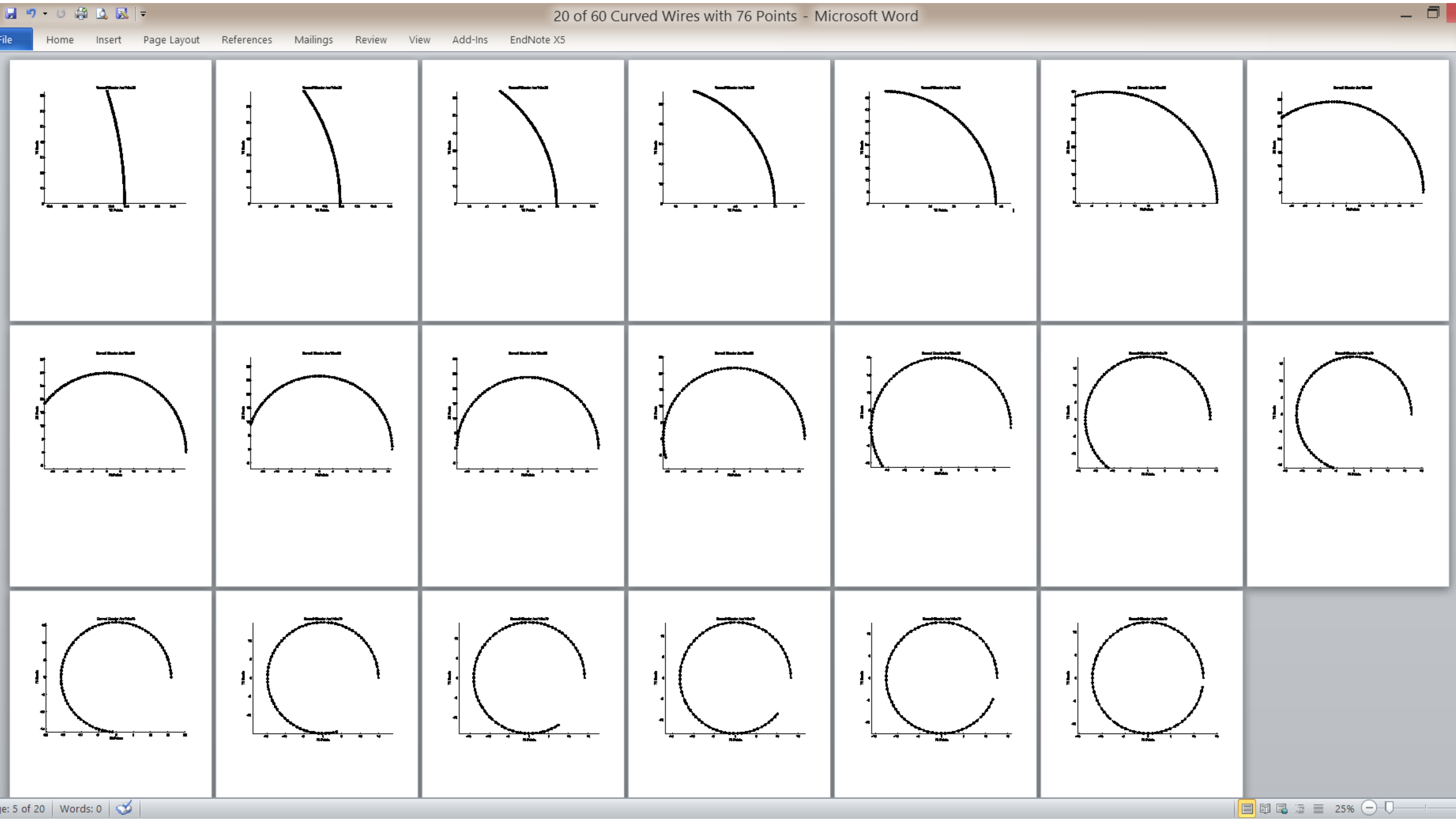








Shape



20 of 60 Curved Wires with 76 Points - Microsoft Word
