Ultracold Physics, Quantum Simulators, and Quantum Simulations

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Co-organizers:

Ignacio Cirac, Max Planck Institute for Quantum Optics

Erich Mueller, Cornell University

David Weiss, The Pennsylvania State University

Outline: Ultracold Physics, Quantum Simulators, and Quantum Simulations

- Motivation and Themes
- Ultracold Physics
- Quantum Simulators for Outstanding Problems in Condensed Matter Physics
- What Can Quantum Simulations on Classical Computers Offer?

Quantum Mechanics is Hard

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- Need approximation methods already in single particle quantum mechanics
  - Hydrogen atom
  - Perturbation Theory, Dyson series, Feynman diagrams
  - Sudden/Adiabatic approximations
  - Etc. etc.
- Hilbert space of many body quantum mechanics scales exponentially
  - L sites, spin-1/2 particles, $\dim(H)=2^L$

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- A Bug is a Feature?
  - Feynman, 1982: Quantum computer to simulate physics
  - Peter Shor's algorithm, 1994: Factor large numbers

Feynman says…

If we suppose that we know all the physical laws perfectly, of course we don't have to pay any attention to computers. It's interesting anyway to entertain oneself with the idea that we've got something to learn about physical laws; and if I take a relaxed view here (after all I'm here and not at home) I'll admit that we don't understand everything. The first question is, What kind of computer are we going to use to simulate physics? Computer theory has been developed to a point where it realizes that it doesn't make any difference; when you get to a *universal computer, it doesn't matter how it's manufactured, how it's actually made.* Therefore my question is, Can physics be simulated by a universal computer?

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Now, what kind of physics are we going to imitate? First, I am going to describe the possibility of simulating physics in the classical approximation, a thing which is usually described by local differential equations. But the physical world is quantum mechanical, and therefore the proper problem is the simulation of quantum physics--which is what I really want to talk about, but I'll come to that later. So what kind of simulation do I mean? There is, of course, a kind of approximate simulation in which you design numerical algorithms for differential equations, and then use the computer to compute these algorithms and get an approximate view of what physics ought to do. That's an interesting subject, but is not what I want to talk about. I want to talk about the possibility that there is to be an exact simulation, that the computer will do exactly the same as nature.

Feynman adds…

The rule of simulation that I would like to have is that the number of computer elements required to simulate a large physical system is only to be proportional to the space-time volume of the physical system. I don't want to have an explosion. That is, if you say I want to explain this much physics, I can do it exactly and I need a certain-sized computer. If doubling the volume of space and time means I'll need an *exponentially larger computer,* I consider that against the rules (I make up the rules, I'm allowed to do that).

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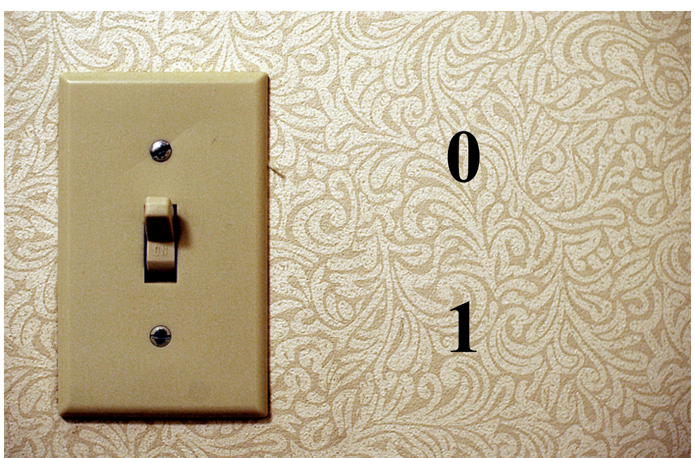

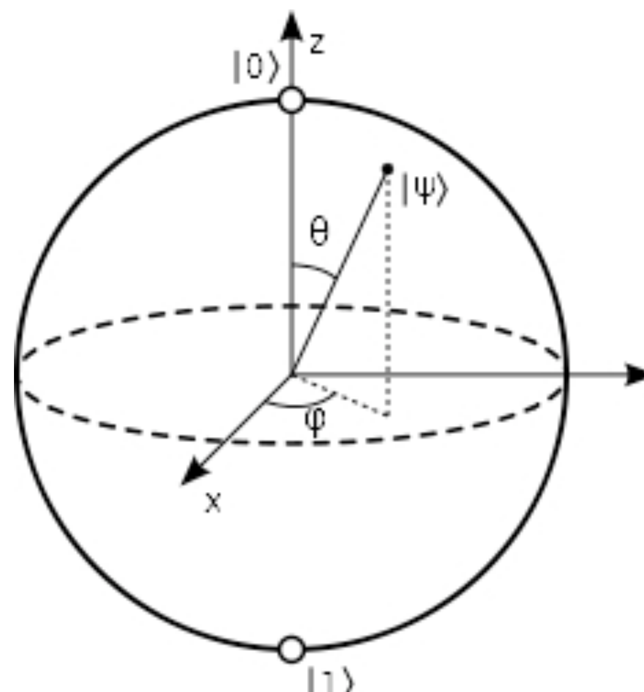

How do we think about this now?

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- Quantum simulator
  - More like an analog device
  - An exact experimental realization of a quantum model
  - Closer to Feynman's idea
- Quantum computer
  - More like a digital device
  - Can perform arbitrary quantum computation
  - Closer to Shor's idea
- Ultracold neutral atoms and molecules provide a promising platform…

Themes of Our Workshop

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- I: What are the key outstanding problems from condensed matter physics which ultracold atoms and molecules can address?

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- II: What new many-body aspects of ultracold atoms and molecules require new techniques and new perspectives, in comparison to "traditional" solid state systems? What new insight can we obtain into issues in fundamental quantum mechanics and quantum information processing?

Themes

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- III: What are the main challenges for simulating quantum systems and using ultracold atoms and molecules for quantum information processing? What new simulation techniques on classical computers can be brought to bear on these challenges?

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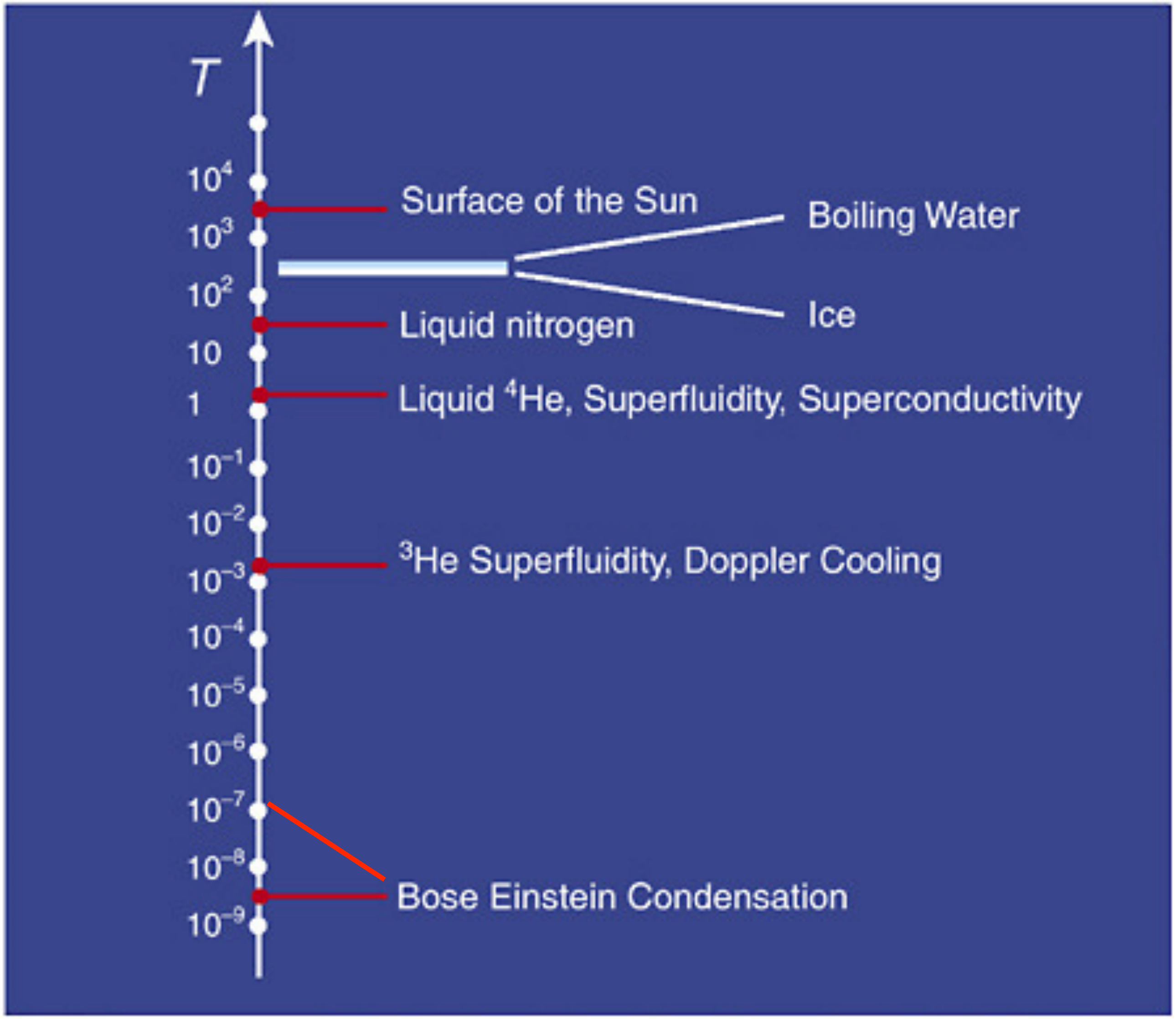
- IV: What is the best way to perform a quantum computation in ultracold atoms and molecules with the appropriate fidelity? How does one then interrogate such a quantum simulation or "read out" the answer from such a quantum computer?

How Cold is Ultracold?



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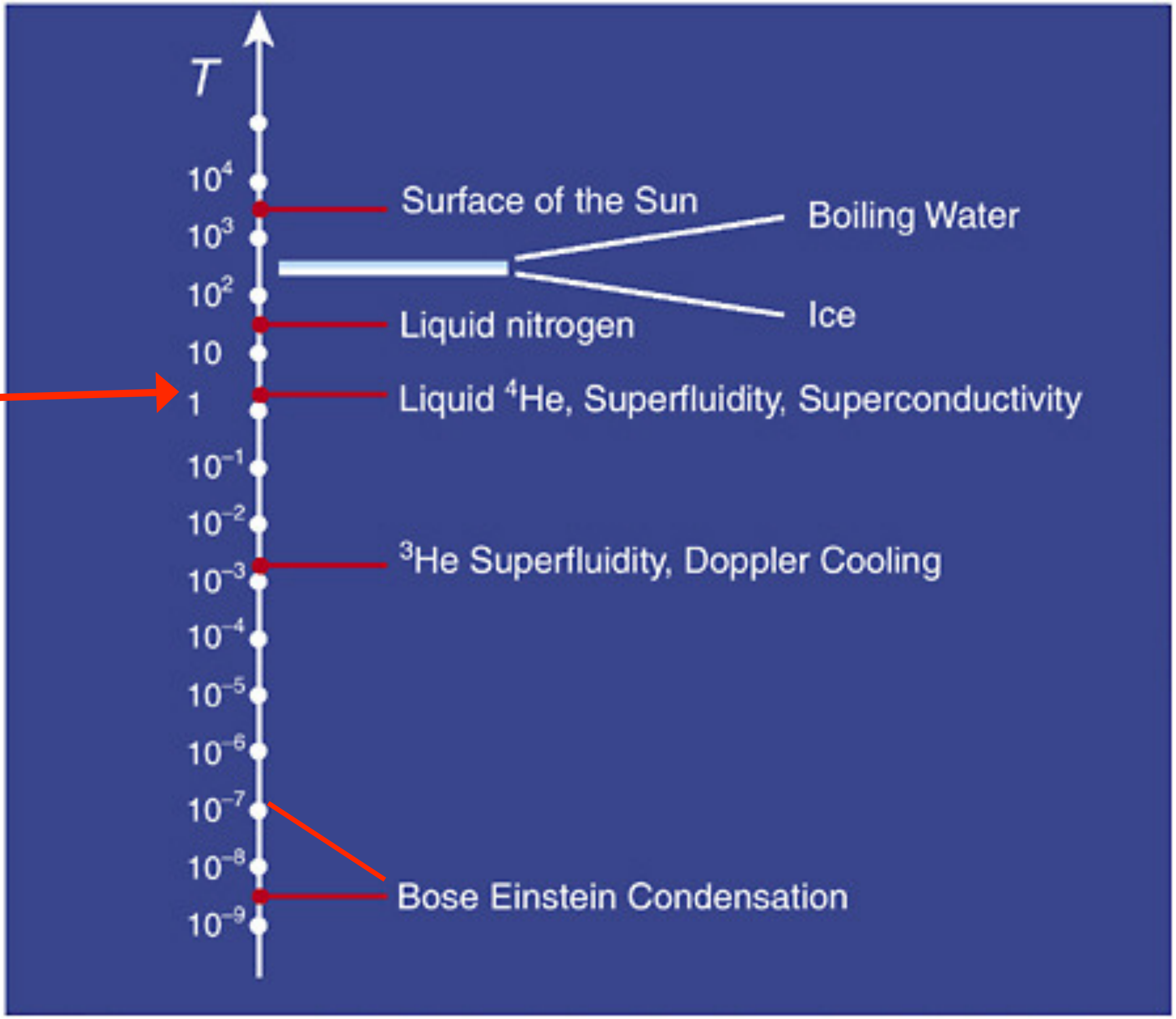
3K Cosmic Microwave Background



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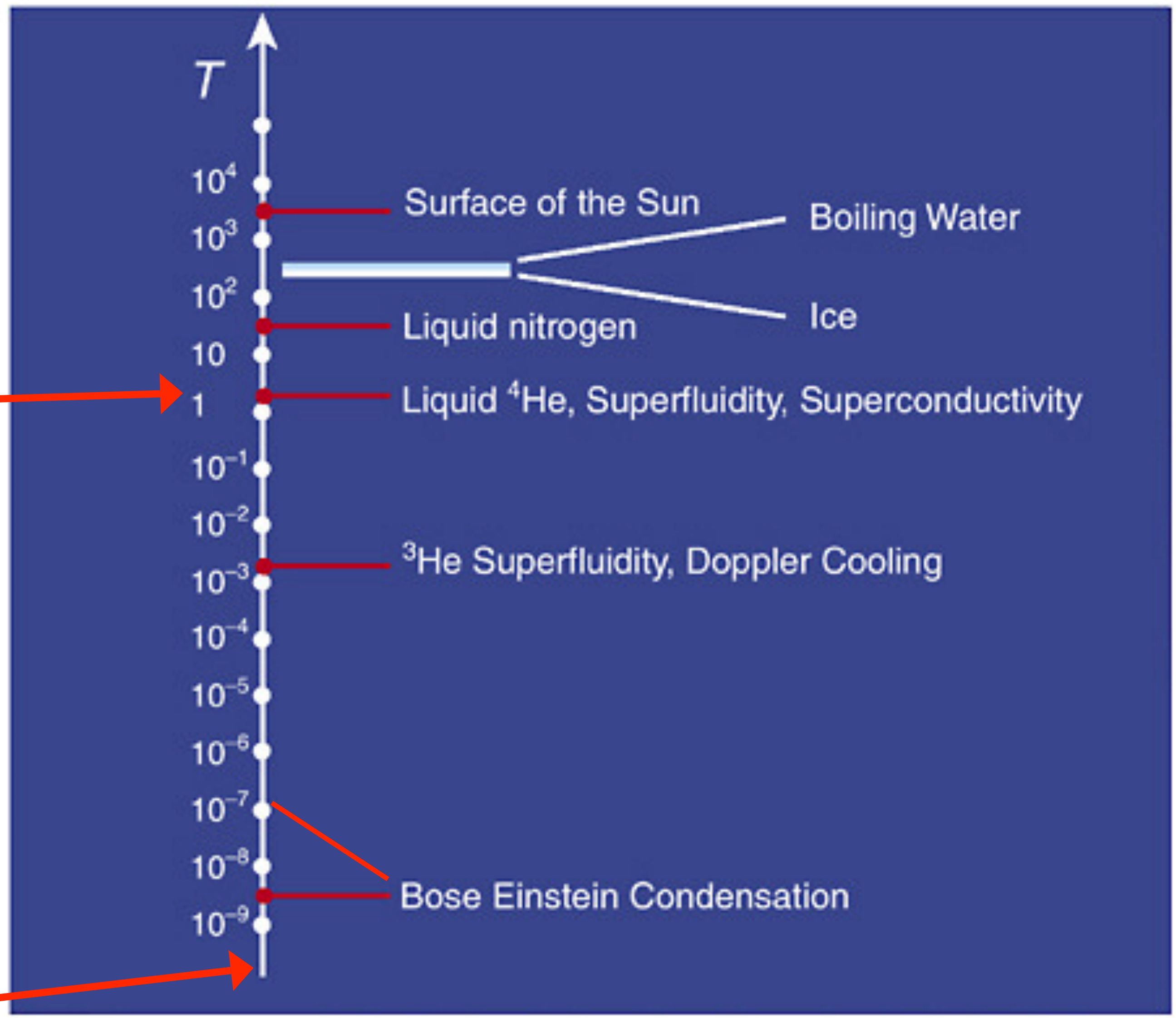
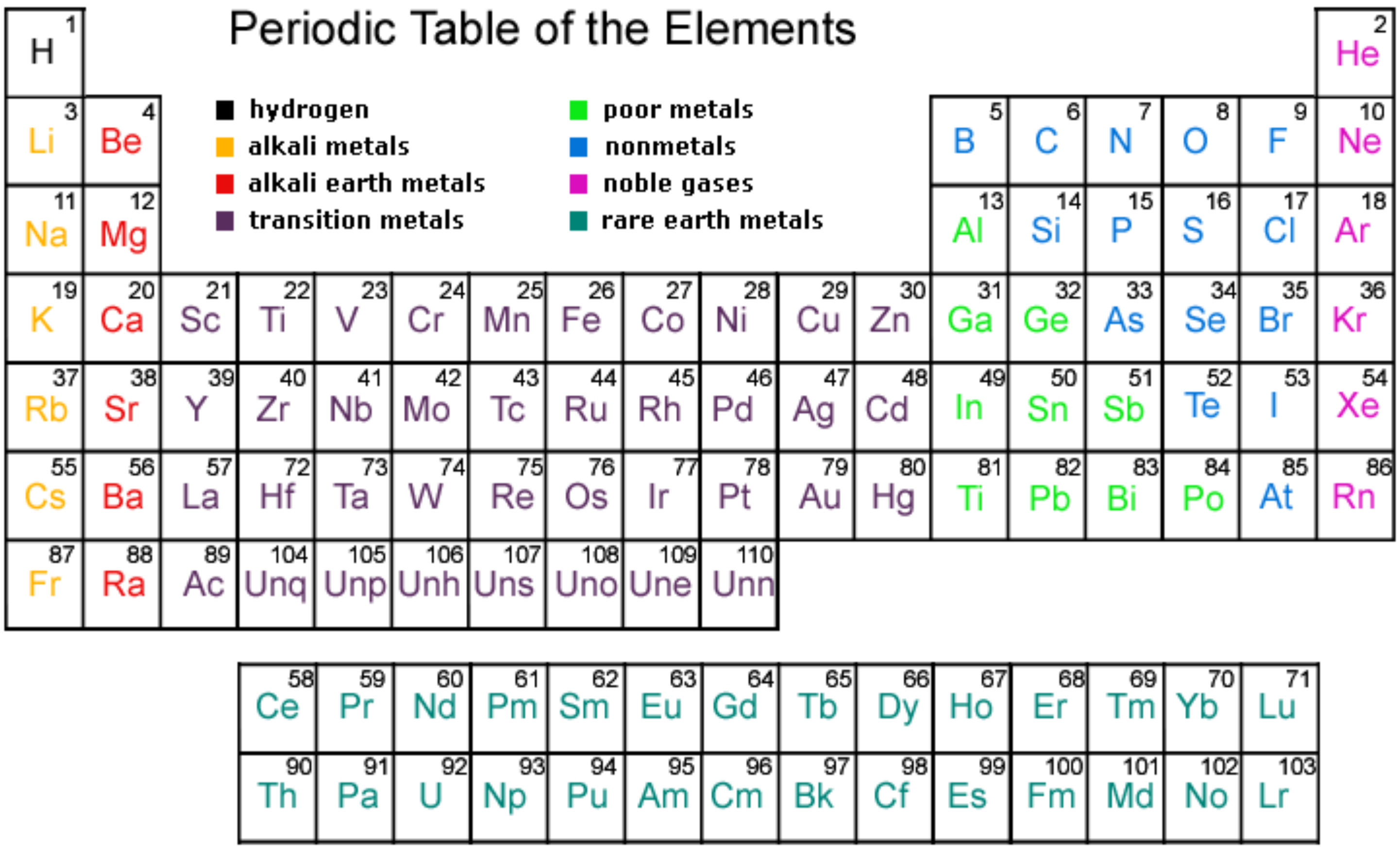


