Correlated quantum systems out of equilibrium

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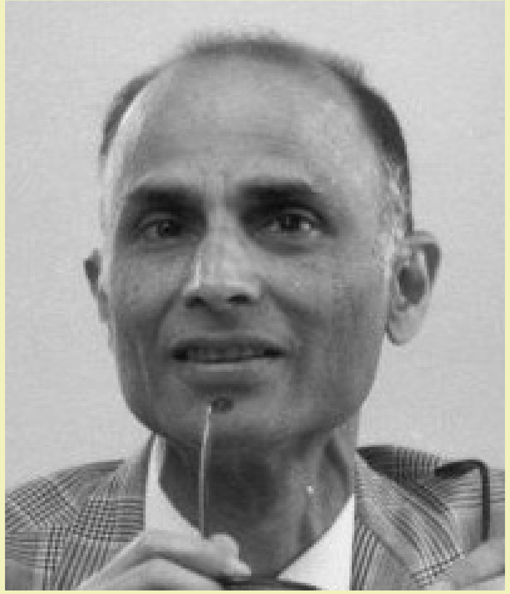
Abdus Salam

HRI



Harish-Chandra

Abdus Salam and Harish-Chandra: similarities and contrasts

- *Salam and Harish-Chandra were born within three years of each other (1926 and 1923) in undivided India.*
- *They were both extremely gifted students. Salam published research in mathematics while a student. HC was recognised by Krishnan and Raman.*
- *Both went to Cambridge for Ph.D in theoretical physics in the late 1940s. HC with Dirac and AS with Kemmer. Then the paths diverged.*
- *HC moved to the US, Columbia then Princeton, and spent his working life there. His work on Representation Theory has been enormously influential but his direct impact on Indian mathematics has been limited.*
- *Salam's work on the Standard Model is one of the pillars of modern physics. He maintained a lifelong connection with Pakistan, encouraging students and developing institutions. He also played a global role in fostering third world science.*

The scientist as lone scholar -vs- the scientist as world citizen.

Our synopsis:

- *At the microscopic level matter follows the laws of quantum mechanics.*
- *The elementary constituents, electrons, also interact among themselves.*
- *This leads to a “quantum many body” or “correlated electron” problem.*
- *Exploring such materials and models has been on the agenda since 1950’s.*
- *The focus was on “equilibrium” - the system settled into a thermal state.*
- *That itself allows a wide variety of phases, transitions, and functionality ..*

What if you push matter out of equilibrium - by pumping extra energy?

- *Intuition - will disrupt or destroy order.. Reality - new order can emerge!*
  - *an insulator can become a superconductor*
  - *an antiferromagnet becomes a ferromagnet ..*
- *For a theorist, the trusted Boltzmann principle no longer works!*

This talk: an overview of the phenomena, and attempts to understand them.

Outline

- *Correlated quantum systems*
- *Nonequilibrium situations*
- *The equilibrium Mott insulator*
- *The ‘driven’ Mott insulator*
- *Lessons?*

Correlated quantum systems

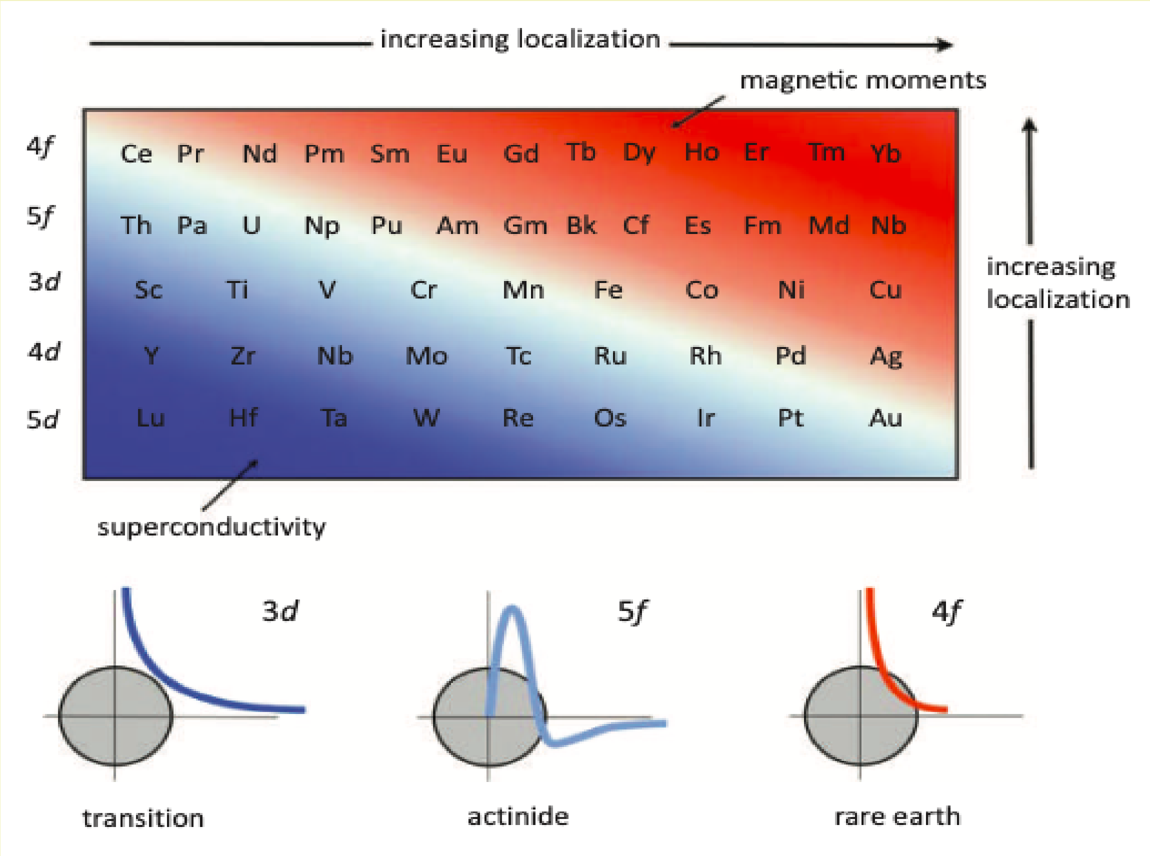
Correlated systems ?!

- *Free electrons have only kinetic energy. A system dominated by kinetic energy is ‘essentially free’ with small corrections to free Fermi behaviour.*
- *There are interacting systems where the energy associated with interactions is comparable to or greater than the kinetic energy.*
- *These ‘correlated’ systems are different, in terms of, typically,*
  - *absence of quasiparticles (quasi free..),*
  - *multiple, competing, ordered phases,*
  - *huge response to perturbations.*

When does this happen? Electron bandwidth $\ll$ local interaction.

In which materials? Next ..

