ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Dissertation ETH Number 21384

Numerical simulations of bosons and fermions in three dimensional optical lattices

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Supervisor: Prof. Matthias TROYER

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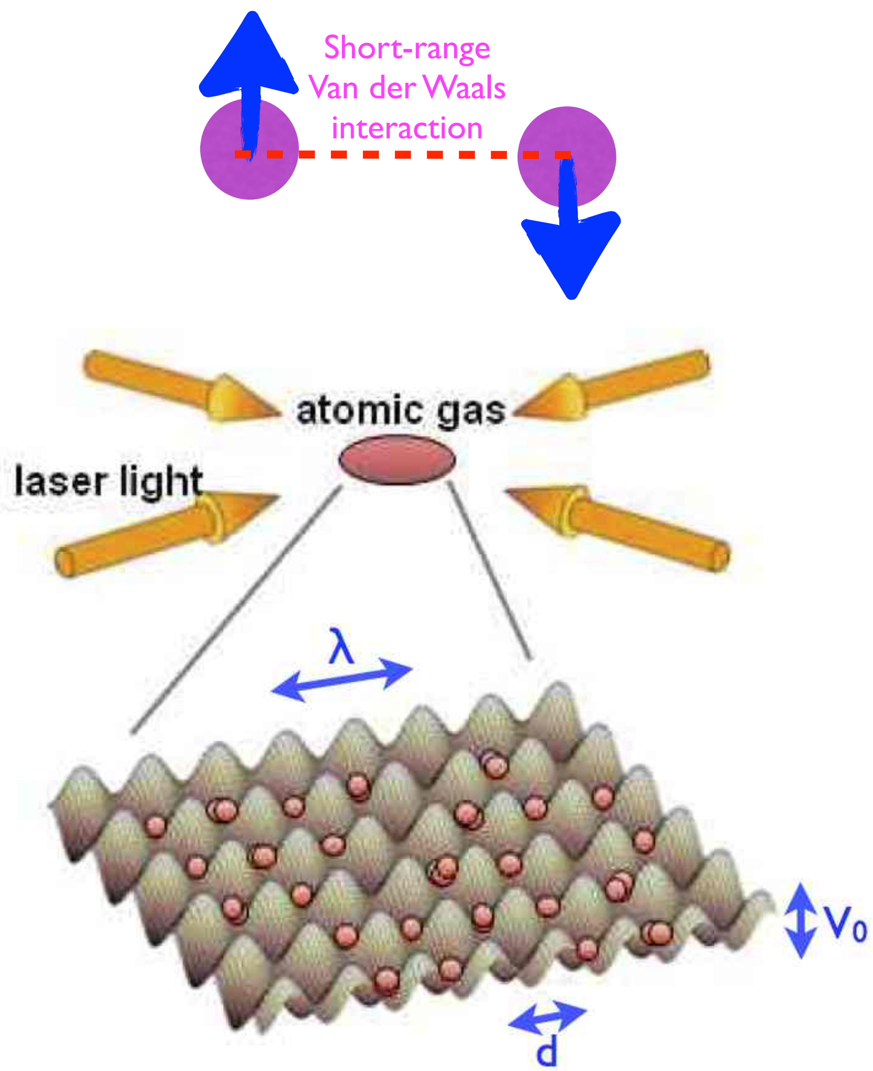
Optical lattices



Cartoon illustration

-- setup by 3 orthogonal pairs of laser beams.

$$V(\mathbf{x}) = \sum_{x^i = x,y,z} V_0 \sin^2(kx^i)$$

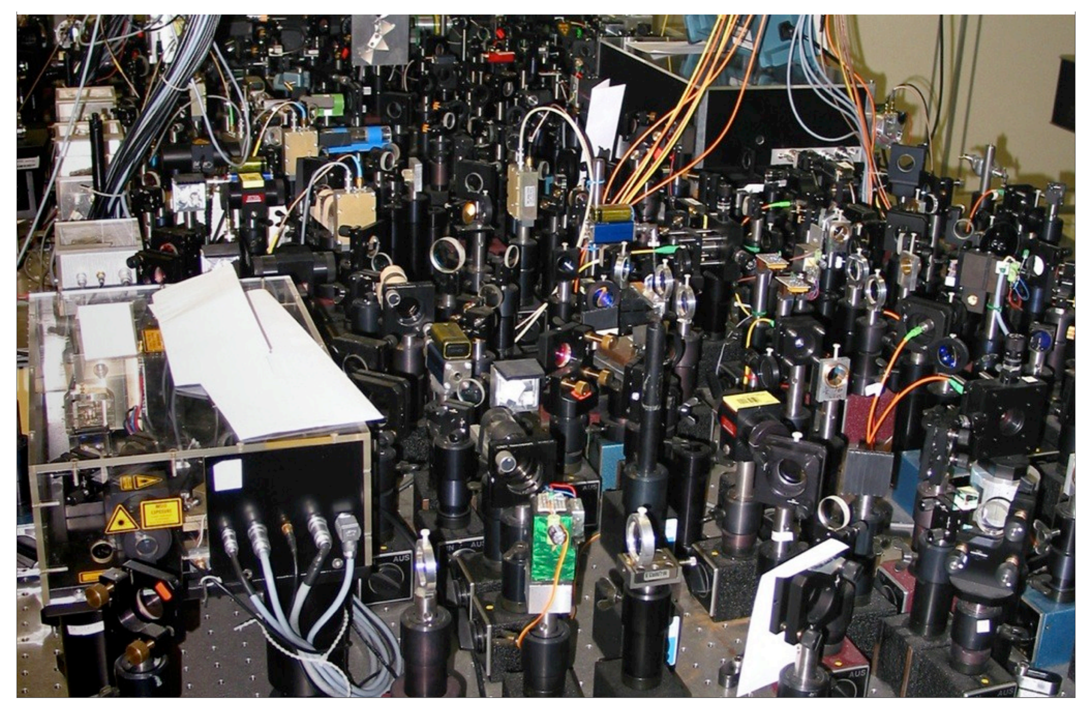
Lattice strength: V_0

Lattice separation: $d = \frac{\lambda}{2}$;

Lattice wavevector: $k = \frac{2\pi}{\lambda} = \frac{\pi}{d}$

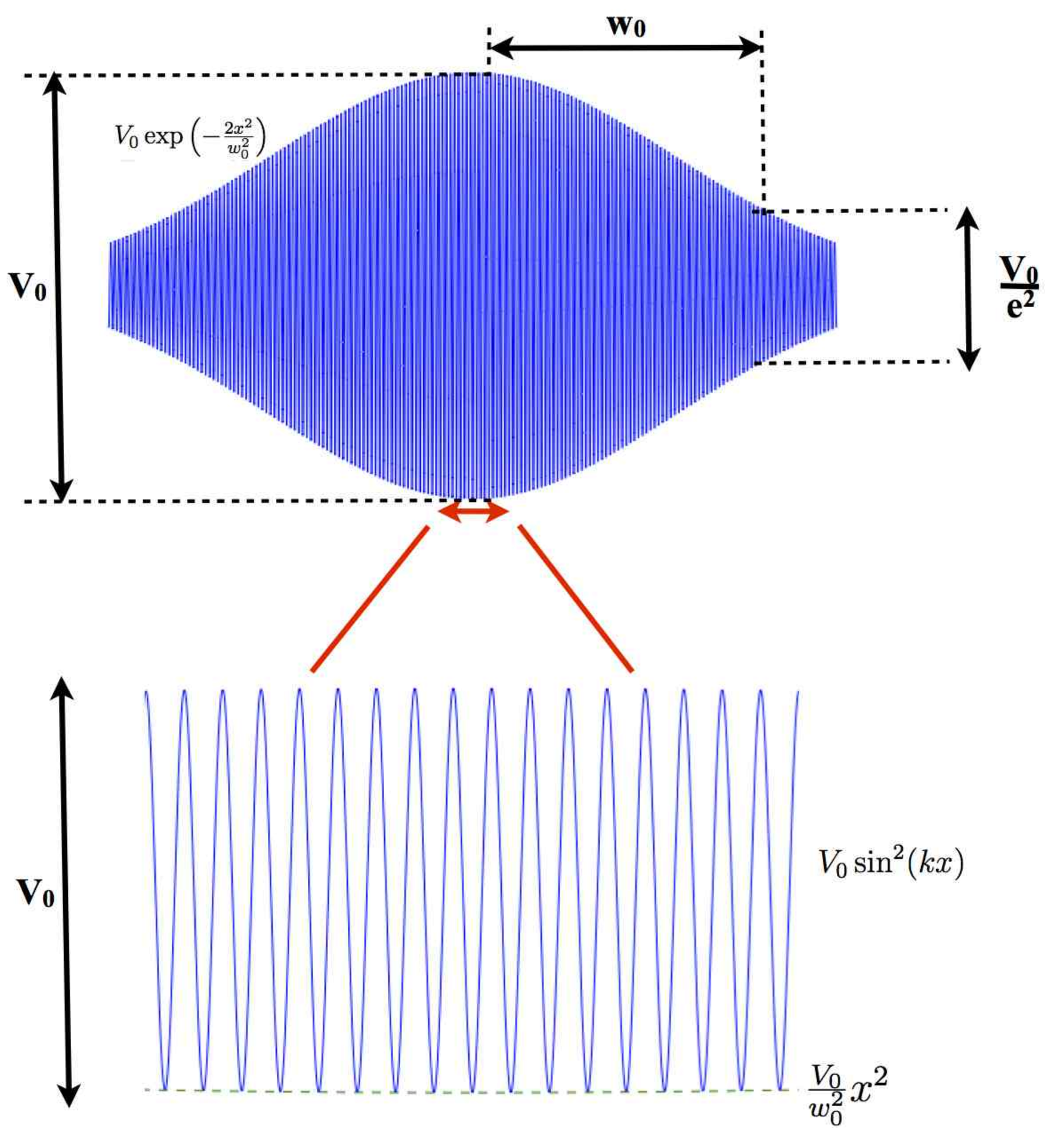
s-wave scattering length: a

-- setup by 3 orthogonal pairs of laser beams.



Immanuel Bloch's laboratory, Max Planck Institute

Optical lattices



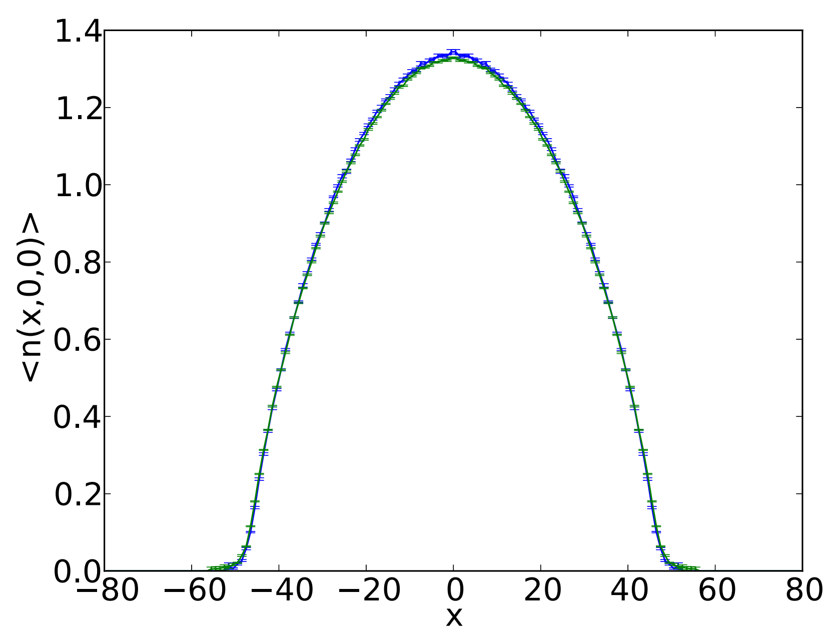
-- Gaussian laser beams induce trapping of atoms.

trapping envelope: $V_0 \exp\left(-\frac{2r^2}{w_0^2}\right)$

-- Current experiments:
Atoms are around the vicinity of the center.

