Quantum Simulation II

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Supported by DARPA, JST/SORST, the Special Coordination Funds for Promoting Science and Technology, FIRST Quantum Information Processing Project

Quantum Simulation

The aim of Quantum Simulation is to provide an alternative method to solving quantum many body problems to simulations on a classical computer.

Feynman, Int. J. Theo. Phys. **21**, 467 (1982)

Idea: Use quantum mechanics to simulate quantum mechanics!

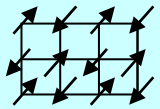
Why aren't classical computers very good at simulation?

N=40 S=1/2 spins need a Hilbert space dimension of $\dim(H) = 2^N \approx 10^{12}$

Applications

Solid state physics

Spin, electronic, bosonic models (e.g. Heisenberg, Hubbard, t-J, etc.),



High energy physics

QCD lattice gauge theory

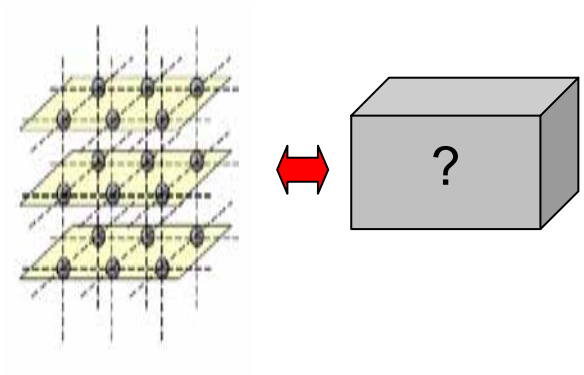
Quantum chemistry

Electronic structure of molecules

Approaches to quantum simulation

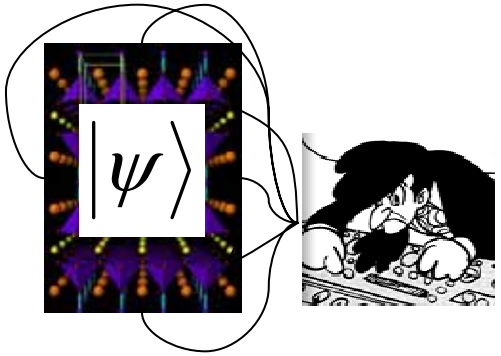
There are two main approaches to quantum simulation, analogue and digital.

“Analogue” QS



In analogue QS, an experimental system with similar properties to a material of interest is created in the laboratory. The created system is studied directly to extract information about the original material.

“Digital” QS

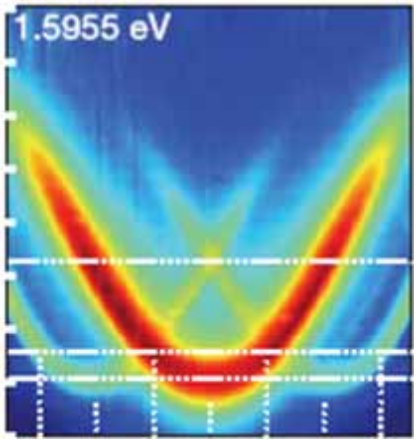


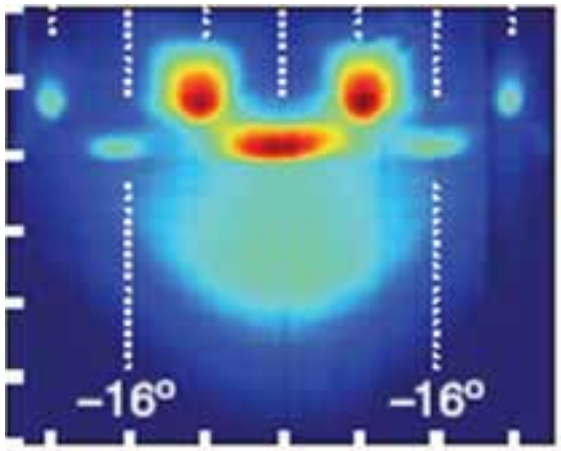
In digital QS, a quantum computer is used to simulate a particular Hamiltonian, much like classical computers simulate systems today. Quantities of interest are calculated using a suitable algorithm.

Outline

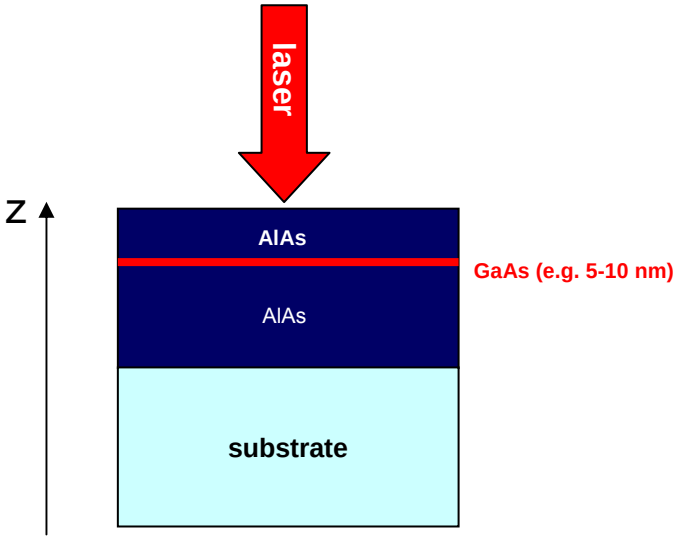
1) Quantum simulation using exciton-polaritons (Analogue)
   - BECs of exciton-polariton introduction
   - Interactions of exciton-polaritons
   - Bose-Hubbard models of exciton-polaritons
   - 1D and 2D arrays
   - BCS-BEC crossover
2) Digital Quantum Simulation
   - Phase estimation algorithm
   - Efficiency
   - Simulatable Hamiltonians
3) Computation by quantum simulation (Analogue)
   - General principle
   - Using BECs to speed up computation
   - Feedback control

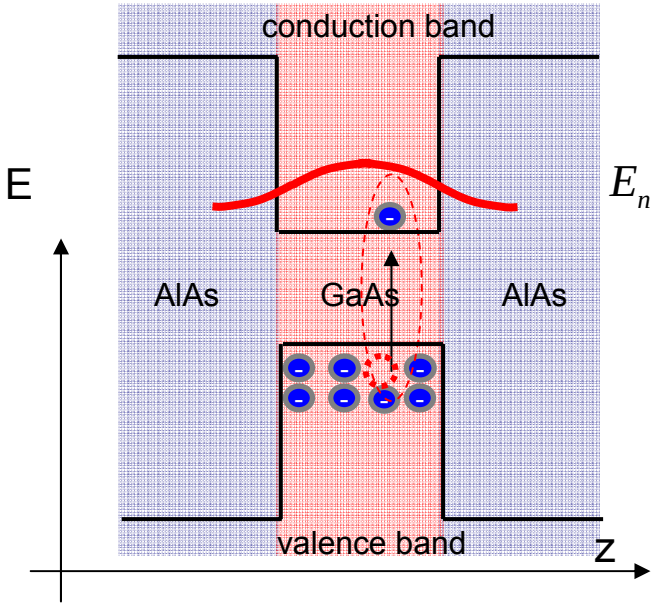
(1) Quantum simulation using exciton-polaritons





Excitons





square well:

$$E_n = \frac{\hbar^2 \pi^2 n^2}{2m^* L^2}$$

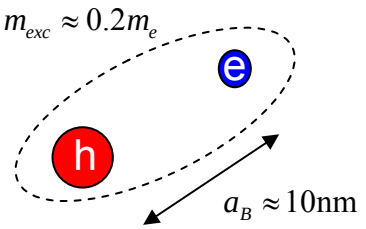
$$\approx (56meV)n^2 \quad (n = 1, 2, \ldots)$$

L=10nm

$m^*=0.067m_0$

A quantum well is produced by sandwiching a narrow band gap material (e.g. GaAs) with a wide band gap material (e.g. AlAs).

Laser excitation forms bound state excitation made of a hole and electron (=exciton)



1 exciton case

Gives an Schrodinger equation for 1 electron and 1 hole

$$\left[-\frac{\hbar^2}{2m_e}\nabla^2-\frac{\hbar^2}{2m_h}\nabla^2+U(x-x')\right]\psi(x,x')=E\psi(x,x')$$

$$U(x)=\frac{e^2}{4\pi\varepsilon x}$$

➡ Same equation as Hydrogen atom in 2D

Lowest energy state (for relative coordinate) is

$$\psi_K(r,R)=e^{iKR}\frac{2}{a_B}e^{-\frac{r}{a_B}}$$

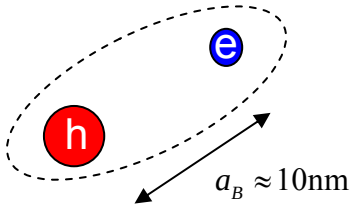
R=center of mass coordinate

r=relative coordinate

Bohr radius $a_B=\frac{4\pi\varepsilon\hbar^2}{2e^2\mu}$ Reduced mass $\mu=\frac{m_e m_h}{m_e+m_h}$

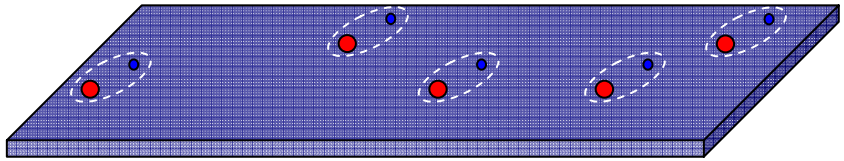
(In 2D, this is ½ the Bohr radius in 3D)

An exciton is a hydrogen atom in a semiconductor made of an electron and a hole



Low density excitons

In the low density limit, we can have many excitons in the same sample



Assuming all the excitons are in their ground states, define an exciton creation operator

$$C_K^+ = \int d^2x d^2x' \psi_K(x,x') e^+(x) h^+(x')$$
$$= \int d^2k \psi_{1s}(k) e^+(K - k/2) h^+(K + k/2)$$

$$\psi_{1s}(k) = \frac{1}{(1+k^2)^2}$$

1s exciton wavefunction

We can write an effective Hamiltonian

$$H_{exc} = \sum_K \frac{\hbar^2 k^2}{2m_{exc}} C_K^+ C_K \qquad m_{exc} = m_e + m_h \approx 0.2 m_0$$

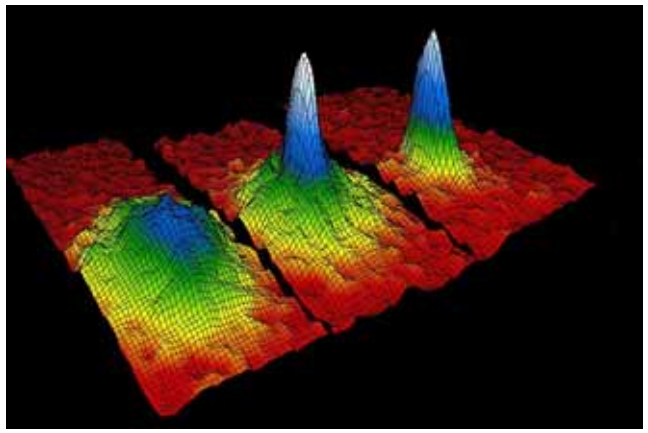
m_0 =free electron mass

Since excitons are composed of two fermions, excitons are approximate bosons:

$$\left[C_K, C_K^+\right] = 1 + O\left(\frac{a_B^2}{A}\right)$$

Bose-Einstein condensation of excitons

Quasi-boson nature of excitons means that they are candidates for BEC!



In 3D, BEC occurs at the critical temperature

$$k_B T = \frac{2\pi\hbar^2}{m}\left(\frac{n}{2.612}\right)^{2/3} \quad \text{or} \quad n\lambda_T^{\,3} = 2.62 \qquad \lambda_T = \sqrt{\frac{2\pi\hbar^2}{mk_B T}}$$

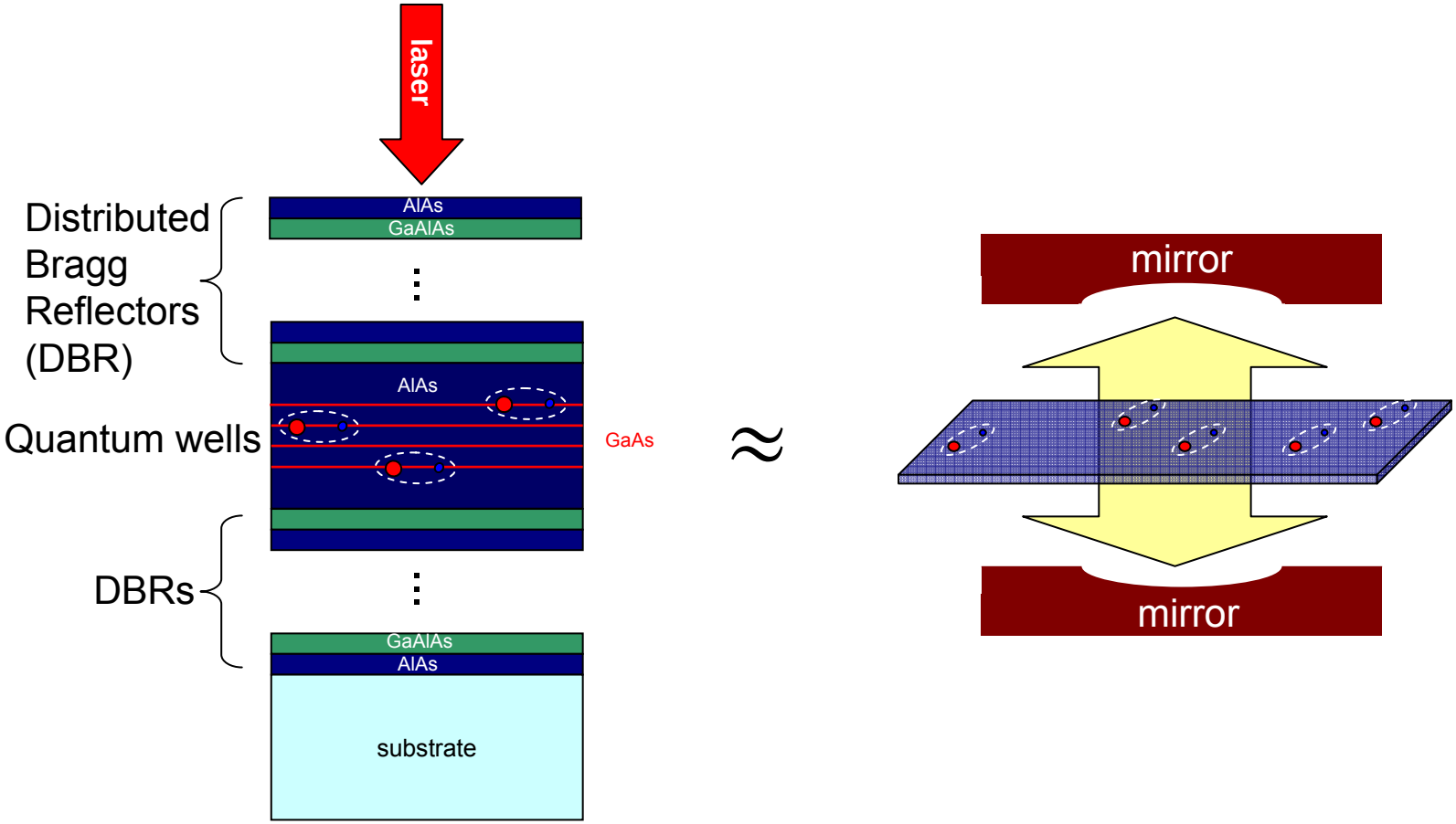
In 2D, BEC doesn't occur for an infinite system, but for a finite system of area L^2

$$n\lambda_T^2 = 2\ln(L/\lambda_T)$$

Enemies of BEC: 1) Anderson localization 2) Disassociation of excitons 3) Mott transition

Bose-Einstein condensation has NOT been observed for excitons, despite many years of trying.

Exciton-polaritons



By placing the exciton in a cavity, we can form a superposition statie of a cavity photon and an exciton. This is an exciton-polariton.

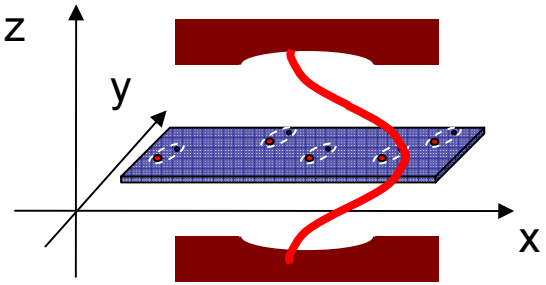
$$\left| polariton \right\rangle = a \left| exciton \right\rangle + b \left| photon \right\rangle$$

Many-body Hamiltonian for exciton-polaritons

Cavity photons

In z-direction, the wavelength is fixed by the cavity resonance

$$E_{ph} = h\nu = \frac{\hbar c|\mathbf{k}|}{n} = \frac{\hbar c}{n}\sqrt{k_z^2 + K^2} \approx \frac{\hbar c k_z}{n} + \frac{\hbar^2 K^2}{2m_{ph}}$$



$$H_{ph} = \sum_K \frac{\hbar^2 K^2}{2m_{ph}} a_K^+ a_K \qquad m_{ph} = \frac{h}{\lambda c}$$

photon acquires a mass!

Excitons

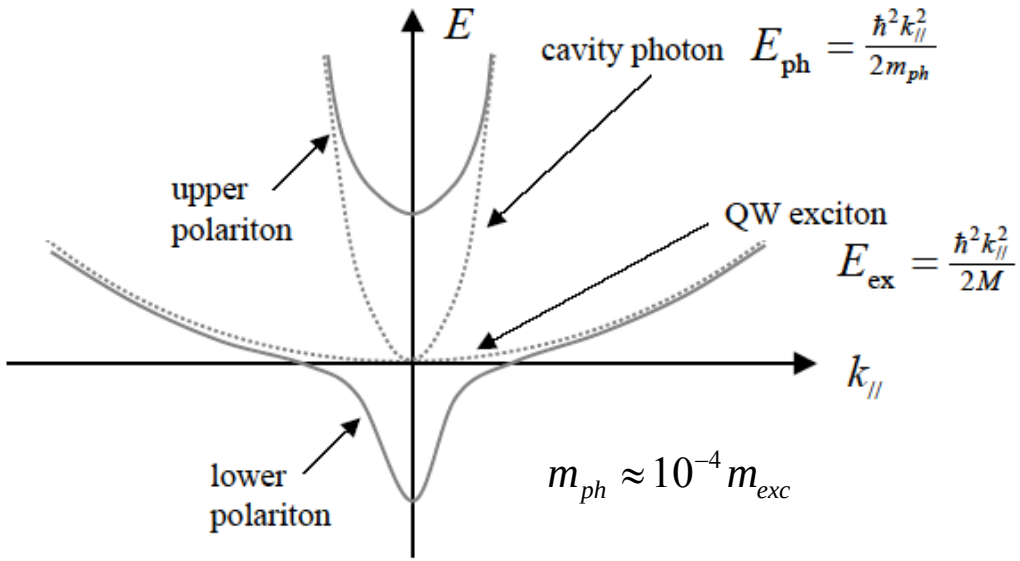
$$H_{exc} = \sum_K \frac{\hbar^2 k^2}{2m_{exc}} C_K^+ C_K$$

Exciton-photon Coupling

$$H_{exc-ph} = \hbar g_K \sum_K C_K a_K^+ + a_K C_K^+$$

Originates from the dipole approximation interaction Hamiltonian

$$H_{\text{int}} = -e\mathbf{r}\cdot\mathbf{E}$$



$$H = H_{exc} + H_{ph} + H_{exc-ph}$$

$$= \sum_K \varepsilon_{LP}(K) p_{LP}^+(K) p_{LP}(K) + \sum_K \varepsilon_{UP}(K) p_{UP}^+(K) p_{UP}(K)$$

$$p_{LP}^+(K) = u_K C_K^+ + v_K a_K^+$$

$$p_{UP}^+(K) = v_K C_K^+ - u_K a_K^+$$

$$m_{pol} = \left[\frac{1}{m_{ph}} + \frac{1}{m_{exc}} \right]^{-1} \approx 10^{-4} m_{exc}$$

Lower and upper polaritons are superposition states of excitons and cavity photons.

