The Hubbard Model (HM): From Solids to Cold Atoms and Back Again

- 1. Origin of Energy Bands in a Solid (noninteracting HM)
- 2. Some Examples (graphene, cuprates, flat bands)
- 3. Mott Insulators and Antiferromagnetism- physics of the HM
- 4. The real world: cuprates and transition metal oxides.
- 5. Simplified Materials i: Optical lattices (to cold atoms)
- 6. Simplified Materials ii: Engineered Silicon (and back again)
- 7. Whither the field?

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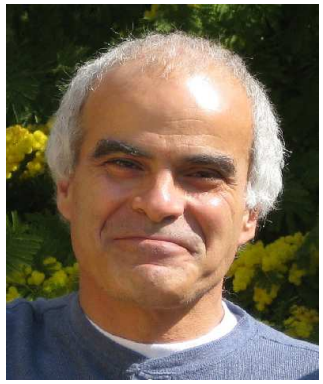

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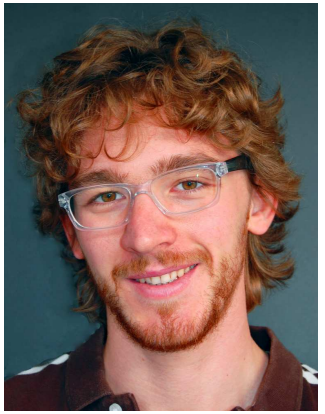

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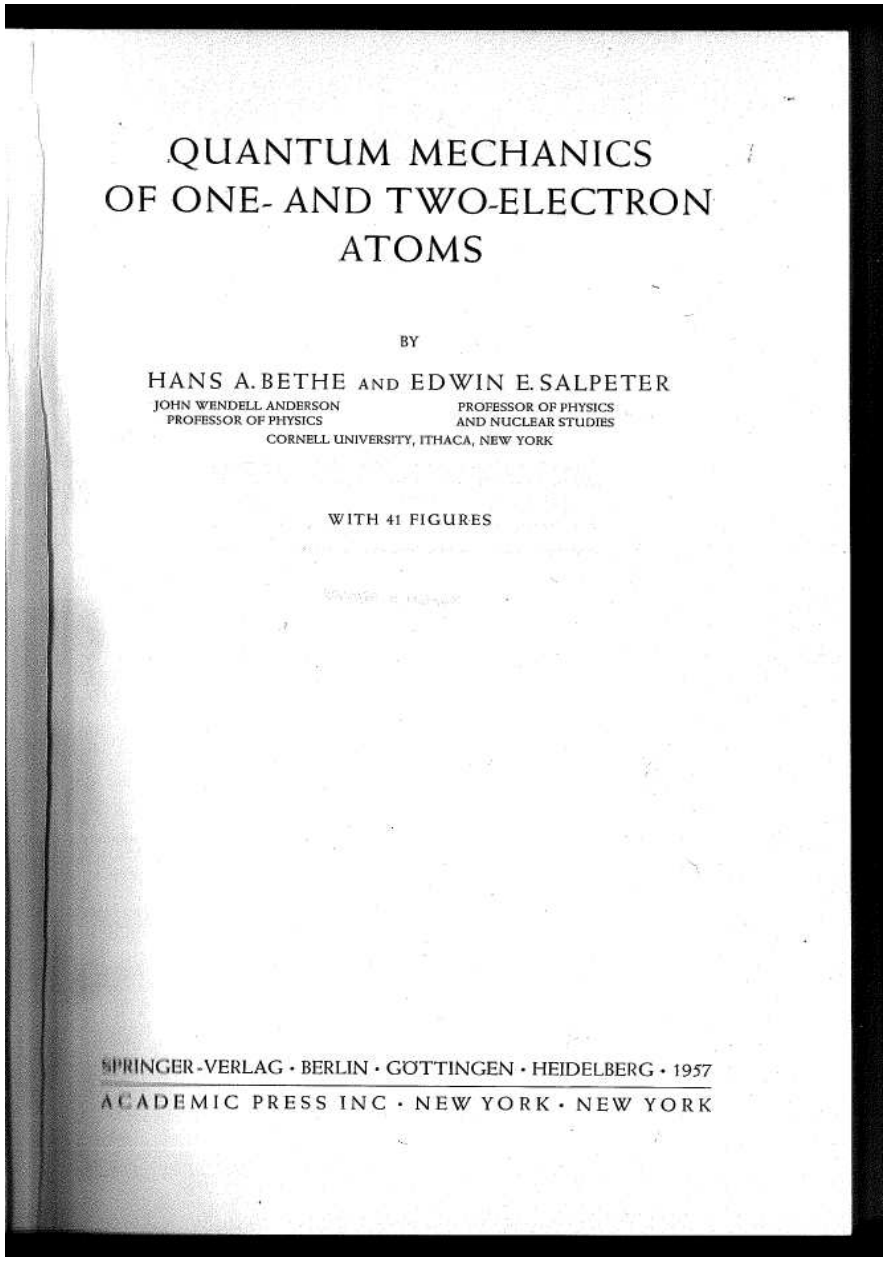

QUANTUM MECHANICS
OF ONE- AND TWO-ELECTRON
ATOMS

BY

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WITH 41 FIGURES

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The aim of this book is two-fold. First, to act as a reference work on calculations pertaining to hydrogen-like and helium-like atoms and their comparison with experiment. However, these calculations involve a vast array of approximate methods, mathematical tricks, and physical pictures $\cdots$.

For atoms and ions with two electrons, such as H^-, He, Li^+, etc., exact analytic solutions are not possible at the present time $\cdots$. (1957, three decades after the invention of quantum mechanics, and still true today!)

What shall we do with solids with 10^{23} electrons?!?!

Instructions to Colloquia Speakers: Therefore, an accessible talk which includes a thorough introduction of the topic of your research is strongly encouraged.

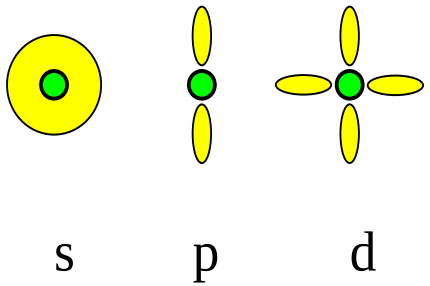
1. Origin of Energy Bands in a Solid (noninteracting HM)

Individual atoms: discrete energy levels

Atoms far apart: electrons are localized on single atom

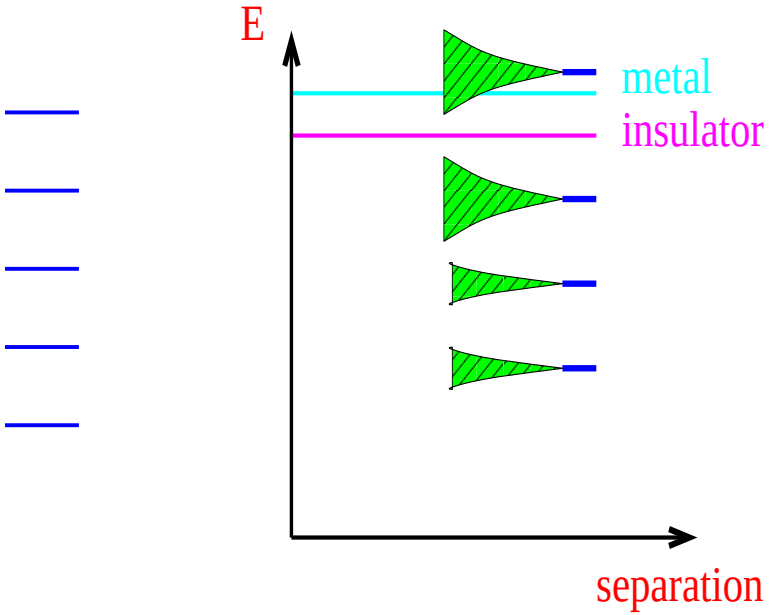
Atoms brought together (solid): degenerate level couple and broaden into a band.

Eigenvectors are delocalized (plane/"Bloch" waves)



$$\phi(r) \sim e^{-r/a_0}$$

$$E_n = -13.6 / n^2$$



Metals and Band Insulators

Energy band completely filled: Insulator

Finite energy gap to next unoccupied level

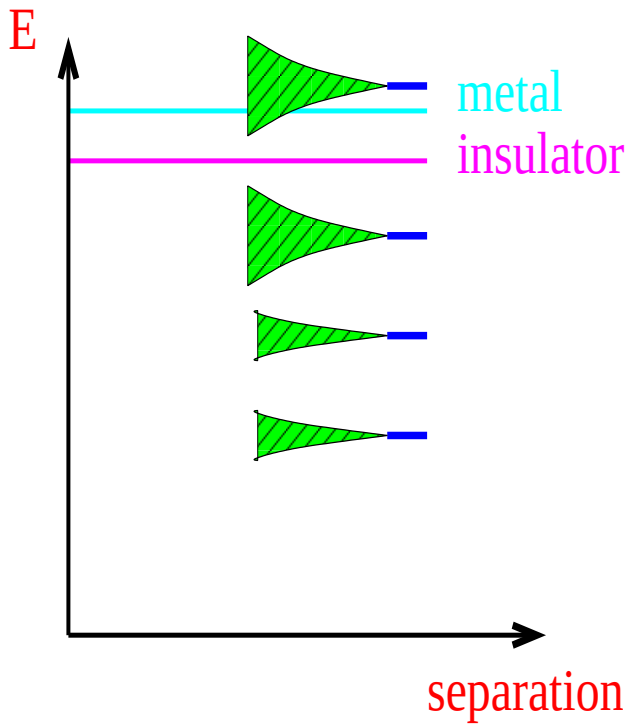
Simple counting arguments predict whether many solids are metallic or insulating!!

k eigenstate can be occupied by two electrons (spin $\uparrow, \downarrow$).

Solids with an odd number of electrons per unit cell must be metallic.

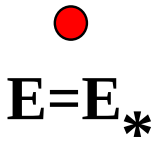
Alkalis (Li, Na, K):
one valence e^-
$(2s^1, 3s^1, 4s^1)$ per unit cell:
Good metals.

Diamond, silicon, germanium (C, Si, Ge):
eight valence electrons
$(2s^2 2p^2, 3s^2 3p^2, 4s^2 4p^2)$: per unit cell
Insulators.

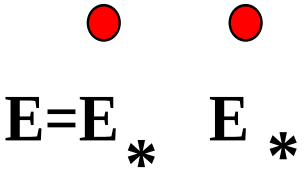


2. Some Examples (graphene, cuprates, flat bands)

- Boils down to diagonalizing a (simple) matrix!



A single atom (site) with energy E_*.



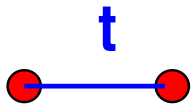
Two independent atoms (sites). Electron can sit on site 1 or 2. Two degenerate levels E_*.

Useful mathematical representation: Matrix H

$$H = \begin{bmatrix} E_* & 0 \\ 0 & E_* \end{bmatrix} \qquad \psi_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad \psi_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

$\psi_{1,2}$: electron localized on site (1,2). Eigenvectors with eigenvalues E_*.

Allow electrons to move between sites.



Two overlapping atoms (sites).

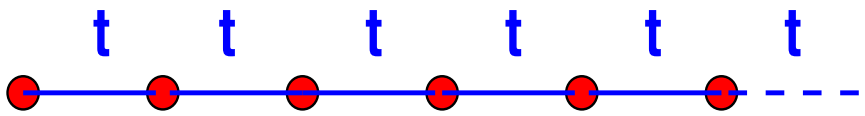
E= ?

$$H = \begin{bmatrix} E_* & -t \\ -t & E_* \end{bmatrix} \qquad (E_* - E)^2 - t^2 = 0 \qquad E = E_* \pm t$$

t is a 'bridge' between atoms: the overlap of wavefunctions on the adjacent atoms.

