UCDAVIS

Harnessing the Sign Problem to study Quantum Magnetism and Metal-Insulator Transitions

- 1. Energy Bands in Solids (noninteracting Hubbard Model)
  Initial Implications for Strongly Correlated Materials
- 2. The Hubbard Model
- 3. Quantum Monte Carlo (Solving the Hubbard Model)
  Powerful (when it works $\cdots$) $\rightarrow$ the Sign Problem
- 4. Making Use of the Sign Problem !!
- 5. An Alternate Approach: Simplified Materials
  Optical lattices and Engineered Silicon
- 6. Some Conclusions

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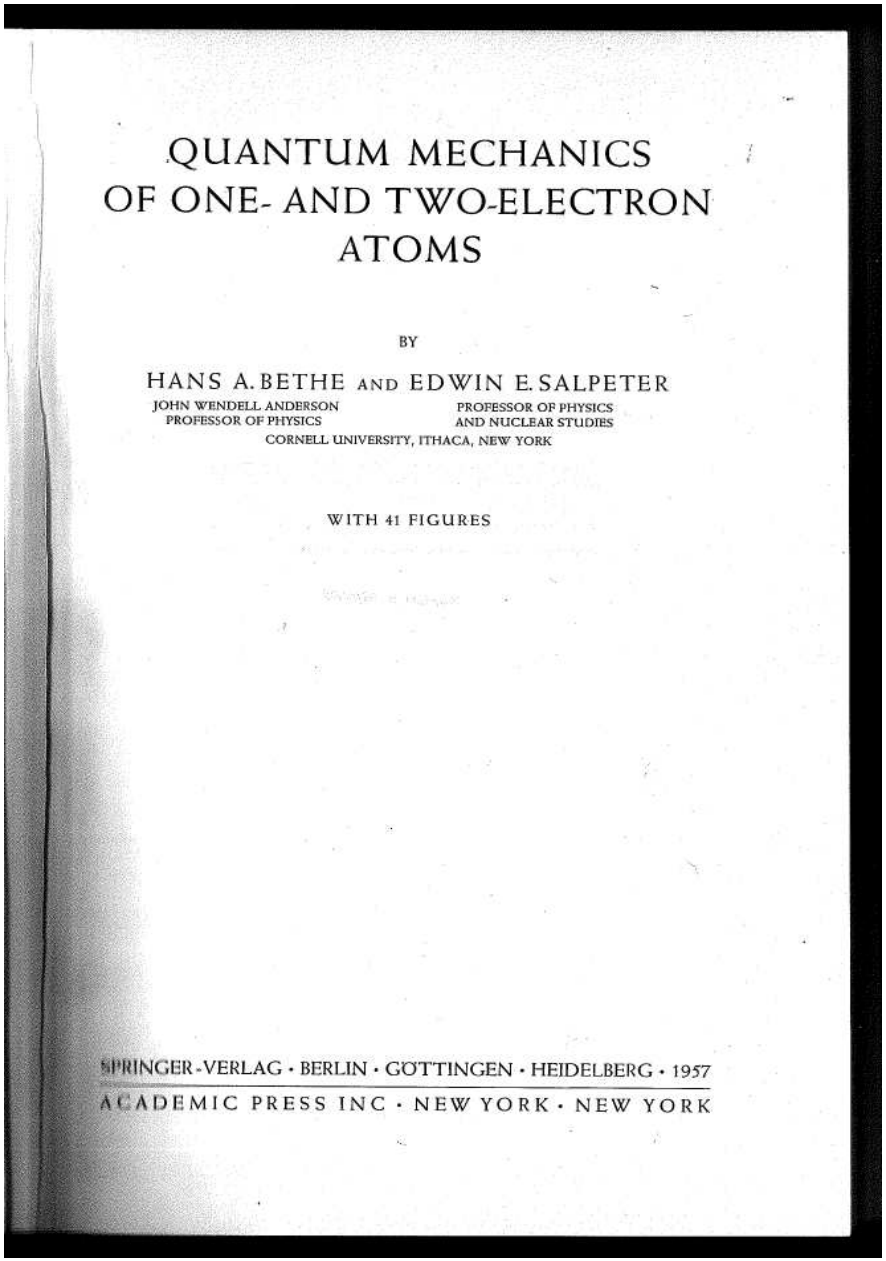

QUANTUM MECHANICS
OF ONE- AND TWO-ELECTRON
ATOMS

BY

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WITH 41 FIGURES

SPRINGER-VERLAG · BERLIN · GÖTTINGEN · HEIDELBERG · 1957
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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?!?!

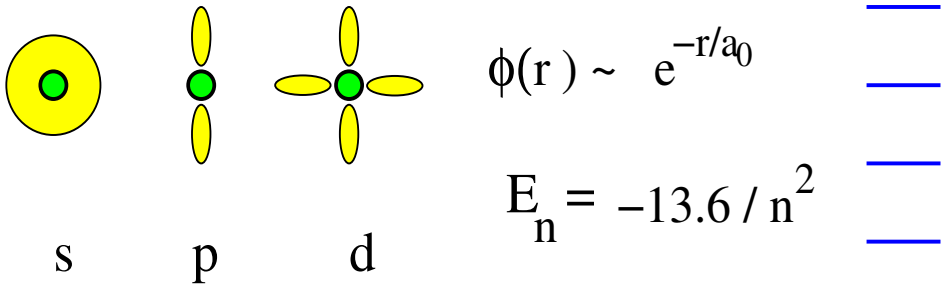
1. Origin of Energy Bands in a Solid (noninteracting HM)

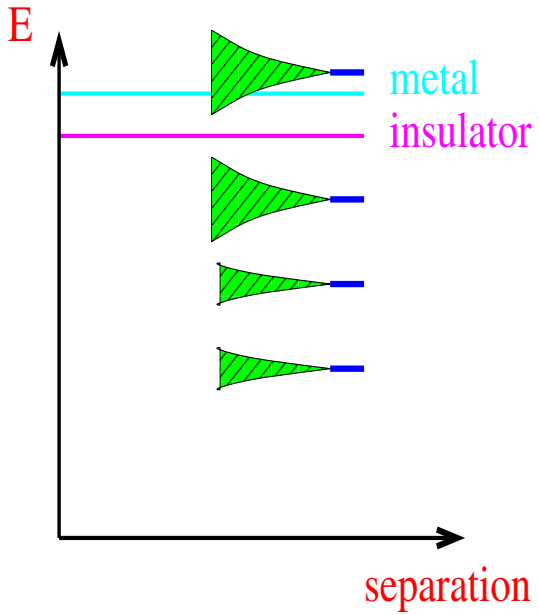
Individual atoms: discrete energy levels

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)





Energy band completely filled: Insulator

Finite energy gap to next unoccupied level

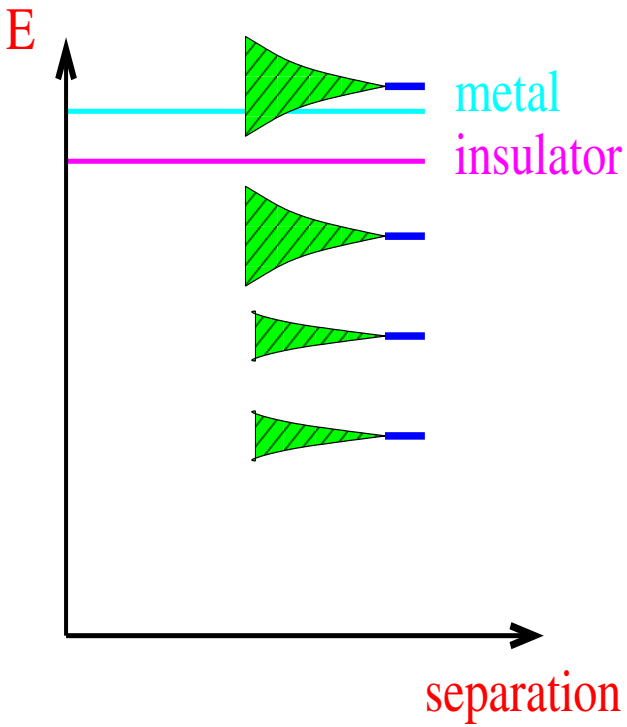
Simple counting arguments predict whether many solids are metallic or insulating!!

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.



Density Functional Theory: Accurate Energy Bands for Real Materials

Tight binding model:

Given a lattice geometry.

Electrons hop on neighboring sites $\langle lj \rangle$:

$$H = -t \sum_{\langle lj \rangle} \left(c_l^\dagger c_j + c_j^\dagger c_l \right)$$

Go to momentum space

$$c_k^\dagger = \frac{1}{\sqrt{N}} \sum_l e^{ikl} c_l^\dagger$$

to diagonalize H:

$$H = \sum_k E_k \, c_k^\dagger c_k$$

Dispersion relation: $E(k)$

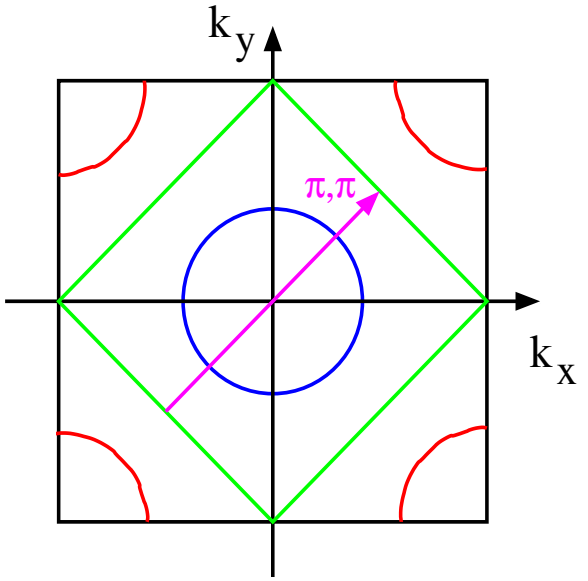
Fermi Surface: constant E_k trajectory.

Density of states:

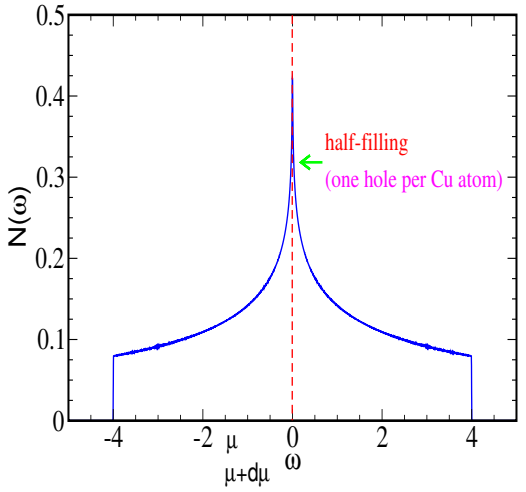
$$N(\omega) = \int dk_x \, dk_y \, \delta\left(\omega - E_k \right)$$