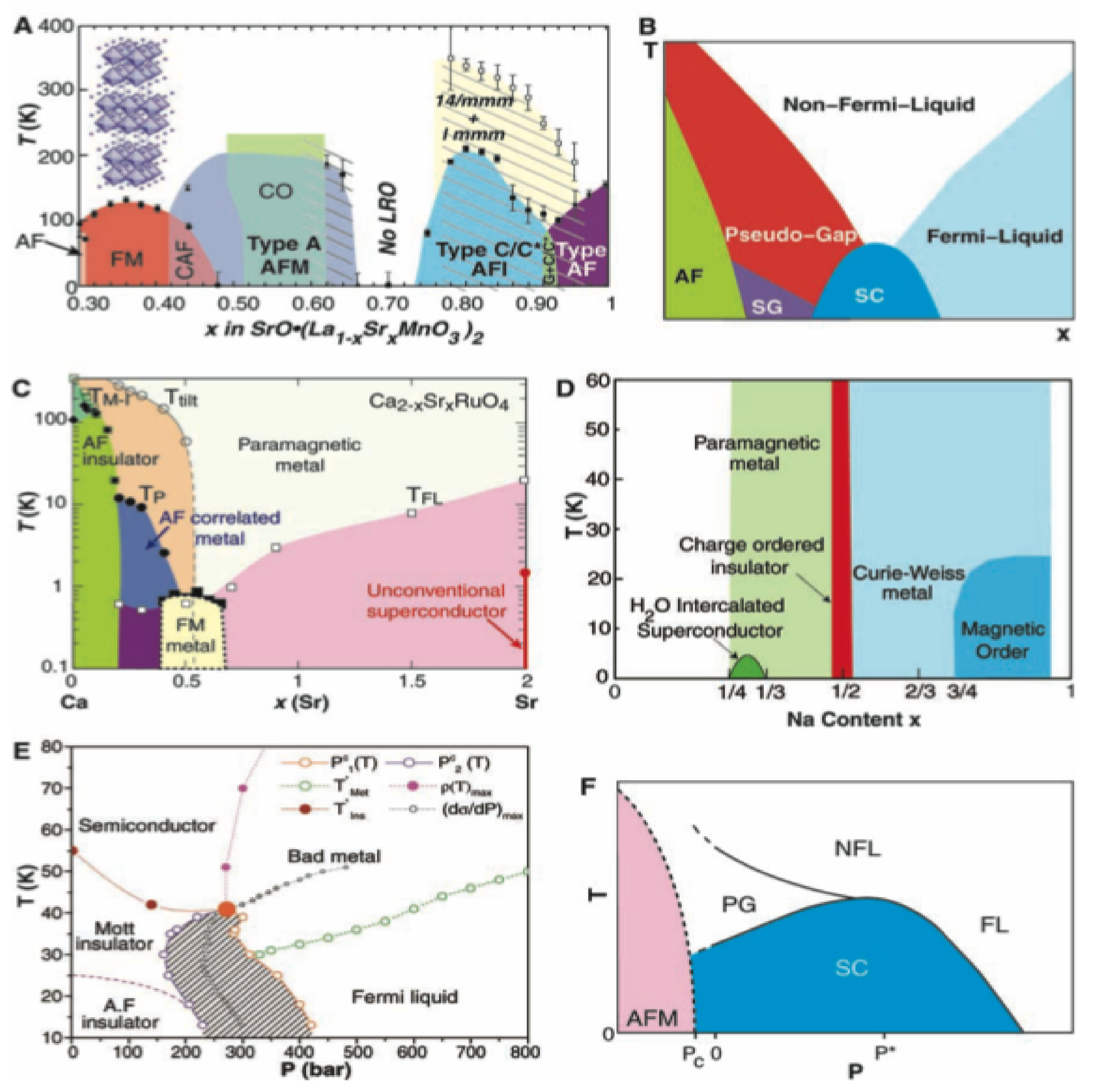
Atomic origin of correlation



The Kmetko-Smith diagram from P. Coleman, "Introduction to many body physics", pp 583.

What happens at strong correlation?

E. Dagotto, Science (2005)



What do we take away?

- *Most of these materials have a “Mott insulating” parent state..*
- *Multiple ordered phases - magnets, superconductors, cdw.. in proximity*
- *‘Bad metals’: unusually high resistivity, sometimes ‘non Fermi liquids’..*
- *Perturbations can sometimes lead to huge response (in resistivity, say..)*

- *And all of these are very different from a ‘benign’ metal, e.g, Cu ..*

Two directions from here:

(i) How do you understand these correlated materials? long story ..

(ii) Our theme: what happens when you push them out of equilibrium..?

We look at experiments on (ii) first, then theories for (i) and (ii) ..

Nonequilibrium situations

Nonequilibrium? not in equilibrium!

Equilibrium: the system is described by a Boltzmann distribution (?!)

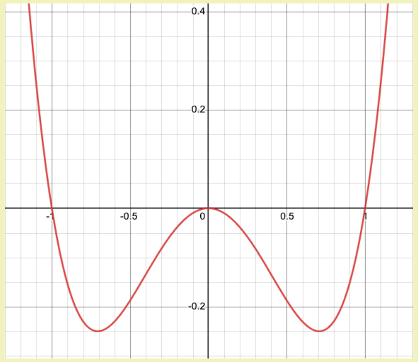
- *The foundational laws of physics are dynamical.*
- *Given an initial condition* $\phi(0)$ *it in principle provides* $\phi(t)$.
- *Poses enormous difficulty:*
  - *typically we have no clue about 'initial conditions'*
  - *even if we knew them, the dynamics problem is too hard*
  - *nonlinear (in classical mechanics), too many variables (QM)..*
- *Any simplification at 'long times'?*

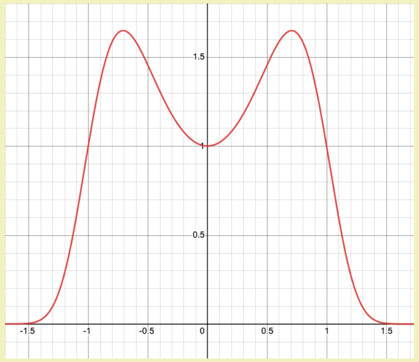
Boltzmann: at temperature T *the probability of being in a state* ϕ *is:*

$$P[\phi] \propto e^{-E[\phi]/k_B T}$$

Simplification afforded by equilibrium: trivial example

Classical particle: double well potential, dissipation, thermal bath.





Start with the particle at some place x_0, then let go: follows Langevin eqn.

$$m\frac{d^2x}{dt^2} = -\frac{dV}{dx} - m\gamma\frac{dx}{dt} + \eta(t)$$

Calc $x(t, x_0, \eta)$, then the probability $P(x, x_0, t)$: no analytic soln possible.

