

Bosons and Fermions in optical lattices

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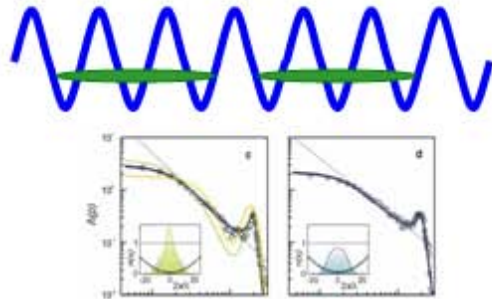
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S. Fölling (Mainz)

TRENTO, March 2004



OUTLINE

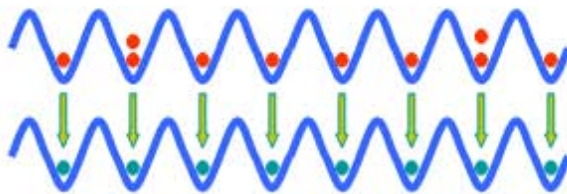
1. Tonks-Girardeau gas in 1D optical lattices:



2. Extensions:

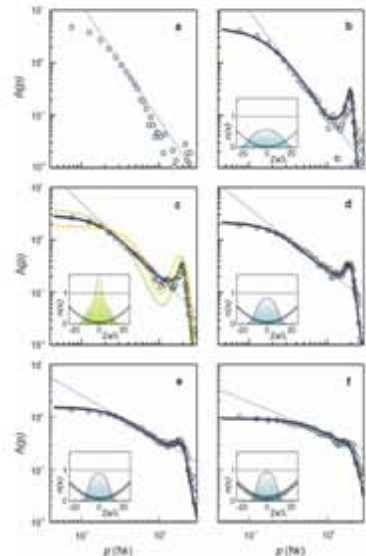
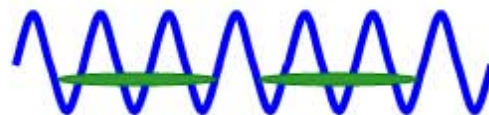


3. Loading optical lattices:



1. Tonks-Girardeau gas in OL

B. Paredes, A. Widera, V. Murg, O. Mandel, S. Fölling,
J.I. Cirac, G. V. Shlyapnikov, T. W. Hänsch & I. Bloch



M. Girardeau, J. Math. Phys. 1, 516 (1960).

Relationship between Systems of Impenetrable Bosons and Fermions in One Dimension.

Other works in the field of Atomic Physics:

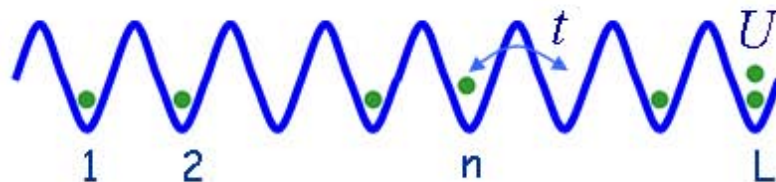
Experiments in the gas phase: NIST and Zürich

Theory in the gas phase: Olshanii et al., Cazalilla, Giorgini et al, Drummond et al, Shlyapnikov et al...

Theory in an optical lattice: Zwerger et al, ...

Fermionization: review

N particles, L sites



Characteristic energies:

t : tunnel

U : On-site interaction

Bose-Hubbard model:
$$H_B = -t \sum_n (a_{n+1}^\dagger a_n + a_n^\dagger a_{n+1}) + U \sum_n (a_n^\dagger)^2 a_n^2$$

bosonic
operators

• We will consider:

- Strong interacting regime: $t \ll U$
- Low temperature: $k_B T \ll U$
- Dilute: $\nu = N/L < 1$

➡ At most one atom per site:

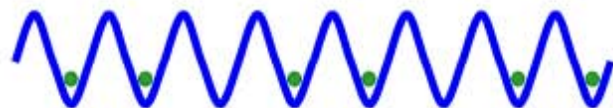


Hard-core bosons.

Fermionization

Hard-core Bosons

Allowed states:



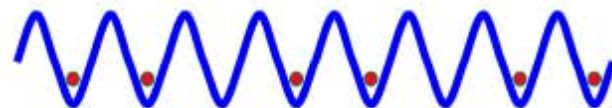
$$|1,1,0,1,1,0,1,1\rangle$$

$$|1,0,1,1,1,0,1,1\rangle$$

etc

Fermions

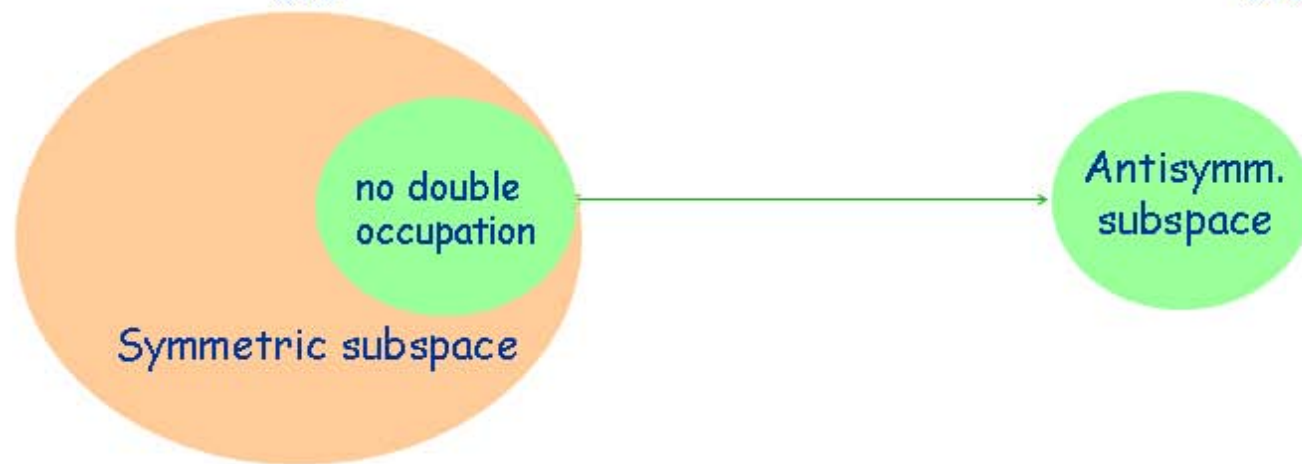
Allowed states:



$$|1,1,0,1,1,0,1,1\rangle$$

$$|1,0,1,1,1,0,1,1\rangle$$

etc



We can establish a one-to-one correspondence

... but we must be careful, since states (H) have different symmetries

JORDAN-WIGNER TRANSFORMATION

Hard-core Bosons

STATES
 $|1,1,0,1,1,0,1,1\rangle$

OPERATORS
 (OBSERVABLES)

$$a_n$$

Fermions

STATES
 $|1,1,0,1,1,0,1,1\rangle$

OPERATORS
 (OBSERVABLES)