$\psi_1 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}$ $\psi_2 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix}$. Lowest energy state is "spread out".

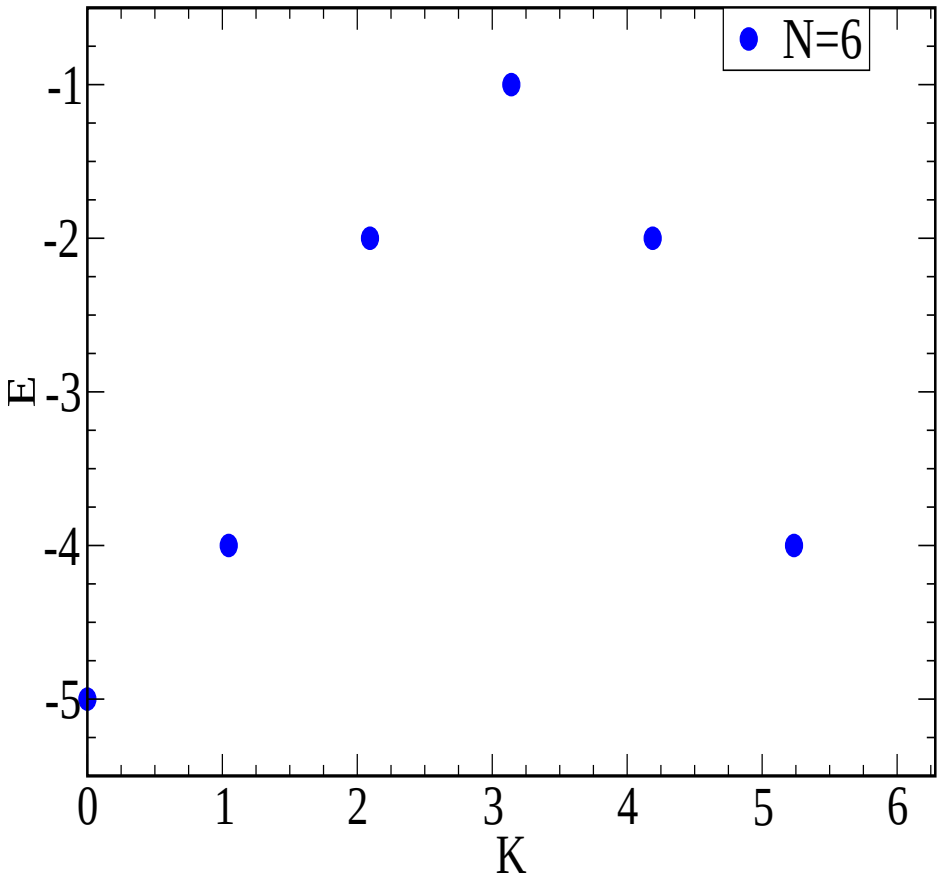
Six atoms (sites) with overlapping orbitals (and periodic boundary conditions):



$$H = \begin{bmatrix} E_* & -t & 0 & 0 & 0 & -t \\ -t & E_* & -t & 0 & 0 & 0 \\ 0 & -t & E_* & -t & 0 & 0 \\ 0 & 0 & -t & E_* & -t & 0 \\ 0 & 0 & 0 & -t & E_* & -t \\ -t & 0 & 0 & 0 & -t & E_* \end{bmatrix} \qquad \psi_1 = \frac{1}{\sqrt{6}} \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} \qquad E_1 = E_* - 2t$$

General rule: N=number of sites.

$E_n = -2t\cos(\,2\pi n/N\,).\qquad n = 1, 2, 3, \cdots N$



Particle moving in

continuous space:

$$E_K = K^2/2m$$

On a lattice $K \leftrightarrow n$

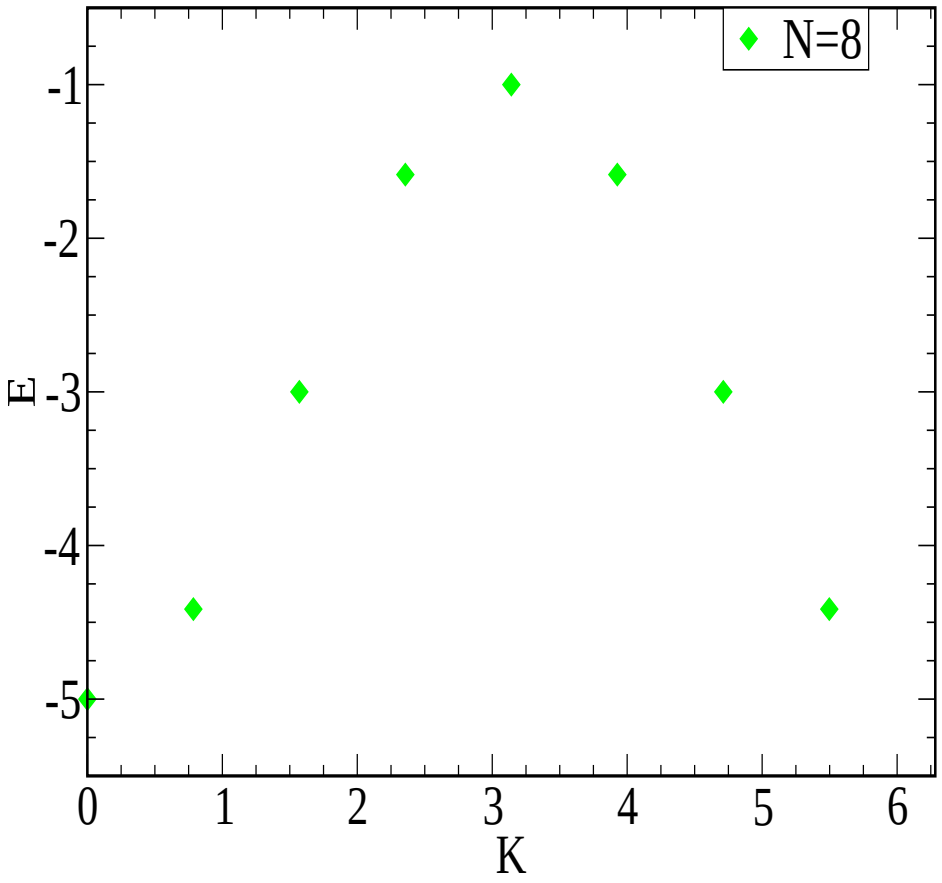
$$K = 2\pi n/N$$

$E_* = -3$

$t = 1$

General rule: N=number of sites.

$E_n = -2t\cos(\,2\pi n/N\,).\qquad n = 1, 2, 3, \cdots N$



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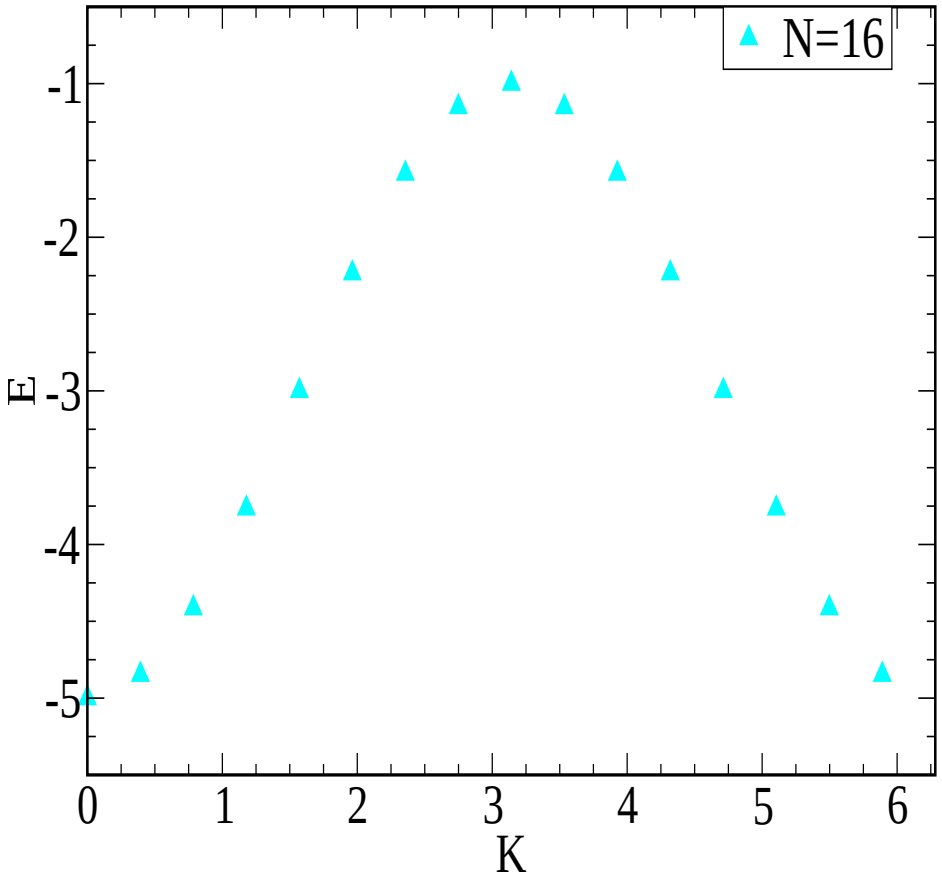

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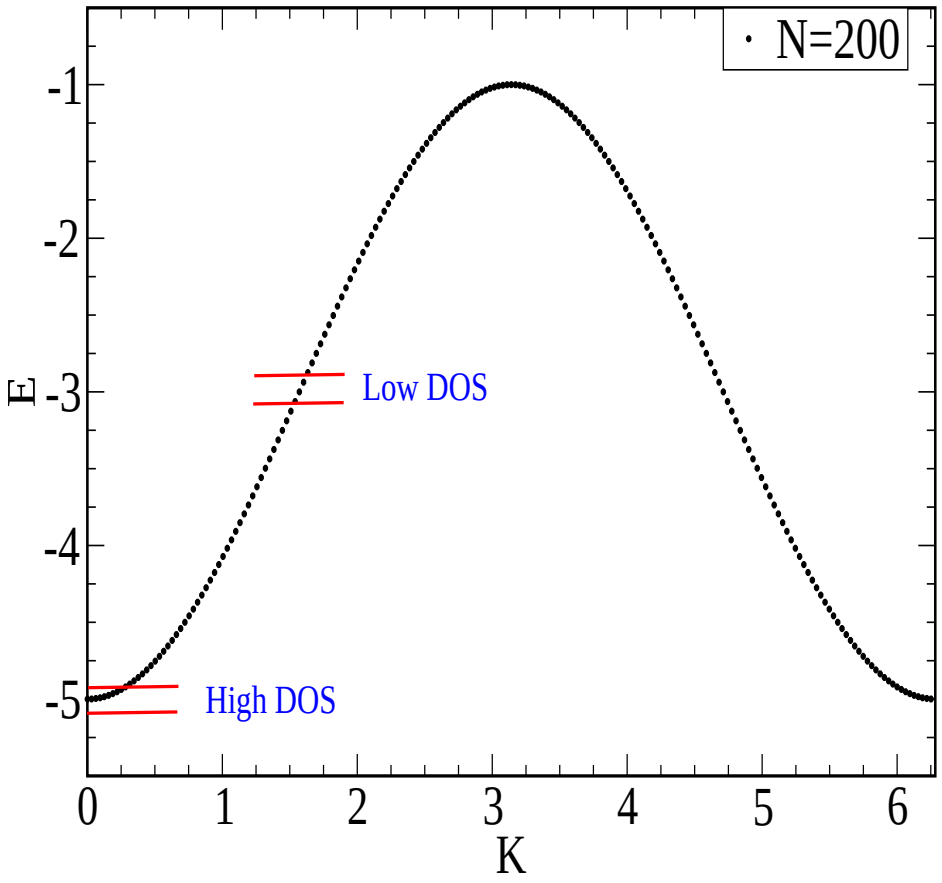


Energy band one dimensional chain of atoms.