~ harmonic trapping: $V_T(\mathbf{x}) = V_T\mathbf{x}^2$

~ waist effects are minimal:



Bosons in an optical lattice. QMC-DWA simulation.
U/t = 8.11, T/t = 1.00, N = 280,000, w_o = 150μm
(Red) Minimal effect seen due to waist corrections.

Optical lattices

For deep lattices, or large V_0:

1. bosons in an optical lattice

$$\hat{H} = -t \sum_{\langle i,j \rangle} \hat{b}_i^\dagger \hat{b}_j + \frac{U}{2} \sum_i n_i (n_i - 1) - \sum_i (\mu - V_T \mathbf{x}_i^2) n_i$$

(boson Hubbard model)

2. fermions in an optical lattice

$$\hat{H} = -t \sum_{\langle i,j \rangle, \sigma} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - \sum_i (\mu - V_T \mathbf{x}_i^2) n_i$$

(Hubbard model)

hopping   onsite interaction

Easy and convenient conversion within ALPS Python:

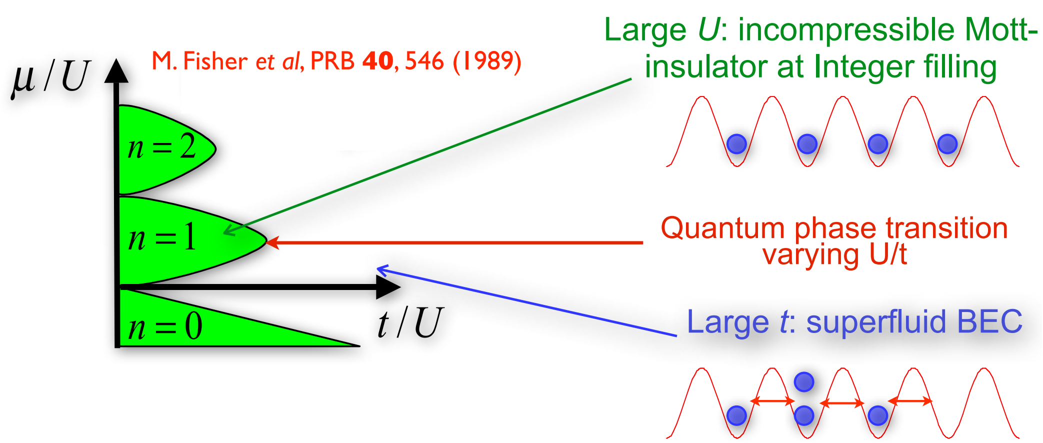
```
>>> import numpy;
>>> import pyalps.dwa;
>>>
>>> V0   = numpy.array([8.805, 8. ,  8. ]); #lattice strength [Er]
>>> wlen = numpy.array([765., 843., 843.]); #laser wavelength [nm]
>>> a    = 101;    #s-wave scattering length [bohr radius]
>>> m    = 86.99;  #mass [a.m.u.]
>>> L    = 160;    #lattice of size L^3
>>>
>>> band = pyalps.dwa.bandstructure(V0, wlen, a, m, L);
>>>
```

```
>>> band

Optical lattice:
================
V0    [Er] = 8.805   8    8
lamda [nm] = 765     843  843
Er2nK      = 188.086     154.89   154.89
L          = 160
g          = 5.51132

Band structure:
===============
t [nK] : 4.77257    4.77051 4.77051
U [nK] : 38.7027
U/t    : 8.1094 8.1129   8.1129
```

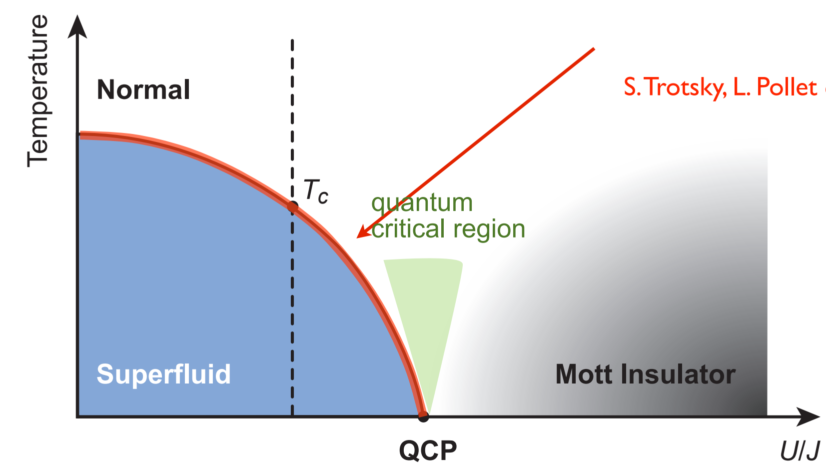
Bosons in an optical lattice

$$\hat{H} = -t\sum_{\langle i,j\rangle}\hat{b}_i^\dagger\hat{b}_j + \frac{U}{2}\sum_i n_i(n_i-1) - \sum_i(\mu - V_T\mathbf{x}_i^2)n_i$$

Phase diagram for homogeneous systems:



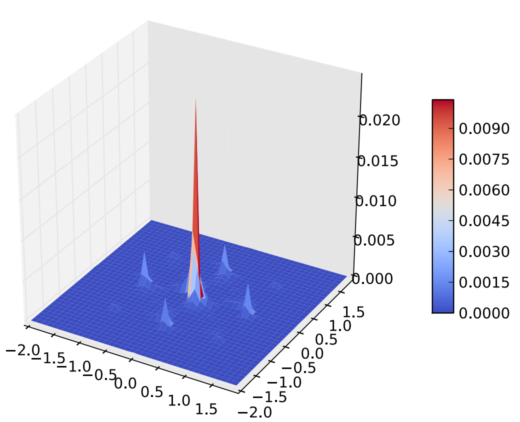
At **zero** temperature

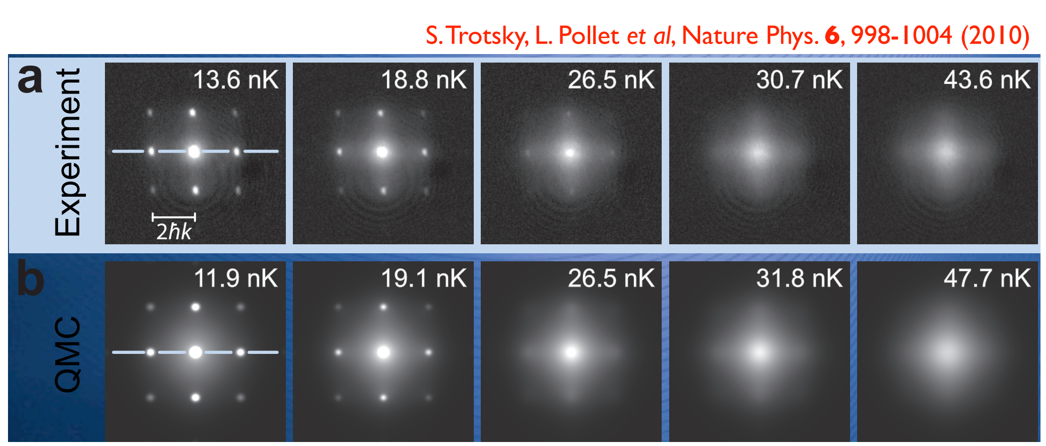


At **finite** temperature

Quantitative validation:

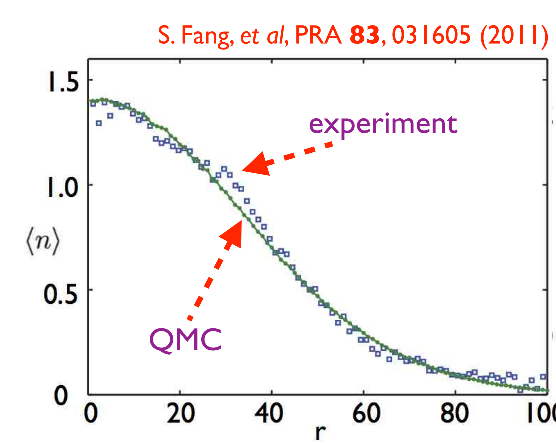
1. on time-of-flight (tof) images:





$V_0/E_R = 8$, $U/t = 8.11$, $N = 280{,}000$

2. on density profiles:



Fermions in an optical lattice

$$\hat{H} = -t \sum_{\langle i,j \rangle, \sigma} \hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - \sum_i (\mu - V_T \mathbf{x}_i^2) n_i$$

Quantum Monte Carlo -- negative sign problem

M. Troyer, U-J. Weise, PRL **94**, 170201 (2005)

$$\begin{aligned} \langle A \rangle &= \frac{\sum_c A(c) p(c)}{\sum_c p(c)} \\ &= \frac{\sum_c A(c) s(c) |p(c)| / \sum_c |p(c)|}{\sum_c s(c) |p(c)| / \sum_c |p(c)|} \equiv \frac{\langle As \rangle'}{\langle s \rangle'} \end{aligned}$$

$$\frac{\Delta s}{\langle s \rangle} = \frac{\sqrt{\left(\langle s^2 \rangle - \langle s \rangle^2\right)/M}}{\langle s \rangle} = \frac{\sqrt{1 - \langle s \rangle^2}}{\sqrt{M}\langle s \rangle} \sim \frac{e^{\beta N \Delta f}}{\sqrt{M}}$$

~ scales exponentially with
1) inverse temperature β, and
2) system size N.

Therefore, phase diagram for fermions is not entirely clear in general

At half-filling, the Hubbard model exhibits antiferromagnetic ground state.