2D square lattice

$$E_k = -2\,t \left(\cos k_x + \cos k_y \right)$$



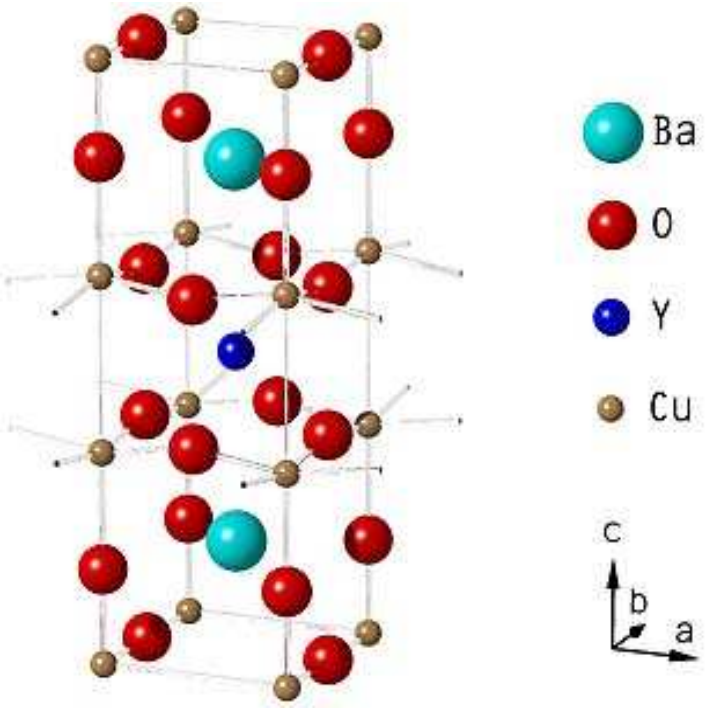
Perfect Nesting

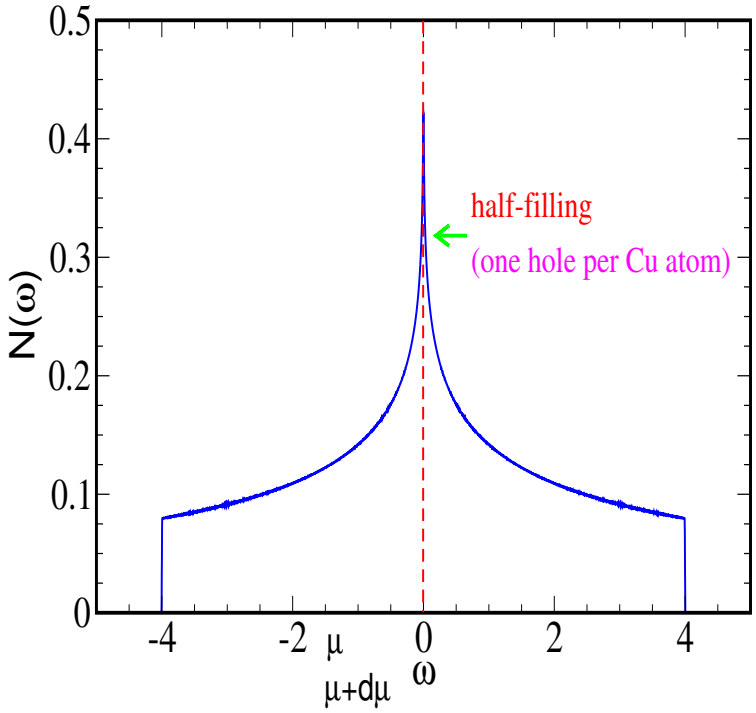


Van Hove singularity

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

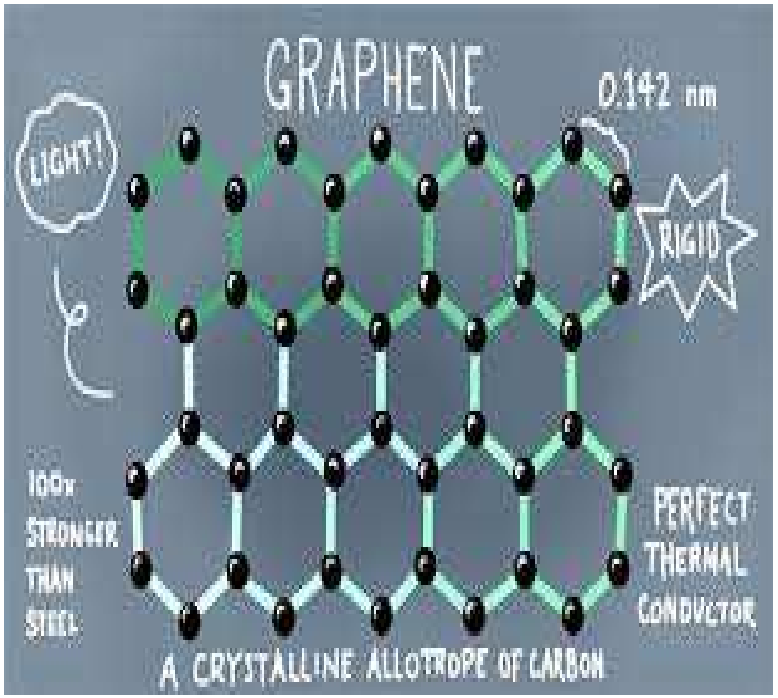
$T_c \sim e^{-1/\lambda N(\omega=0)}$ $\Rightarrow$ T_c is high.

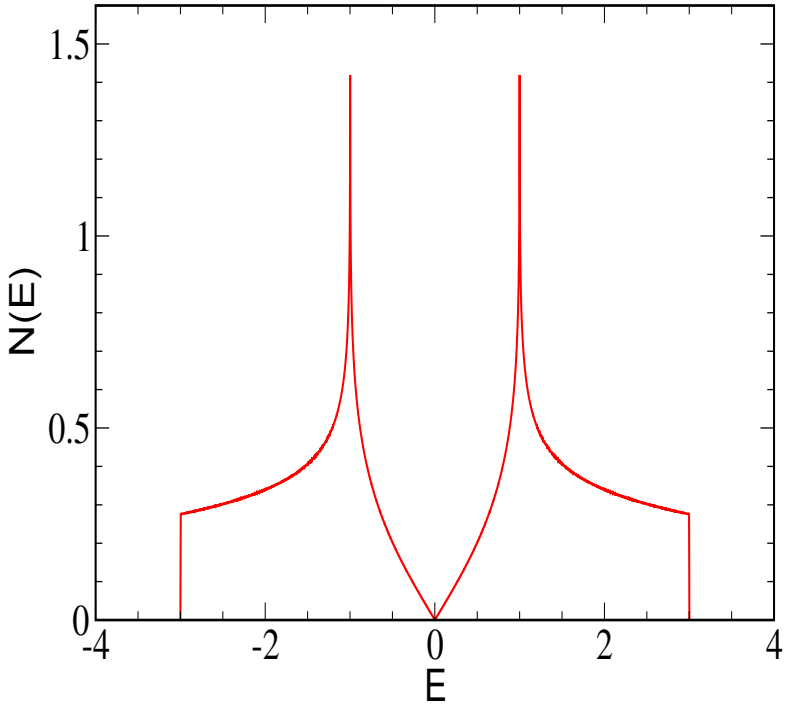
Previous superconductors: $\lambda N(\omega = 0) \sim 1/4$.

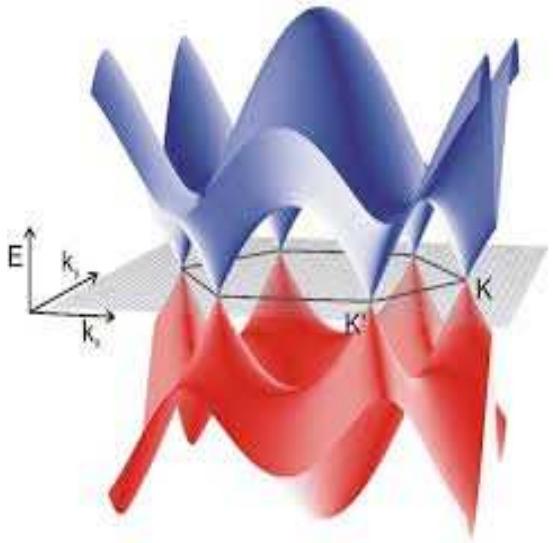
Critical coupling $U_c = 0$ for antiferromagnetic (AF) order.

$\chi(q,T) = \frac{\chi_0(q,T)}{1-\mathbf{U}\chi_0(q,T)}$

Graphene (Honeycomb lattice)







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

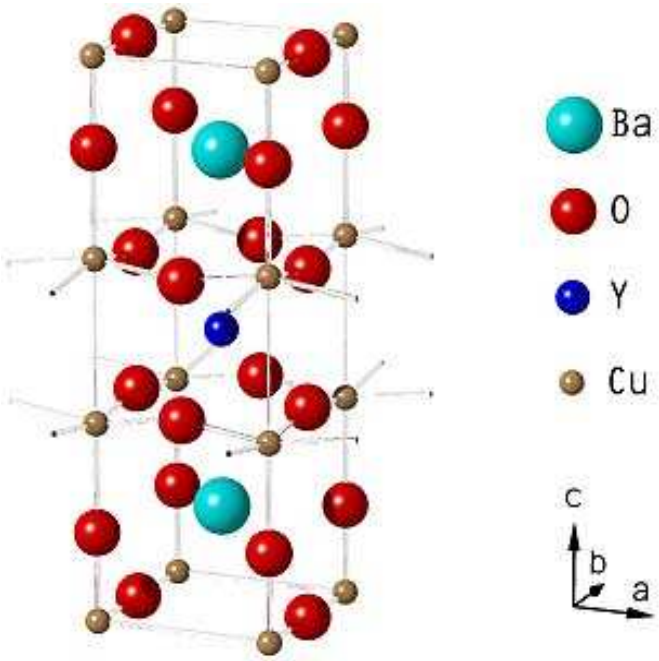
Tied to 'Dirac cones' $E(\mathbf{k}) = v\,|\mathbf{k}|$.

$N(E) = 0 \to U_c \neq 0$ for AF order

Trouble in Paradise $\cdots$

Parent compounds of cuprate superconductors:

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

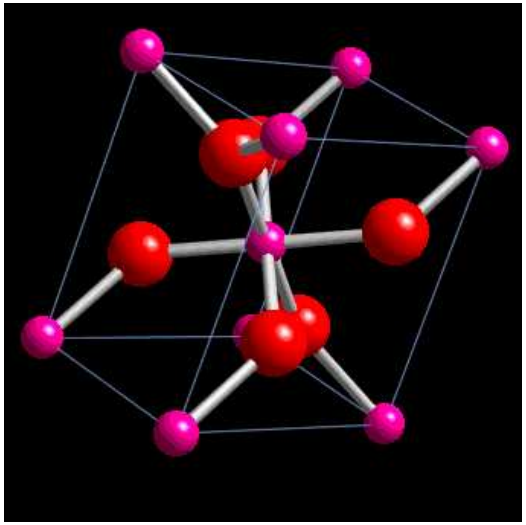


Transition metal monoxides (MnO, FeO, CoO):

(Many oxides in earth's interior.)

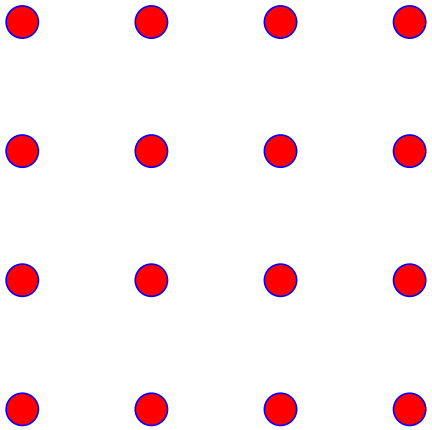
MnO: Mn^{2+} d band half-filled (d^5: odd # electrons)

- Why are they antiferromagnetic insulators?!

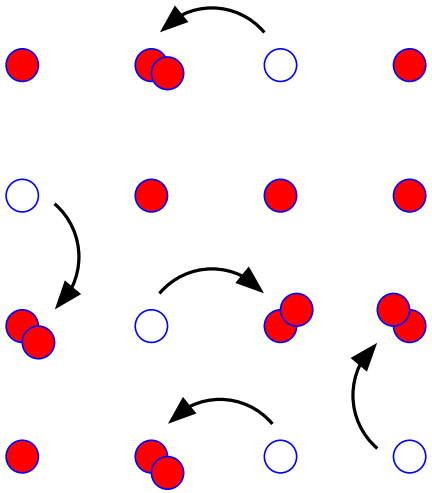


2. The Hubbard Hamiltonian

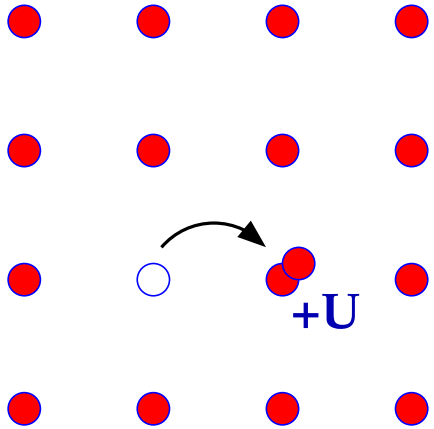
(A different type of Insulator)



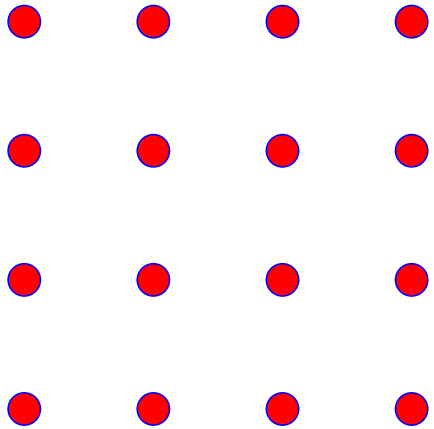
Consider a lattice of sites with
"commensurate filling":
The average number of particles
is one per site.



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.)

