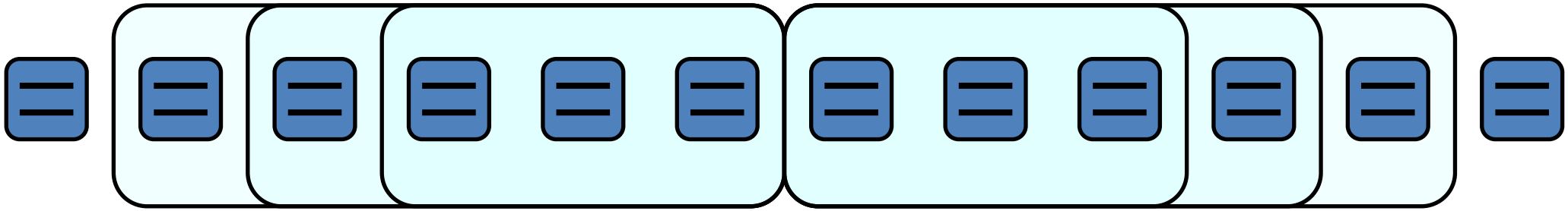
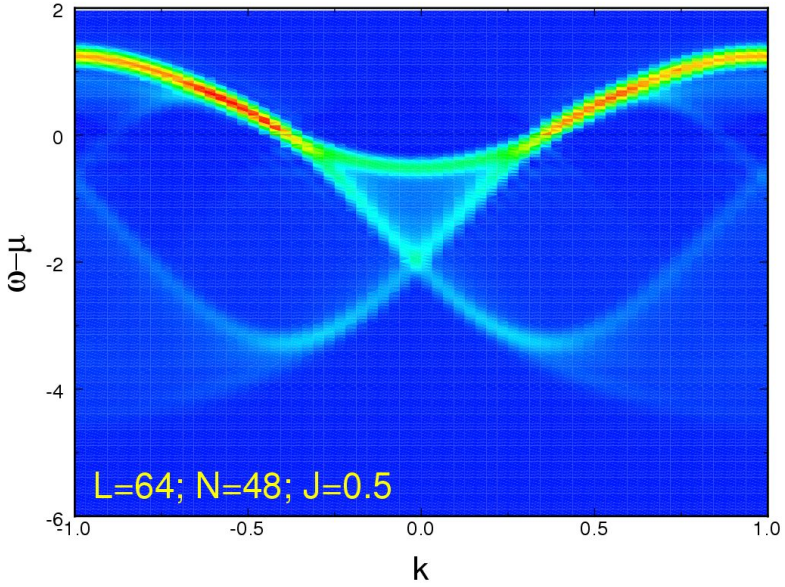
Understanding strongly correlated quantum matter

Adrian Feiguin





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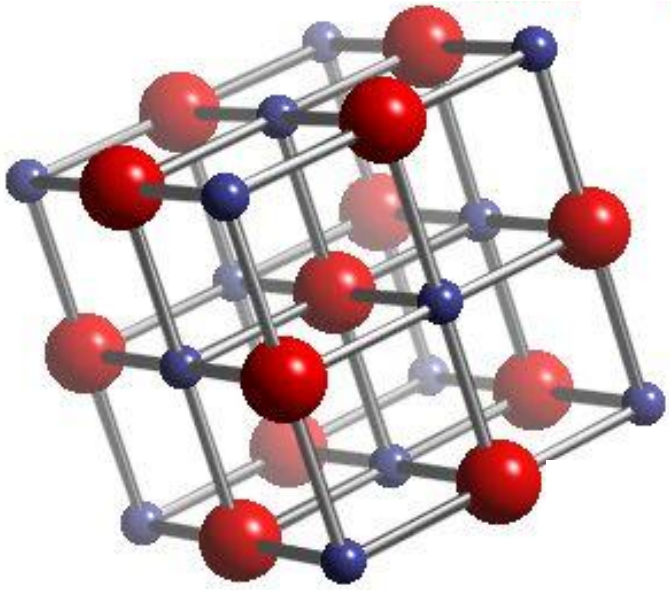
Condensed matter

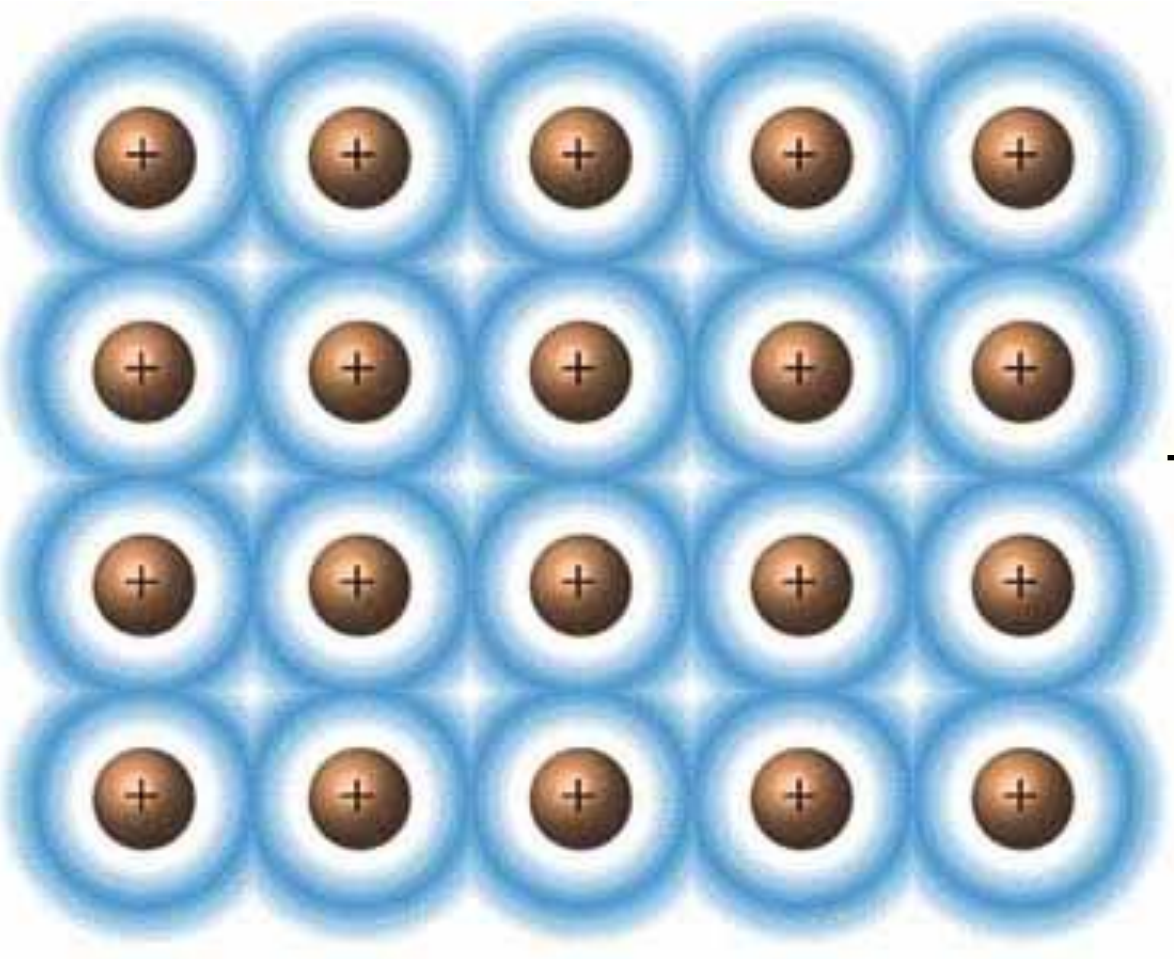
-Phenomena emerging from the collective behavior of a large number of degrees of freedom inside a solid.

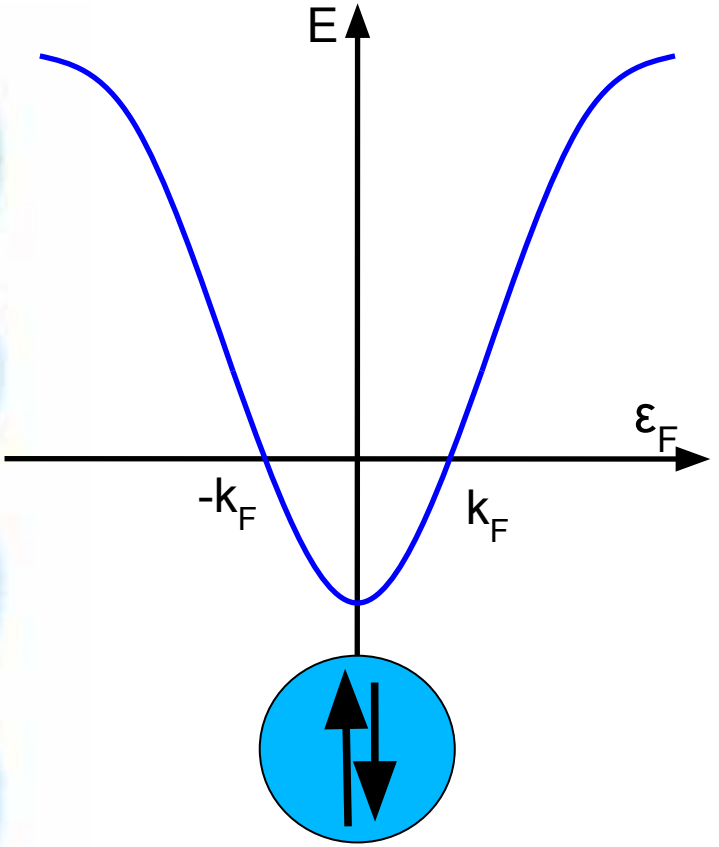
-We start with putting together single constituents (particles) with well defined properties (mass, spin, charge), and turning on interactions.

-We observe different phases of matter, and transitions between them.