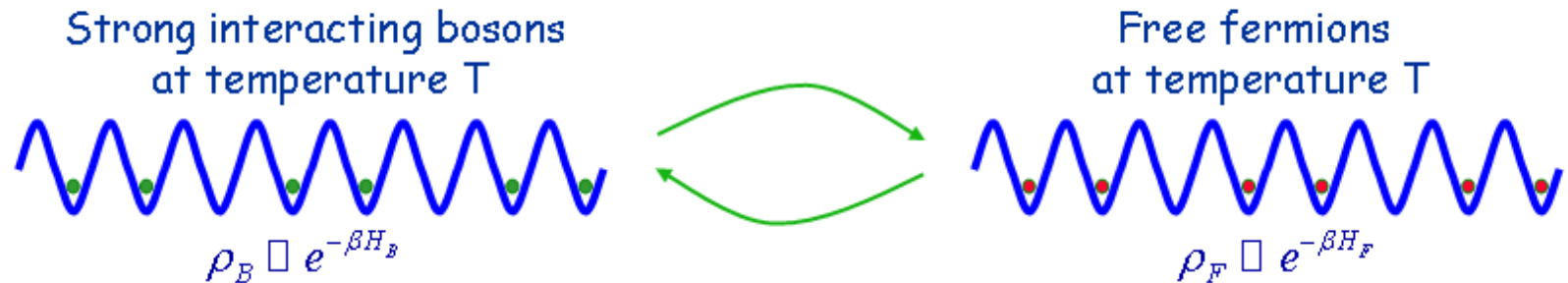
$$(-1)^{\sum_{m < n} c_m^\dagger c_m} c_n$$

It ensures that $\langle \Psi_B | O_B | \Psi_B \rangle = \langle \Psi_F | O_F | \Psi_F \rangle$



STATE IN THERMAL EQUILIBRIUM

	a_n	$\longleftrightarrow$	$(-1)^{\sum_{m<n} c_m^\dagger c_m} c_n$
Density:	$a_n^\dagger a_n$	$\longleftrightarrow$	$c_n^\dagger c_n$
Tunnel:	$a_{n+1}^\dagger a_n$	$\longleftrightarrow$	$c_{n+1}^\dagger (-1)^{c_n^\dagger c_n} c_n = c_{n+1}^\dagger c_n$
Hamiltonian:	$H_B = -t \sum_n (a_{n+1}^\dagger a_n + a_n^\dagger a_{n+1}) + U \sum_n (a_n^\dagger)^2 a_n^2$	$\longleftrightarrow$	$H_F = -t \sum_n (c_{n+1}^\dagger c_n + c_n^\dagger c_{n+1})$
Density operator:	$\rho_B \propto e^{-\beta H_B}$	$\longleftrightarrow$	$\rho_F \propto e^{-\beta H_F}$



TONKS-GIRARDEAU GAS

OBSERVABLES



A) The observable has the same expression:

Density:	$a_n^\dagger a_n$	$\longleftrightarrow$	$c_n^\dagger c_n$
Tunnel:	$a_{n+1}^\dagger a_n$	$\longleftrightarrow$	$c_{n+1}^\dagger c_n$
Hamiltonian:	$H_B = -t \sum_n (a_{n+1}^\dagger a_n + a_n^\dagger a_{n+1})$	$\longleftrightarrow$	$H_F = -t \sum_n (c_{n+1}^\dagger c_n + c_n^\dagger c_{n+1})$

Examples:

Density and density fluctuations
 Kinetic energy
 Total energy and energy fluctuations
 Spectrum
 Density of states
 Entropy
 Etc.

For strong int. Bosons at temperature T
are the same as
for free Fermions at temperature T .

OBSERVABLES



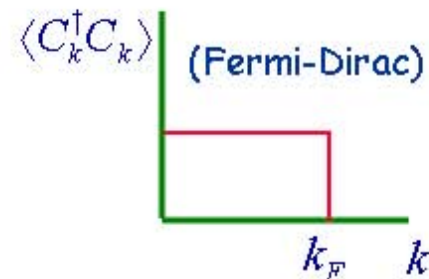
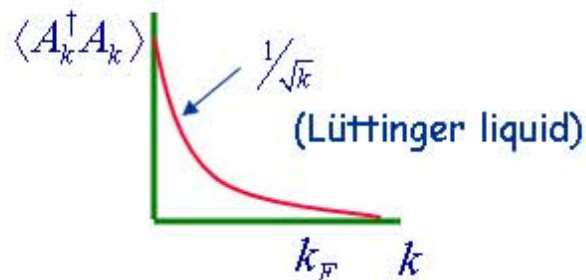
B) The observable has a different expression:

Correlation: $a_m^\dagger a_n \longleftrightarrow c_m^\dagger (-1)^{\sum_{n < m} c_l^\dagger c_l} c_n \neq c_m^\dagger c_n$

Momentum: $A_k^\dagger A_k \longleftrightarrow \dots \neq C_k^\dagger C_k$

These properties are different for hard core bosons and free fermions.

- For an infinite, homogeneous lattice at $T=0$:



In some aspects, they behave like free fermions.
 In other aspects, they are totally different.

Quasi-momentum distribution:

$$\langle A_k^\dagger A_k \rangle = \text{DFT}[\underbrace{\langle a_n^\dagger a_m \rangle}_{\rho_B}]$$

$$\langle c_m^\dagger (-1)^{\sum_{n \leq m} c_i^\dagger c_i} c_n \rangle_{\rho_F}$$

Wick's
theorem

$$\sum \prod \langle c_\alpha^\dagger c_\beta \rangle_{\rho_F} = \det[\langle c_\alpha^\dagger c_\beta \rangle_{\rho_F}]$$

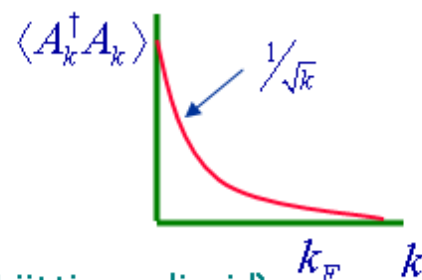
Töplitz
determinant

small
systems

Numerically:
Determinant of
 $L \times L$ matrix
(efficient)

$$|\alpha - \beta| \ll 1$$

$$\frac{1}{\sqrt{|\alpha - \beta|}}$$



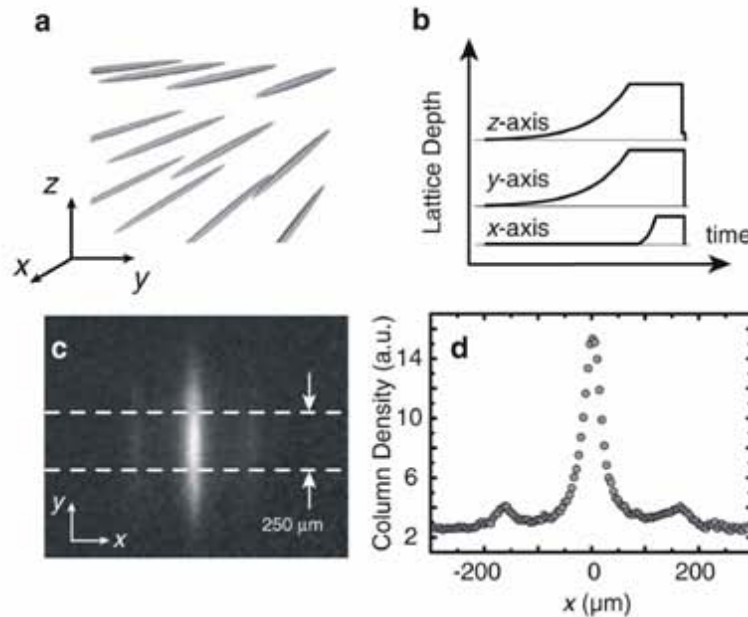
(Shortcut: Luttinger liquid)