However, at long times, when equilibrium attained: $P_{eq}(x, t) \sim e^{-V(x)/k_B T}$

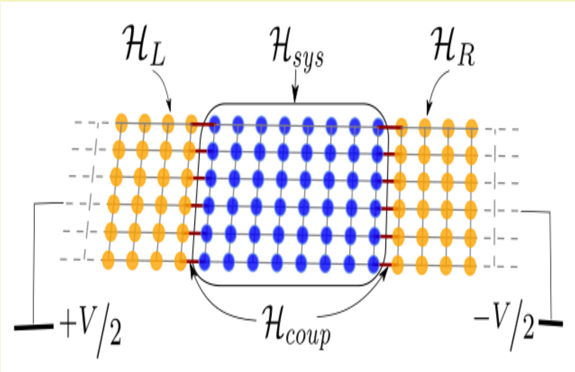
This was just one classical particle.

For many interacting quantum particles, the equil-noneq diff is much worse..

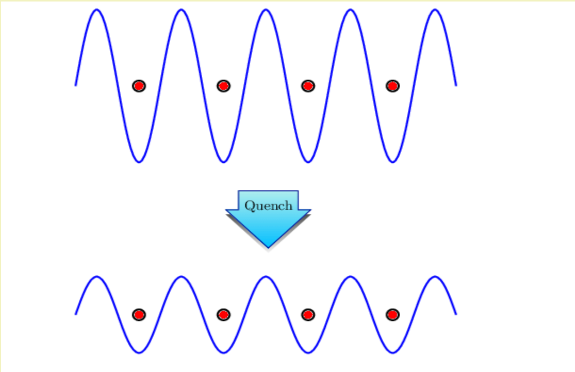
There are various ways in which one can drive matter out of equilibrium..

Possibilities:

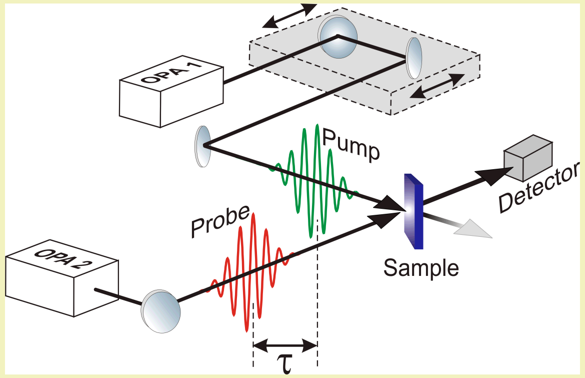
- *Put a large voltage or T bias across the system.. ‘currents’ flow..*
- *Use strong radiation at a high frequency .. ‘Floquet’ phenomena ..*
- *Change parameters abruptly - well depth in cold atom systems ..*
- *‘Pump’ using a short laser pulse, ‘probe’ the transient dynamics ..*



DC bias

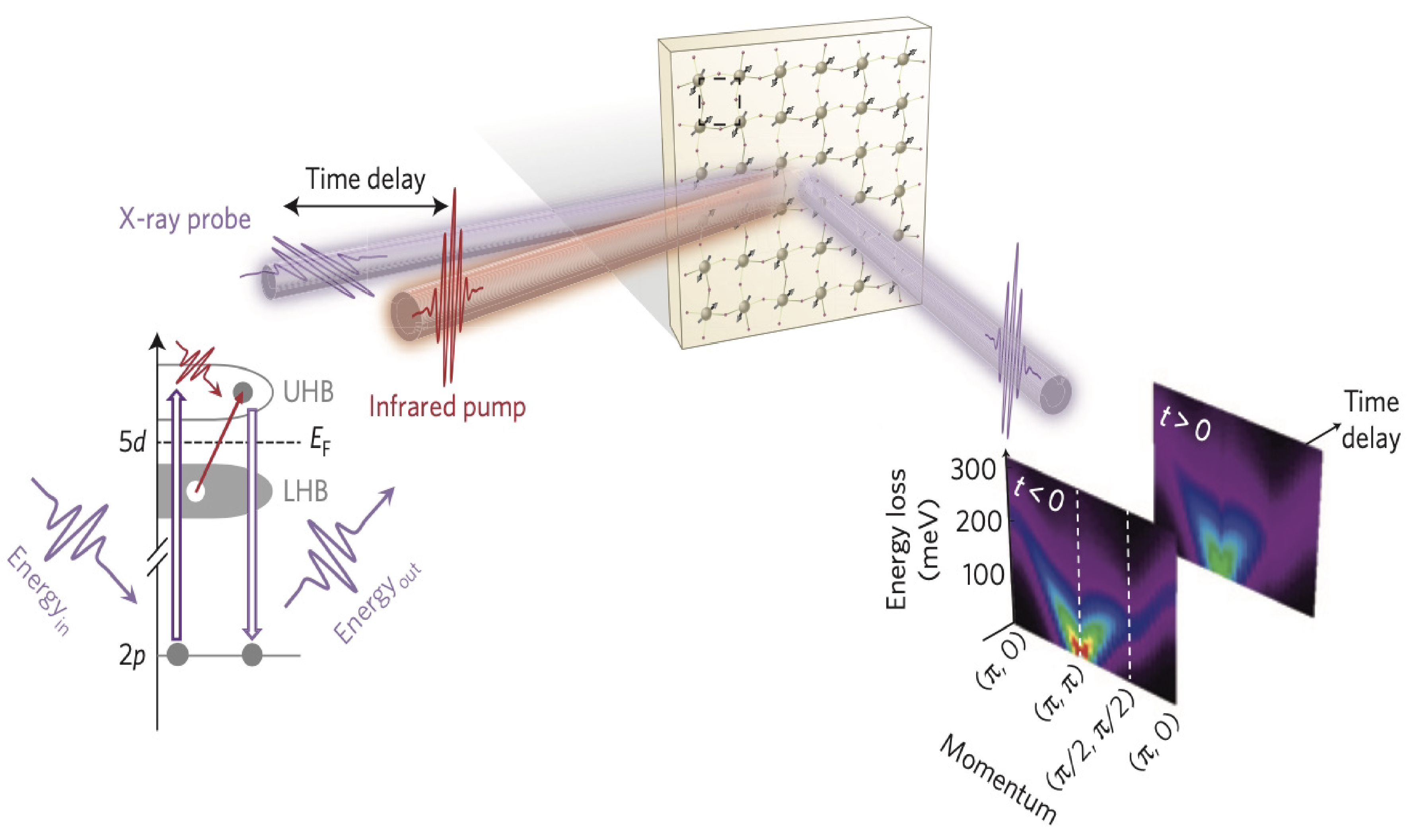


Parameter quench



Pump-probe

We focus on pump-probe experiments



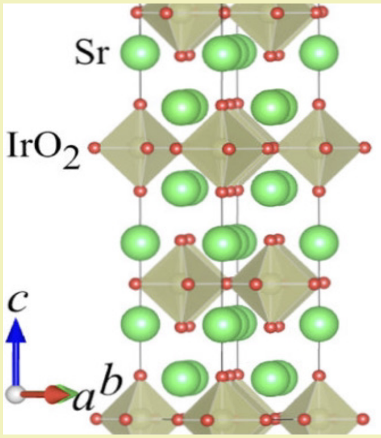
Schematic from Dean et al., Nat Materials (2016).