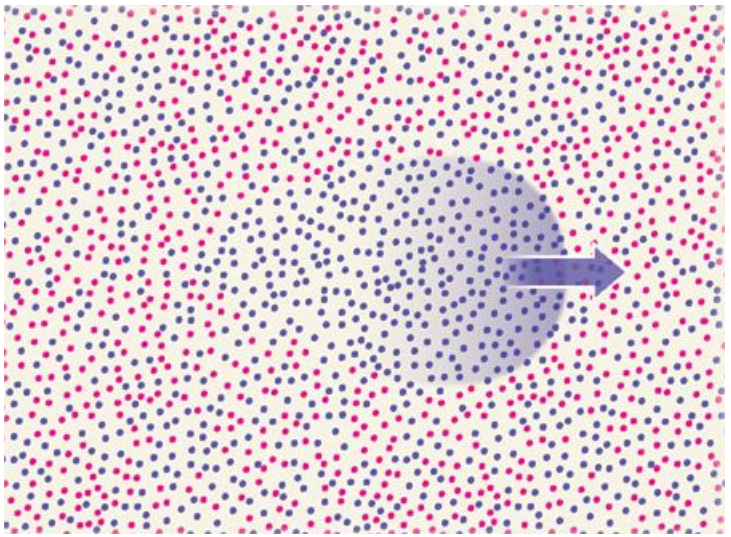
The Fermi Sea





Weakly interacting electrons

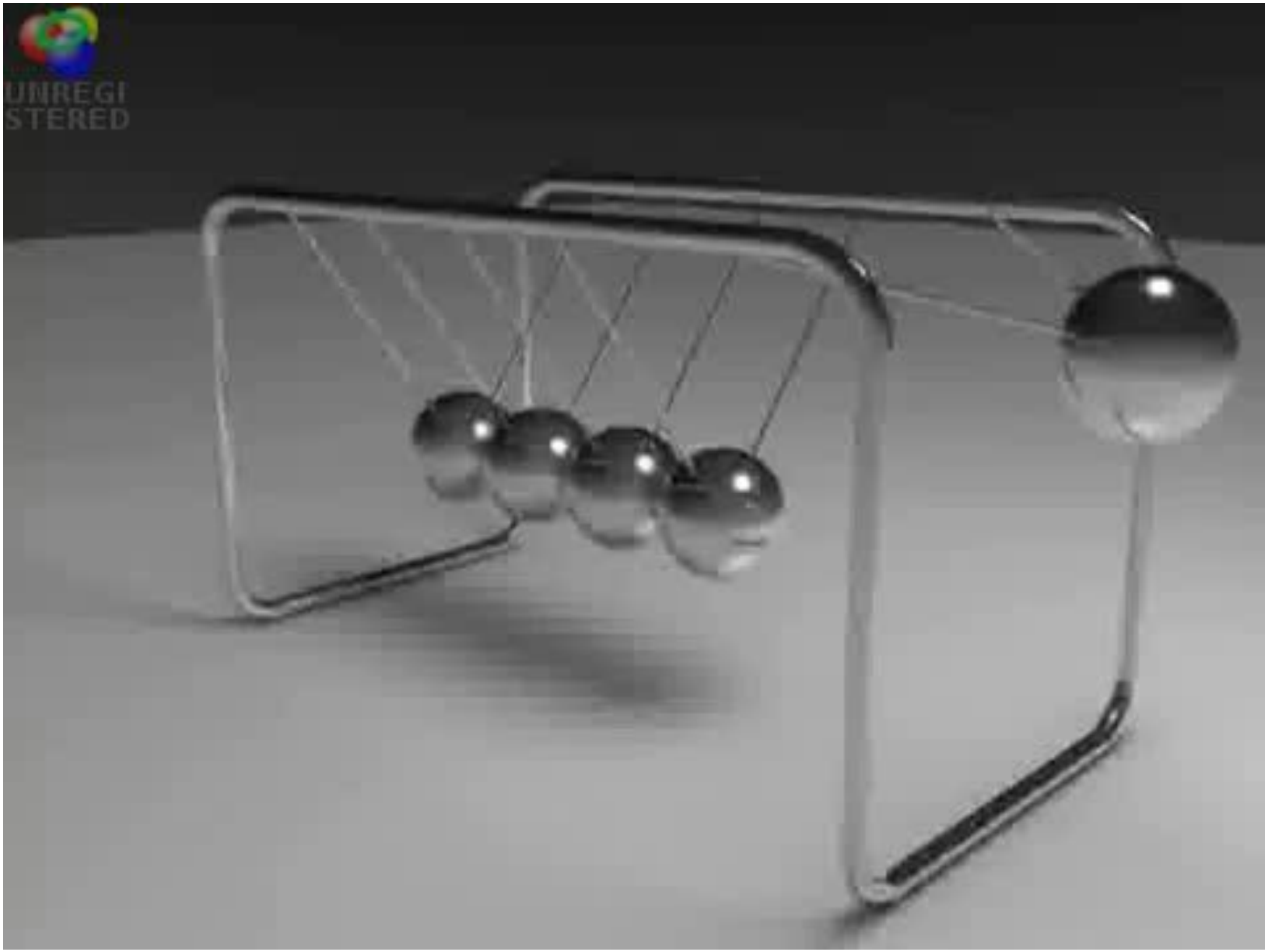
Electrons in solids:
We think “quasi-particles”



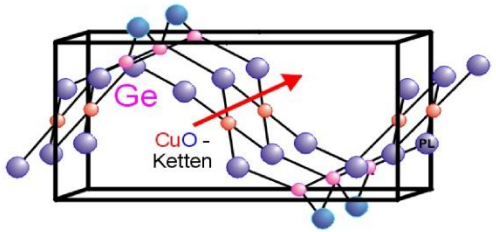
In a normal Fermi liquid, each constituent particle (dots) is surrounded by a polarization cloud of particles (blue shading) that is dragged along by its motion (arrow). The constituent particle and 'dressing cloud', which together form what is known as a quasi-particle, act like weakly interacting particles.

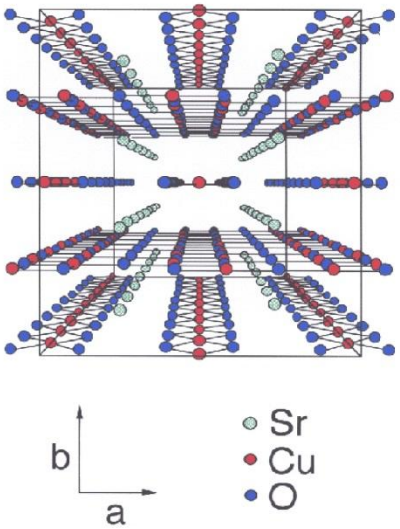
Collective behavior

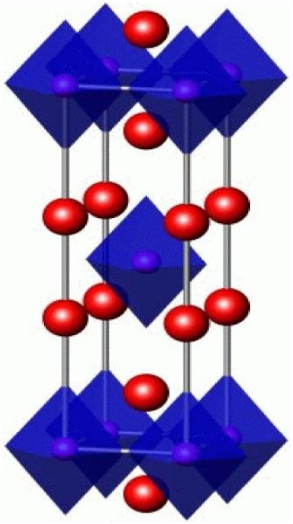
What happens in one dimension?



Low dimensional compounds







$CuGeO_3$

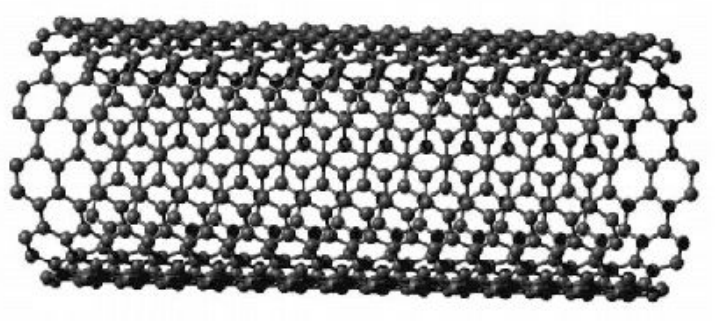
(chains)

$Sr_{14}Cu_{24}O_{41}$

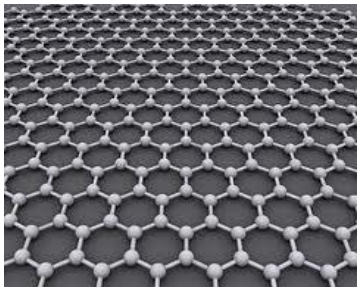
(ladders)

La_2CuO_4

(planes)



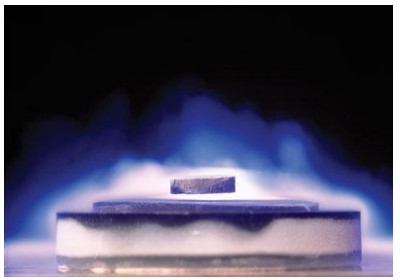
carbon nanotubes

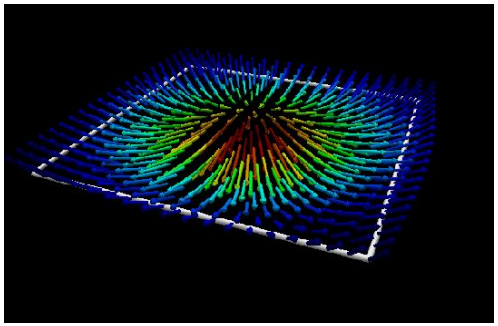


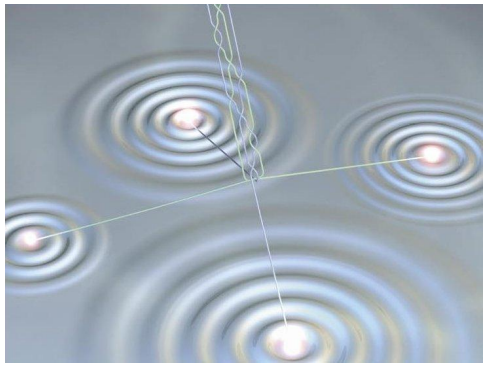
graphene

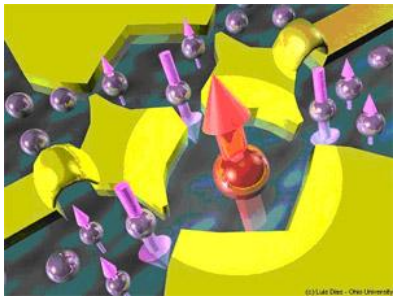
Strongly correlated problems

- High temperature superconductivity
- Colossal magnetoresistance (Manganites)
- Mott-Hubbard transition
- Non Fermi liquid behaviour
- Anderson and Kondo impurity problems
- Transport in low dimensions (quantum dots)
- Fractional Quantum Hall Effect
- Spin liquids; topological phases (novel quantum phases)









Emergent behavior defies intuition!

Areas of interest

- Exotic phases of matter of quantum origin: quantum magnetism, superconductivity…
- Quantum transport and non-equilibrium physics. “Mottronics” and molecular devices. Materials for light harvesting applications.
- Spintronics, using spin for logical gates and computing. NV centers in diamond.
- Basic understanding of quantum phenomena using cold atoms.
- New computational algorithms for quantum chemistry and condensed matter.

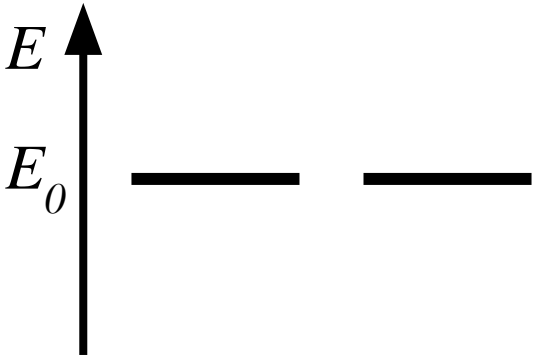
Why we need numerical methods?