Magnetism

Time Line

2009 — Stoner ferromagnetism experimentally detected in (ultracold) **gases.**

$$\hat{H} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} \hat{c}^\dagger_{\mathbf{k}} \hat{c}_{\mathbf{k}} + \frac{1}{2}\frac{U}{N} \sum_{\substack{\mathbf{k}_1\mathbf{k}_2 \\ \mathbf{q}\neq 0}} \hat{c}^\dagger_{\mathbf{k}_1+\mathbf{q}\uparrow} \hat{c}^\dagger_{\mathbf{k}_2-\mathbf{q}\downarrow} \hat{c}_{\mathbf{k}_2\downarrow} \hat{c}_{\mathbf{k}_1\uparrow}$$

Magnetism in gases

Magnetism in solids

1965 — Kohn-Sham DFT:

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) + V^{\mathrm{HXC}}_{\sigma}(\rho_\uparrow, \rho_\downarrow; \mathbf{r})\right)\phi^\sigma_n = \epsilon^\sigma_n \phi^\sigma_n$$

1. many-body → effective single-body quantum problem
2. largely successful in electronic structure problems
3. inadequate to explain (strong) magnetism

1947: Birth of the transistor

1928: Quantum mechanics appiled to solids
Birth of Heisenberg model

1926 — Quantum Mechanics (Schrodinger equation):

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{x},t) = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x},t)\right)\psi(\mathbf{x},t)$$

1887 — Classical electromagnetism (Maxwell's equations):

$$\nabla\cdot\mathbf{E} = \frac{\rho}{\varepsilon_0}$$

$$\nabla\cdot\mathbf{B} = 0$$

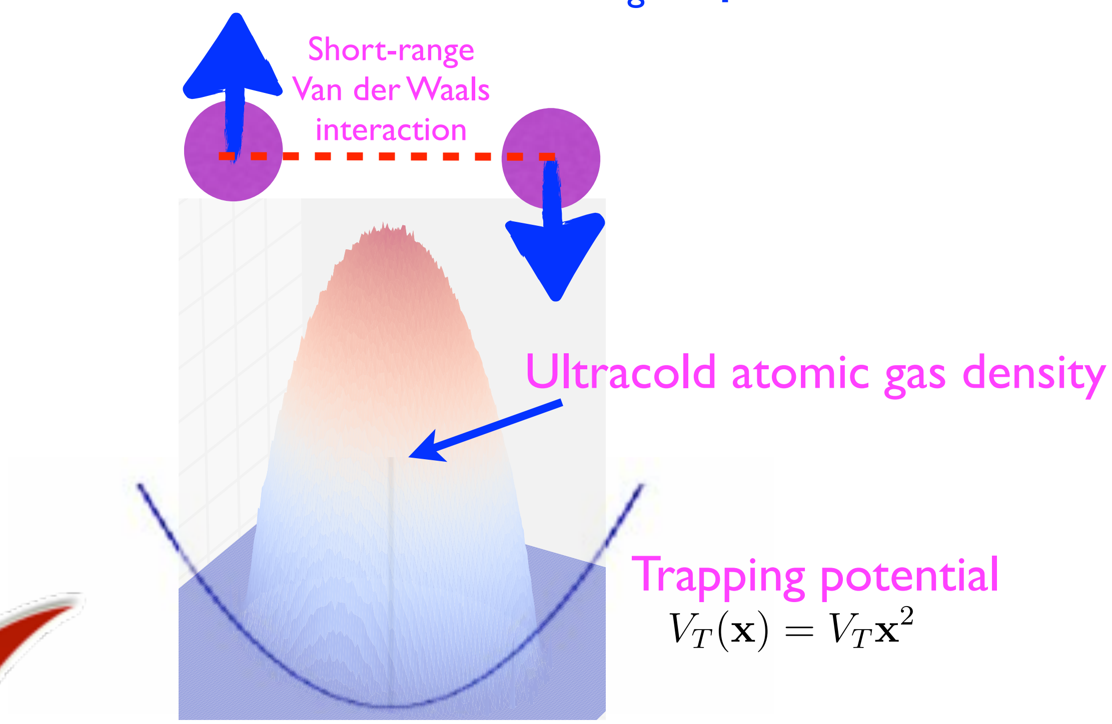
$$\nabla\times\mathbf{E} = -\frac{\partial\mathbf{B}}{\partial t}$$

$$\nabla\times\mathbf{B} = \mu_0\mathbf{J} + \mu_0\varepsilon_0\frac{\partial\mathbf{E}}{\partial t}$$

585 B.C. — " ... loadstone attracts iron because it has a soul."
— Thales of Miletus, ~ *585 B.C.*

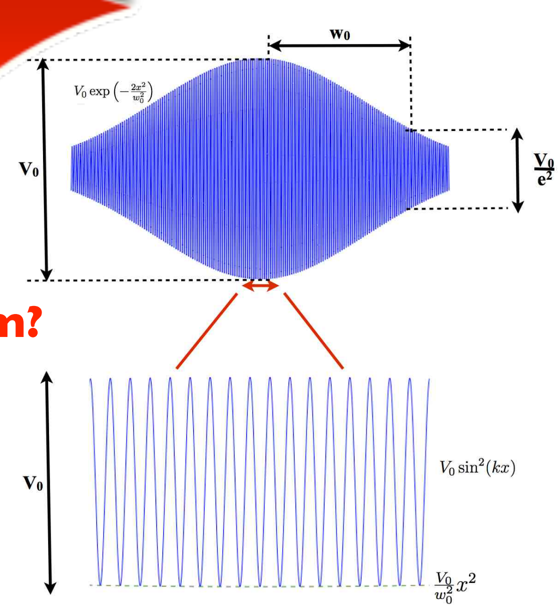
Magnetism in (ultracold) gases

Interaction strength: $\mathbf{k_F a}$



Cartoon illustration

setup an optical lattice



Q: Magnetism?

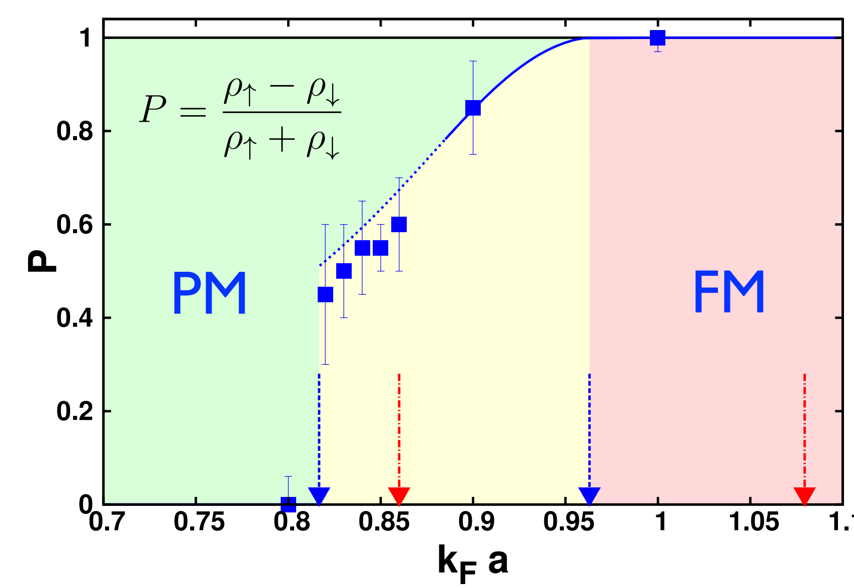
Stoner ferromagnetism:

$$\hat{H} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} \hat{c}^\dagger_{\mathbf{k}} \hat{c}_{\mathbf{k}} + \frac{1}{2}\frac{U}{N} \sum_{\substack{\mathbf{k}_1\mathbf{k}_2 \\ \mathbf{q}\neq 0}} \hat{c}^\dagger_{\mathbf{k}_1+\mathbf{q}\uparrow} \hat{c}^\dagger_{\mathbf{k}_2-\mathbf{q}\downarrow} \hat{c}_{\mathbf{k}_2\downarrow} \hat{c}_{\mathbf{k}_1\uparrow}$$

-- first observed experimentally in an ultracold ^{6}Li gaseous cloud in 2009.

G-B. Jo, et al,
Itinerant ferromagnetism in a Fermi gas of ultracold atoms,
Science **325**, 5947 (2009).

-- phase diagram

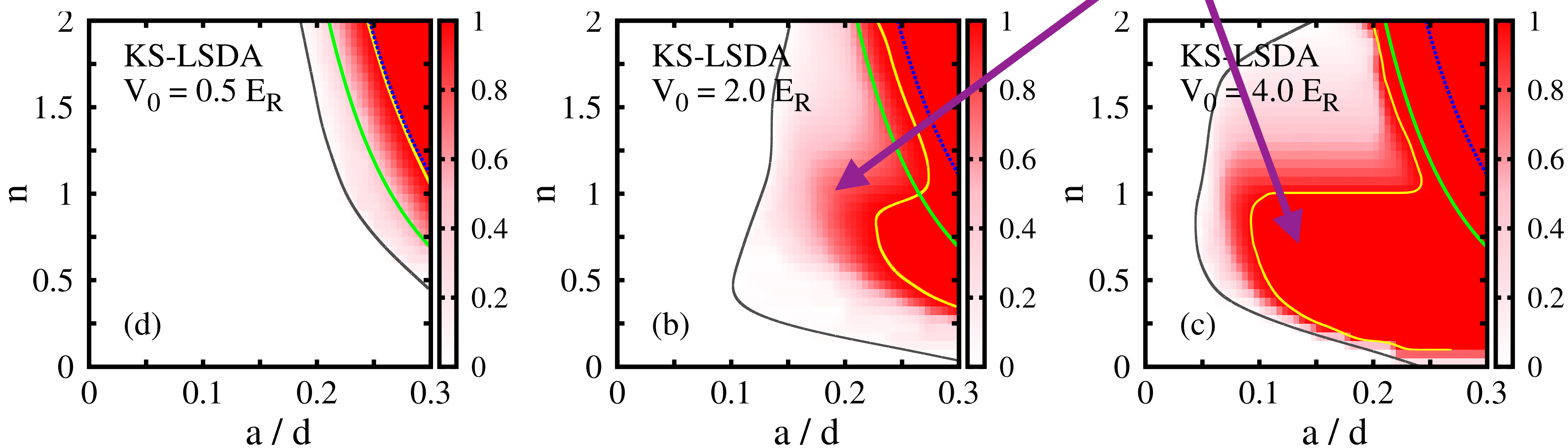


S. Pilati, G. Bertaina, S. Giorgini, and M. Troyer,
Itinerant ferromagnetism of a repulsive atomic Fermi gas: a quantum Monte Carlo study
Phys. Rev. Lett. **105**, 030405 (2010).

Magnetism in optical lattices

Ferromagnetism is enhanced by optical lattice (band structure effects):

$$P = \frac{\rho_\uparrow - \rho_\downarrow}{\rho_\uparrow + \rho_\downarrow}$$



Kohn-Sham density functional theory (KS-DFT):

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) + V_\sigma^{\mathrm{HXC}}(\rho_\uparrow, \rho_\downarrow; \mathbf{r})\right)\phi_n^\sigma = \epsilon_n^\sigma\,\phi_n^\sigma$$

-- KS-DFT is exact only with exact h.x.c. potential:

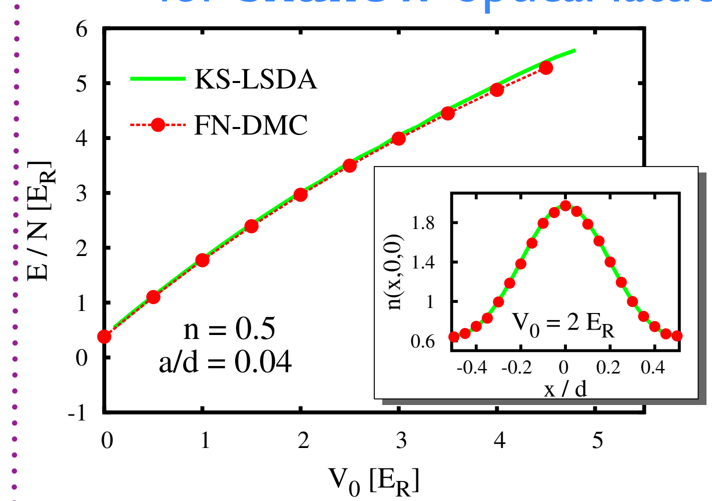
$$V_\sigma^{\mathrm{HXC}}(\rho_\uparrow, \rho_\downarrow; \mathbf{r}) = \frac{\delta}{\delta\rho_\sigma(\mathbf{r})}\left[\epsilon_{\mathrm{HXC}}(\rho_\uparrow, \rho_\downarrow; \mathbf{r})\right]$$

-- Local density approximation (LDA) to h.x.c. potential

(See appendix B in thesis.)