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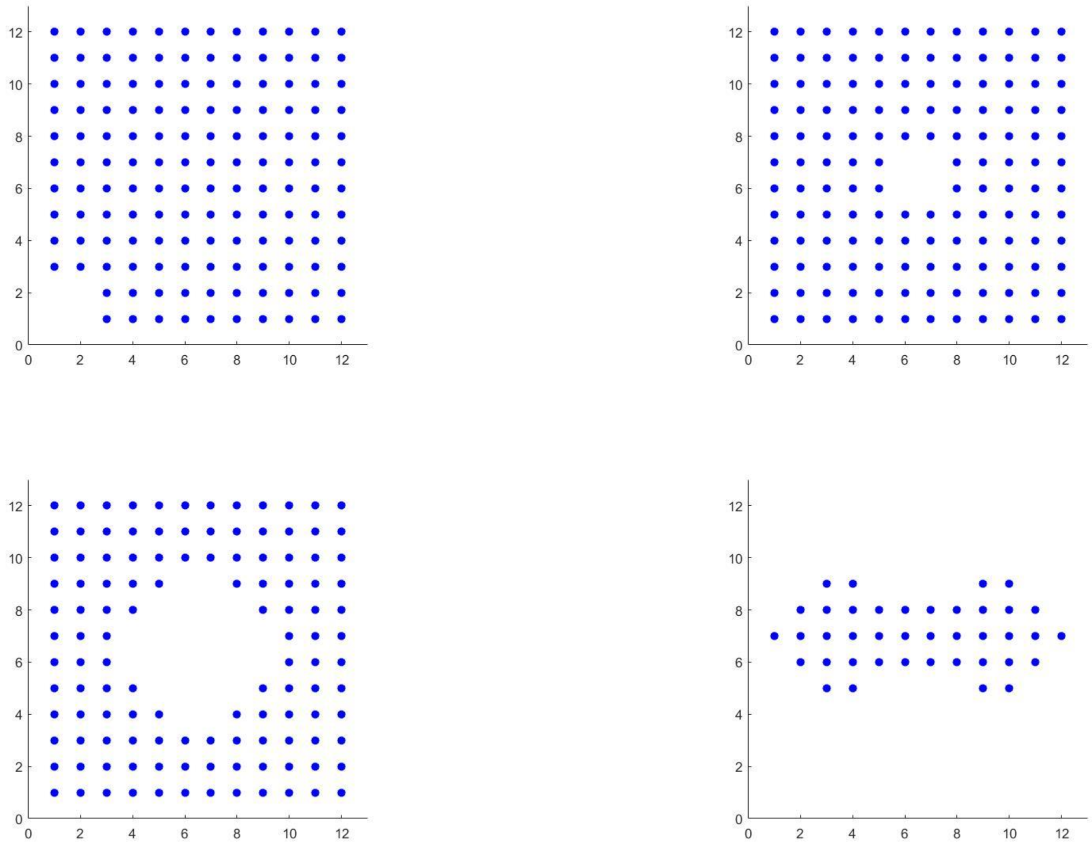
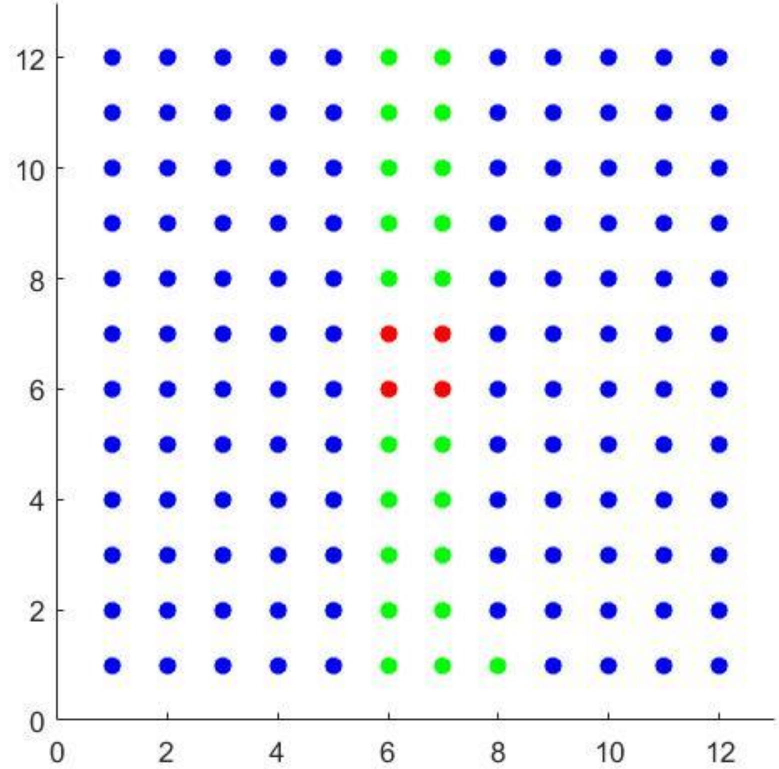
Shape