- Analytical methods are no longer reliable!
- We need numerical methods to:
  - Validate predictions from theory
  - Understand the physics when theory fails
  - Compare competing orders (phases)
  - Find new phases
  - Make quantitative predictions for experiments

“Hydrogen” molecule

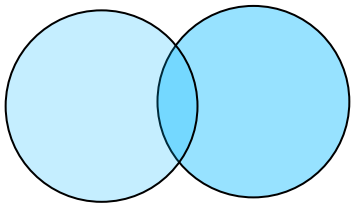
Case 1: atoms are far apart

$$H = \begin{bmatrix} E_0 & 0 \\ 0 & E_0 \end{bmatrix}$$

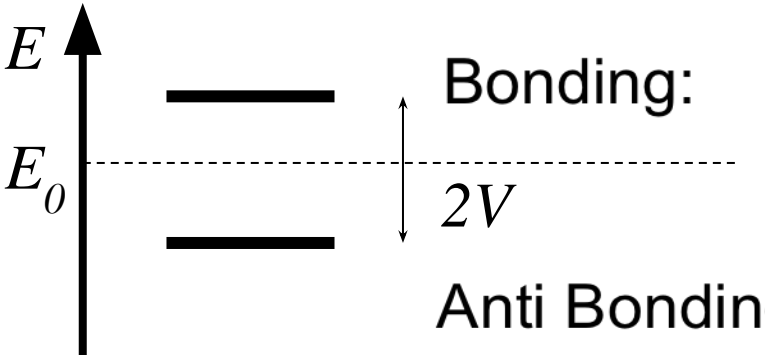


“Hydrogen” molecule

Case 2: we bring atoms closer together



$$H = \begin{bmatrix} E_0 & V \\ V & E_0 \end{bmatrix}$$

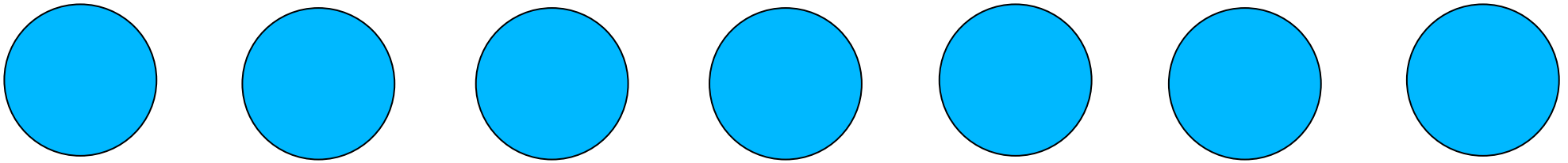


Bonding: $|+\rangle = |1\rangle + |2\rangle = |1\rangle + e^{i0}|2\rangle$

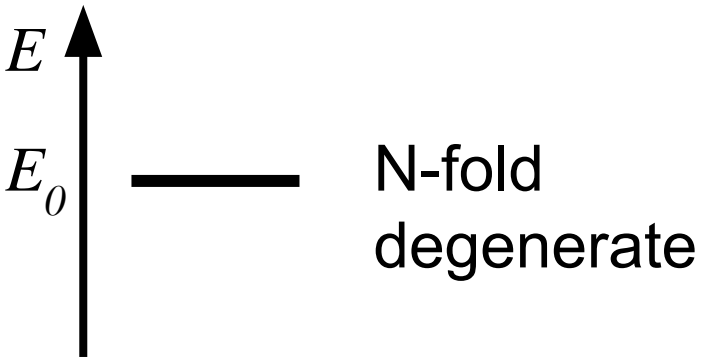
Anti Bonding: $|-\rangle = |1\rangle - |2\rangle = |1\rangle + e^{i\pi}|2\rangle$

We can classify these states as $|k\rangle = |1\rangle + e^{ik}|2\rangle$ with $k=0,\pi$

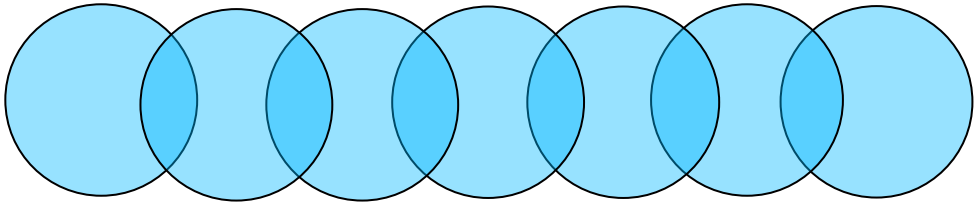
“Hydrogen” chain



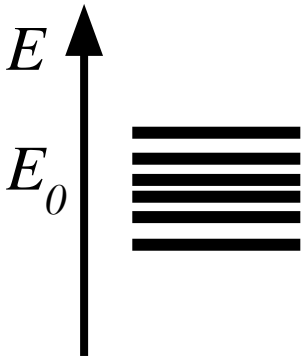
$$H = \begin{pmatrix} E_0 & 0 & \cdots & 0 \\ 0 & E_0 & & 0 \\ \vdots & & \ddots & \vdots \\ 0 & 0 & \cdots & E_0 \end{pmatrix}$$

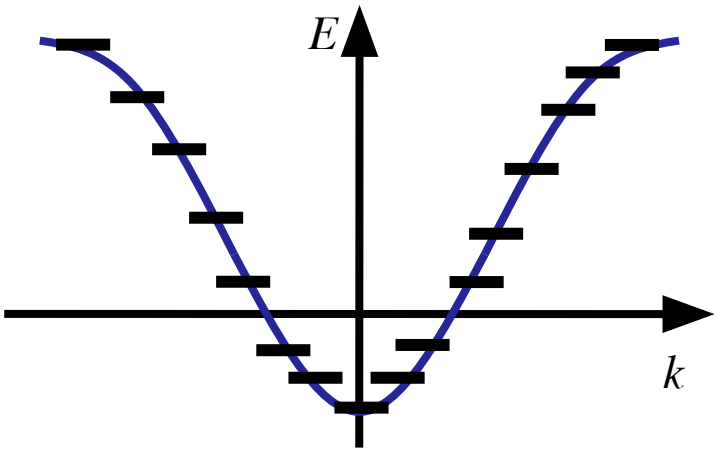


“Hydrogen” chain



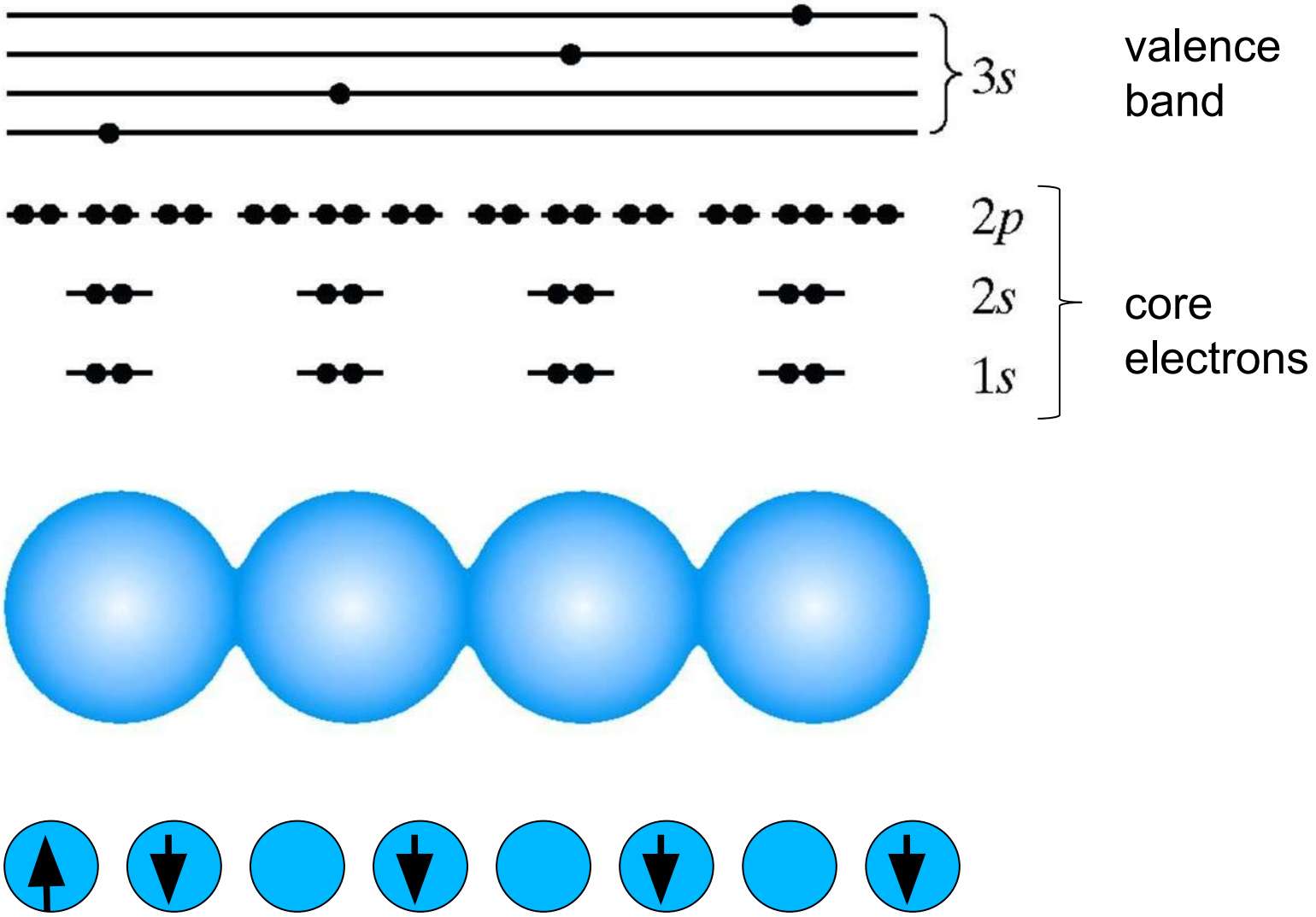
$$H = \begin{bmatrix} E_0 & V & 0 & \dots & 0 & 0 \\ V & E_0 & V & & & 0 \\ 0 & V & E_0 & & & 0 \\ \vdots & & & \ddots & & \vdots \\ 0 & & & & E_0 & V \\ 0 & 0 & & \dots & V & E_0 \end{bmatrix}$$





State now lie on an “energy band”

Effective models



Basis of states

Occupation number representation

(1 orbital per site, spin ½)

Empty | Spin up | Spin down | Double occupied

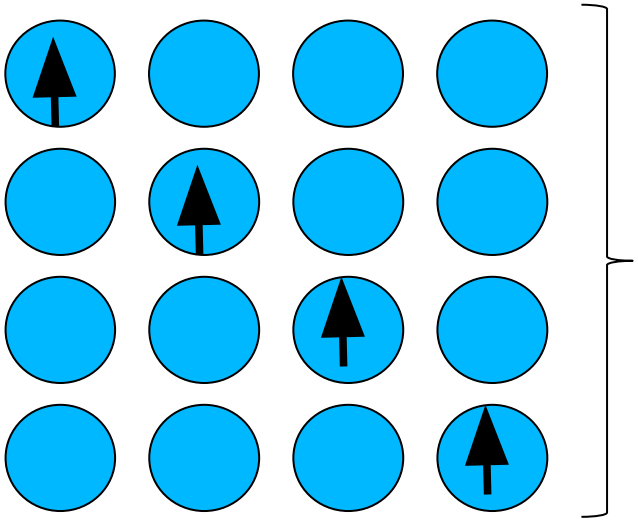
$|0\rangle$ $|\uparrow\rangle$ $|\downarrow\rangle$ $|2\rangle$

States $|x\rangle = |x_1\rangle|x_2\rangle|x_3\rangle$ $|x_4\rangle....|x_N\rangle$

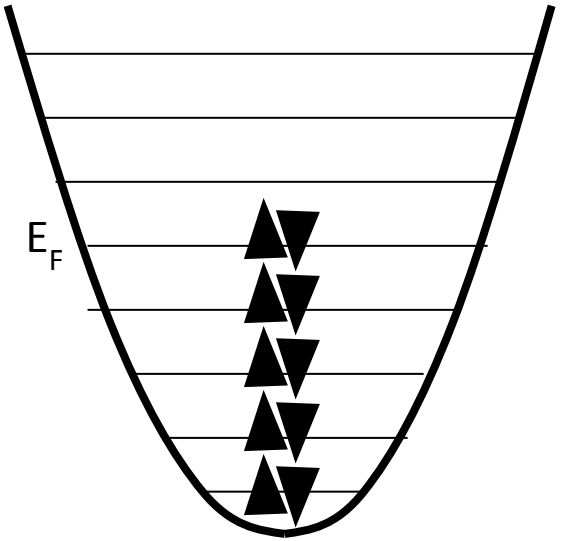
Dimension = number of configurations = 4^N