Q: How valid is KS-DFT?

A: KS-DFT works (quantitatively) for **shallow** optical lattice



Magnetism in optical lattices

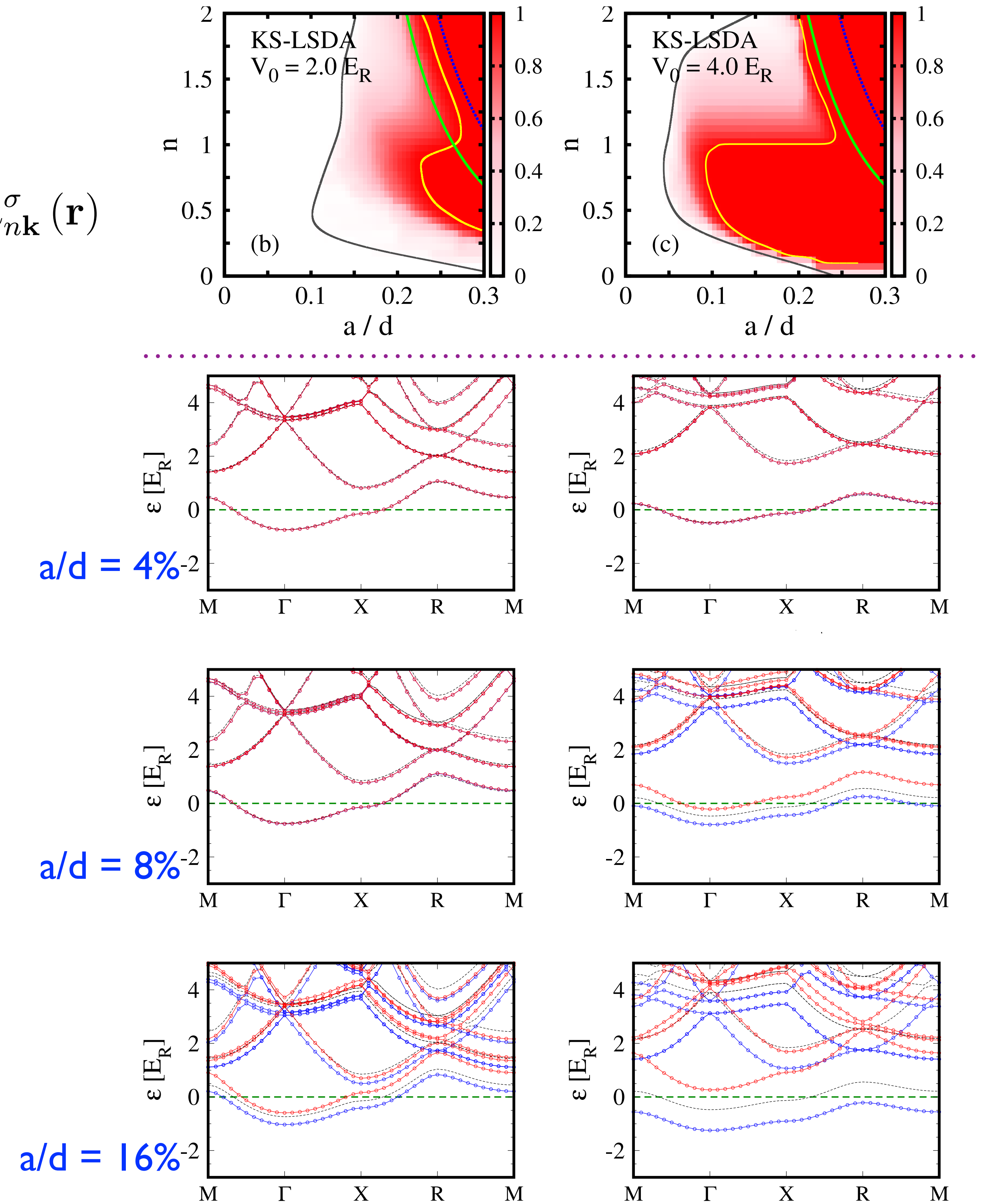
KS-DFT:

$$\left[\frac{1}{\pi^2}\left(-i\nabla+2\pi\mathbf{k}\right)^2+V_\sigma^{\rm eff}\left(\rho_\uparrow,\rho_\downarrow;\mathbf{r}\right)\right]u_{n\mathbf{k}}^\sigma\left(\mathbf{r}\right)=\epsilon_{n\mathbf{k}}^\sigma u_{n\mathbf{k}}^\sigma\left(\mathbf{r}\right)$$

simple cubic (sc) lattice:

$$\mathbf{b}_1=\hat{\mathbf{x}}\ ,\ \mathbf{b}_2=\hat{\mathbf{y}}\ ,\ \mathbf{b}_3=\hat{\mathbf{z}}$$

Notation	$\mathbf{k}$-point
Γ	(0, 0, 0)
X	(1/2, 0, 0)
M	(1/2, 1/2, 0)
R	(1/2, 1/2, 1/2)



Conclusion:

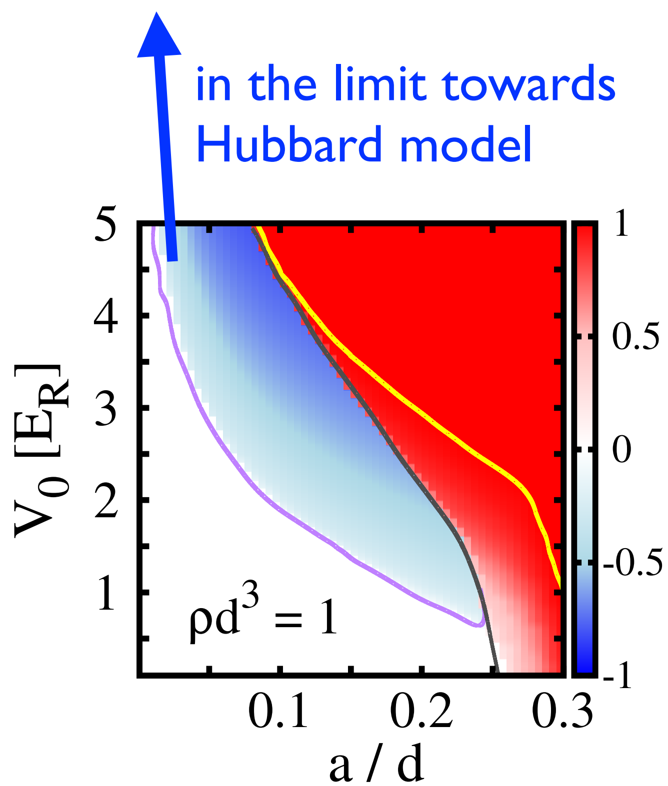
Band structure effects **stablizes** ferromagnetism.

Magnetism in optical lattices

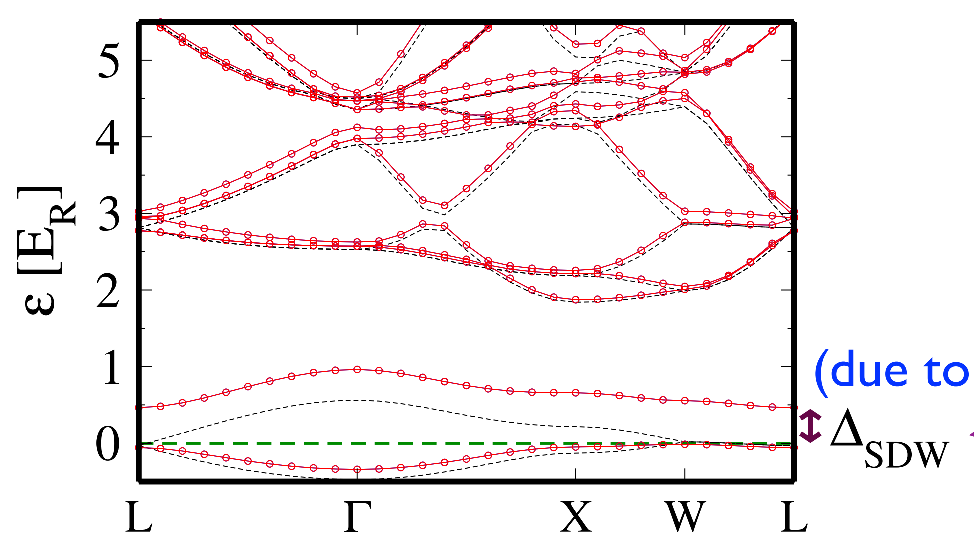
Antiferromagnetism:

fcc lattice:

Notation	**k**-point
Γ	(0, 0, 0)
X	(1/2, 0, 0)
W	(1/4, 1/2, 0)
L	(1/4, 1/4, 1/4)



$V_0/E_R = 4$, a/d = 8% :



-- qualitatively correct (AFM ground state) towards the Hubbard limit.

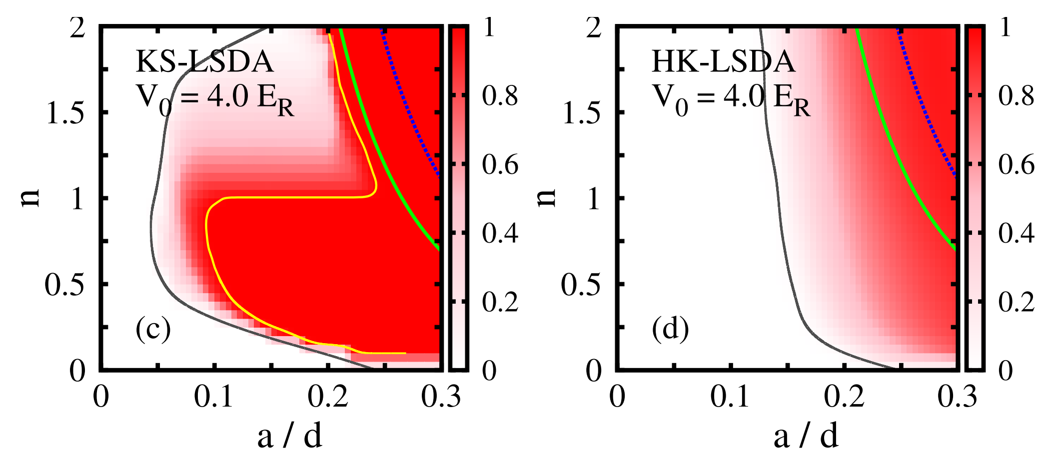
-- AFM phase can be deduced indirectly by probing Δ_{SDW}

-- Cooling towards GS is an experimental challenge!