Ground-state wavefunction:

$$\Psi_B(x_1, x_2, \dots, x_N) = \langle x_1, x_2, \dots, x_N | \Psi \rangle = |\Psi_F(x_1, x_2, \dots, x_N)| = \prod_{i < j} |\sin(\pi(x_i - x_j)/L)|$$

Slater determinant

Comparison with experiment



Facts to be taken into account:

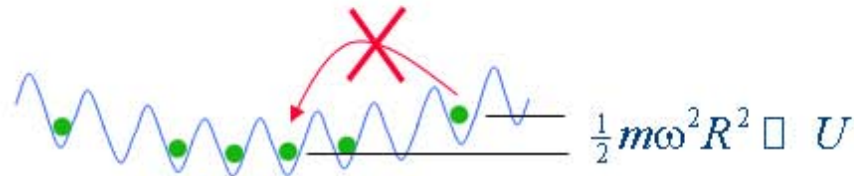
- External harmonic potential.
- Number of atoms is different in the tubes.
- Finite temperatures.

Other issues:

- Is the momentum distribution affected during expansion?

External harmonic potential:

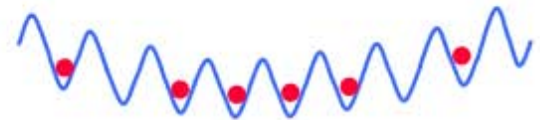
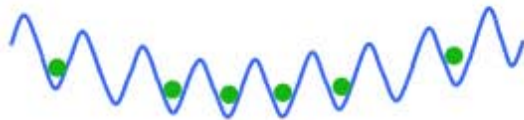
- Extra condition for the JW mapping.



Hamiltonian:

$$H_B = -t \sum_n (a_{n+1}^\dagger a_n + a_n^\dagger a_{n+1}) + b \sum_n n^2 a_n^\dagger a_n \longleftrightarrow H_F = -t \sum_n (c_{n+1}^\dagger c_n + c_n^\dagger c_{n+1}) + b \sum_n n^2 c_n^\dagger c_n$$

Density operator: $\rho_B \propto e^{\beta H_B} \longleftrightarrow \rho_F \propto e^{\beta H_F}$



TONKS-GIRARDEAU GAS

In the gas phase: Olshanii et al., Cazalilla, Giorgini et al, Drummond et al, Shlyapnikov et al...

Some properties coincide with those of free fermions:

Density: $n(x) \stackrel{TF}{=} \frac{1}{\pi} \arccos \left(\max \left[\frac{\mu - bx^2}{-2t}, -1 \right] \right) \longrightarrow \text{size of the cloud } R \longrightarrow \text{condition } \frac{1}{2} m \omega^2 R^2 \leq U$

Energy, excitation frequencies, entropy, etc.

Other properties are different:

Quasi-momentum distribution:

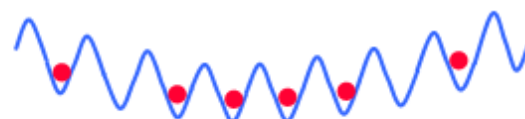
$$\langle A_k^\dagger A_k \rangle = \text{DFT} \left[\underbrace{\langle a_n^\dagger a_m \rangle}_{\rho_F} \right]$$

$$\langle c_m^\dagger (-1)^{\sum_{n < m} c_i^\dagger c_i} c_n \rangle_{\rho_F}$$

$\xrightarrow{\text{Wick's theorem}}$

$$\sum \prod \langle c_\alpha^\dagger c_\beta \rangle_{\rho_F} = \det[\langle c_\alpha^\dagger c_\beta \rangle_{\rho_F}]$$

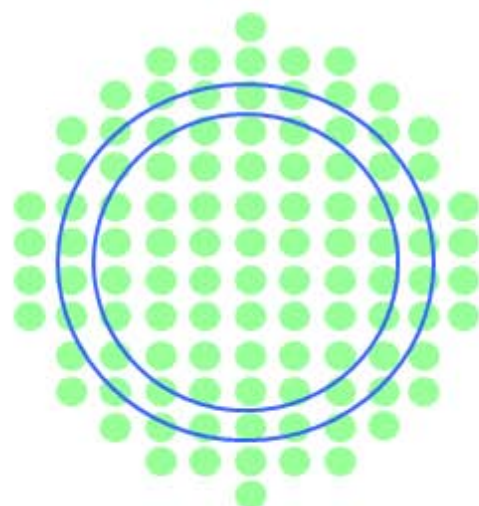
Töplitz determinant



This can be efficiently evaluated

Number distribution in the 1D tubes:

At some point the tubes get isolated and the number of atoms remains fixed.



$$E = \sum_{\text{tubes}} E_t^{1D}(N_t) + N_t V_t - \mu N_t$$

1D Thomas-Fermi Lagrange multiplier

2D Harmonic trap

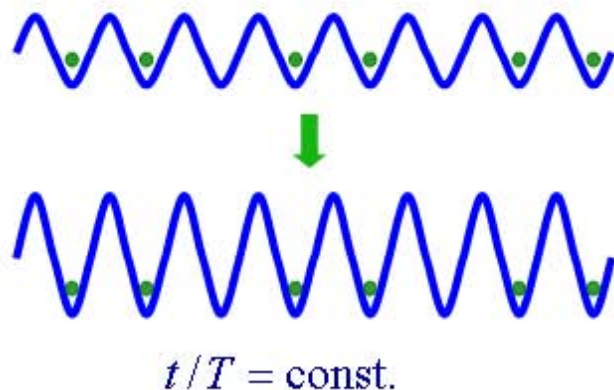
$$\frac{\partial E}{\partial N_t} = 0 \Rightarrow P(N) = \frac{K}{N^{1/3}}$$

Normalization $\int_0^{N_0} P(N) dN = 1$

The distribution is completely fixed by N_0

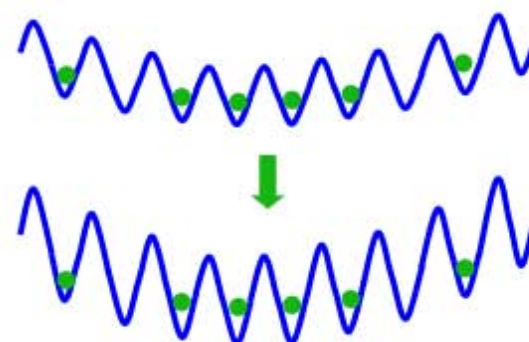
↑
Fitting parameter

Finite temperature:



- Eigenfunctions remain invariant.
- Energies are proportional to t :

$$H_F = -t \sum_n \left(c_{n+1}^\dagger c_n + c_n^\dagger c_{n+1} \right)$$



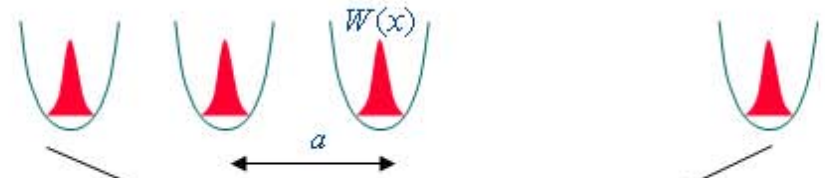
- The process is adiabatic.
- The entropy remains constant.
- The entropy is that of free fermions

We fit the initial temperature T_0

Expansion:

Ideal case:

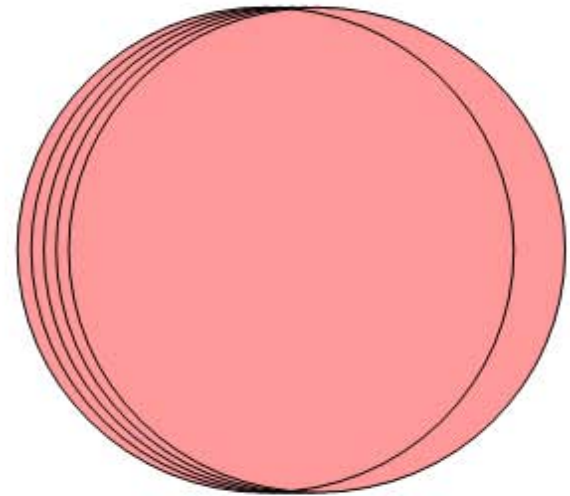
$$\Psi(x, 0) = \sum_n c_n W(x - an)$$



$$\Psi(x, t) = \sum_n c_n W(x - an, t)$$

$$\Psi(x = p\hbar t / ma, t) \xrightarrow{t \rightarrow \infty} \sum_n c_n e^{-ipn} \bar{W}(p)$$

$$n(x = p\hbar t / ma, t) \xrightarrow{t \rightarrow \infty} \underbrace{|\bar{W}(p)|^2}_{\text{envelope}} \underbrace{\left| \sum_n c_n e^{-ipn} \right|^2}_{\text{Momentum distribution}}$$



Effects of interactions:

- The envelope is practically unaffected.
- The phase of the coefficients may be affected.

Taking Gaussian Wannier function, this can be easily estimated.



Change of the phase of a coefficient due to the interactions with the rest of the atoms < 0.02

Momentum distribution:

$$\hat{n}_{M_k, T_k}(p) = \left| \overline{W}(p) \right|^2 \sum_{\ell, \ell'=-\infty}^{\infty} e^{-ip(\ell-\ell')} \left\langle a_{\ell}^{\dagger} a_{\ell'} \right\rangle_{\rho_B}$$

↓ J-W Transformation

$$\left\langle c_{\ell}^{\dagger} (-1)^{\sum_{\ell' < m < \ell'} c_m^{\dagger} c_m} c_{\ell'} \right\rangle_{\rho_F} \quad \text{with} \quad \rho_F \propto e^{-\beta H - \mu N}$$

↓ W. Theorem

$$|\ell - \ell'| \times |\ell - \ell'| \quad \text{Töplitz determinant} \\ \text{in terms of} \\ \left\langle c_k^{\dagger} c_{k'} \right\rangle_{\rho_F}$$

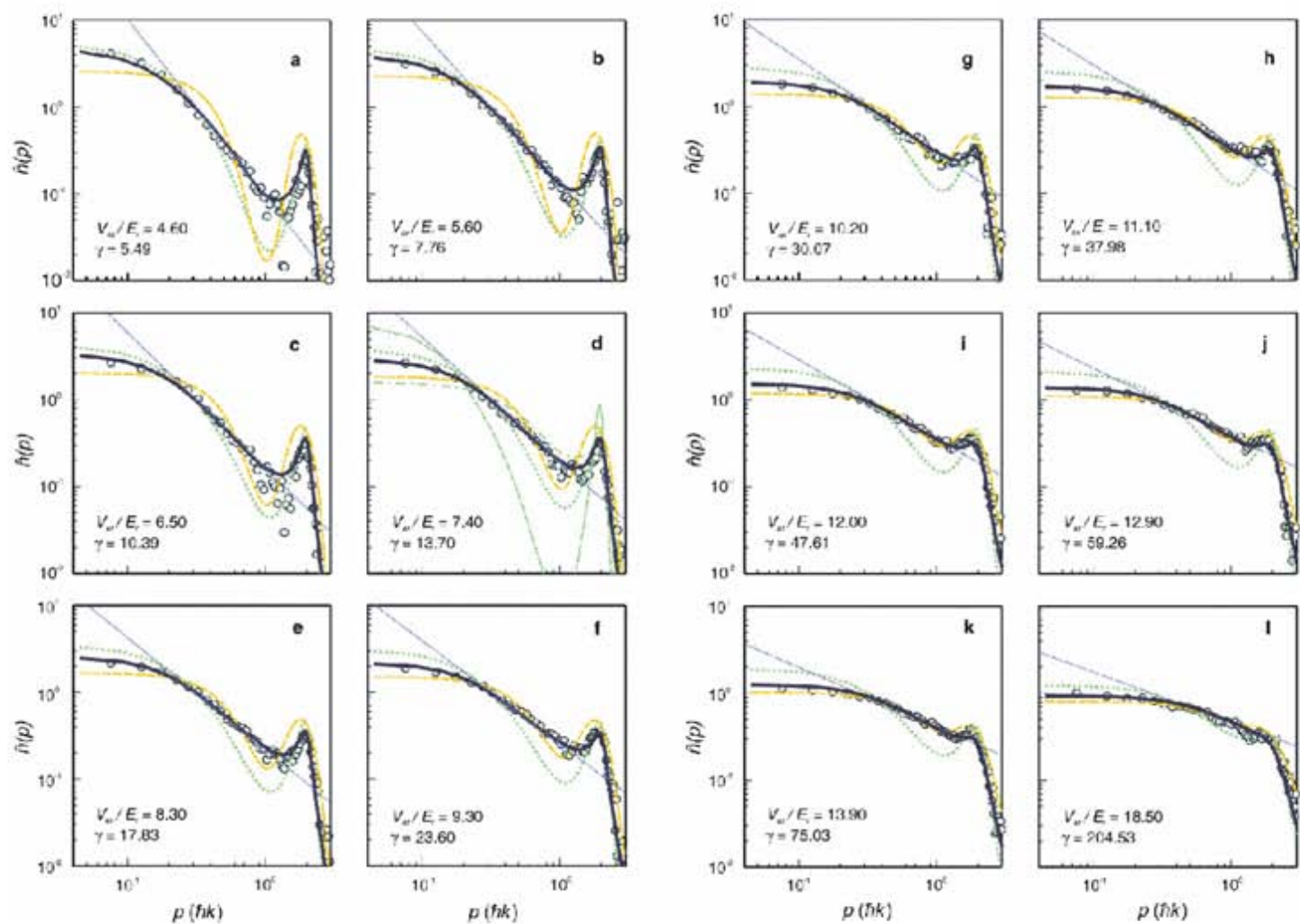


free Fermions

We have to average with respect to the tubes:

- Number of atoms.
- Temperature.