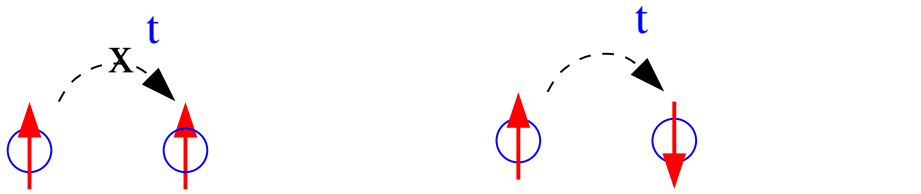
Two ways to destroy Mott Insulator:

* 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.



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

Mott insulating behavior and antiferromagnetism go hand-in-hand.
Qualitative picture of cuprate physics before doping.

Surprisingly, square lattice Hubbard Model captures physics of doped cuprates:

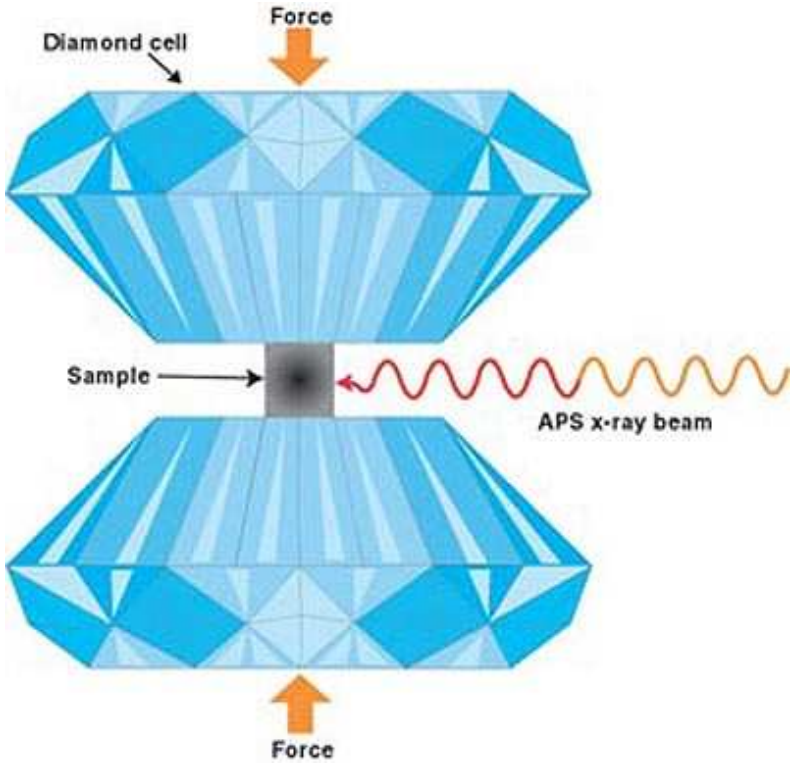
Spin gap and strange metal behavior, stripes, d-wave pairing $\cdots$

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

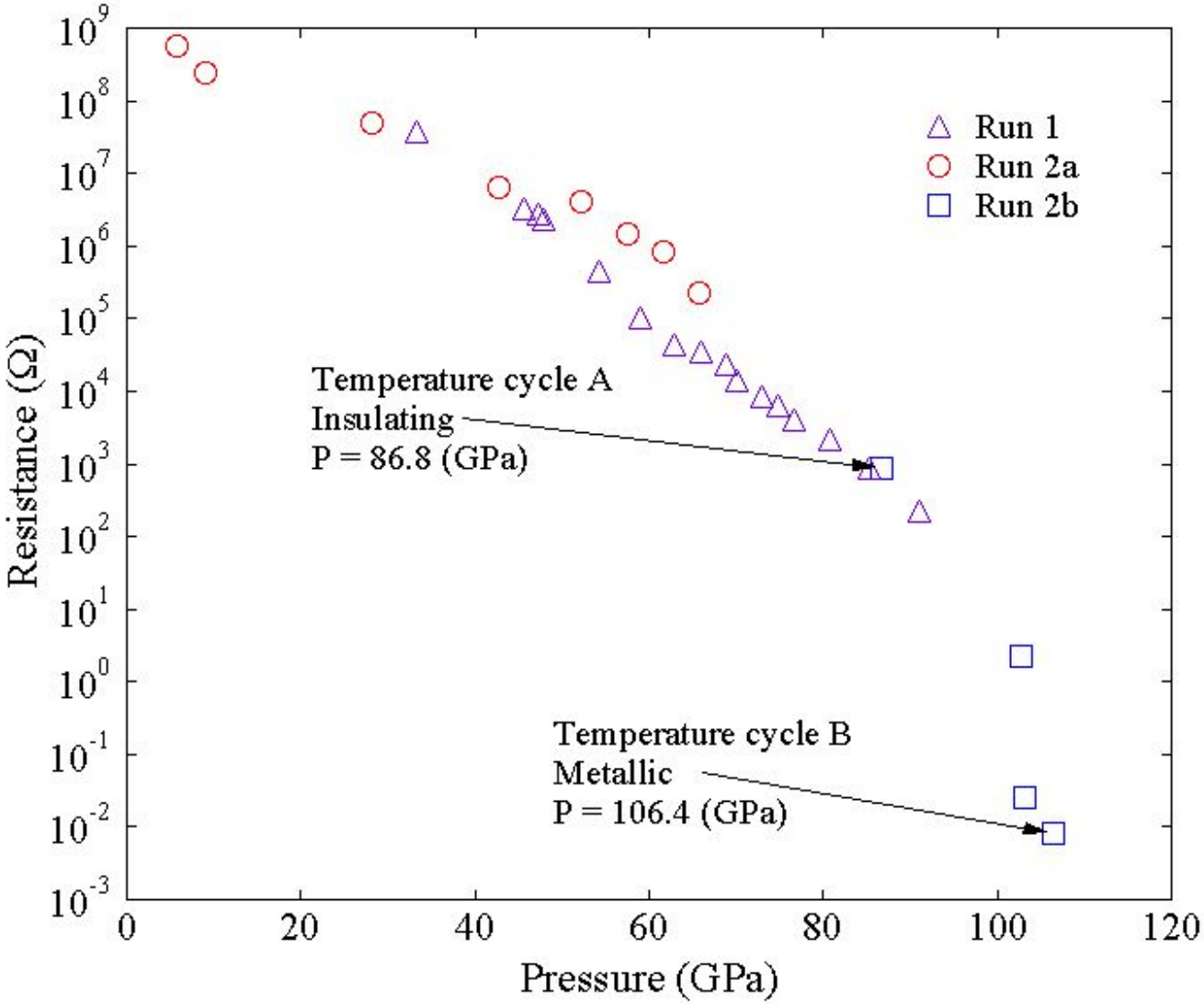
Diamond Anvil Cell

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.

Determinant Quantum Monte Carlo

Compute operator expectation values

$$\begin{aligned} \langle \hat{A} \rangle &= Z^{-1} \text{ Tr } [\hat{A} e^{-\beta \hat{H}}] \\ Z &= \text{Tr } [e^{-\beta \hat{H}}] \end{aligned}$$

Hubbard Hamiltonian

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

- Inverse Temperature discretized: $\beta = L \Delta \tau$

$$Z = \text{Tr } [e^{-\beta \hat{H}}] = \text{Tr } [e^{-\Delta \tau \hat{H}}]^L$$

- Suzuki-Trotter Approximation

$$e^{-\Delta \tau \hat{H}} \approx e^{-\Delta \tau \hat{K}} e^{-\Delta \tau \hat{P}}$$

Extrapolation to $\Delta \tau = 0$.

- (Discrete) Hubbard-Stratonovich Fields (Hirsch) decouple interaction:

$$e^{-\Delta\tau U(n_{\mathbf{i}\uparrow}-\frac{1}{2})(n_{\mathbf{i}\downarrow}-\frac{1}{2})} = \frac{1}{2}e^{-U\Delta\tau/4}\sum_{S_{\mathbf{i}\tau}} e^{\Delta\tau\lambda S_{\mathbf{i}\tau}(n_{\mathbf{i}\uparrow}-n_{\mathbf{i}\downarrow})} = e^{-\Delta\tau\mathcal{P}_{\mathbf{i}}(\tau)}$$

where $\cosh(\Delta\tau\lambda) = e^{U\Delta\tau/2}$.

- Quadratic Form in fermion operators: Do trace analytically

$$\begin{aligned} Z &= \sum_{\{S_{\mathbf{i}\tau}\}} \mathrm{Tr}\,[e^{-\Delta\tau\hat{K}}e^{-\Delta\tau\hat{\mathcal{P}}(1)}e^{-\Delta\tau\hat{K}}e^{-\Delta\tau\hat{\mathcal{P}}(2)}e^{-\Delta\tau\hat{K}}\ldots e^{-\Delta\tau\hat{\mathcal{P}}(L)}] \\ &= \sum_{\{S_{\mathbf{i}\tau}\}} \det M_\uparrow(\{S_{\mathbf{i}\tau}\})\det M_\downarrow(\{S_{\mathbf{i}\tau}\}) \end{aligned}$$

$\dim(M_\sigma)$ is the number of spatial sites. For multi-band models dimension is (number of spatial sites)x(number of orbitals per site).

- Sample HS field stochastically.

$$\begin{aligned} S_{\mathbf{i_0}\tau_0} &\rightarrow -S_{\mathbf{i_0}\tau_0} \\ \det M_\sigma(\{S_{\mathbf{i}\tau}\}) &\rightarrow \det M_\sigma(\{S_{\mathbf{i}\tau}\}') \end{aligned}$$

Algorithm is order $N^3 L$.

$N \sim \quad 10^2 - 10^3$ lattice sites/electrons

$L = \beta/\Delta\tau \sim$ a hundred imaginary time slices (low temperatures).

- Measurements

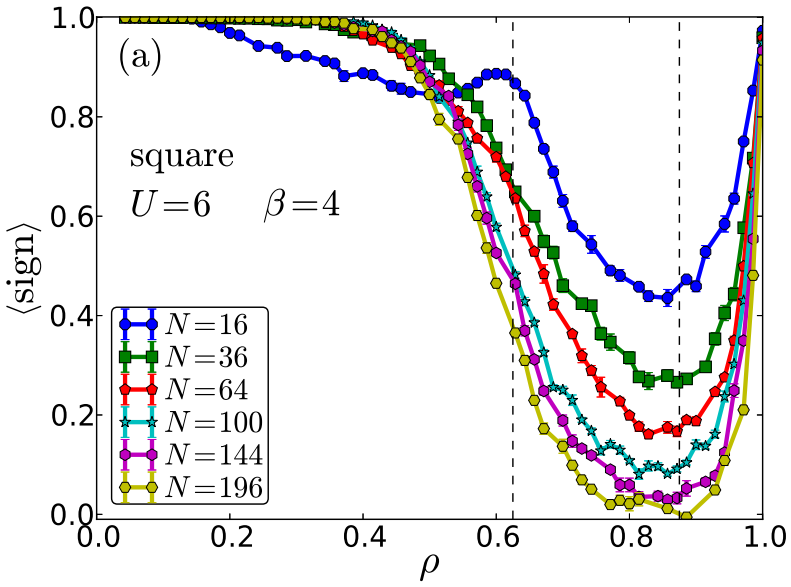
$$\langle c_{\mathbf{i}\sigma} c^\dagger_{\mathbf{j}\sigma} \rangle \leftrightarrow \langle [M_\sigma^{-1}]_{\mathbf{ij}} \rangle = \langle [G_\sigma]_{\mathbf{ij}} \rangle$$

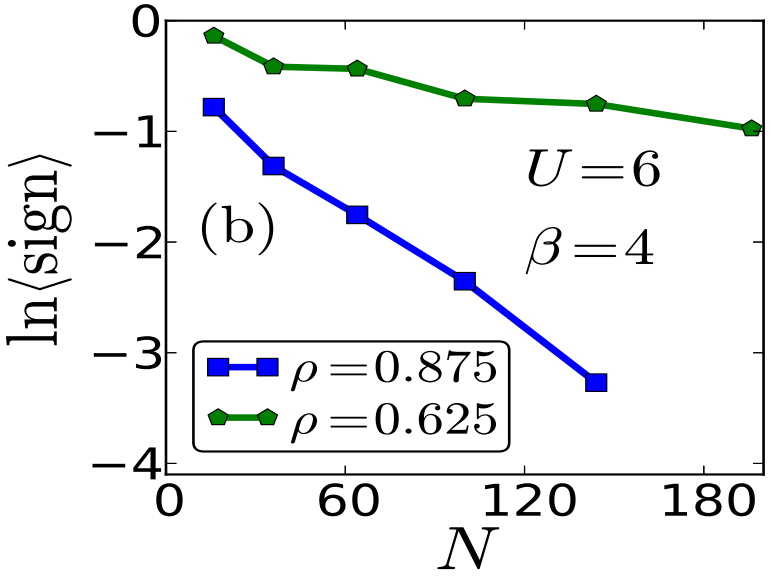
- Sign Problem

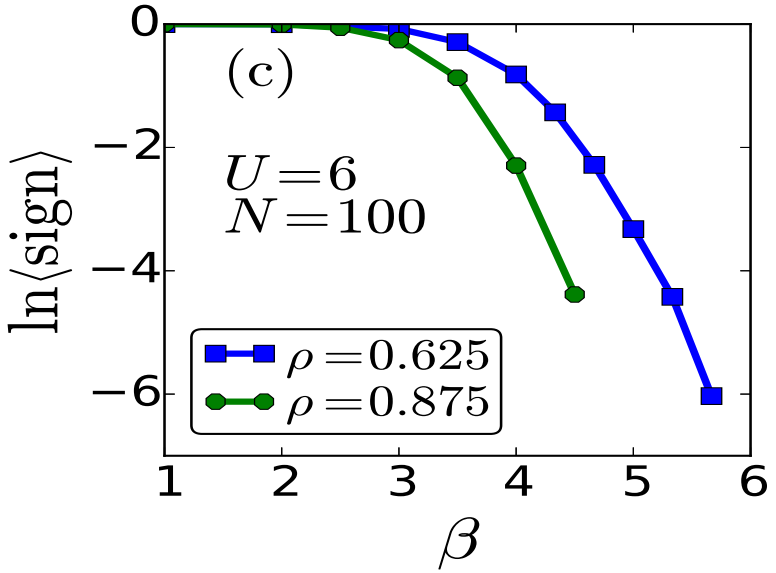
At low temperature $\det M_\sigma$ can go negative.