N: number of lattice sites

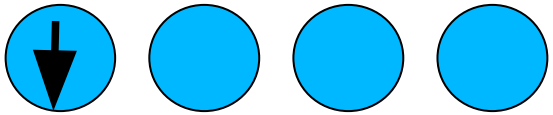
Single particle vs. many body picture



4 configurations
4x4 matrix

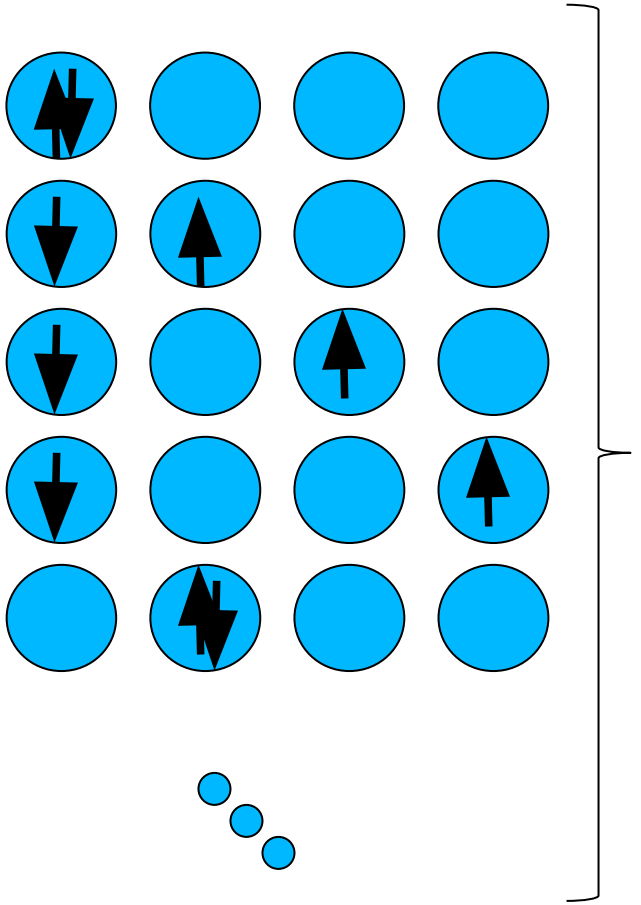


And similarly for the “down” electrons



The state of the system is a “product state” of single particle states. We only need to solve the one-particle problem.

Single particle vs. many body picture



16 configurations
16x16 matrix

The state of the system is “highly entangled”. It cannot be written as a “product state”, and the behavior of each electron is dictated by the behavior of the rest.

Numerical methods

- Quantum Monte Carlo
- Exact Diagonalization (Lanczos)
- Density Matrix Renormalization Group

Exact diagonalization

"<u>brute force</u>" diagonalization of the Hamiltonian matrix.

Schrödinger's Equation:

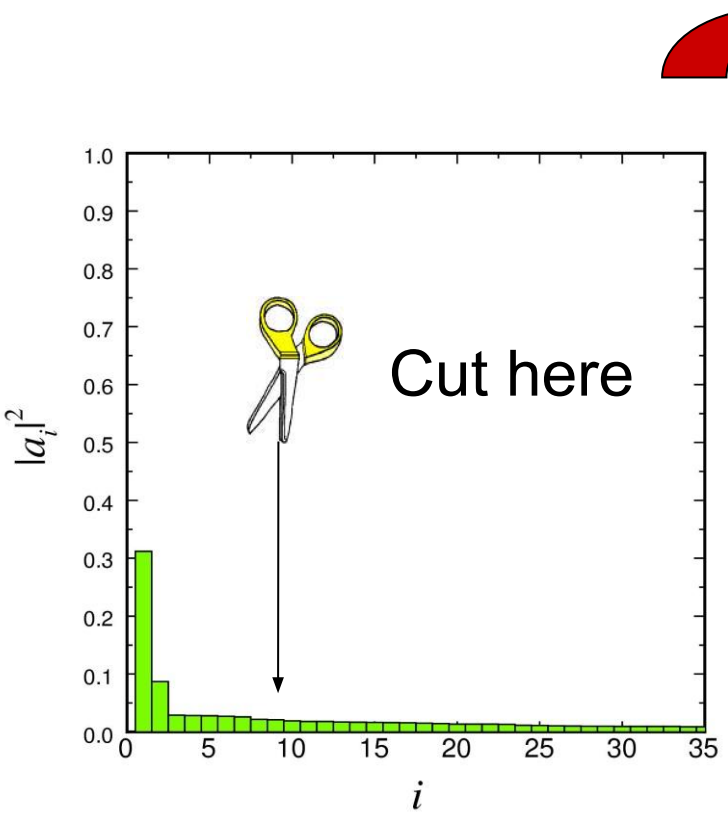
$$H\,|x\rangle = E\,|x\rangle$$

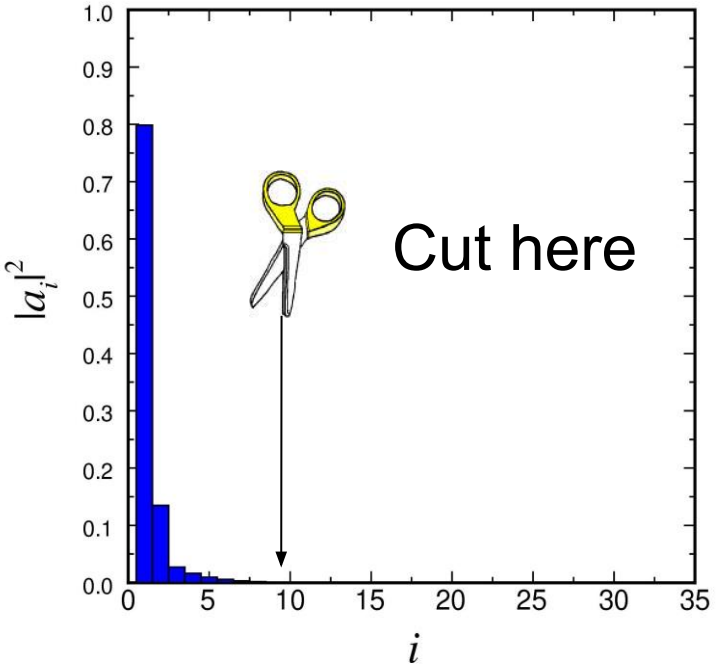
H : Hamiltonian operator
$|x\rangle$: eigenstate
E : eigenvalue (ENERGY)

- *Direct evaluation of the ground state of the full Hamiltonian..*
- *Excitation energies (gaps).*
- *Correlation functions.*
- *… anything you want to know about the state…* ***but… only small systems***

Truncating the Hilbert space

Can we rotate our basis to one where the weights are more concentrated, to minimize the error?





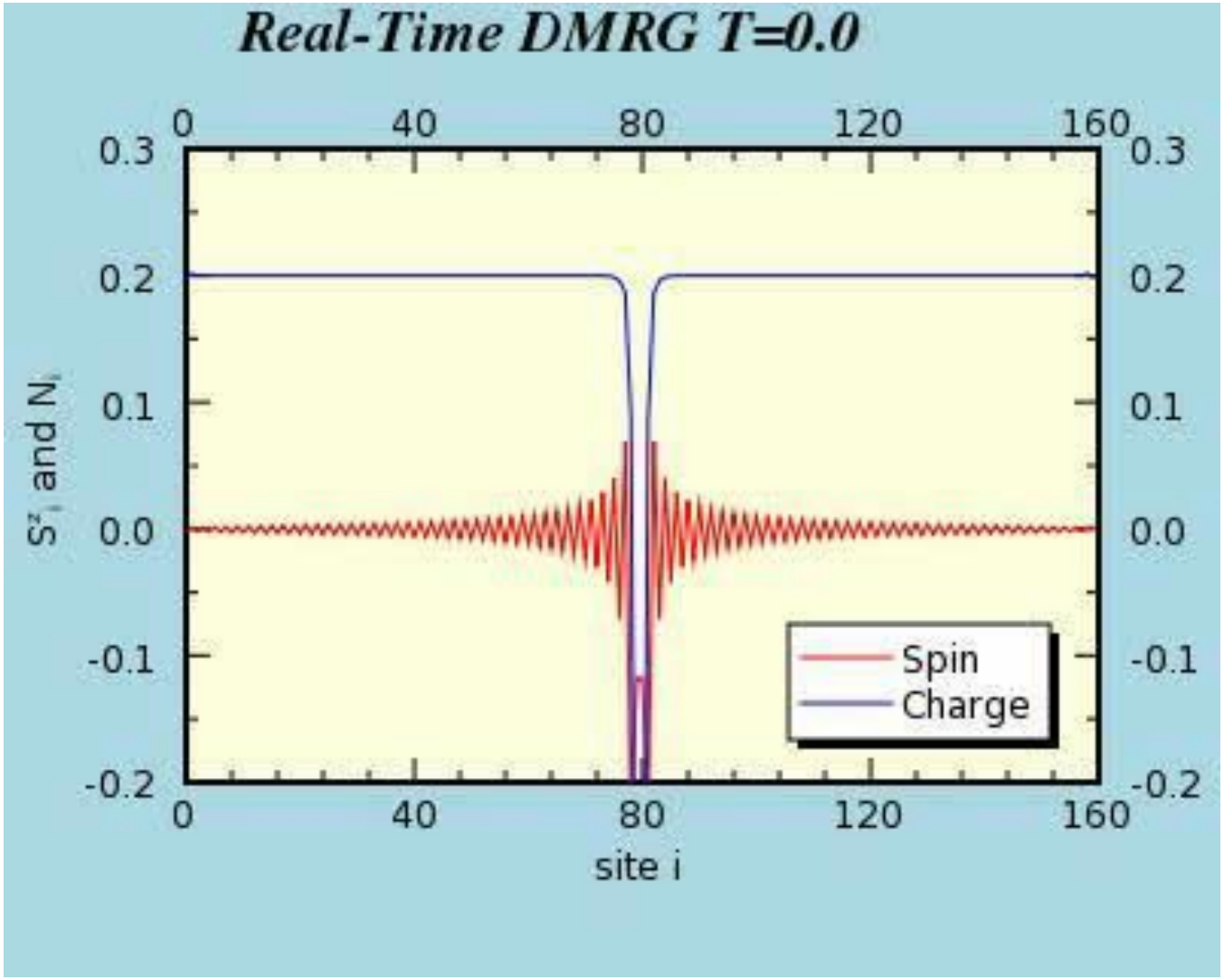
$$|\mathrm{gs}\rangle = \sum a_i |x_i\rangle \quad , \sum |a_i|^2 = 1 \Rightarrow Error = 1 - \sum' |a_i|^2$$

“Classical” analogy
Image compression algorithms (e.g. Jpeg)

We want to achieve “lossless compression”
… or at least minimize *the loss of information*