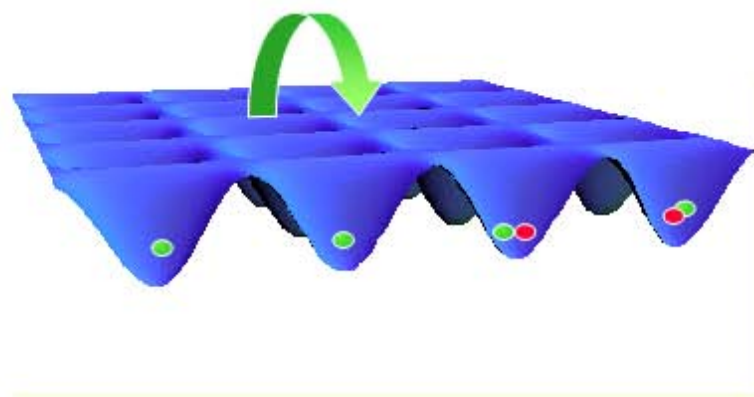
$$\hat{n}(p) = \int_0^{N_0} P(M) \hat{n}_{M, T_M}(p) dM$$



Fitting parameters: N_0, T_0

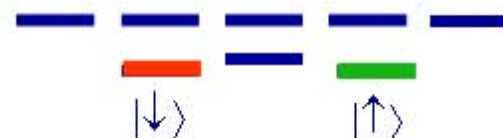
2. Extensions

B. Paredes and G. Shlyapnikov



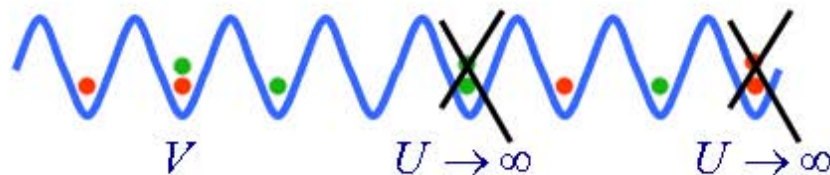
2.1. Two-component Bosons

(B. Paredes and J.I. Cirac, 2003)



• We will consider:

- Strong interacting regime: $t, |V| \ll U$
- Low temperature: $k_B T \ll U$
- Dilute: $\nu_i = N_i/L < 1$



may behave, in some aspects, as interacting spin $\frac{1}{2}$ Fermions

JORDAN-WIGNER TRANSFORMATION

Hard-core Bosons

OPERATORS
(OBSERVABLES)

$$a_{n,\sigma}$$

Fermions

OPERATORS
(OBSERVABLES)

$$(-1)^{\sum_{m < n} c_m^\dagger c_m} c_{n,\sigma}$$

Hamiltonian:

$$H_B = -t \sum_{n,\sigma} (a_{n+1,\sigma}^\dagger a_{n,\sigma} + a_{n,\sigma}^\dagger a_{n+1,\sigma}) + \sum_{n,\sigma} E_{n,\sigma} a_{n,\sigma}^\dagger a_{n,\sigma} + V \sum_n a_{n,\uparrow}^\dagger a_{n,\uparrow} a_{n,\downarrow}^\dagger a_{n,\downarrow} \longleftrightarrow H_F = -t \sum_{n,\sigma} (c_{n+1,\sigma}^\dagger c_{n,\sigma} + c_{n,\sigma}^\dagger c_{n+1,\sigma}) + \sum_{n,\sigma} E_n c_{n,\sigma}^\dagger c_{n,\sigma} + V \sum_n c_{n,\uparrow}^\dagger c_{n,\uparrow} c_{n,\downarrow}^\dagger c_{n,\downarrow}$$

Density operator: $\rho_B \propto e^{-\beta H_B}$

$$\rho_F \propto e^{-\beta H_F}$$

Strong interacting bosons
at temperature T



$$\rho_B \propto e^{-\beta H_B}$$

Interacting fermions
at temperature T



$$\rho_F \propto e^{-\beta H_F}$$

- Strong interacting bosons behave as interacting fermions in several aspects.

For example:

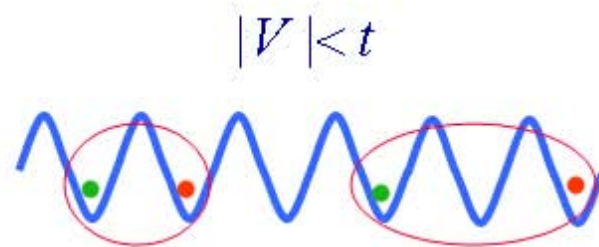
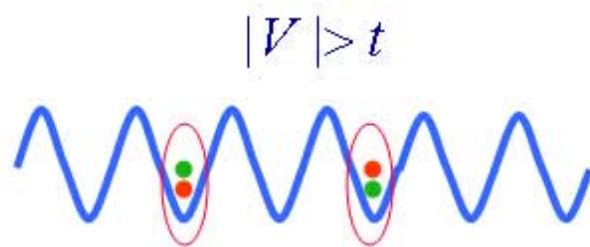
- Density-density correlations: $\langle n_{x+\Delta} n_x \rangle$
 - Spin-spin correlations: $\langle S_{x+\Delta} S_x \rangle$
- where
- $$n_x = a_{x,\uparrow}^\dagger a_{x,\uparrow} + a_{x,\downarrow}^\dagger a_{x,\downarrow}$$
- $$S_x = a_{x,\uparrow}^\dagger a_{x,\uparrow} - a_{x,\downarrow}^\dagger a_{x,\downarrow}$$

For $V < 0$ these functions reflect the appearance of „Cooper“ pairs.

- In other aspects, the behavior will be different.

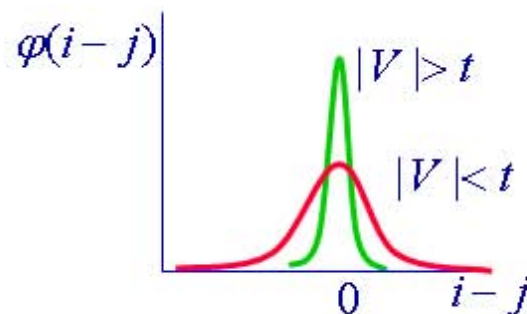
Let us consider $V < 0$

- Correlation functions: Cooper-pair formation
- Depending on the ratio $t/|V|$, we have localized/delocalized pairs.

