

Quantum Simulation *Theory*



**Find an interesting “Quantum effect”
poorly known (non-perturbative
regimes)**

topology, frustration, lattice gauge theories



**Derive/Guess the easiest model
(Hamiltonian) where this quantum
effect (you hope) will occur**

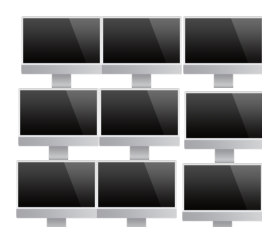
kinetic energy + interactions (Hubbard-like,
Heisenberg-like) i.e.

$$H = -J \sum_i (b_i^\dagger b_{i+1} + h.c.) + U \sum_i n_i(n_i - 1)$$



**Design a quantum simulator where
your results can be tested**

ultracold atoms/ions in optical lattice/tweezer



**Perform numerical analysis
of the model**

*Matrix-product-state (quasi exact
ground state in 1D and 2D)*



**Ask experimentalists to realize the
model you designed (and hope your
ideas are not wrong)**

*choose the atoms (alkaline, earth alkaline,
lanthanide) + detection schemes*

Choose the type of atom and its statistics

PERIODIC TABLE OF ELEMENTS

Chemical Group Block

[illegible]

Alkali (Li, Cs, K, Na, Rb) short-range interaction

$$U_{int}(r, r') \propto a_s \delta(r - r')$$

Alkali earth (Yb, Sr) short-range interaction

$$U_{int}(r, r') \propto a_s \delta(r - r')$$

Lanthanide (Er, Dy) long-range (dipolar) interaction

$$U_{int}(r, r') \propto a_s \delta(r - r') + \frac{1 - 3 \cos^2 \theta}{|r - r'|^3}$$



Atom Cooling

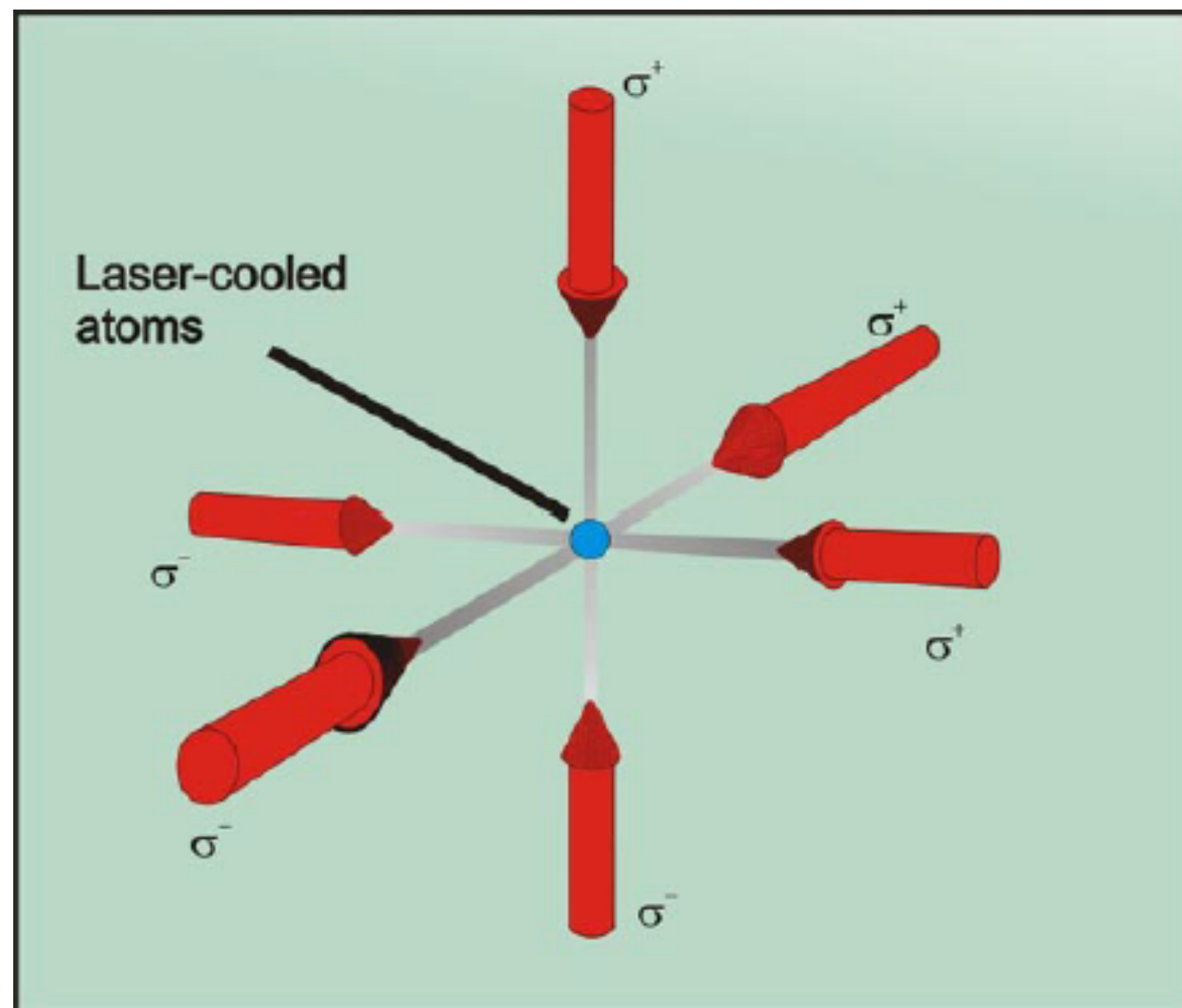
What do we mean by the “cooling” of atoms? Normally, atoms in a gas move with a speed that is related to their temperature. For example, at room temperature, the atoms and molecules in air move at an average speed of about 4000 km/hour. The atoms can be slowed down by lowering their temperature. At normal atmospheric pressure, gases will condense and turn into a liquid and then a solid as they are cooled. If the gas is cooled in a vacuum, it will remain a gas, and the individual properties of the atoms (rather than the properties of atoms in liquids or solids) can be studied. So “cooling” atoms can be interpreted as “slowing them down. How do we do it? we use light....

Properties (in brief) of light

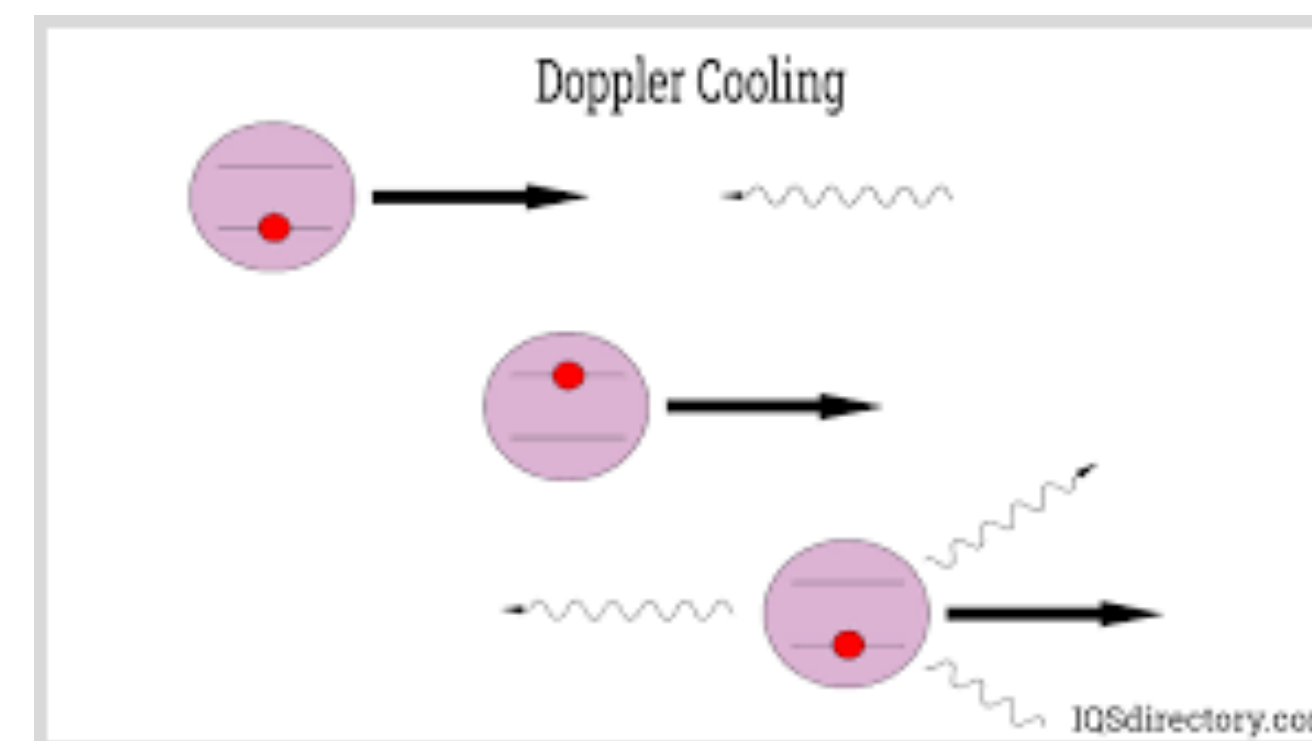
- Light is an oscillating electromagnetic wave. We denote the frequency of oscillation with ν
- Light consists of particles, which we call photons. Each photon corresponds to a quanta of energy. The amount of energy E in each quanta is related to the frequency ν by the formula $E = h\nu$
- Lasers are made of photons with the same frequency ν , i.e. they are coherent light, and momentum $p = E/c$
- Doppler shift: When the direction of propagation of the light is the same as the direction of the relative motion of the source and observer, the shift in frequency is given by: $\Delta\nu = \nu - \nu_0 = \nu \frac{v}{c}$ where ν_0 is the frequency observed when the source is at rest relative to the observer, and ν is the frequency observed when the source is moving towards the observer with velocity v . If the source is moving away from the observer, replace v by $-v$

Laser Cooling (1997 Nobel prize)

6 laser beams consist of three orthogonal pairs; the beams in each pair are pointing straight at each other