$E(K) = E_* - 2\,t\cos(\,K\,)$

$= -3 - 2\cos(\,K\,)$

N large $\rightarrow$ K continuous.

Density of States: Count number of energy levels (k values) in given energy window.

All the associated eigenvectors are "delocalized". "Bloch's Theorem"

The electron has an equal probability to live on any site!

$$\psi_N = \frac{1}{\sqrt{N}} \begin{bmatrix} +1 \\ +1 \\ +1 \\ +1 \\ \vdots \\ +1 \\ +1 \end{bmatrix} \qquad \psi_{3N/4} = \frac{1}{\sqrt{N}} \begin{bmatrix} +1 \\ -i \\ -1 \\ i \\ \vdots \\ -1 \\ i \end{bmatrix} \qquad \psi_{N/2} = \frac{1}{\sqrt{N}} \begin{bmatrix} +1 \\ -1 \\ +1 \\ -1 \\ \vdots \\ +1 \\ -1 \end{bmatrix}$$

Very similar to plane wave solutions of Schroedinger Eq. in continuous space!

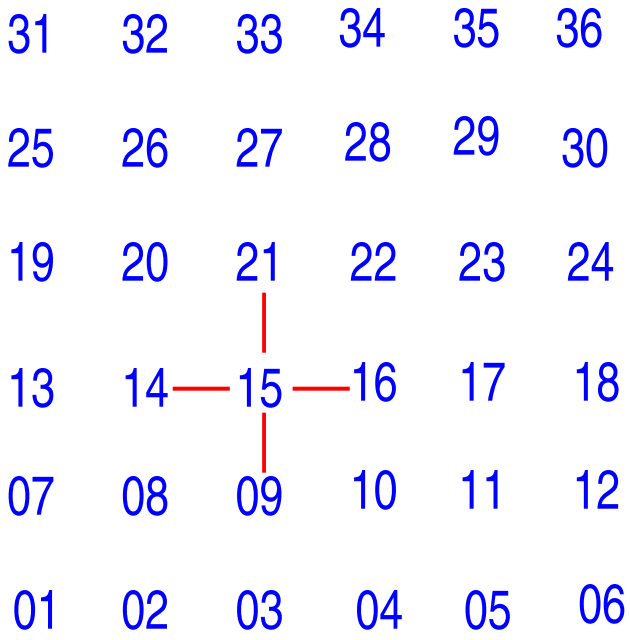
$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\,\psi(x) = E\,\psi(x) \qquad\qquad \psi(x) \sim e^{iKx}$$

(Compare ψ_N with $e^{i\,(K=0)\,x}$.) Motivates identification $n \leftrightarrow K$.

In fact, in finite box, $K = \pi n/L$ gets discretized, just as in our 1D lattice.

In higher dimension:

Label sites in lattice. If two sites i, j adjacent: corresponding $H_{ij} = H_{ji} = -t$.



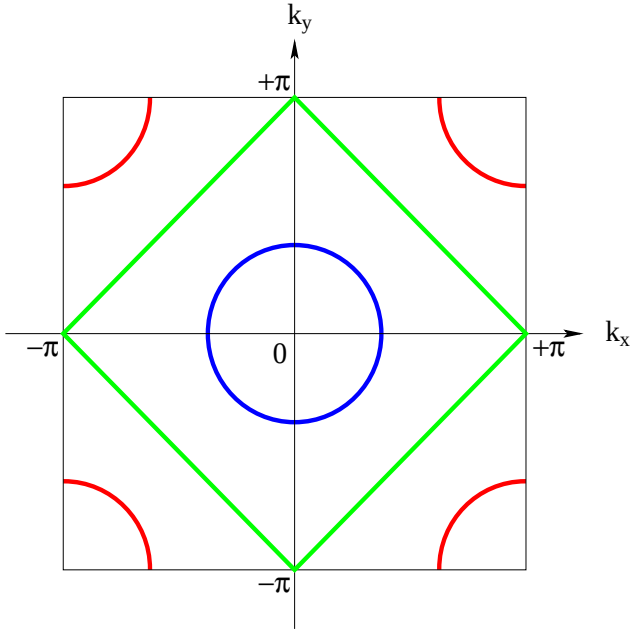
$$H_{9,15} = H_{15,9} = -t$$
$$H_{14,15} = H_{15,14} = -t$$
$$H_{16,15} = H_{15,16} = -t$$
$$H_{21,15} = H_{15,21} = -t$$

2D band structure $\leftrightarrow$ diagonalize H.

$E(\mathbf{k}) = -2\,t\,\big(\cos k_x + \cos k_y\,\big)$

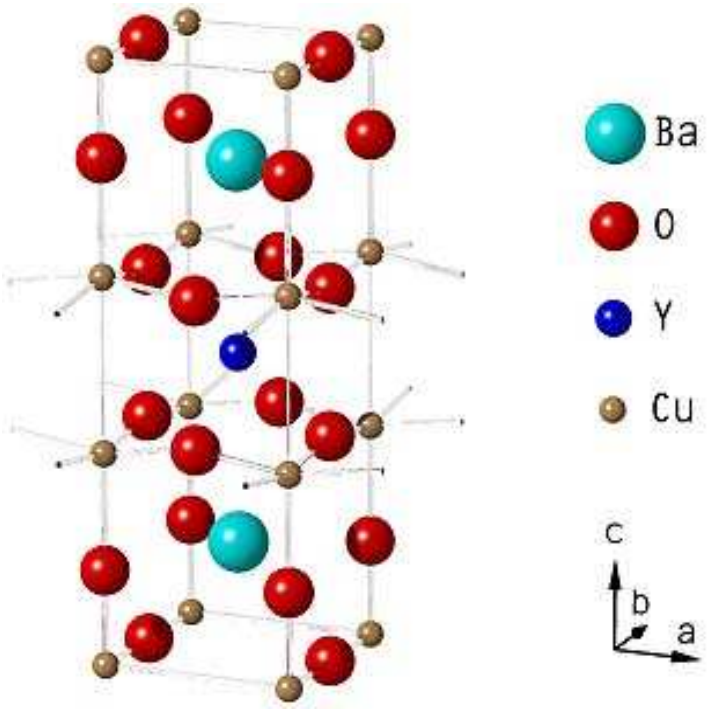
$N(\omega) = \int dk_x\, dk_y\, \delta\big(\,\omega - E(k)\,\big)$

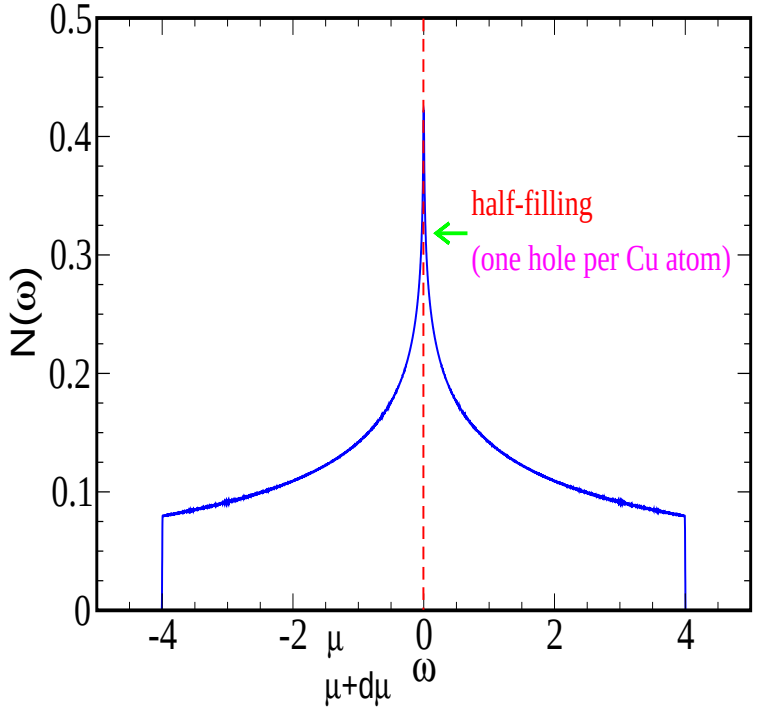
Fermi Surface: trajectory of constant $E(\mathbf{k})$.



Simplest picture of cuprate (high temperature) superconductors. (Nobel Prize 1987)

Focus on square array of copper atoms in CuO_2 sheets.





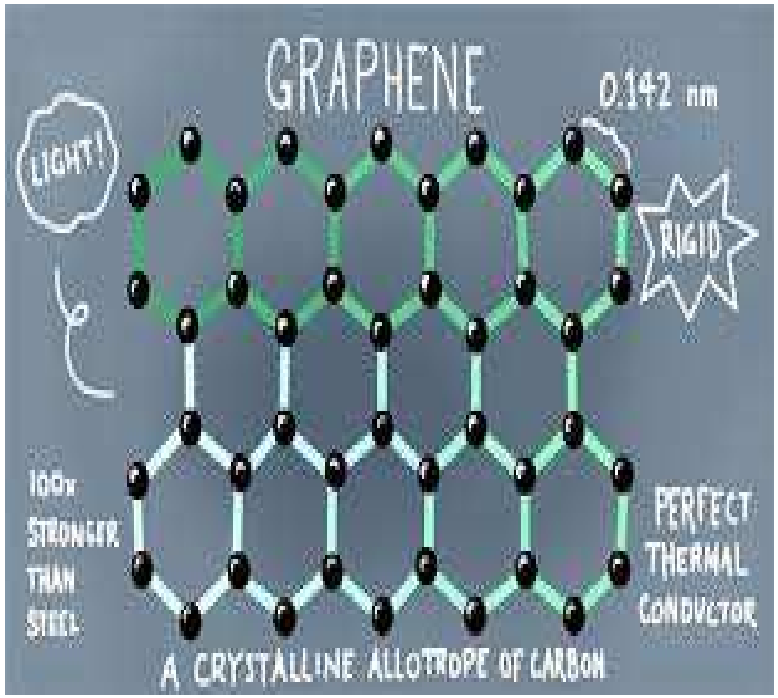
VanHove singularity of DOS: $N(\omega = 0)$ diverges.

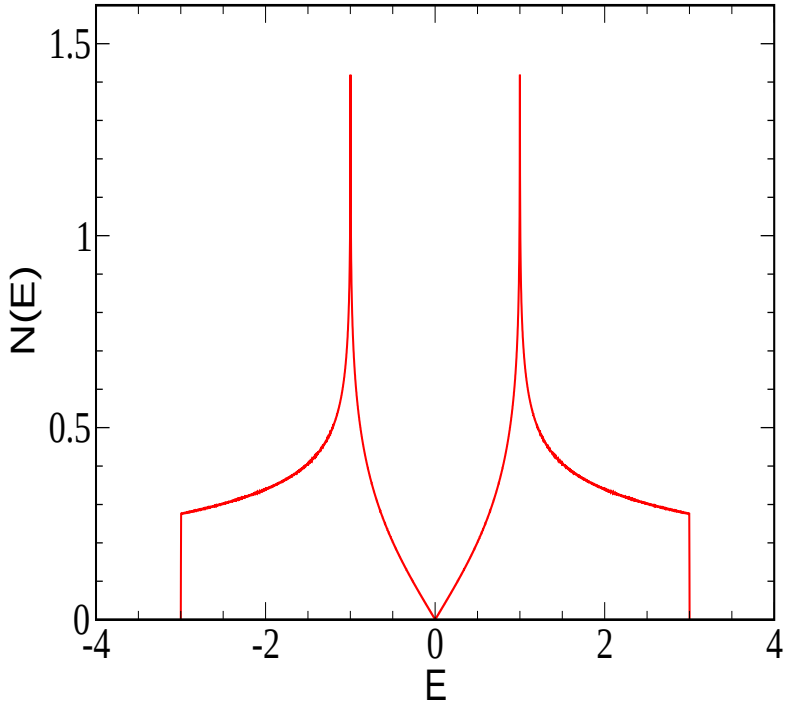
Early theory of high Tc

$T_c \sim e^{-1/\lambda N(\omega=0)}$ $\Rightarrow$ T_c is high.