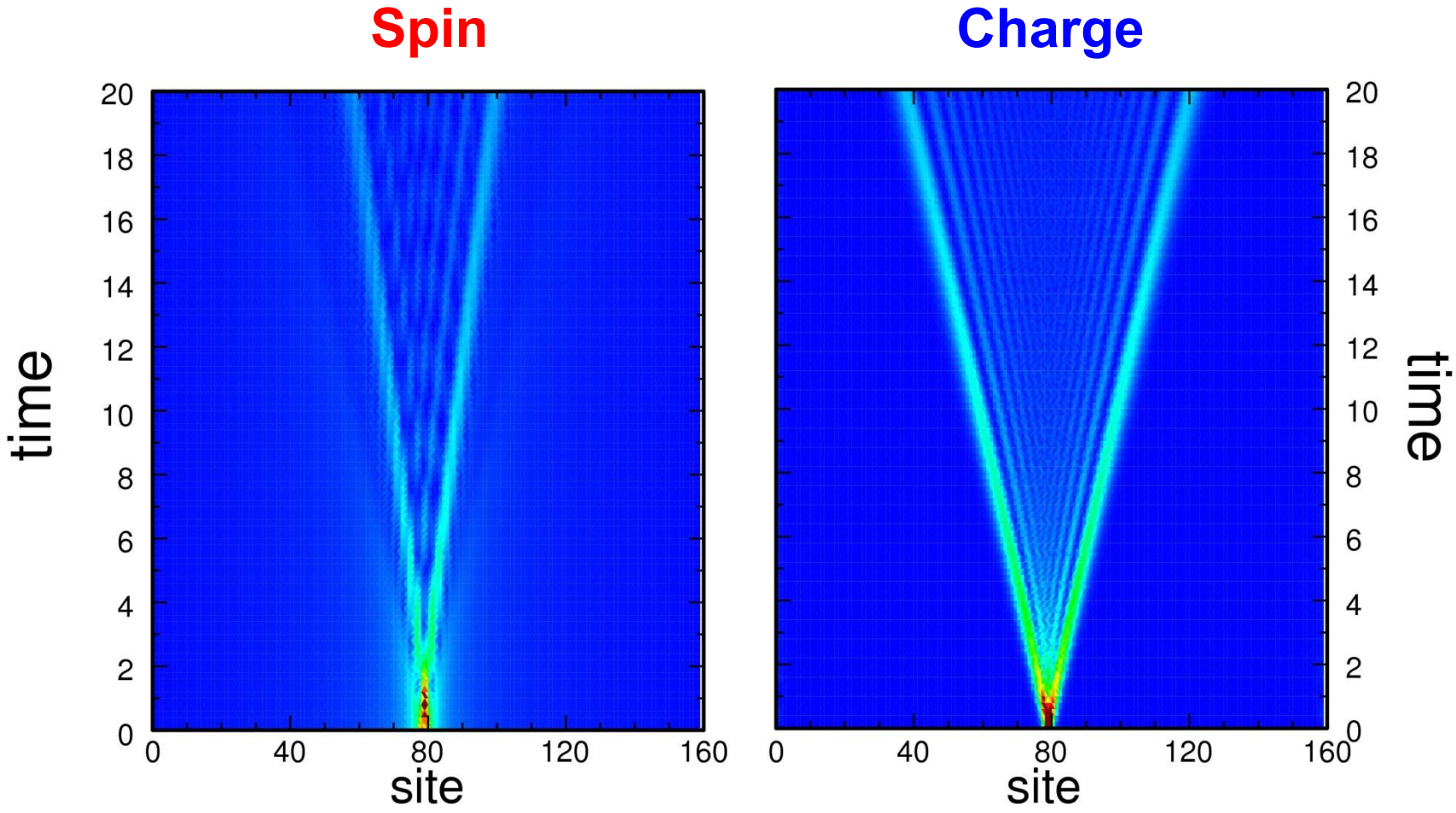
Real-time simulation

Half-filled Hubbard model (L=160, U=4)



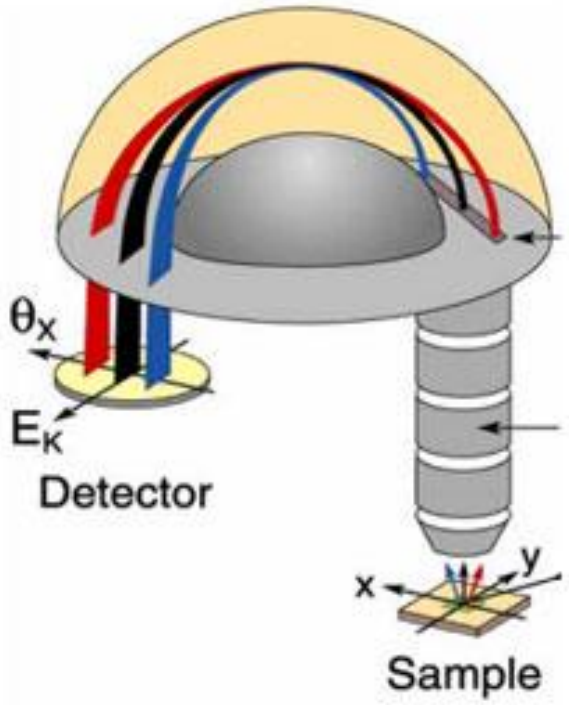
S.R.White and AEF, PRL (2004), Daley et al, J. Stat. Mech.: Theor. Exp. (2004); AEF and S.R.White, PRB (2005), Rapid Comm.

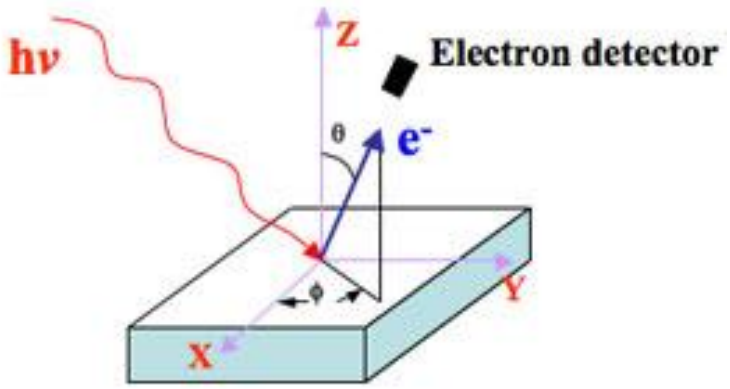
Lightcones



Spin and charge propagate at different velocities

ARPES


θx
EK
Detector
x
y
Sample


hν
z
Electron detector
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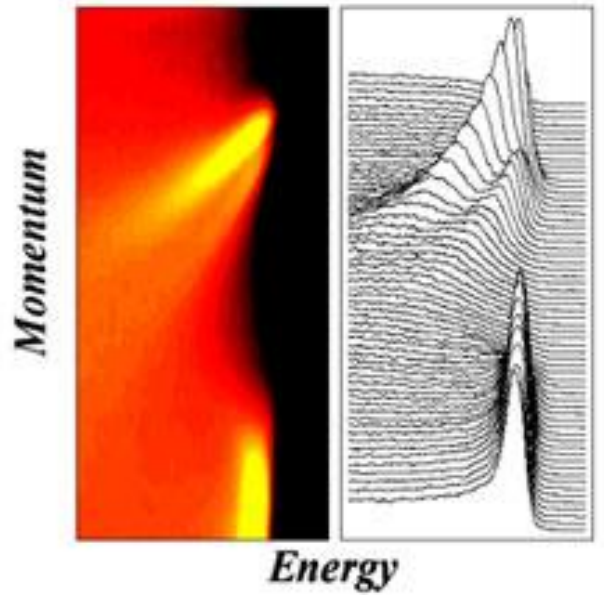
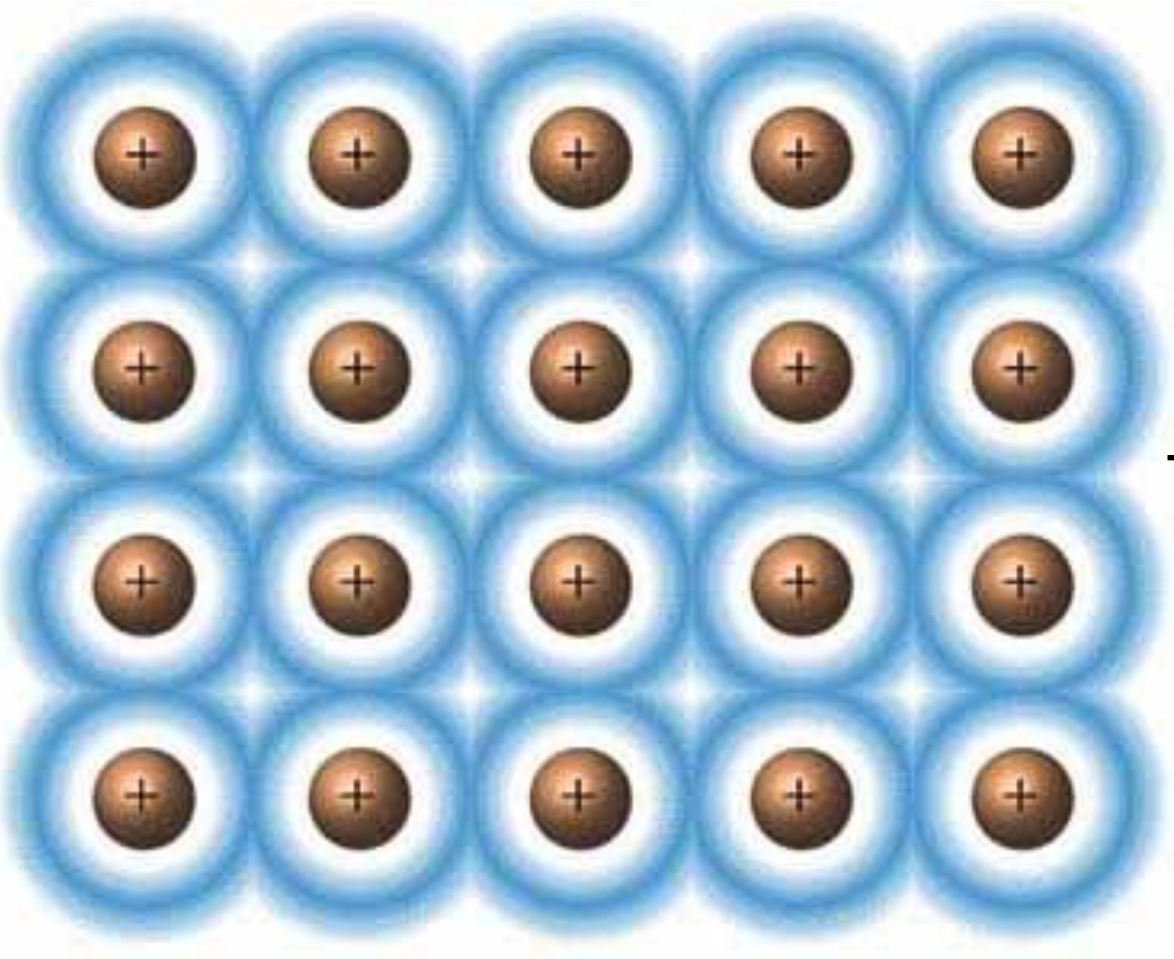
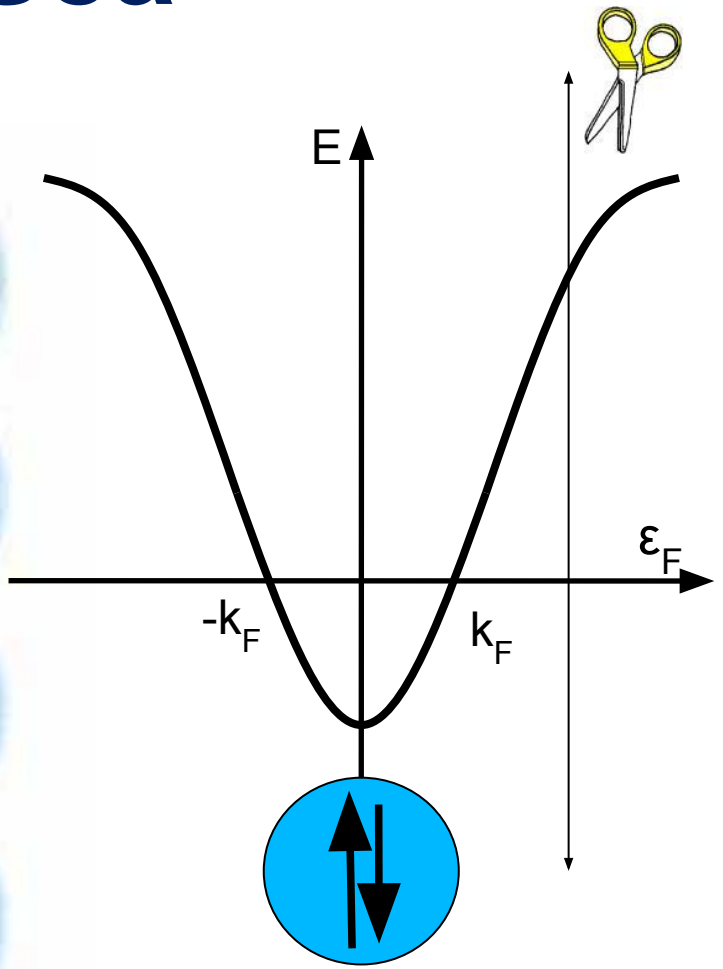
e-
y
x