What happens when you hit an ‘ordered state’ with a laser pulse?

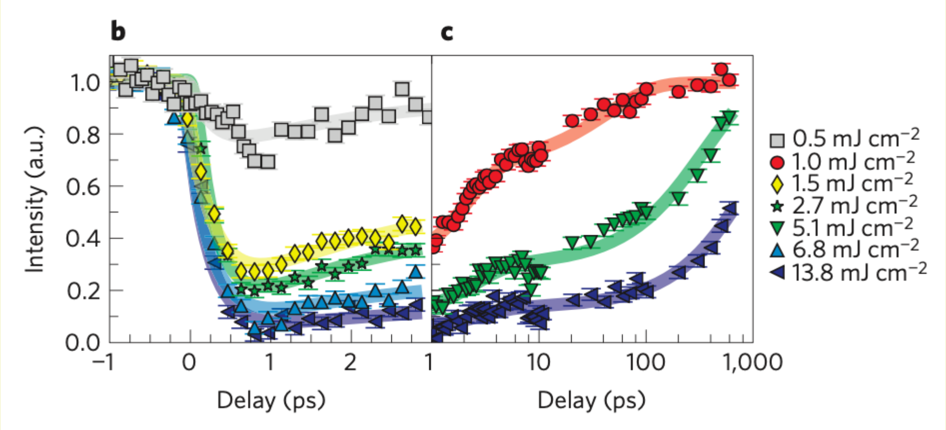
- *At short time: it will disrupt the order, maybe even destroy it.*
- *At long times?*
  - *if the system is coupled to a thermal bath:*
    - *extra energy dissipates, old order recovers*
  - *if the system is thermally ‘isolated’:*
    - *a suppressed version of the old order can appear*
    - *the system could be disordered at long times..*
    - *the system may exhibit altogether different order!*

We look at two experiments probing these phenomena.

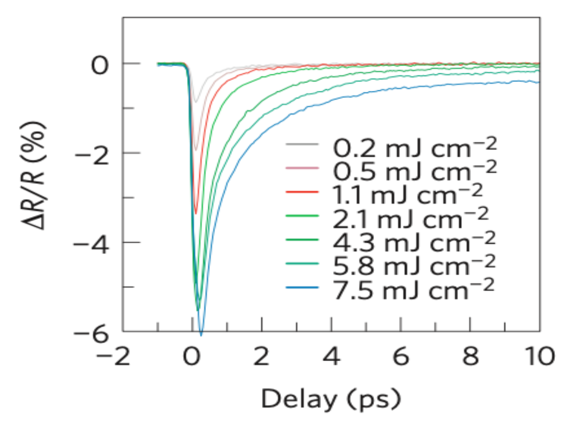
(A) Laser pumping an antiferro Mott insulator, Sr_2IrO_4 (Nat Matl. 2016)



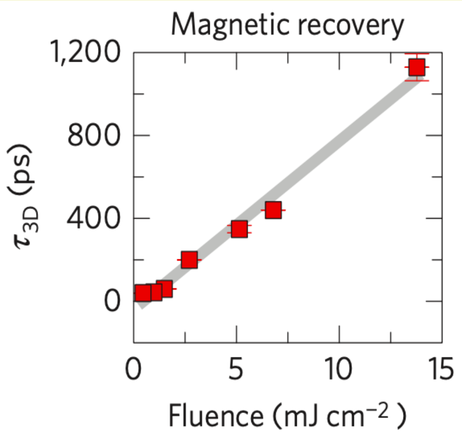
structure



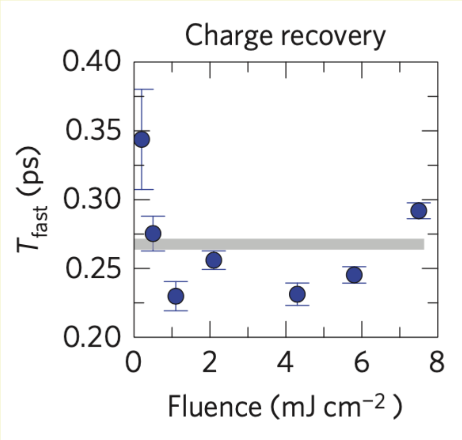
loss and recovery of magnetic order



electronic response



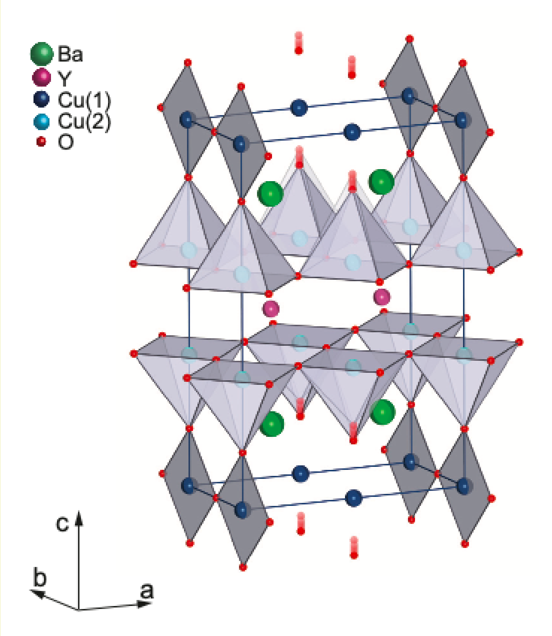
magnetic recovery, τ_m



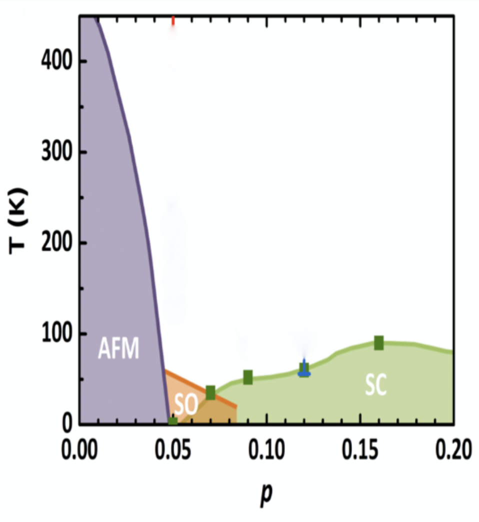
electron timescale, τ_{el}

(B) Pump induced high T_c superconductivity: $YBa_2Cu_3O_{6+\delta}$ (PRB 2014)

YBCO is one of the earliest discovered "high T_c" cuprate superconductors. It has a complex structure, and maximum $T_c \sim 100K$ at hole doping ~ 0.16.