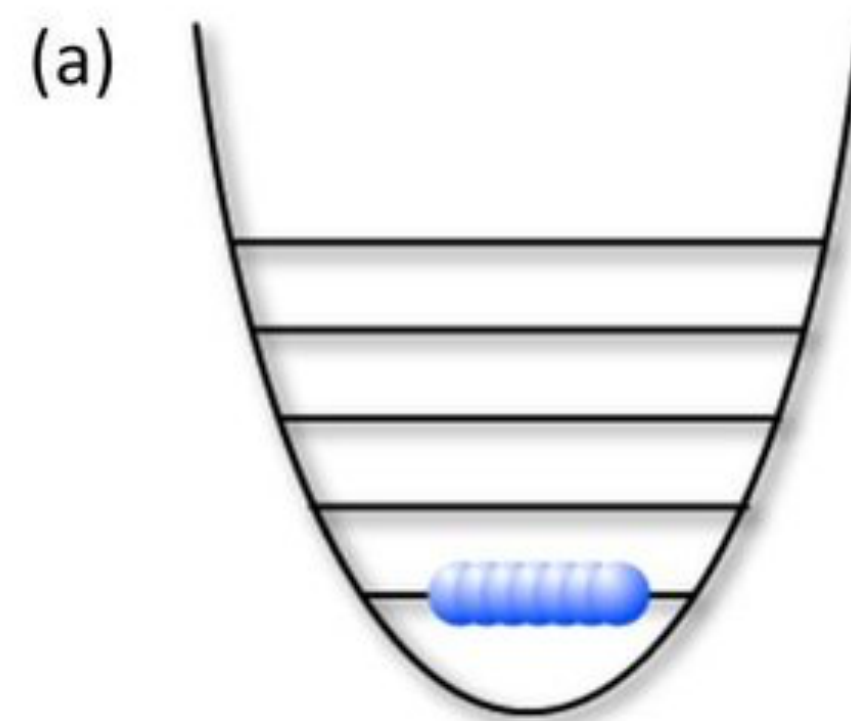
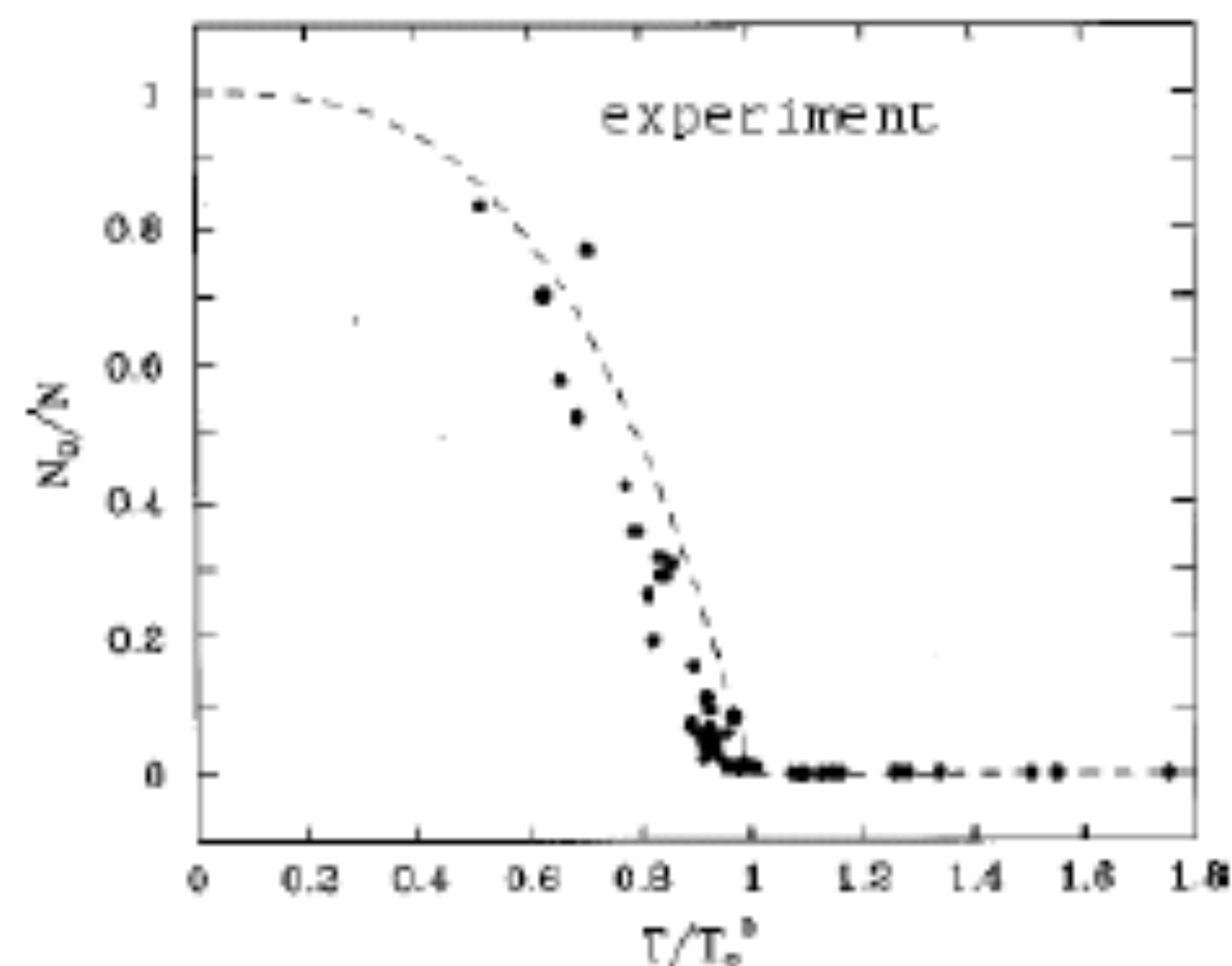
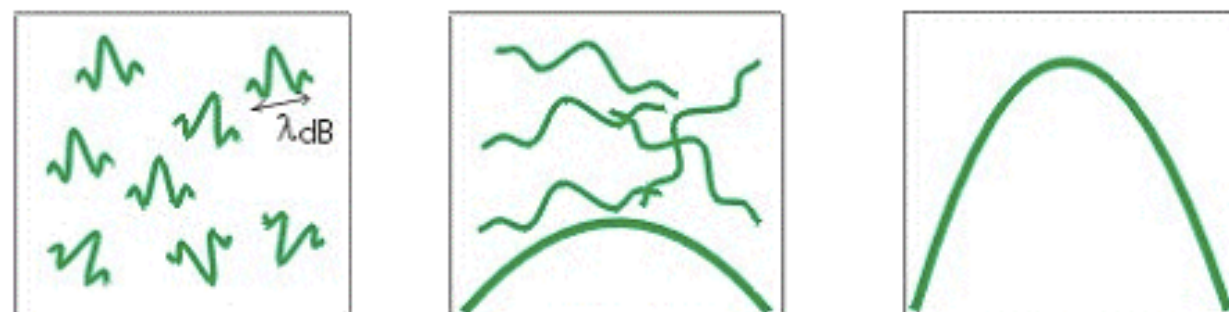


- *First consider just one incident beam. If the energy (or frequency) of the photons in the laser beam corresponds to the difference between the ground state and an excited state of the atom, then the atom can absorb the photon.*
- *Once it has absorbed the photon, the atom is in an excited state.*
- *It will soon drop back into its ground state, emitting a photon of the same energy that it absorbed, but in a random direction*
- *When an atom absorbs an incoming photon of light, giving the atom a “kick” that starts it moving in the direction of the photon. Re-emitting the light also gives the atom a kick, but in a random direction. Over many cycles, these random kicks cancel out and the net effect is a force in the direction of the light*