Momentum
Energy

The Fermi Sea





Electrons in solids:
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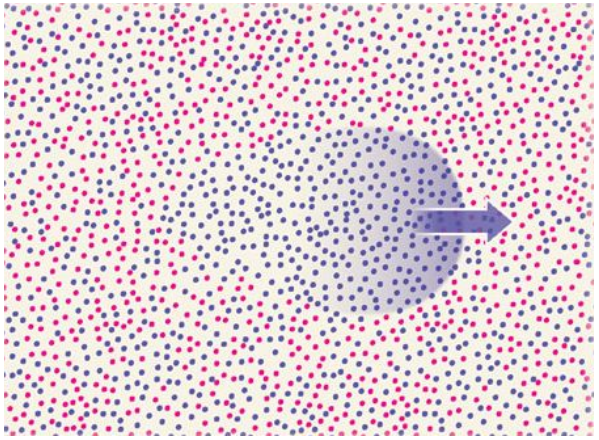

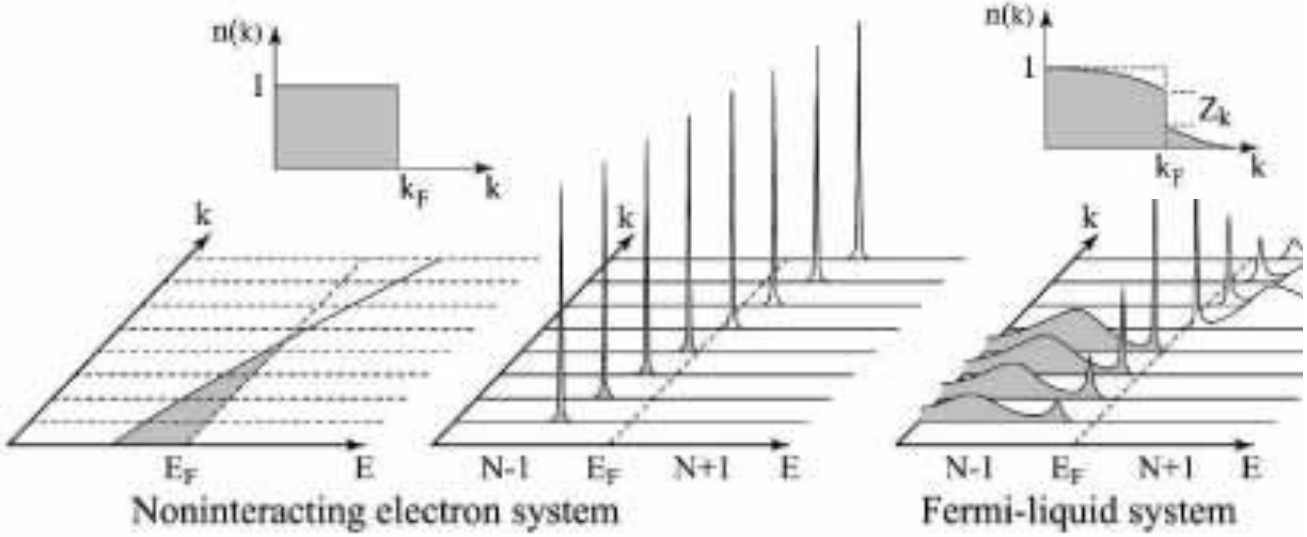

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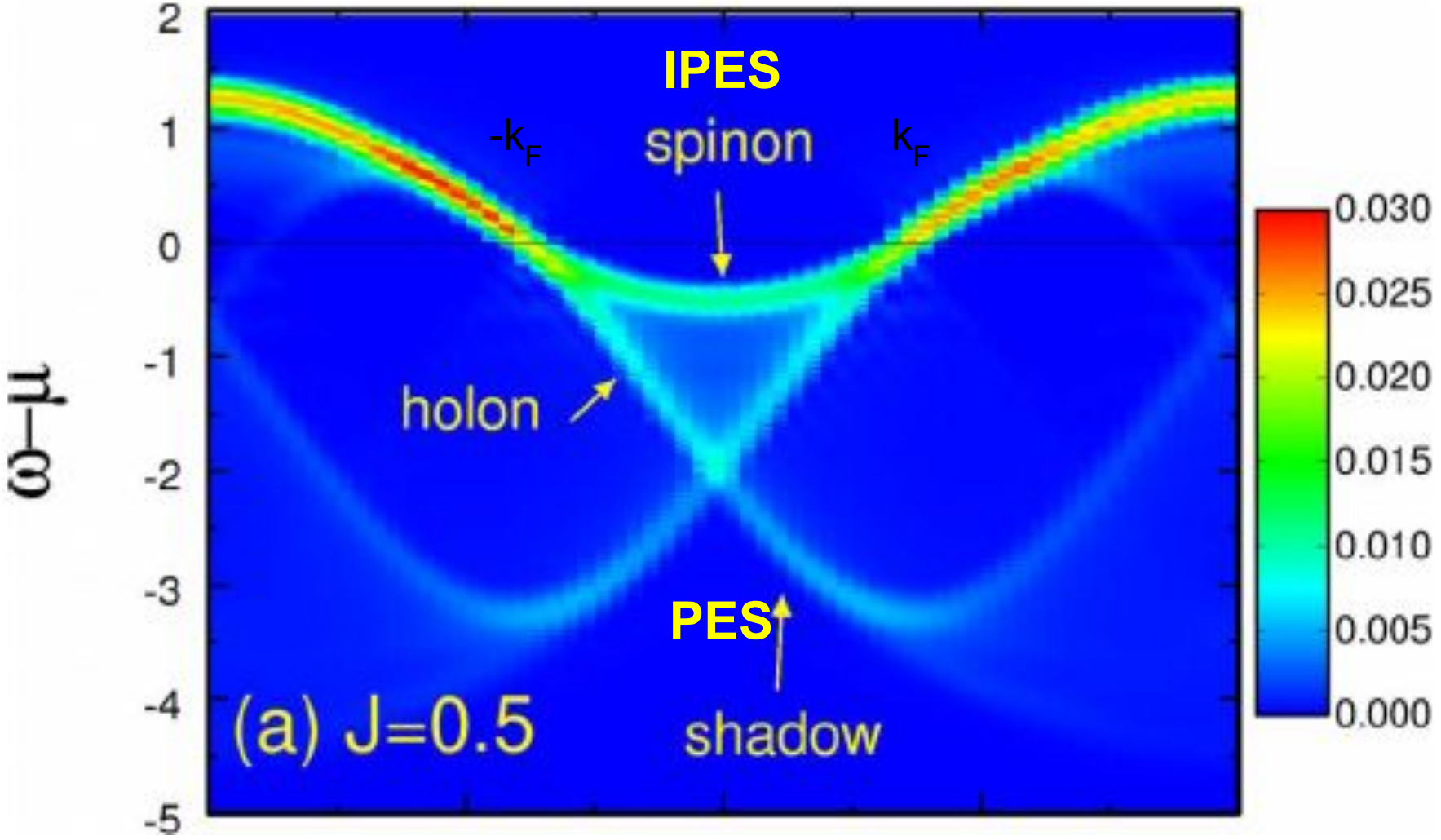
ARPES at T=0

1D t-J model (J=0.5)



Variational Neural Networks

$$|\psi\rangle = \sum_{\{\sigma_1 \ldots \sigma_N\}} \psi_{\sigma_1 \ldots \sigma_N} \, |\sigma_1 \ldots \sigma_N\rangle$$

$$\psi(\vec{\sigma}^z, \vec{a}, \vec{b}, W) = \sum_{h_1, h_2, \cdots, h_M} e^{-E(\vec{\sigma}, \vec{h})},$$

with -

$$-E(\vec{\sigma}, \vec{h}) = \sum_{i=1}^{N} a_i \sigma_i^z + \sum_{i=1}^{N} b_i h_i + \sum_{i=1}^{N} \sum_{j=1}^{M} W_{ij} \sigma_i^z h_j,$$

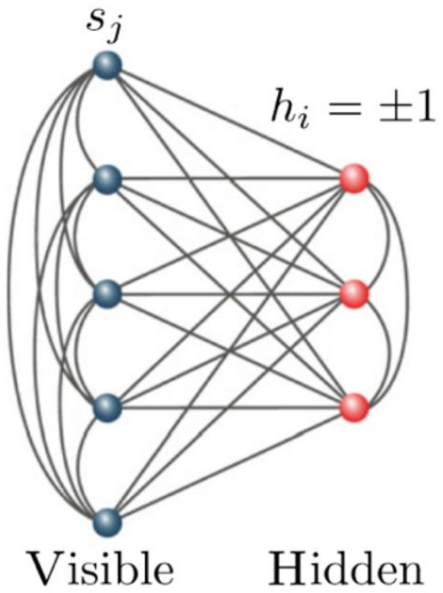


Figure 1: A restricted Boltzmann machine. Physical degrees of freedom are represented by the visible layer.

where h_i={-1,1} are "hidden variables", W's are weights and a,b are biases

"Training" the NN corresponds a "variational minimization": finding the weights and biases a,b and W that minimize the "energy functional"

$$E = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle}$$

We use "Variational Monte Carlo"

Excited states (spectrum)

We want to calculate the "Green's function"

$$G_{ij}(z) = \langle\psi|A_i^\dagger \frac{1}{z-\hat{H}} A_j|\psi\rangle$$

where A is some operator of interest and $z = E_0 + \omega + i\eta$

We introduce auxiliary states:

$$|A_i\rangle = \hat{A}_i|\psi\rangle$$
$$|\chi_j(z)\rangle = \frac{1}{z-\hat{H}}|A_j\rangle,$$

where $|\chi_j(z)\rangle$ is called the "correction vector". Explicitly, $|\chi_j(z)\rangle$ can be obtained by solving the equation:

$$(z-\hat{H})|\chi_j(z)\rangle = \hat{A}_j|\psi\rangle = |A_j\rangle.$$

The spectral function is defined as the imaginary part of the Green's function, $A_{ij}(\omega) = -\frac{1}{\pi}\mathrm{Im}G_{ij}(z)$, or:

$$A_{ij}(\omega) = -\frac{1}{\pi}\mathrm{Im}\langle A_i|\chi_j(z)\rangle.$$

The calculation has to be carried out using Monte Carlo for each value of frequencies z!!!