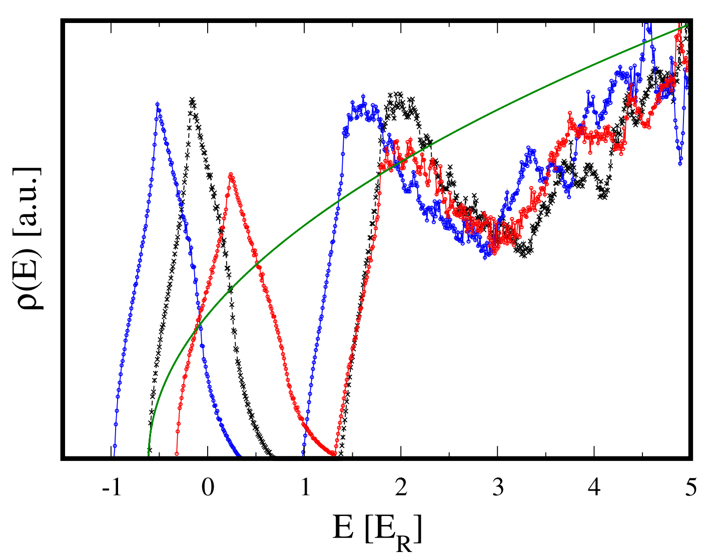
Magnetism in optical lattices

Inadequacy of Hohenberg-Kohn DFT (HK-DFT):

Phase diagram:

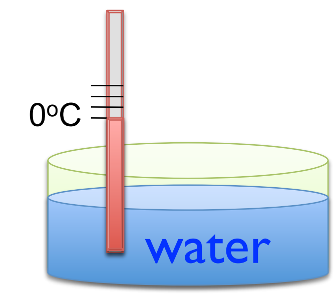


Density-of-states:



Thermometry

mercury thermometer

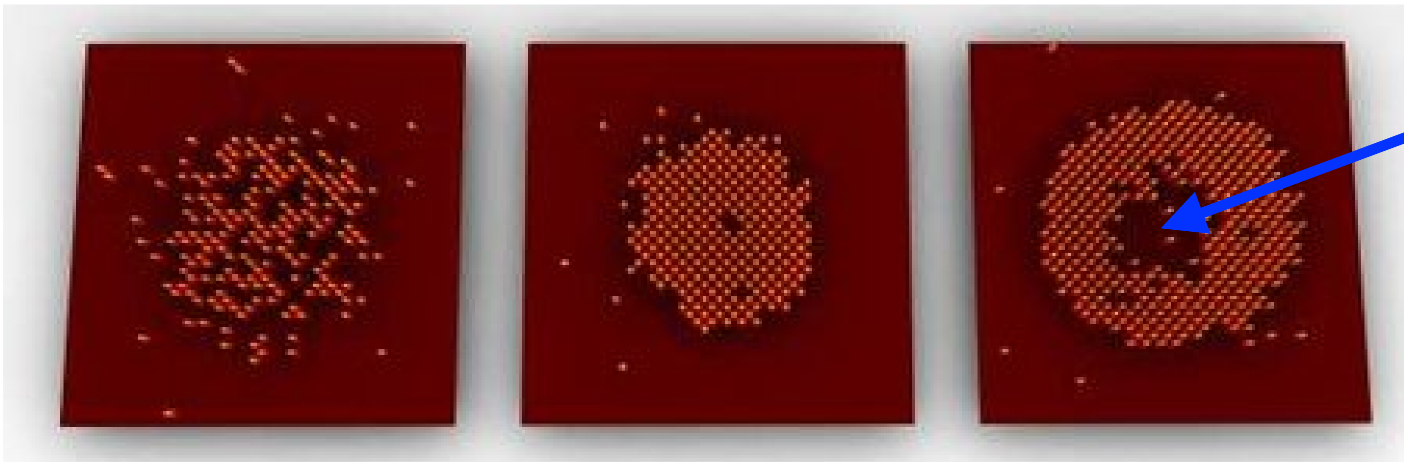


non-destructive measurement

In-situ density images:

J. F. Sherson, *et al*, Nature **467**, 68 (2010)

destructive measurement



Unable to distinguish a doublon

Fluorescence experiment: a single measurement of atom distribution of bosons in an optical lattice. Single-site resolution

We can then collect a timeseries of density measurements, thereby able to evaluate density-related observables, for instance:

1. average density , i.e. $\langle n(r)\rangle$
2. density correlations , i.e. $\langle n(r)n(r')\rangle - \langle n(r)\rangle \langle n(r')\rangle$

Fluctuation-Dissipation Thermometry

Fluctuation-dissipation theorem:

$$\frac{\partial\langle n(\vec{r})\rangle}{\partial\mu} = \beta\left[\langle n(\vec{r})N\rangle - \langle n(\vec{r})\rangle\langle N\rangle\right]$$

Local Density Approximation

($V(\mathbf{r}) = {}^1/_2 M\omega^2\mathbf{r}^2$)

$$n(\mathbf{r};T,\mu) = n_o(\mu(\mathbf{r}),T)$$, where $\mu(\mathbf{r}) = \mu - V(\mathbf{r})$

(Thereby, we have $\frac{d\mu(\mathbf{r})}{dr} = -M\omega^2 r$ and $\frac{\delta\langle n(\mathbf{r})\rangle}{\delta\mu(\mathbf{r})} = -\frac{1}{M\omega^2 r}\frac{\partial\langle n(\mathbf{r})\rangle}{\partial r}$.)

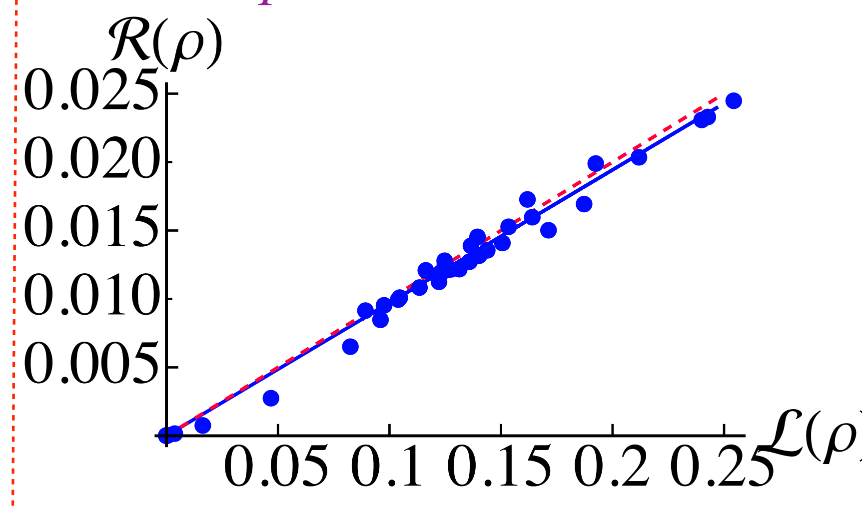
Universal Thermometry:

$$\boxed{-\frac{k_B}{M\omega^2 r}\frac{\partial\langle n(\vec{r})\rangle}{\partial r}} \times T = \boxed{\langle n(\vec{r})N\rangle - \langle n(\vec{r})\rangle\langle N\rangle}$$

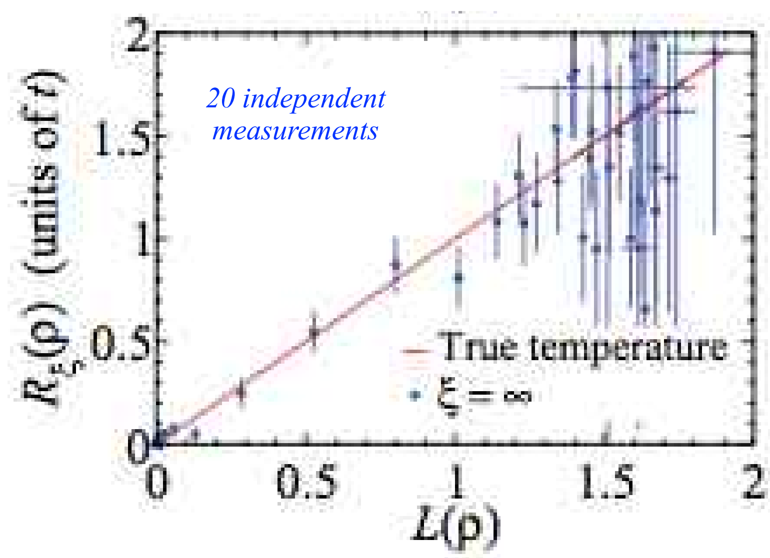
or : $\boxed{L(r)} \times T = \boxed{R(r)}$

Q. Zhou, T-L. Ho,
Universal thermometry for quantum simulation,
Phys. Rev. Lett **106**, 225301 (2011)

1200 non-interacting fermions, 2D optical lattice, T/t = 0.1



125 000 interacting bosons, 3D optical lattice, T/t = 1.0



Uncontrolled statistical noise!

Fluctuation-Dissipation Thermometry

Window-sizing:

$$R_\xi(\boldsymbol{\rho}) = \int d\boldsymbol{\rho}' \{\langle n(\boldsymbol{\rho}) n(\boldsymbol{\rho}')\rangle - \langle n(\boldsymbol{\rho})\rangle\langle n(\boldsymbol{\rho}')\rangle\}\theta(\xi - |\boldsymbol{\rho} - \boldsymbol{\rho}'|)$$

$$L(\rho) = -\frac{1}{M\omega^2\rho}\frac{\partial\langle n(\rho)\rangle}{\partial\rho}$$