Bose-Einstein condensation of polaritons

There is an increasing concensus that a BEC of exciton-polaritons has been realized

Vol 443|28 September 2006|doi:10.1038/nature05131 nature

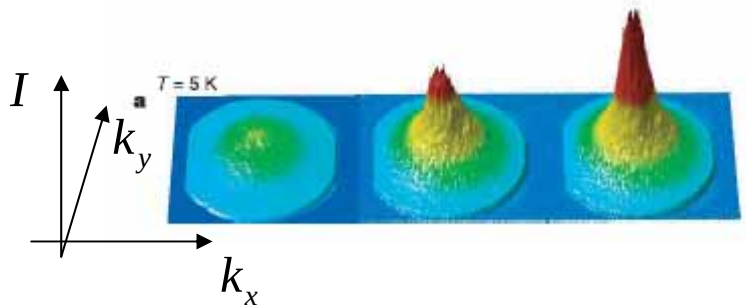
Bose–Einstein condensation of exciton polaritons

J. Kasprzak[1], M. Richard[2], S. Kundermann[2], A. Baas[2], P. Jeambrun[2], J. M. J. Keeling[3], F. M. Marchetti[4], M. H. Szymańska[5], R. André[1], J. L. Staehli[2], V. Savona[2], P. B. Littlewood[4], B. Deveaud[2] & Le Si Dang[1]

www.sciencemag.org SCIENCE VOL 298 4 OCTOBER 2002 199

Condensation of Semiconductor Microcavity Exciton Polaritons

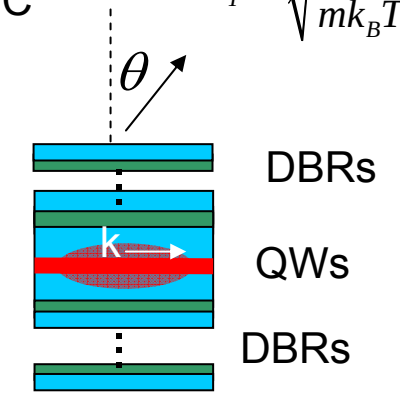
Hui Deng,[1*] Gregor Weihs,[1,2] Charles Santori,[1] Jacqueline Bloch,[3] Yoshihisa Yamamoto[1,4]



$$n\lambda_T^2 = 2\ln(L/\lambda_T)$$

$$\lambda_T = \sqrt{\frac{2\pi\hbar^2}{mk_BT}}$$

- $m_{pol} \approx 10^{-4} m_{exc}$ allows for Tc~10-100K and lower critical density for BEC
- Can overcome localization due to disorder in semiconductors
- Can read out k-distribution of condensate due to momentum conservation of in x-y plane.

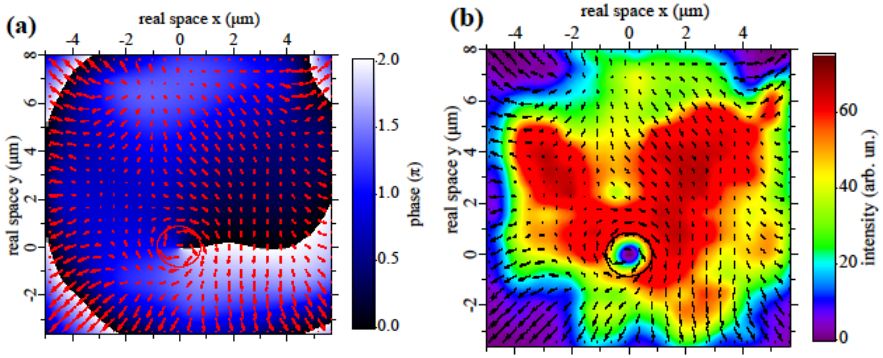


The controversy: Due to short polariton lifetime $\tau_{pol} \sim 10\text{ps}$, condensation is dynamical

Properties of exciton-polariton BECs

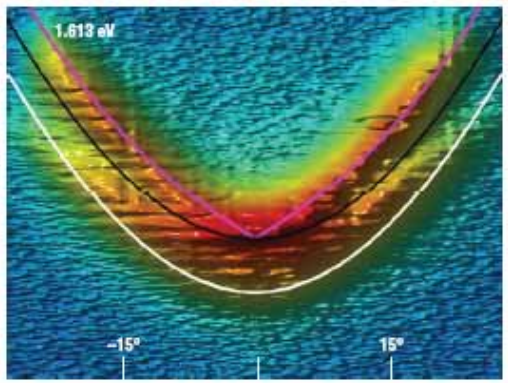
A variety of BEC related phenomena have already been observed

Vortices



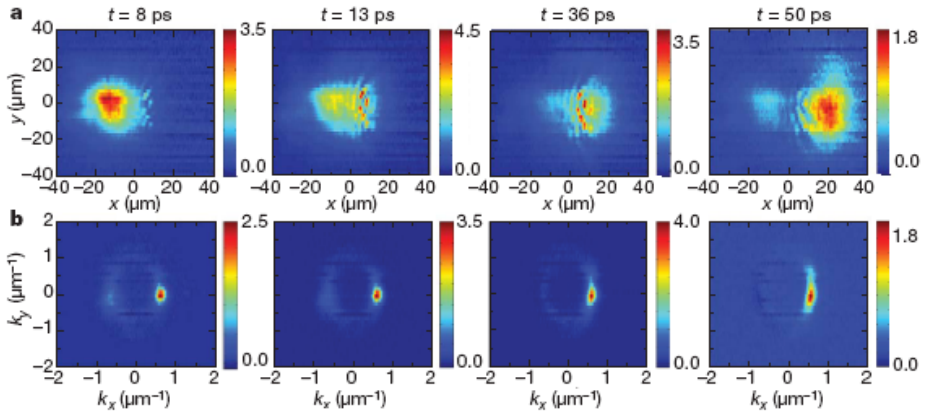
Lagoudakis et al. Nature Phys. **4**, 706 (2008)

Bogoliubov excitations



Utsunomiya et al. Nature Phys. **4**, 700 (2008)

Superfluidity



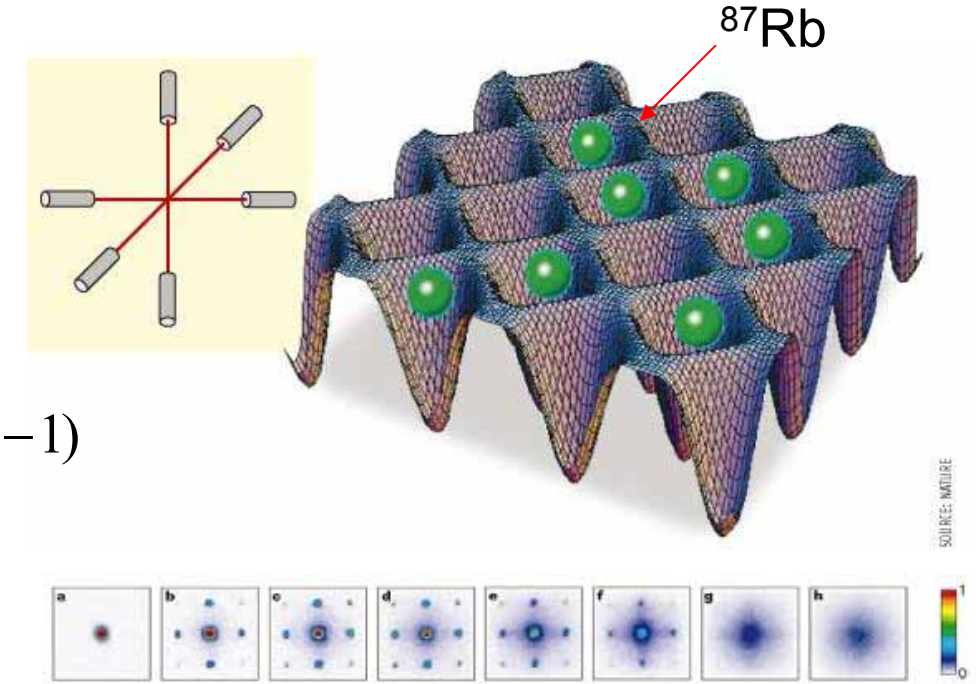
Amo et al. Nature **457**, 291 (2009)

Opens door for many atomic physics-type quantum simulation experiments

Bose-Hubbard model

Application to quantum simulation:

Perform analogue of optical lattice superfluid to Mott insulator quantum phase transition experiment:



$$H_{BH} = -t\sum_{ij}\left(b_i^+ b_j + b_j^+ b_i\right) + \frac{U}{2}\sum_i n_i(n_i - 1)$$

M. Greiner et al. Nature **415**, 39 (2002)

We need two main ingredients for this:

1) Strong enough trapping potential so that we can make the Hubbard model approximation in the first place

2) Interactions strong enough that U/t>23 in 2D

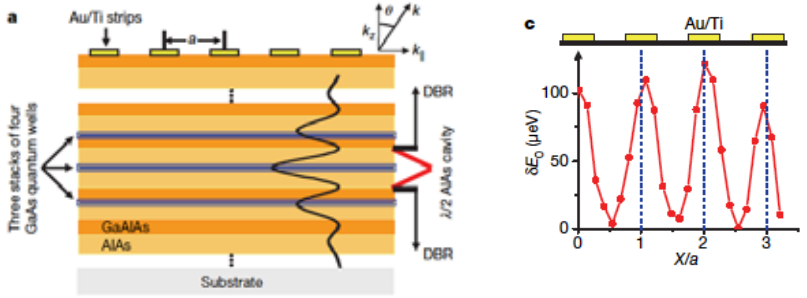
In 1 dimension, with large enough interactions a Fermi-like Tonks gas is formed.

Paredes et al. Nature **429** 277 (2004)

Trapping potentials

Metal gate

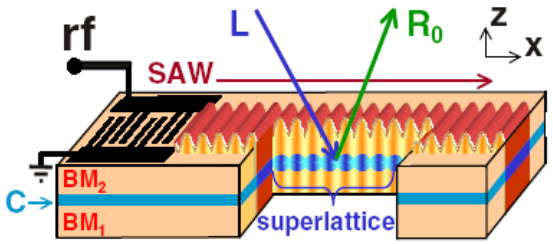
Lai et al. Nature **450**, 529 (2007)
Young Phys. Stat. Sol. (b), **245**, 1076 (2008)



Metal patterning on surface modifies photonic boundary conditions, effectively creating a potential

Surface acoustic wave (SAW)

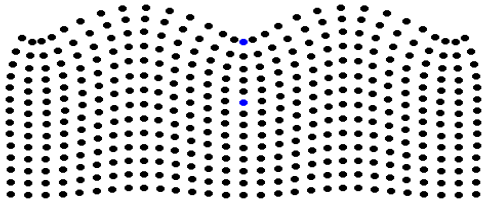
Lima et al. PRL 97, 045501 (2006)



refractive index of material changed, as well as physical microcavity thickness.

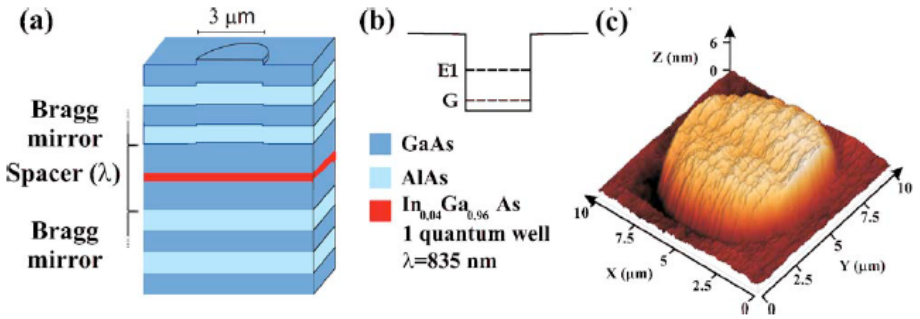
$$\frac{\Delta\varepsilon_{ph}}{\varepsilon_{ph}} = \frac{\Delta\lambda_c}{\lambda_c}$$

$$\varepsilon_{ph} = \frac{\hbar c 2\pi}{n_c \lambda_c}$$



Cavity etching

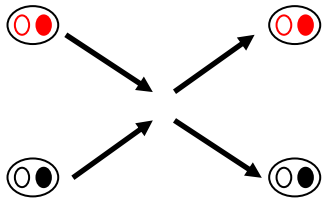
Daif Appl. Phys. Lett. 88, 061105 (2006)
Loffler Appl. Phys. Lett 86, 111105 (2005)



Interactions of exciton-polaritons

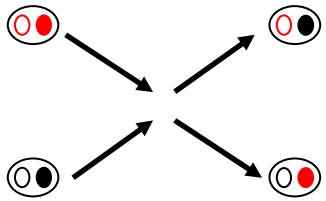
The interaction of polaritons originate from the non-linear interaction of the exciton components.

The effective interaction results from electron-electron and hole-hole exchange effects:



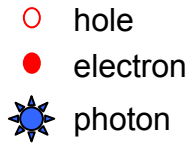
Direct contribution

$$\langle \psi(r_e', r_h')\psi(r_e, r_h) | H_{Coul} | \psi(r_e, r_h)\psi(r_e', r_h') \rangle$$

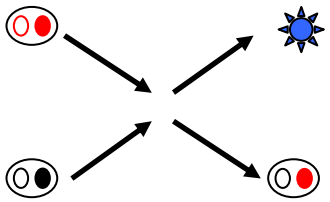


Exchange contribution

$$\langle \psi(r_e', r_h)\psi(r_e, r_h') | H_{Coul} | \psi(r_e, r_h)\psi(r_e', r_h') \rangle$$



With the presence of a microcavity, there is also a contribution due to anomalous recombination of electron hole pairs



"Saturation" contribution

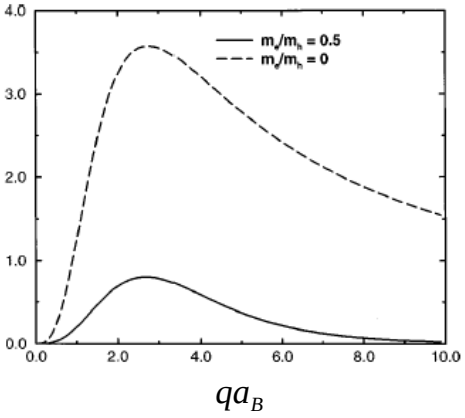
$$\langle \psi(r_e', r_h)a | H_{ph} | \psi(r_e, r_h)\psi(r_e', r_h') \rangle$$

$$H_{Coul} = \frac{1}{2}\sum_{k,k',q}\left[V_q^{ee} e^{\dagger}_{k'-q} e^{\dagger}_{k'+q} e_{k'} e_k - 2V_q^{eh} e^{\dagger}_{k+q} h^{\dagger}_{k'-q} h_{k'} e_k + V_q^{hh} h^{\dagger}_{k'-q} h^{\dagger}_{k'+q} h_{k'} h_k\right]$$

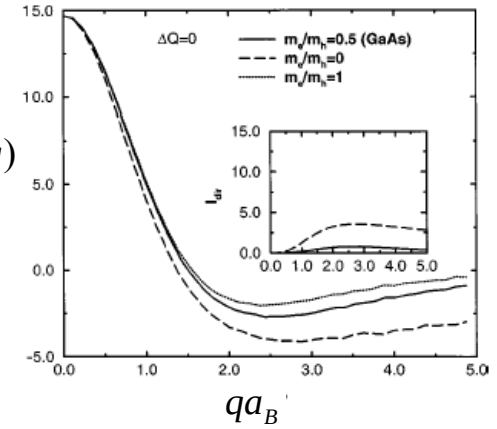
$$H_{ph} = \Omega\sum_k e_k^{\dagger} h_{-k}^{\dagger} a + a^{\dagger} h_{-k} e_k + \omega a^{\dagger} a$$

Hubbard parameters

$I_{dir}(q)$



$-I_{exch}(q)$



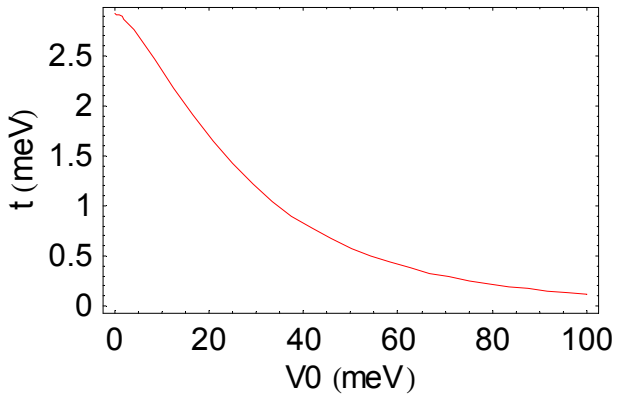
Ciuti et al. PRB **58**, 7926 (1998)
de-Leon PRB **63**, 125306 (2001)
Rochat PRB **61**, 13856 (2000)

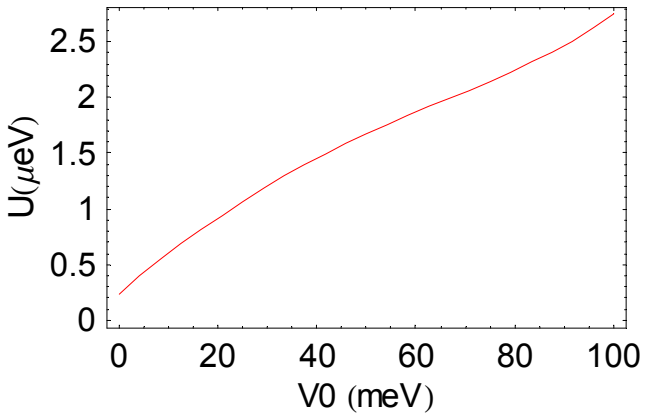
$$H_{exc}(Q,Q',q)=\frac{4e^2a_B}{A\varepsilon\pi^2}\left[I_{dir}(q)+I_{dir}(\sqrt{(Q-Q')^2+q^2-2(Q-Q')q\cos\theta})-I_{exch}(Q-Q',q,\theta,m_e/M)-I_{exch}(Q-Q',q,\theta,m_h/M)\right]$$

direct | exciton-exciton exchange | electron exchange | hole exchange

Using standard derivation of Hubbard parameters via wannier functions

$$t=\int d^2x w(x)H_{kin}w(x-\lambda) \qquad U\approx|u|^4 H_{exc}(0,0,0)\int d^2k\,|w(k)|^4$$





Putting in current experimental parameters we get U/t<<1.

zero detuning

$\lambda = 5\mu m$

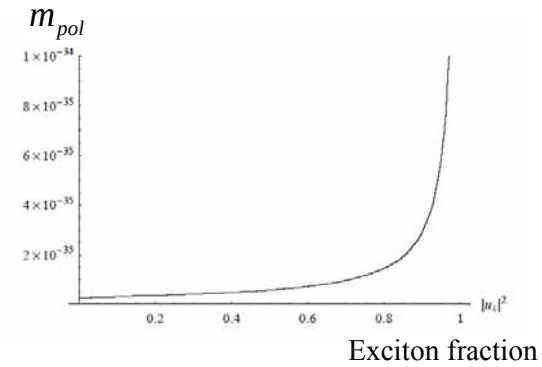
$m_{pol}\approx 6\times10^{-6}m_0$

Reaching the transition point

Does reducing λ improve this ratio?

$$U \approx \frac{e^2 a_B |u|^4}{\varepsilon \lambda^2} \qquad t \approx \frac{\hbar^2}{m_{pol} \lambda^2}$$