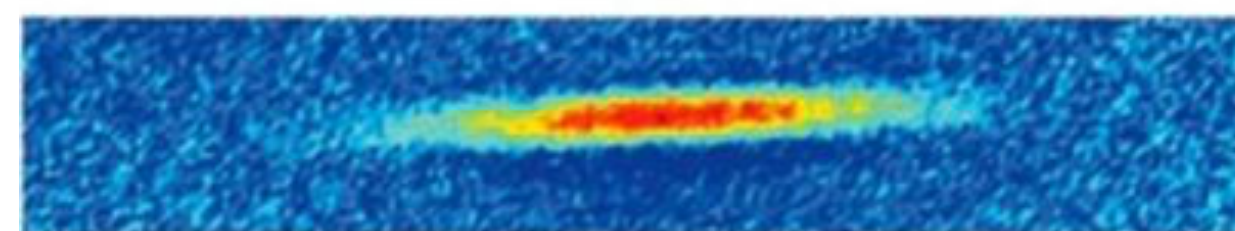


Bose-Einstein Condensate

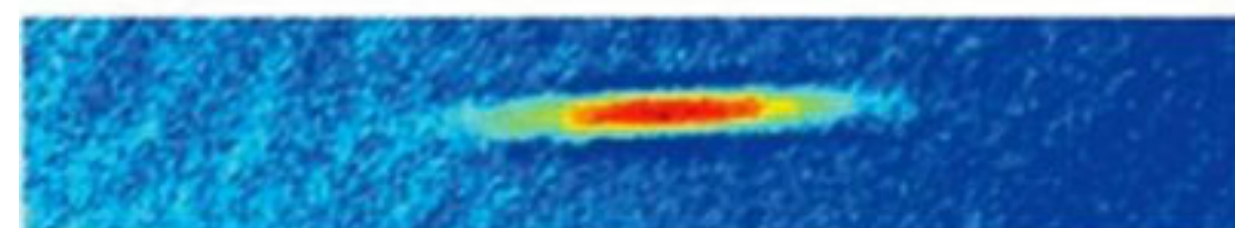
Nobel prize 2001



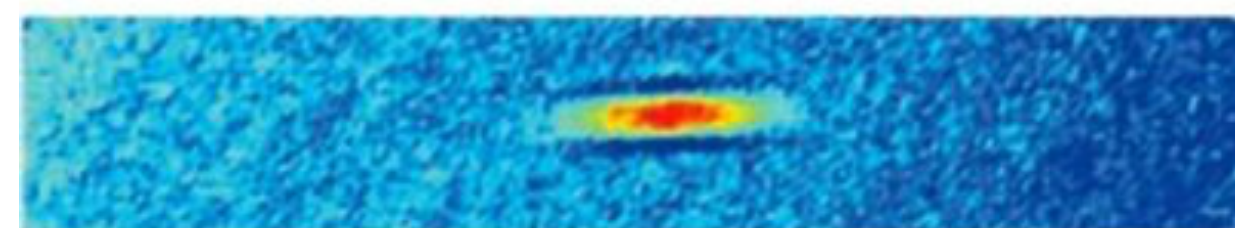
(c) ^7Li



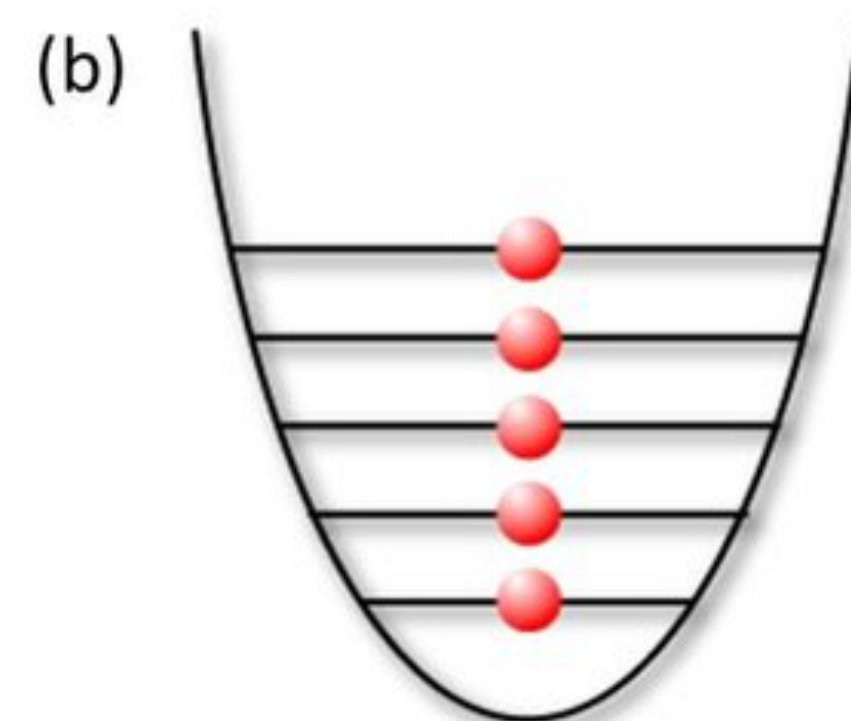
$T = 810 \text{ nK}$



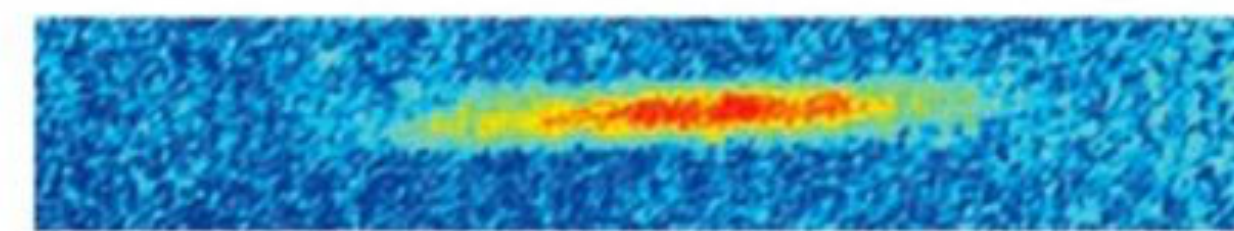
$T = 510 \text{ nK}$



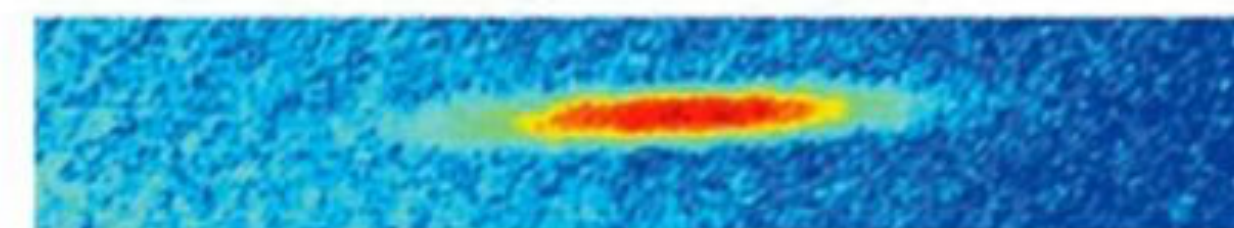
$T = 240 \text{ nK}$



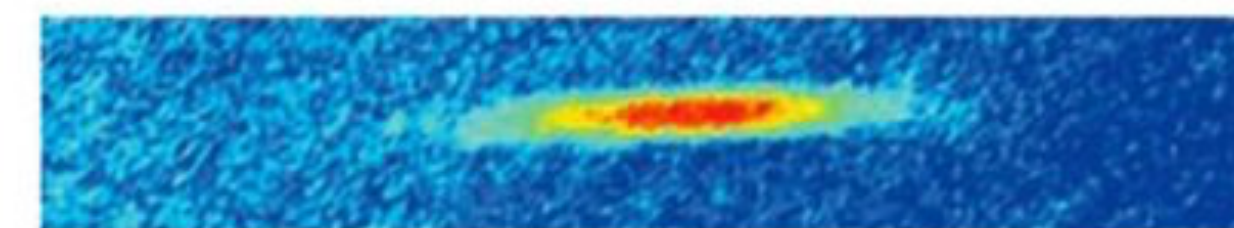
(d) ^6Li



$T/T_F = 1.0$



$T/T_F = 0.56$



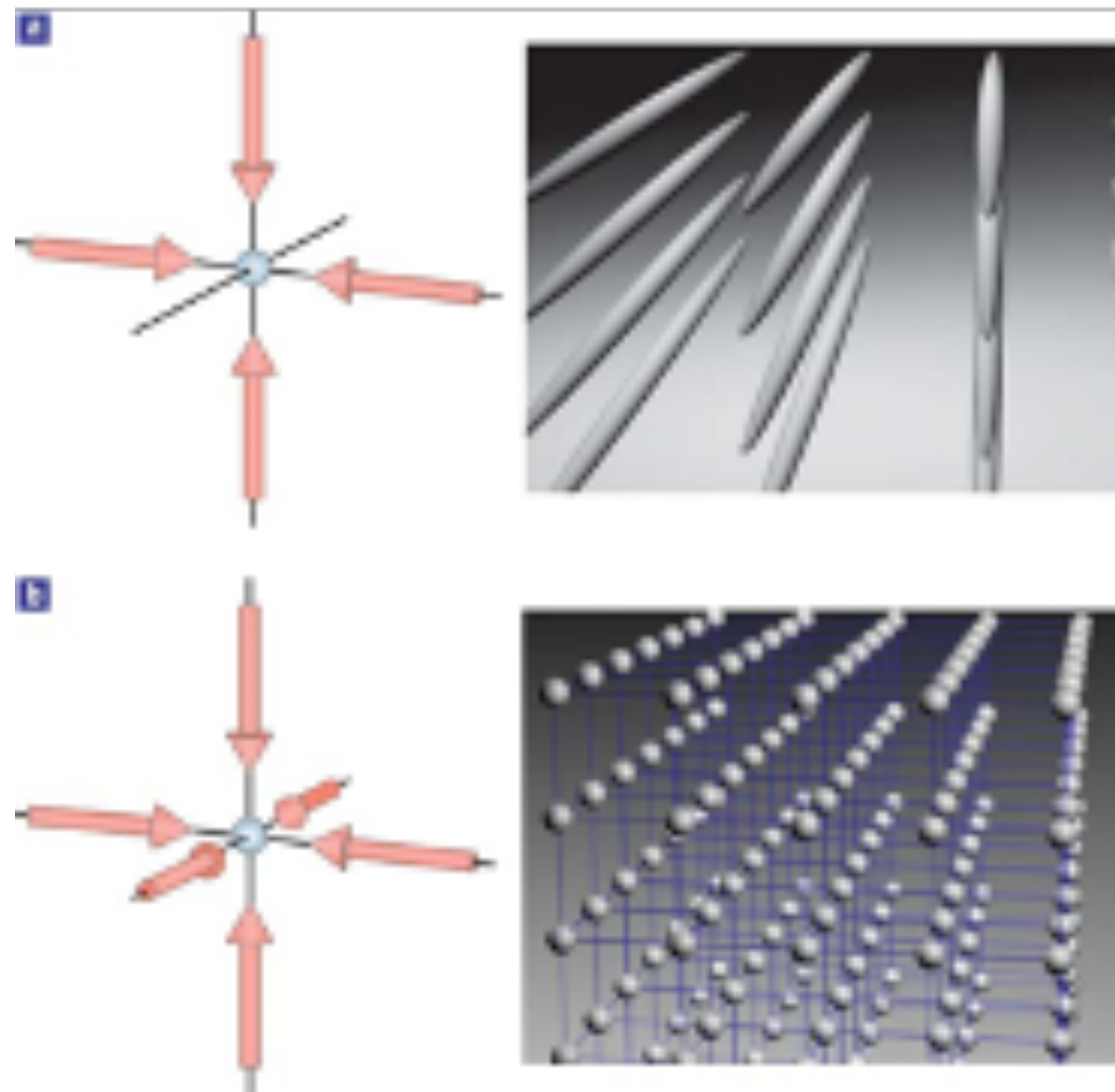
$T/T_F = 0.25$

Optical lattices

Two or more intersecting laser beams can combine and “interfere” to form a standing wave, an array of peaks and valleys of light intensity

$$V(r) = V_{o,r} \cos^2 \vec{k} \vec{r} \quad k_i = \frac{2\pi}{\lambda_i}, \quad i = x, y, z$$

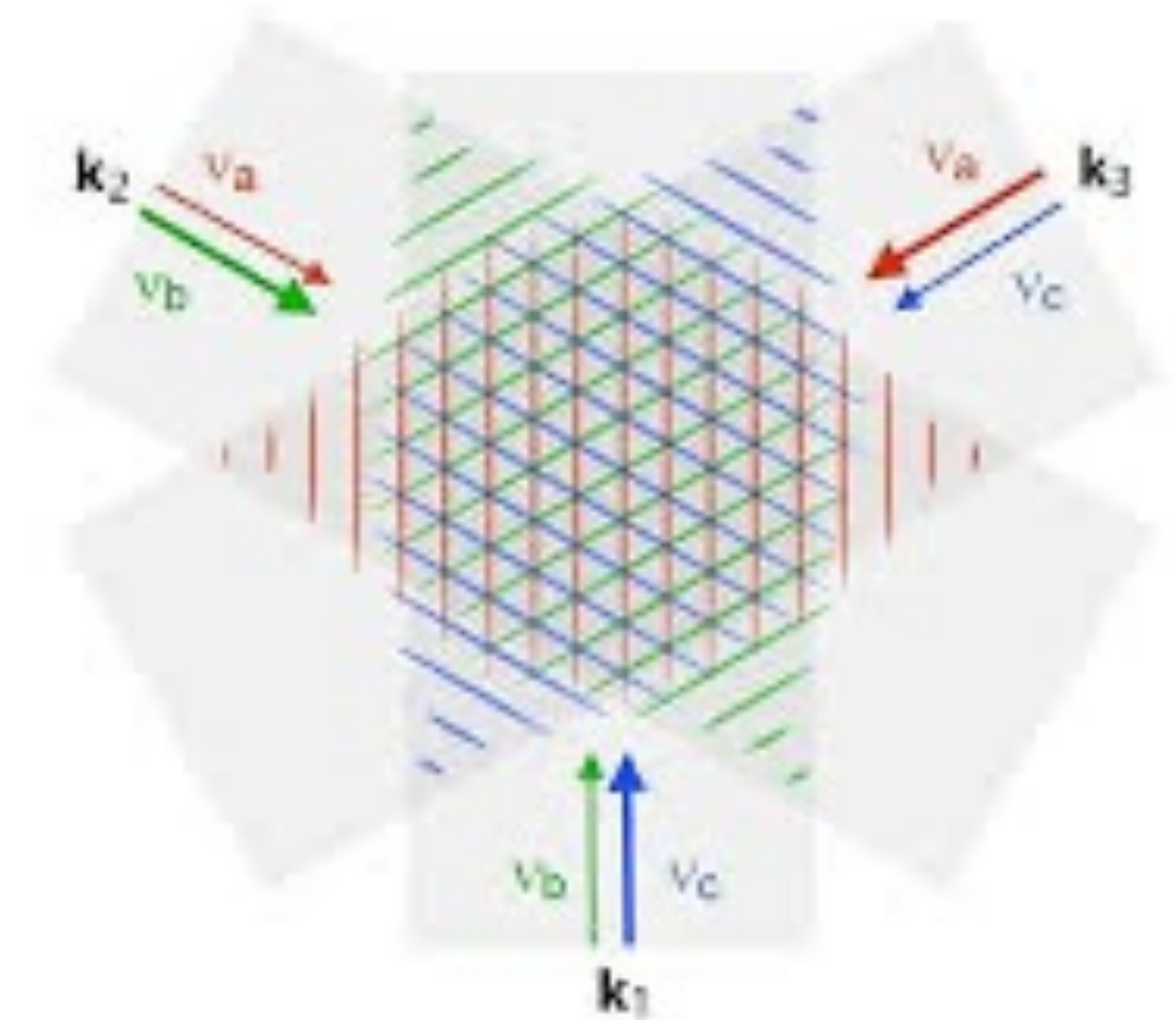
triangular, honeycomb, kagome, sawtooth, etc etc