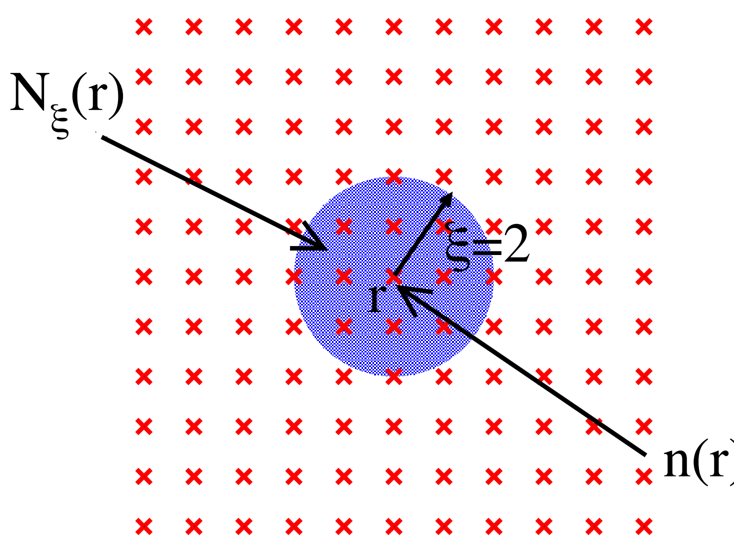
-- **density-density correlation length**
-- unknown in reality
-- yet can be "*obtained*" by *slowly enlarging the "window size"*

where the 3D density is integrated along the line-of-sight:

$$\langle n(\boldsymbol{\rho})\rangle = \int dz \langle n(\mathbf{r})\rangle,$$

$\boldsymbol{\rho}(\rho,\phi)$

$\mathbf{r}(\rho,\phi,z)$



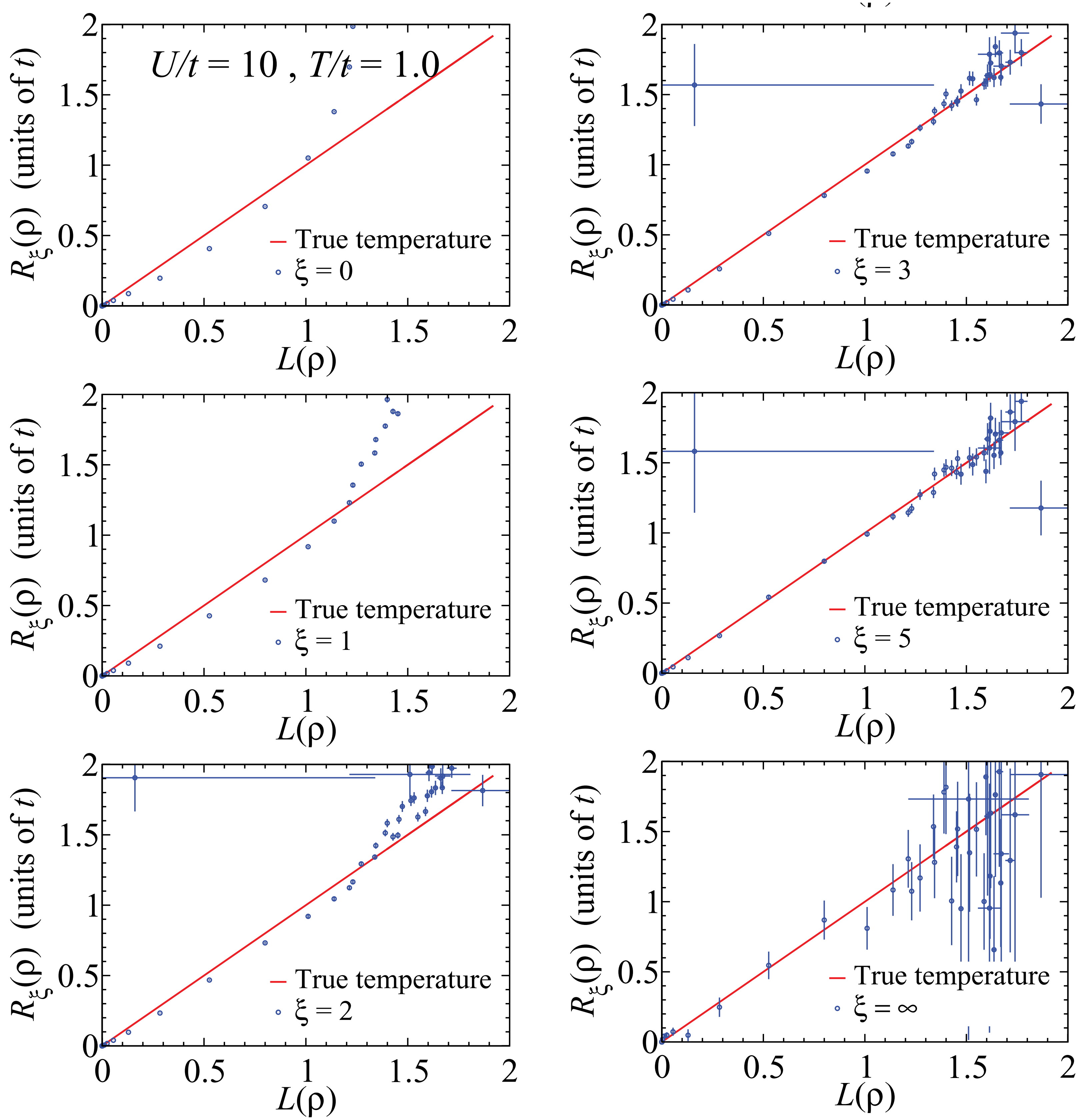
Graphical illustration of $\xi = 2$

Systematic error arises due to lack of correlations

0

1

2



3

5

∞

Statistical noise arises with increasing ξ

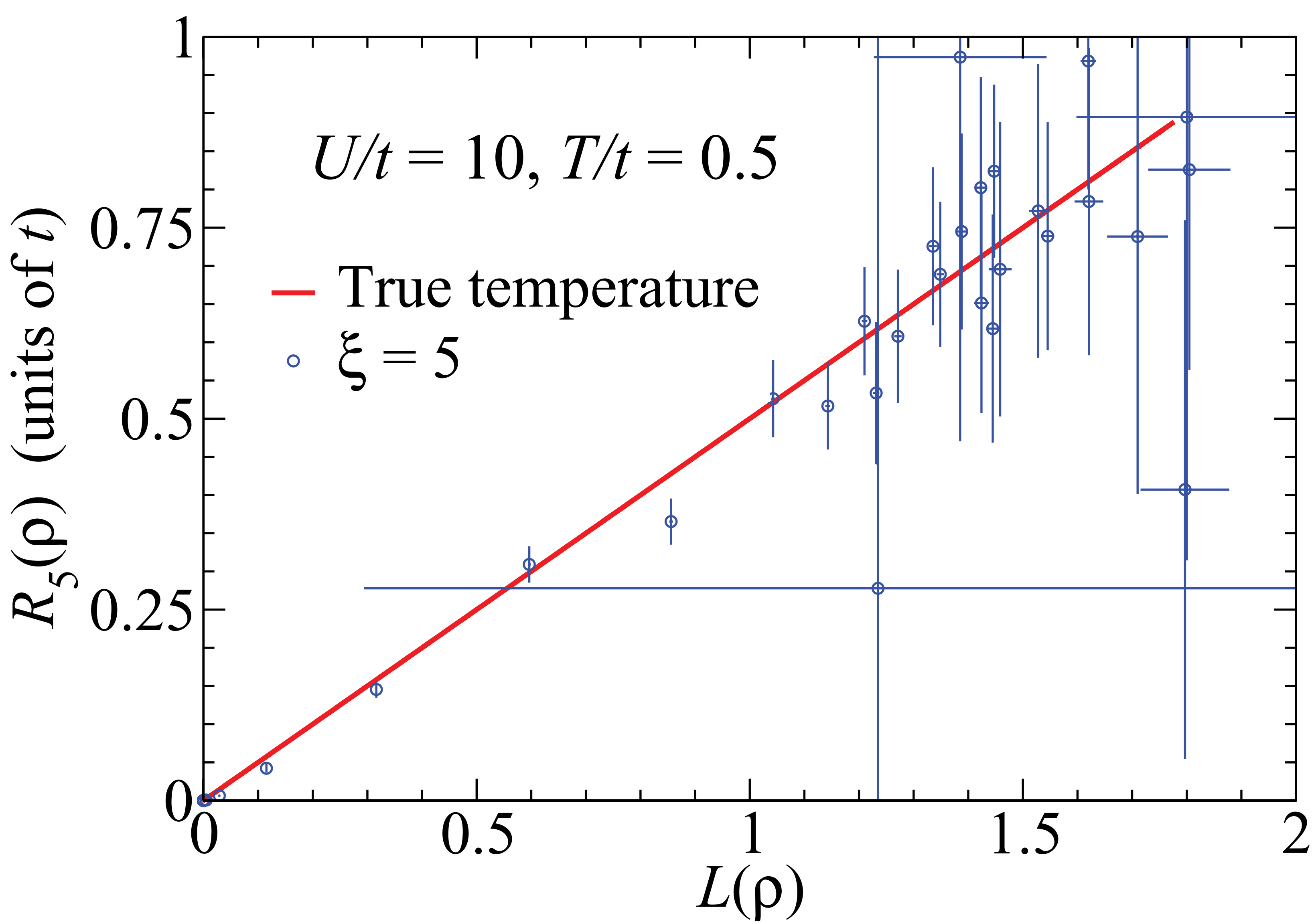
Number of independent shots required to estimate the temperature within 5% accuracy

System	Number of shots $\xi = 3$	Number of shots $\xi = \infty$
$U/t = 10$, $T/t = 1$	20	$O(10^4)$
$U/t = 10$, $T/t = 3$	14	$O(10^4)$
$U/t = 50$, $T/t = 1$	21	$O(10^4)$
$U/t = 50$, $T/t = 3$	12	$O(10^4)$

-- The simple trick of "*window-sizing*" leads to orders-of-magnitude improvement!
-- Statistical noise is drastically reduced.

-- Fluctuation-dissipation thermometry will remain a feasible tool so long as the *density-density correlation length remains short* !

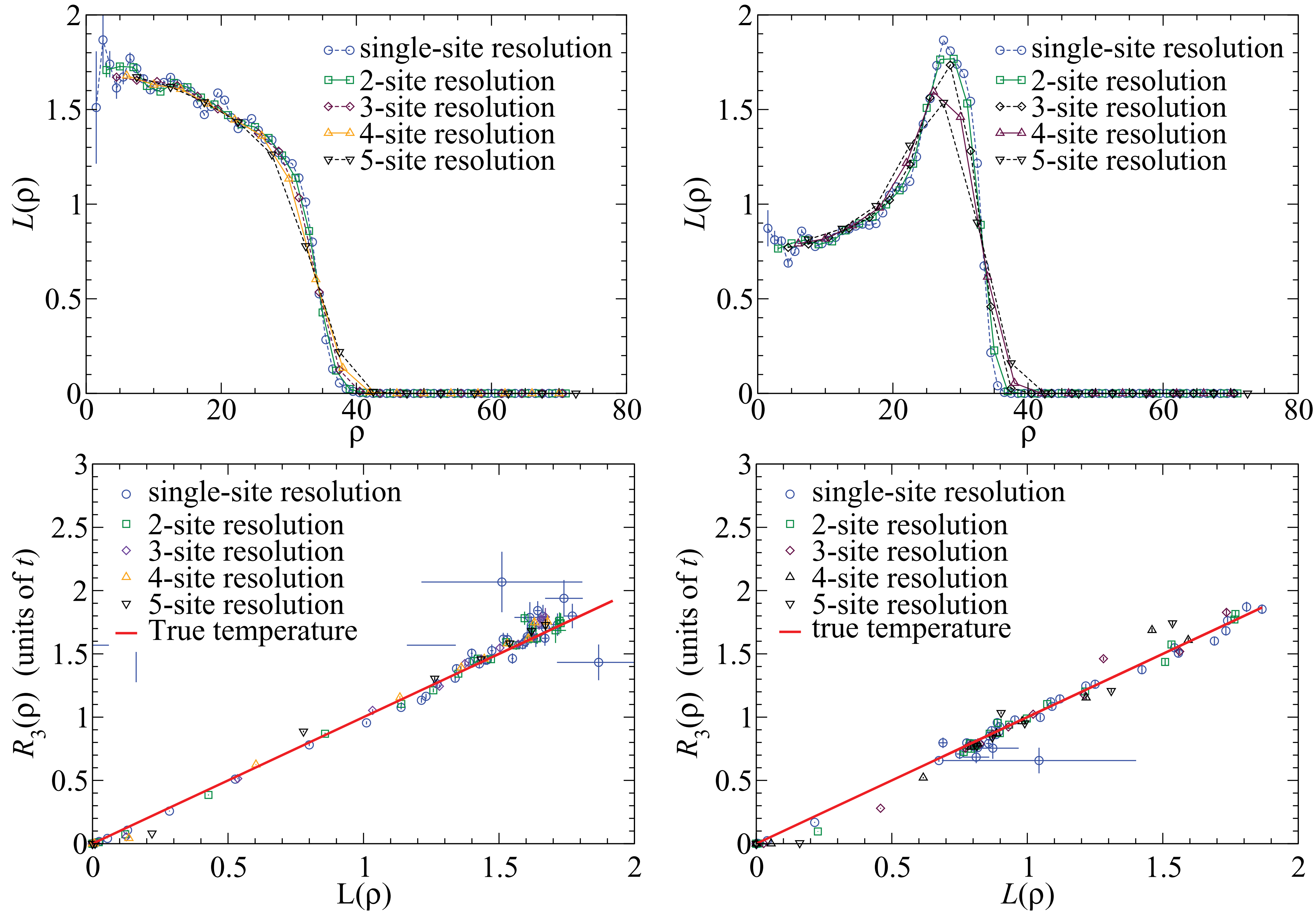
At a lower temperature, a larger window is needed due to increasing correlation length :