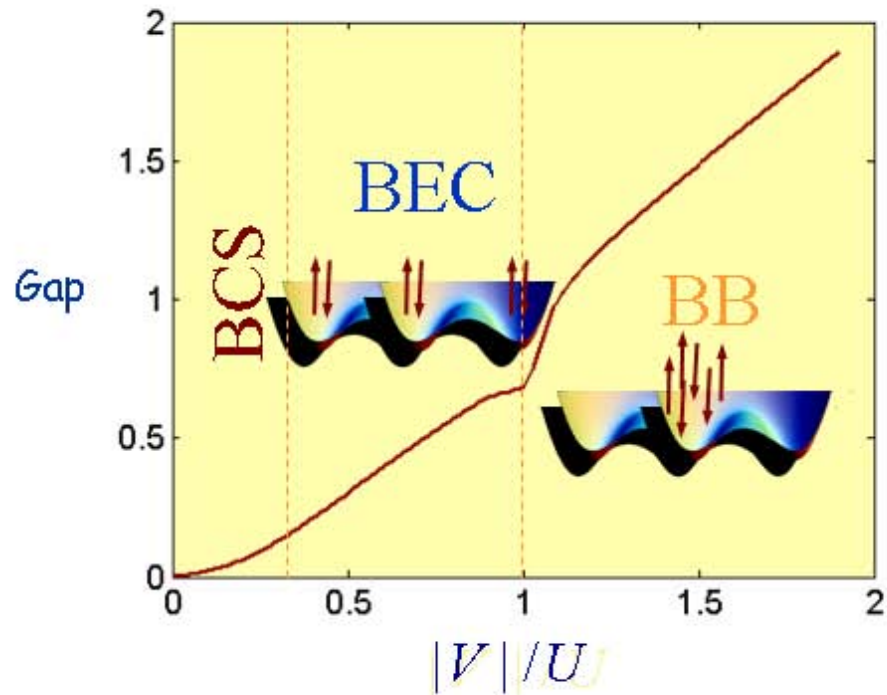
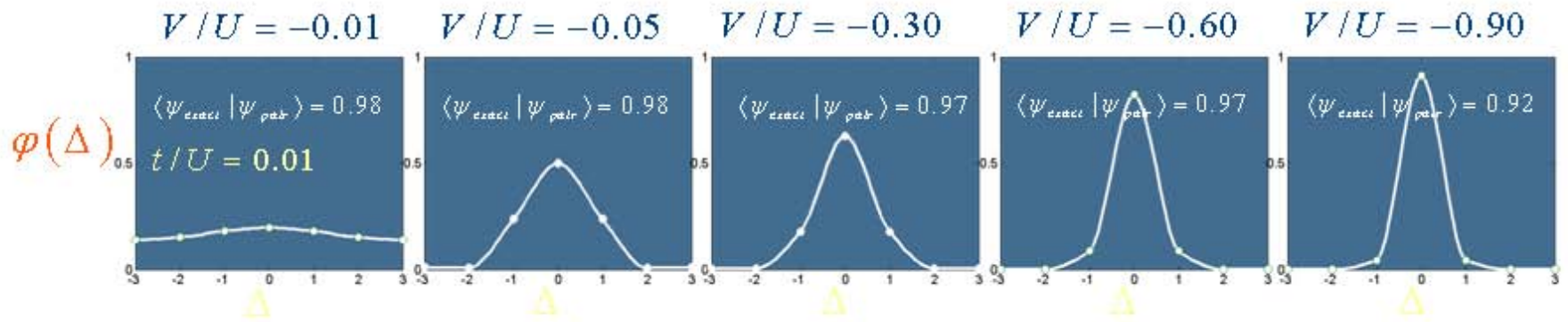


Qualitative behavior: BCS wavefunction

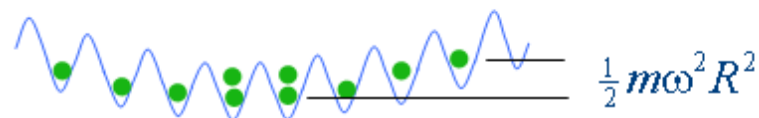
$$|\Psi_F\rangle \propto A \left\{ \prod \left[\sum_{i,j} \varphi(|i-j|) |i,j\rangle \right]^{\otimes N/2} \right\}$$



Numerical results

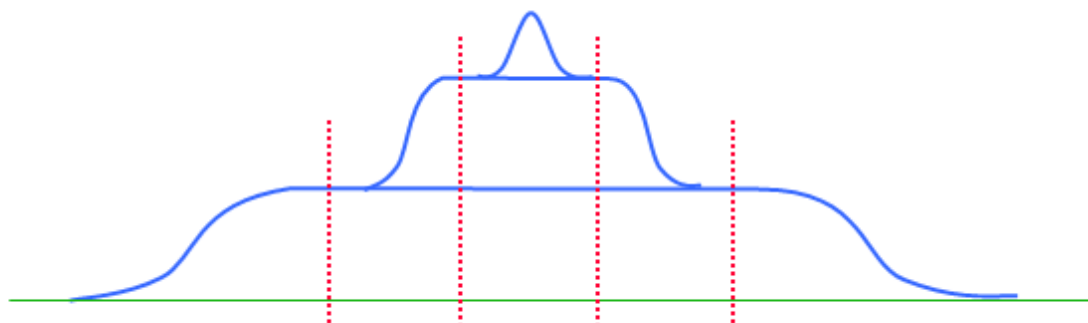


2.2. Higher filling factors:

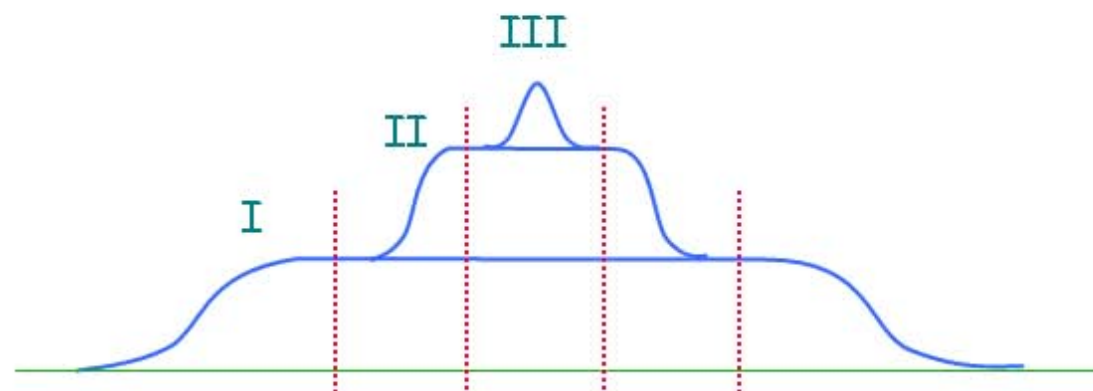


- Strong interacting regime: $t \ll U$
- Low temperature: $k_B T \ll U$
- Not-dilute: $\frac{1}{2}m\omega^2 R^2 \geq U$

We have different layers of Tonks-Girardeau gases:



Description.