Ultracold neutral atom quantum computer?

What are they made of?



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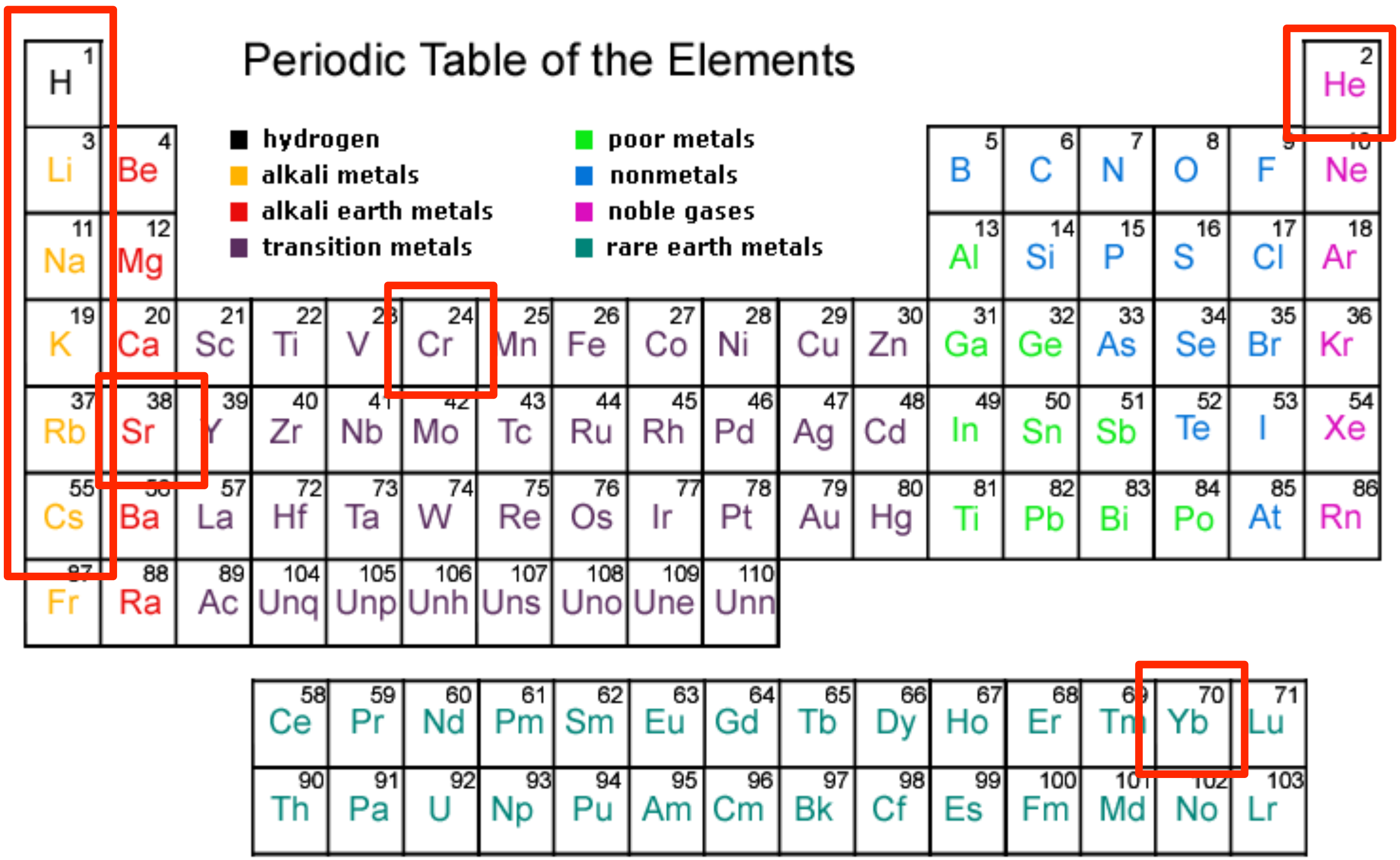
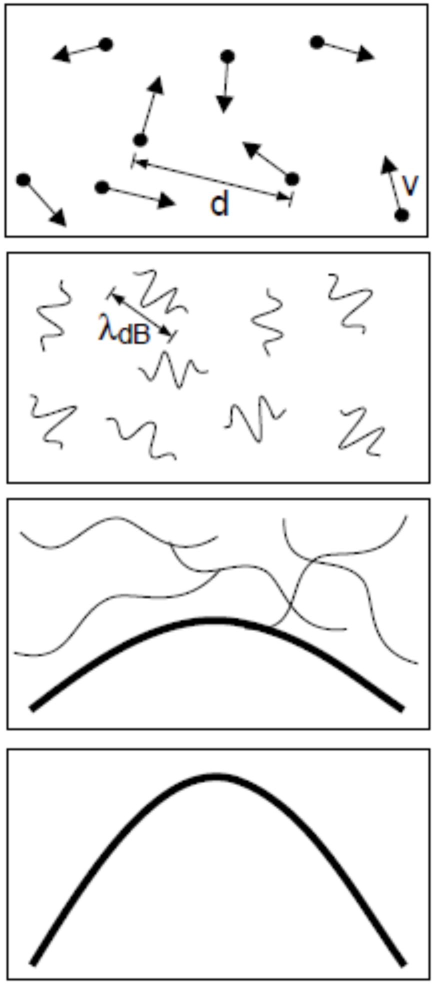


Dilute Quantum Gases



High Temperature T:

thermal velocity v

density d^{-3}

"Billiard balls"

Low Temperature T:

De Broglie wavelength

$\lambda_{dB}=h/mv \propto T^{-1/2}$

"Wave packets"

$T=T_C$:

BEC

$\lambda_{dB} \approx d$

"Matter wave overlap"

T=0:

Pure Bose condensate

"Giant matter wave"

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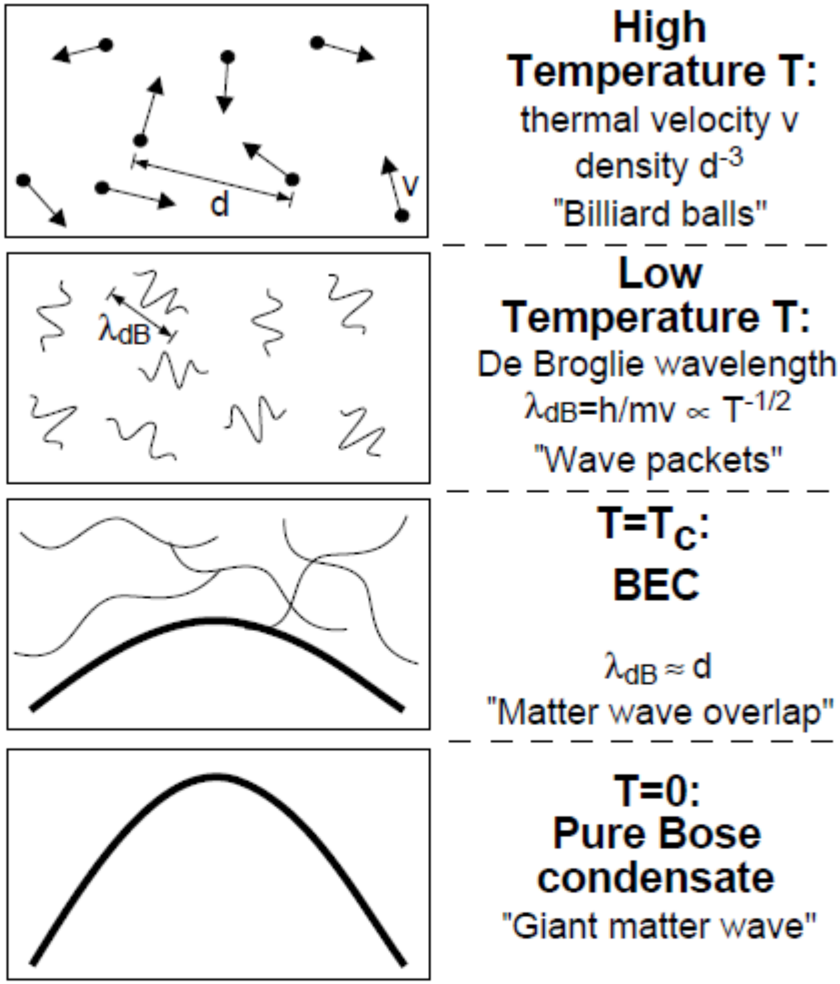

$$\Omega = n \times \lambda_{\mathrm{dB}}^3$$

$$\lambda_{\mathrm{dB}} = h/\sqrt{2\pi m k_B T}$$

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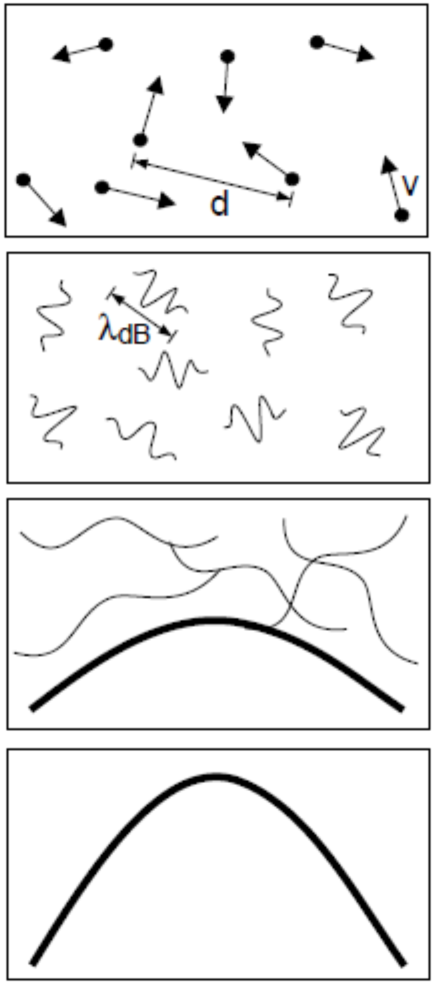

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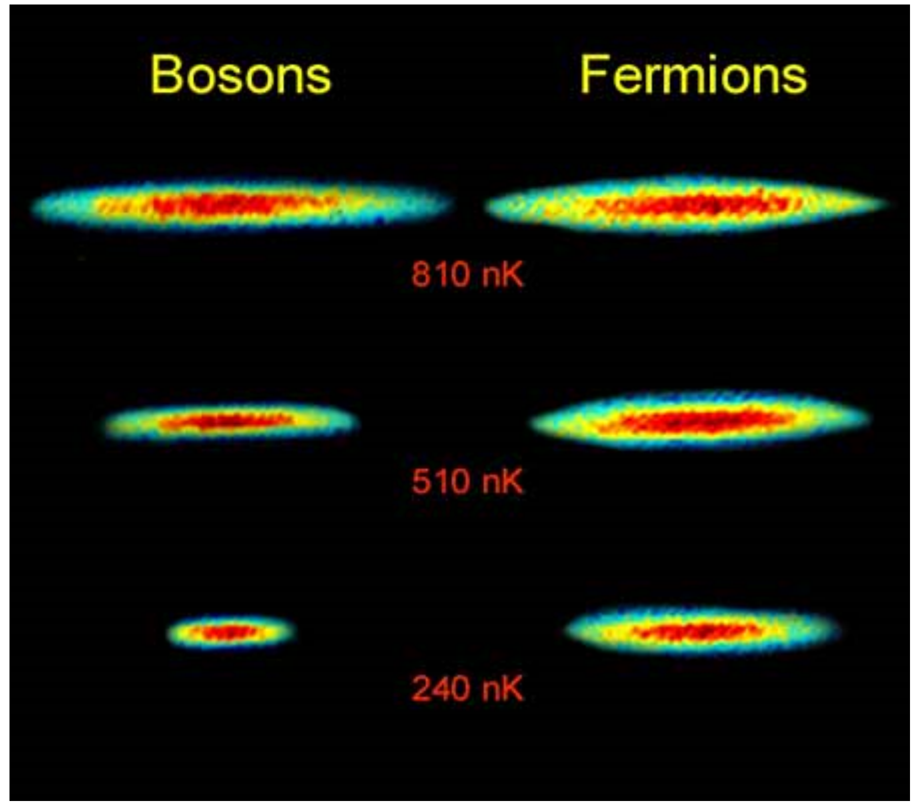

Truscott *et al*., Hulet Group, Science **291**, 2570 (2001)