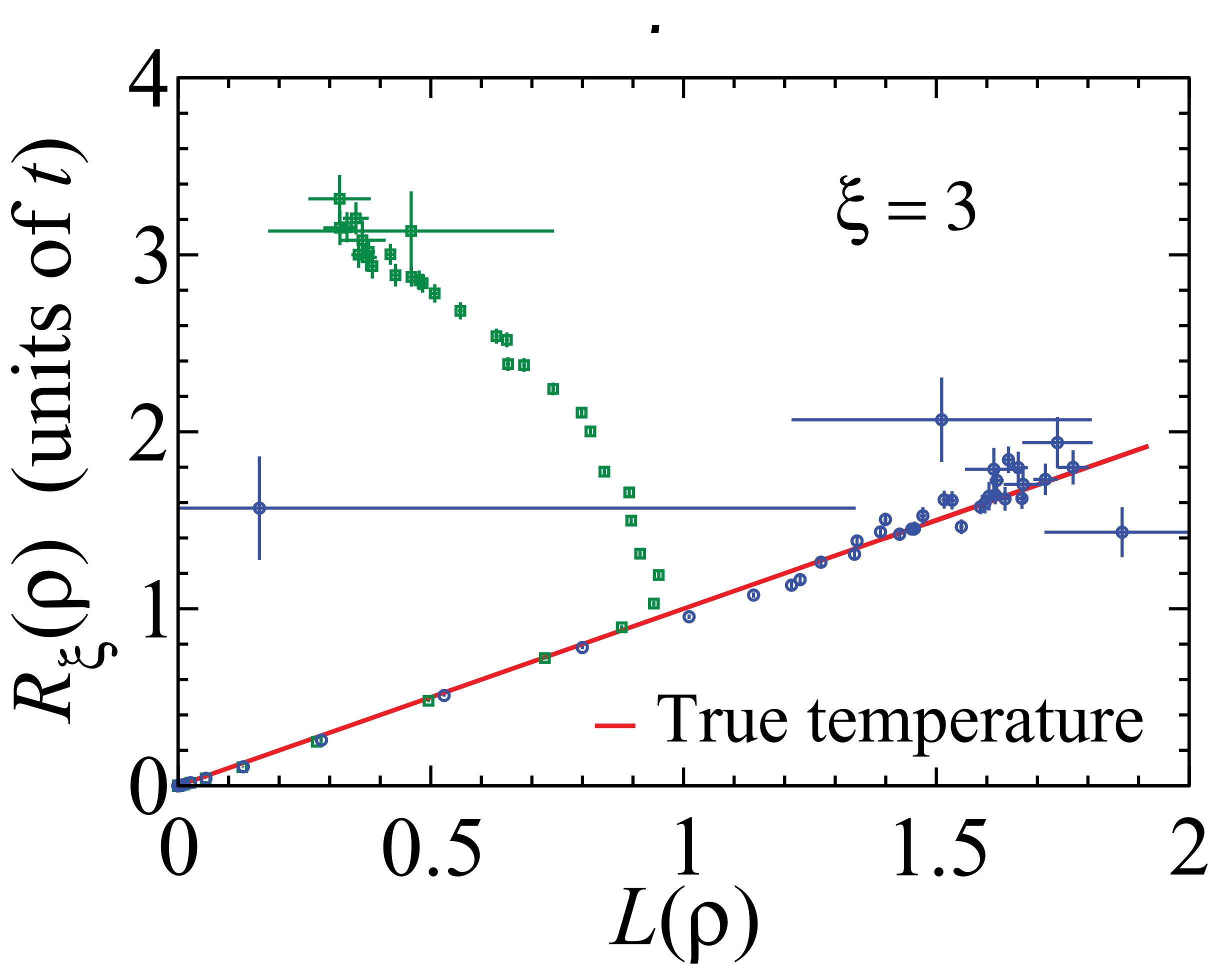
100 shots

Lower Resolution

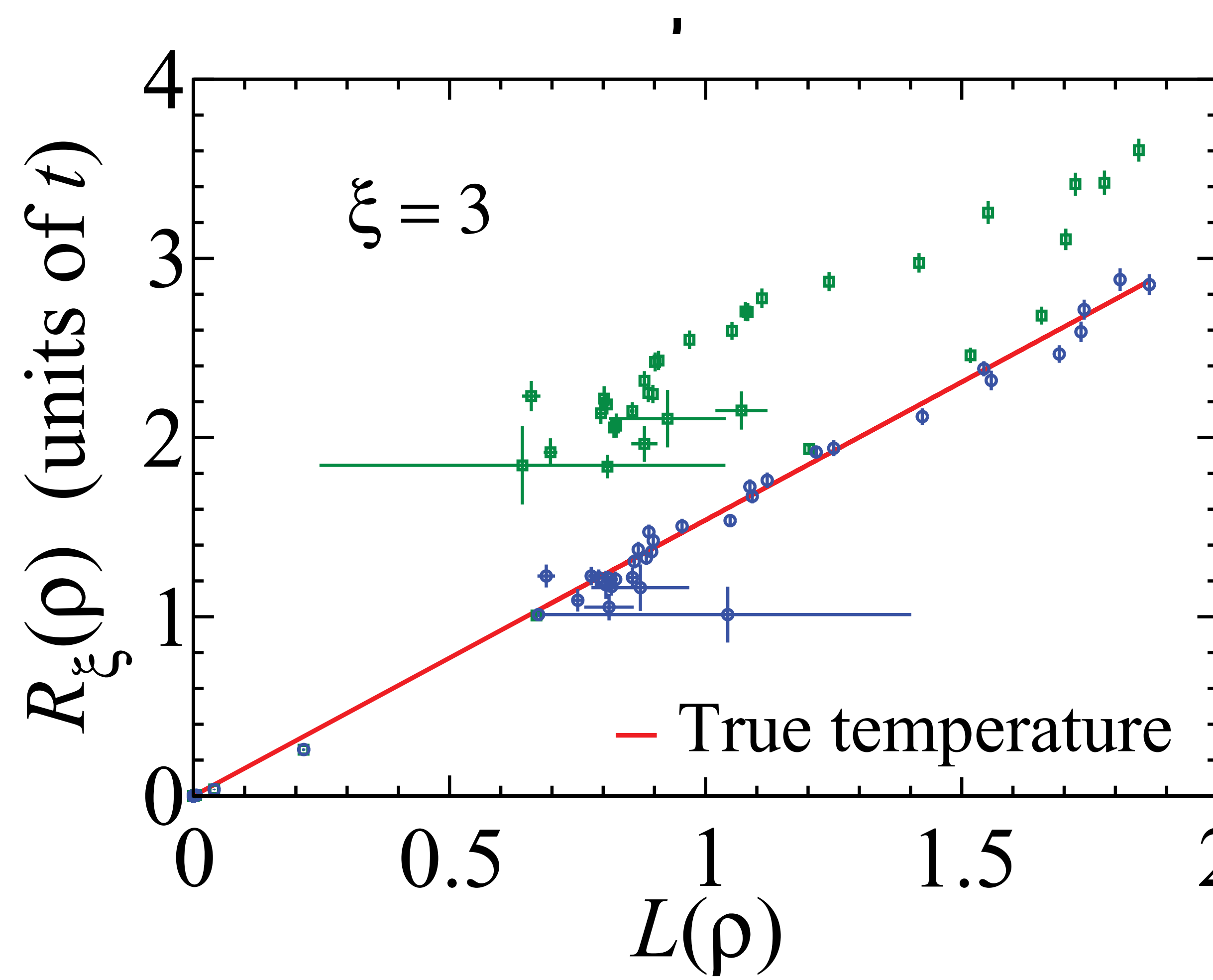
U/t = 10 ,T/t = 1.0 *U/t = 50 ,T/t = 1.0*



Fluorescence experiments can only detect parity densities



U/t = 10 ,T/t = 1.0



U/t = 50 ,T/t = 1.0

Can only trust mesurements with densities <~ 0.4 ...