1D $V_{0,x} \ll V_{0,y}, V_{0,z}$

2D $V_{0,x}, V_{0,y} \ll V_{0,z}$

3D $V_{0,x} \approx V_{0,y} \approx V_{0,z}$





Hamiltonian derivation

Bosons

$$H = \int d^3r d^3r' \psi^\dagger(\mathbf{r}) \left[-\frac{\hbar^2 \nabla^2}{2m} + V(\mathbf{r}) + \frac{g}{2} \psi^\dagger(\mathbf{r}') \psi(\mathbf{r}') - \mu \right] \psi(\mathbf{r})$$

$\frac{4\pi\hbar^2 a_s}{m} \delta(r-r')$

Fermions

$$H = \sum_{\sigma} \int d^3r d^3r' \psi_{\sigma}^{\dagger}(\mathbf{r}) \left[-\frac{\hbar^2 \nabla^2}{2m} + V(\mathbf{r}) + \frac{g}{2} \psi_{\sigma}^{\dagger}(\mathbf{r}') \psi_{\sigma}(\mathbf{r}') - \mu \right] \psi_{\sigma}(\mathbf{r})$$

$\frac{4\pi\hbar^2 a_s}{m} \delta(r-r')$

Bloch Theorem

$$\psi(\mathbf{r}) \sum_{\mathbf{k}} \phi_{\mathbf{k}} a_{\mathbf{k}} = \sum_i w(\mathbf{r} - \mathbf{R}_i) b_i \quad [b_i, b_j^{\dagger}] = \delta_{i,j}$$

$$\psi(\mathbf{r}) \sum_{\mathbf{k}} \phi_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} = \sum_i w_{\sigma}(\mathbf{r} - \mathbf{R}_i) c_{i,\sigma} \quad \{c_{i,\sigma}, c_{j,\sigma'}^{\dagger}\} = \delta_{i,j} \delta_{\sigma,\sigma'}$$

Space discretization

Bose-Hubbard

$$H_{BH} = -J \sum_i b_i^{\dagger} b_{i+1} + h.c. + \frac{U}{2} \sum_i n_i(n_i - 1) - \mu \sum_i n_i$$

$$J = - \int d^3r w^*(\mathbf{r} - \mathbf{R}_i) \left[-\frac{\hbar^2 \nabla^2}{2m} + V(\mathbf{r}) \right] w(\mathbf{r} - \mathbf{R}_{i+1}) \propto V_{0,r}^{3/4} e^{\sqrt{V_{0,r}}}$$

$$U = \int d^3r |w(\mathbf{r} - \mathbf{R}_i)|^4 \propto a_s V_{0,r}^{3/4}$$

Fermi-Hubbard

$$H_{FH} = -J \sum_{\sigma} \sum_i c_{i,\sigma}^{\dagger} c_{i+1,\sigma} + h.c. + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_i n_i$$

$$J = - \int d^3r w_{\sigma}^*(\mathbf{r} - \mathbf{R}_i) \left[-\frac{\hbar^2 \nabla^2}{2m} + V(\mathbf{r}) \right] w_{\sigma}(\mathbf{r} - \mathbf{R}_{i+1}) \propto V_{0,r}^{3/4} e^{\sqrt{V_{0,r}}}$$

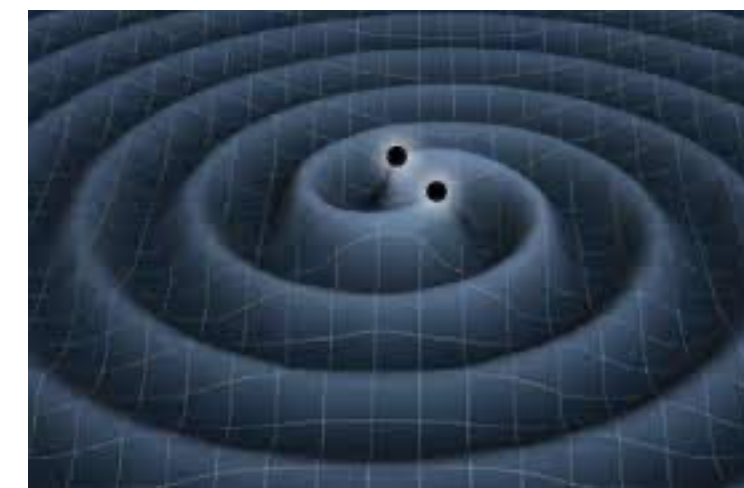
$$U = \int d^3r |w_{\uparrow}(\mathbf{r} - \mathbf{R}_i)|^2 |w_{\downarrow}(\mathbf{r} - \mathbf{R}_i)|^2 \propto a_s V_{0,r}^{3/4}$$

Tunable!!!

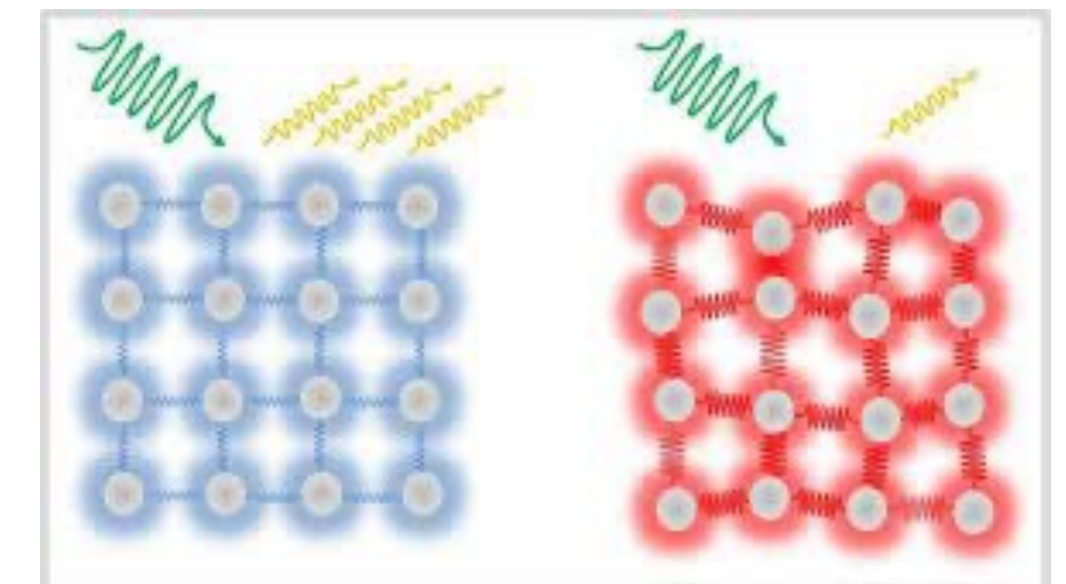
Efficient and much more accurate
quantum simulation of real
materials

Quantum Simulation of Bosonic
systems

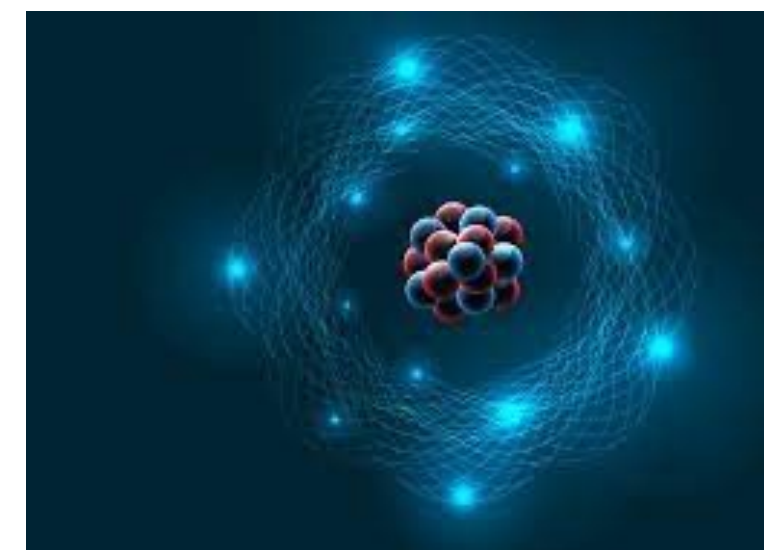
gravitons (gravity)