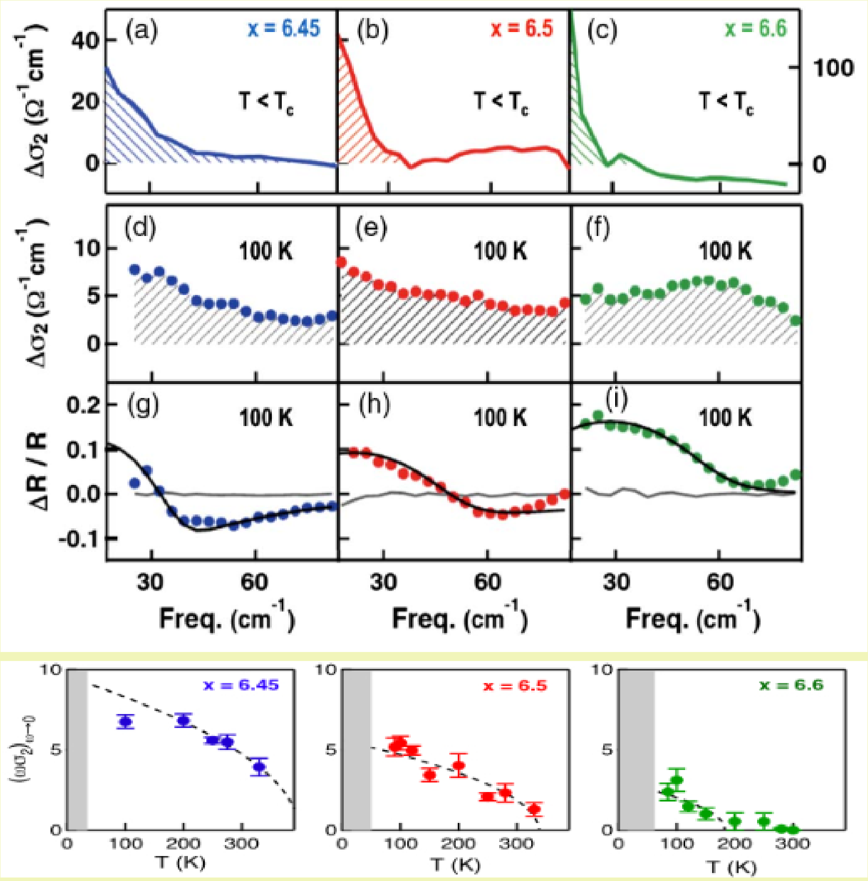
Structure



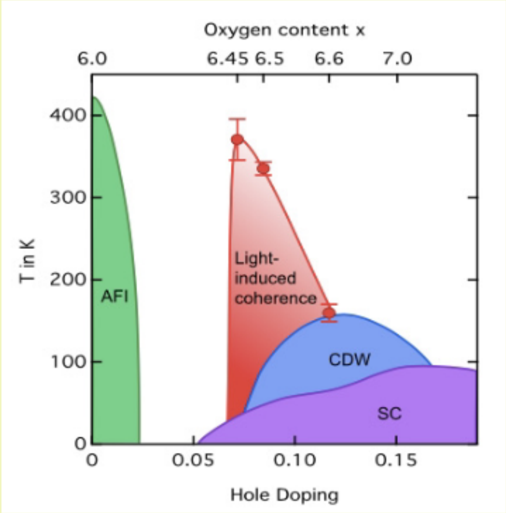
Phase diagram

Above the SC dome one probably has "preformed pairs" but no coherence. What does optical excitation do to such a system?

Kaiser et al., Phys. Rev. B (2014)



laser induced pairing enhancement



transient 'phase diagram'

The laser excites a c-axis mode, which enhances in plane superconductivity..

The effect is transient, the 'light induced coherence' lasts for a few pico sec..

General lessons from these experiments:

Order parameter control by choice of ampl or frequency of the laser.

Suppression, or strongly delayed recovery in some cases (iridate Mott)..

Emergence of transient ordered phase well above equilibrium T_c (YBCO)..

The new ordered phases have short lifetimes $\sim$ few ps

In general allows control of electronic couplings, populations,

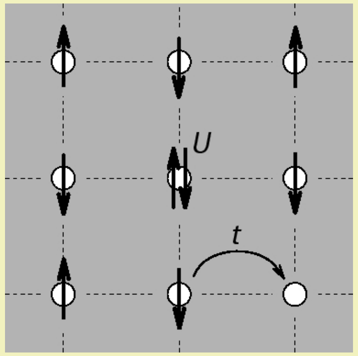
Let us address the Mott example.

First equilibrium, then pump..

The equilibrium Mott state

The simplest description is in terms of the Hubbard model

$$H = -t \sum_{\langle ij \rangle, \sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$



- *Model parameters:* U/t *and electron density:* $n = N_{el}/N_{site}$.

Remaining at $n = 1$, *half up, half down..*

$U \ll t$? *..extended states, wavelike behaviour, Fermi sea*

$U \gg t$? *..localised electrons, 'particle like', Mott state*

Intuitively obvious, hard to formulate a full quantum theory..

Build a picture:

- *The role of U? suppress double occupancy.. penalise $|\uparrow\downarrow\rangle$..*
- *At half-filling this promotes the $|\uparrow\rangle$ & $|\downarrow\rangle$ states, 'local moments'..*
- *Effectively $\equiv$ 'test particle' + self-generated magnetic background*

Formalise: introduce an auxiliary variable $\vec{m}_i$ .. 'Hubbard-Stratonovich'..

Effective Hamiltonian at half filling: electrons coupled to a vector field $\vec{m}_i$.

$$H_{el} = \sum_{ij,\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} - \frac{U}{2} \sum_i \vec{m}_i.\vec{\sigma}_i$$

What decides the $\{\vec{m}_i\}$ background?

$$\begin{aligned} H_m &= F_{el}\{\vec{m}\} + \frac{U}{4} \sum_i m_i^2 \\ &\approx \sum_{ij} J^{(2)}_{ij} \vec{m}_i.\vec{m}_j + \sum_{ijkl} J^{(4)}_{ijkl} (\vec{m}_i.\vec{m}_j)(\vec{m}_k.\vec{m}_l) + ... \frac{U}{4} \sum_i m_i^2 \end{aligned}$$

Structure:

- non interacting electrons in a magnetic background..

- the backgrounds are determined by the electron free energy..