Previous superconductors: $\lambda N(\omega = 0) \sim 1/4$.

Graphene (Nobel Prize 2010)

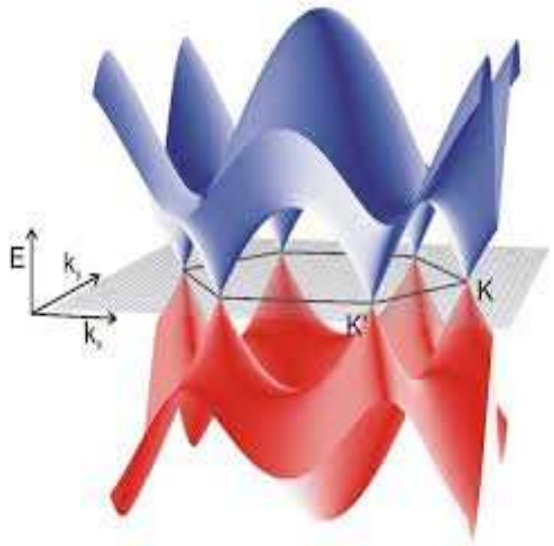




Density of states vanishes linearly at $\omega \to 0$.

Tied to 'Dirac cones' $E(\mathbf{k}) = v\,|\mathbf{k}|$.

(Zhe Fei, graphene nonribbons, etc)



RECAP:

- Understand Na,Li,K (metal) versus C,Si,Ge (insulator)
  Partially versus completely filled bands.
  No electron-electron interactions!

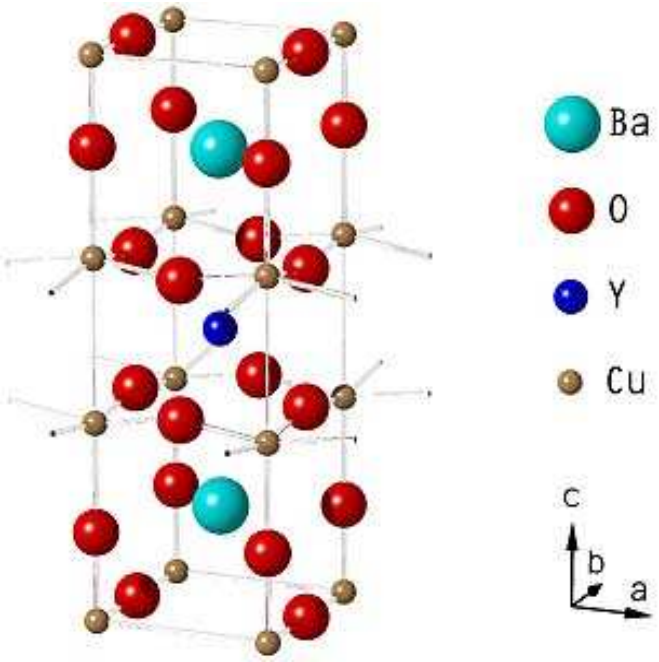
- Initial insight into strongly correlated materials.
  [1] Non-interacting DOS on square lattice (Cu atoms in cuprates)
  van Hove singularity $\Rightarrow$ high T_c
  [2] Non-interacting DOS on honeycomb lattice (graphene)
  Dirac fermions.
  [3] Topological insulators:
  Interconversion (spin-orbit) terms between spin up and spin down.
  Hopping between 'spin up sites' and 'spin down sites'.

- Band structure: diagonalizing a matrix!
  (non-interacting Hubbard Model)

Trouble in Paradise $\cdots$

Parent compounds of cuprate superconductors:

- 1 hole/Cu
- Fermi level cuts middle of band.
- Why are they antiferromagnetic insulators?!

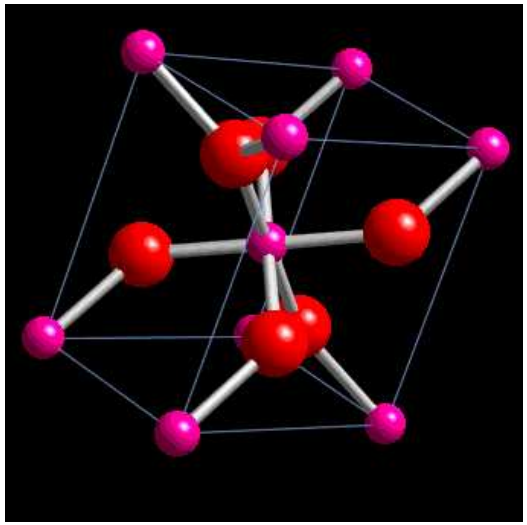


Transition metal monoxides (MnO, FeO, CoO):

(Many oxides in earth's interior.)

MnO: Mn^{2+} d band half-filled (d^5: odd # electrons)

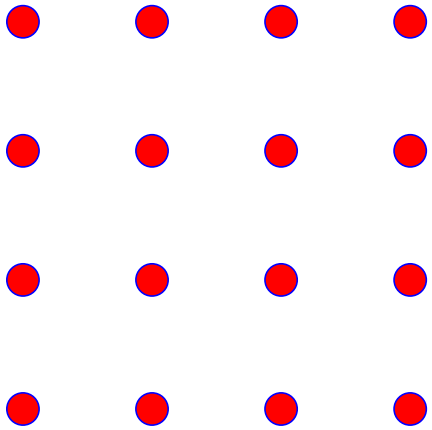
- Why are they antiferromagnetic insulators?!



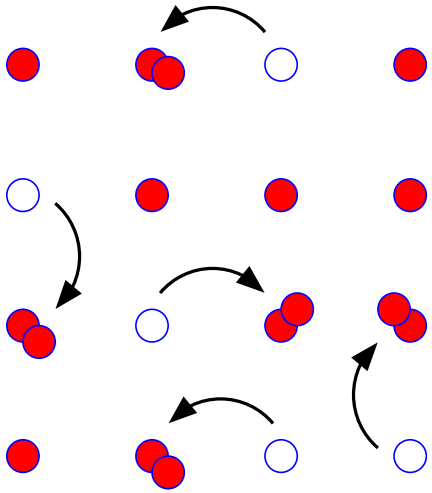
(Jigang Wang: Insulating AF Manganites)
(Rebecca Flint: AF in Heavy Fermions)
(John Van Dyke: $CeCoIn_5$)
(Yuriy Sizyuk: AF in Na_2IrO_3)
(Paul Canfield: Correlated Electron Materials)

3. Mott Insulators and Antiferromagnetism- The Hubbard Hamiltonian

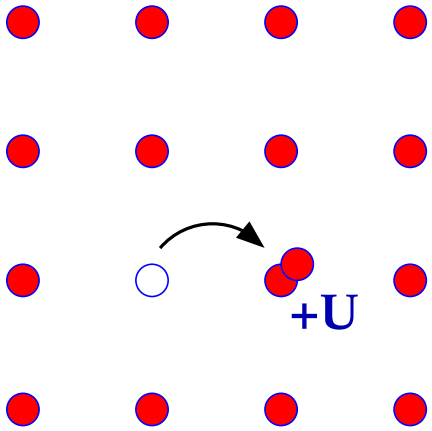
(A different type of Insulator)



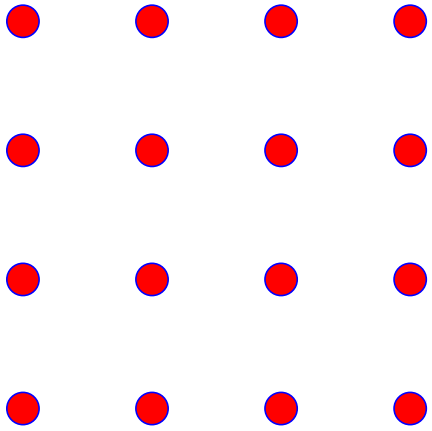
Consider a lattice of sites with
"commensurate filling":
The average number of particles
is one per site.



Kinetic energy and entropy both
favor particles moving around lattice.
Metal: odd number (one) particle per cell/site.
(Like cuprate superconductors.)



But what if there were a large repulsive interaction U between particles on the same site?



A Mott Insulator forms.
Basic physics of parent compounds of cuprate superconductors!
(Also other solids: FeO, CoO, MnO.)

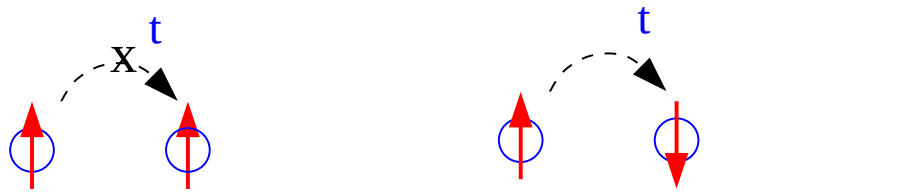
Two ways to destroy Mott Insulator:

* Decrease U/t: By applying pressure (MnO)
* Shift $\langle n \rangle \neq 1$: Dope chemically (cuprate superconductors)

What is optimal spin arrangement?

Hopping of neighboring parallel spins forbidden by Pauli.

Antiparallel arrangement lower in second order perturbation theory.



$\Delta E^{(2)} = 0$ $\Delta E^{(2)} \propto -t^2/U = -J$

Mott insulating behavior and antiferromagnetism go hand-in-hand.

Qualitative picture of cuprate physics before doping.

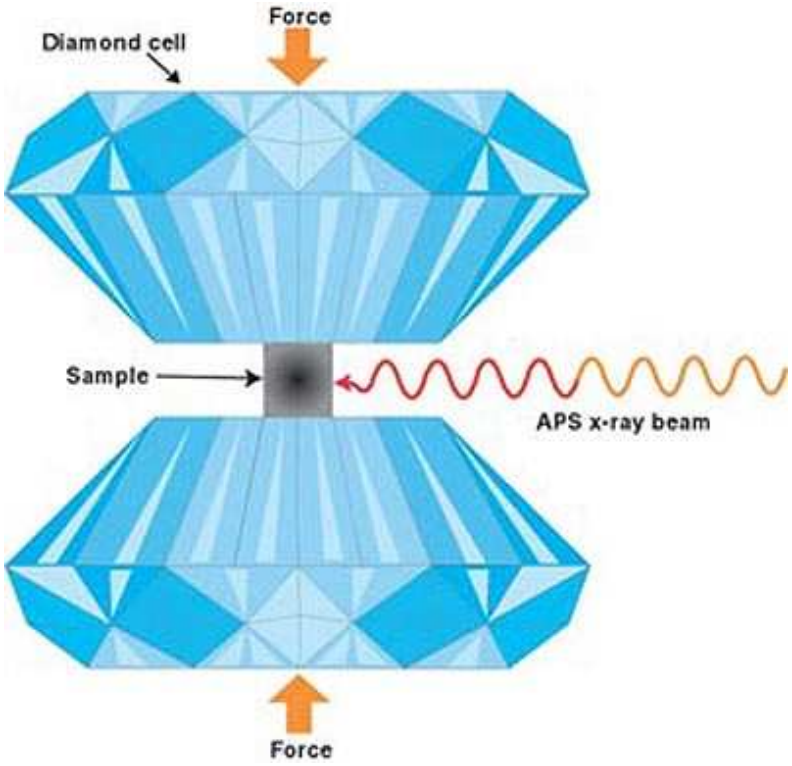
Still do not really understand why cuprates become superconducting after doping.