Trapping Technology

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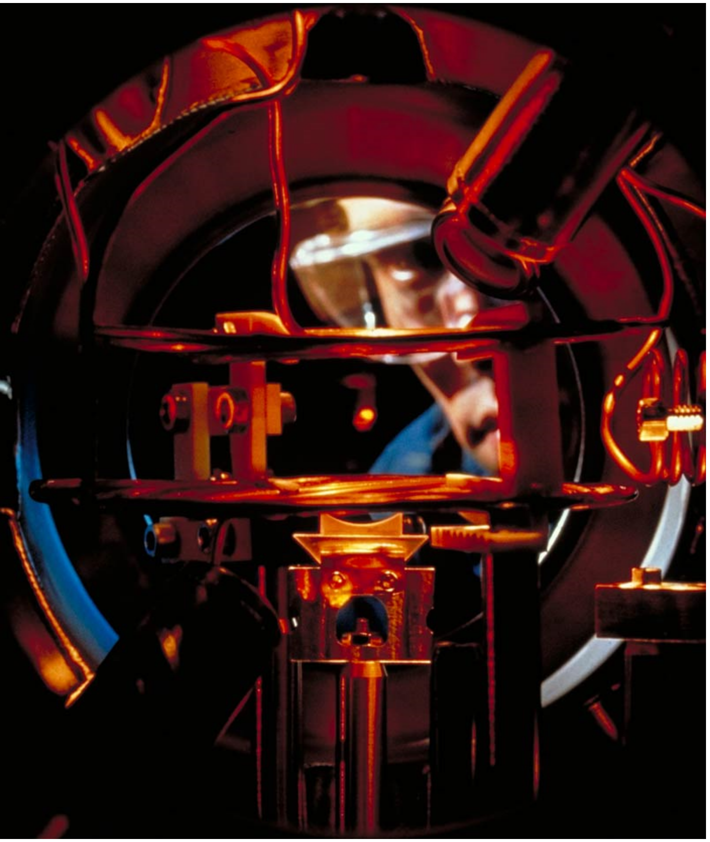
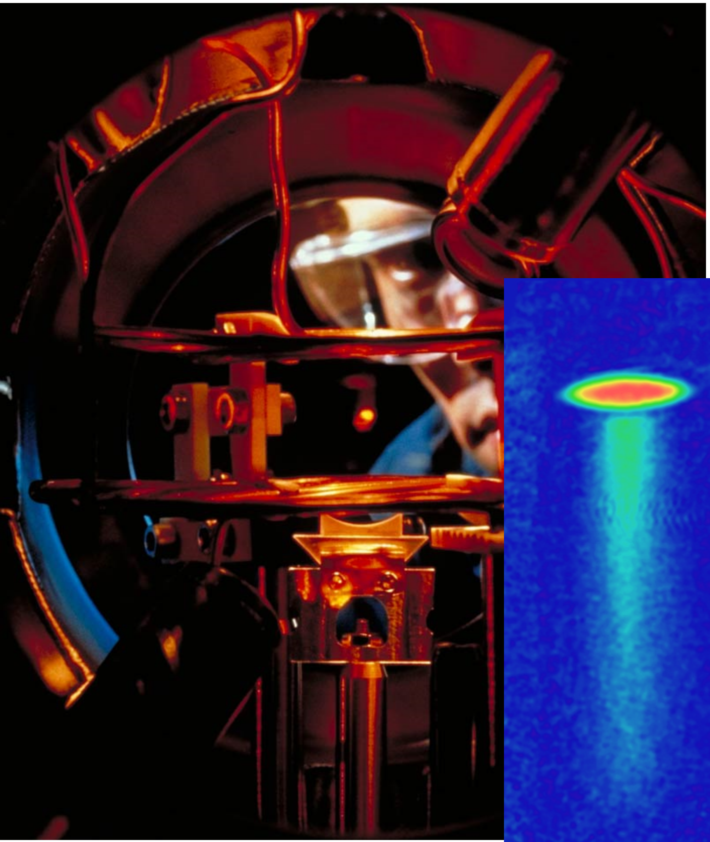


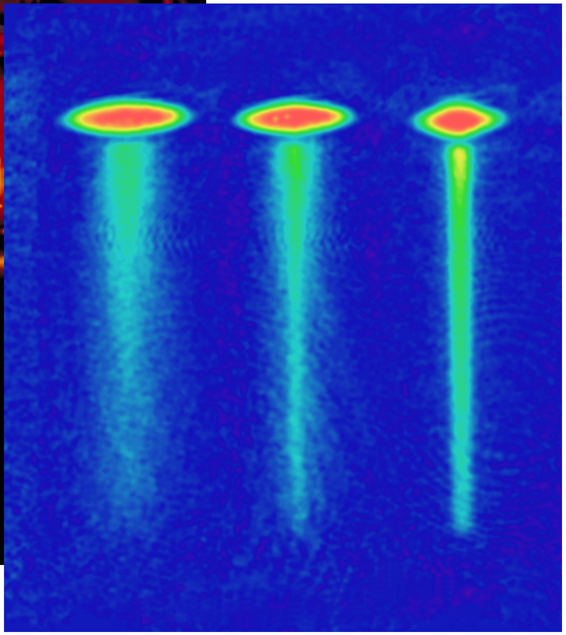
Magnetic traps

Trapping Technology

Magnetic traps

Atom laser





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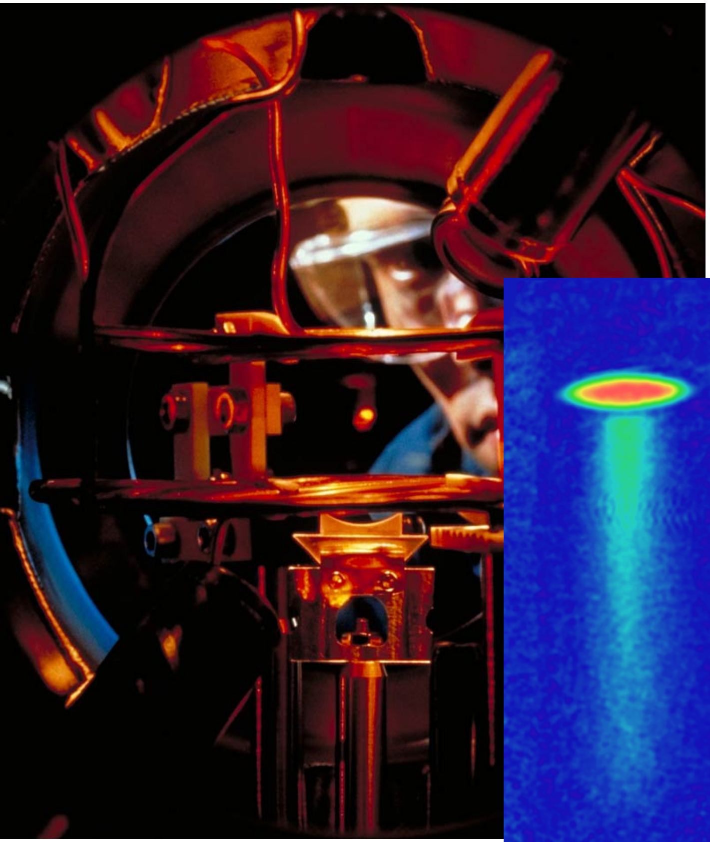

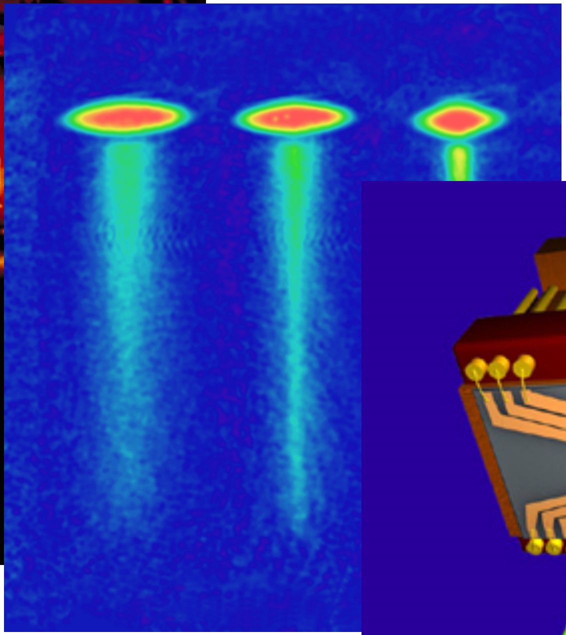

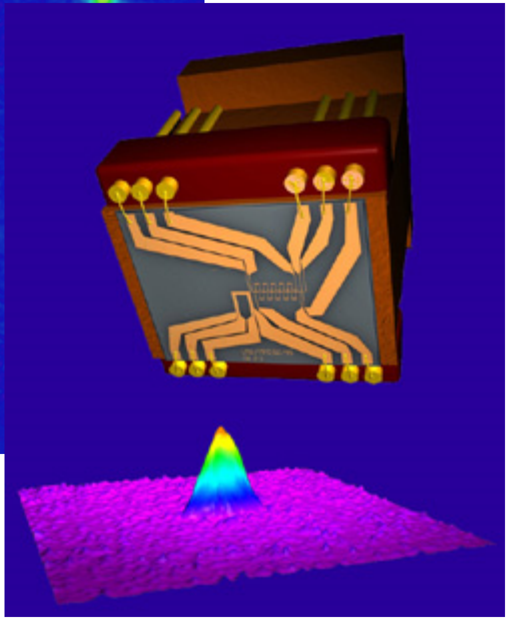

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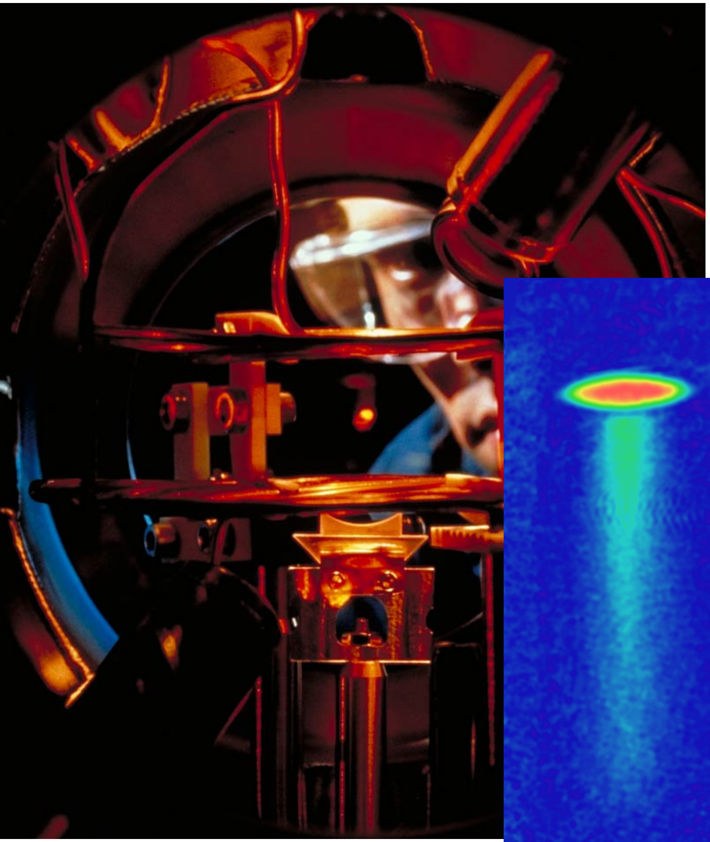
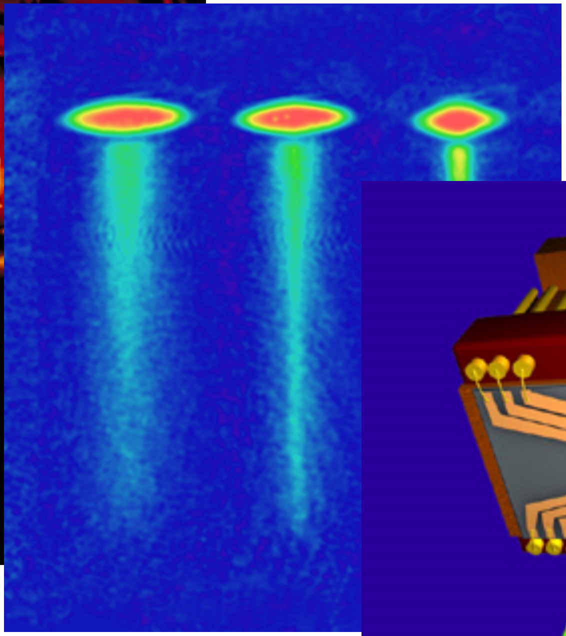
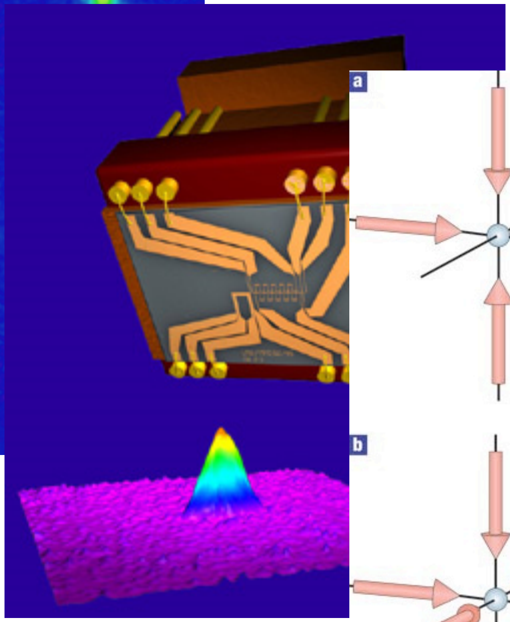
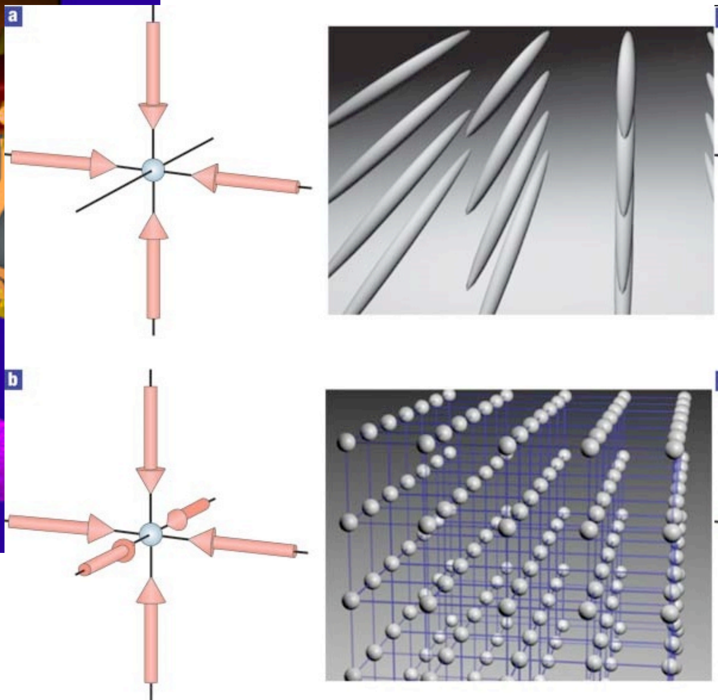
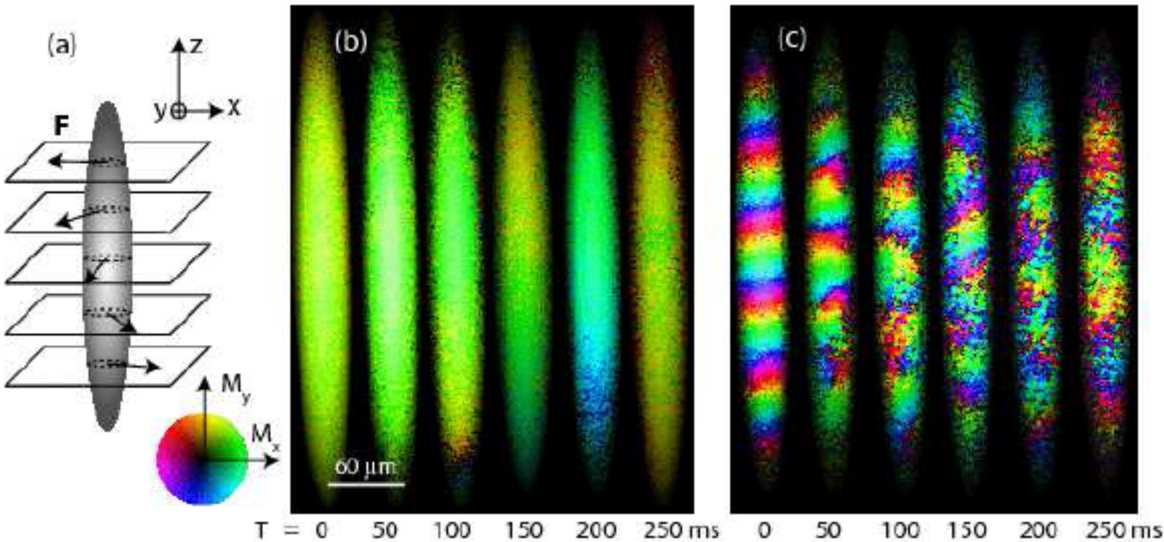
Optical Lattices