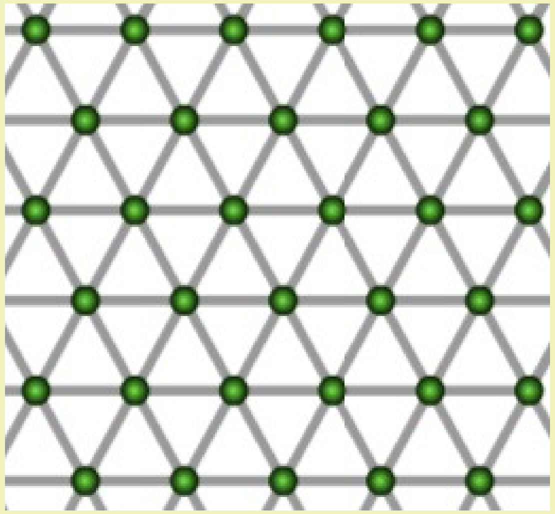
- self-consistency ..

How do you solve this?

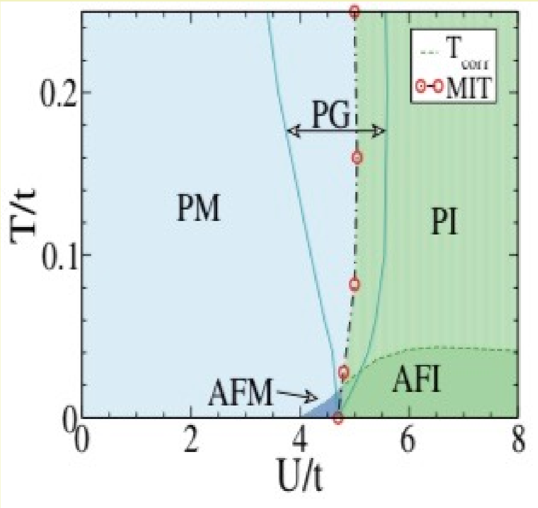
- *Monte Carlo:*
  - *Sample* $\{\vec{m}\}$ *configs with weight* $\propto e^{-\beta H_m}$
  - *Involves diagonalisation of the electron* H *for every move ..*
  - *Calculate electronic properties after attaining equilibrium ..*

- *Langevin dynamics:*
  - *Write an eqn of motion for* $\vec{m}_i$ *with torque derived from* $\frac{\partial H_m}{\partial m_i}$
  - *Add thermal noise and damping satisfying flucn-dissipation*
  - *Can access both 'static' and dynamical correlations ..*

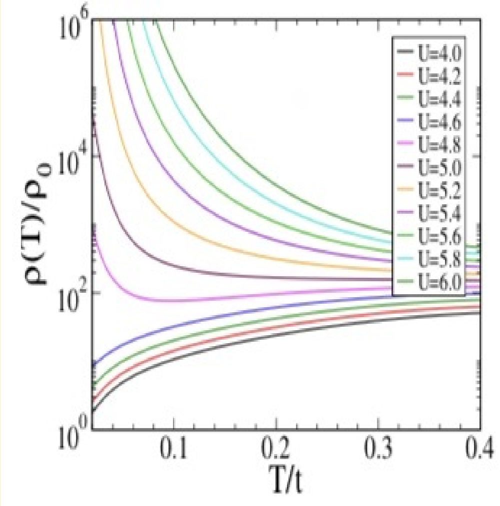
Does it work? the triangular lattice Mott transition..



lattice



phase diagram



resistivity

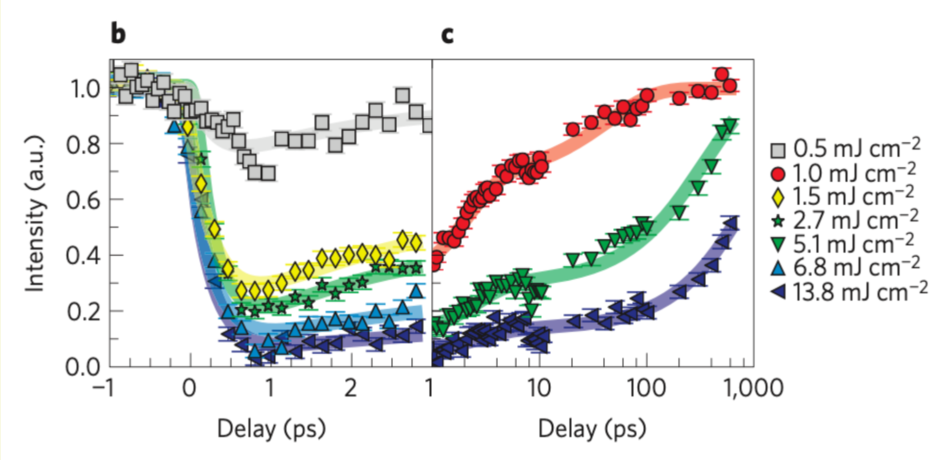
Intuitively correct, matches reasonably with QMC..

How do you generalise to nonequilibrium situations?

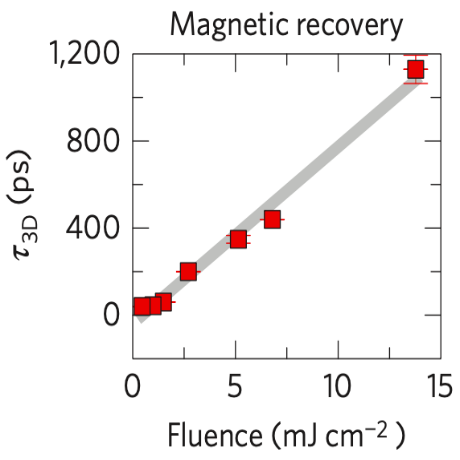
Back to the pump-probe Mott problem..

The ‘driven’ Mott insulator

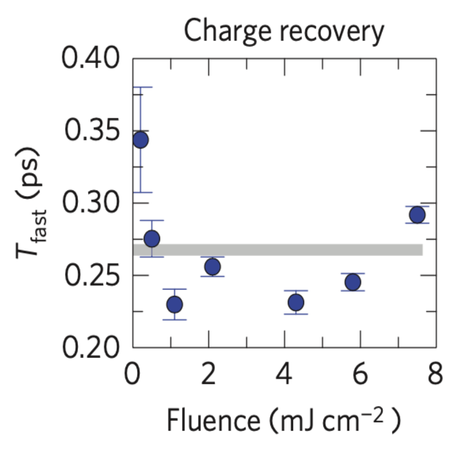
At the risk of repetition .. the iridate expt again.



loss and recovery of magnetic order



magnetic recovery, τ_m



electron timescale, τ_{el}

Mystery?