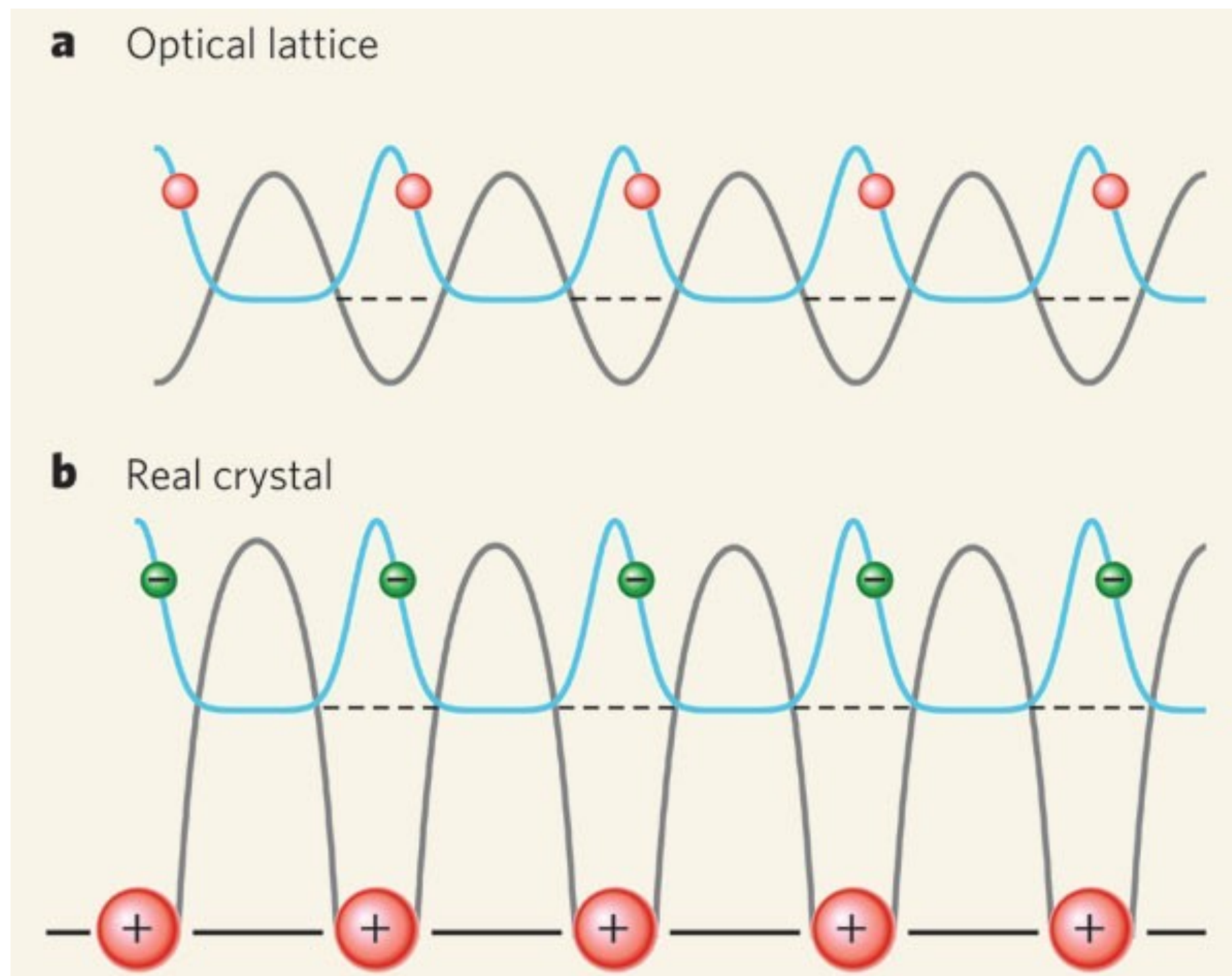
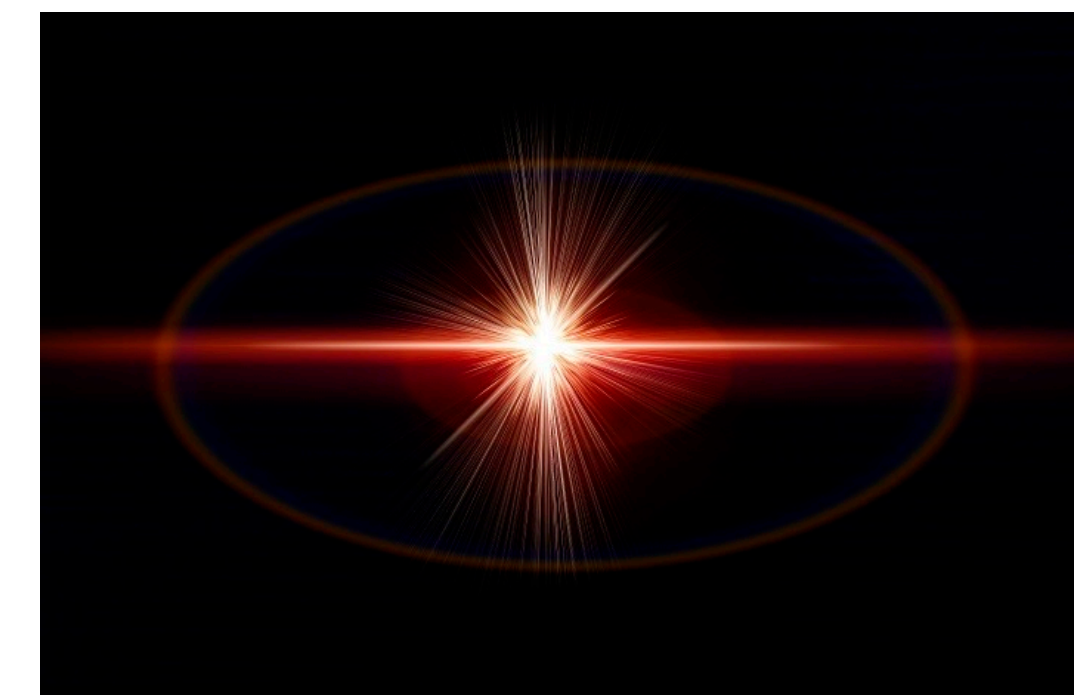
phonons (solids)



gluons&mesons (nuclei)



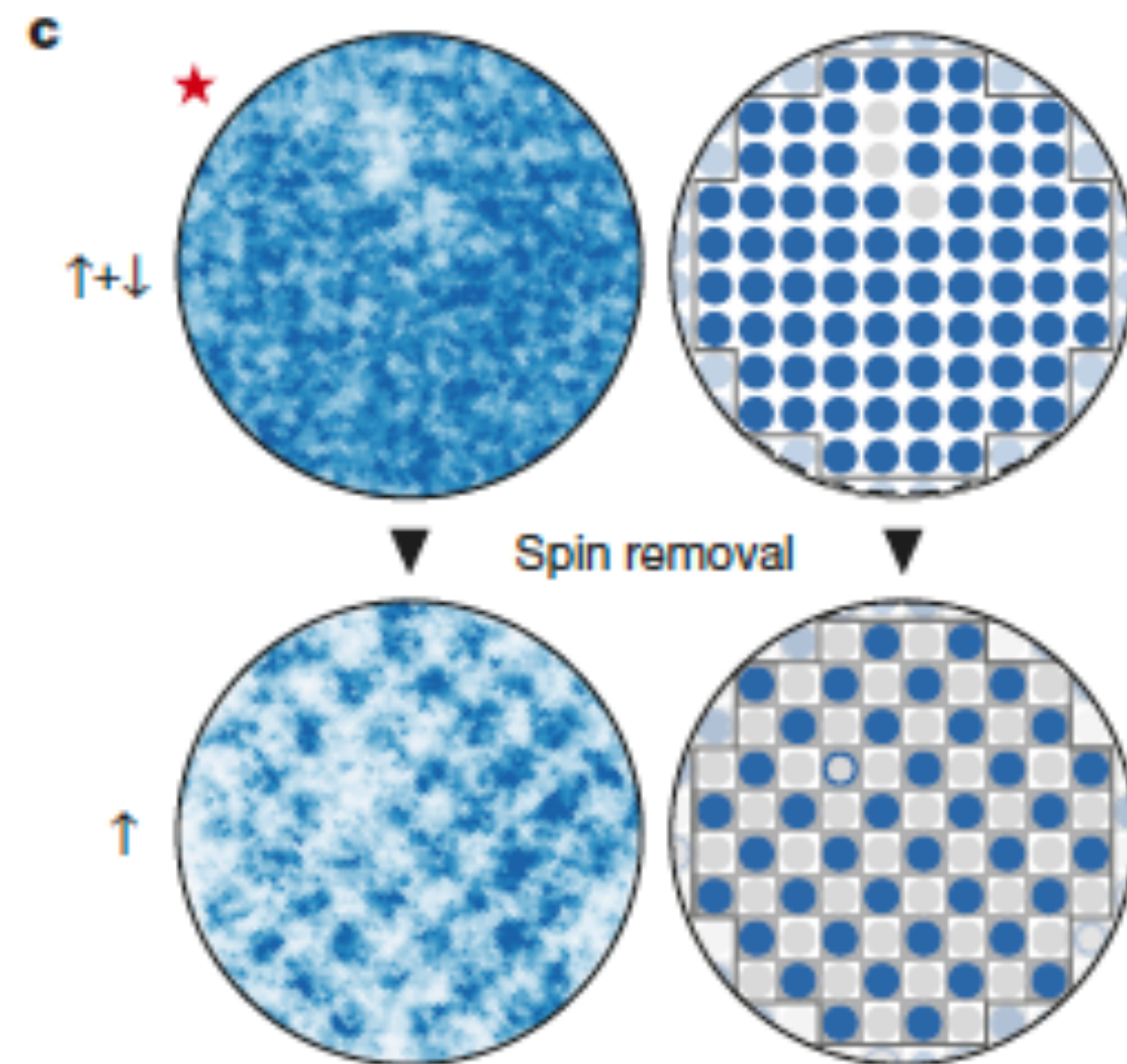
photons (light)



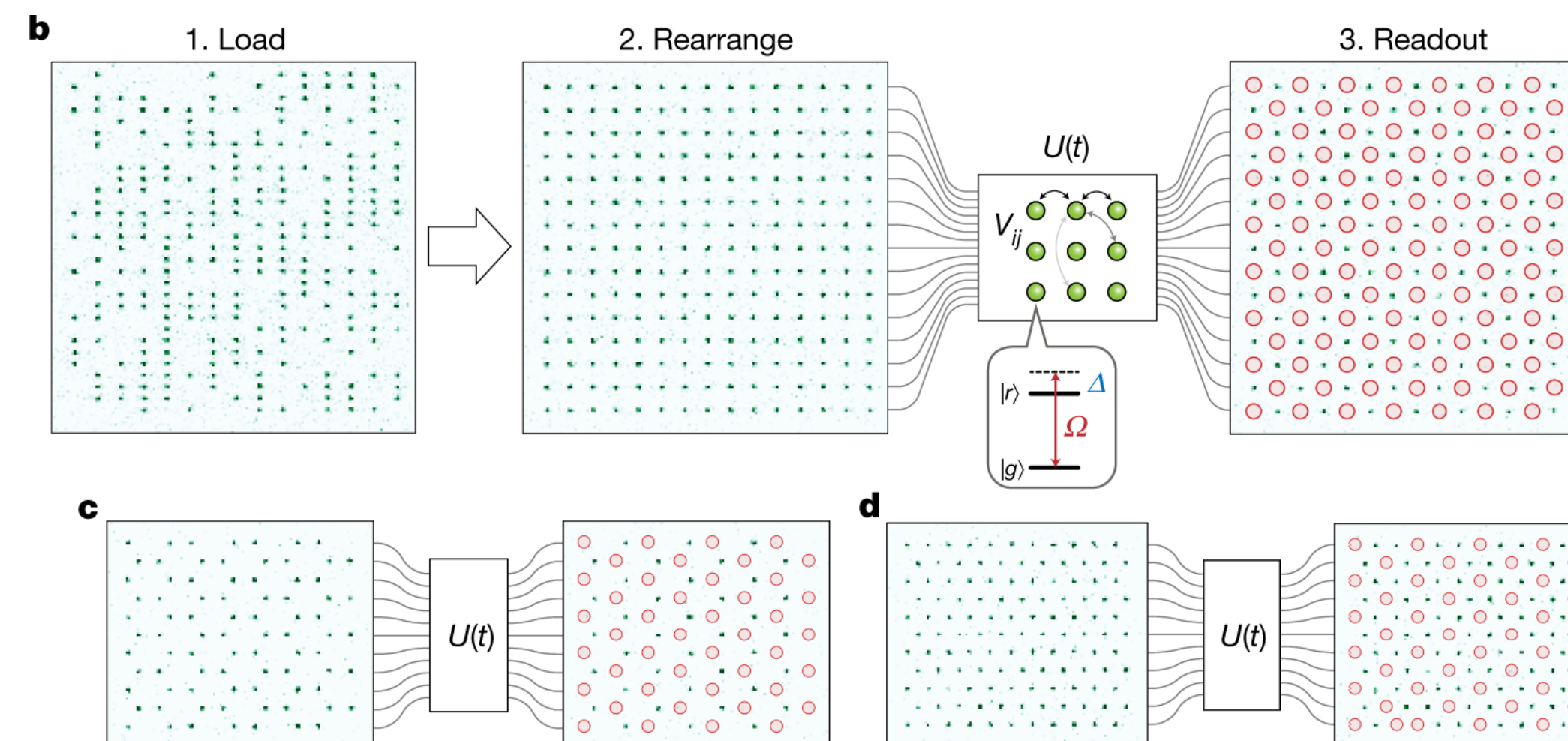
Detection scheme (output)