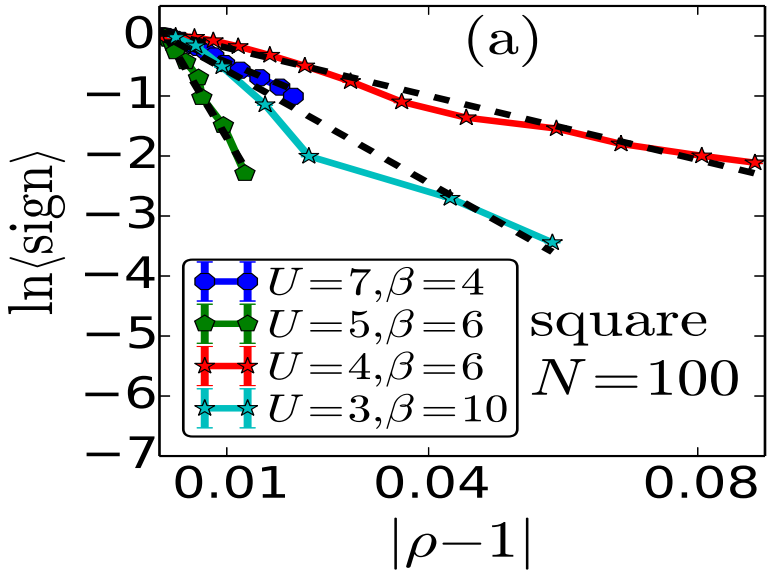
CPU time grows exponentially in L (β).

QMC limited to $T \gtrsim t/4$.









Special symmetry points (half-filling $\rho = 1$) $\det M_\uparrow = \det M_\uparrow$. No Sign Problem!

Kolodrubetz at al, The Journal of Chemical Physics 138, 024110 (2013).

DQMC is really nice (when it works $\cdots$)

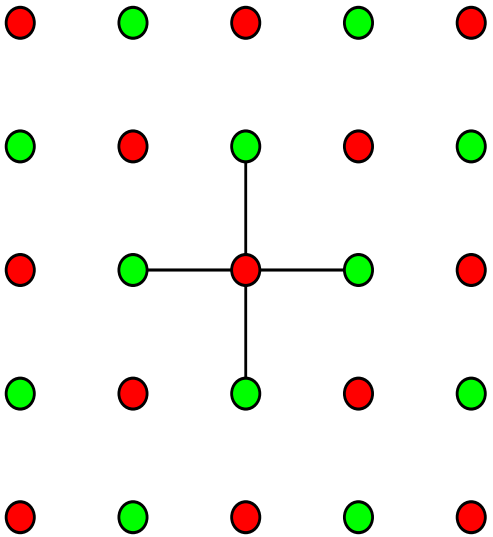
The Square Lattice at Half filling

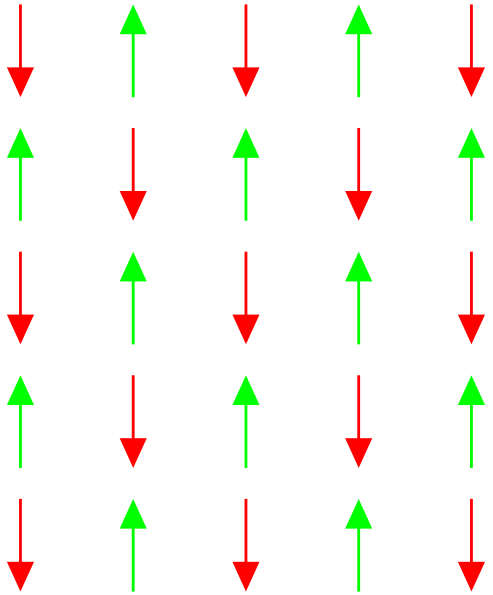
Electron spins on two neighboring sites like to be antiparallel.

Bipartite lattices are a natural for long range antiferromagnetic order

where this up-down pattern extends over entire lattice.

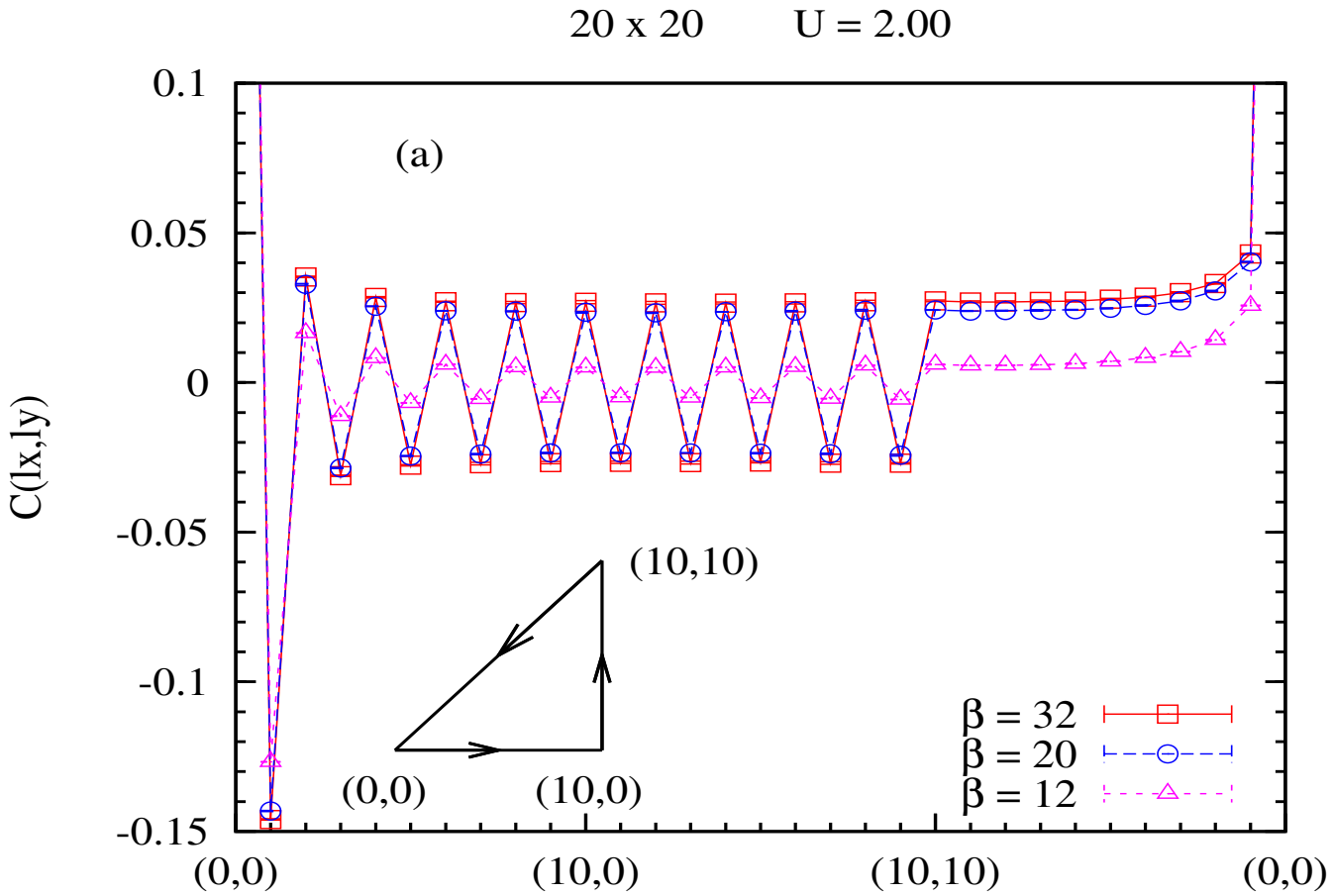
Especially square lattice: Perfect nesting





Antiferromagnetic spin correlations

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

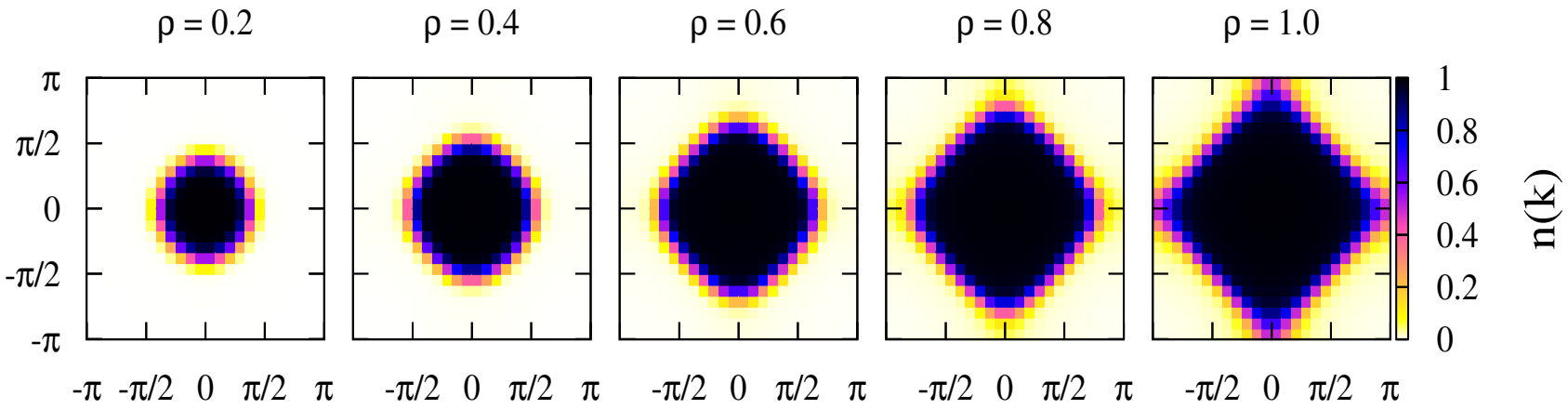


There is long range antiferromagnetic order!

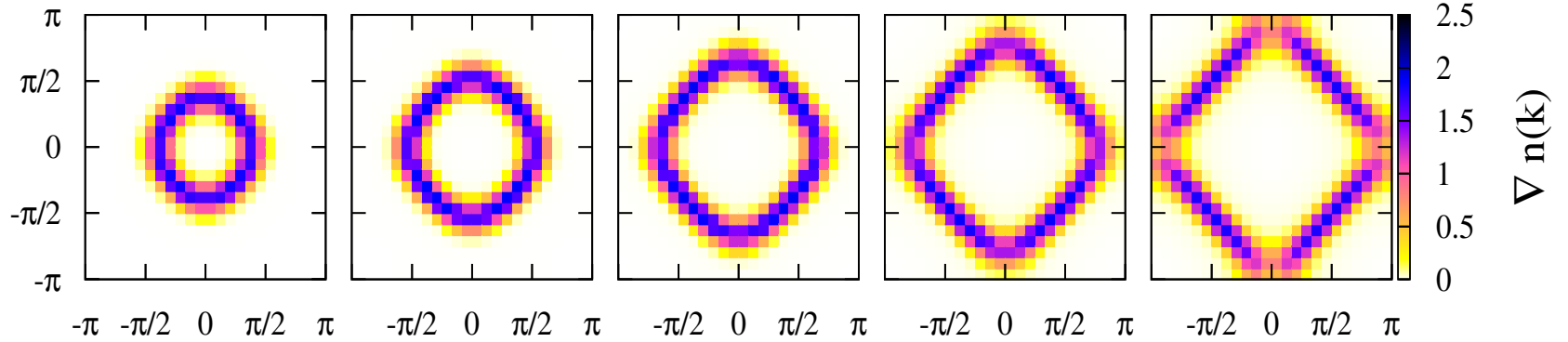
"Quantum Monte Carlo Study of the 2D Fermion Hubbard Model at Half-Filling", C.N. Varney, C.R. Lee, Z.J. Bai, S. Chiesa, M. Jarrell, and RTS, Phys. Rev. B80, 075116 (2009).