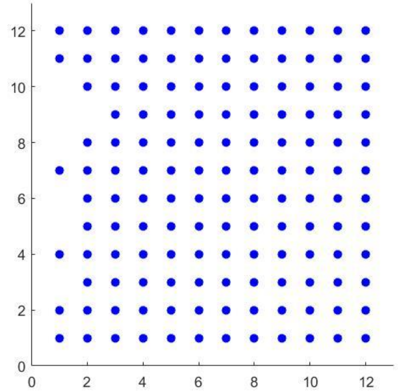


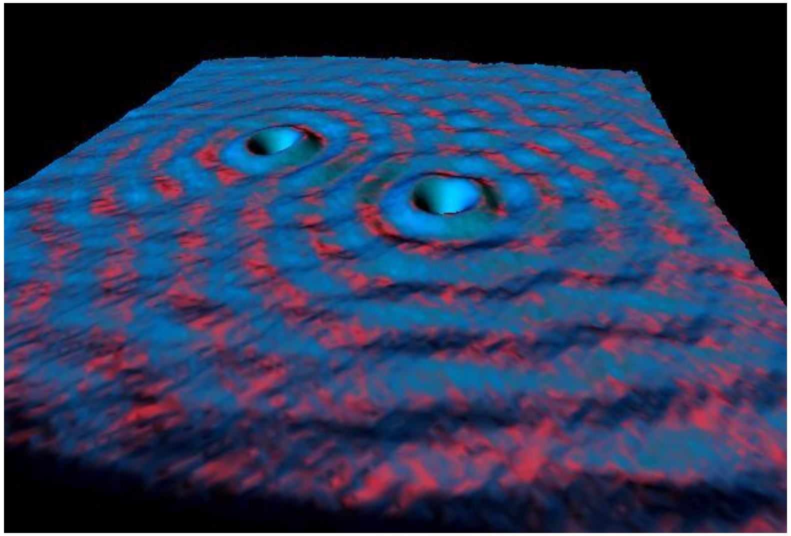
Transitions

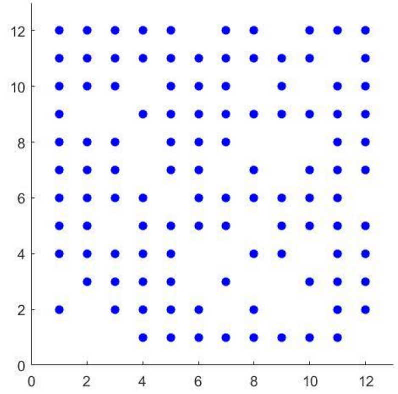


Disorder

- Impurities
- Hamiltonian

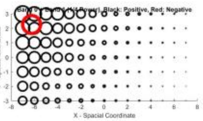
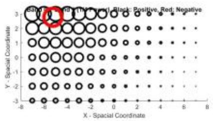
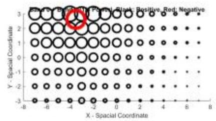
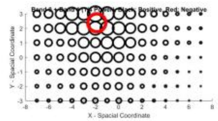
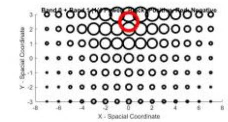


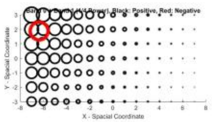


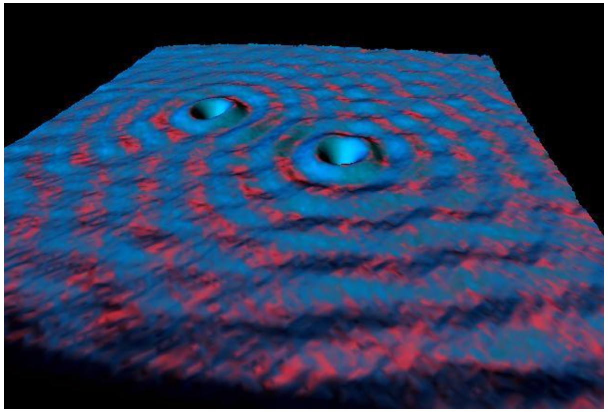


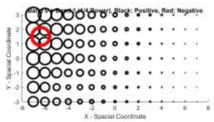
In this scanning tunneling microscope (STM) image, electron density waves are seen to be breaking around two atom-sized defects on the surface of a copper crystal. The resultant standing waves result from the interference of the electron waves scattering from the defects. Courtesy, Don Eigler, IBM.