Can however make MnO have the expected metallic behavior...

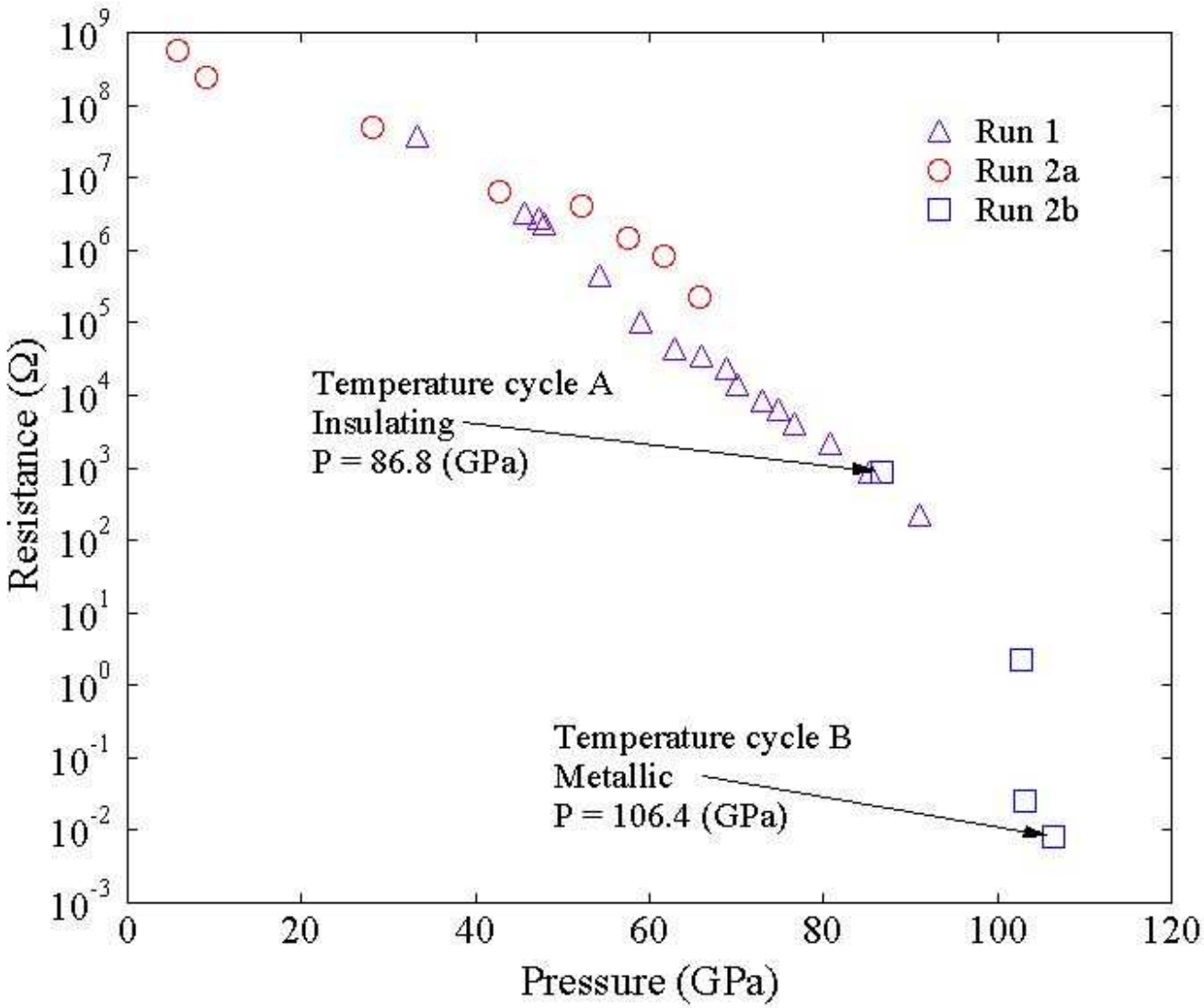
Diamond Anvil Cell

Apply pressure (and lots of it!) to push atoms closer.

* Direct measurement of resistance
* Probe magnetic moments with synchotron radiation (APS at Argonne)



Resistance drops to typical metallic values at $P \approx 100$ GPa.



J.R. Patterson *etal.*, Phys. Rev. B69, 220101(R) (2004).

(Single band) Hubbard Hamiltonian

$$\hat{H} = -t \sum_{\langle \mathbf{ij} \rangle \sigma} (c^{\dagger}_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + c^{\dagger}_{\mathbf{j}\sigma} c_{\mathbf{i}\sigma}) + U \sum_{\mathbf{i}} (n_{\mathbf{i}\uparrow} - \frac{1}{2})(n_{\mathbf{i}\downarrow} - \frac{1}{2}) - \mu \sum_{\mathbf{i}\sigma} (n_{\mathbf{i}\sigma} + n_{\mathbf{i}\sigma})$$

- Two spin species $\sigma = \uparrow, \downarrow$.
- Kinetic energy t describes hopping between near-neighbor sites $\langle \mathbf{ij} \rangle$.
- On-site repulsion U discourages double occupancy
- Chemical potential μ controls filling.
- Half-filling ($\rho = 1$) at $\mu = 0$.

Cuprate materials (LaSrCuO, YBaCuO, . . .) drive interest in 2D square lattice:

Cu atoms in CuO_2 sheets are in that geometry.

Ignore bridging O atoms.

Ignore La, Sr, Y, Ba between layers.

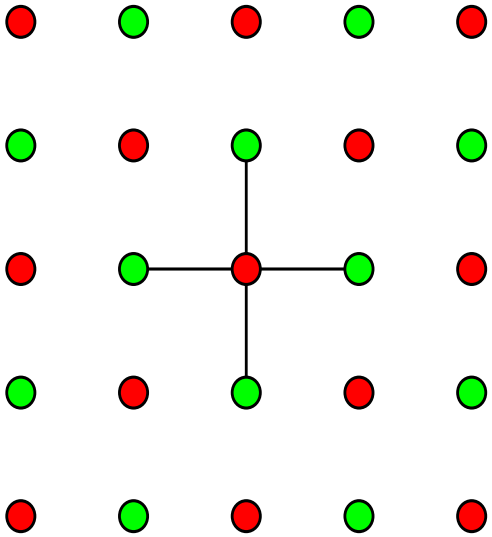
Graphene → honeycomb lattice.

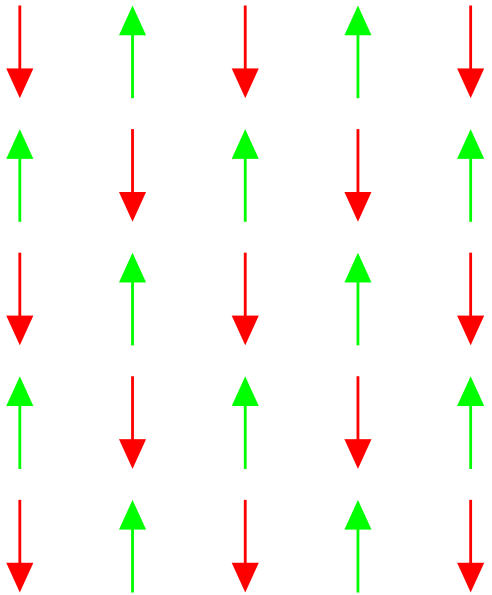
Illustration: The Square Lattice

Electron spins on two neighboring sites like to be antiparallel.

Bipartite lattices are a natural for long range antiferromagnetic order

where this up-down pattern extends over entire lattice.



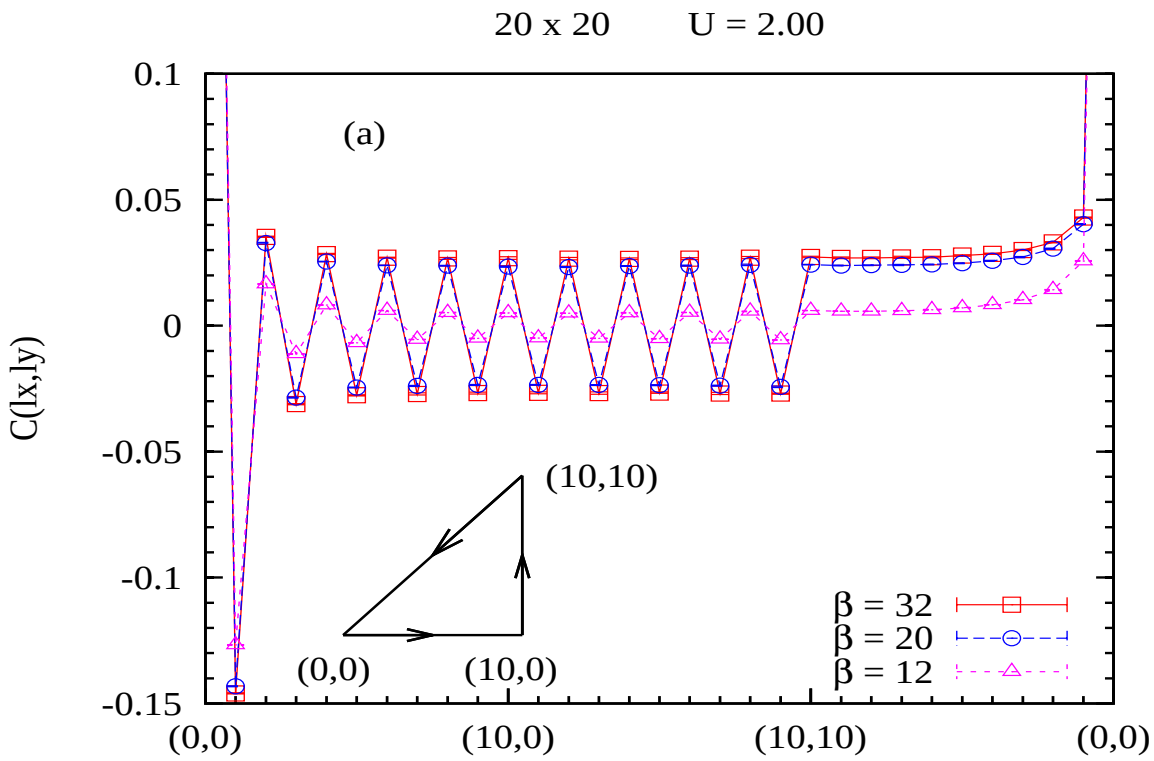


But does it really happen?!

Quantum Monte Carlo Simulations

Antiferromagnetic spin correlations

$$c(l_x, l_y) = \left\langle \left(n_{lx,ly,\uparrow} - n_{lx,ly,\downarrow} \right) \left(n_{0,0,\uparrow} - n_{0,0,\downarrow} \right) \right\rangle$$

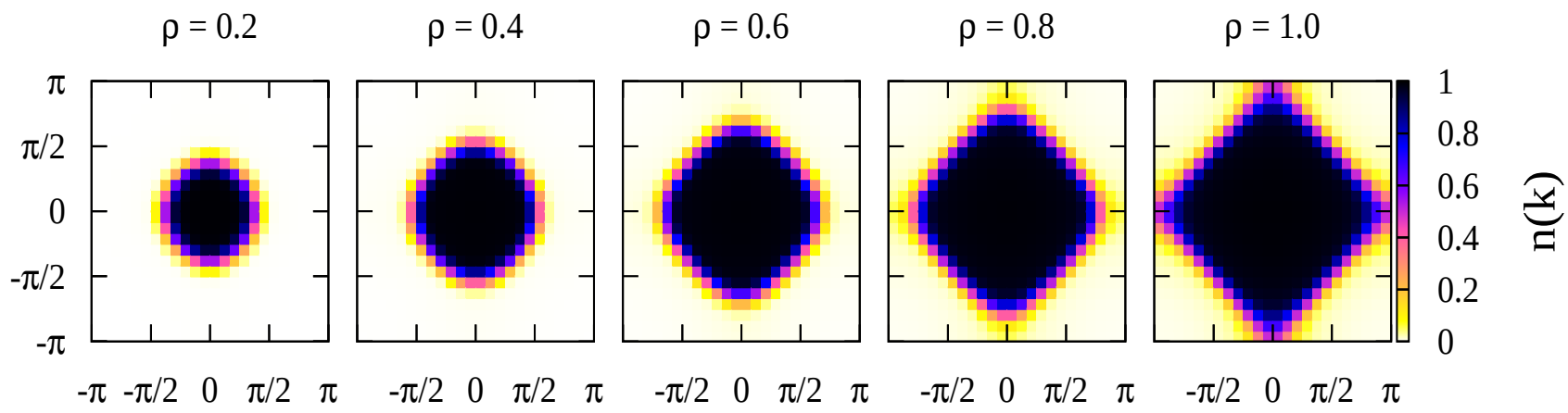


There is long range antiferromagnetic order!