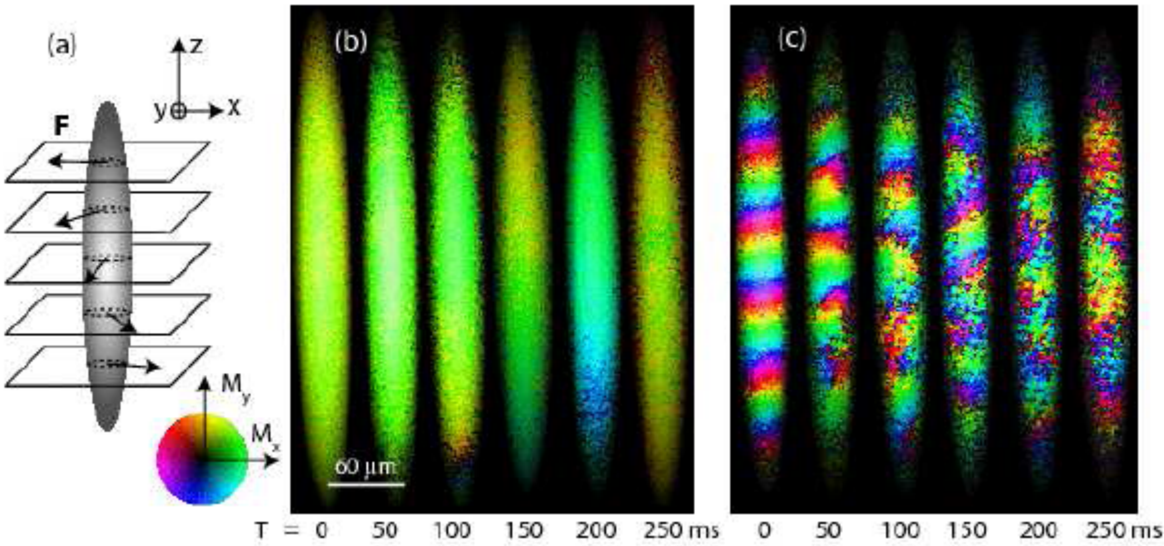





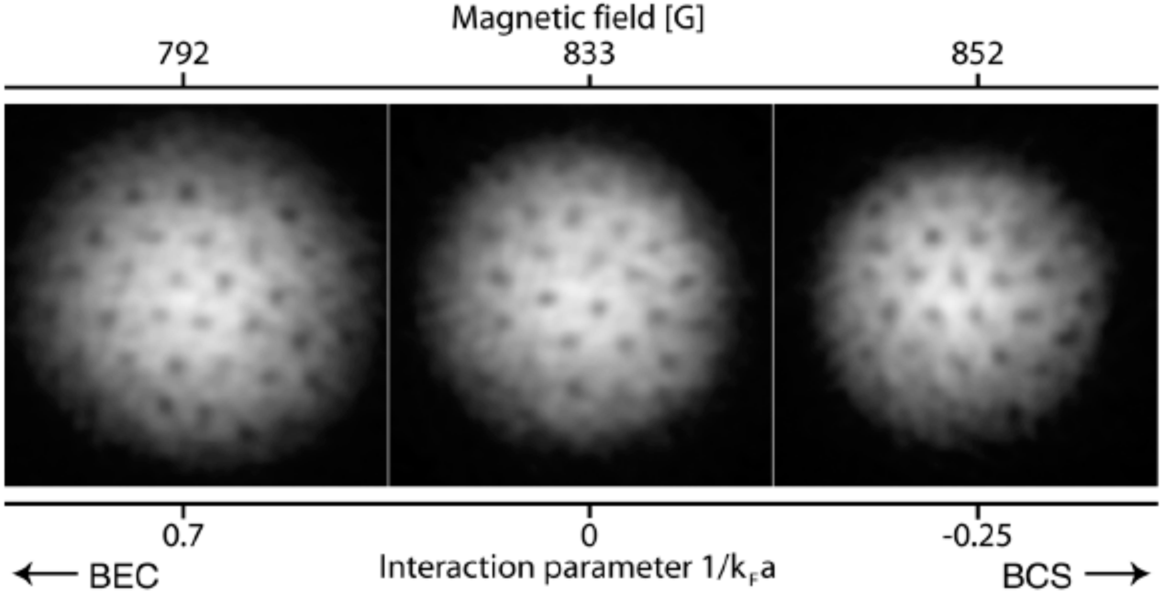
Internal States and Spin



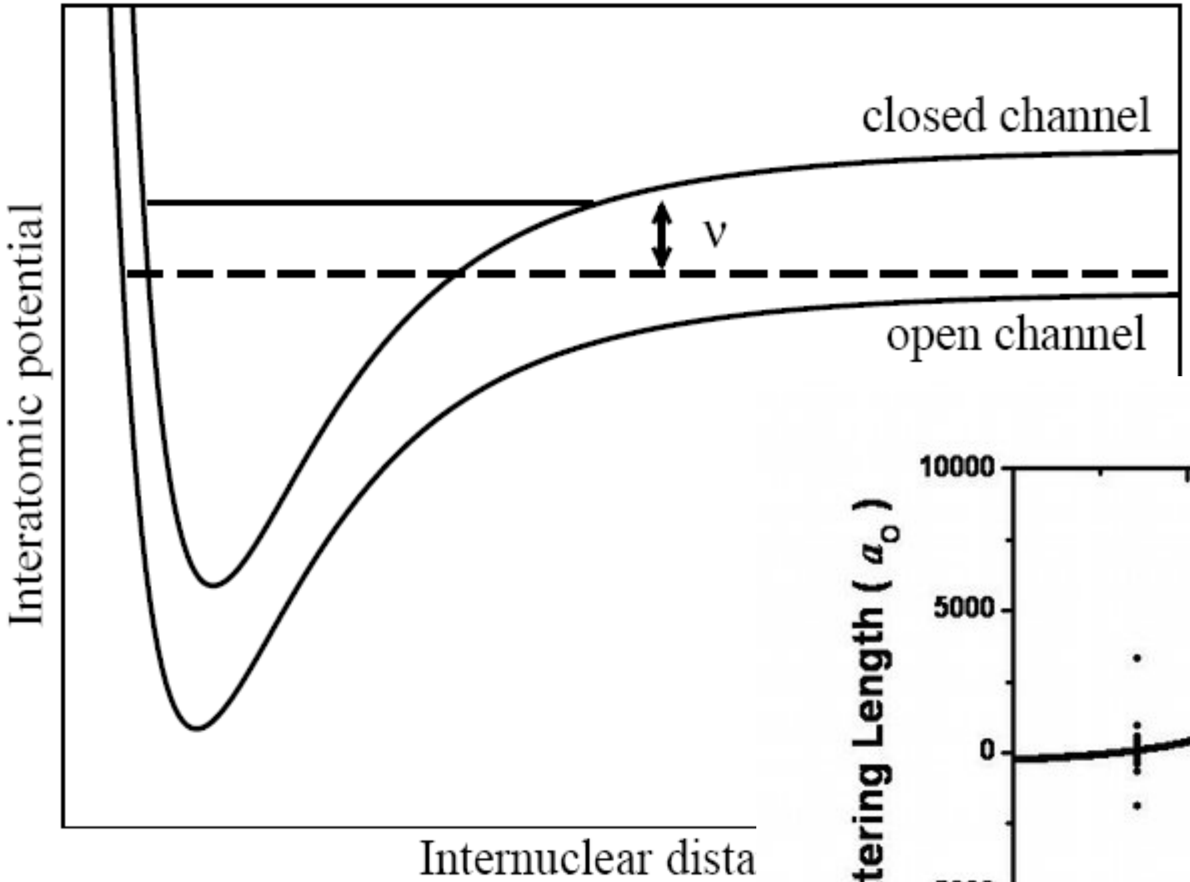
Internal States and Spin

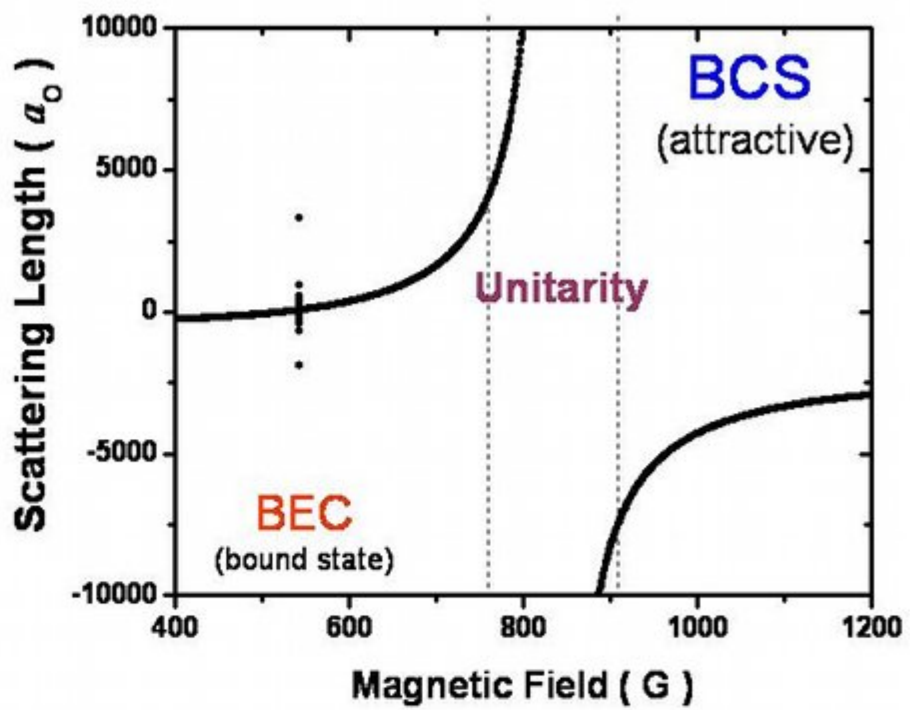
- Boson: 87Rb
  - F=2, F=1
  - Vengalatorre *et al.*, Stamper-Kurn group, Phys. Rev. Lett. **100**, 170403 (2008)
- Fermion: 6Li
  - F=3/2, F=1/2
  - Zwierlein *et al.*, Ketterle group, Nature **435**, 1047 (2005)





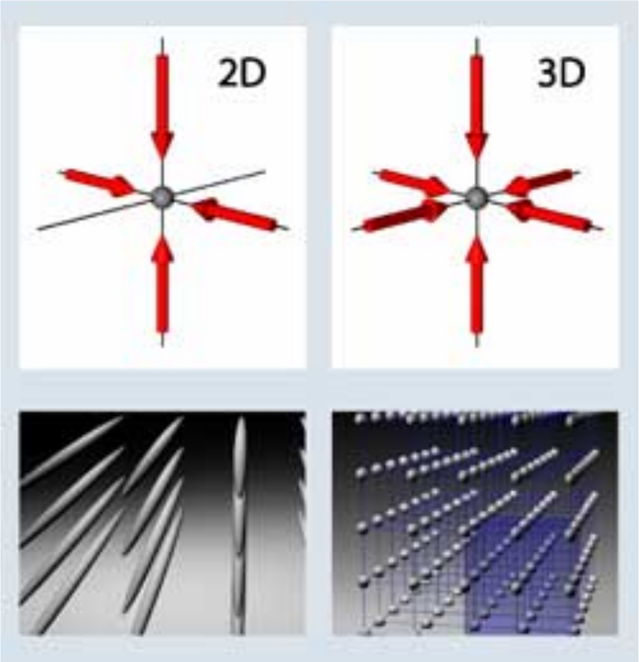
Control of Interactions





Quantum Phase Transitions

- Optical Lattices



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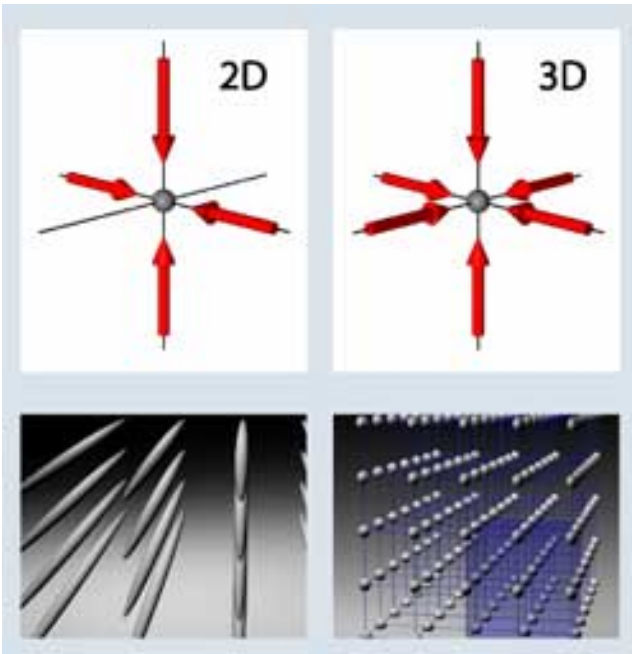
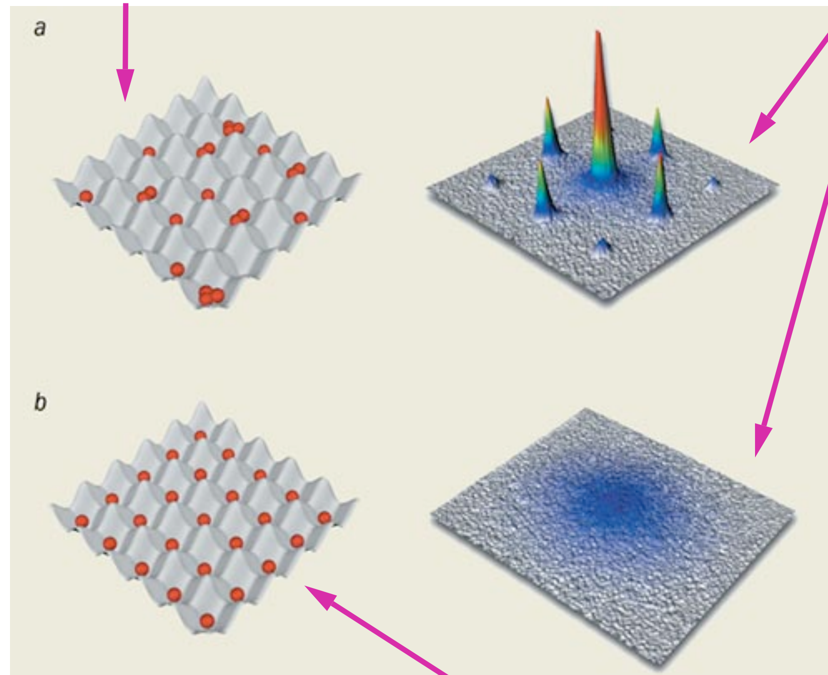


Superfluid

Density image after expansion



Mott Insulator

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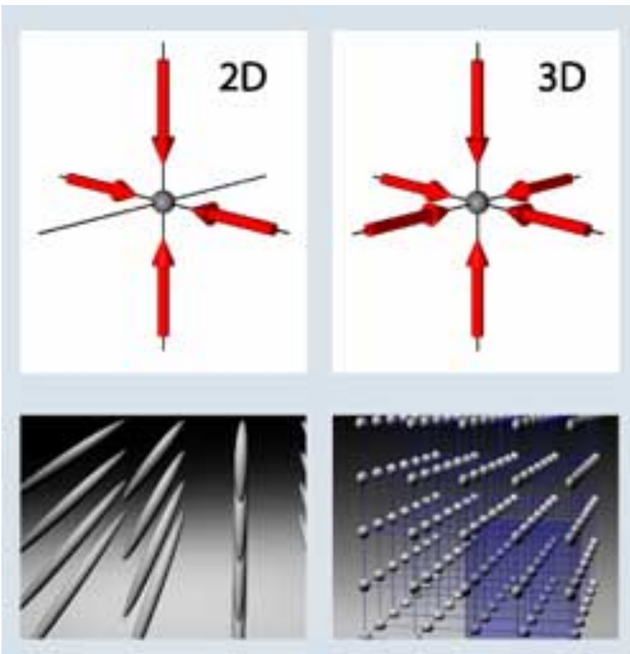

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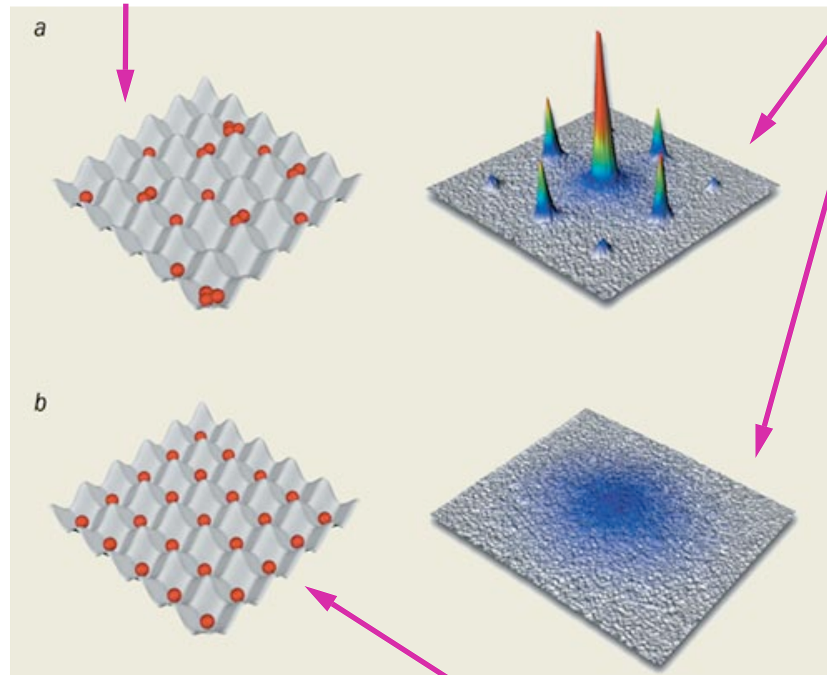