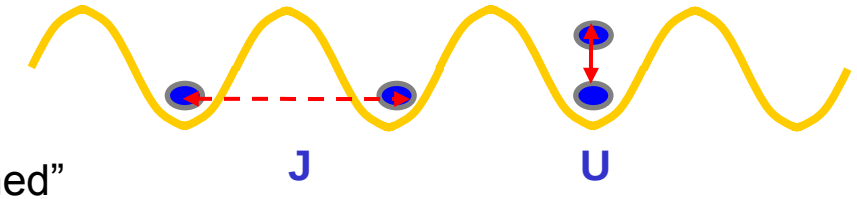
Doesn't help U/t ratio



So we have two choices remaining

1) Increase the lattice potential

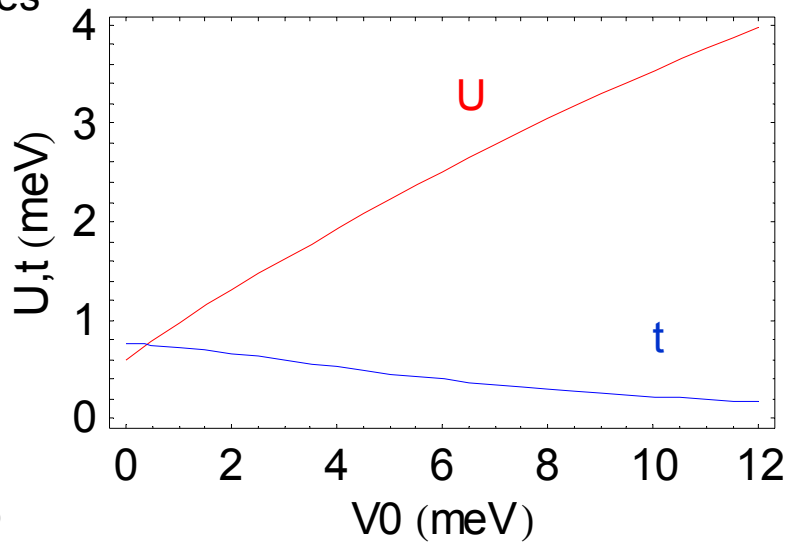
2) Make the polariton mass heavier

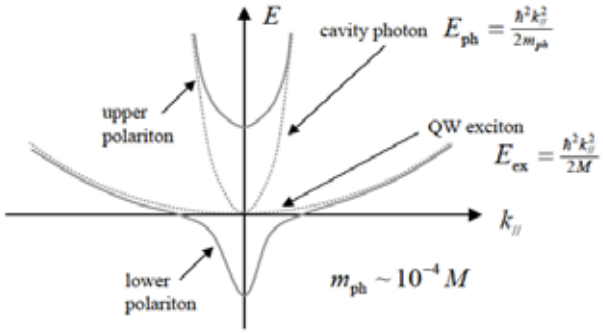


for small potentials we require heavy "blue-detuned" polaritons with masses

$$m_{pol} \approx 0.01 m_{exc}$$

$$\lambda = 0.1 \mu m$$





$$m_{pol} = \left[\frac{|u|^2}{m_{ph}} + \frac{|v|^2}{m_{exc}} \right]^{-1}$$

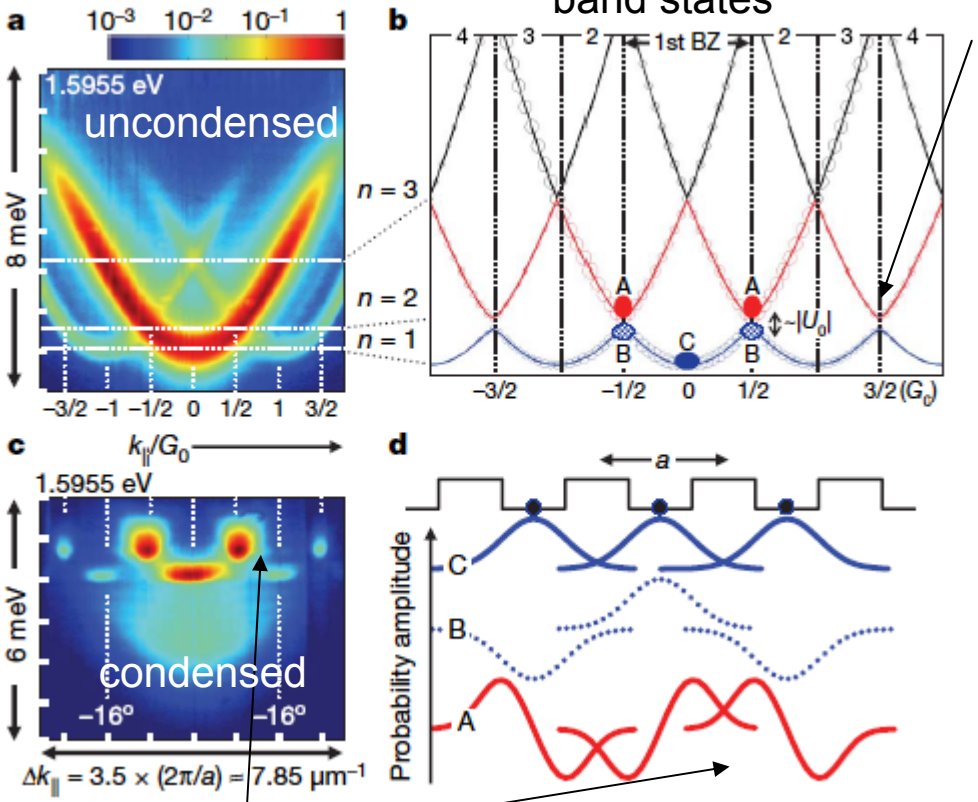
Byrnes, Recher, Yamamoto, Phys. Rev. B **81**, 205312 (2010)

p-state condensation in periodic potentials

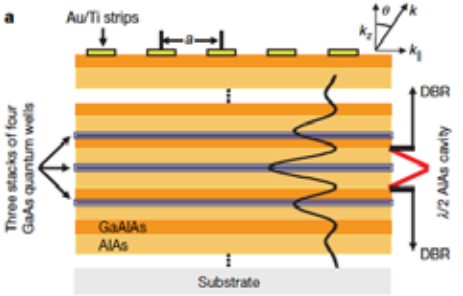
Using the metal trapping technique, a metastable condensate was formed

Band gap causes metastable condensation in 1st excited band states

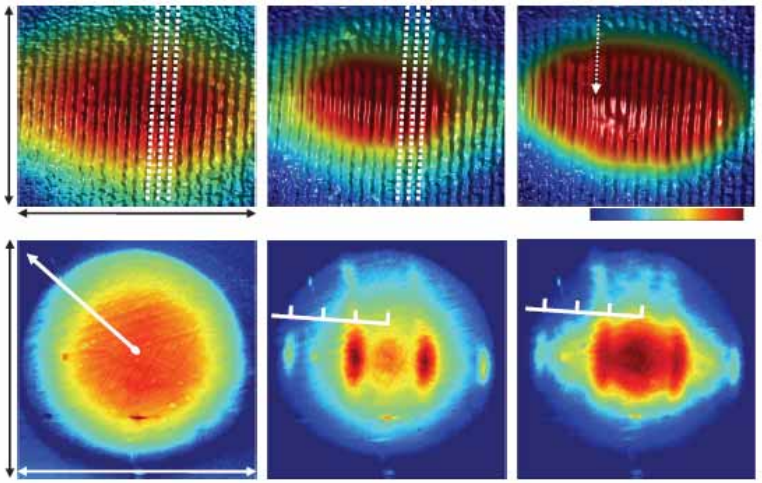
Lai et al. Nature **450**, 529 (2007)



adjacent states are pi out of phase



Increasing density



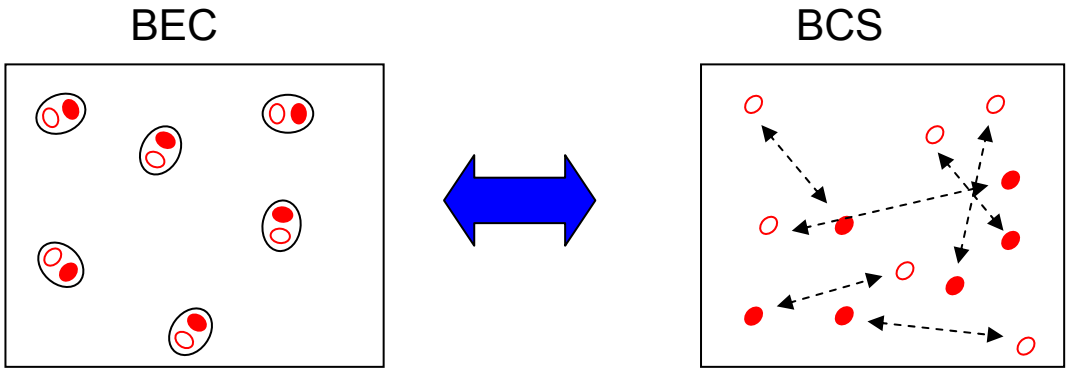
Uncondensed

Bottleneck metastable condensate (p-state)

Ground state condensate (s-state)

BCS-BEC crossover

For an excitonic system, it is known that as the density is increased in the system crosses over from tightly bound exciton pairs to loosely bound Cooper pairs



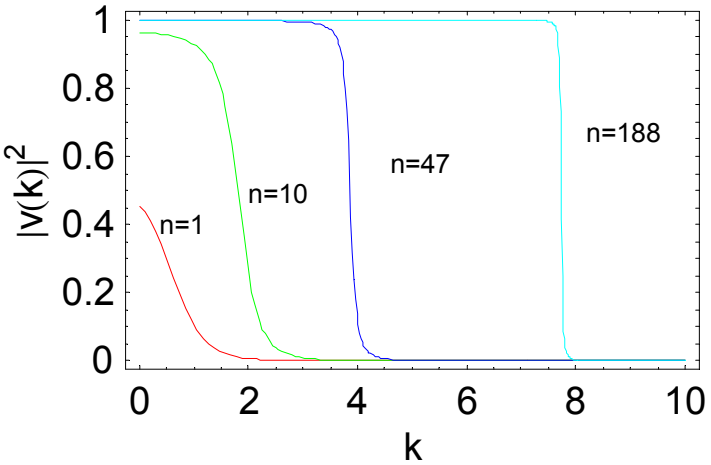
Kjeldysh Sov. Phys. JETP 27, 521 (1968)

Comte J. Physique 43, 1069 (1982)

$$|\Phi\rangle = \prod_k \left[u_k + v_k e_k^\dagger h_{-k}^\dagger \right] |0\rangle$$

By adjusting the fermionic interaction by Feshbach resonances, the BCS-BEC crossover in atomic gases has been observed:

Regal. Adv. Atom. Mol. Opt. Phys. 54, 1 (2006)



polariton BCS-BEC crossover theory

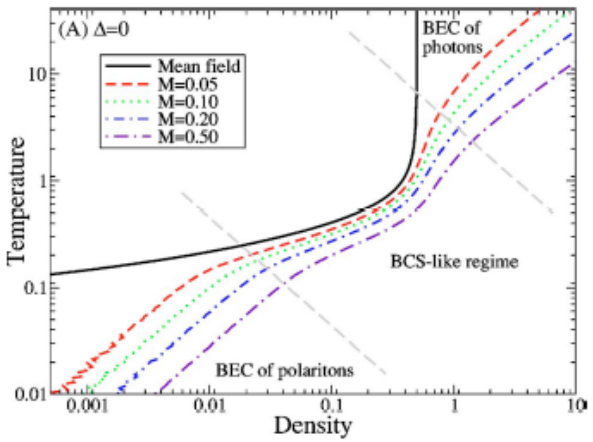
We can extend this to a coupling to cavity photon field by simply adding

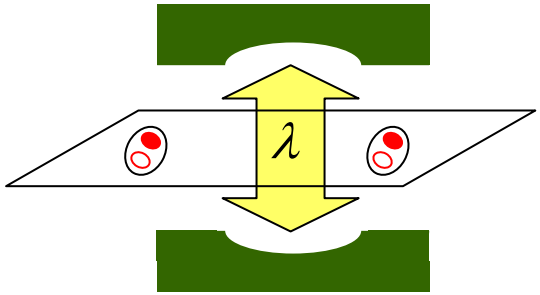
$$|\Phi\rangle = \exp[\lambda a^\dagger]\prod_k \left[u_k + v_k e_k^\dagger h_{-k}^\dagger\right]|0\rangle \qquad H = H_{exc} + H_{ph}$$

With respect to the Hamiltonian

$$H_{exc} = \sum_k \left[\left(\frac{\hbar^2 k^2}{2m_e} - \mu\right) e_k^\dagger e_k + \left(\frac{\hbar^2 k^2}{2m_h} - \mu\right) h_k^\dagger h_k\right] + \frac{1}{2}\sum_{k,k',q}\left[V_q^{ee} e_{k'-q}^\dagger e_{k'+q}^\dagger e_{k'} e_k - 2V_q^{eh} e_{k+q}^\dagger h_{k'-q}^\dagger h_{k'} e_k + V_q^{hh} h_{k'-q}^\dagger h_{k'+q}^\dagger h_{k'} h_k\right]$$

$$H_{ph} = (\omega - \mu) a^\dagger a + \Omega \sum_k e_k^\dagger h_{-k}^\dagger a + a^\dagger h_{-k} e_k$$



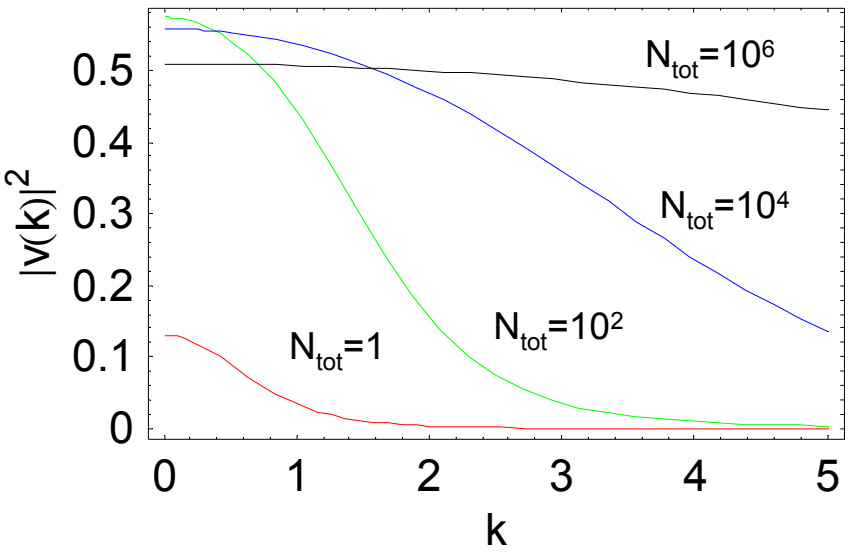


BEC ⟺ BCS-like state ⟺ photon BEC

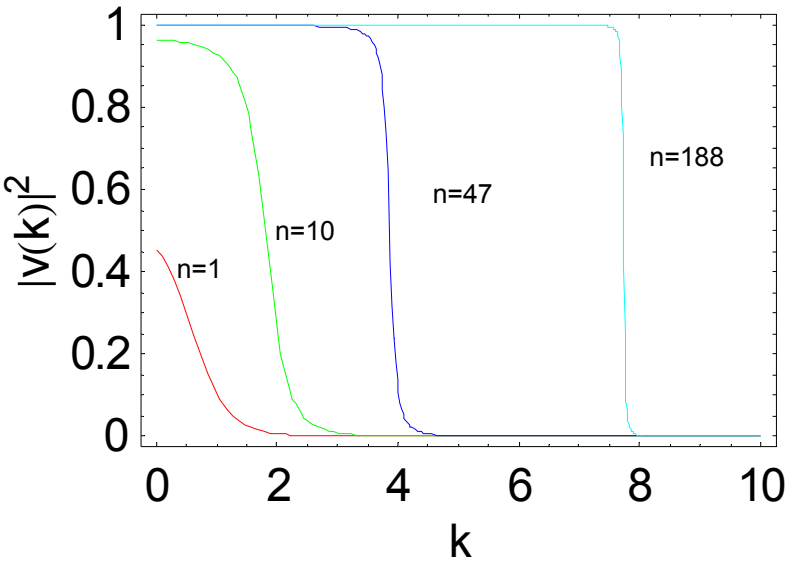
Keeling Phys. Rev. B 72, 115320 (2005)
Eastham Phys. Rev. B 64, 235101 (2001)
Byrnes, Horikiri, Ishida, Yamamoto arxiv 1005.3141

Including Coulomb interactions

exciton-polaritons

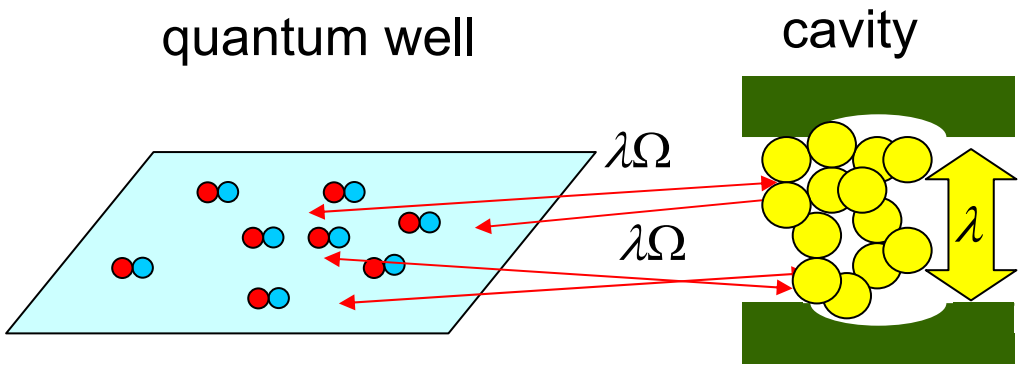


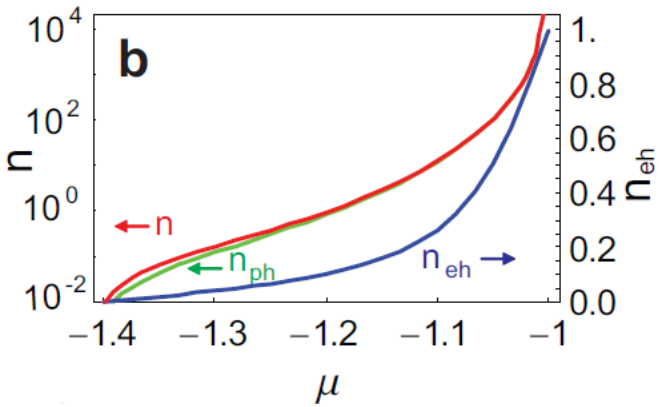
c.f. excitons



$$|\Phi\rangle = \exp[\lambda a^\dagger] \prod_k \left[u_k + v_k e_k^\dagger h_{-k}^\dagger \right] |0\rangle$$

Why the flat distribution?





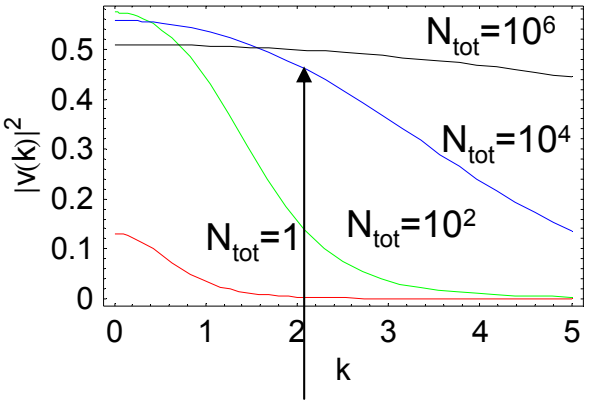
Due to saturation effect, there are many more photons than excitons. Enhanced Rabi splitting due to bosonic statistics.