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

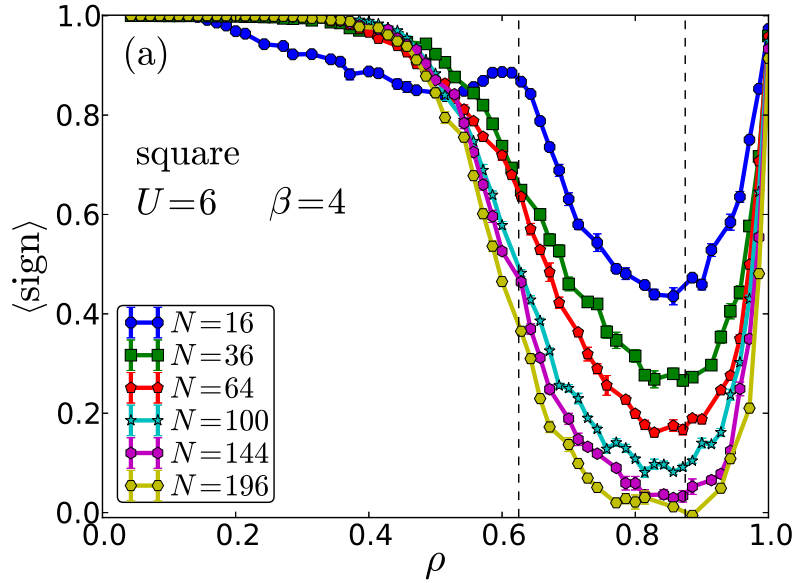
$U = 2$ Fermi function:



$U = 2$ Gradient of Fermi function:



4. Making Use of the Sign Problem



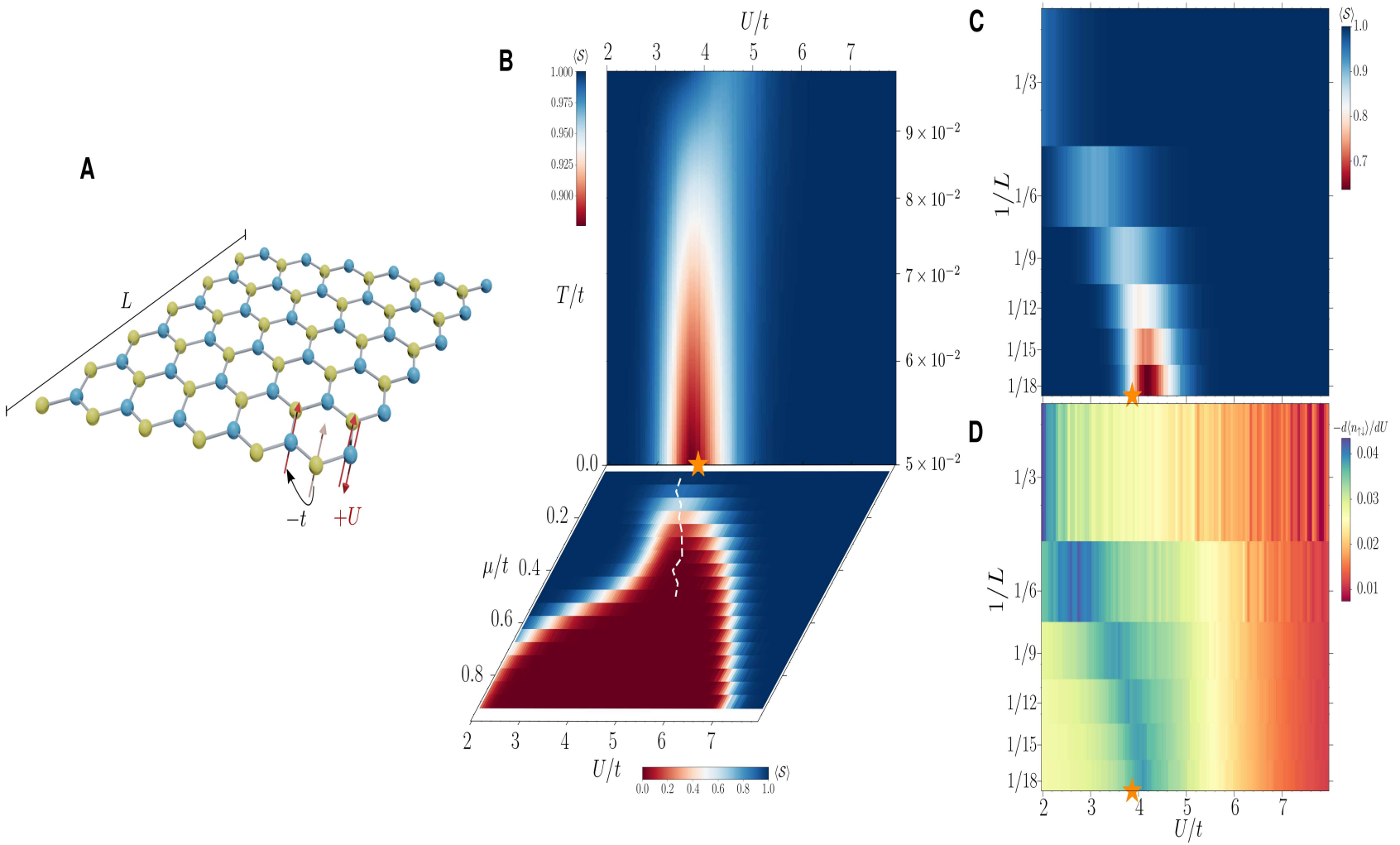
Is it a coincidence that the sign problem in the 2D Hubbard model is worst at density $\rho \sim 0.87$ precisely where T_c is highest?

Examine the behavior of $\langle \mathcal{S} \rangle$ for models whose critical points are known *known*.

Example 1: spinful Hubbard model on a honeycomb lattice.

Vanishing of $N(E=0)$ (semi-metal) gives $U_c/t \sim 3.869$ for semi-metal to AF QCP.

"Absence of a Spin Liquid Phase in the Hubbard Model on the Honeycomb Lattice", S. Sorella, Y. Otsuka, and S. Yunoki, Sci. Rep. 2, 992 (2012).



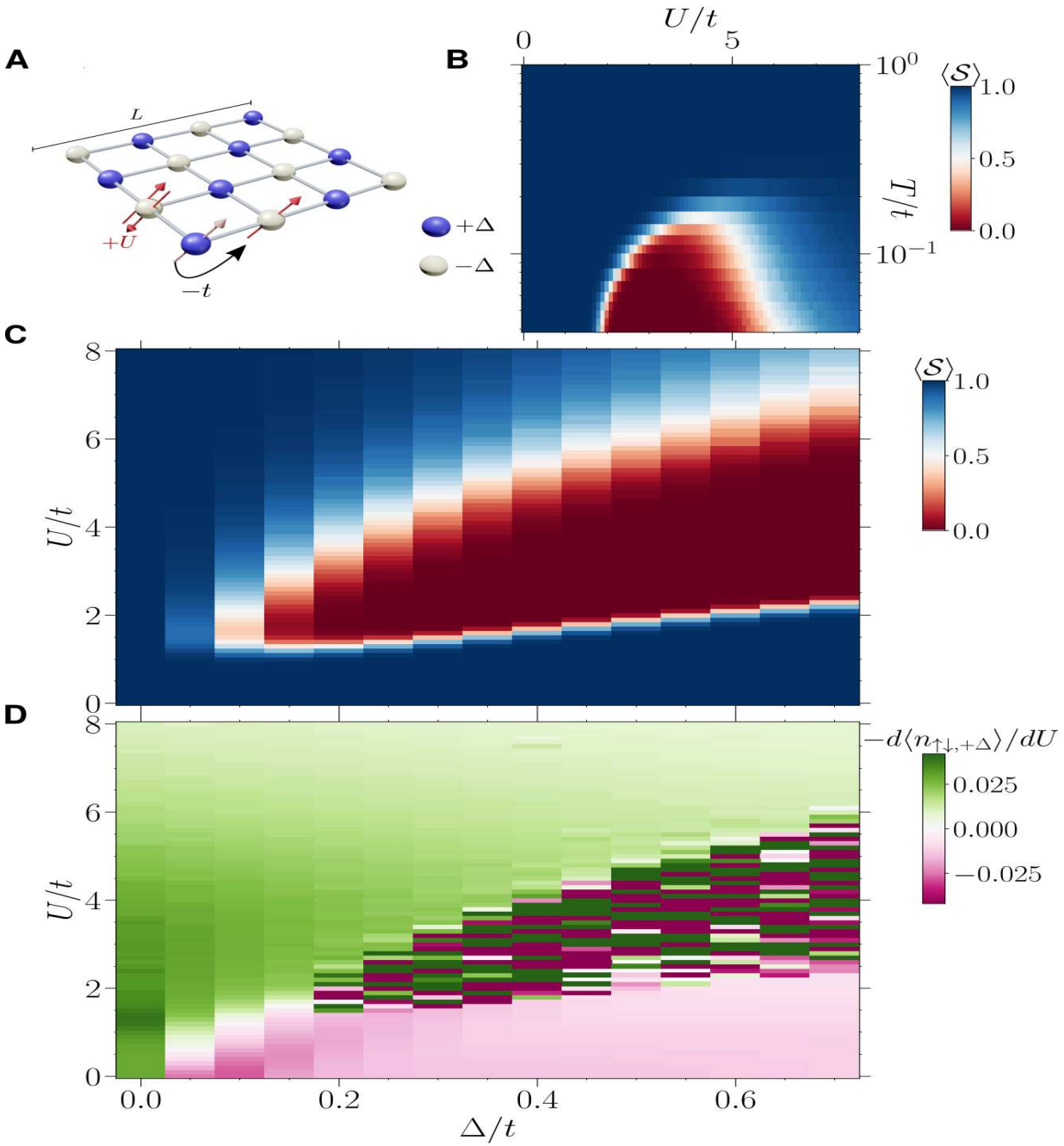
B upper(lower): $\langle \mathcal{S} \rangle$ in T/t-U/t (μ/t-U/t) planes.

C: $\langle \mathcal{S} \rangle$ extrapolated in linear system size L at $T/t = 1/20$ and $\mu/t = 0.1$.

D: Derivative of double occupancy

Star Marker: known QCP from 'traditional' observables. (eg. AF structure factor).

"Quantum Critical Points and the Sign Problem", R. Mondaini, S. Tarat, and R.T. Scalettar.



Example 2: Square lattice Ionic Hubbard model

Site energy $\pm\Delta$
on sublattices A/B
$\rightarrow$ Band gap opens.