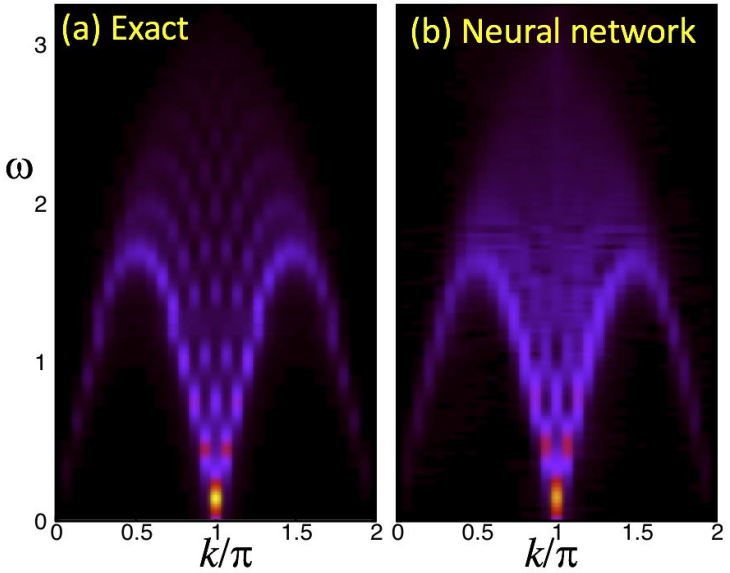
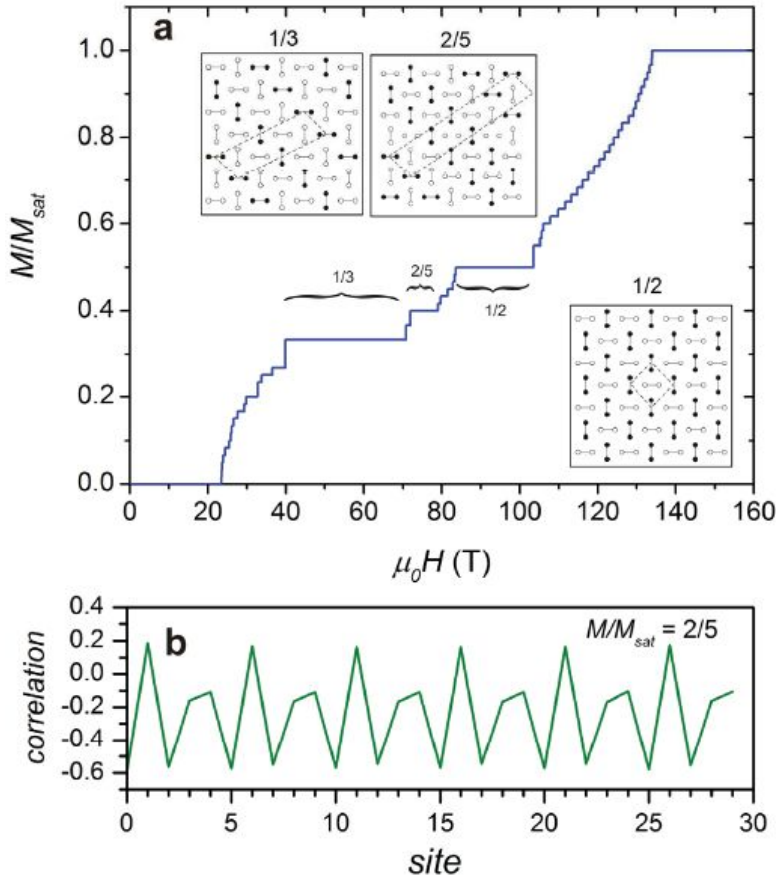


Figure 2: Excitation spectrum of a quantum spin chain using quantum ML (Ref.[5]), compared to the exact result.

Applications (experiments)

Quantum magnetism

On-going collaborations with experimental groups in LANL (M. Jaime), ETH Zurich (H. Ott and F. Casola), PSI (C. Ruegg)



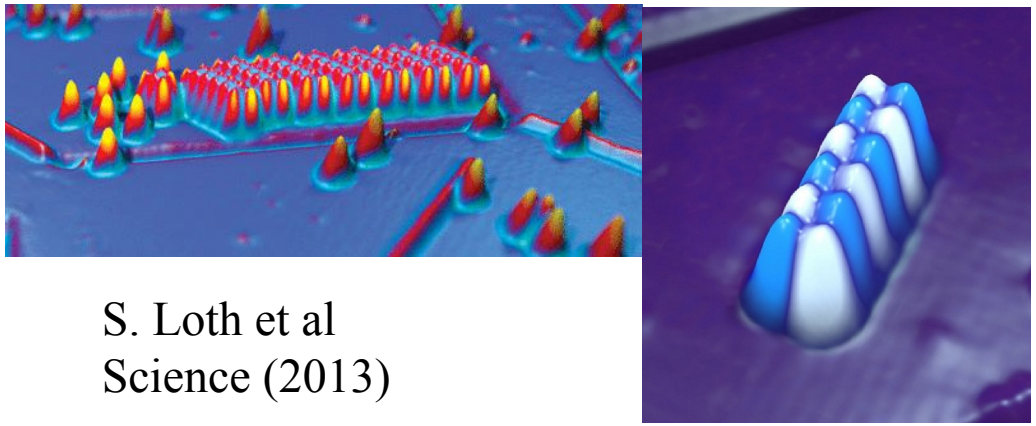
Magnetostriction and magnetic texture to 100.75 Tesla in frustrated $SrCu_2(BO_3)_2$

Marcelo Jaime[a,b,1], Ramzy Daou[c,d], Scott A. Crooker[a,b], Franziska Weickert[b], Atsuko Uchida[a,b], Adrian E. Feiguin[e], Cristian D. Batista[f], Hanna A. Dabkowska[g], and Bruce D. Gaulin[g,h]

PNAS (2012)

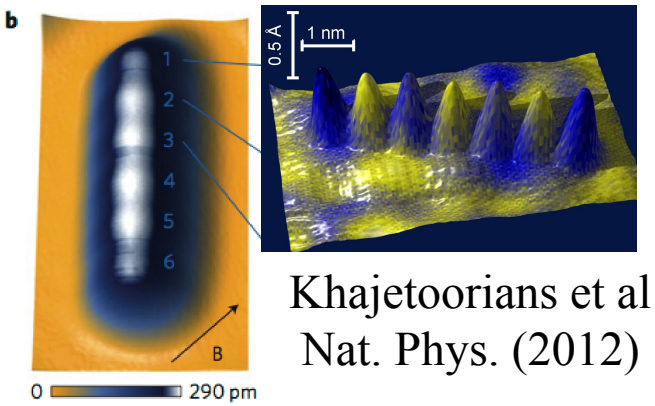
Atomic scale magnetic structures

Ladders and magnetic clusters



S. Loth et al
Science (2013)

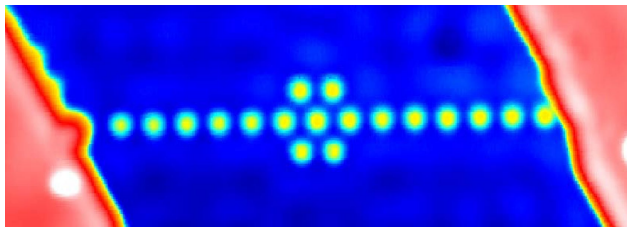
Spin chains



Khajetoorians et al
Nat. Phys. (2012)

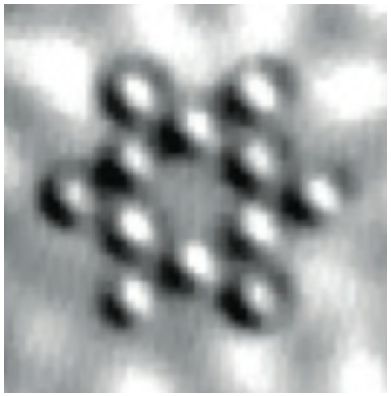
Spinelli et al
Nat. Mat. (2014)

Magnetic devices



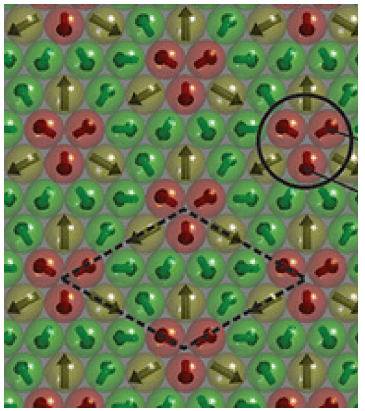
Khajetoorians et al
Science (2011)

Frustration



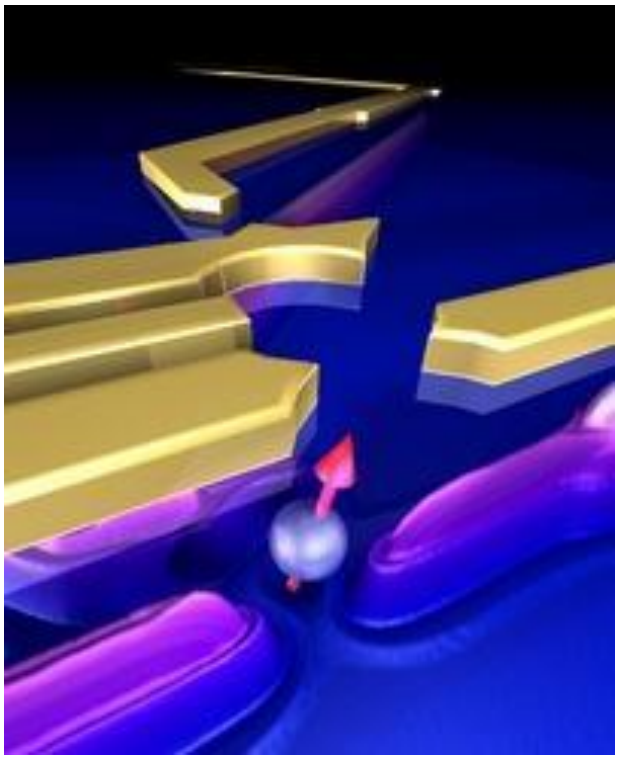
Khajetoorians et al
Science (2011)

Skyrmions



Von Bergmann
Nano. Lett. (2015)

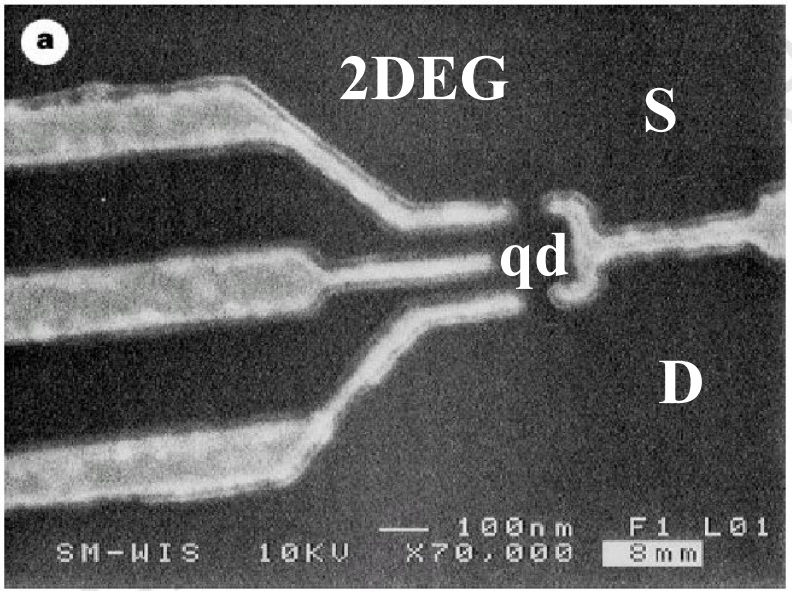
Quantum Transport



References: PRB **78**, 195317 (2008); PRA **78**, 013620 (2008) ; PRL **100**, 166403 (2008) ; PRB **73**, 195304 (2006); New. J. of Phys (2010)