Dominant part of Hamiltonian:

$$H = (\omega - \mu) a^\dagger a + \Omega \sum_k e_k^\dagger h_{-k}^\dagger a + a^\dagger h_{-k} e_k$$

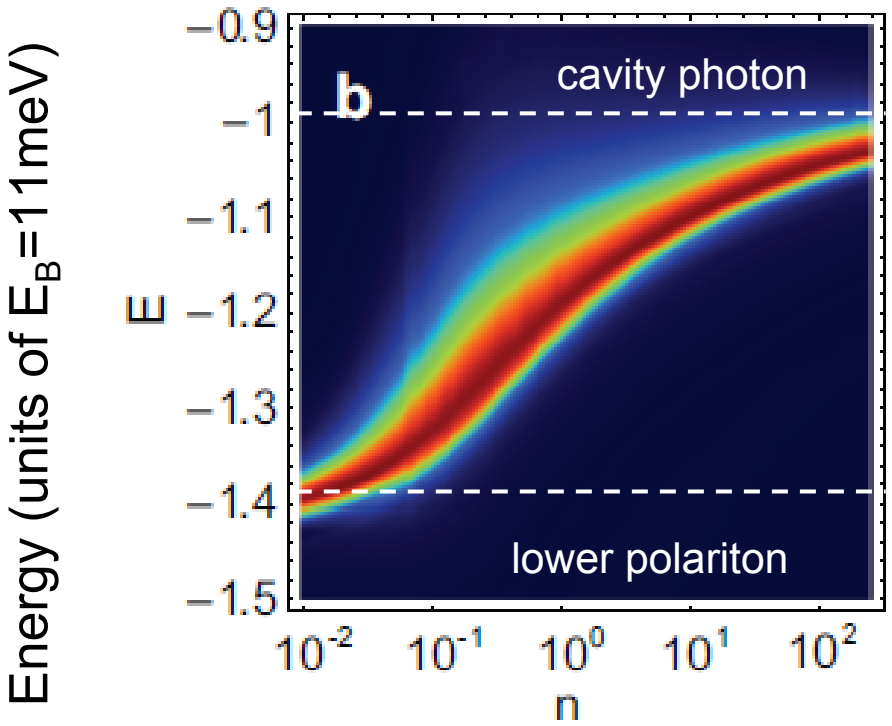
We are in a regime where $E_{binding} < \lambda\Omega$

The excitonic wavefunction is overwhelmed by the cavity coupling



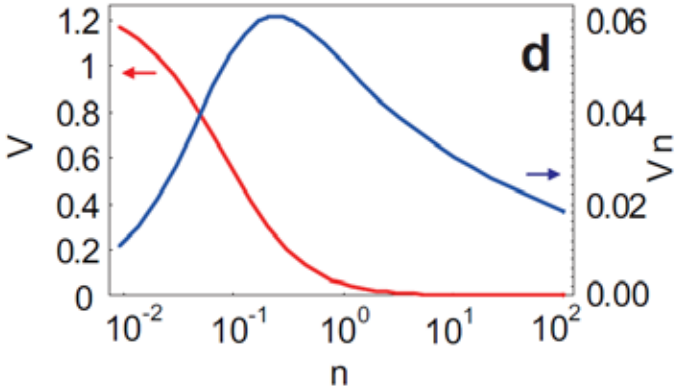
Flat distribution of electron and hole momenta

PL spectrum including interactions



Extracting single and two particle energy from BCS calculation gives

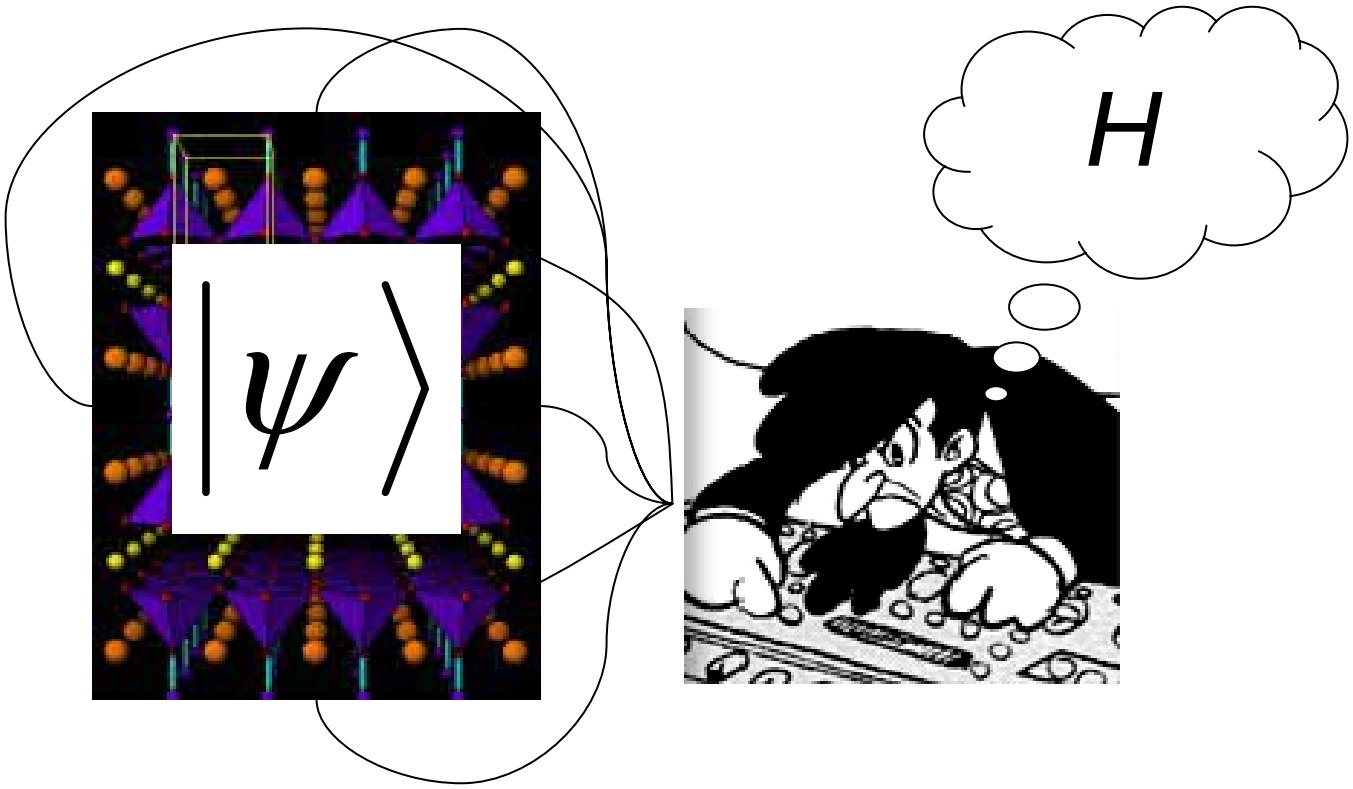
$$\mu = \frac{dE}{dn} \qquad Vn = \frac{d^2E}{dn^2}$$



Using simple single particle theory with interactions
(Porras PRB **67**,161310(R) (2003))

- peak energy gradually shifts from LP to cavity photon energy
- linewidth increases at first, but then decreases.

(2) “Digital” Quantum Simulation



Algorithm approach to solving quantum many-body physics

Assumptions (necessary)

• A quantum computer is available (full unitary control and measurements are possible)

• Operation is perfect (i.e. error correction is already implemented)

Assumptions (not necessary, but typical)

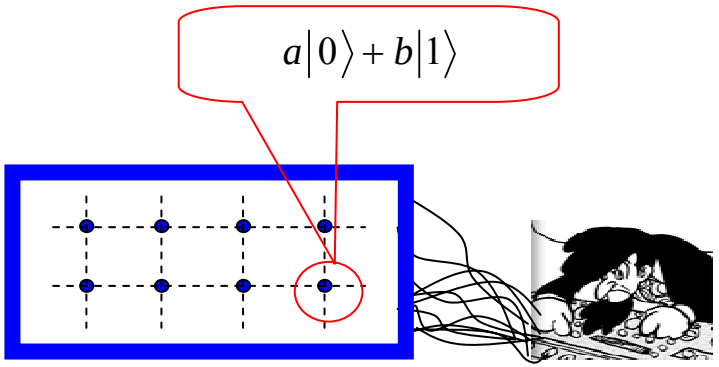
• Control of the quantum computer is via one and two qubit gates

• Quantum computer is made of qubits (as opposed to qudits or other schemes)

Aim

Simulate a given quantum Hamiltonian and extract quantities of interest

Provide an alternative to simulations on classical computers, in the style of Feynman's original idea



Simulating on a classical computer

What does “simulate and extract quantities of interest” mean exactly?

Usually this means the task is to diagonalize a given Hamiltonian H and obtain its eigenvalues and eigenvectors

From eigenvalues and eigenvectors we can extract everything we want to know: correlation functions, time evolution, etc..

Example

Typical quantum many body problem: transverse Ising model

$$H = J\sum_{<ij>}\sigma_i^z\sigma_j^z + \lambda\sum_i \sigma_i^x$$

1) Choose a basis (for two sites: $\uparrow\uparrow$ $\downarrow\uparrow$ $\uparrow\downarrow$ $\downarrow\downarrow$)
2) Contruct Hamiltonian in matrix form
3) Diagonalize!

$$H = \begin{array}{c} \begin{matrix} \uparrow\uparrow & \downarrow\uparrow & \uparrow\downarrow & \downarrow\downarrow \end{matrix} \\ \begin{pmatrix} J & \lambda & \lambda & 0 \\ \lambda & -J & 0 & \lambda \\ \lambda & 0 & -J & \lambda \\ 0 & \lambda & \lambda & J \end{pmatrix} \end{array} \begin{matrix} \uparrow\uparrow \\ \downarrow\uparrow \\ \uparrow\downarrow \\ \downarrow\downarrow \end{matrix}$$

Hamiltonian matrix scales exponentially with lattice size

No. matrix elements for
N=25 sites $\left(2^{25}\right)^2 \approx 10^{15}$

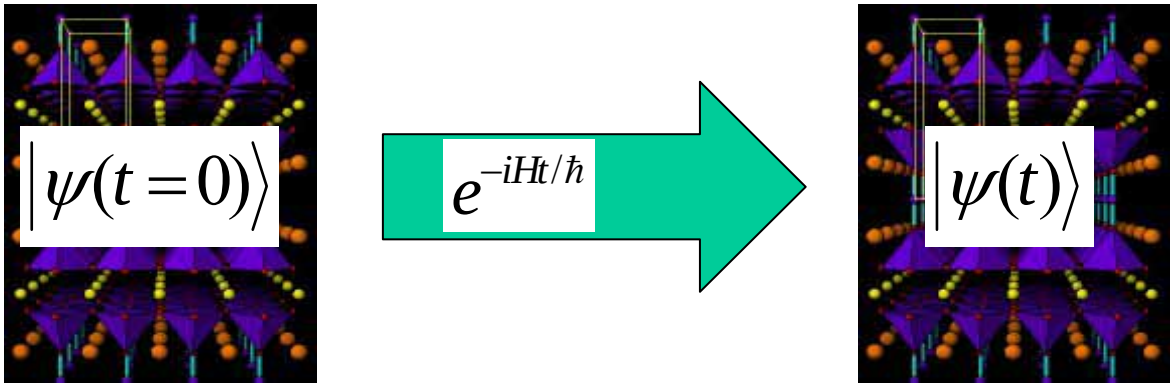
360 TB Memory=3.6 x 10^{14} B
1750 teraflops =1.75 x 10^{15} flops

Jaguar Oak Ridge supercomputer
(No. 1 on top 500 6/2010)

Simulating Hamiltonians using quantum gates

Assuming we have a quantum computer, how do we use it for simulation?

Simplistic approach: Evolve the system in time according to the Hamiltonian



We can't directly do this since the target Hamiltonian H can be quite complicated (assumption of using only one and two qubit gates)

e.g. $$H = J\sum_{<ij>}\sigma_i^z\sigma_j^z + \lambda\sum_i \sigma_i^x$$

Trotter decomposition

We can however approximately perform the evolution

$$U(t) = e^{-iHt} \approx \left(e^{-iH_1 t/m} e^{-iH_2 t/m} \cdots e^{-iH_M t/m} \right)^m + O\left(\frac{t^2}{m} \right)$$

where $H = \sum_i H_i$ and H_i are simulatable Hamiltonians

Example

Say we would like to simulate $H = J \sum_{<ij>} \sigma_i^z \sigma_j^z + \lambda \sum_i \sigma_i^x$

$$U(t) = e^{-iHt/\hbar} \approx \exp[-i\sigma_1^z \sigma_2^z \Delta t/\hbar] \exp[-2i\sigma_1^x \Delta t/\hbar]$$
$$\exp[-2i\sigma_2^x \Delta t/\hbar] \exp[-i\sigma_1^z \sigma_2^z \Delta t/\hbar]$$

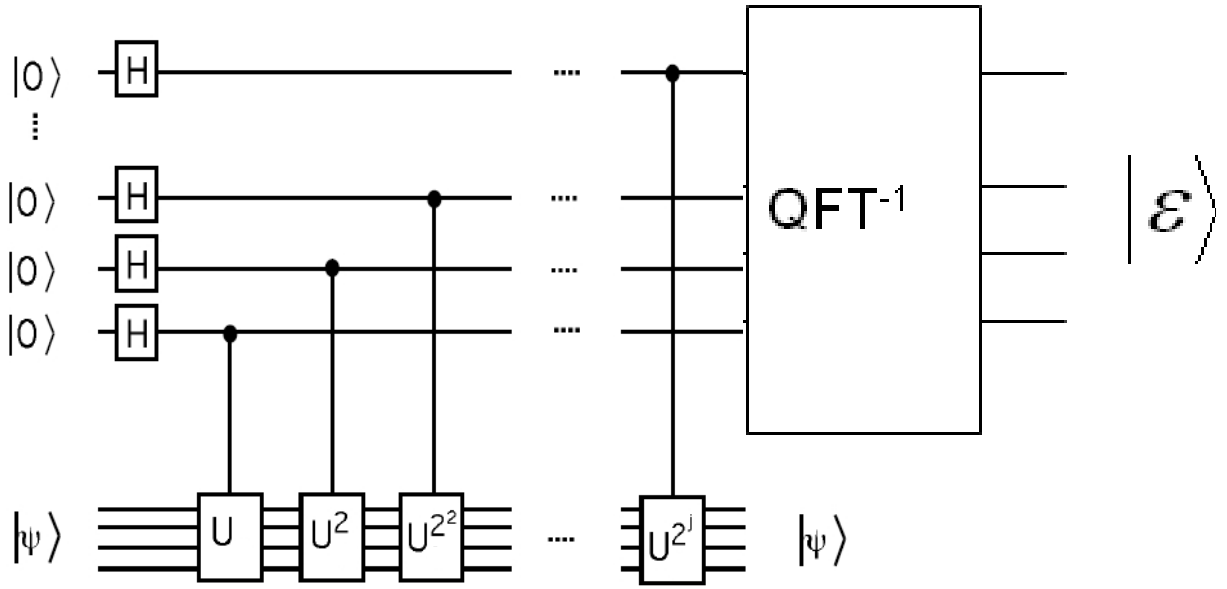
$$\Delta t = t/2$$

By making Δt small we can get arbitarily good precision of the evolution

Ok, we can evolve the system just like the real system. But how do we get what we want (i.e. eigenvalues & eigenvectors) out of it?

Method 1: Phase Estimation Algorithm

The phase estimation algorithm is a way of reading out the phase of a given operator



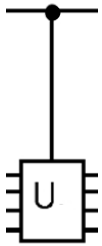
Assume we can prepare qubits in an eigenstate $|\psi\rangle$ of H

The phase estimation algorithm estimates the phase

$$\exp[iHt]|\psi\rangle = \exp[i\varepsilon t]|\psi\rangle$$

Taking an inverse Quantum Fourier Transform gives the energy ε

Phase Estimation Algorithm components



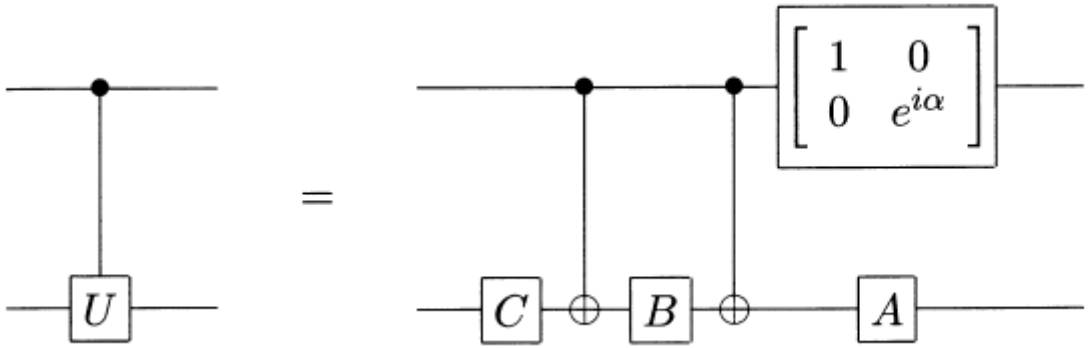
= Controlled-U gate

$$U = \exp[2\pi i H t]$$

This is performed using the Trotter decomposition

(factor of 2π for convenience)

A single qubit controlled-U is performed by the decomposition (p.181 Nielsen & Chuang)



$$ABC = 1$$

$$AXBXC = R_z(\beta)R_y(\gamma)R_z(\delta)$$

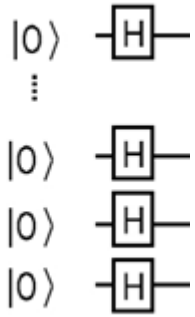
$$A = R_z(\beta)R_y(\gamma/2)$$

$$B = R_y(-\gamma/2)R_z(-(\delta+\beta)/2)$$

$$C = R_z((\delta-\beta)/2)$$

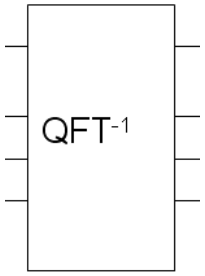
An arbitrary U can be performed by the decomposition $U = e^{i\alpha}R_z(\beta)R_y(\gamma)R_z(\delta)$

2-qubit controlled-U by similar techniques



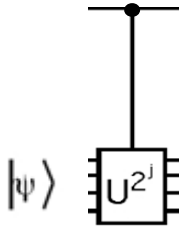
$$|00\rangle \rightarrow \frac{1}{2}\left(|0\rangle+|1\rangle\right)\left(|0\rangle+|1\rangle\right)=\frac{1}{2}\left[|00\rangle+|01\rangle+|10\rangle+|11\rangle\right]$$

superposition of every binary combination



= Inverse Quantum Fourier Transform

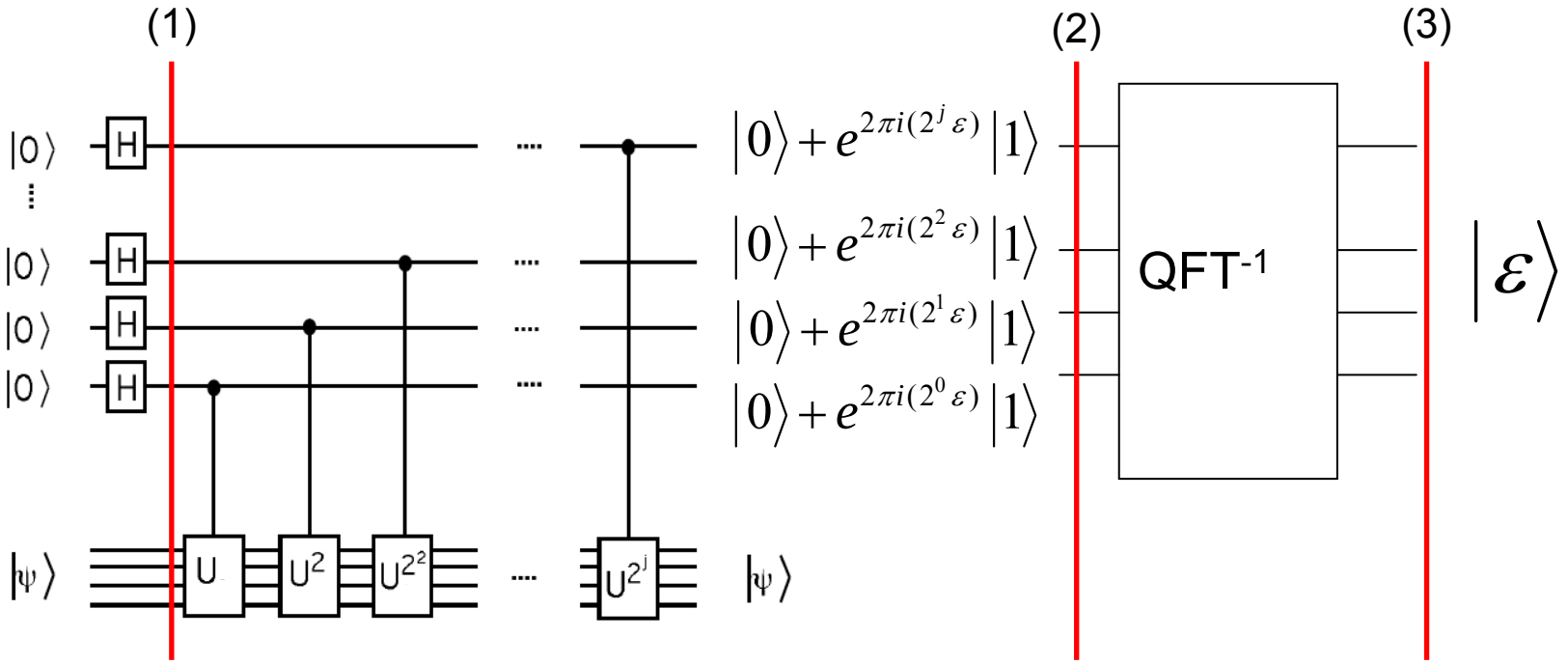
$$\frac{1}{\sqrt{N}}\sum_{k=0}^{N-1} e^{i\frac{2\pi n}{N}k}\left|k\right\rangle \rightarrow \left|n\right\rangle$$



$|\psi\rangle$ is an eigenstate of H with energy ε

$$U^{2^j}\left|\psi\right\rangle = \exp[2\pi i H t]^{2^j}\left|\psi\right\rangle = \exp[2\pi i 2^j \varepsilon t]\left|\psi\right\rangle$$

Phase Estimation Algorithm



(1) $\left[|0\rangle+|1\rangle\right]|\psi\rangle=|0\rangle|\psi\rangle+|1\rangle|\psi\rangle$

(2) $|0\rangle|\psi\rangle+|1\rangle U|\psi\rangle=\left[|0\rangle+e^{2\pi i\varepsilon}|1\rangle\right]|\psi\rangle$

(3) $\prod_{l=1}^{n}\left[|0\rangle+\exp[2\pi i\left(2^{l}\varepsilon\right)]|1\rangle\right]=\sum_{k}\exp\left[i2\pi\varepsilon k\right]|k\rangle\overset{QFT^{-1}}{\rightarrow}|\varepsilon\rangle$

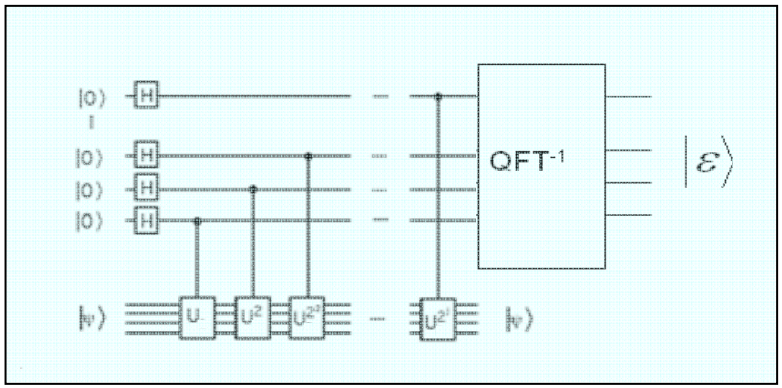
Initial state

The phase estimation algorithm gives the energy given the eigenstate.
But we usually don't know the eigenstate!!