Quantum gas microscopy to perform measurements of correlation functions

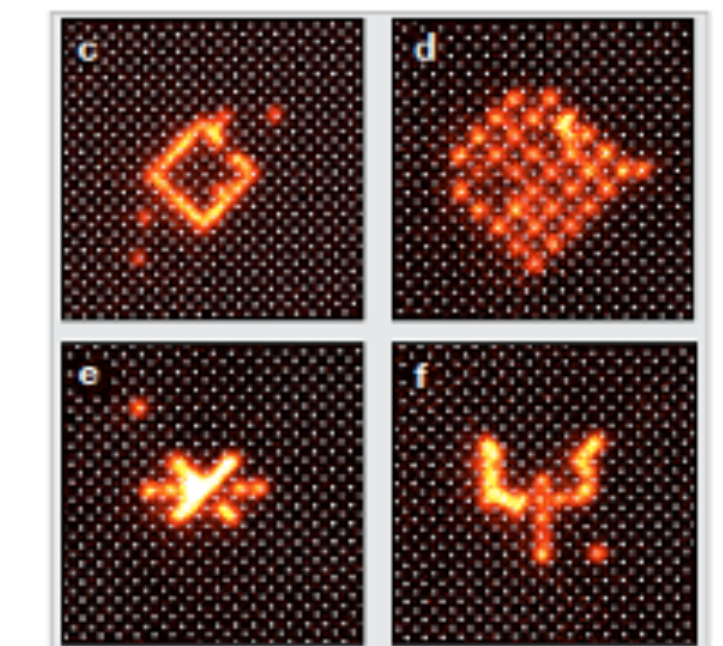
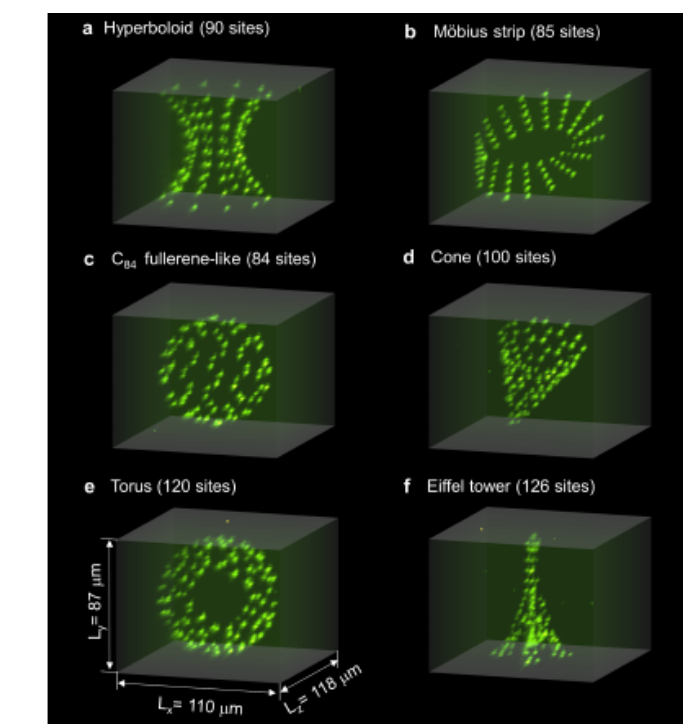
Antiferromagnetism



Logical gates



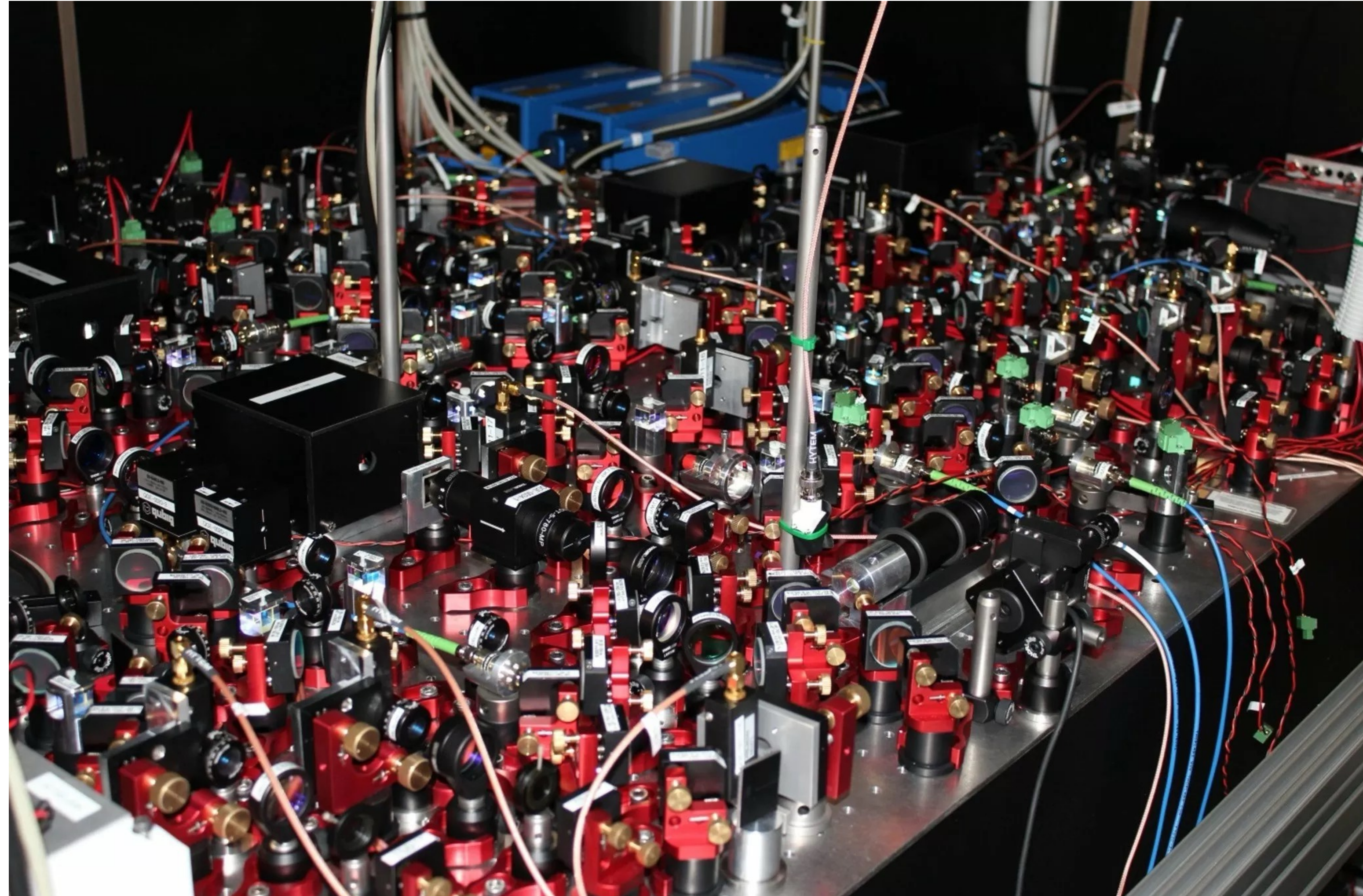
Exotic geometries





Politecnico
di Torino

QTCM computational lab on quantum simulation

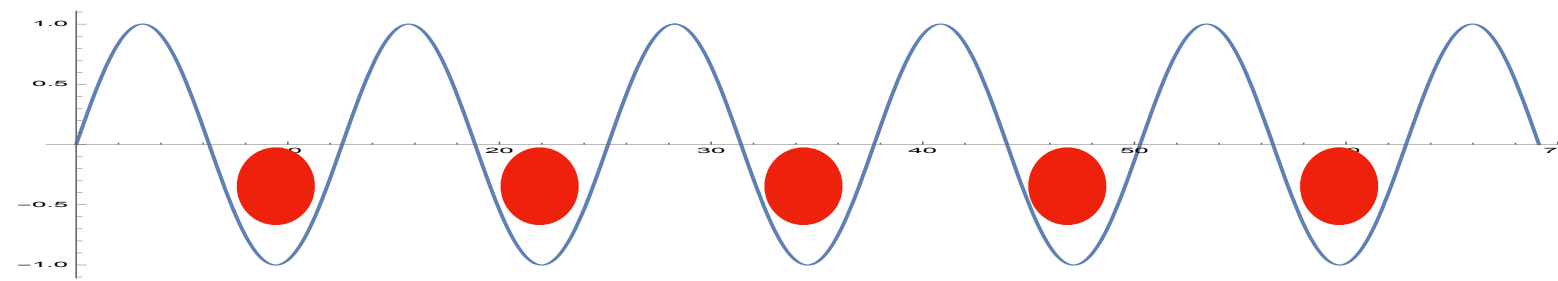


1D Bose-Hubbard

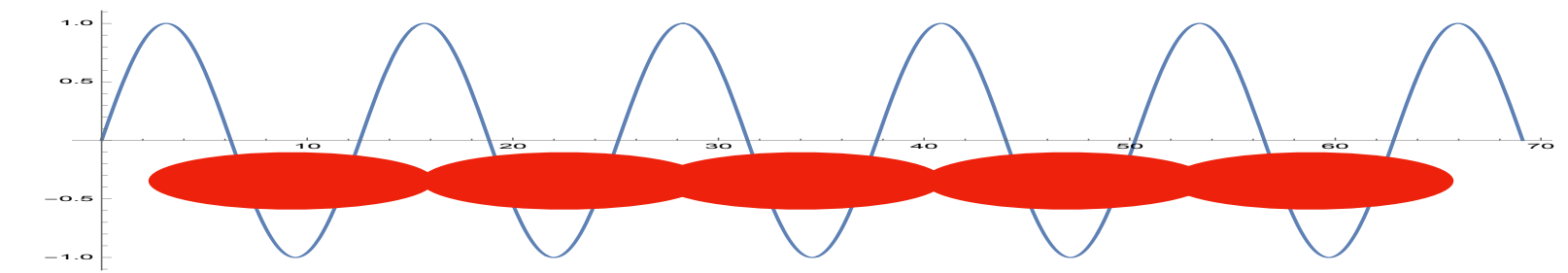
$$H_{BH} = -J \sum_i (b_i^\dagger b_{i+1} + b_i b_{i+1}^\dagger) + \frac{U}{2} \sum_i n_i(n_i - 1)$$