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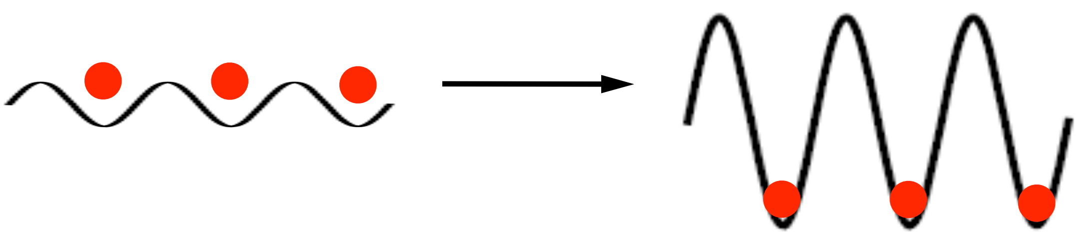
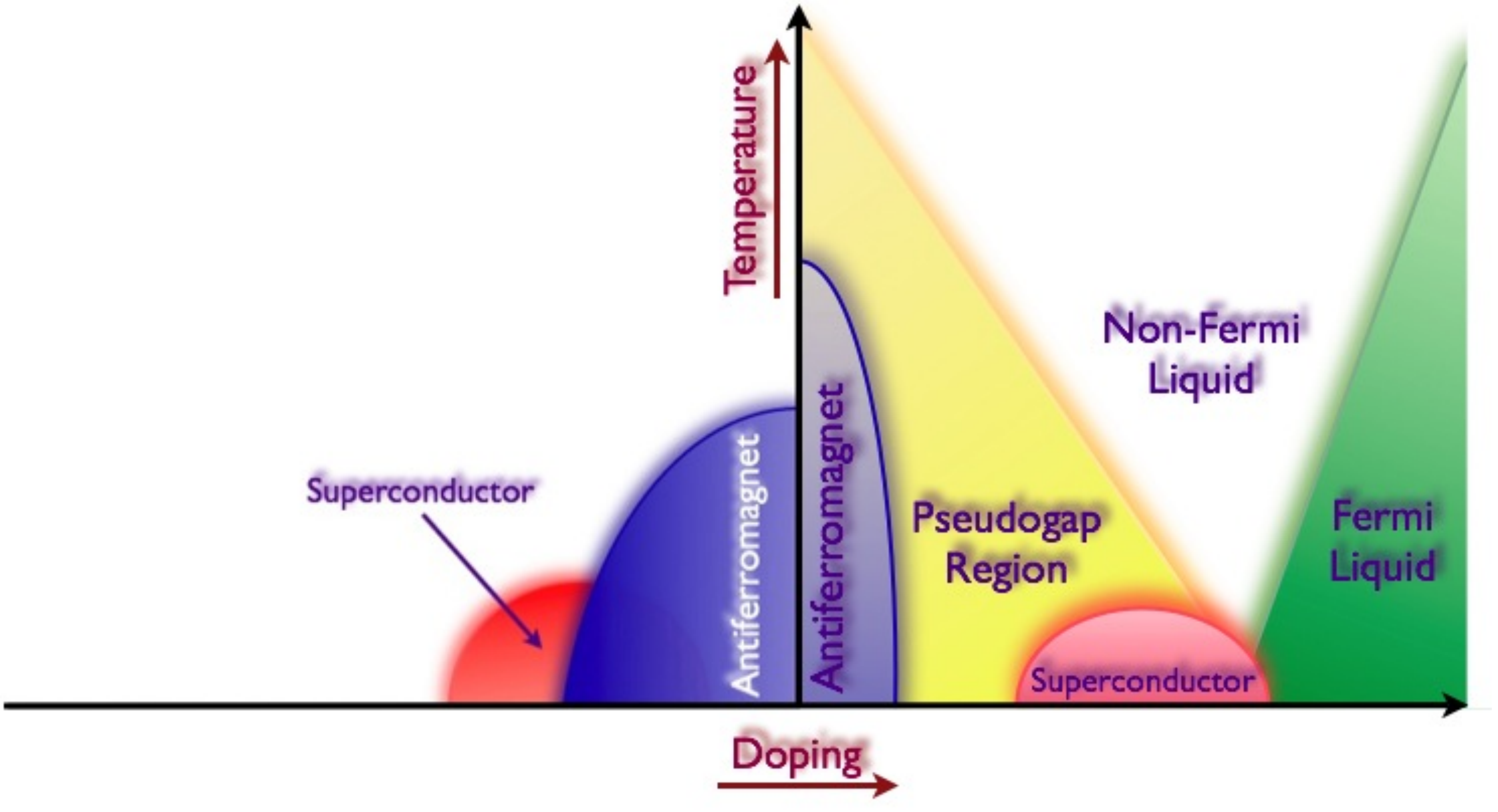


$$\Delta n \Delta \phi \geq 1$$

A Little History…

- 1925 Bose-Einstein condensation proposed (Bose and Einstein)
- 1995 BEC realized (Cornell and Wieman, Ketterle, Hulet)
- 1999 Quantum degenerate fermions realized (Deborah Jin)
- 2002 BEC in an Optical Lattice (Greiner and Bloch)
  - Dynamics of Quantum Phase Transition
- 2004 BCS-BEC Crossover (Jin, Grimm)
  - Turns over 20 years of many body theory
- 2006 imbalanced fermions (Ketterle, Hulet)
  - Never seen in solid state – hope to see FFLO soon…
- 2007 Single site imaging, CNOT gates (Weiss, Porto, Bloch)
- 2008 Quantum Degenerate Cold Molecules (Jin and Ye, Grimm)

Outstanding problem in condensed matter physics



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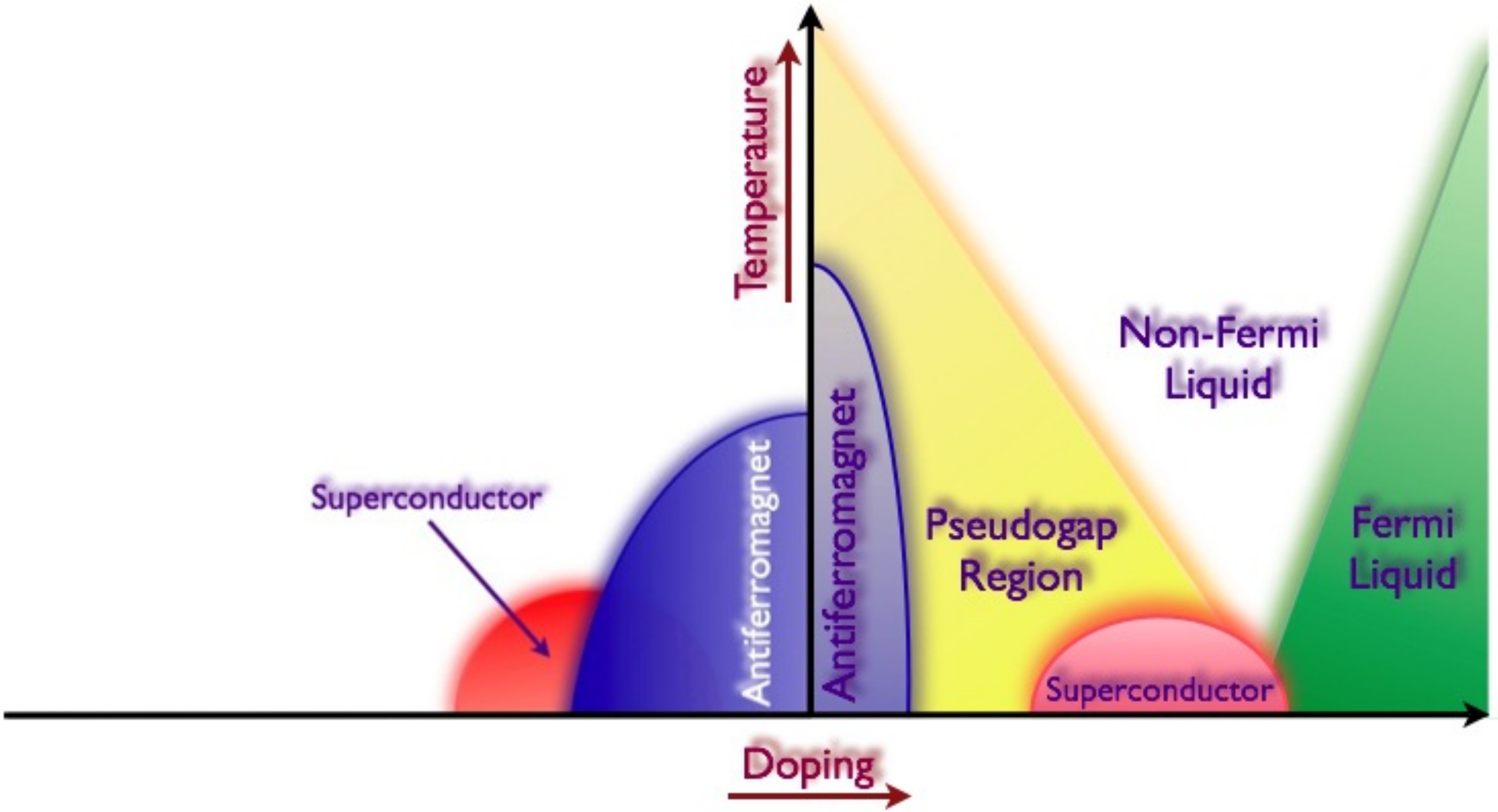

Can some or all of this behavior be reproduced by a simple model?

Hubbard Hamiltonian

$$\hat{H} = -t \sum_{<i,i'>,\sigma} \left(\hat{a}^{\dagger}_{i\sigma} \hat{a}_{i'\sigma} + \text{h.c.} \right) + \frac{U}{2} \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

Hubbard Hamiltonian

- Minimal Lattice Hamiltonian

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  - U= on-site interaction
  - <i,i'> = nearest neighbor
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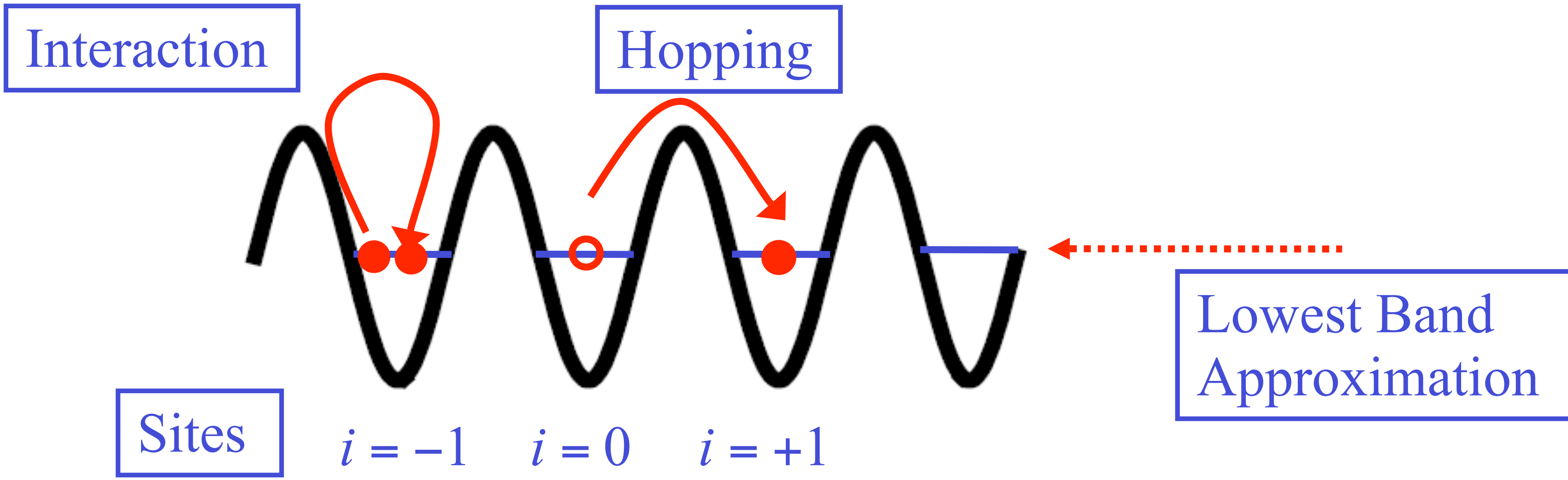
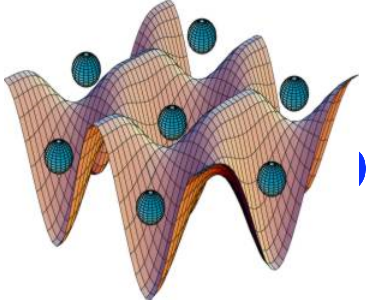
- Model in CM, First Principles for cold atoms

Sketch of Hubbard Hamiltonian Mathematics





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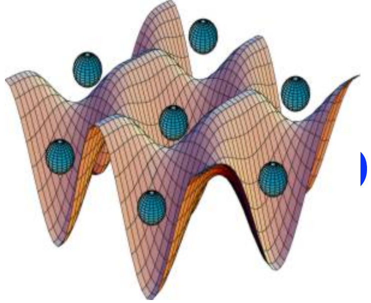

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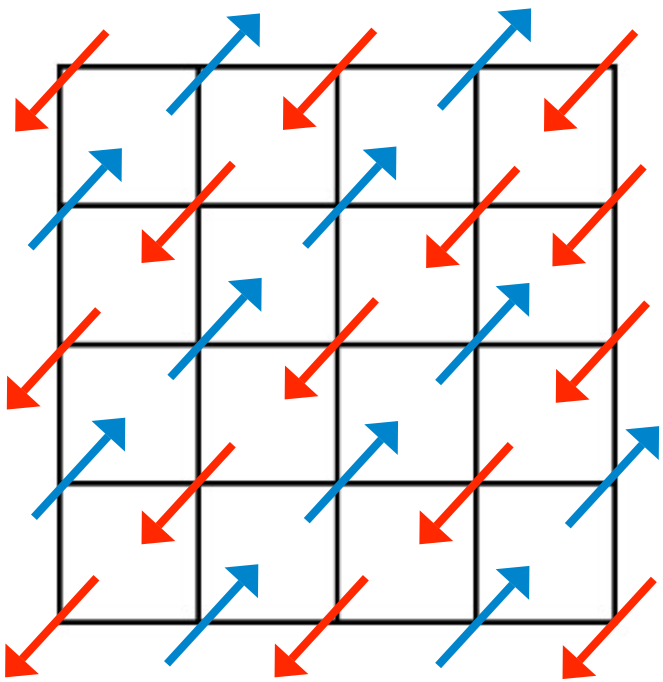
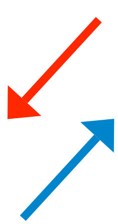
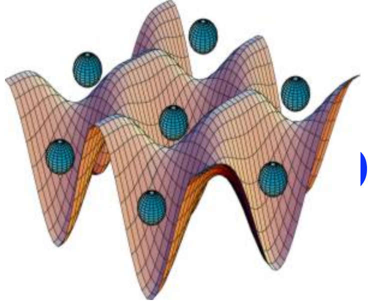
Half-filled Hubbard Model





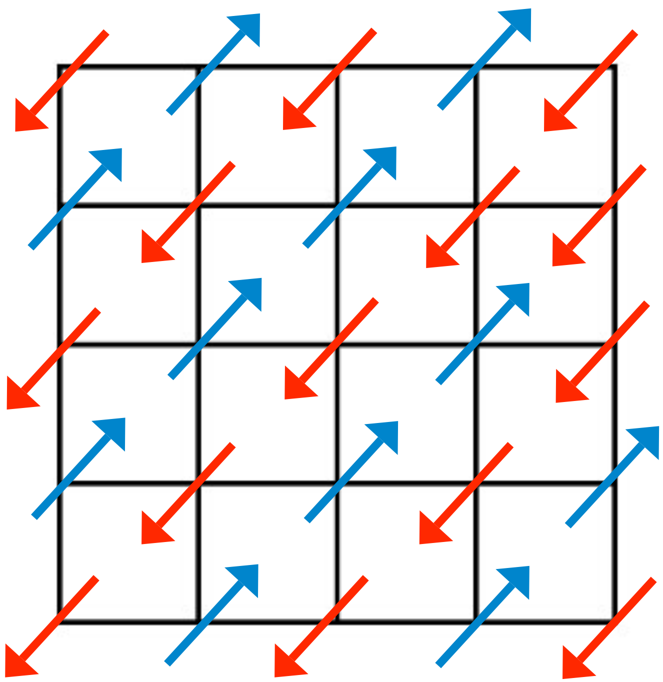
= internal state |1>

= internal state |2>

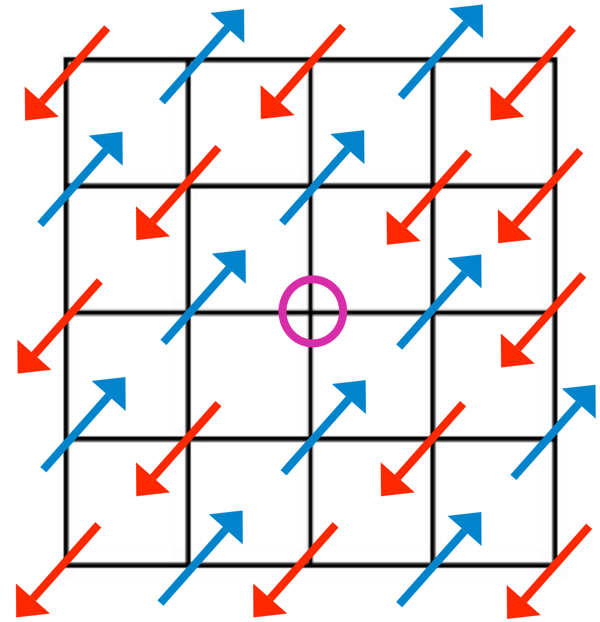


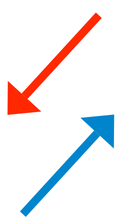
ard Hamiltonian in Cold Atoms

Half-filled
Hubbard Model



Hole-
doping





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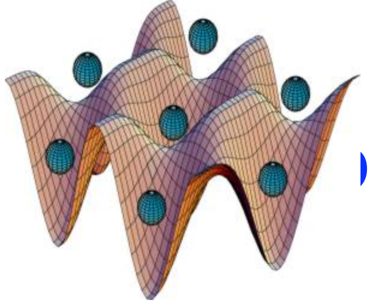

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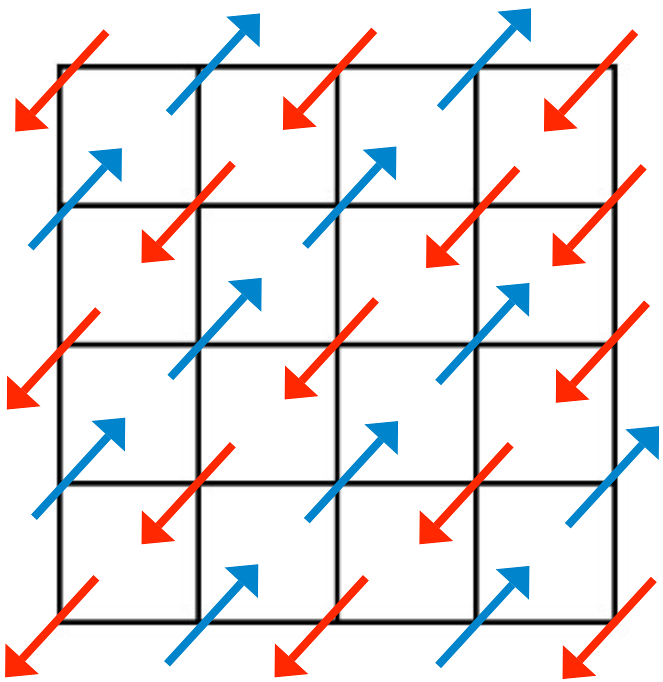