- *What are the qualitative effects at play in this system?*
- *Why is the order parameter recovery time* $\tau_m \ggg \tau_{el}$*?*

- *Set up a model:*
  - *The iridate is a 'spin-orbit coupled' sq lattice Mott insulator.*
  - *Can be modeled via an effective Hubbard model with* $U \sim 3t$.
  - *Peierls couple an external laser field to the electrons ..*

$$H = \sum t_{ij} (e^{i \int \vec{A}(t).\vec{dl}} c^{\dagger}_{i\sigma} c_{j\sigma} + h.c) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

- *How to solve this?!*
  - *Write the Heisenberg equation for* $\rho^{\alpha\beta}_{ij}(t) = \langle c^{\dagger}_{i\alpha}(t) c_{j\beta}(t) \rangle$..
  - *'Close' by factorising the interaction term in terms of* ρ.
  - *Energy conserving evolution after passage of the pulse.*

What do we see? Let us move slowly ..

- *First, the nature of the correlated reference state:*
  - *repulsion U betn electrons prevents 'up+down' occ of sites.*
  - *singly occupied sites behave as immobile magnetic moments.*
  - *the state is insulating, and the moments show antiferro order.*
  - *magnetic order can be suppressed by*
    - *destroying spatial correlations betn moments, or*
    - *suppressing moments by creating ↑↓ occupancy.*

- *Next, expected effect of a laser pulse:*
  - *a weak pulse would excite the 'normal modes' of the antiferromagnet.*
  - *a strong pulse can create large double occ, killing the moments ..*
  - *at intermed pulse strength ones see mom reduction + angular disorder*

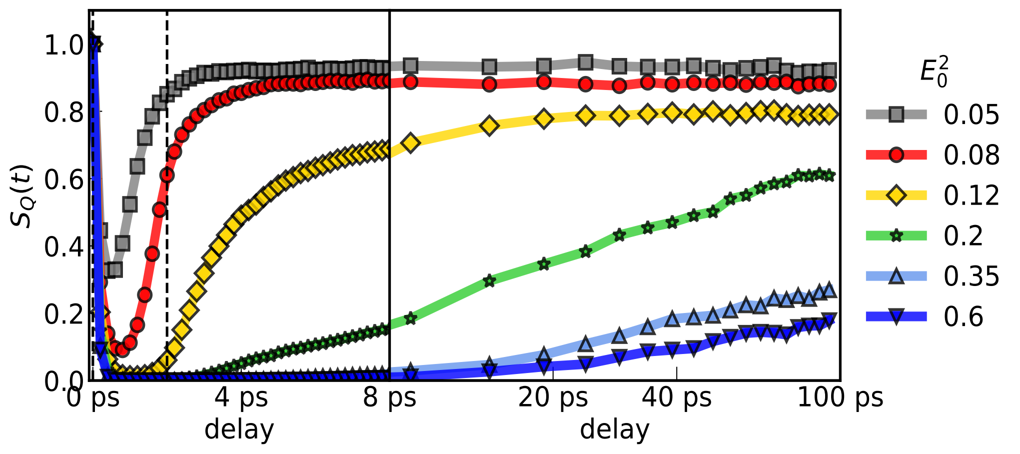
- *Computational complexity:*

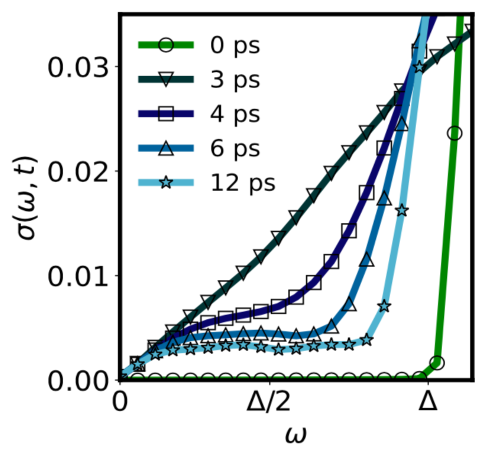
  - *equilibrium mean field theory requires just one number* m*: ord param.*
  - *steady state in biased Mott insulator requires a field* $\vec{m}_i$*, i.e, O(N)..*
  - *resp to laser pulse requires* $\rho_{ij}^{\alpha\beta}(t)$*, i.e,* $O(N^2)$ *time dependent fns.*

Despite the 'mean field' like closure this is a vastly more complex scheme.

What do we see?