Quantum dots

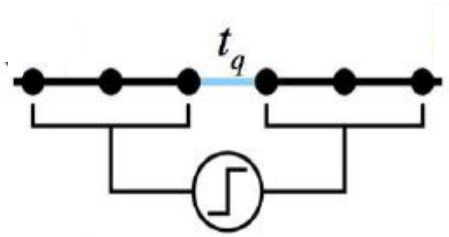
Lateral dot

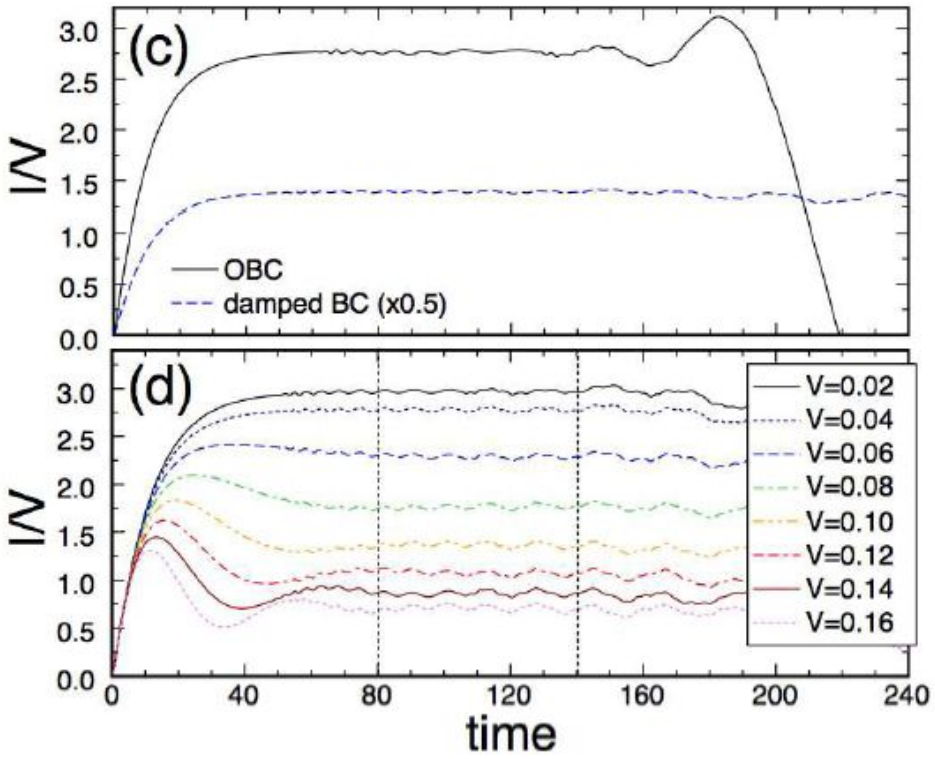


D. Goldhaber-Gordon, Hadas Shtrikman, D. Mahalu, David Abusch-Magder, U. Meirav and M. A. Kastner, Nature **391** (1998) 156

- Semiconductor heterostructure
- 0-d system
- Droplet of few confined electrons
- Very precise control and tuning
- Single electron transistors
- Size quantization: “Artifical atoms”

Example: transport in 1d





Interacting spinless fermions

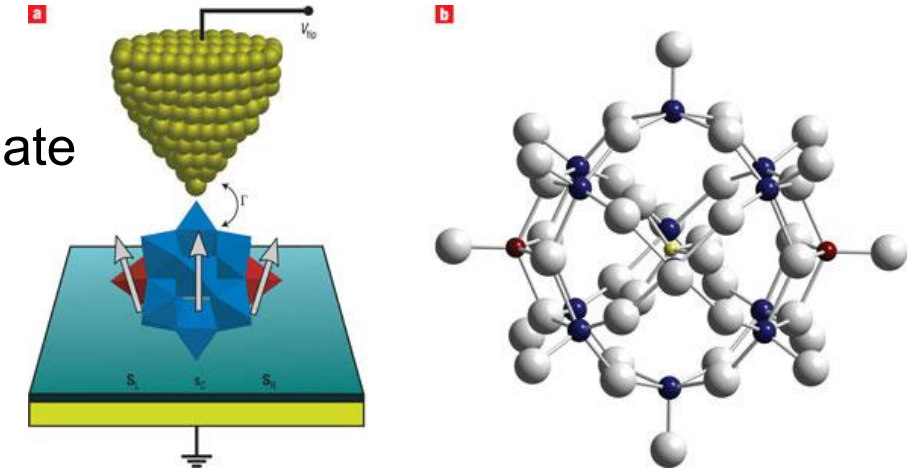
Typical behavior:

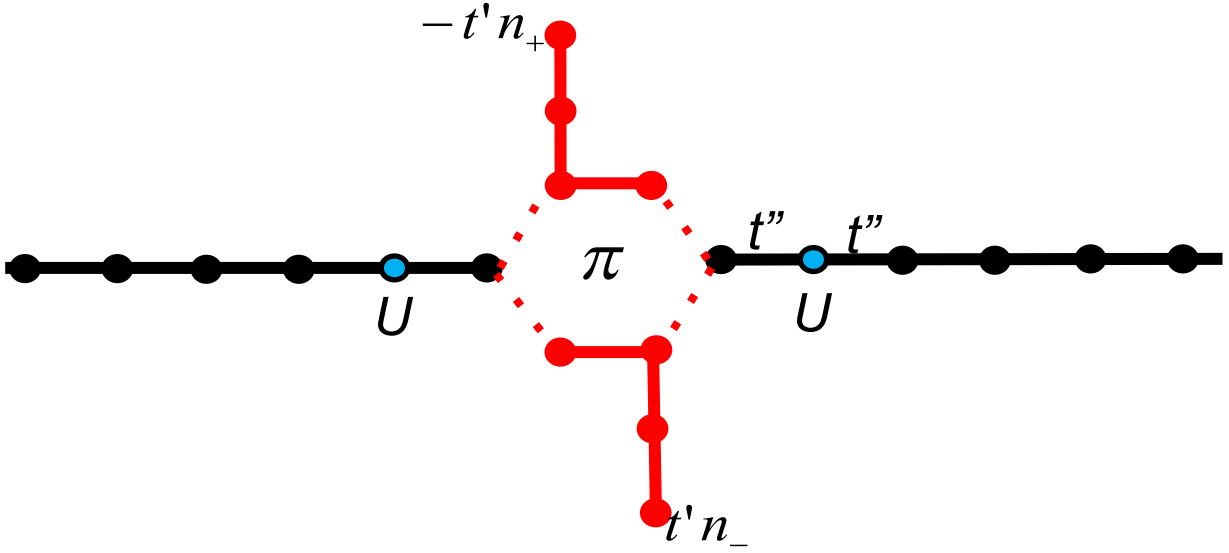
1) Short time transient
2) Plateau (we measure!)
3) Reflection at the boundaries. Current changes sign.

AEF, P. Fendley, MPA Fisher, C. Nayak, PRL

Molecular devices: multi-terminal devices and logical gates

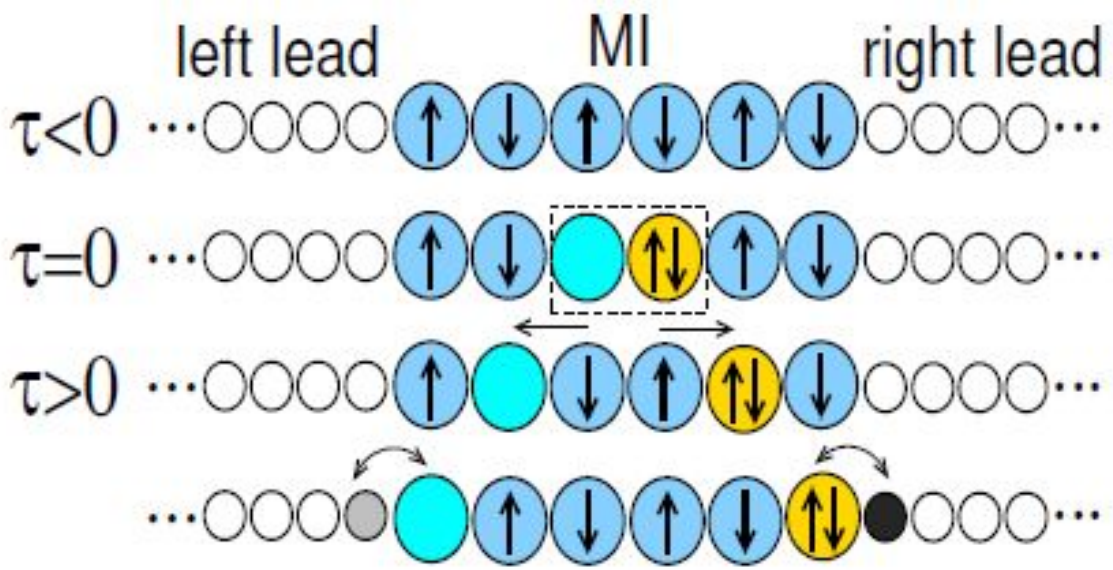
Polyoxometalate

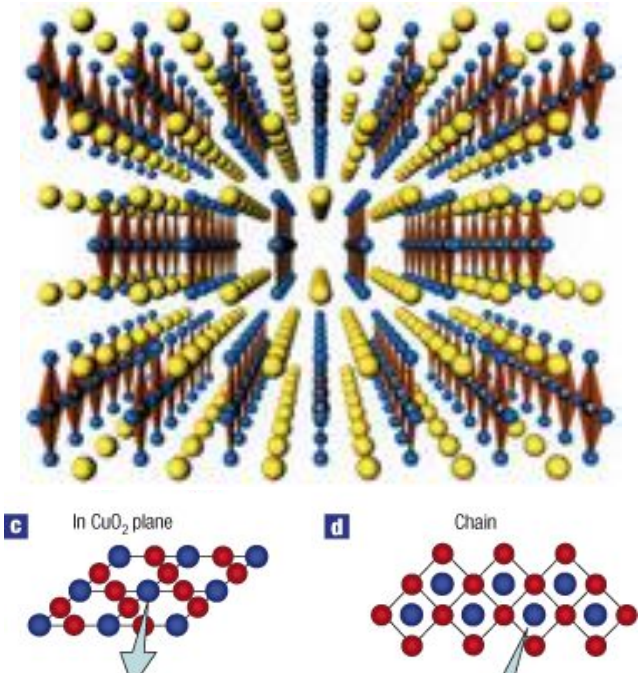




J. Lehmann et al, Nature, Nanotech. 2, 312 (2007), C. A. Busser and AEF (2012)

Exciton creation and recombination: many-body effects in light harvesting materials

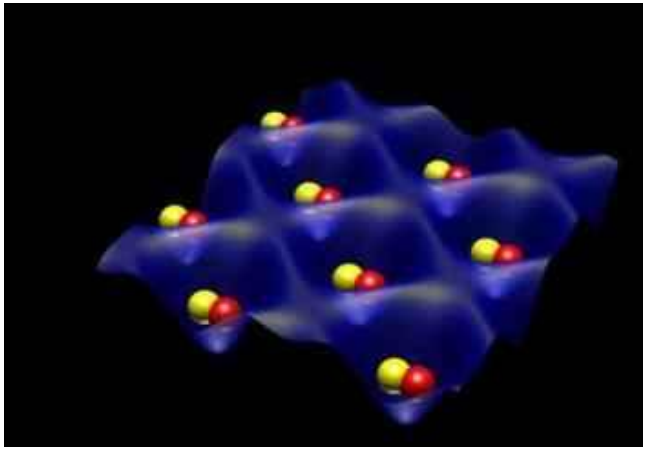




Sr_2CuO_3

Phys. Rev. B **81**, 125113 (2010); Phys. Rev. Lett. **100**, 166403 (2008)

CM phenomena in cold atom systems



Condensed Matter

- Bulk
- Disordered
- Unknown interactions

Cold Atoms

- Finite, trapped
- Fine tuned interactions
- Quantum coherence
- Engineered Hamiltonians
- “Artificial” quantum phases
- Free of dislocations or defects
- No phonons

Areas of interest

- Exotic phases of matter of quantum origin: quantum magnetism, superconductivity…
- Quantum transport and non-equilibrium physics. “Mottronics” and molecular devices. Materials for light harvesting applications.
- Spintronics, using spin for logical gates and computing. NV centers in diamond.
- Basic understanding of quantum phenomena using cold atoms.
- New computational algorithms for quantum chemistry and condensed matter.