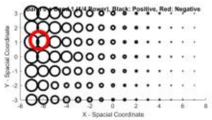
Robustness

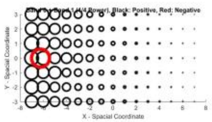




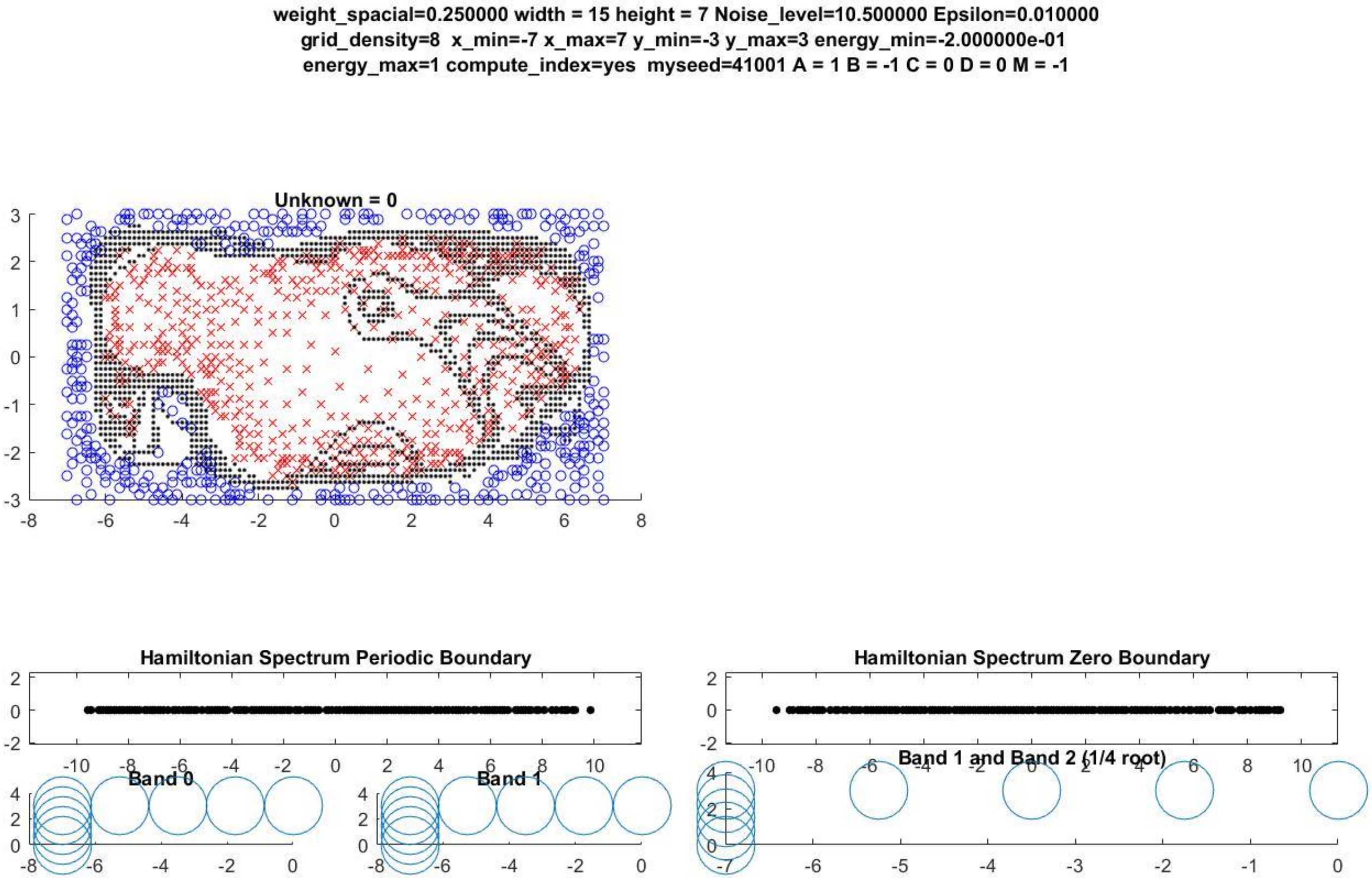




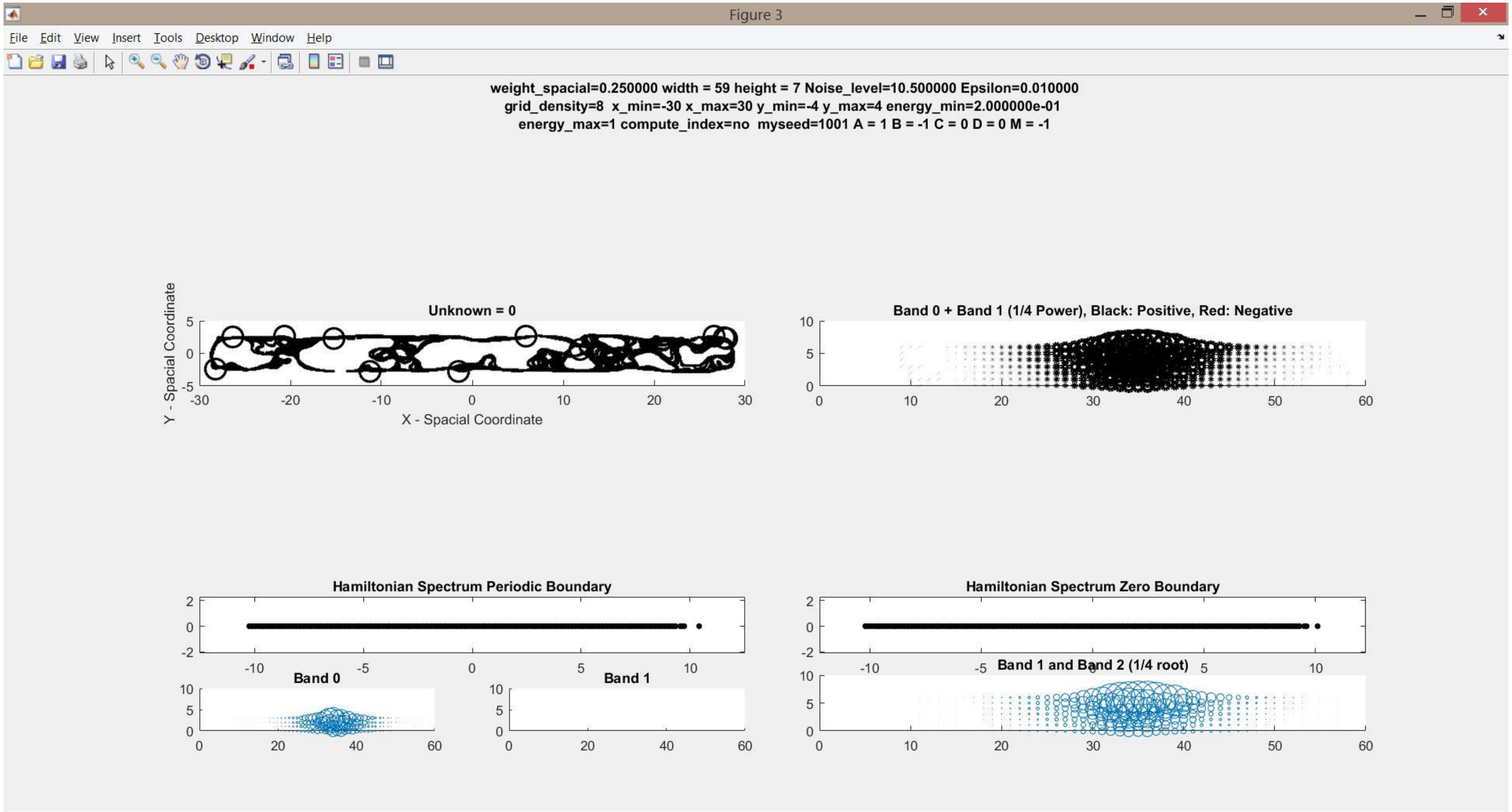
In this scanning tunneling microscope (STM) image, electron density waves are seen to be breaking around two atom-sized defects on the surface of a copper crystal. The resultant standing waves result from the interference of the electron waves scattering from the defects. Courtesy, Don Eigler, IBM.



Numerical Experiments



Numerical Experiments



How will it Get Done?

Year	2016									2017											
Month	4	5	6	7	8	9	10	11	12	1	2	3	4	5	6	7	8	9	10	11	12
Shape Experiment																					
Disorder Experiment																					
Robustness																					
Shape Manuscript																					
Disorder Manuscript																					
Robustness Manuscript																					
New Hamiltonian, Dimension or Disorder																					
Dissertation																					
Final Defense																					

What Good is the Research?

- More Efficient Prototyping
- Less Expensive Design
- Faster Time to Development
- Increased Knowledge of Shape, Size and Disorder on Topological Insulator Properties of the Edge, Meso and Bulk Regions
- Local Manufacture

Questions?