Approximate method

Prepare state of high overlap with states of interest.

$$\left|\Psi_{init}\right\rangle = \sum_n \Lambda_n \left|E_n\right\rangle$$

$\left|\Psi_{init}\right\rangle\left|0000\right\rangle$ 

$\sum_n \Lambda_n \left|E_n\right\rangle\left|\varepsilon_n\right\rangle$

estimated energy

Performing a measurement on the computational basis on ancilla qubits gives the correct result with probability $\left|\Lambda_n\right|^2$

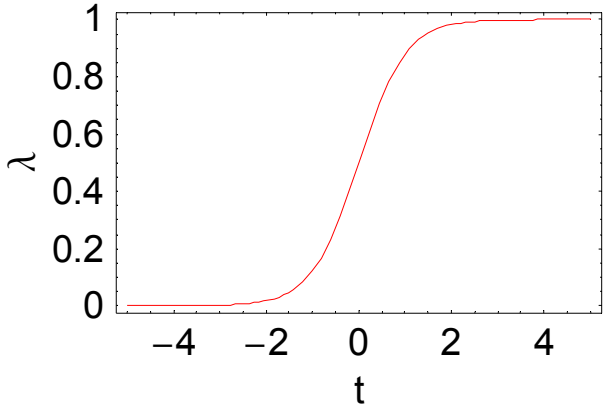
Methods for preparing the initial state

(1) Use some analytical or numerical approximation scheme

- Mean field theory
- Approximate wavefunction
- Numerical schemes (Monte Carlo/DMRG etc.)

(2) Perform a quantum adiabatic evolution initially

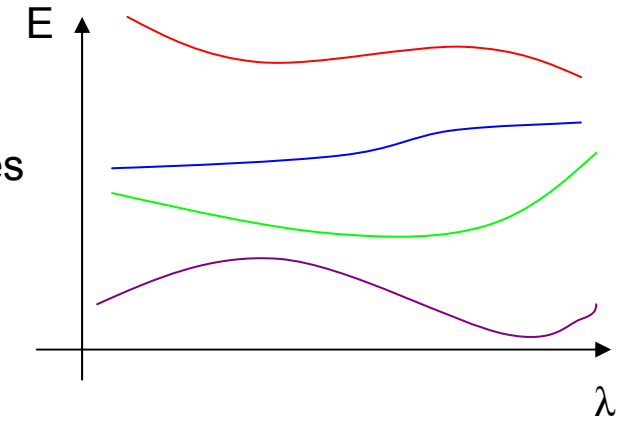
$$H = \lambda(t) H_{prob} + (1 - \lambda(t)) H_{known}$$



H_{prob} = problem Hamiltonian

H_{known} = a Hamiltonian where the ground state is known

1) Prepare qubits in ground state of H_{known}
2) Slowly sweep $\lambda(t)$ such that at the Hamiltonian changes from H_{known} to H_{prob}
3) By the adiabatic theorem, the final state should be in the ground state of H_{prob}



Method 2: Post processing Fourier transform

The second method is similar, but performs the Fourier transform classically.

1) Prepare initial state $\left|\Psi_{init}\right\rangle$

2) By repeated measurements for various t, find function

$$f(t) = \left\langle \Psi_{init} \left| \exp[-iHt] \right| \Psi_{init} \right\rangle$$

(if we prepare $\left|\Psi_{init}\right\rangle$ perfectly)

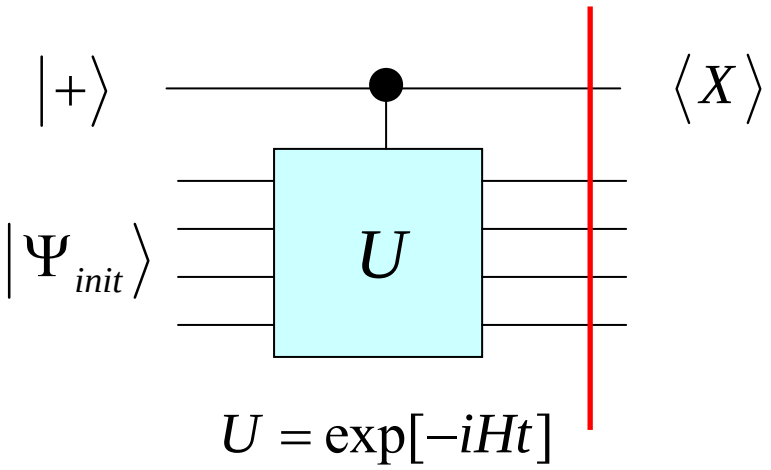
3) Take Fourier transform of f(t)

How to measure f(t)?

$$\frac{1}{\sqrt{2}}\left|0\right\rangle\left|\Psi_{init}\right\rangle + \frac{1}{\sqrt{2}}\left|1\right\rangle U\left|\Psi_{init}\right\rangle$$

$$= \frac{1}{\sqrt{2}}(1+e^{-i\varepsilon t})\left|+\right\rangle\left|\Psi_{init}\right\rangle + \frac{1}{\sqrt{2}}(1-e^{-i\varepsilon t})\left|-\right\rangle\left|\Psi_{init}\right\rangle$$

$$\left\langle X \right\rangle = 2\cos\varepsilon t$$



Somma et al. PRA **65**, 042323 (2002)

What if we don't have the perfect eigenstate?

Again, use a guess state:

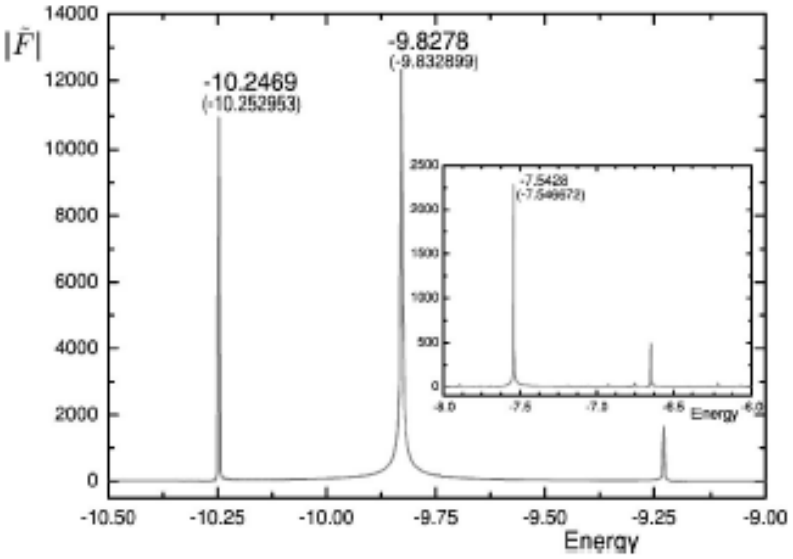
$$\left|\Psi_{init}\right\rangle = \sum_n \Lambda_n \left|E_n\right\rangle$$

Then

$$f(t) = \left\langle \Psi_0 \left| \exp[-iHt] \right| \Psi_0 \right\rangle = \sum_n \left|\gamma_n\right|^2 e^{-i\varepsilon_n t}$$

Hubbard model 4x2 lattice, U=4, t=1

$$\Delta t = 0.05$$



Peaks give the energy levels.

Somma et al. PRA **65**, 042323 (2002)

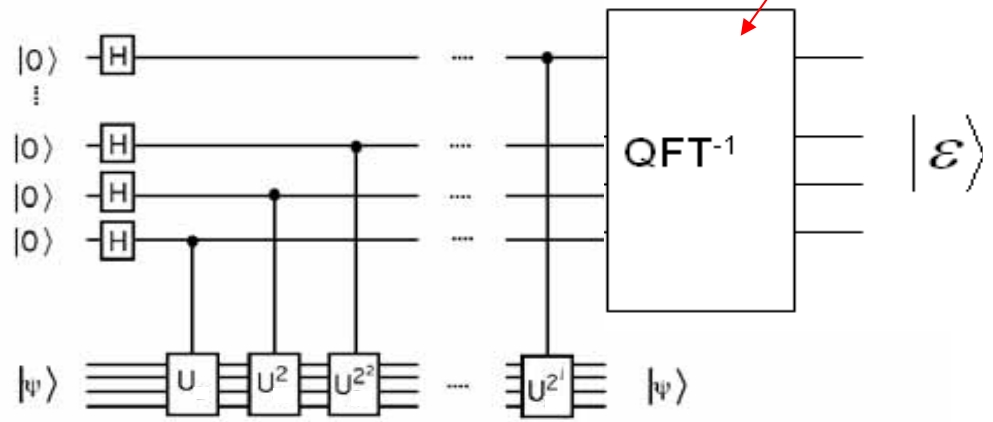
Efficiency with respect to site number

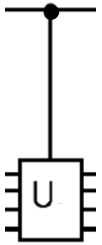
The algorithm is polynomial in the number of sites

QFT is polynomial with no. sites

no qubits=no of digits of binary precision

no qubits=no of sites to be simulated





U is Trotter decomposed individual gates.

$$U = e^{-iHt} = \left(e^{-iH_1 t/m} e^{-iH_2 t/m} \cdots e^{-iH_M t/m} \right)^m$$

Number of gates $\propto$ No. terms in Hamiltonian (scales polynomially with no. sites)

The algorithm itself has an exponential speedup over classical computers

Efficiency with respect to error

Repeated measurements are necessary for the Fourier transform step (N steps)

Estimated function

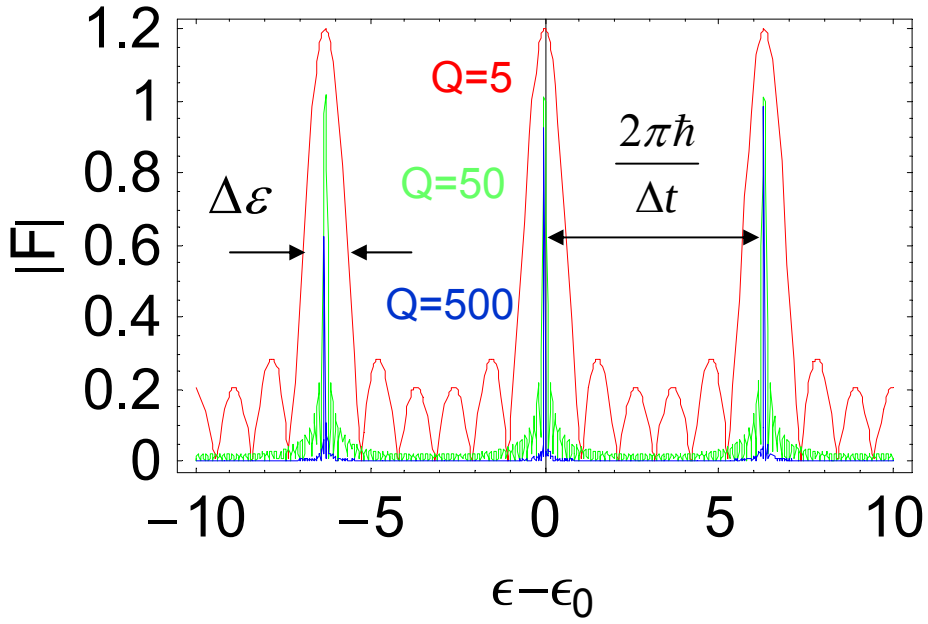
$$F_n = \exp[-i\varepsilon_0 \Delta t n]$$

Fourier transform

$$F(\varepsilon) = \frac{1}{Q}\sum_{n=0}^{Q} F_n \exp[-i\varepsilon \Delta t n]$$

Width of peak of energy estimate

$$\Delta\varepsilon \sim \frac{2\pi\hbar}{Q\Delta t}$$



Error scaling due to Trotter decomposition

$$e^{i(A+B)\Delta t} = \left(e^{iA\Delta t/k} e^{iB\Delta t/k}\right)^k + O\left[\frac{\Delta t^2}{k}\right]$$

Number of gates $\sim 2k$

To get an M extra digits of precision, we need exponentially increasing Q and an exponential number of gates

Brown et al. Phys.Rev. Lett. **97**, 050504 (2007)

Fermionic Hamiltonians

Up to now we have assumed spin based Hamiltonians. What about other forms?

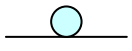
Example

$$H_{Hubbard} = -t\sum_{<nm>} c^{+}_{n\sigma}c_{m\sigma} + c^{+}_{m\sigma}c_{n\sigma} + U\sum_{m} n_m{}^{\uparrow} n_m{}^{\downarrow} \qquad \left\{c_i^{\dagger}, c_j\right\} = \delta_{ij}$$

Use a Jordan-Wigner tranformation map fermionic Hamiltonian onto spin Hamiltonian

Jordan-Wigner transform

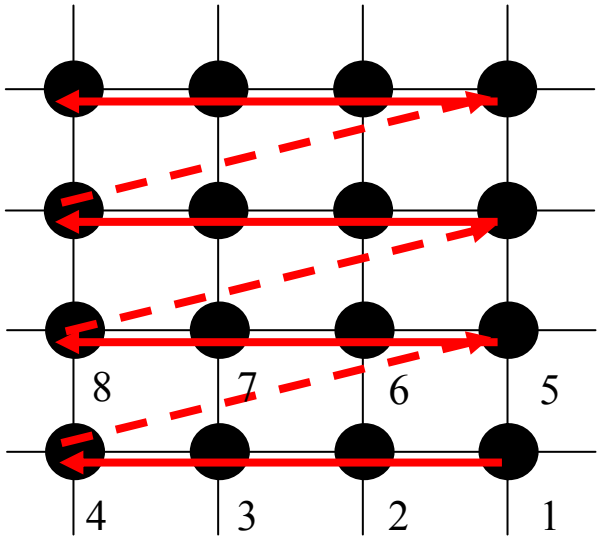
$$c_i^{\dagger} = \prod_{j<i} -\sigma_j^z \sigma_i^+$$

electron $c^{\dagger}|0\rangle$ 

no electron $|0\rangle$

$|\uparrow\rangle$

$|\downarrow\rangle$

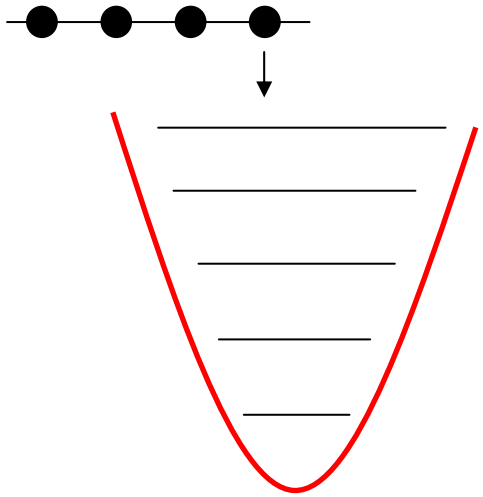


Ortiz et al. PRA **64**, 022319 (2001)

e.g. $c_1^{\dagger}c_5 = \sigma_1^{+}\sigma_2^{z}\sigma_3^{z}\sigma_4^{z}\sigma_5^{-}$

Bosonic Hamiltonians

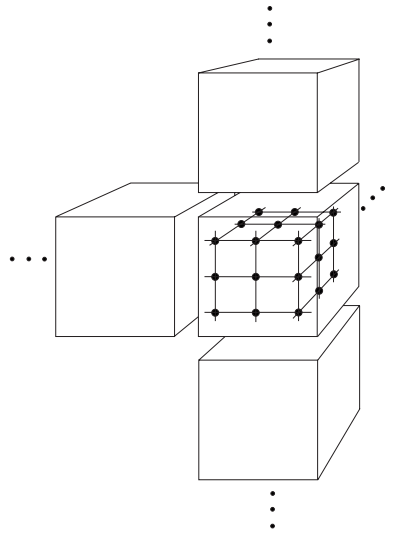
$$H_{Bose-Hubbard} = -t \sum_{<nm>} b_n^+ b_m + b_m^+ b_n + \frac{U}{2} \sum_m n_m (n_m - 1) \qquad [b_i^\dagger, b_j] = \delta_{ij}$$



$$|3\rangle = (b^\dagger)^3 |0\rangle$$
$$|2\rangle = (b^\dagger)^2 |0\rangle$$
$$|1\rangle = b^\dagger |0\rangle$$
$$|0\rangle$$

Keep track of state on each site by qubit register

$$|\downarrow\downarrow\downarrow\uparrow\rangle$$
$$|\downarrow\downarrow\uparrow\downarrow\rangle$$
$$|\downarrow\uparrow\downarrow\downarrow\rangle$$
$$|\uparrow\downarrow\downarrow\downarrow\rangle$$



$$b_n^\dagger \leftrightarrow \sum_j \sqrt{j+1}\,\sigma_{j,n}^- \sigma_{j+1,n}^+ \qquad n_m \leftrightarrow \sum_j j \frac{(\sigma_{m,j}^z + 1)}{2}$$

Somma et al., quant-ph 0304063 (2003)

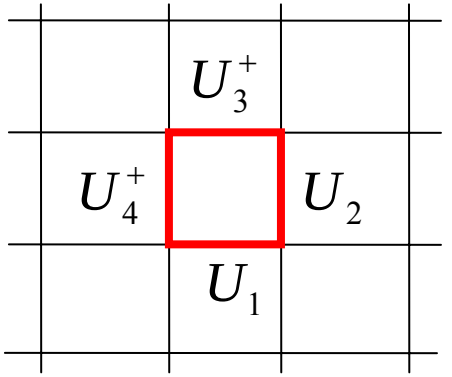
More exotic Hamiltonians

U(1) Lattice gauge theory

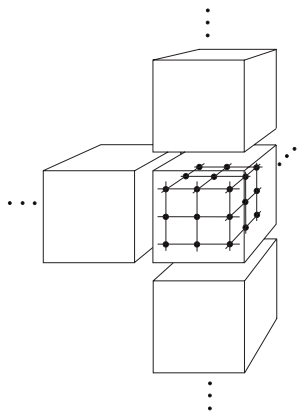
$$H_{U(1)} = \sum_{n \in links} E^2(n) - x \sum_{p \in plaquettes} \left(Z(p) + Z^+(p) \right)$$

$$Z(p) = U_1 U_2 U_3^+ U_4^+ \qquad U_i = \exp[igA_i]$$

$$[E_i, A_j] = i\delta_{ij}$$



qubit implementation



each link is a qubit register, and use the mapping

$$\tilde{U} = \sum_{n=-e_{\max}}^{e_{\max}} \sigma_n^- \sigma_{n+1}^+ \qquad \tilde{E}^2 = \sum_{n=-e_{\max}}^{e_{\max}} n^2 (\sigma_i^z + 1)/2$$

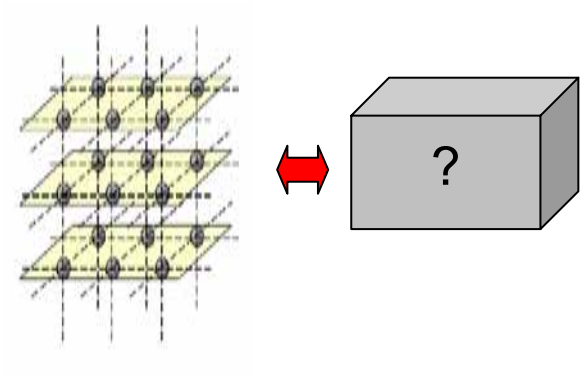
SU(2) and SU(3) Lattice gauge theories can also be implemented. SU(3) theory with fermions is thought to be the theory of strong interactions

Byrnes & Yamamoto, Phys. Rev. A **73**, 022328 (2006)

Comparison of analogue and digital quantum simulation

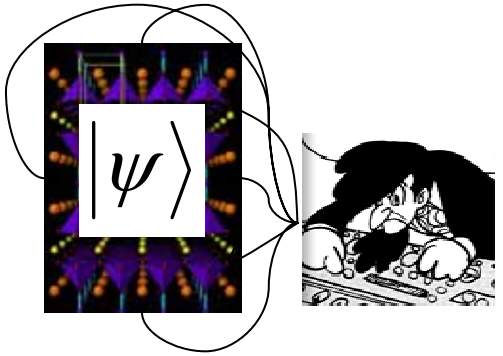
We have seen two different approaches of simulation. What are their differences and similarities?