"Traditional Observables":

$S_{\mathrm{af}}, \rho_{\mathrm{dc}}, A(\omega), \quad \langle n_{\uparrow\downarrow}\rangle$

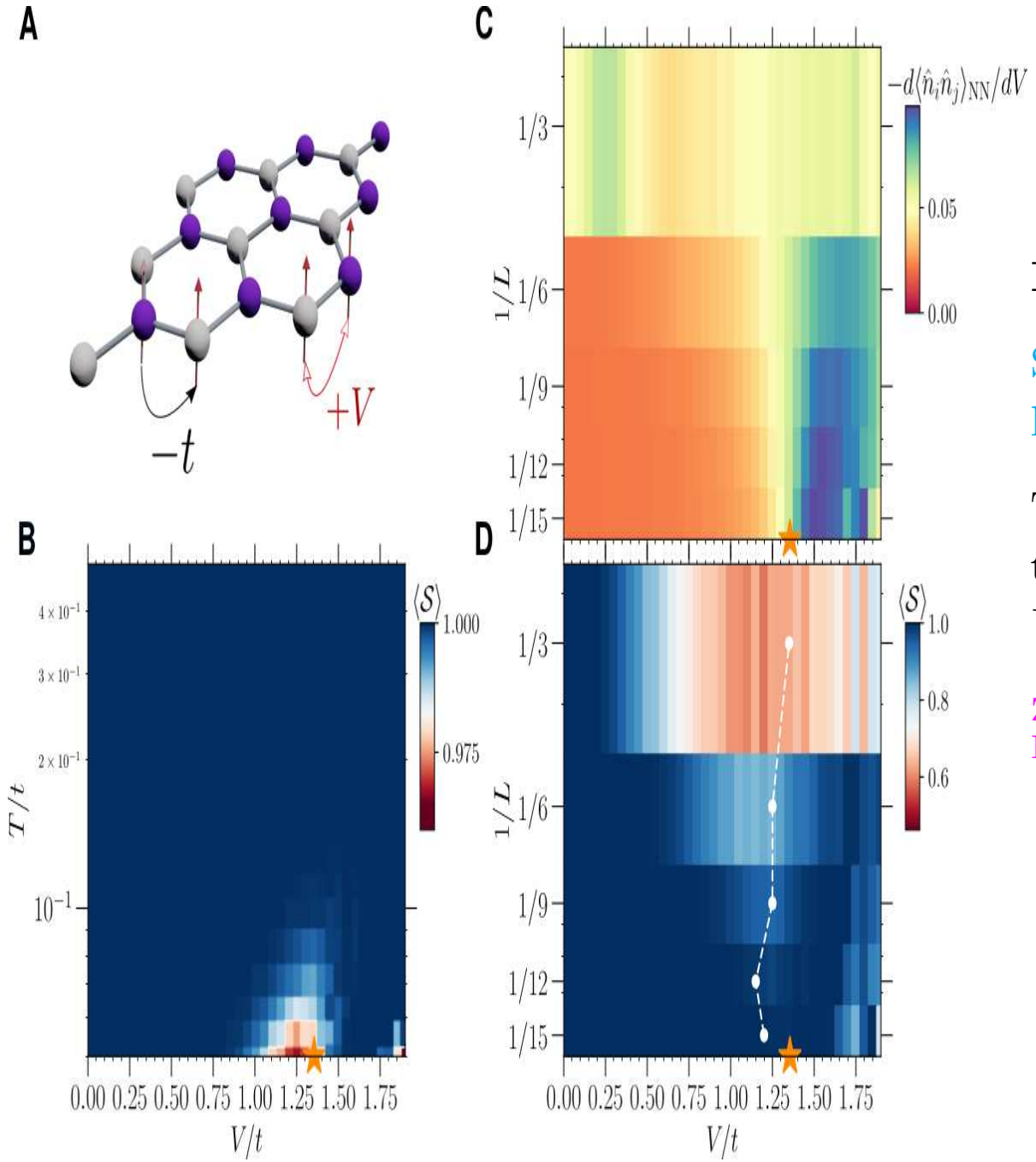
Band insulator $U/t \lesssim 2$.

Mott insulator $U/t \gtrsim 5$.

Metallic phase intervenes.

$\langle \mathcal{S} \rangle$ reproduces known PD.

Fermionic superlattices:
Chuanwei Zhang,
Phys. Rev. A100, 023616 (2019)



Example 3:

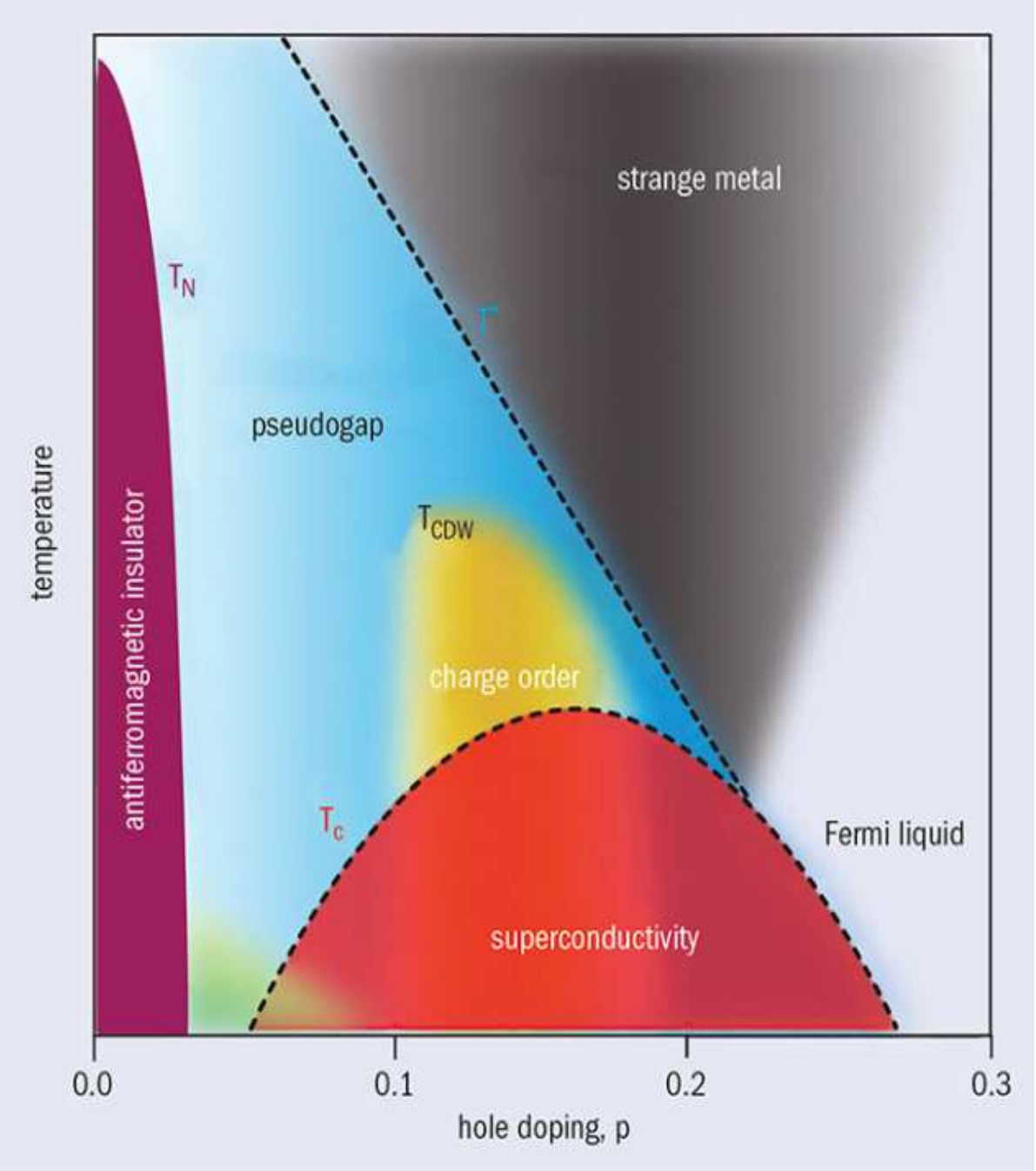
Spinless fermions on honeycomb lattice, intersite V

Transition from Metal to charge density wave

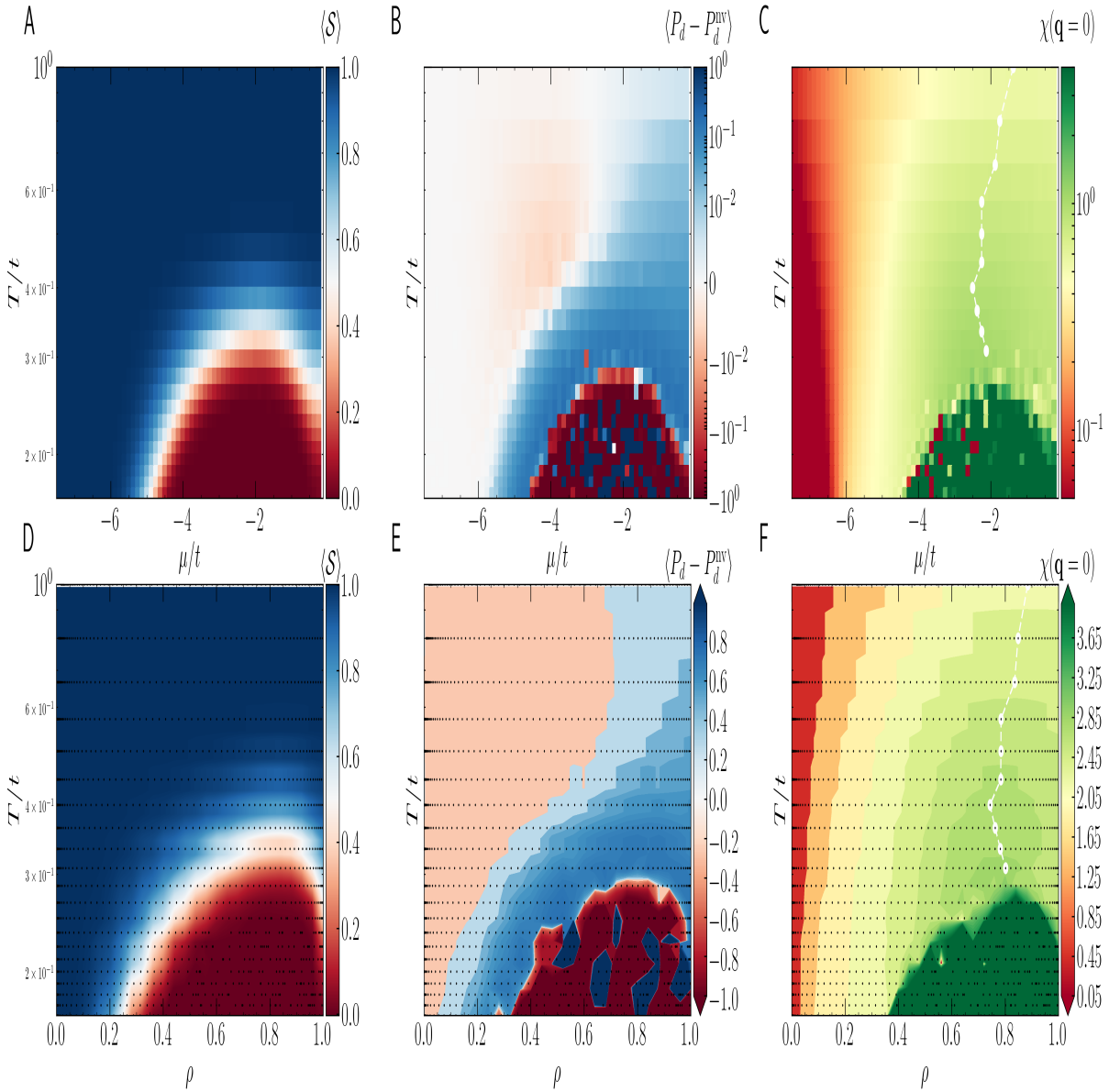
$V_c/t = 1.35$

Z.X. Li, Y.F. Jiang, and H. Yao, Phys. Rev. B91, 241117 (2015).