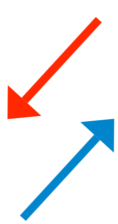

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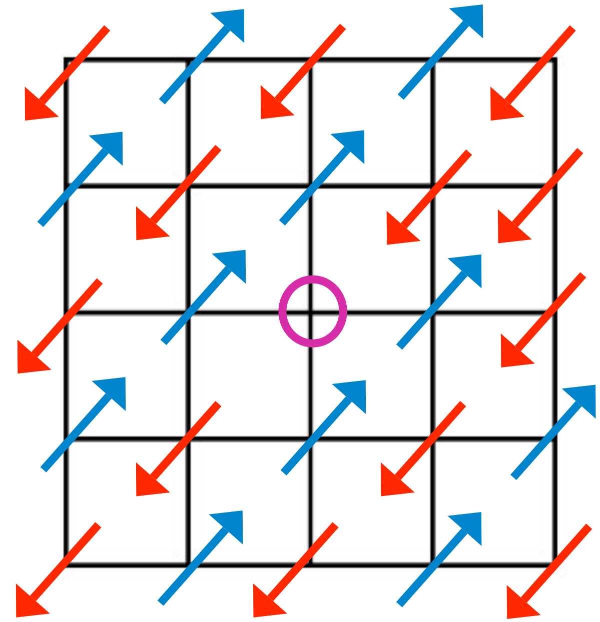
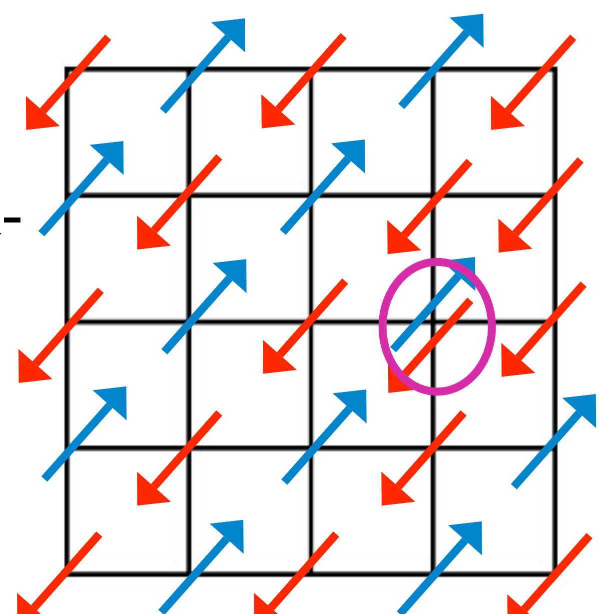
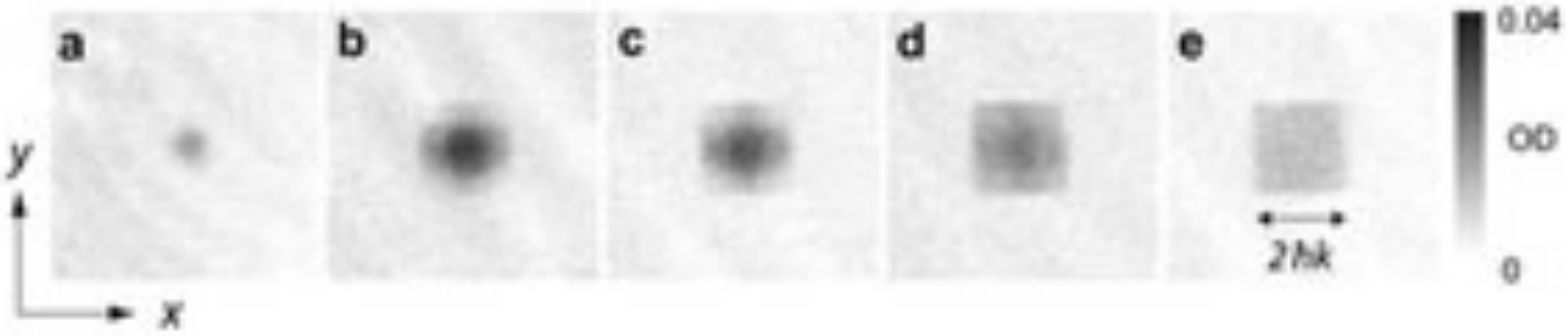
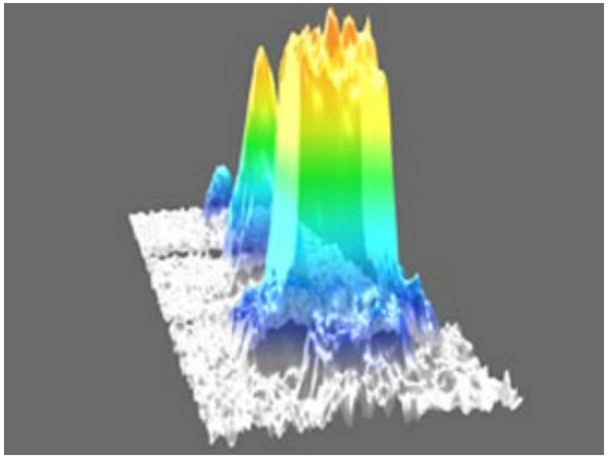


Electron-
doping



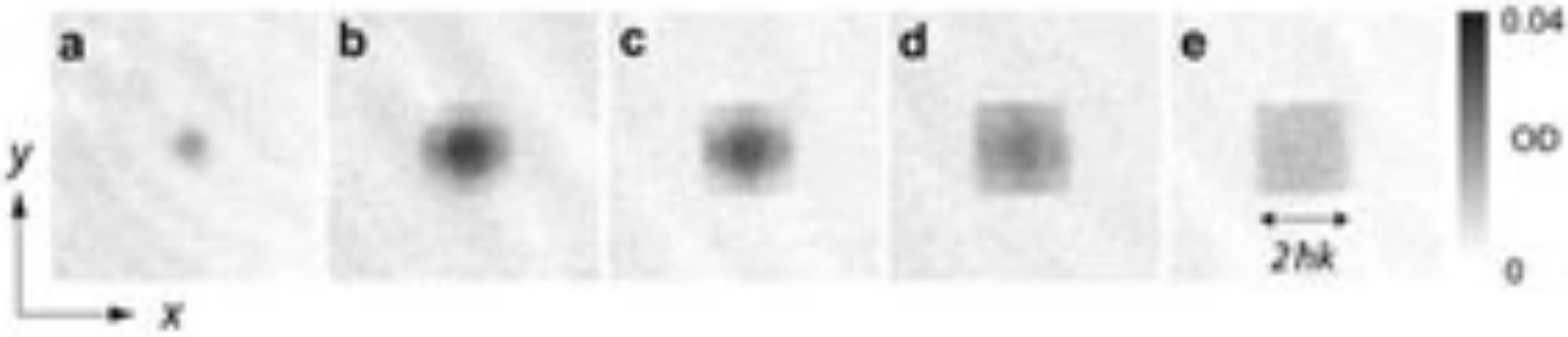
Early Fermi-Hubbard Data

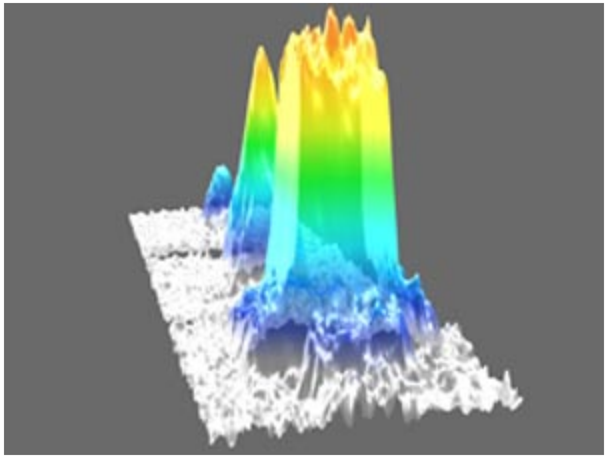


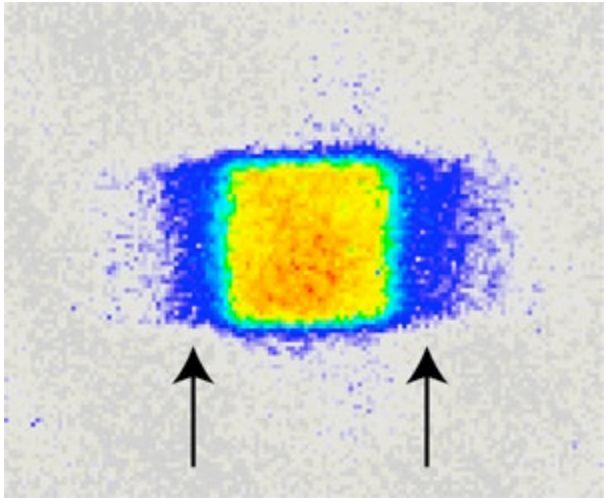


M. Köhl *et* al., Esslinger group, Phys. Rev. Lett. 94, 080403 (2005)

Early Fermi-Hubbard Data

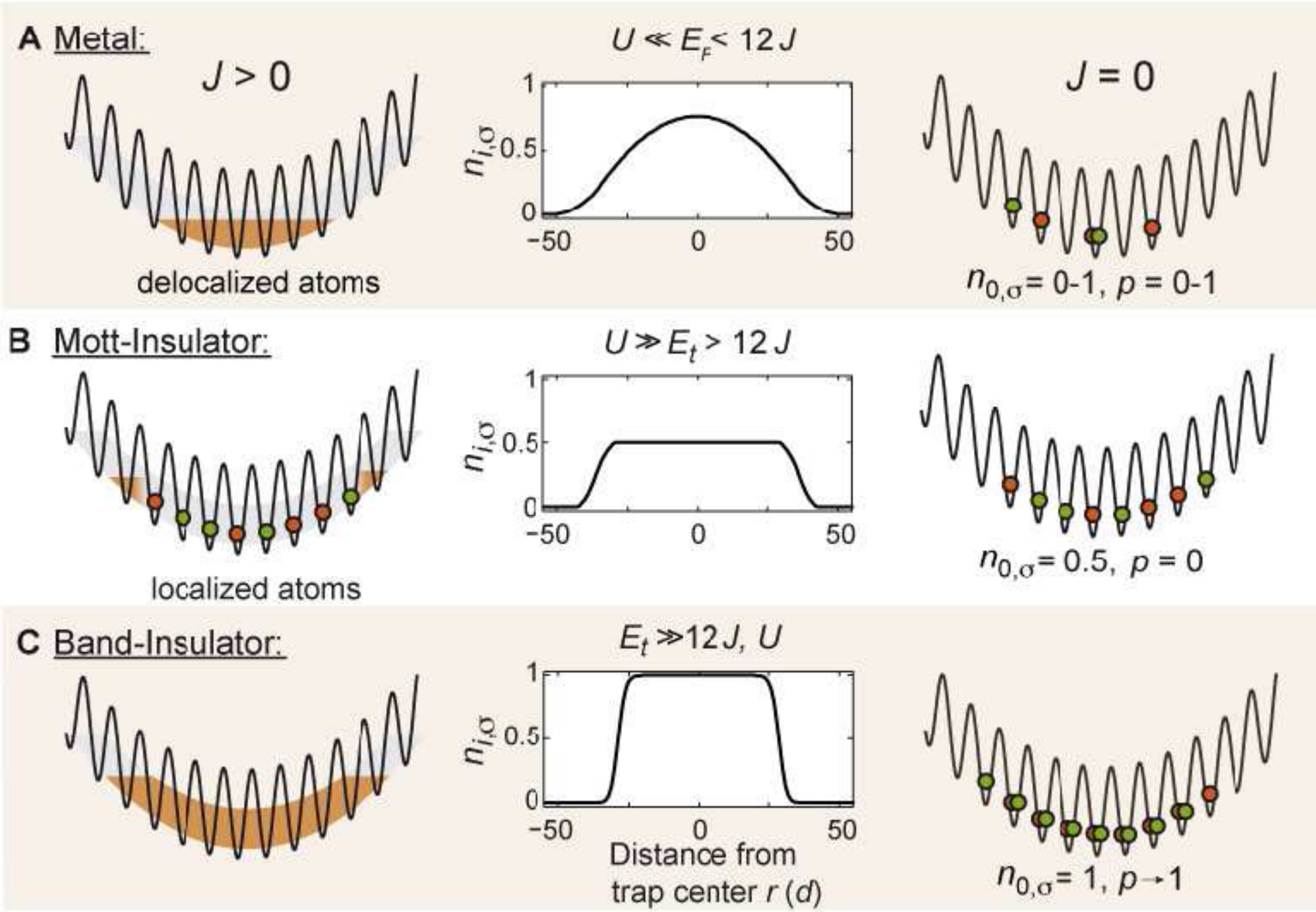






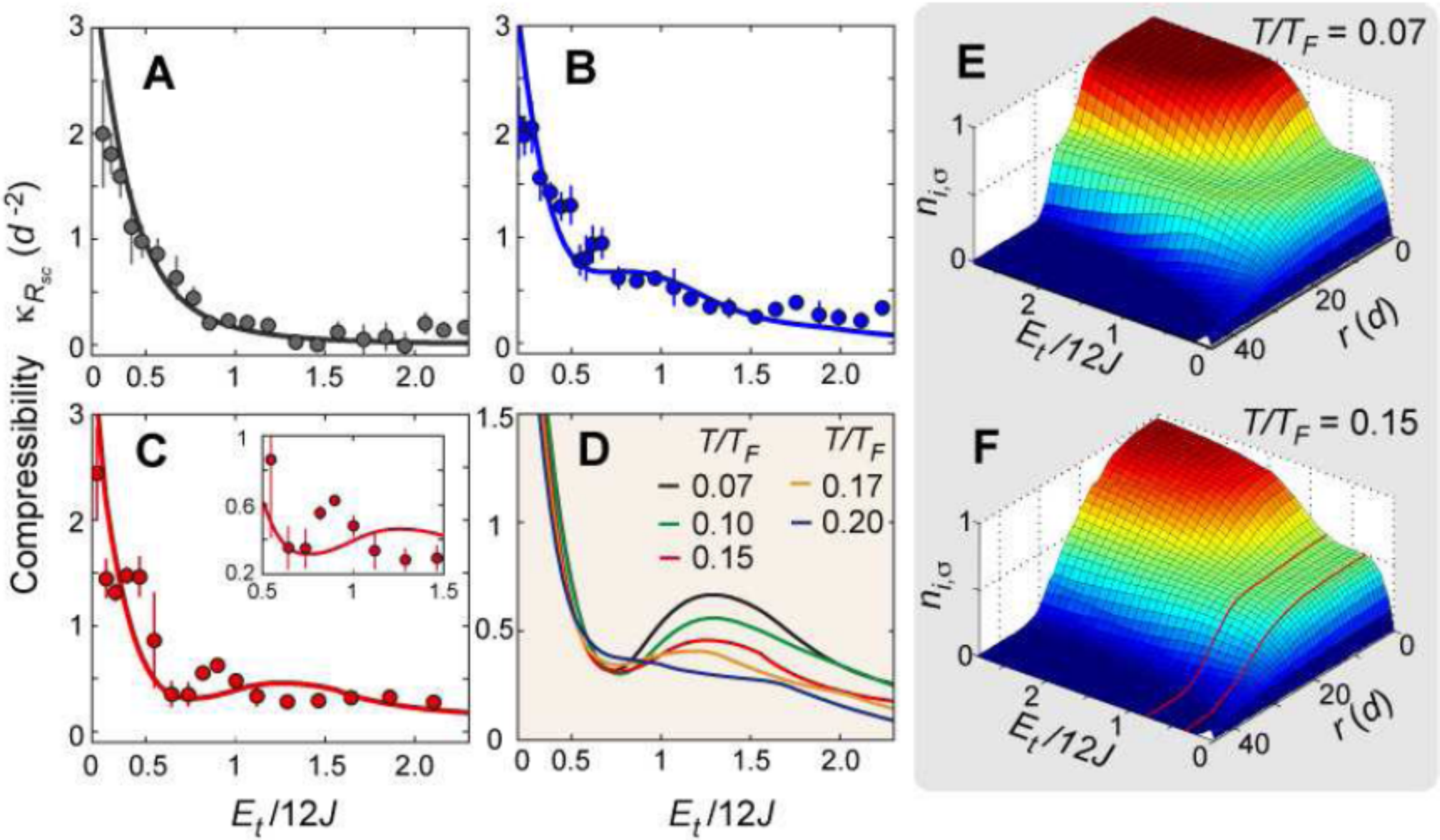
M. Köhl *et* al., Esslinger group, Phys. Rev. Lett. 94, 080403 (2005)

Recent Fermi-Hubbard Data



*R. Jordens et al., Esslinger group, Nature **455**, 204 (2008)*
*U. Schneider et al., Bloch group, Science **322**, 1520 (2008)*

Recent Fermi-Hubbard Data II



Compressibility: A=non-interacting, B=Moderate Interactions, C=Strong Interactions, D=Calculated; E,F = Density

Quantum Simulators of the (near) future

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- 1D Physics – a good starting point
- Spin models – alkali earth atoms, spin liquid
- Interplay between interactions and disorder
  - Beyond Anderson Localization

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- Recent reviews:
  - Lewenstein *et al.*, Adv. Phys. **56**, 243 (2006)
  - Bloch *et al.*, Rev. Mod. Phys. **80**, 885 (2008)

How can quantum simulations help?