"Analogue" QS



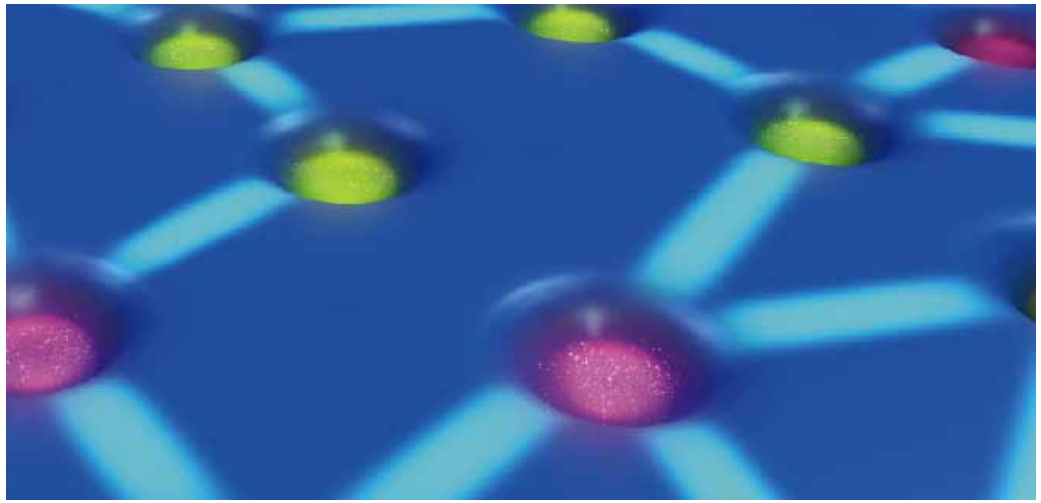
- Experimentally duplicate system of interest
- Open system
- One simulator per model
- No need for individual qubit control, so is easier to realize than quantum computer..

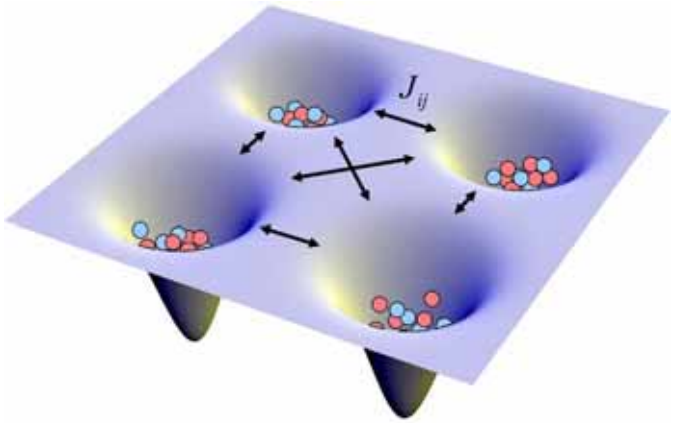
"Digital" QS



- Use a quantum algorithm to solve Hamiltonian
- Closed system
- Can simulate (just about) any system
- Requires a quantum computer so is experimentally challenging.

(3) Computing by quantum simulation



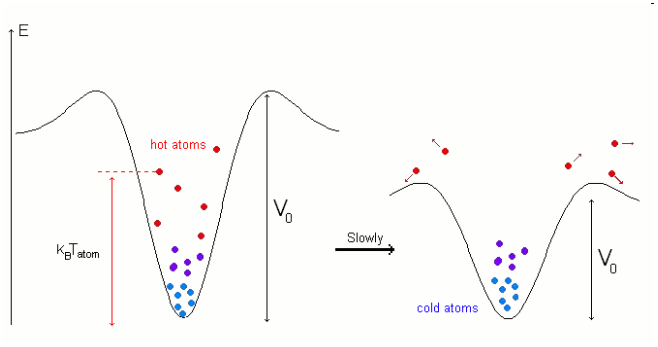


Where is the computation in analogue quantum simulation?

In the ideal case, both analogue and digital quantum computation “solves” a given Hamiltonian.

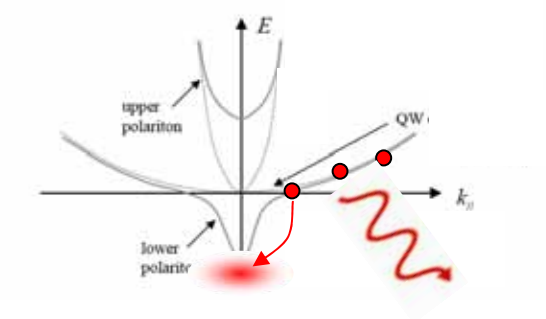
How does analogue quantum computation find the ground state exactly?

Cold atoms

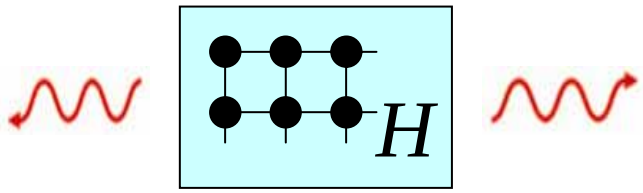


- Laser & evaporative cooling
- Adiabatic evolution to desired Hamiltoinan

Exciton-polaritons



- Cooling via phonon emission
- Stimulated scattering to ground state



$k_B T < |H|$

Both procedures involves a cooling, i.e. dissipation to an environment. So the “computation” being done by the reservoir.

Computation by analogue quantum simulation

This kind of scheme is attractive from a technological perspective because

- Easier experimental realization than building a quantum computer. Having an open system is in fact a necessary part of the operation.
- No complicated algorithms need to be invented.

Is it possible to extend this kind of idea to a more general setting?

Can we perform a computation using the ideas of quantum simulation?

In analogue quantum simulation, typically only one Hamiltonian can be simulated per device.

Is it possible to extend this so that we can control more than just one (or a few) parameters?

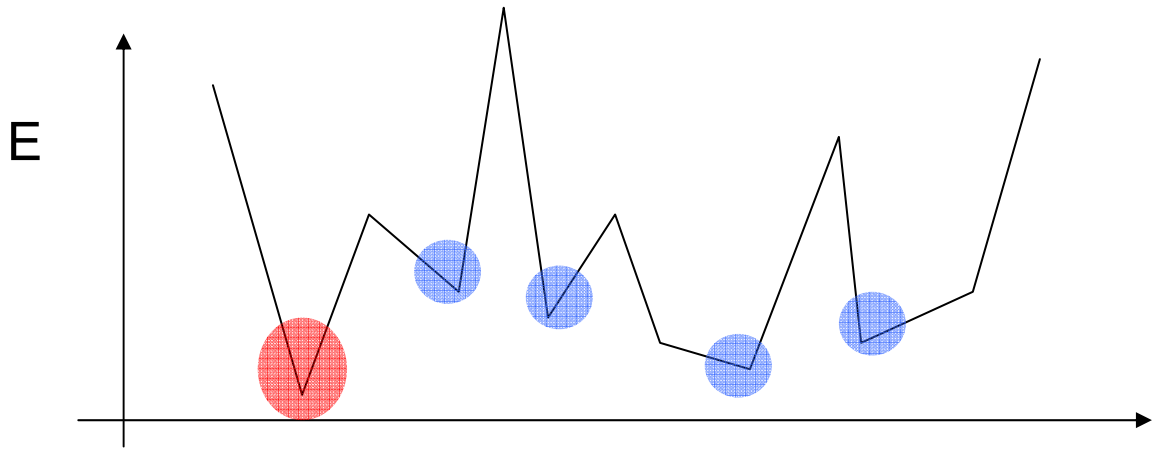
Computational problems as optimization

Many difficult computation problems (including NP-complete problems) can be formulated as an optimization problem

For example, the travelling salesman problem is known to be NP-complete

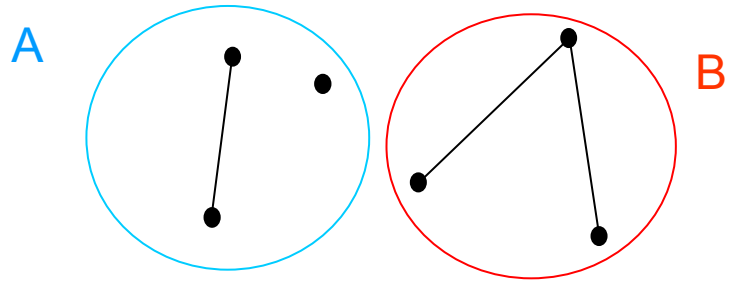
These problems can be mapped onto a combinatorial cost function (Hamiltonian) to be minimized

$$H = \sum_{i<j} J_{ij} \sigma_i^z \sigma_j^z$$



Example: the Graph Partitioning Problem

Given 2*N* points with arbitrary connections between them, the objective is to divide the points into two groups (A and B) of *N* points, minimizing the number of connections between them.



This can be recast into a cost function to be minimized

Label each site i and assign a variable $\sigma_i = \begin{cases} 1 & \text{if site } i \text{ in group A} \\ -1 & \text{if site } i \text{ in group B} \end{cases}$

Define a connectivity matrix $J_{ij} = \begin{cases} J & \text{if } i \text{ and } j \text{ connected} \\ 0 & \text{otherwise} \end{cases}$

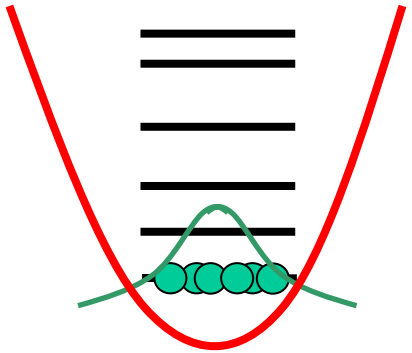
Given a particular pair (i,j), the pair is

$$\sigma_i \sigma_j = \begin{cases} 1 & \text{if (i,j) are in the same group} \\ -1 & \text{if (i,j) are in different groups} \end{cases}$$

The cost function is

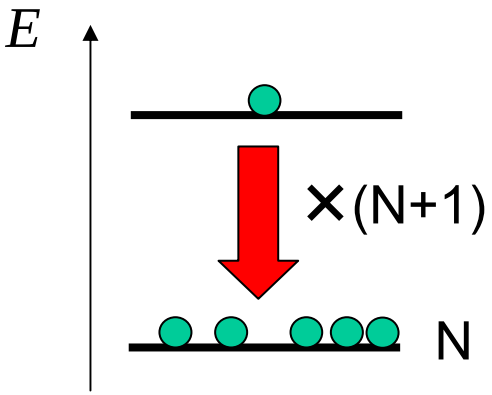
$$H_{GPP} = \sum_{i<j} J_{ij}(1-\sigma_i^z \sigma_j^z) = -\sum_{i<j} J_{ij}\sigma_i^z \sigma_j^z + const.$$

Fundamental properties of bosons



We know that in a BEC, the system has a large concentration of particles in the system ground state.

→ Bosonic particles “like” to accumulate in the ground state



Bosonic particles also possess the property of final state stimulation. Given N particles in the final state, the transition rate is enhanced by a factor N+1.

→ Bosonic particles have an enhanced cooling rate

Can these properties of bosons be used to find the ground state of a given Ising model problem?

Bosonic Ising model

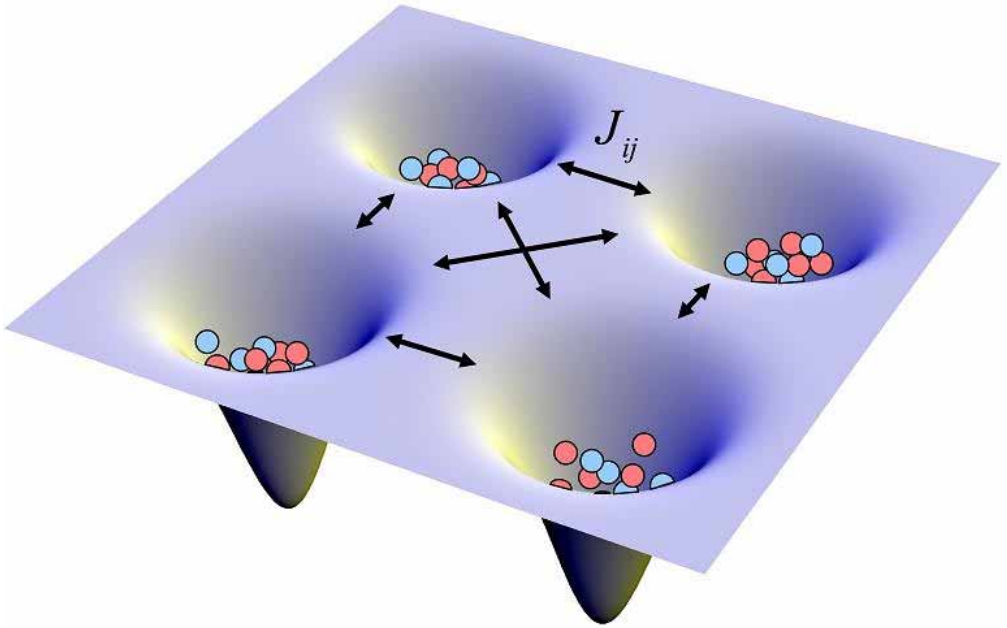
Each site of Ising model has N bosons, each which can be in one of two states (red/blue).

Interactions between sites are modified externally such as to follow the Hamiltonian

$$H = \sum_{i,j=1}^{M} J_{ij} S_i^z S_j^z$$

$$S_i = \sum_{k=1}^{N} \sigma_i^k$$

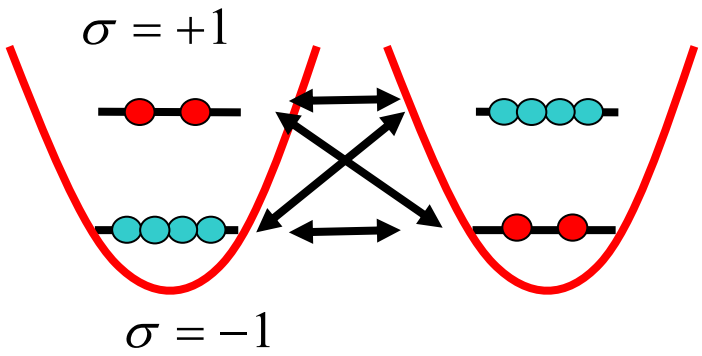
$$\sigma_i^k = \pm 1$$



For now, assume the Hamiltonian is “magically” put into place. Later, I will discuss a feedback control implementation.

Energy spectrum of Bosonic Ising model

Look at a two site system at thermal equilibrium



$$S_i = \sum_{k=1}^{N} \sigma_i^k$$

$$H = -JS_1S_2 - \lambda N\,(S_1 + S_2)$$

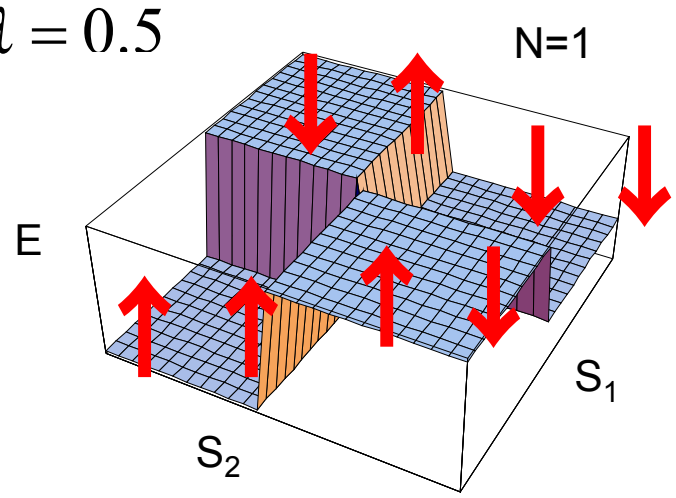
Look at 2 site model, for the parameters

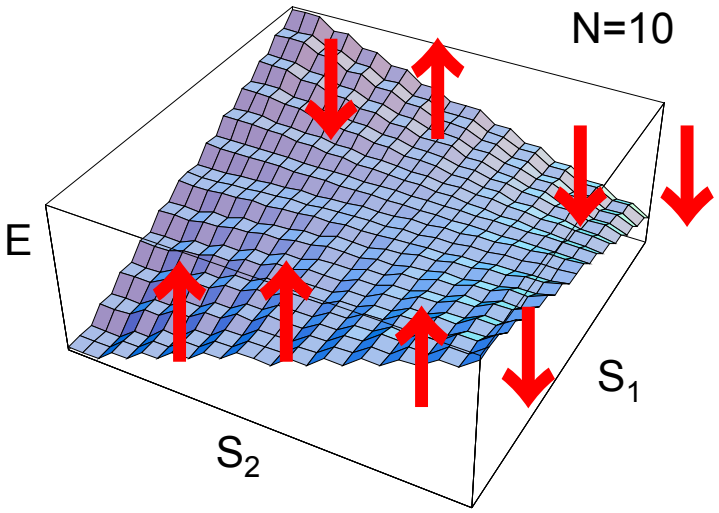
$J = 10$ $\lambda = 0.5$

the "solution" is ↑ ↑

The ground spin configuration of the original Ising model is the ground state of the bosonic Ising model

Energy spectrum:





Properties at thermal equilibrium

Calculate the average spin of the system at thermal equilibrium

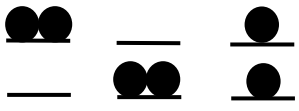
To see the effect of using bosons, compare usage of normal distinguishable particles