Example 4: Square Lattice– Cuprate Phase Diagram



Example 4 (cont'd): Square lattice Hubbard model

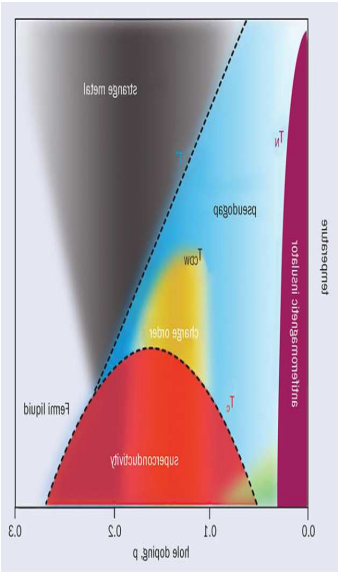


A: $\langle \mathcal{S} \rangle$ in T-μ plane

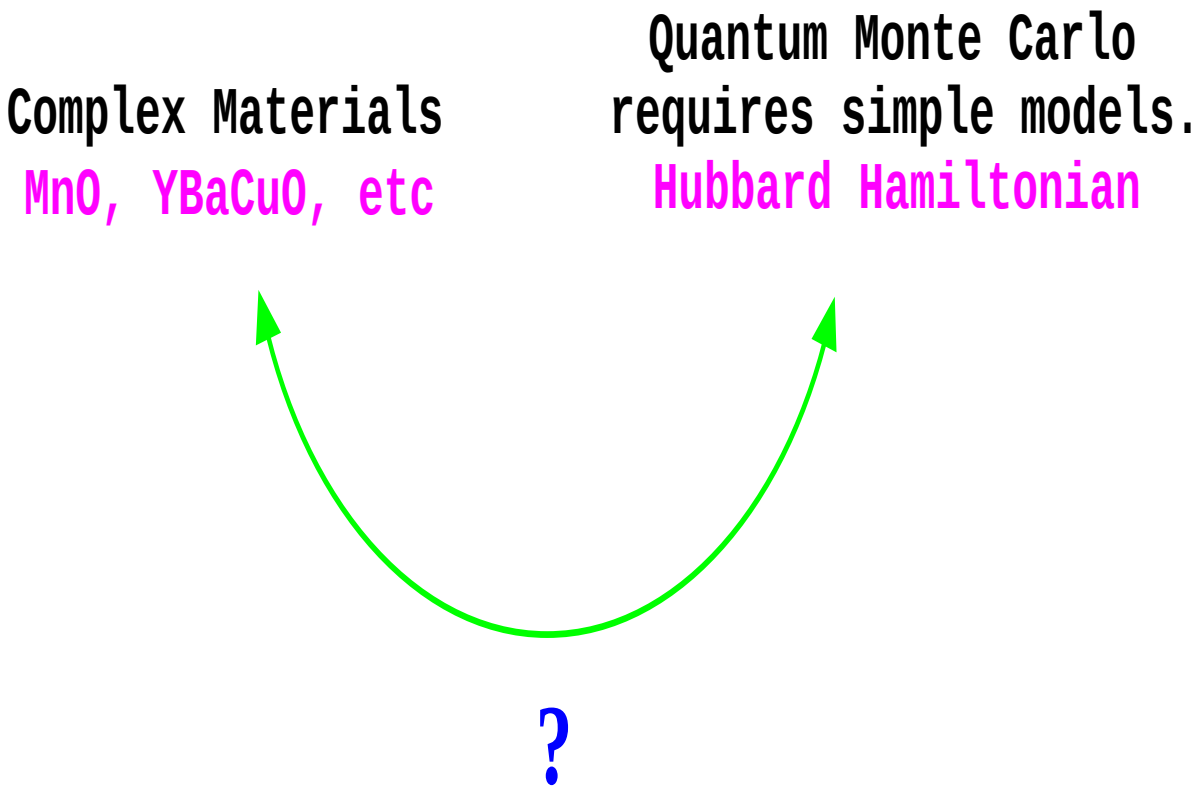
B: Enhancement of d-wave pairing.

C: Magnetic susceptibility.

D, E, F: Same quantities in T-ρ plane.

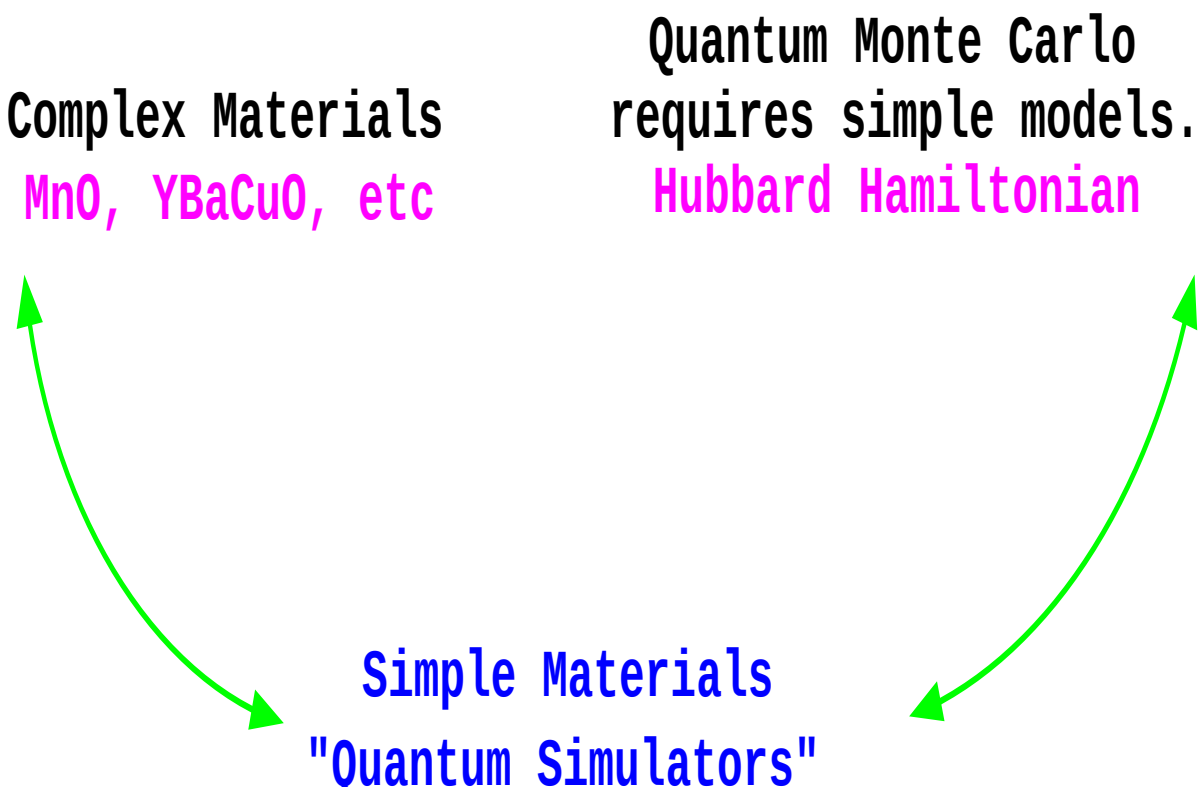


5. Simplified Materials



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.

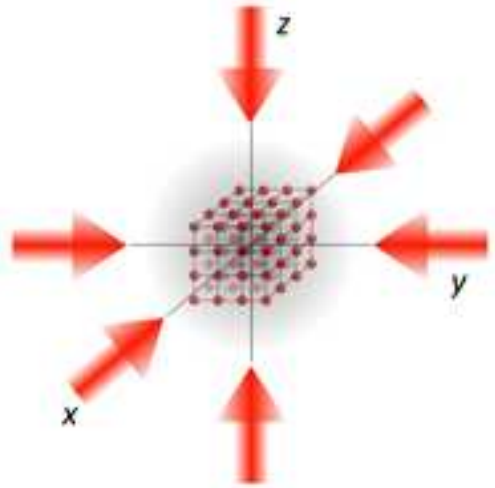
Iulia Buluta and Franco Nori, "Quantum Simulators" Science 326 pp.108-111, (2009). DOI: 10.1126/science.1177838

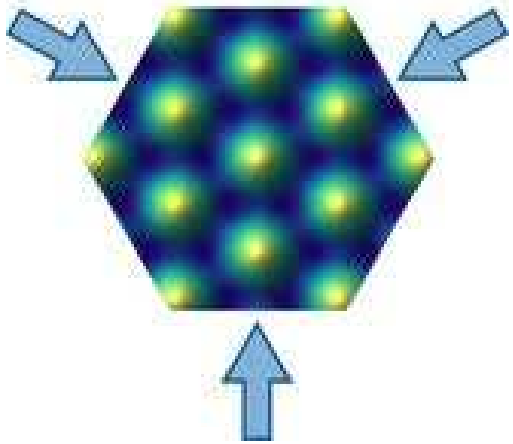
i: Optical Lattices

Lattice formed by interference of counterpropagating laser beams.

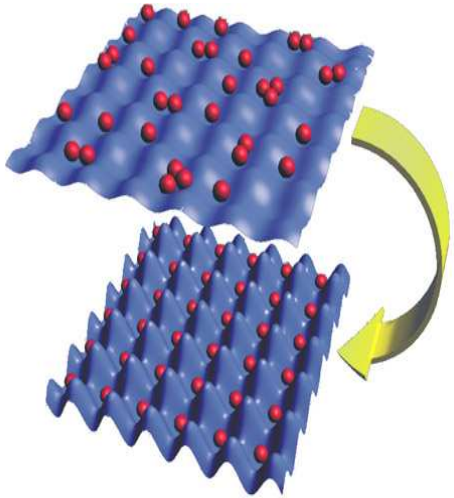
Atoms $\left(o(10^5)\right)$ trapped by Stark shift. Cool evaporatively $\cdots$.

Different geometries accessable (e.g. cubic, honeycomb, $\cdots$)



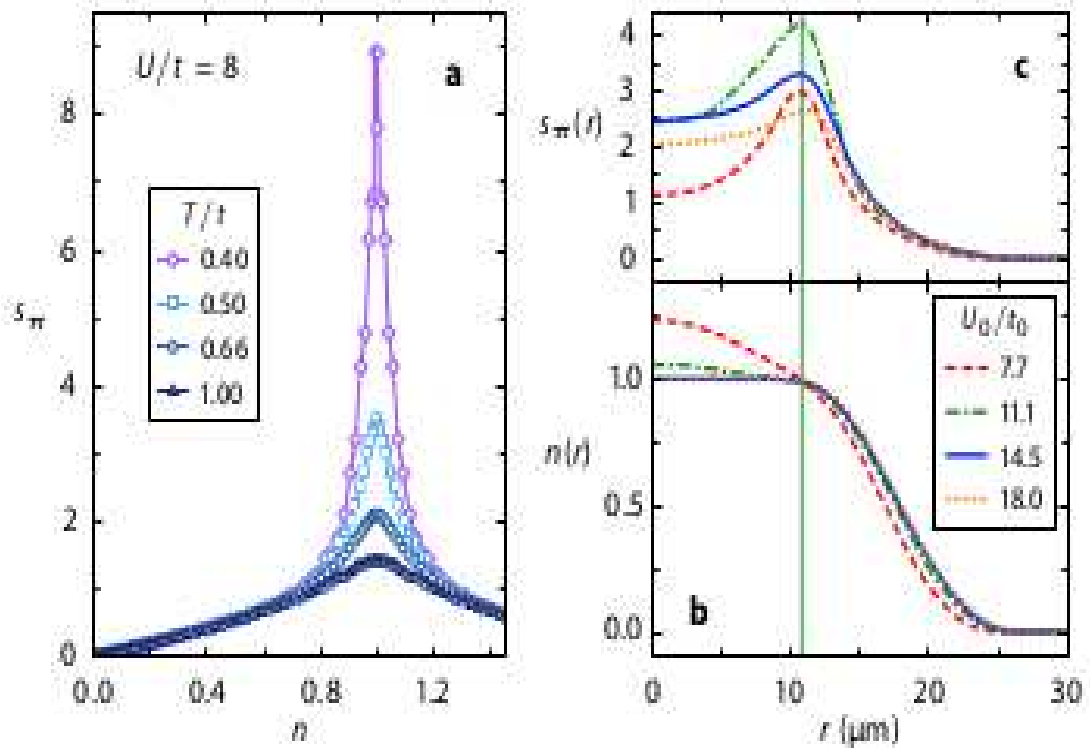


Control hopping t, interactions U
much more easily than solids.
Use, e.g. to drive Mott insulator.



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.

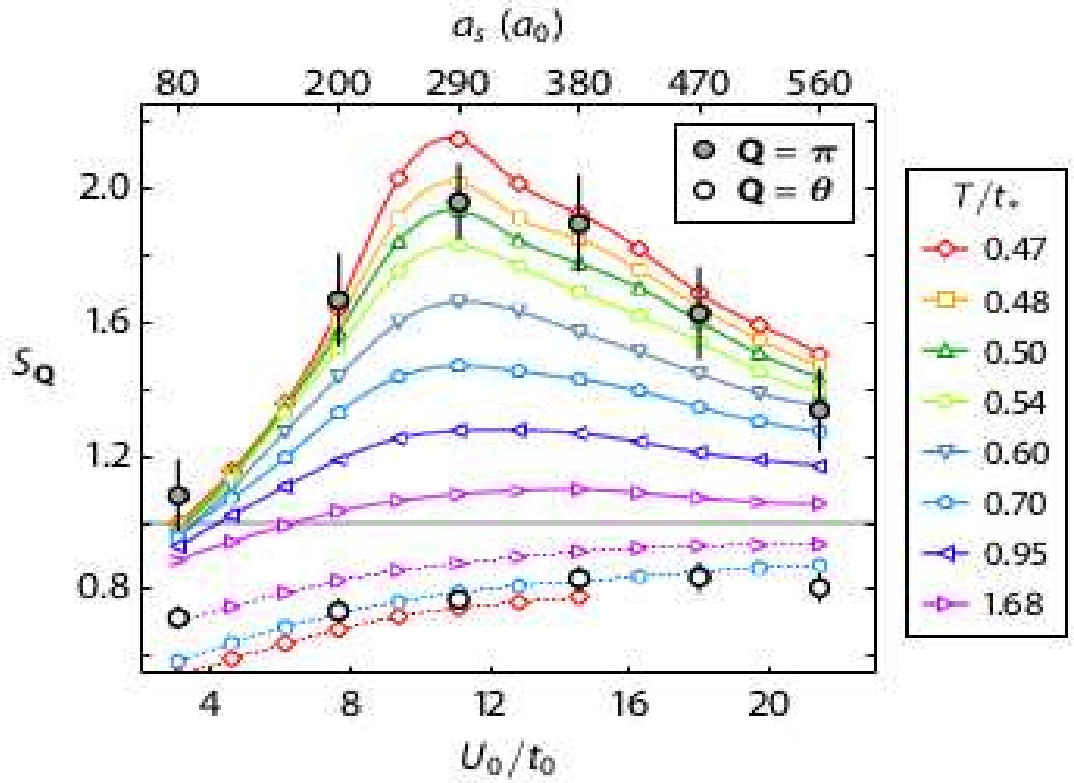
Local Mott/AF regions coexist with paramagnetic metal.