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- Statics:
  - Quantum Monte Carlo
  - Dynamical Mean Field Theory
  - Density Matrix Renormalization Group Methods
- Dynamics
  - Projected Entangled Pair States (PEPS) and variations
  - Vidal's Time Evolving Block Decimation (TEBD) Algorithm
    - Cut-off in entanglement, i.e., Schmidt number χ
      - χ = # of non-zero eigenvalues in reduced density matrix
      - Conserved under local unitary operations
    - Algorithm scales as $\sim L \chi^3 d^3$
    - Recall L sites, spin-1/2 particles, $\dim(H)=2^L$.
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      - L = system size
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Is there a simple idea behind these new dynamical methods?

How much information is in a matrix?

```
imgArray = Import["C:\Professional\Presentations\2009\Toronto2009\EntangledTurtle.jpg"];
Show[imgArray]
```

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Singular Value Decomposition

- An m x n matrix M can be factorized as
  - $M = U \Sigma V^{\dagger}$
  - U is an m x m unitary matrix
  - Σ is an m x n diagonal matrix with non-negative real numbers on the diagonal
  - $V^{\dagger}$ is a conjugate transpose of n x n unitary matrix V

- **Convert to lists**

```
In[5]:= bb = imgArray /. Graphics -> List;

In[6]:= pixelvals = bb[[1, 1]];

        Dimensions[pixelvals]
        Dimensions[pixelvals][[1]] * Dimensions[pixelvals][[2]]

        {300, 416}

        124 800
```

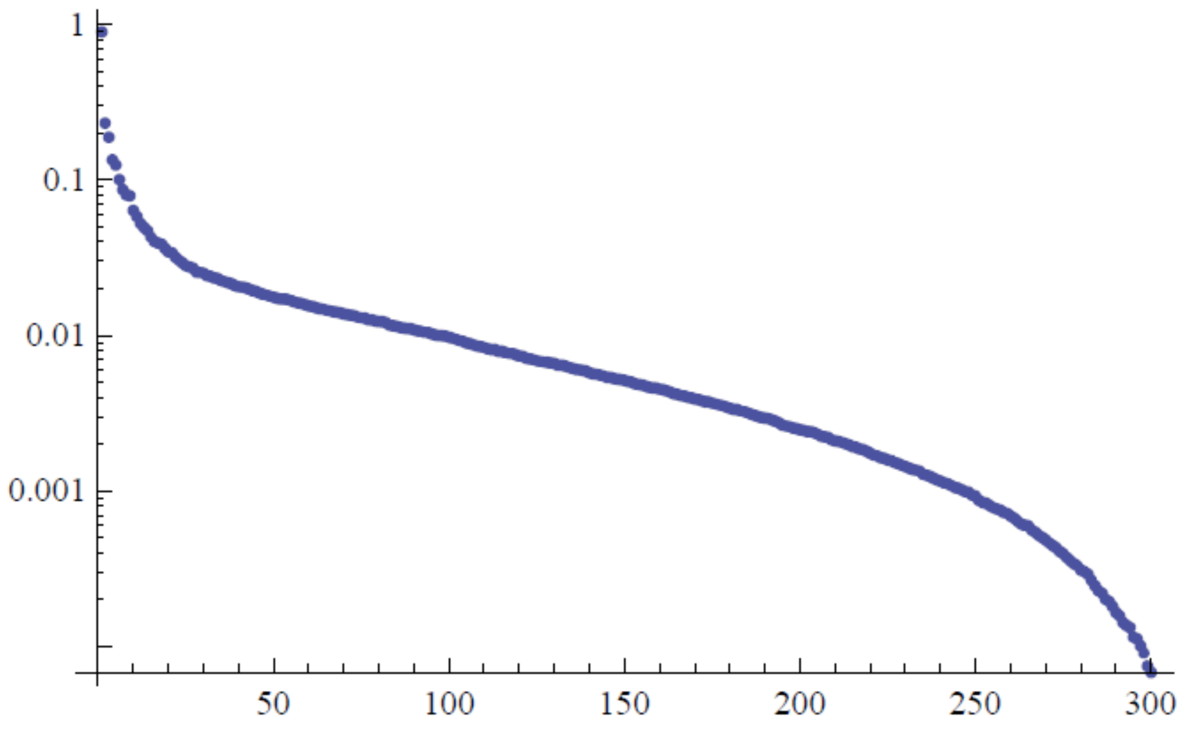
Turtle Singular Values Plot

- **Find the Singular values and normalize them**

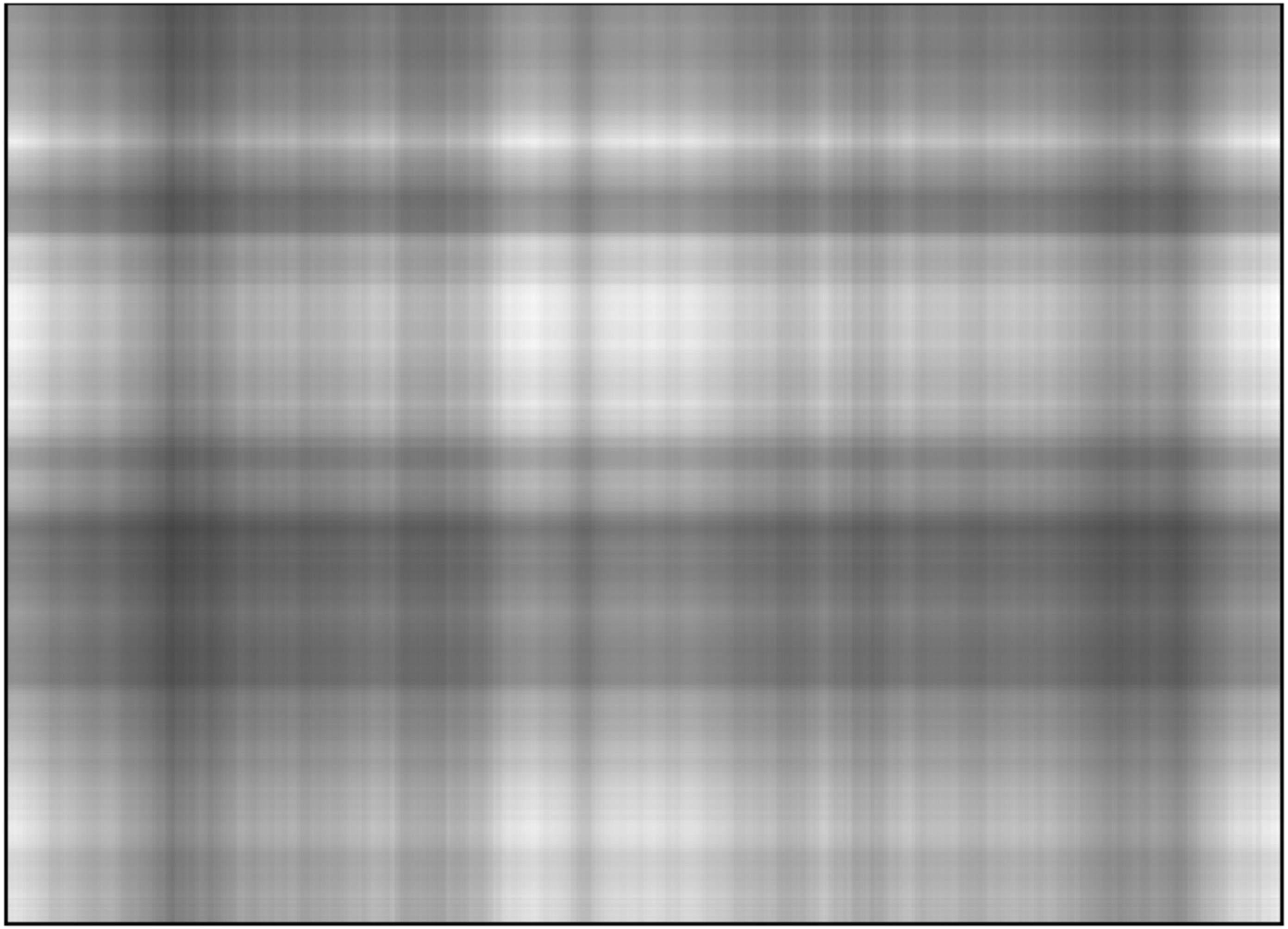
```
In[7]:= svlist = SingularValueList[N[pixelvals]];
        norm = svlist.svlist;
```

In[9]:= ListLogPlot$\left[\frac{1}{\text{Sqrt[norm]}}\text{ SingularValueList[N[pixelvals]]}\right]$

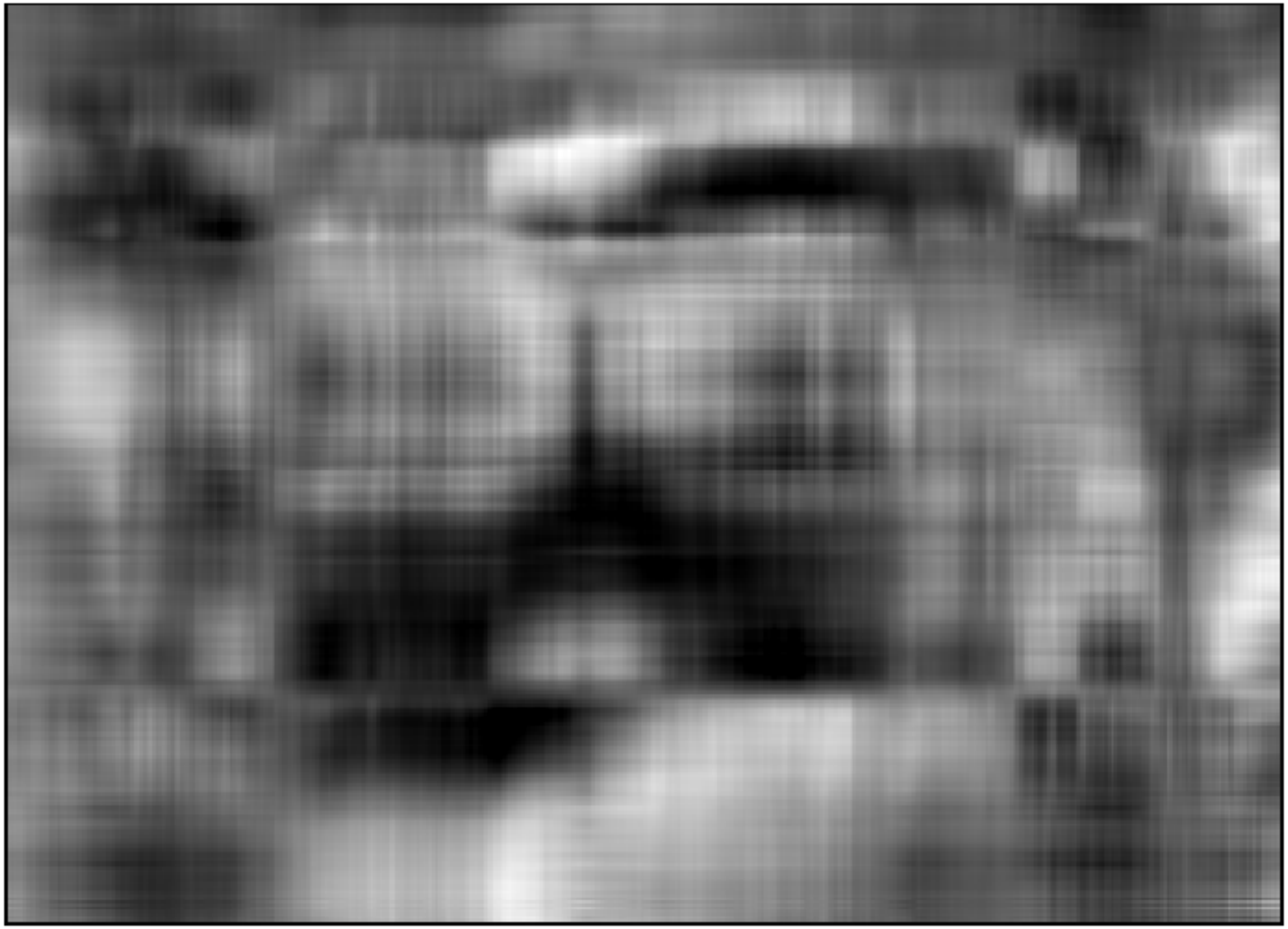
Out[9]=



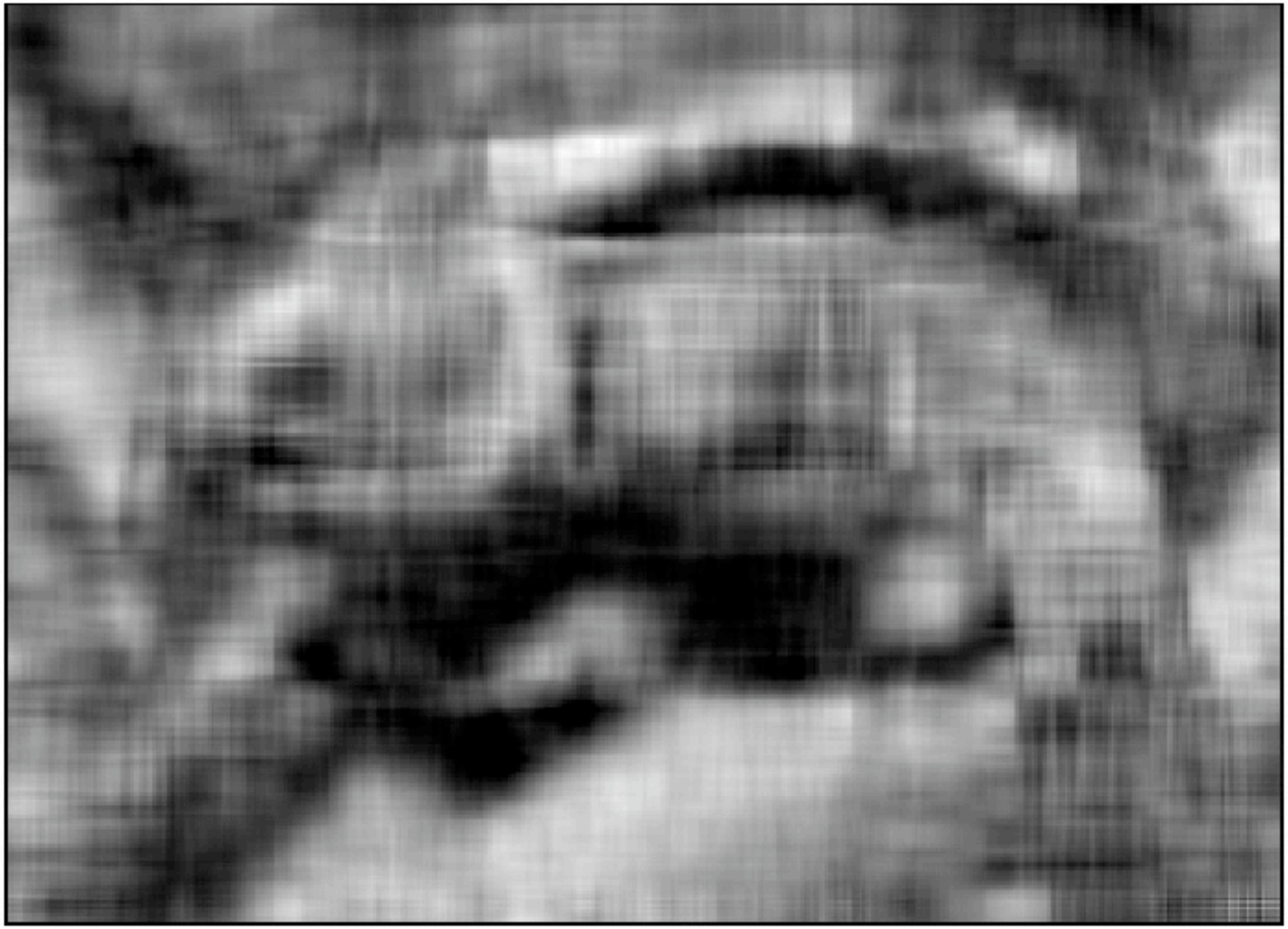
Approximate Turtle: χ=1 singular value



Approximate Turtle: χ=5 singular values



Approximate Turtle: χ=10 singular values



Approximate Turtle: χ=25 singular values

Approximate Turtle: χ=50 singular values

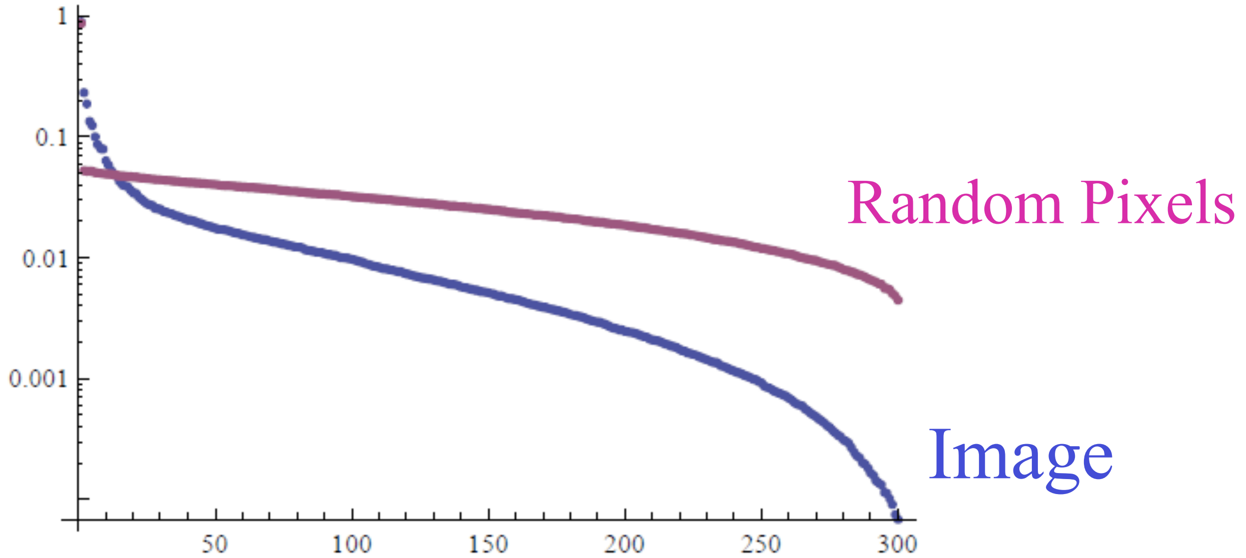
Approximate Turtle: χ=100 singular values

Why does this work?