Density=1 i.e. $N/L=1$

$U \gg J$ Mott insulator

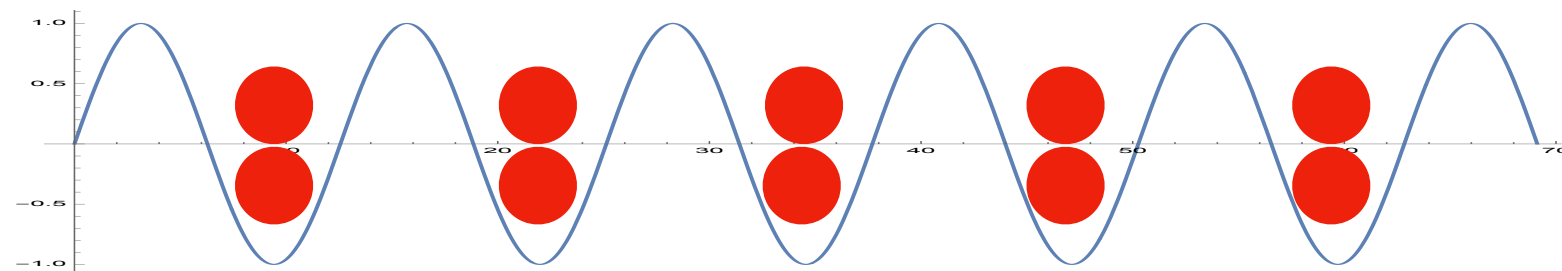


$U \ll J$ superfluid

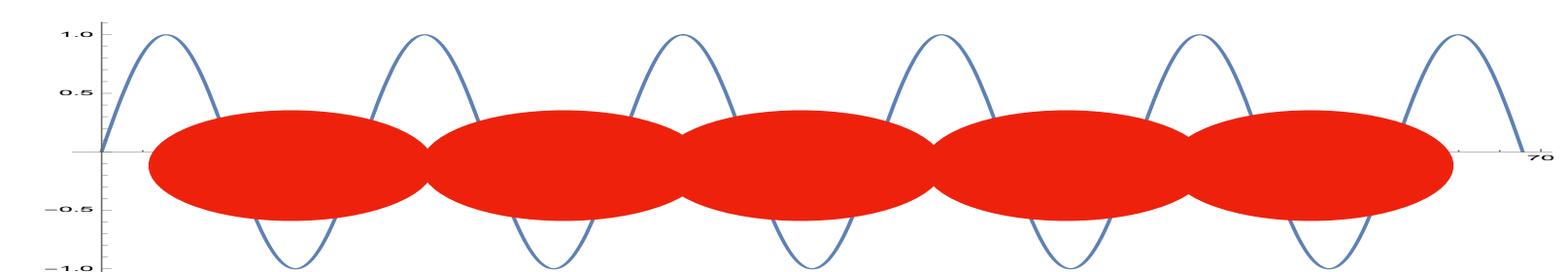


Density=2 i.e. $N/L=2$

$U \gg J$ Mott insulator

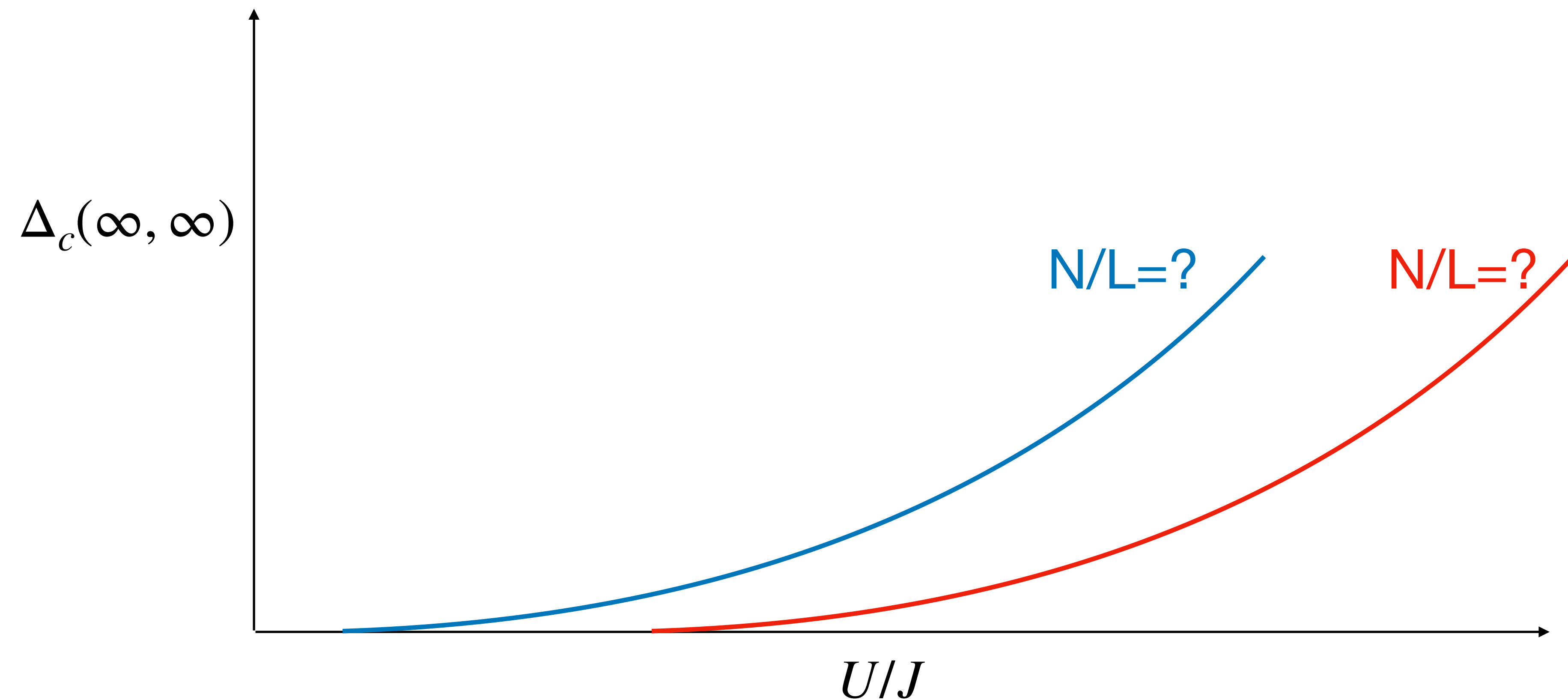


$U \ll J$ superfluid



Phase diagram

It is always possible to distinguish SF and MI through a gap analysis $\Delta_c(N, L) = E_{GS}(N+1, L) + E_{GS}(N-1, L) - 2E_{GS}(N, L)$, i.e. the energy cost in adding/removing one boson

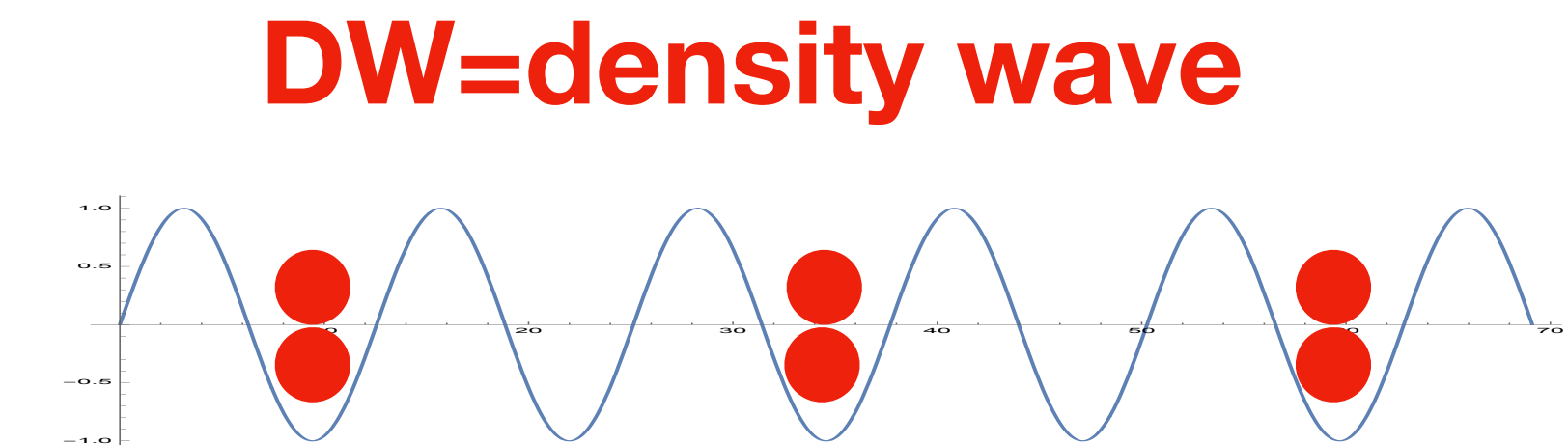
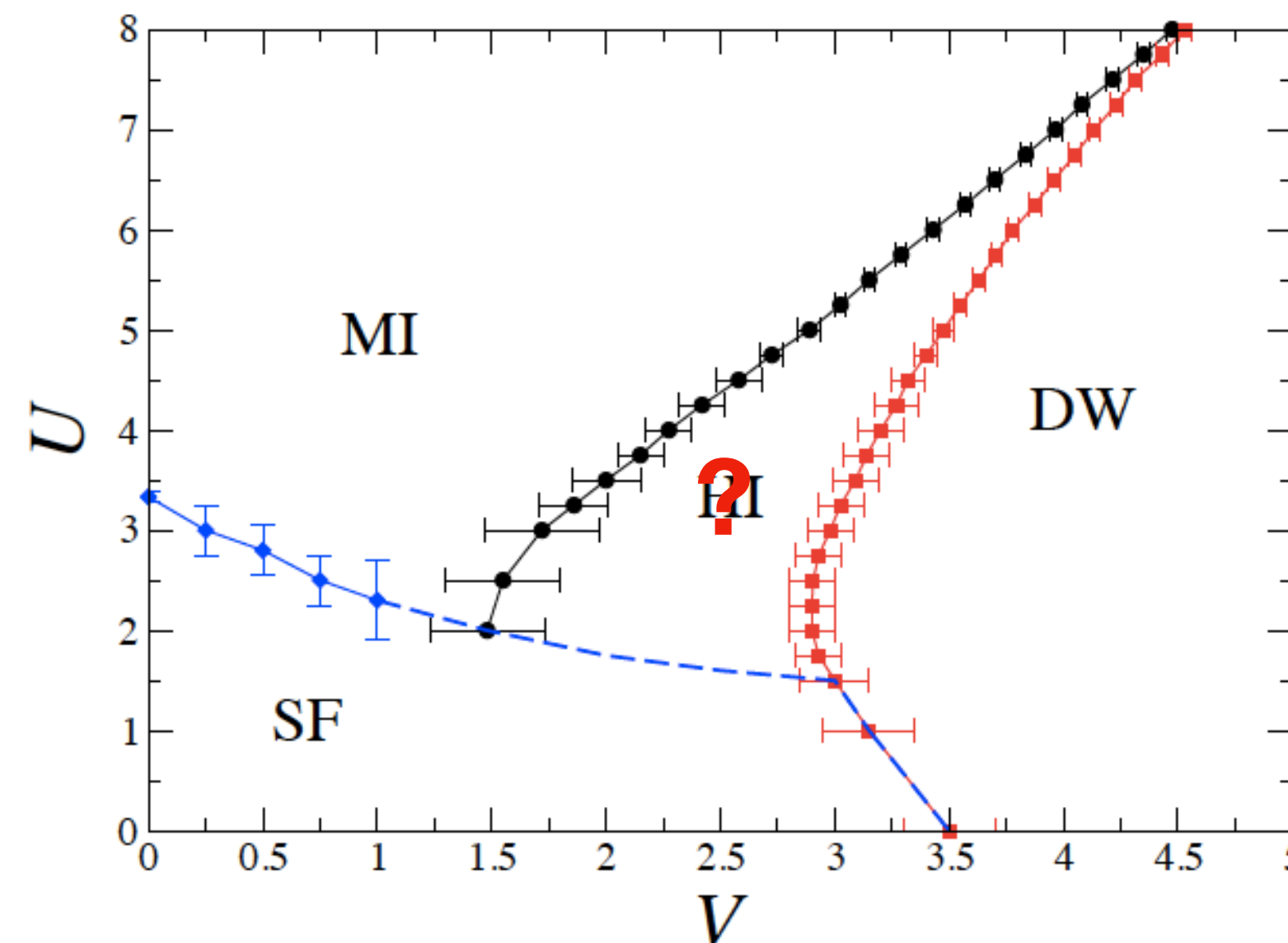