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.

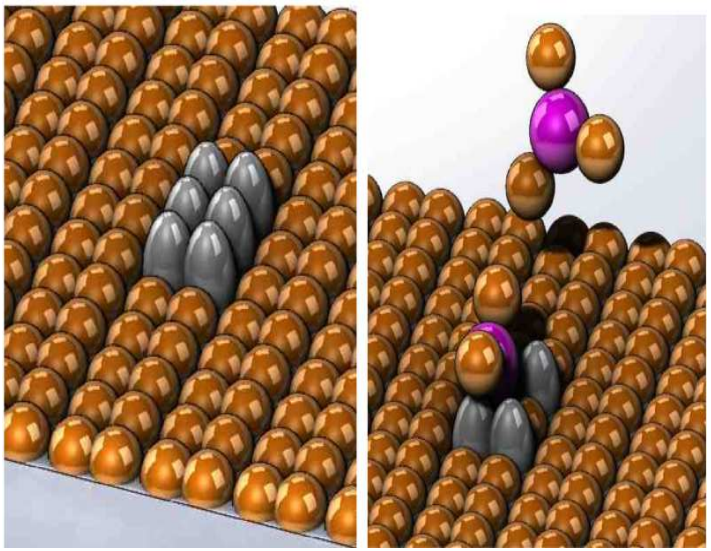
$\Rightarrow$ T/t is not small!

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.



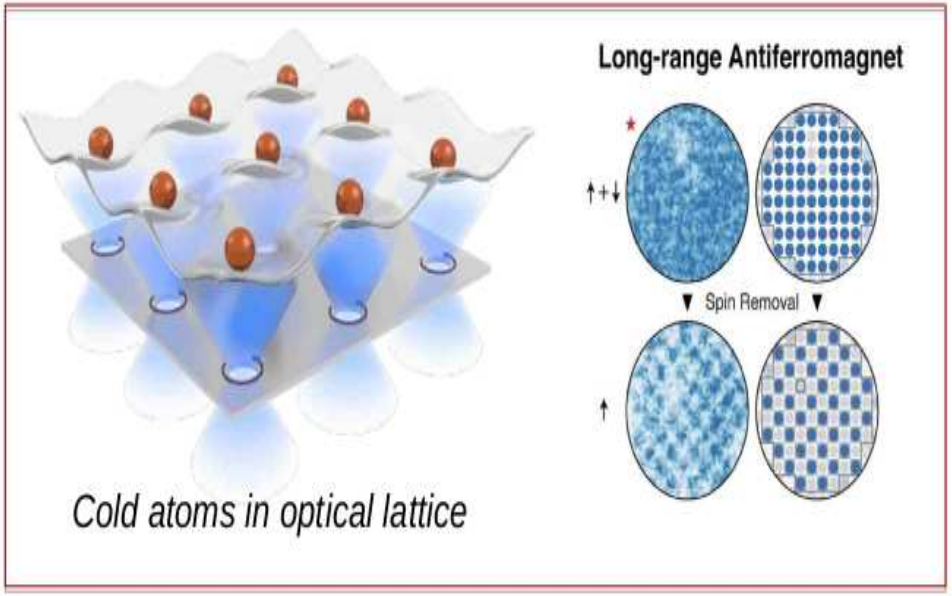
Like optical lattices:

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

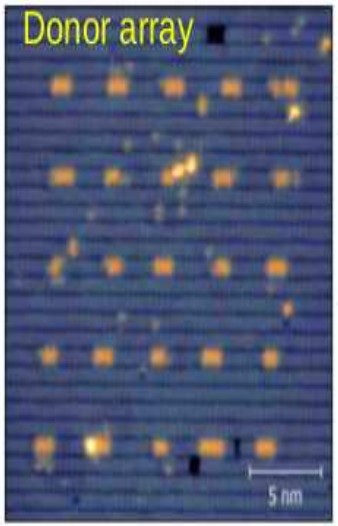
$\Rightarrow$ Basic ingredients for a tunable Fermi-Hubbard system.

Temperatures (much) lower than optical lattice systems!

J. Randall, J. Owen, W. Kirk, R. Moheimani, R. Silver, J. Lyding, I. Kuljianishvili, D. Natelson, S. Misra

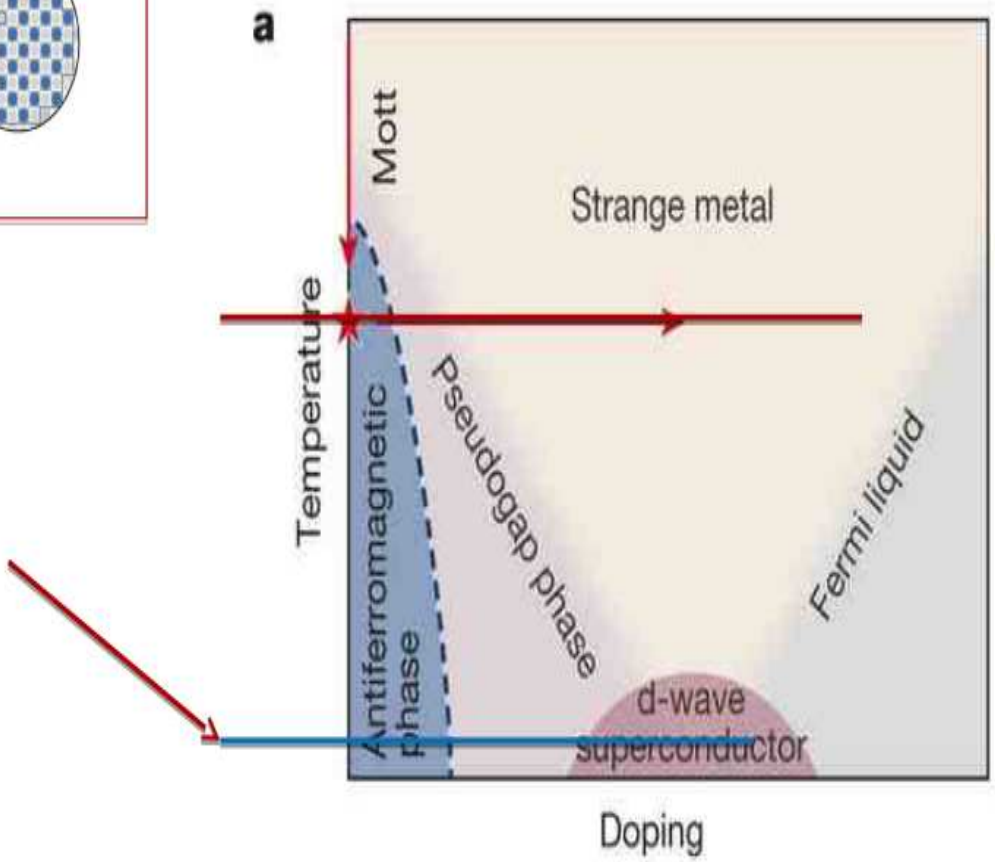


Fermi-Hubbard in Li
U/t ~ 7 (strongly interacting)
T/t~ 0.25 (moderate temperature)



Donors

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



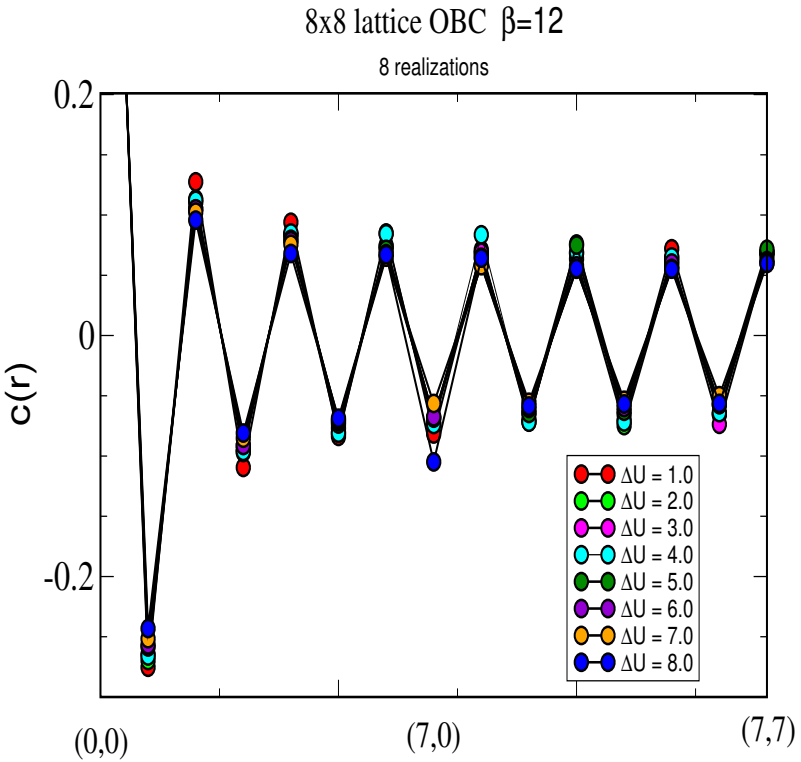
Despite 'precision,' the disorder can be pronounced.

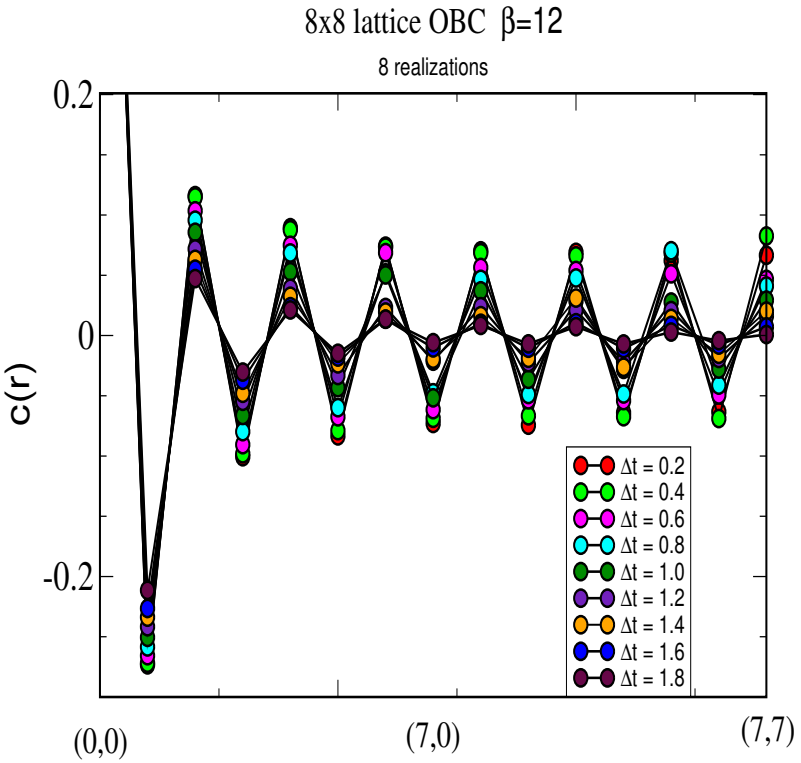
(Unclear, as yet, what other obstacles will arise.)

Quantum Monte Carlo tests of effect of disorder on AF.

Left: Disorder in interaction strength U

Right: Disorder in hopping t





6. Some Conclusions

- Hubbard Model: a way to understand many-body effects in solids
  Mott insulators, magnetic order, exotic superconductivity $\cdots$
- **But:** Sign Problem is show-stopper for low T QMC in most situations.
  "The Hubbard model cannot be solved"
- This has opened up the field of quantum emulators:
  Ultracold atoms; Engineered Silicon
- It is possible to exploit the sign problem to investigate quantum criticality.