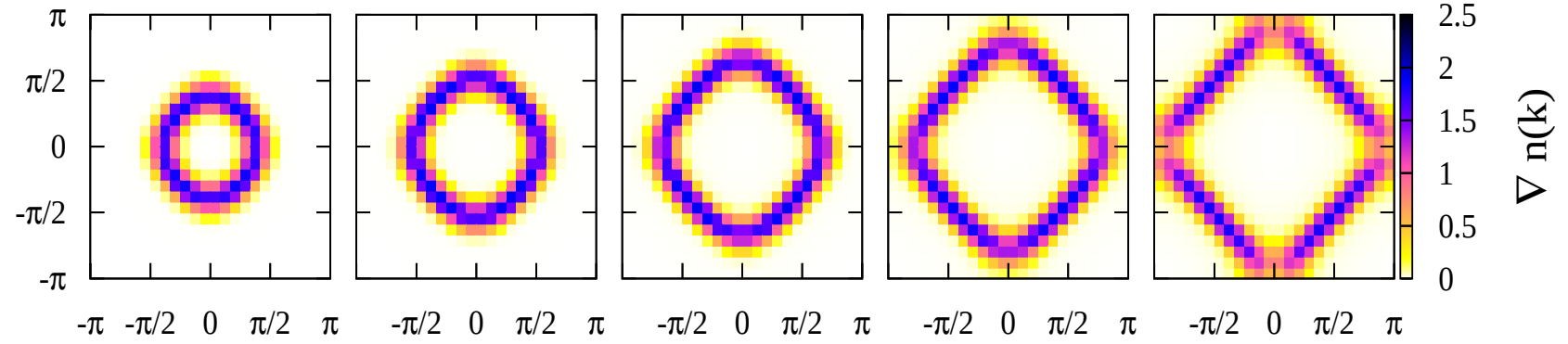
"Quantum Monte Carlo Study of the 2D Fermion Hubbard Model at Half-Filling", C.N. Varney, C.R. Lee, Z.J. Bai, S. Chiesa, M. Jarrell, and RTS, Phys. Rev. B80, 075116 (2009).

DQMC results- Fermi distribution $n(k_x, k_y)$

$U = 2$ Fermi function:

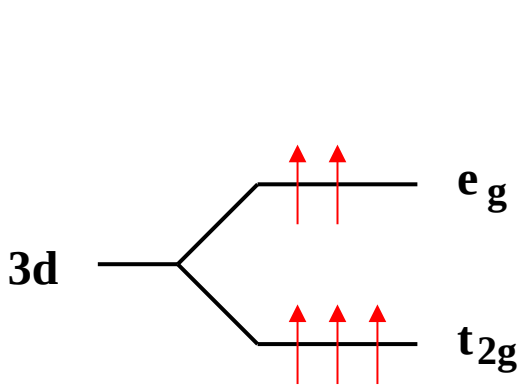


$U = 2$ Gradient of Fermi function:

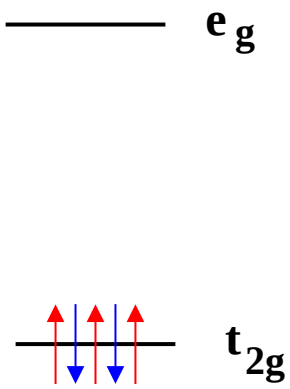


Transition Metal Monoxides - The Whole Story ?

Kinetic Energy	$3d$ bandwidth	t_d
Correlation Energy	On-site Coulomb	U_d
Multiple orbitals	Hund's rule (exchange)	J_H
Both Mn and O atoms	Charge transfer energy	$E_{3d} - E_{2p}$
Mn in cubic environment	Crystal field splitting	$E_{e_g} - E_{t_{2g}}$



Exchange splitting
>
crystal field



crystal field
>
Exchange splitting

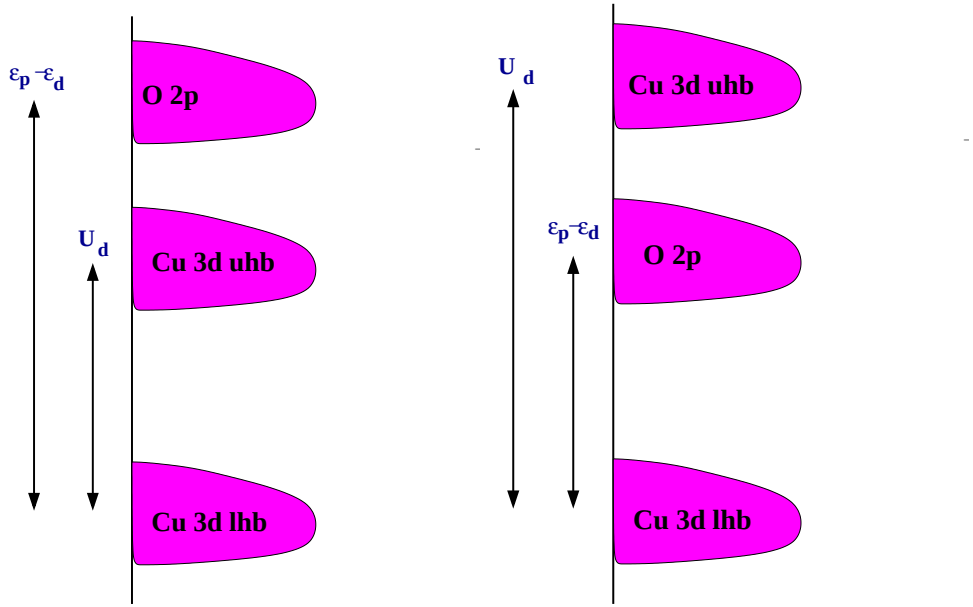
Loss of moment transition actually a "high-spin to low spin transition"?
Crystal field splitting decreases below exchange splitting as pressure applied.

Cuprate Superconductors - The Whole Story ?

Again, many 'real life' complications

Like TMOs: Oxygen orbitals. 3-band ('Emery') model.

Charge transfer versus Mott-Hubbard Insulator



Role of number of layers and interlayer atoms

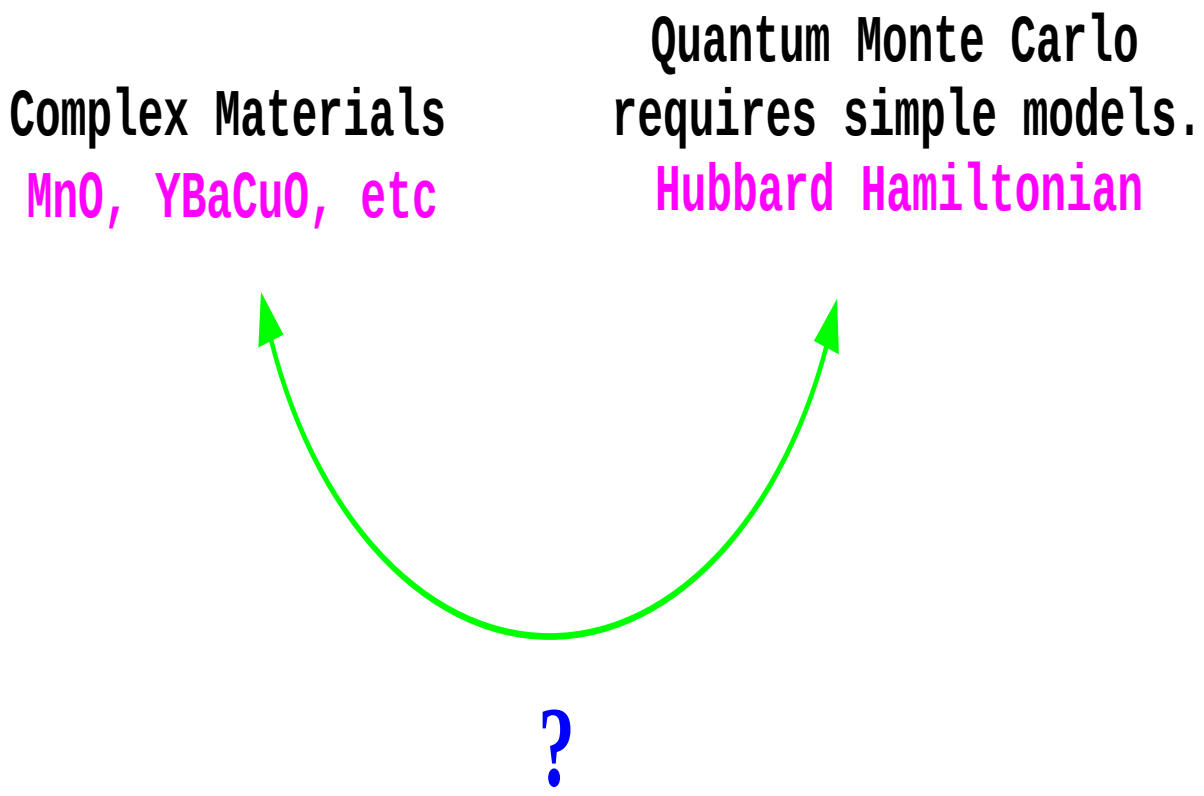
$La_{1-x}Sr_xCuO_2$: $T_c \approx 35^\circ K$.

$Y_1Ba_2Cu_3O_{7-\delta}$: $T_c \approx 90^\circ K$.

Hubbard Hamiltonian 'particle-hole' symmetry.