Suppose to consider lanthanides (eg Er or Dy) with strong dipolar interaction $\propto \frac{1 - 3\cos^2\theta}{|r - r'|^3}$, is the approximation of contact interaction correct?

NO! terms like $V = \int d^3r |w(\mathbf{r} - \mathbf{R}_i)|^2 |w(\mathbf{r} - \mathbf{R}_{i+1})|^2$ become relevant

1D Extended Bose-Hubbard

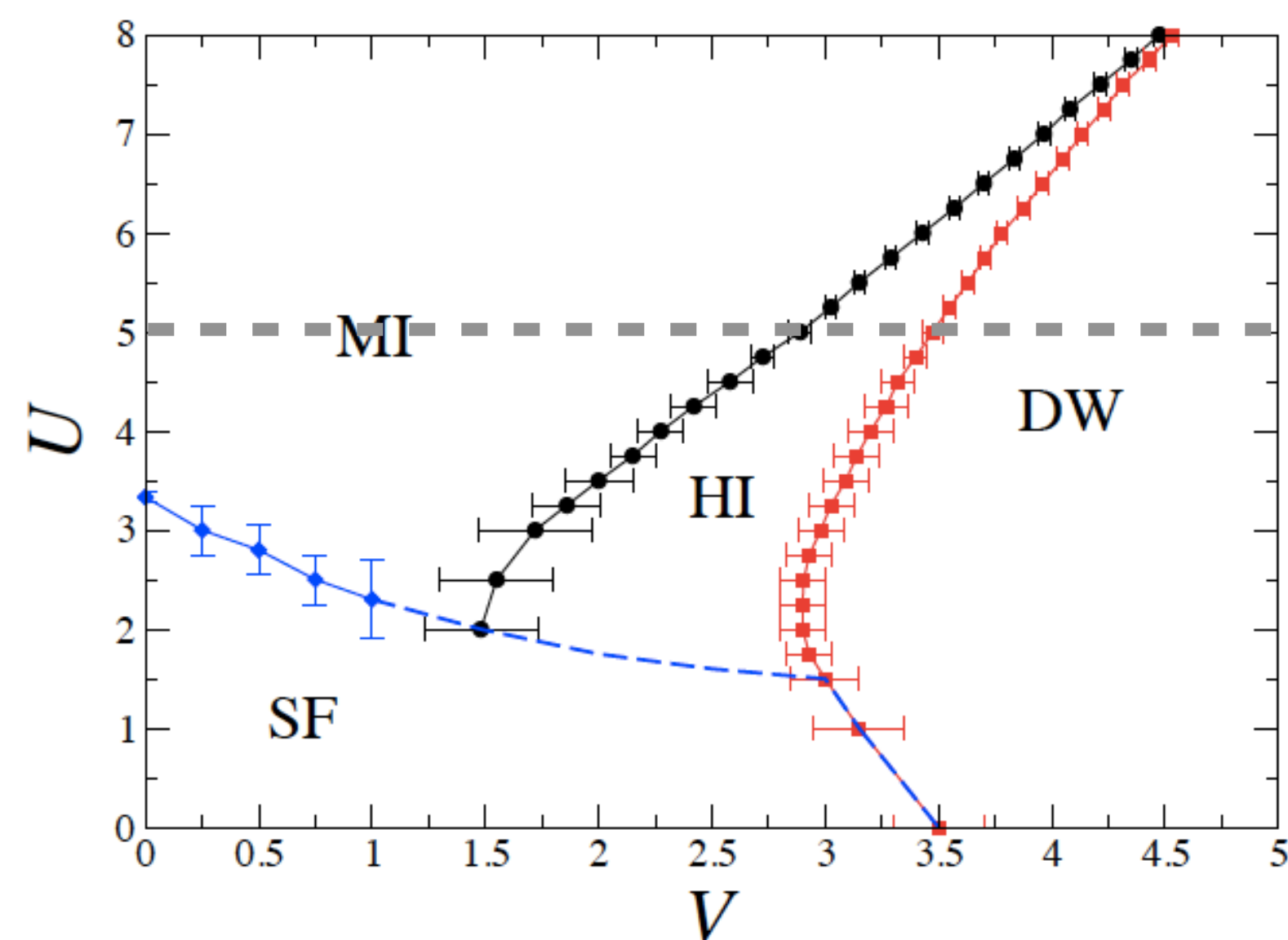
$$H_{BH} = -J \sum_i (b_i^\dagger b_{i+1} + b_i b_{i+1}^\dagger) + \frac{U}{2} \sum_i n_i(n_i - 1) + V \sum_i n_i n_{i+1} \quad \text{Density}=1 \text{ i.e. } N/L=1$$



Gap analysis

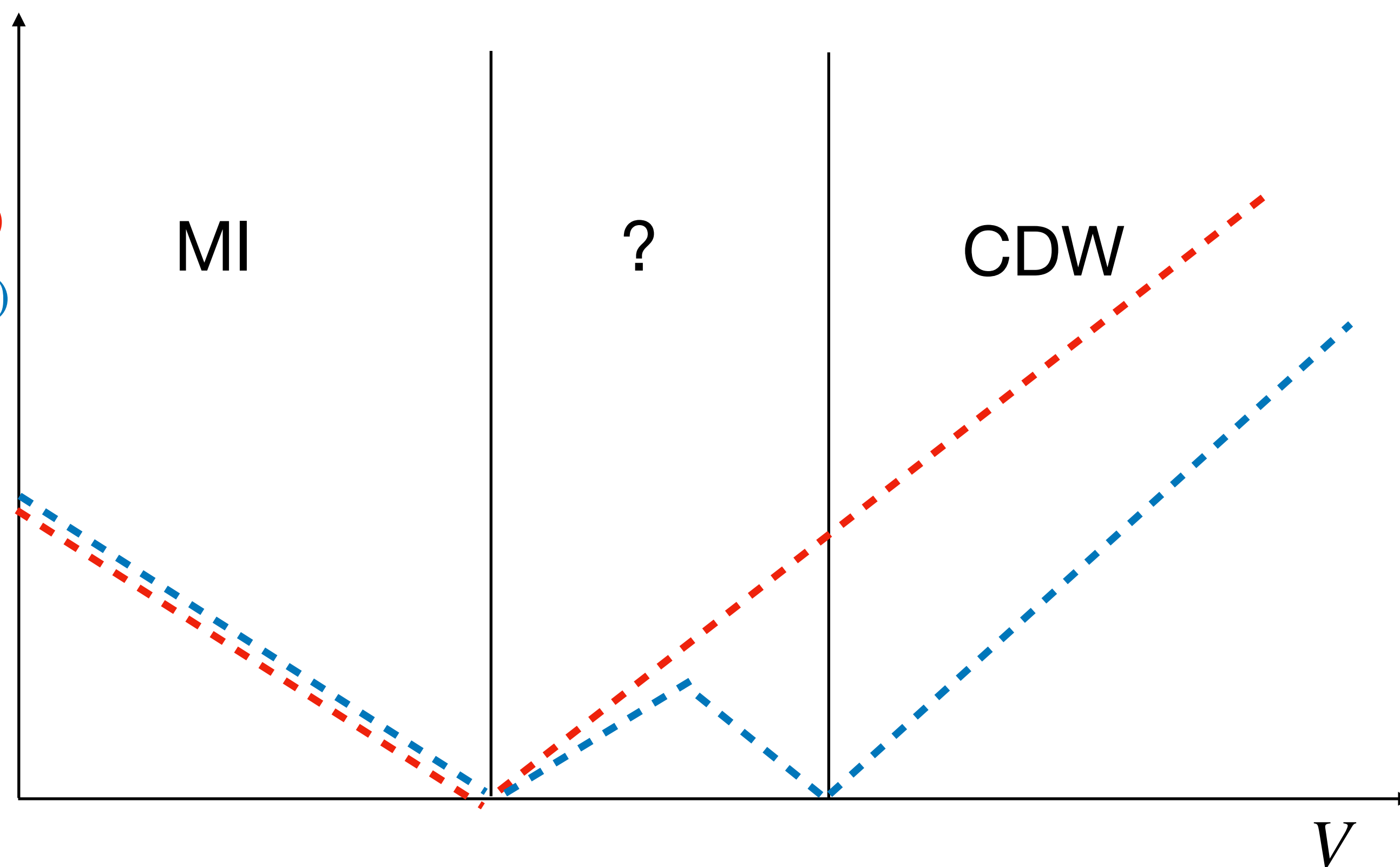
$$\Delta_c(N, L) = E_{GS}(N+1, L) + E_{GS}(N-1, L) - 2E_{GS}(N, L)$$

$$\text{neutral gap } \Delta_N(N, L) = E_1(N, L) - E_{GS}(N, L)$$



$$\Delta_c(\infty, \infty)$$

$$\Delta_N(\infty, \infty)$$





Equivalence between EBH model and XXZ spin-1/2

$$H_{BH} = -J \sum_i (b_i^\dagger b_{i+1} + b_i b_{i+1}^\dagger) + \frac{U}{2} \sum_i n_i(n_i - 1) + V \sum_i n_i n_{i+1}$$

Density=0.5 i.e. $N/L = \bar{n} = 1/2$ and $U \approx \infty \rightarrow$ local Hilbert space $|0\rangle, |1\rangle$

$$b_i^\dagger = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = S_i^+ \quad b_i = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = S_i^-$$

Holstein-Primakoff transformation $S_i^z = (\bar{n} - n_i) = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix} - \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 1/2 & 0 \\ 0 & -1/2 \end{pmatrix}$

$$H_{BH} = H_{XXZ} + \text{irrelevant terms}$$

Particle occupation can act as an effective qubit!!!!