Fermionization:

Hard-core Bosons

Fermions

Zone I:



$$|1, 1, 0, 1, 1, 0, 1, 1\rangle$$

$$-t \sum_n (a_{n+1}^\dagger a_n + a_n^\dagger a_{n+1})$$



$$|1, 1, 0, 1, 1, 0, 1, 1\rangle$$

$$-t \sum_n (c_{n+1}^\dagger c_n + c_n^\dagger c_{n+1})$$

Zone II:



$$|2, 2, 1, 2, 2, 1, 2, 2\rangle$$

$$-t \sum_n (a_{n+1}^\dagger a_n + a_n^\dagger a_{n+1})$$

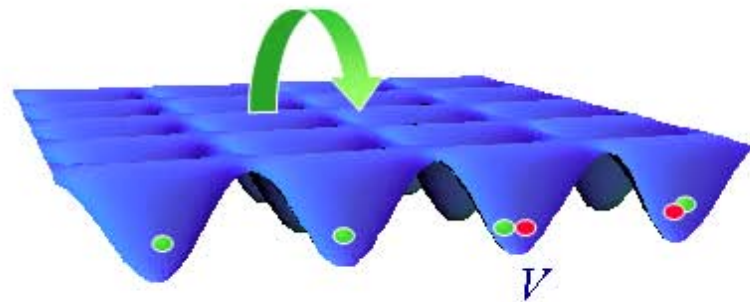


$$|1, 1, 0, 1, 1, 0, 1, 1\rangle$$

$$-\sqrt{2}t \sum_n (c_{n+1}^\dagger c_n + c_n^\dagger c_{n+1})$$

The zones are determined variationally.

2.3. Higher dimensions



- Strong interacting regime: $t \ll U$
- Low temperature: $k_B T \ll U$
- Dilute: $\nu = N/L < 1$

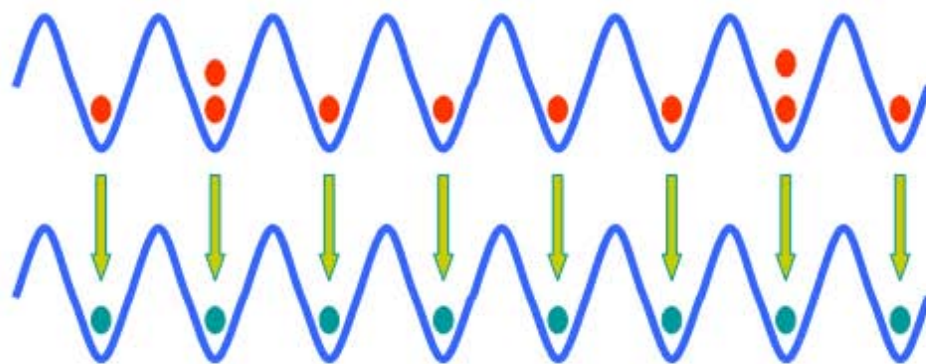
Still, the physics is similar but the fermionization procedure does not work.

- Cooper pairing.
- Analogon of high- T_c superconductivity.
- ???

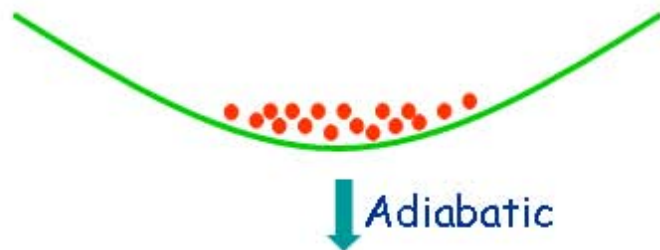
In 2D, in the weak interacting limit: M. Kagan et al.

3. Loading optical lattices

[P. Rabl, A.J. Daley, P.O. Fedichev, J.I. Cirac, and P. Zoller, 2003]



Problem: Trapping single atoms:



In reality:

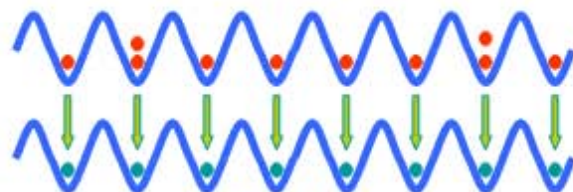


- Atoms/sites not commensurable.
- Temperature is finite.
- Residual potential.

Solutions:

1. Lower the temperatures
or count the atoms: **Hard!**

2. Coherently filter the state:



3. Redefine qubits and use new techniques:

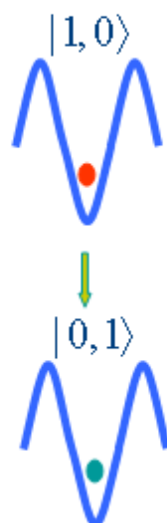


Pattern loading

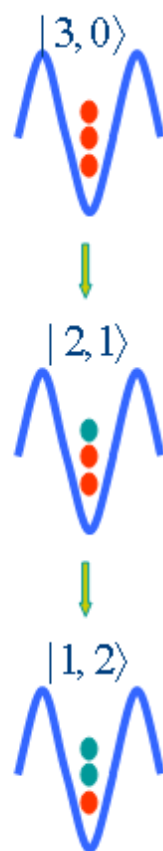
[P. Rabl, A.J. Daley, P.O. Fedichev, J.I. Cirac, and P. Zoller, 2003]

- Tunneling is switched off (raising the lattice potential). We can treat sites individually.
- Consider a particular site and two internal states:

1 particle

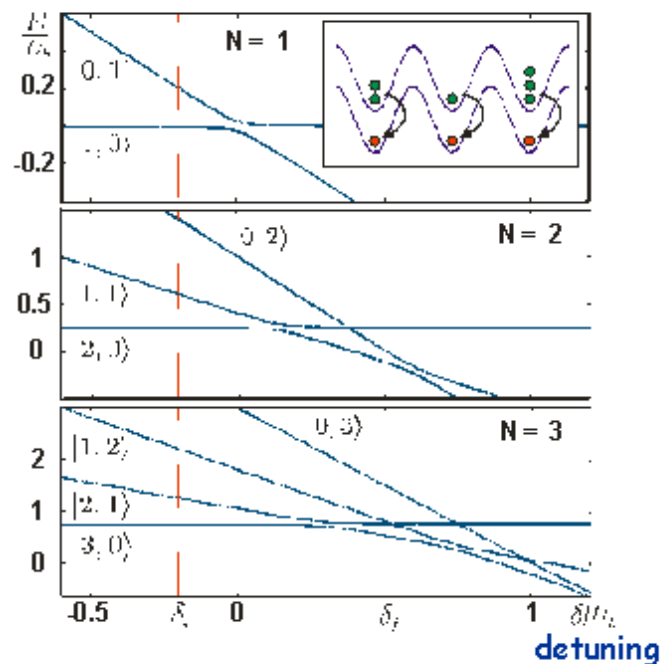


3 particles



Ideas:

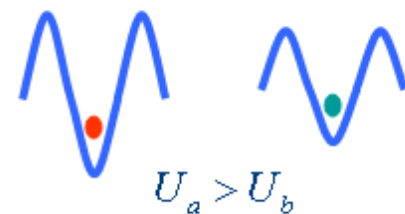
- Interaction energy blocks transfer of more particles.
- Resonance frequency depends on the number of atoms, which is unknown.
- Use adiabatic passage to overcome this problem.