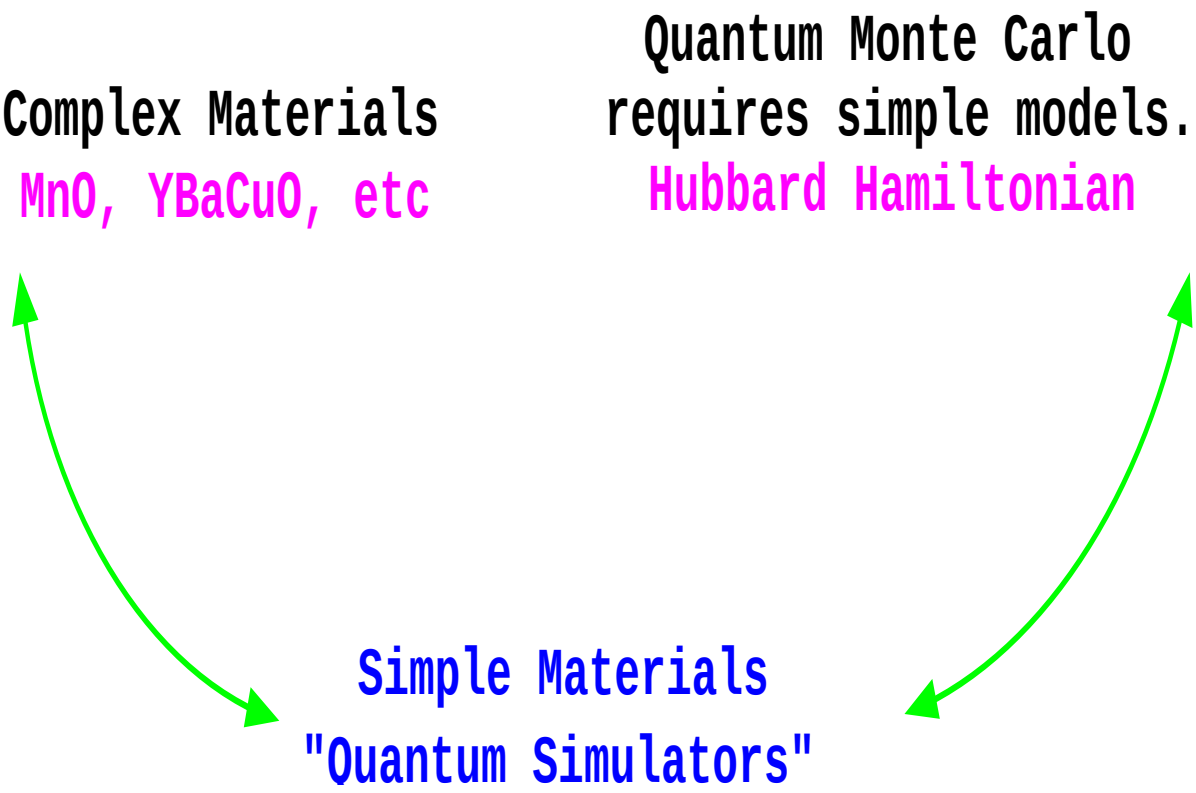
Cuprate superconductors: electron doped $\neq$ hole doped.

Role of phonons



The direct simulation of quantum systems on classical computers is very difficult because of the huge amount of memory required to store the explicit state of the quantum system. This is due to the fact that quantum states are described by a number of parameters that grows exponentially with the system size.

Iulia Buluta and Franco Nori, Quantum Simulators Science 326 pp.108-111, (2009). DOI: 10.1126/science.1177838

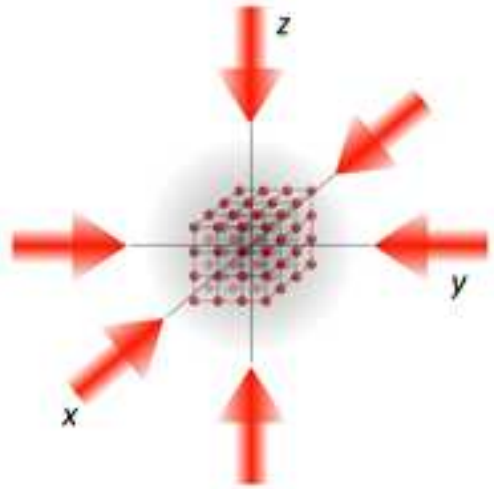


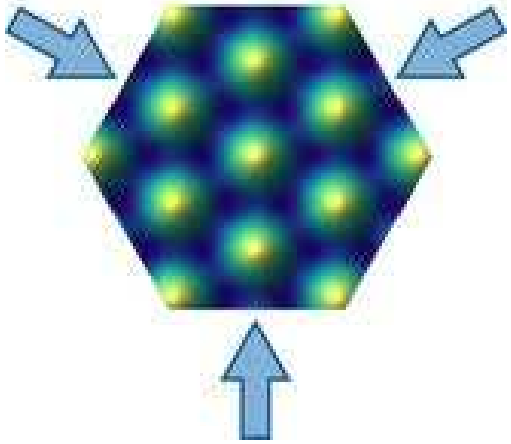
Quantum simulators are controllable quantum systems that can be used to simulate other quantum systems.

Iulia Buluta and Franco Nori, Quantum Simulators Science 326 pp.108-111, (2009). DOI: 10.1126/science.1177838

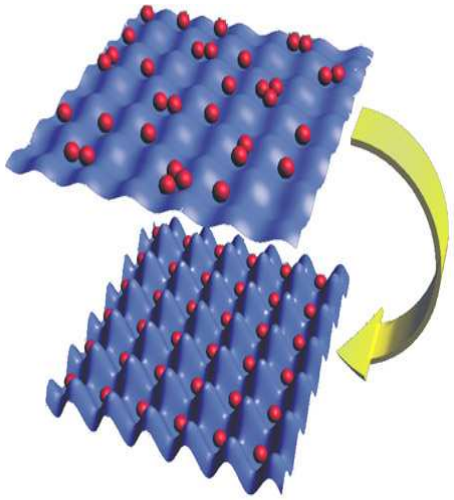
5. Simplified Materials i: Optical Lattices (Peter Orth)

Lattice formed by interference of counterpropagating laser beams.
Atoms $\left(o(10^5)\right)$ trapped by Stark shift. Cool evaporatively $\cdots$.
Different geometries accessable (e.g. cubic, honeycomb, $\cdots$)



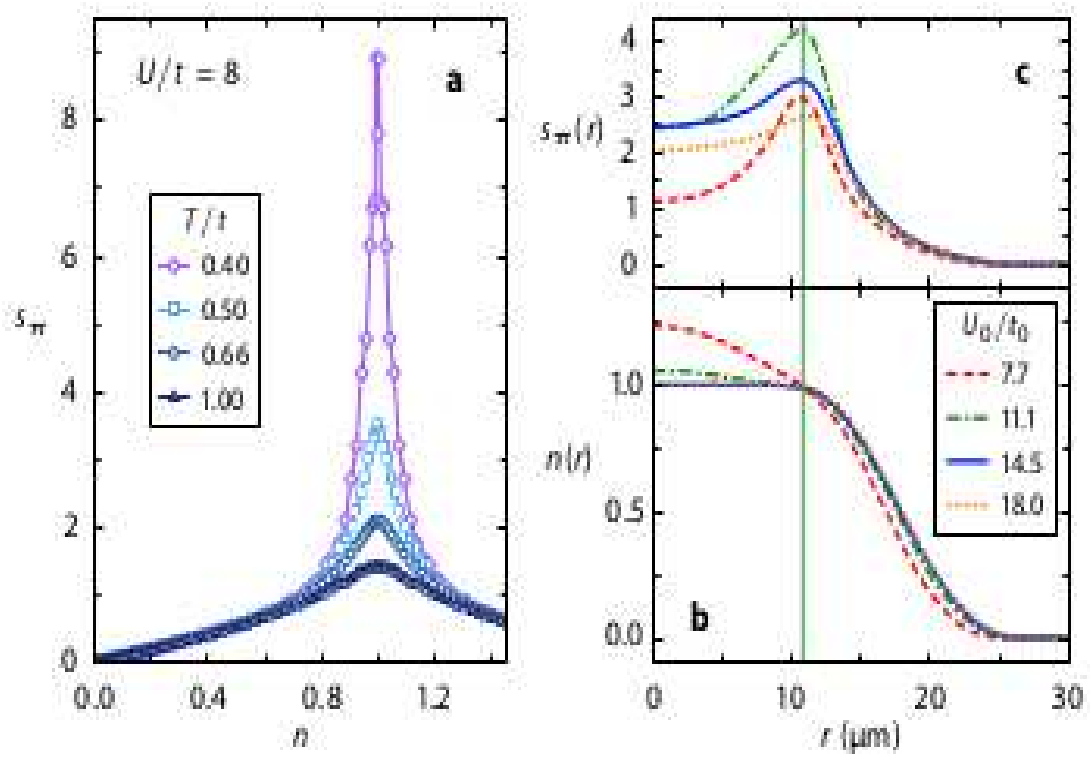


Control hopping t, interactions U
much more easily than solids.
Use, e.g. to drive Mott insulator.



Tune laser wavelength
or Feshbach resonance.

Quantum Monte Carlo Simulations of Hubbard Model with Confining potential.



Illustrates first challenge: Confining potential leads to inhomogeneous density.

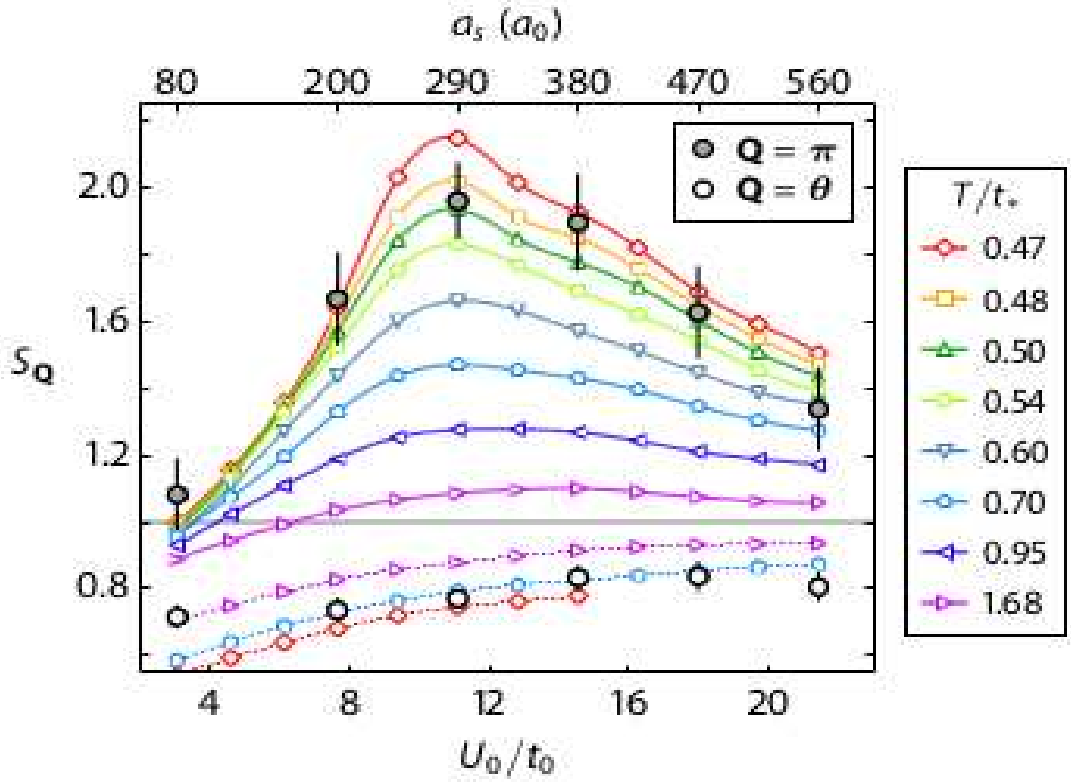
Local Mott/AF regions coexist with paramagnetic metal.

How to disentangle?

"Observation of antiferromagnetic correlations in the Hubbard model with ultracold atoms", R.A. Hart, P.M. Duarte, T. Yang, X. Liu, T. Paiva, E. Khatami, RTS, N. Trivedi, D.A. Huse and R.G. Hulet, Nature 519, 211 (2015).

"Compressibility of a fermionic Mott insulator of ultracold atoms," P.M. Duarte, R.A. Hart, T-L. Yang, X. Liu, T. Paiva, E. Khatami, RTS, N. Trivedi, and R.G. Hulet, Phys. Rev. Lett. 114, 070403 (2015).

Comparison of experiment and Quantum Monte Carlo



Illustrates second challenge:

Limitations on ability to cool.

Temperatures: nanoKelvins, but so are hopping t and interaction U:

Comparison with QMC provides thermometer.