- **Compare the singular value spectrum with that of a random pixel array**

```
In[16]:= f[i_, j_] := RandomReal[1];
randamp = Array[f, {Dimensions[pixelvals][[1]], Dimensions[pixelvals][[2]]}];
randsvlist = SingularValueList[N[randamp]];
norm2 = randsvlist.randsvlist;
ListLogPlot[
 {1/Sqrt[norm] SingularValueList[N[pixelvals]], 1/Sqrt[norm2] SingularValueList[N[randamp]]}]
```

Out[20]=



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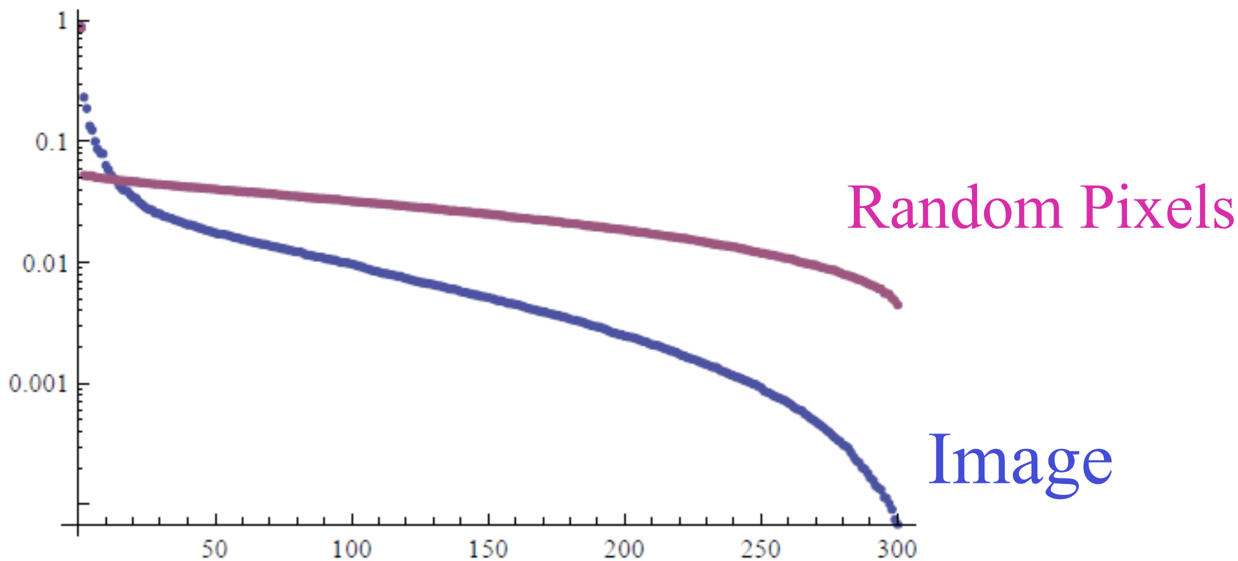
In[16]:=
```
f[i_, j_] := RandomReal[1];
randamp = Array[f, {Dimensions[pixelvals][[1]], Dimensions[pixelvals][[2]]}];
randsvlist = SingularValueList[N[randamp]];
norm2 = randsvlist.randsvlist;
ListLogPlot[
 {1/Sqrt[norm] SingularValueList[N[pixelvals]], 1/Sqrt[norm2] SingularValueList[N[randamp]]}]
```

Out[20]=



Google "Open Source TEBD" to get our free code

A New Platform: Ultracold Molecules

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- Molecules at edge of quantum degeneracy
  - 87Rb-40K, JILA
  - Absolute ground state
- New “handles” compared to atoms
  - Dipole
  - Rotational states

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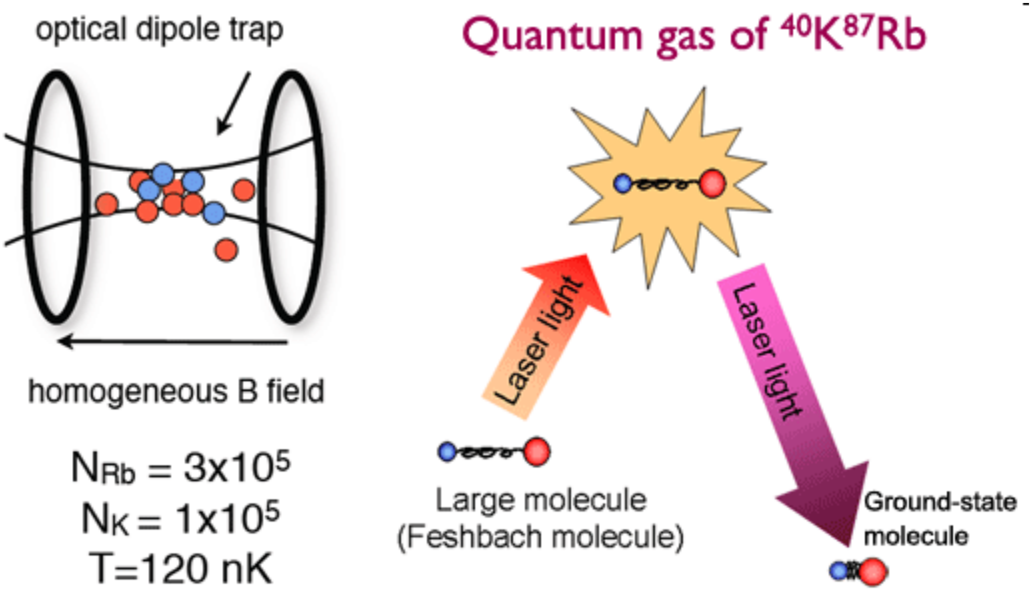

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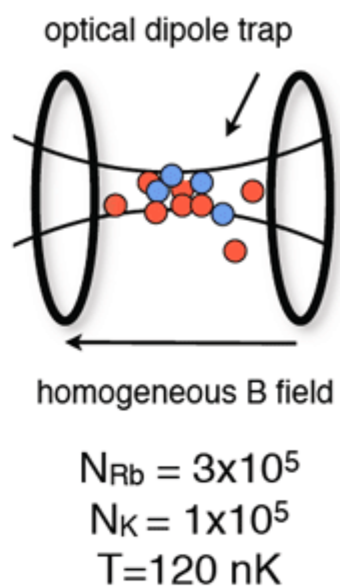
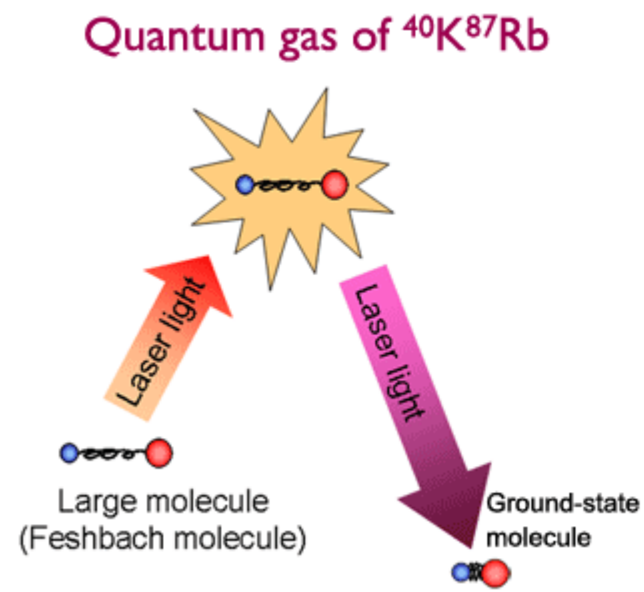
L. D. Carr, David DeMille, Roman V. Krems, and Jun Ye, "Cold and Ultracold Molecules: Science, Technology, and Applications," New J. Phys. **11**, 055049 (2009)





See Lincoln Carr and Jun Ye, "Editorial: Focus on Cold and Ultracold Molecules," New J. Phys. **11**, 055009 (2009)

Conclusions

- Ultracold physics a new platform for quantum simulators
  - High Tc as one example among many
- Quantum simulations have new methods to follow entangled dynamics
  - Many advances in static methods also
- Quantum computing will be discussed in public lecture…

The End

PEPS scalings *(from Ignacio Cirac)*

- In 1D
  - Open boundary conditions (coincides with TEBD): $\approx L^2 d^2 \chi^3$ (S. White, 1991)
  - Periodic boundary conditions: $\approx L^2 d^2 \chi^5$ (Porras, Verstraete, and IC, 2005)

    $\approx L^2 d^2 \chi^3$ (White et al, 2008)
- In 2D
  - Open boundary conditions: $\approx L^2 d^2 \chi^{10}$
  - Periodic boundary conditions: $\approx L^2 d^2 \chi^{14}$
- In 3D $\approx L^2 d^2 \chi^{20}$

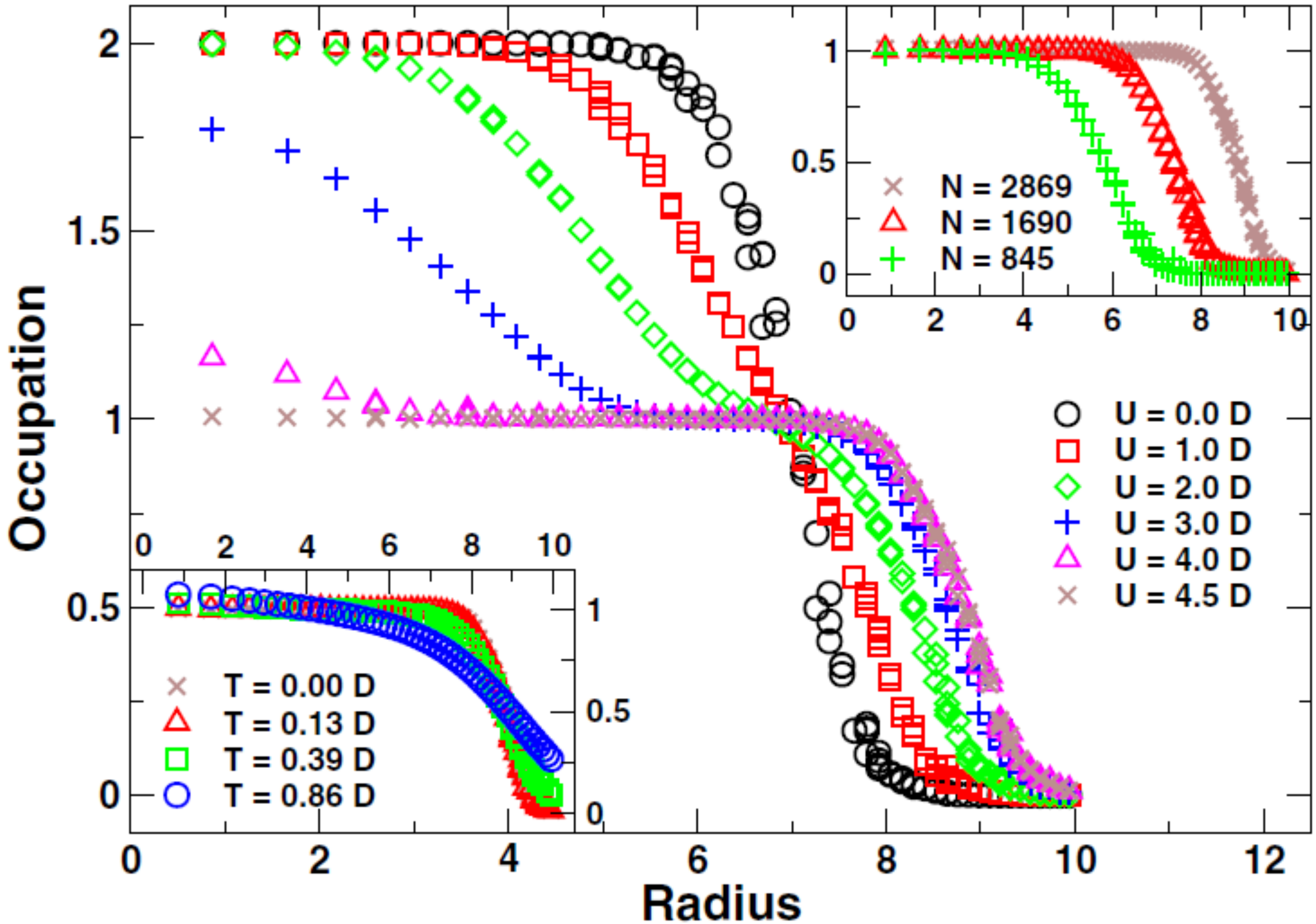
… and it is not easy to parallelize

Combine with Monte Carlo

(Schuch, Wolf, Verstraete,and IC, 2008)

(see also the work of Sandvik and Vidal)

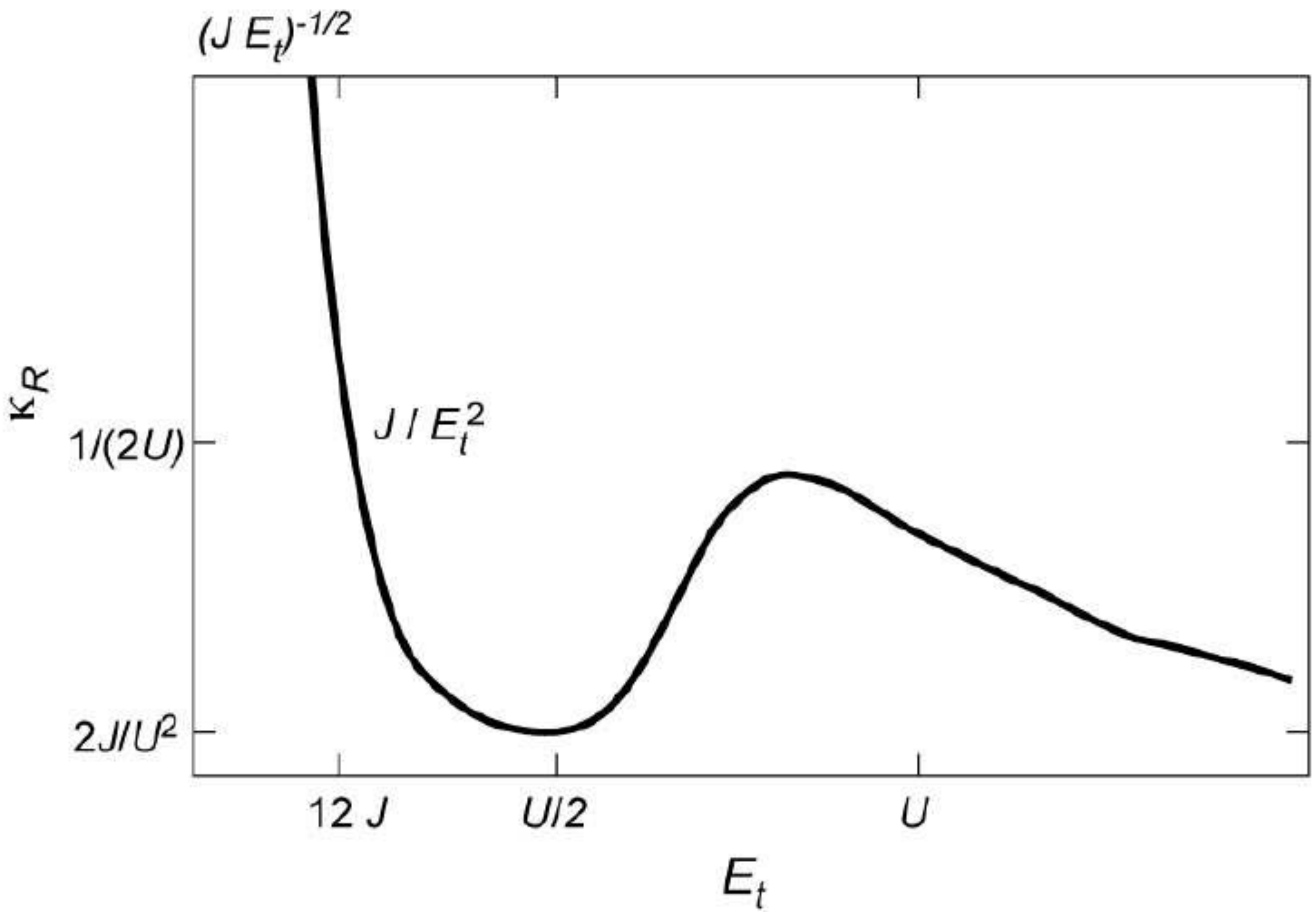
Fermi Wedding Cake



Helmes, Costi, and Rosch, Phys. Rev. Lett. ***100****, 056403 (2008)*

Compressibility: Definition and DMFT Calculations

$$\kappa_R = -\frac{1}{R^3}\frac{\partial R}{\partial V_t} \quad = \quad \frac{1}{3NR^4}\int (r^2 - r_0^2) r^2 \frac{\partial n}{\partial \mu} d^3 r$$



More Recent Fermi-Hubbard Data