Conditions:

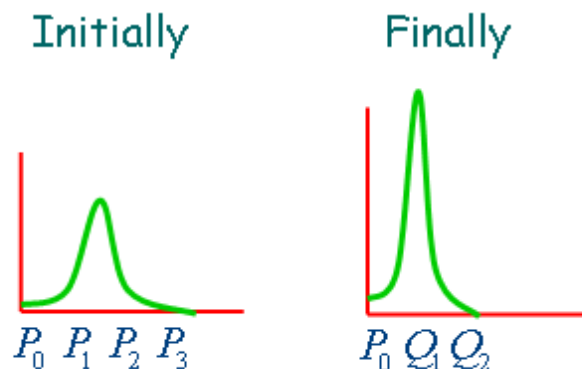
- $U_a \neq U_b$ since otherwise crossings take place at the wrong place.

This can be achieved by having different potentials for a and b.



- Adiabaticity:

Results: atom-number distribution

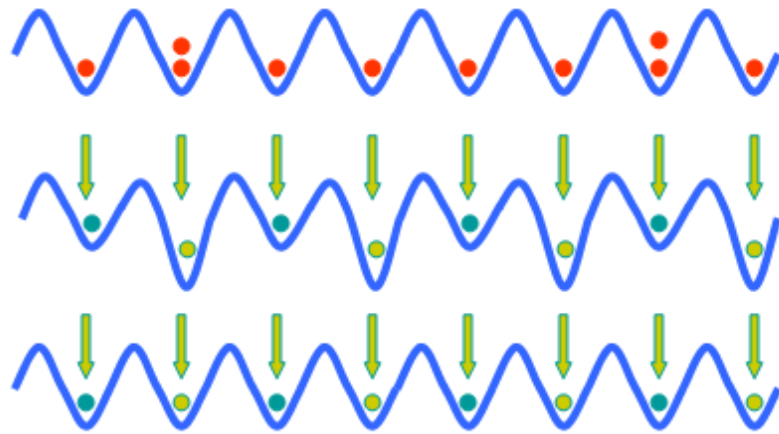


- Using a Grand-canonical distribution for the initial state with

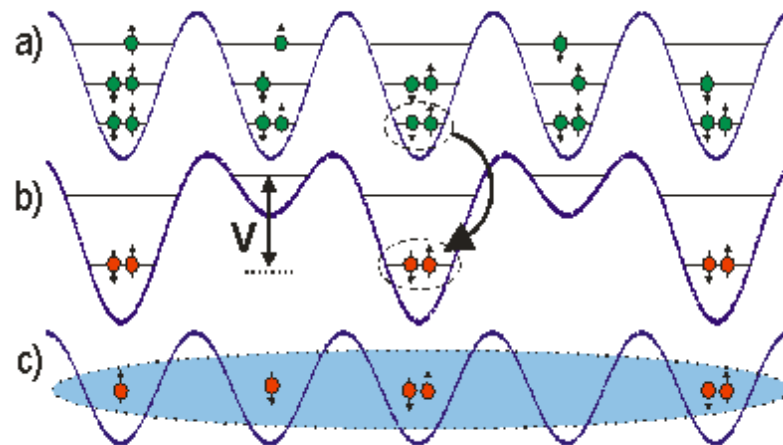
- Temperature such that there is 1 defect every 10 sites.
- 2 atoms per well (in average).

one obtains 1 defect every 10,000 sites.

Also: quantum state engineering...



With Fermions: Cooper pairs

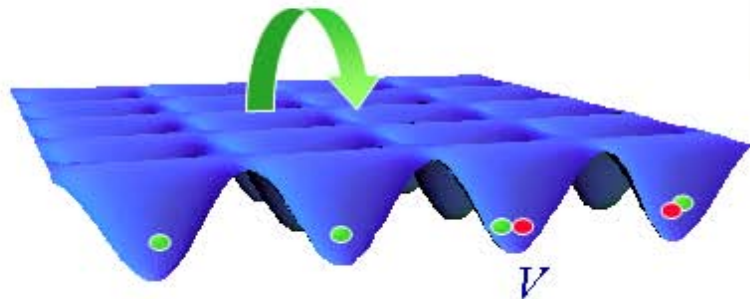


COLD ATOMS IN OPTICAL LATTICES

Fermions

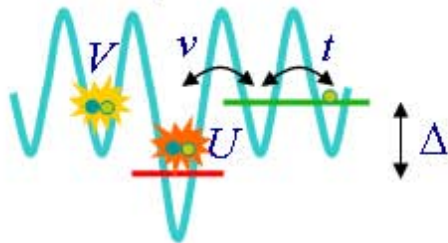
Hubbard model in 2D.

W. Hofstetter, J.I. Cirac, P. Zoller,
E. Demler, and M. Lukin



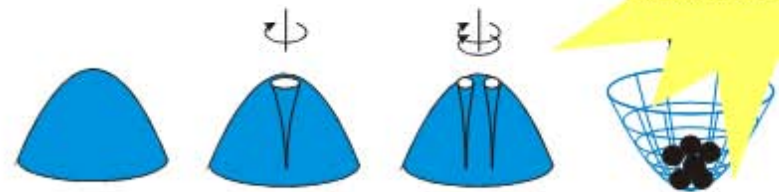
Anderson super-lattices.

B. Paredes, C. Tejedor, and J.I. Cirac



Atoms in rotating traps.

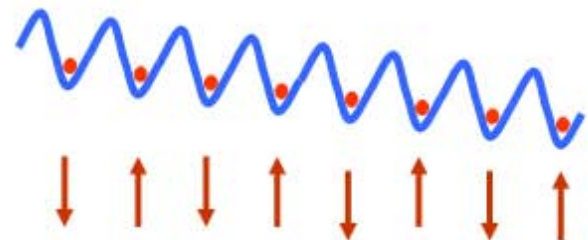
M. Popp, B. Paredes, and J.I. Cirac



See poster by
Markus Popp

Spin systems.

J. Garcia-Ripoll, M.A. Martin-Delgado,
and J.I. Cirac

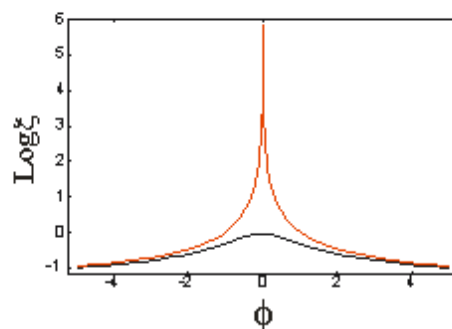


$$X_{k,k+1} \propto \lambda_1 \left[(\vec{S}_k \cdot \vec{S}_{k+1}) + \beta (\vec{S}_k \cdot \vec{S}_{k+1})^2 \right] + (-1)^k \lambda_2 S_k^z$$

QUANTUM INFORMATION THEORY AND CONDENSED MATTER

Diverging entanglement length.

F. Verstraete, M. Popp, M.A. Martin-Delgado,
and J.I. Cirac



Numerical simulation methods.

F. Verstraete, D. Porras, and J.I. Cirac