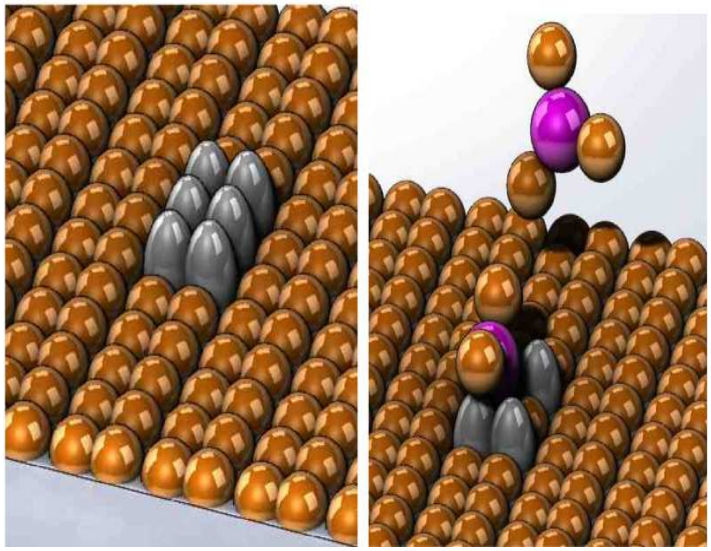
$\Rightarrow$ T/t is not small!

6. Simplified Materials ii: Engineered Silicon

Arrays of dopants in semiconductors,
placed with atomic precision.

Procedure:

- Silicon surface terminated with atomically-ordered layer of H.
- STM tip selectively removes surface H: patterned chemically active sites.
- Dopants chemisorb to lithographically patterned regions.
- Silicon is overgrown to protect atomically-patterned layer.

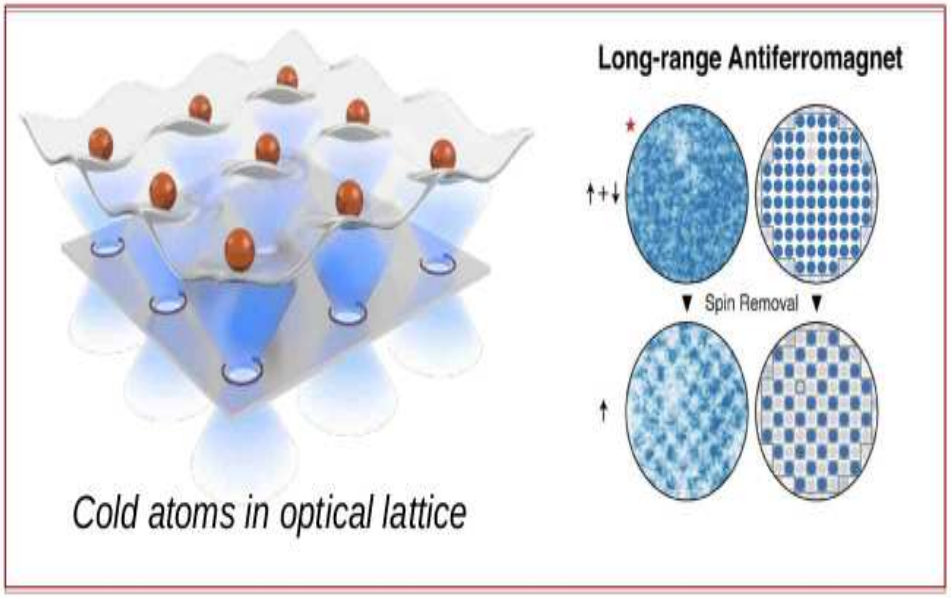


Like optical lattices:

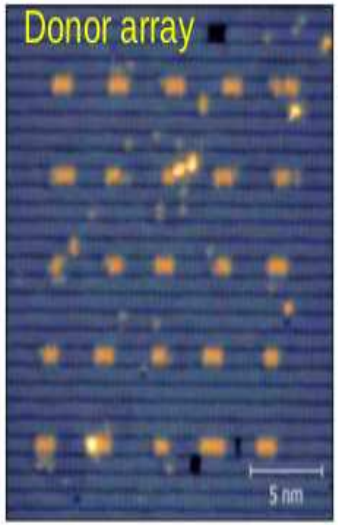
- Control over array symmetry, spacing, carrier density, bandwidth and filling.
- Manipulation of the number of dopants in a node controls interaction strength.

$\Rightarrow$ Basic ingredients for a tunable Fermi-Hubbard system.

Temperatures (much) lower than optical lattice systems!

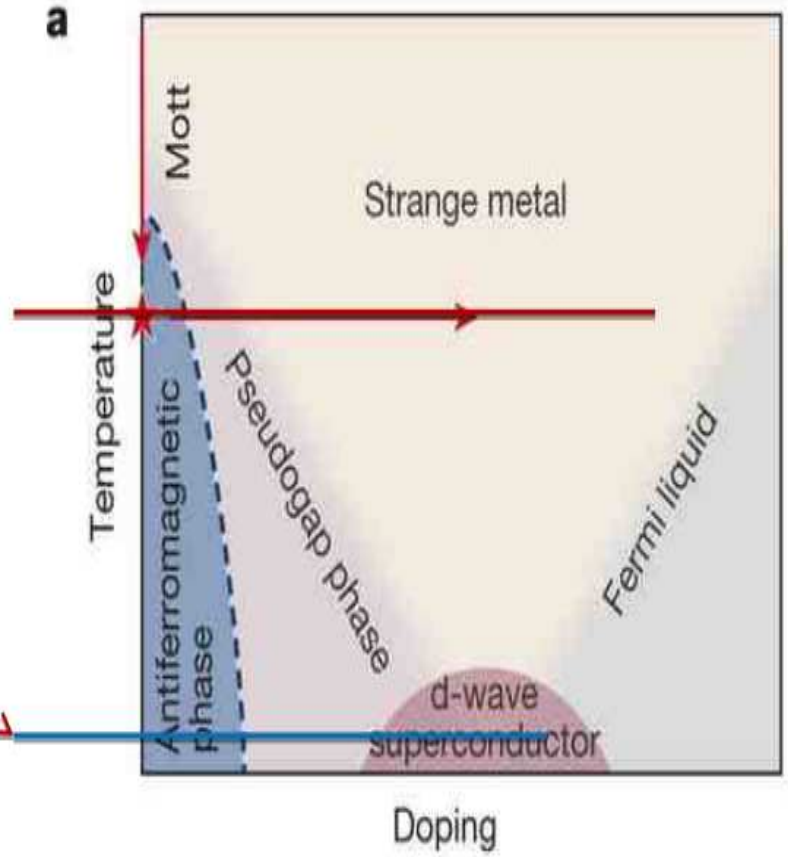


Fermi-Hubbard in Li
U/t ~ 7 (strongly interacting)
T/t~ 0.25 (moderate temperature)



Donors

- Strongly interacting
  U/t ~ 5-100
- Low temperature
  T/t ~ 0.02

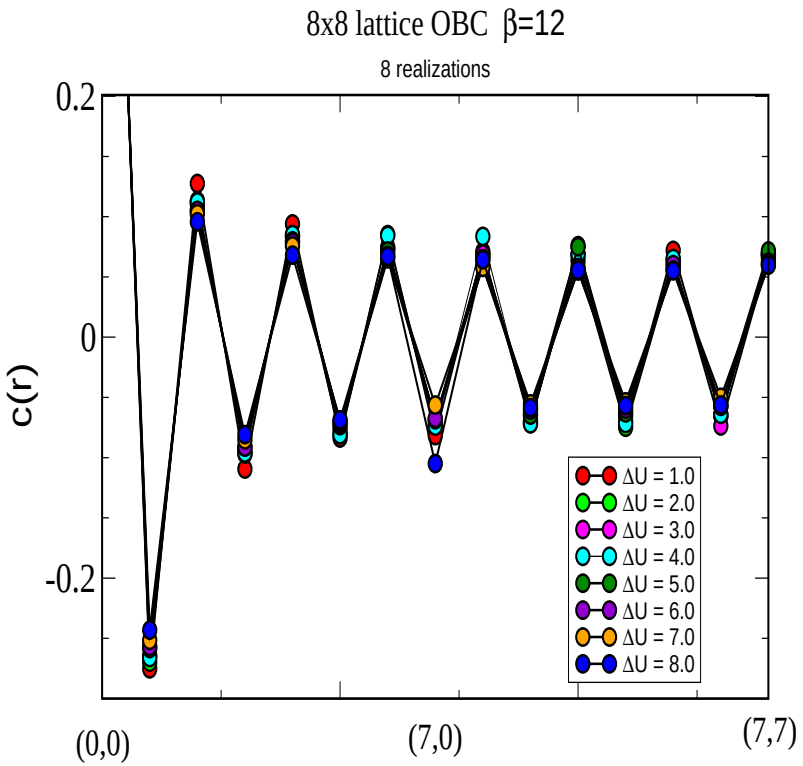


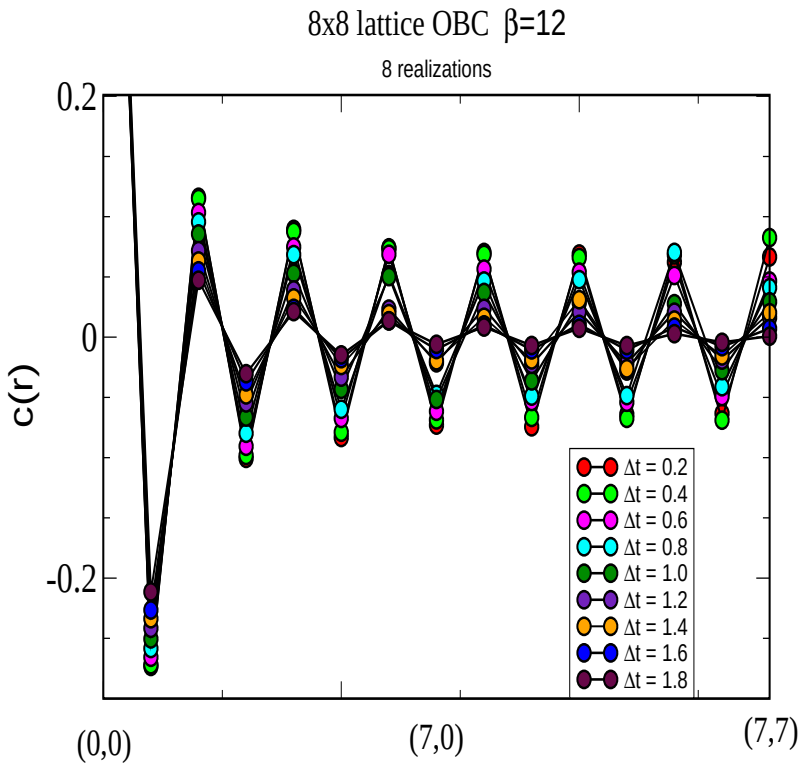
Despite 'precision,' the disorder can be pronounced.
(Unclear, as yet, what other obstacles will arise.)

Quantum Monte Carlo tests of effect of disorder on AF.

Left: Disorder in interaction strength U

Right: Disorder in hopping t





7. Summary/Whither the Field?

- Band Structure: qualitative pictures of weakly interacting electrons.
- Interactions: Essential to understand strongly correlated materials
- Hubbard Model: quantitative picture of role of interactions. Oversimplified!
- Beyond (present) numeric capabilities to solve more complex Hubbard models.
- Search for simpler materials!
- Optical lattices. Enormous successes, but limitations on temperature.
- Engineered silicon might be a new frontier.

"Quantum simulators may become a reality in the near future as the required technologies are now within reach. Quantum simulators, relying on the coherent control of neutral atoms, ions, photons, or electrons, would allow studying problems in various fields including condensed-matter physics, high-energy physics, cosmology, atomic physics, and quantum chemistry.

Iulia Buluta and Franco Nori, Quantum Simulators Science 326 pp.108-111, (2009). DOI: 10.1126/science.1177838