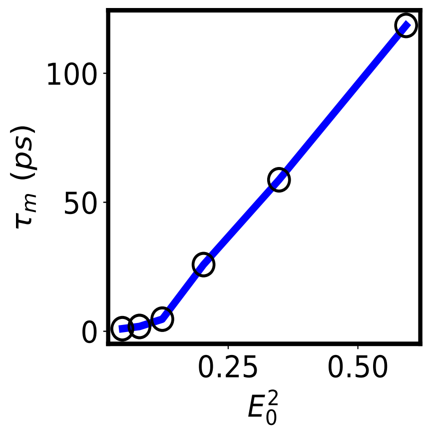
- *Dynamics:*

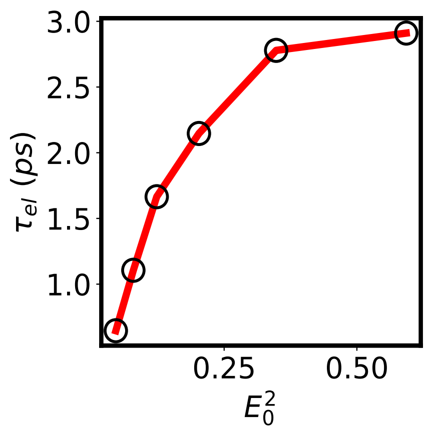




Order parameter dynamics *Time dependence of optics*

- *Timescales:*

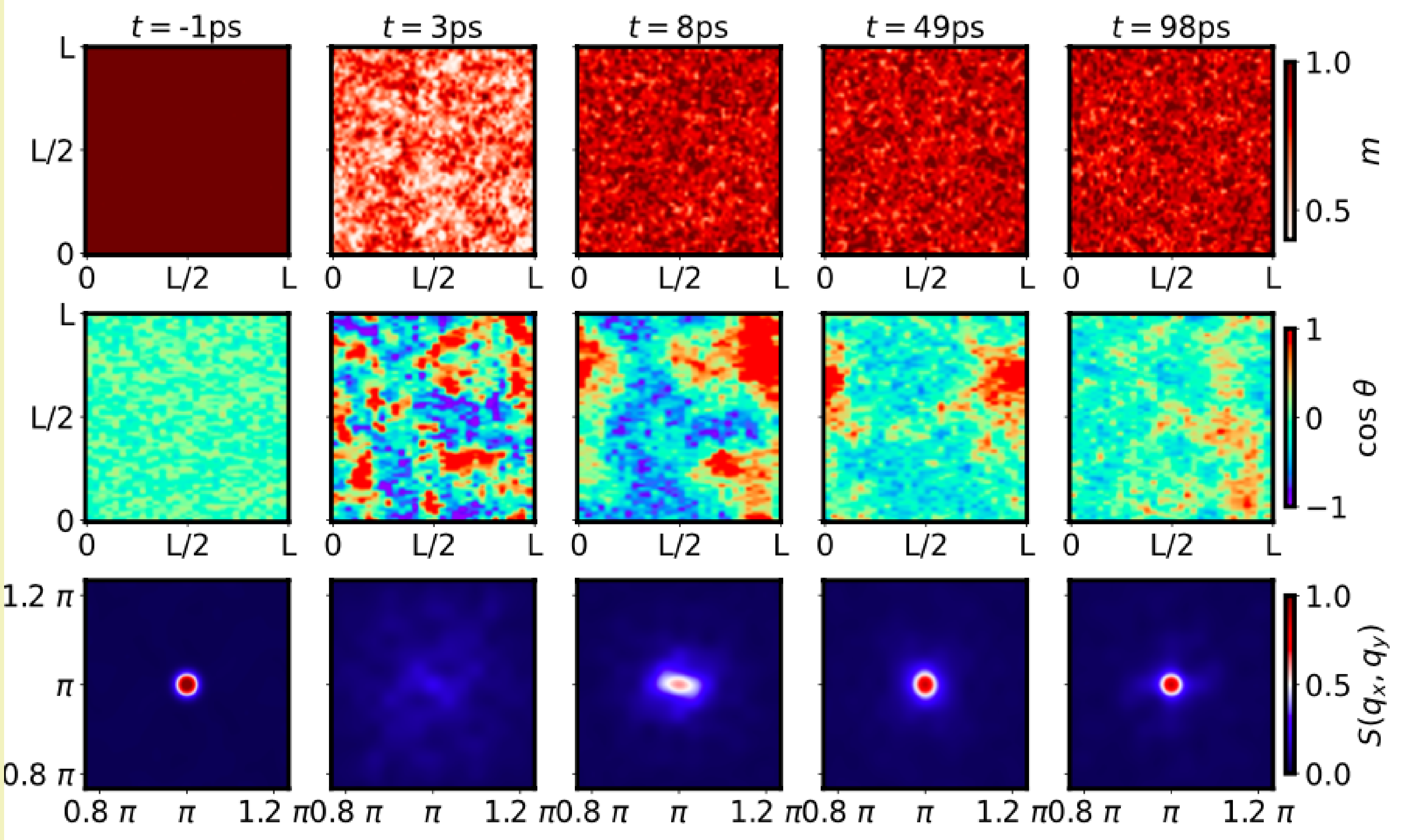




Magnetic recovery *Electronic recovery*

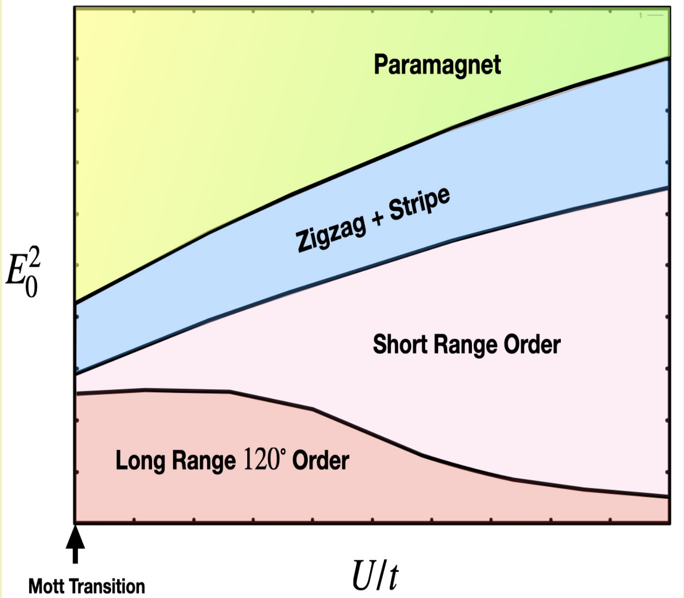
- *Why the differing timescales?*
  - *- electron motion occurs on the 'hopping' timescale:* $\tau_{el} \sim 1/t_{hop}$.
  - *- this can lead to doubly occupied configs, 'killing' a magnetic moment ..*
  - *- conversely, the recovery of the moment* m_i *involves the same timescale..*
  - *- global magnetic order, however, requires large scale reorganisation..*
  - *- this timescale increases with system size..*
- *Visualised (next slide), and known in phase ordering kinetics.*
- *Overall:*
  - *- electronic properties are dictated mainly by double occ,* m_i
  - *- magnetic order dictated by spatial correlations over large dist..*

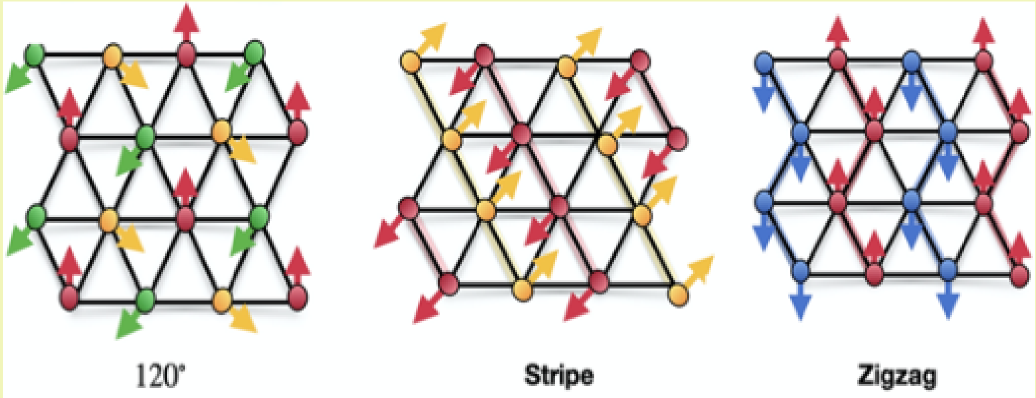
Spatial maps:



Can a completely different kind of order emerge?

Same process on a triangular lattice: more exciting..





Nonequilibrium 'phase diagram'

reference state

emergent order

On the triangular lattice the Mott antiferromagnet has 120° order.

However, there are also competing phases close by in energy (see fig).

Laser excitation creates non-eq electron population, changing exchanges.

As long as the non-eq population sustains, the new order is visible.

Lessons

Where does this lead us?

- *Many body quantum systems have multiple competing phases..*
- *Extra energy is not just a 'disordering agent' unlike temperature. It can:*
  - *create nonequilibrium populations*
  - *modify effective couplings*
  - *stabilise order not possible at equil..*
- *These phases are metastable, make longer lived through pump protocol.*
- *Allows a completely new approach to 'engineering' new phases.*
- *It also pushes the challenge for theorists to the next level.*

There is much to explore!

Thanks