These have different counting factors

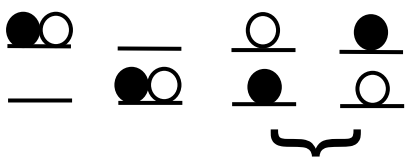
Example

N=2 bosons in a single two level site

bosons



distinguishable



Calculate $\langle S_i \rangle$ using partition function

extra ${}^2C_1$ combinations

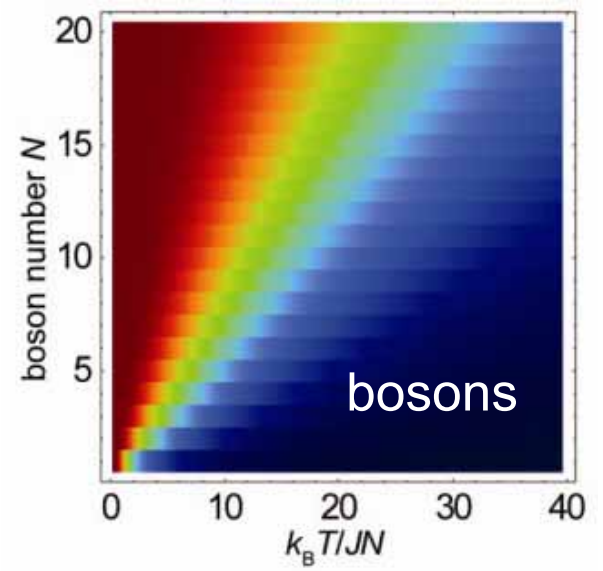
$$Z = \sum_{k_1,k_2=1}^{N} \exp\left[-\beta H(k_1,k_2)\right] C(k_1,k_2)$$

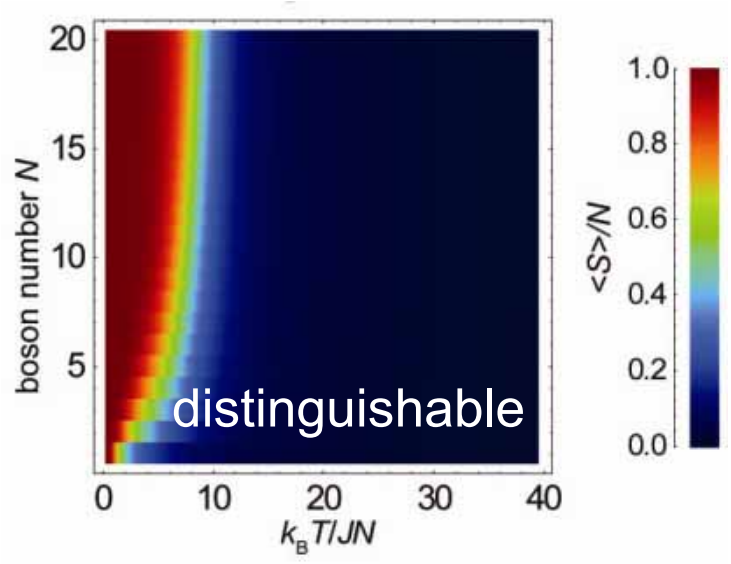
$$C(k_1,k_2) = \begin{cases} 1 & \text{(bosons)} \\ \binom{N}{k_1}\binom{N}{k_2} & \text{(distinguishable particles)} \end{cases}$$

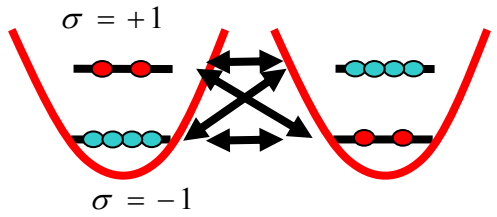
$$H = -JS_1S_2 - \lambda N\,(S_1 + S_2)$$

$$S_i = N - 2k_i$$

Properties at thermal equilibrium

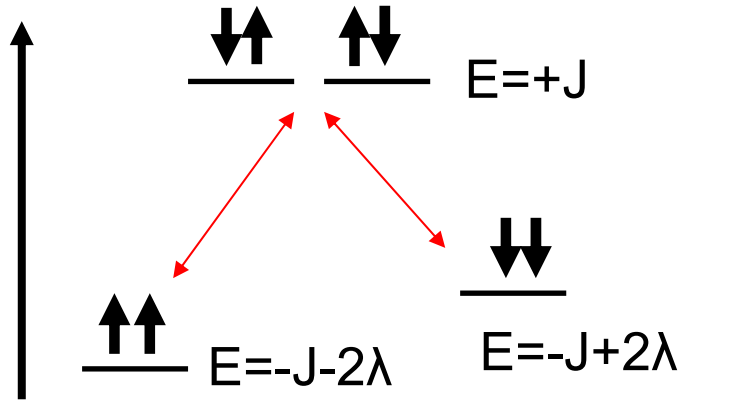






For the same temperature, Bosons have an enhanced ground state population, similar to BEC effect

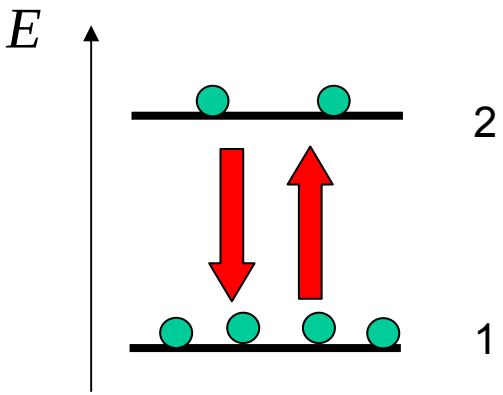
This gives a improved signal-to-noise ratio for the ground state.



$$H = -JS_1S_2 - \lambda N\left(S_1 + S_2\right)$$

Cooling to ground state

Look at time required from cooling from T=∞ state.



Simplest example: 2 levels.

$$\frac{dn_1}{dt} = -\alpha(1+\gamma)(n_2+1)n_1 + \alpha(1-\gamma)(n_1+1)n_2$$

(1→2 on the first term; 2→1 on the second term)

$$\frac{dn_2}{dt} = -\alpha(1-\gamma)(n_1+1)n_2 + \alpha(1+\gamma)(n_2+1)n_1$$

(2→1 on the first term; 1→2 on the second term)

n+1 amplification factors originate from bosonic final state stimulation

$$a^\dagger \left| N \right\rangle = \sqrt{N+1} \left| N+1 \right\rangle$$

Transition rates determined from Fermi's golden rule

$$T_{i\to f} = \frac{2\pi}{\hbar} \left| \left\langle f \left| H_{transition} \right| i \right\rangle \right|^2 \rho$$

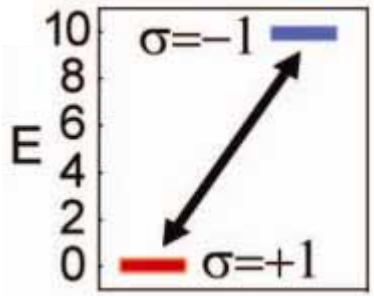
γ factors determined such that the levels are occupied with the thermal equilibrium distributions for

$$\frac{dn_i}{dt} = 0$$

$$\gamma = \frac{p_1 - p_2}{2Np_1p_2 + p_1 + p_2}$$

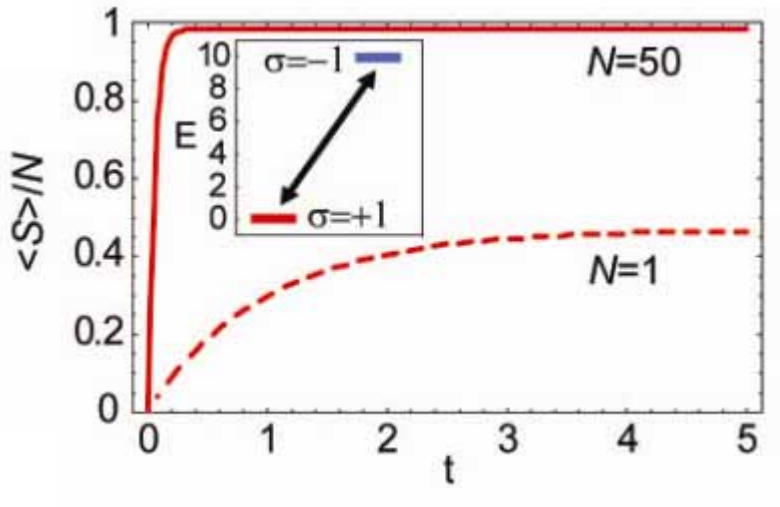
p_i=probability of occupation of level i

2 level system

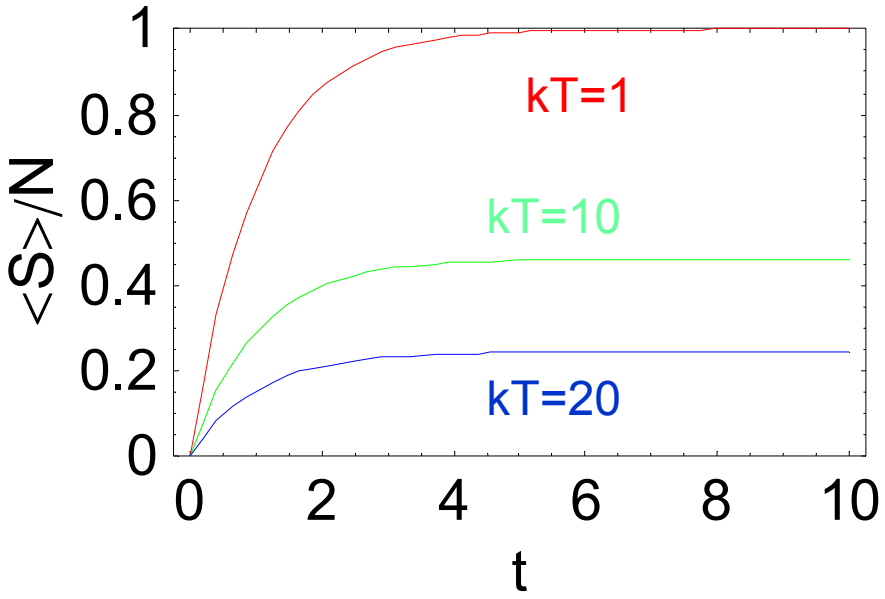


Using large boson numbers N, we get both an accuracy and time improvement.

Fixed temperature (kT=10)



Fixed N=1



Without the use of bosons the equilibriation time is independent of temperature

Simulation of Ising models

To study the two level system we evolved just the populations on each of the sites.

This is ok for one site, but fails for more than one site

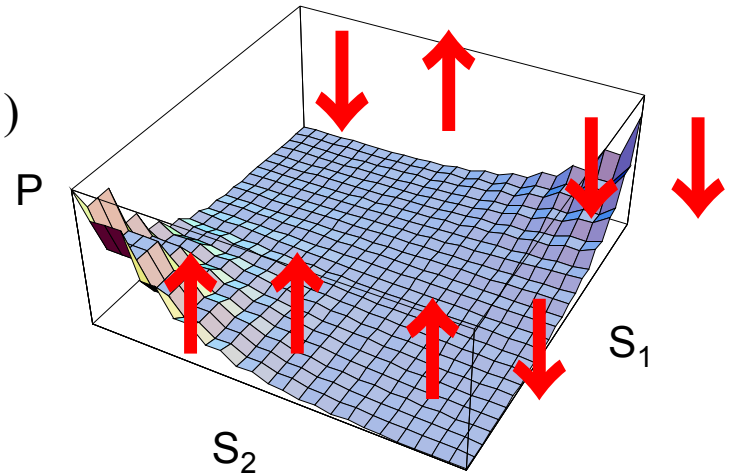
➡ Use Glauber's kinetic Ising model theory

Glauber, J. Math. Phys. **4**, 294 (1963)

Instead of a fixed population, assign a probability distribution to each state

For the pure Ising model case, evolve probability distribution in time according to

$$\frac{dp(\sigma_1,\sigma_2)}{dt} = -w_{\sigma_1,\sigma_2\to-\sigma_1,\sigma_2}\,p(\sigma_1,\sigma_2) - w_{\sigma_1,\sigma_2\to\sigma_1,-\sigma_2}\,p(\sigma_1,\sigma_2)$$
$$+w_{-\sigma_1,\sigma_2\to\sigma_1,\sigma_2}\,p(-\sigma_1,\sigma_2) + w_{\sigma_1,-\sigma_2\to\sigma_1,\sigma_2}\,p(\sigma_1,-\sigma_2)$$



Choose transition rates according to thermal equilibrium

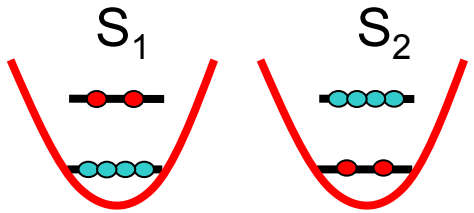
$$\frac{dp(\sigma_1,\sigma_2)}{dt} = 0 \qquad \frac{w_{\sigma_1,\sigma_2\to-\sigma_1,\sigma_2}}{w_{-\sigma_1,\sigma_2\to\sigma_1,\sigma_2}} = \frac{p_{equil}(-\sigma_1,\sigma_2)}{p_{equil}(\sigma_1,\sigma_2)}$$

from partition function

Simulation of bosonic Ising model

Now want to simulate equilibration of

$$H = \sum_{i,j=1}^{M} J_{ij} S_i S_j$$

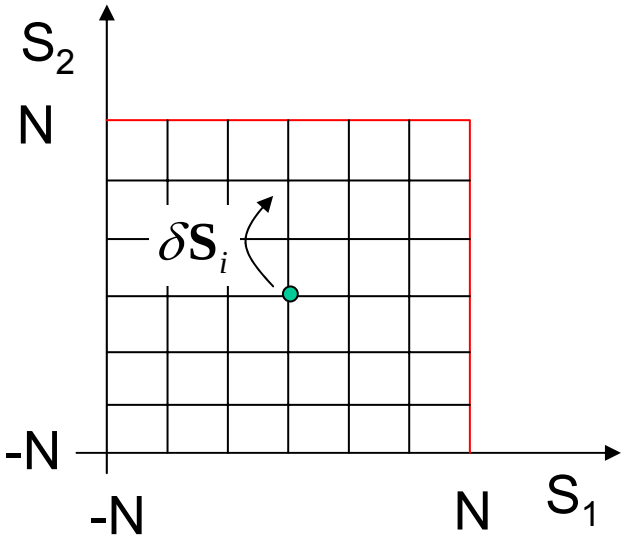


A general state is written

$$\left|\mathbf{S}\right\rangle = \left|S_1, S_2, S_3 \ldots\right\rangle$$

The probability distribution evolves according to

$$\frac{dp_{\mathbf{S}}}{dt} = \sum_i \sum_{\delta S_i} -w(\mathbf{S}, \delta\mathbf{S}_i)\, p_{\mathbf{S}} + w(\mathbf{S}+\delta\mathbf{S}_i, -\delta\mathbf{S}_i)\, p_{\mathbf{S}+\delta\mathbf{S}_i}$$



Final state stimulation factors in transition rates are calculated from Fermi's golden rule

$$w(\mathbf{S}, \delta\mathbf{S}_i) = \alpha \underbrace{\left(1+\gamma_i(\delta S)\right)}_{\text{detailed balance}} \underbrace{\frac{\xi^{\delta S-1}}{((\delta S-1)!)^2} \underbrace{\left|\left\langle \mathbf{S}+\delta\mathbf{S}_i \left| H_t^{\,\delta S} \right| \mathbf{S} \right\rangle\right|^2}_{\text{final state stimulation}}}_{\text{Fermi golden rule}}$$

ξ=suppression coefficient of higher order transitions

$$\gamma_i(\delta S) = \tanh[-\frac{\delta S}{k_B T} \sum_j J_{ij} S_j] \qquad H_t = \sum_{i\sigma} a_{i\sigma}^{\dagger} a_{i-\sigma}$$

Faisal, J. Phys. B: Atom. Molec. Phys. **9**, 3009 (1976).

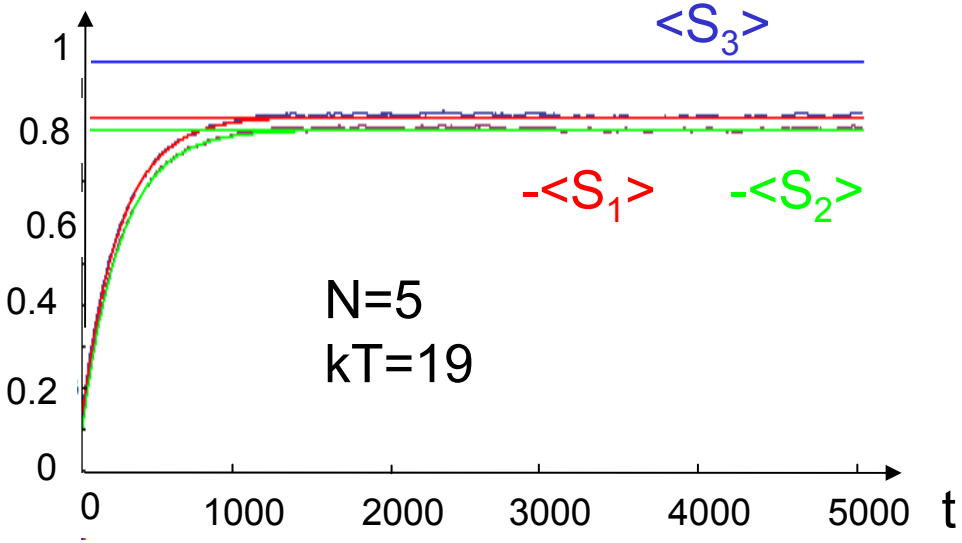
Typical kinetic Monte Carlo datasets

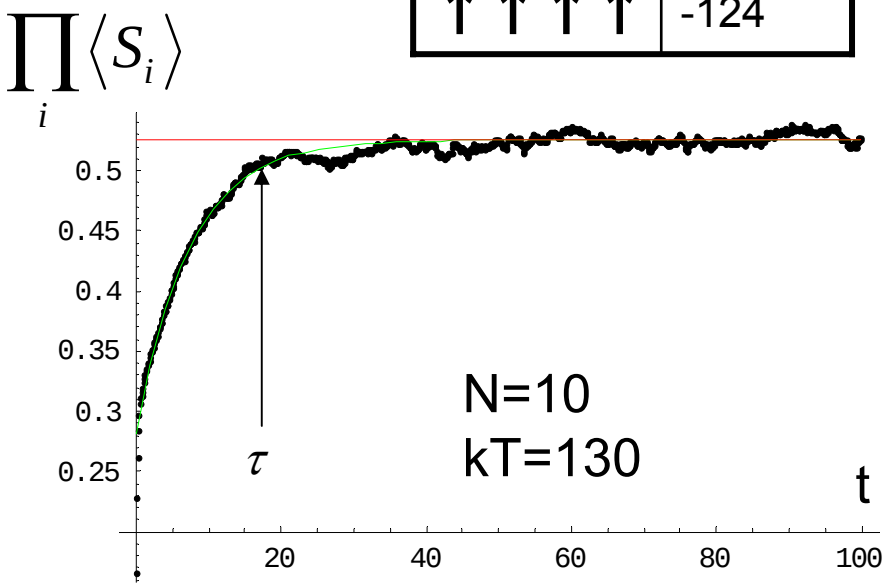
$J_{ij} = 10 \qquad \lambda = 1$

To break S→-S symmetry, introduce second term

$$H = \sum_{i,j} J_{ij} S_i S_j + \lambda N \sum_i S_i$$

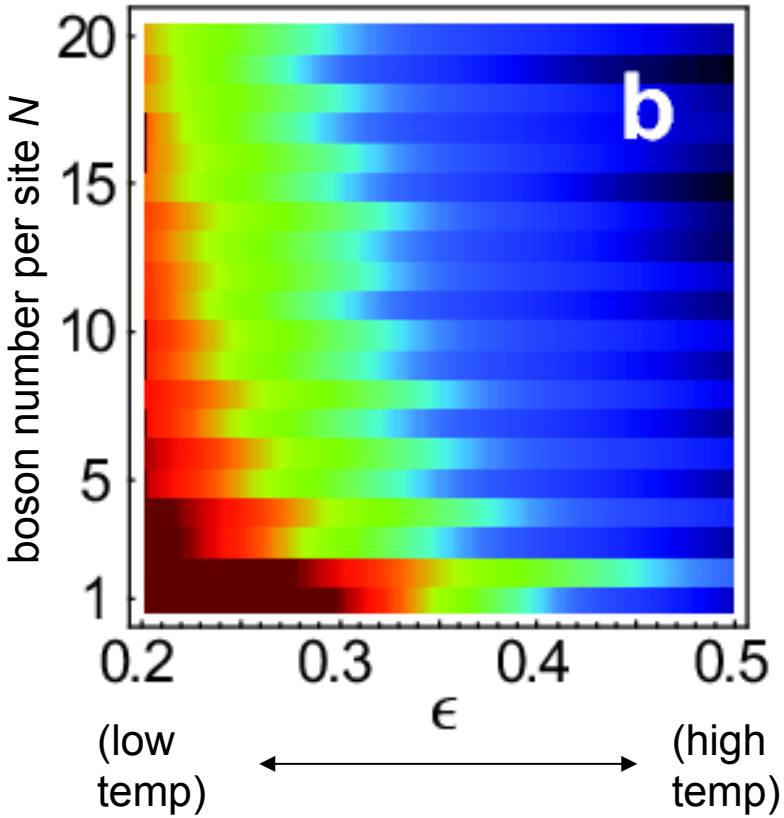
state	energy
↑ ↑ ↓ ↓ +5 others	40
↓ ↓ ↓ ↑ + 3 others	2
↑ ↑ ↑ ↓ + 3 others	-2
↓ ↓ ↓ ↓	-116
↑ ↑ ↑ ↑	-124

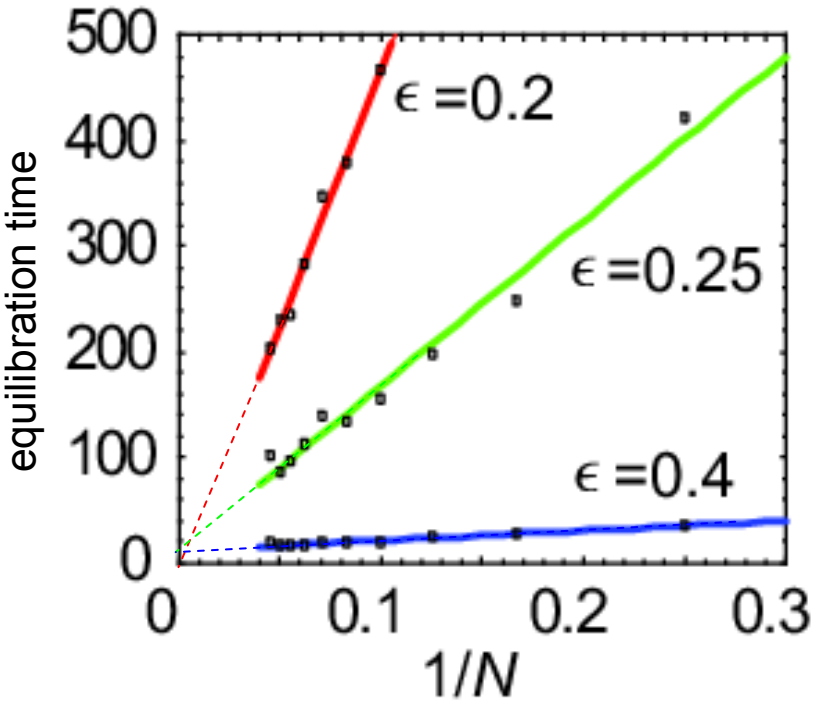




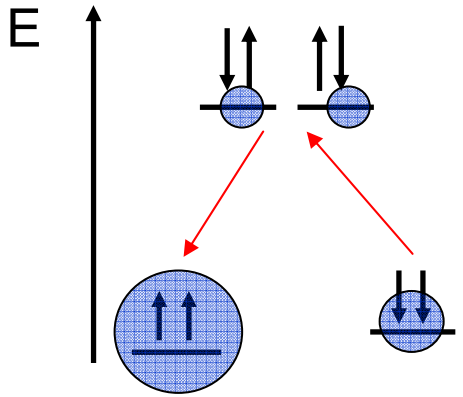
90% equilibrium defines τ

Simulation of 4 site bosonic Ising model





times increase at low temperature due to local minimum effect



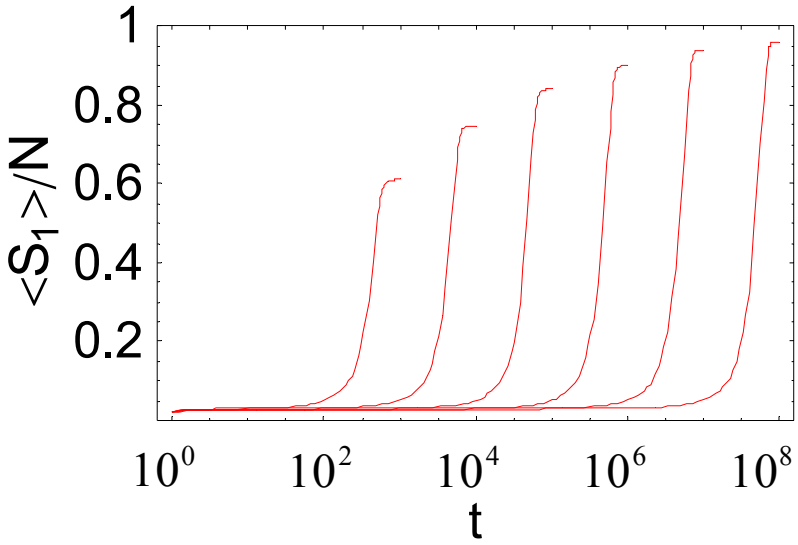
Annealing

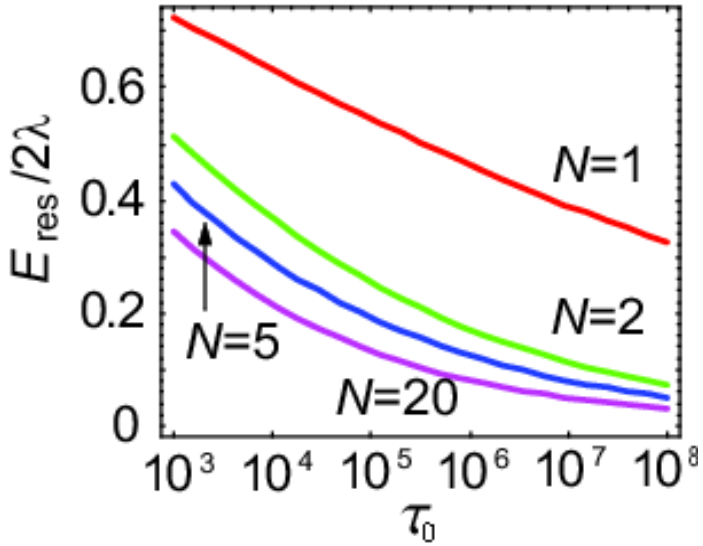
Perform annealing of temperature according to schedule:

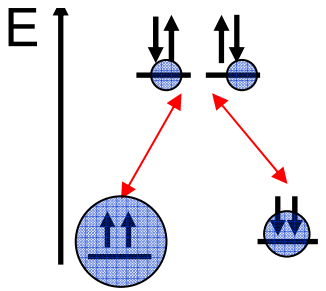
$$T(t) = T_0(N)\exp(-t/\tau_0)$$

$T_0(N)$ = temperature corresponding to error rate of $\varepsilon = 0.7$

2 site Ising model: $J = 10 \quad \lambda = 0.5$





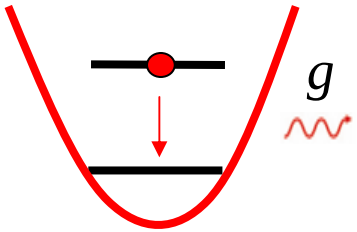


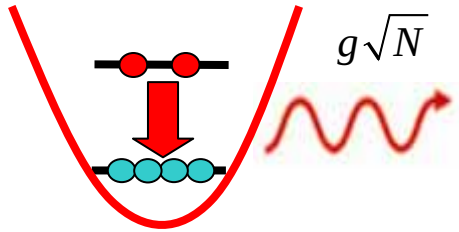
residual energy= average energy above ground state post-annealing

What is the origin of the speedup?

1) Energy scales

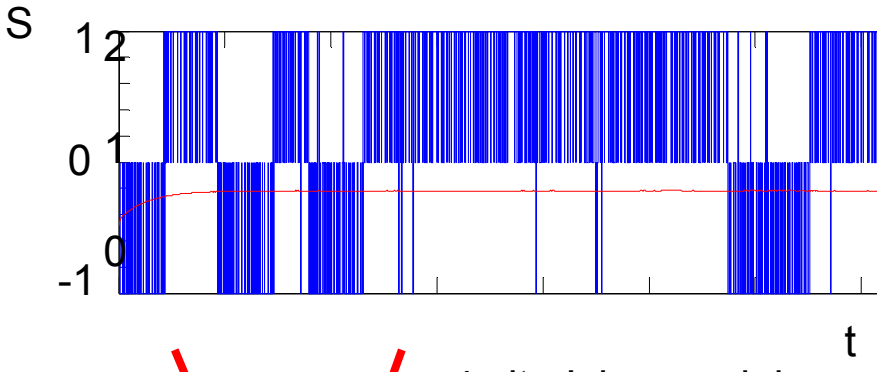
By increasing the number of bosons from 1 to N we increase the overall energy scale of the problem.



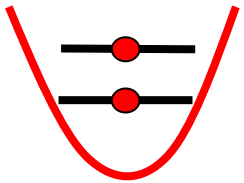


2) Spin flip time

Just because one site cools faster doesn't mean the whole goes to equilibrium faster

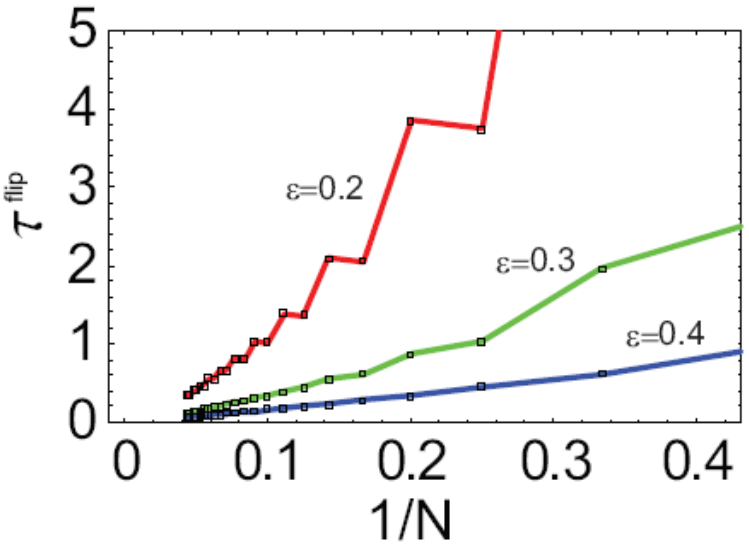


N=2



4 site Ising model

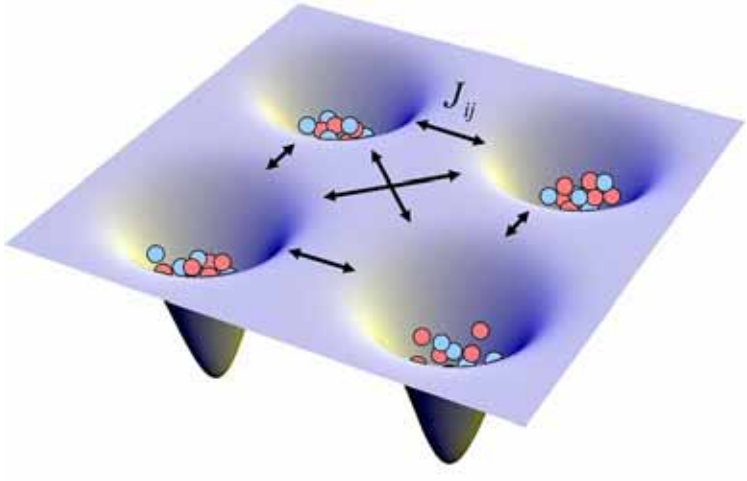
J=10 λ=1



How to implement H?

Everything until now assumed that we have a perfect implementation of the Hamiltonian

$$H = \sum_{i,j=1}^{M} J_{ij} S_i^z S_j^z$$

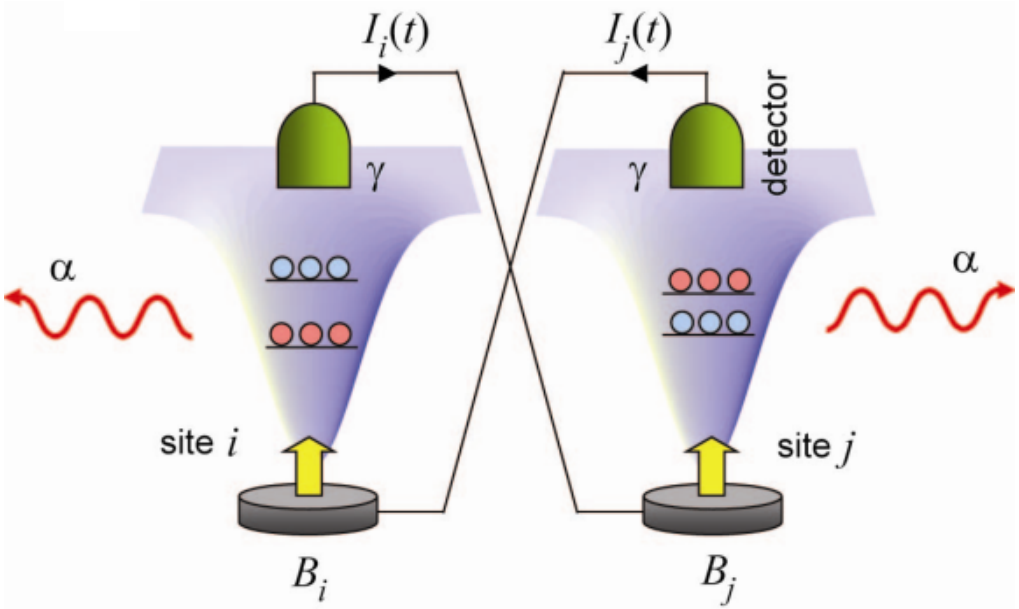


How to do this?

Proposal: Feedback control.

$$H = \sum_{i,j=1}^{M} J_{ij} S_i(t) S_j(t) = \sum_{i=1}^{M} B_i(t) S_i(t)$$

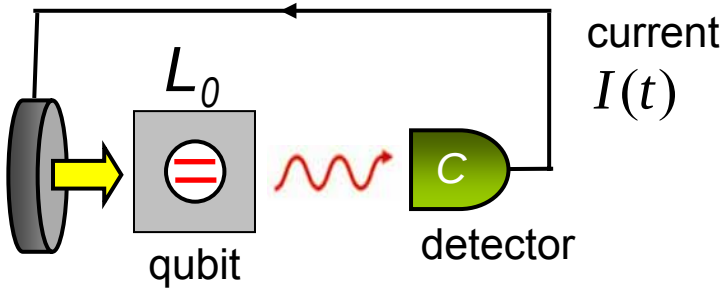
$$B_i(t) = \sum_{j=1}^{N} J_{ij} S_j(t)$$



Quantum feedback control

The quantum state of a system can be controlled by a method of continuous measurement and feedback

$H_{FB} = I(t)F$ applied control



Wiseman, and Milburn, *Phys. Rev. Lett.* **70**, 548 (1993).

In a Markovian approximation with respect to the feedback, the equation of motion is determined by the Wiseman-Milburn feedback master equation

Wiseman, et al, *Phys. Rev. A.* **66**, 013807 (2002).

$$\frac{d\rho}{dt} = L_0\rho + D[C]\rho - i\sqrt{\eta}[F, M\rho] + D[F]\rho$$

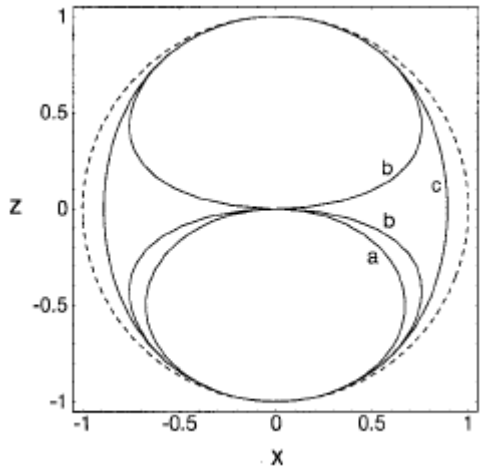
bare system evolution

decoherence due to measurement

induced evolution due to feedback

$$D[C]\rho = C\rho C^\dagger - \{C^\dagger C, \rho\}/2$$

M = Back action operator



using y-driving field and dissipation

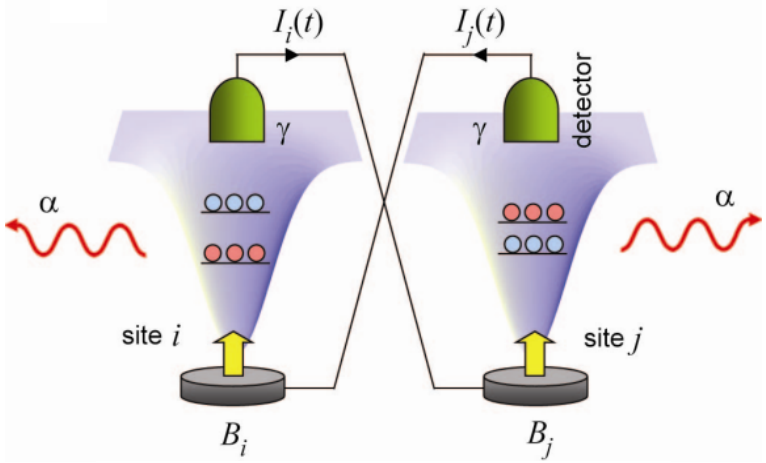
Simulating interaction by feedback

In our case, we wish to affect the state on site busing the measurement result on **another** site

In the Wiseman-Milburn feedback equations we have

Measurement of the z-component of the spin: $C = \sqrt{\gamma} S_i^z$

Back action operator due to z-measurement: $\mathcal{M}\rho = S_i^z \rho + \rho S_i^z .$



Applied feedback Hamiltonian: $F \propto S_i^z .$

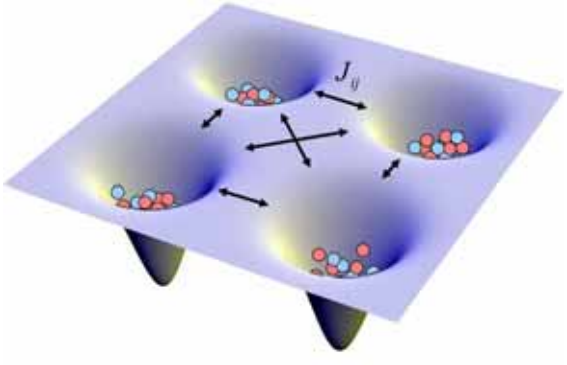
$$H_{\mathrm{fb}}(t) = \lambda \sum_{i,j\neq i} S_i^z J_{ij} I_j(t)$$

Equation of motion

$$\frac{d\rho}{dt} = \sum_i \left[\gamma D[S_i^z]\rho - i\sqrt{\eta} \sum_{j\neq i} \left[\lambda J_{ij} S_i^z, S_j^z \rho + \rho S_j^z \right] + \lambda^2 \sum_{j\neq i} J_{ij} D[S_i^z]\rho + \Omega^-(I_j) D[S_i^-] + \Omega^+(I_j) D[S_i^+] \right]$$

$$= -i\lambda\sqrt{\eta}[H,\rho] + \sum_i \Omega^-(I_j) D[S_i^-] + \Omega^+(I_j) D[S_i^+] + \sum_i \left(\lambda^2 \sum_{j\neq i} J_{ij}^2 + \gamma \right) D[S_j^z]\rho \qquad H = \sum_{i,j=1}^{M} J_{ij} S_i S_j$$

Is this a kind of “quantum” computer?



$$H = \sum_{i,j=1}^{M} J_{ij} S_i S_j$$

Although this is a computational device that uses quantum effects (indistinguishability), it is not a “quantum” computer as we normally think since:

- No entanglement present between sites
- An electrical feedback loop (a classical circuit) could simulate this in principle

→ The equilibriation time is most probably still exponential in the number of sites M.

Introducing coherence improves scaling?

Summary

- Introduced two types of quantum simulation: analogue and digital. Review: Buluta & Nori Science **326**, 108 (2009)
- Analogue quantum simulation is technologically easier than digital quantum simulation. Digital quantum simulation is technologically difficult, but can in principle simulate any system.
- Exciton-polaritons are promising for quantum simulation with many similar applications to cold atoms in optical lattices. For observing the Mott transition, need heavy exciton-polaritons.
- Proposed a method of computing optimization problems with BECs using quantum simulation ideas.