- *normal measurements*
- *parity measurements*

Wing Thermometry

- To fit the wings of 2D cross sectional density profile against HTE2 *(or better)* density.
- Expand the partition function exact up to $(\beta t)^2$

HTE0 :

$$\left\langle n_i^{(0)} \right\rangle = \frac{1}{Z_i^{(0)}} \sum_{\{n_i\}} n_i e^{-\beta(D_i - \mu_i n_i)}$$

$$Z_i^{(0)} = \sum_{\{n_i\}} e^{-\beta(D_i - \mu_i n_i)}$$

$$D_i = \frac{U}{2} n_i (n_i - 1)$$

-- only valid deep in the normal phase

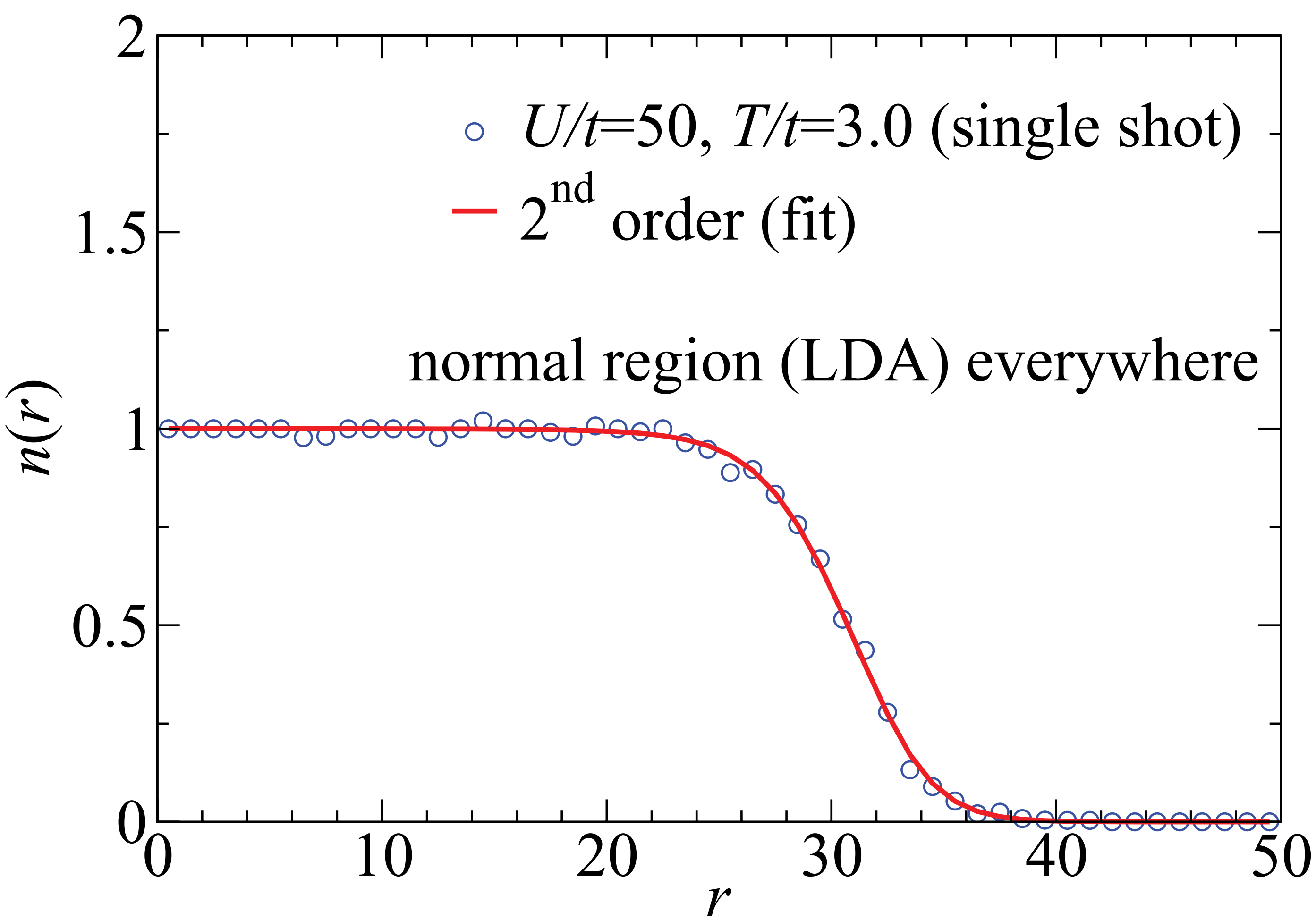
HTE2 :

$$\langle n_i \rangle = \left\langle n_i^{(0)} \right\rangle + \sum_{\langle i,j \rangle} \frac{(-\beta t)^2}{Z_i^{(0)} Z_j^{(0)}} \times \left[\sum_{\{n_i,n_j\}}^{(-,+)} \left(\delta n_i + \frac{\chi_{ij}^\delta}{\Gamma_{ij}^\delta} \right) n_i n_j^\delta e^{-\beta\left(D_i + D_j - \mu_i n_i - \mu_j n_j\right)} \Gamma_{ij}^\delta + \sum_{\{n_i,n_j\}}^{(+,-)} \left(\delta n_i - \frac{\chi_{ji}^\delta}{\Gamma_{ji}^\delta} \right) n_i^\delta n_j e^{-\beta(D_i + D_j - \mu_i n_i - \mu_j n_j)} \Gamma_{ji}^\delta \right]$$

$$\Gamma_{ij}^\delta = \frac{1 - e^{\beta \gamma_{ij}^\delta}}{(\beta\gamma_{ij}^\delta)(\beta\gamma_{ji})} - \frac{1 - e^{\beta\left(\gamma_{ij}^\delta + \gamma_{ji}\right)}}{(\beta\gamma_{ij}^\delta + \beta\gamma_{ji})(\beta\gamma_{ji})}$$

$$\chi_{ij}^\delta = \frac{e^{\beta\gamma_{ij}^\delta}}{(\beta\gamma_{ij}^\delta)(\beta\gamma_{ji})} + \frac{1 - e^{\beta\left(\gamma_{ij}^\delta + \gamma_{ji}\right)}}{(\beta\gamma_{ij}^\delta + \beta\gamma_{ji})(\beta\gamma_{ji})^2} - \frac{(1 - e^{\beta\gamma_{ij}^\delta})(\beta\gamma_{ij}^\delta - \beta\gamma_{ji})}{(\beta\gamma_{ij}^\delta)^2(\beta\gamma_{ji})^2},$$

Wing Thermometry

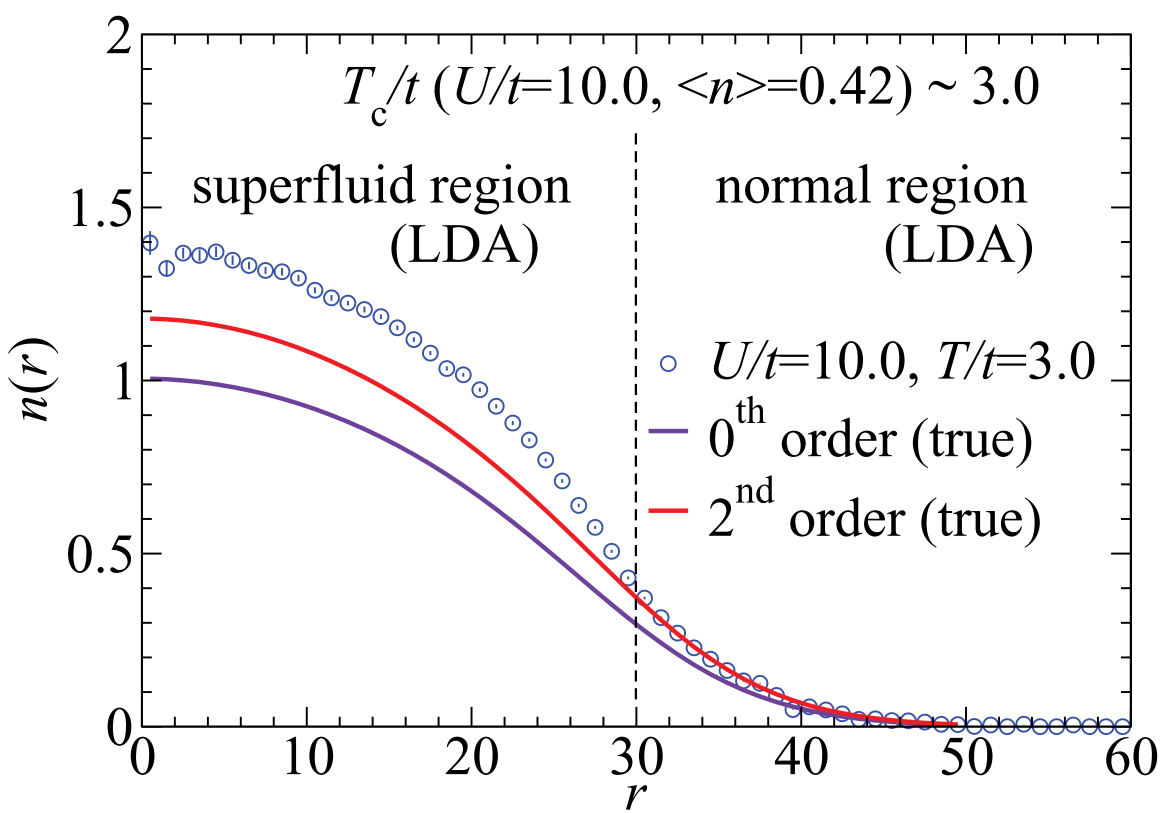


-- Should the entire system be in the normal phase, no more than **a single measurement** is needed to estimate the temperature accurately!

-- Whenever possible, HTE2 is the choice of preference for thermometry.

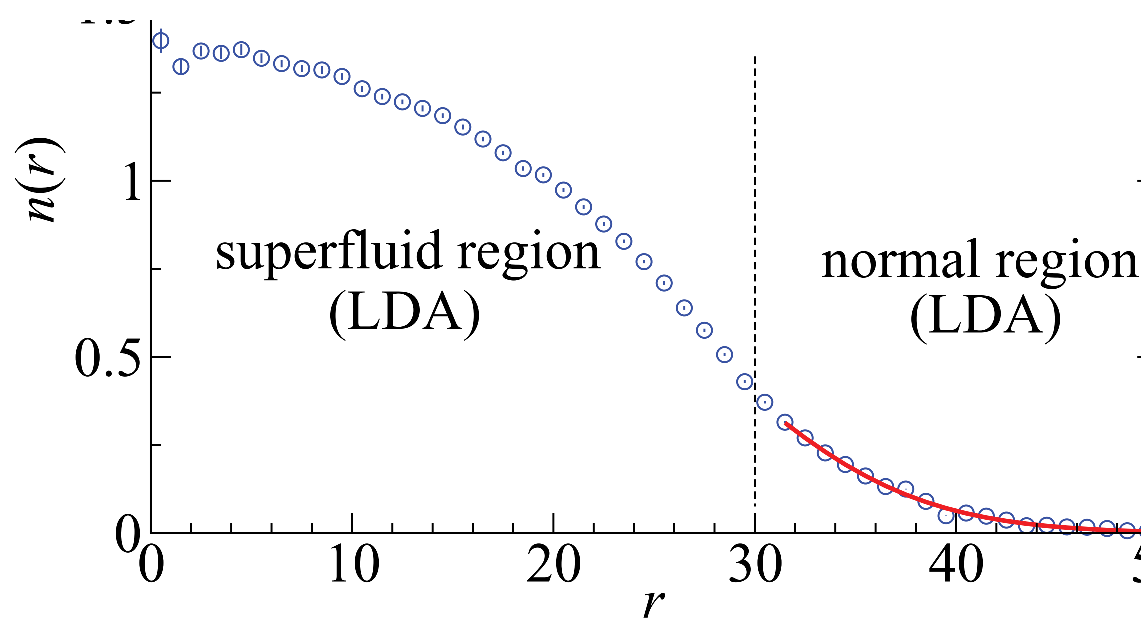
Wing Thermometry

HTE0 / HTE2 Theory in a Picture



- HTE0 works poorly.
- HTE2 captures the entire normal phase.
- *HTE2 works better with larger normal region.*

Fitting density "wings" to HTE2



- The wings of 2D cross sectional density profile is fitted to HTE2 density.

Directed worm algorithm

$$\hat{H}_0 = \frac{U}{2}\sum_i n_i(n_i - 1) - \sum_i \mu_i n_i$$
$$\hat{V} = t\sum_{\langle i,j\rangle} \hat{b}_i^\dagger \hat{b}_j \ ,$$
$$\hat{H}_0|i\rangle = \epsilon_i|i\rangle$$
$$V_{ij} = \langle i|\hat{V}|j\rangle$$

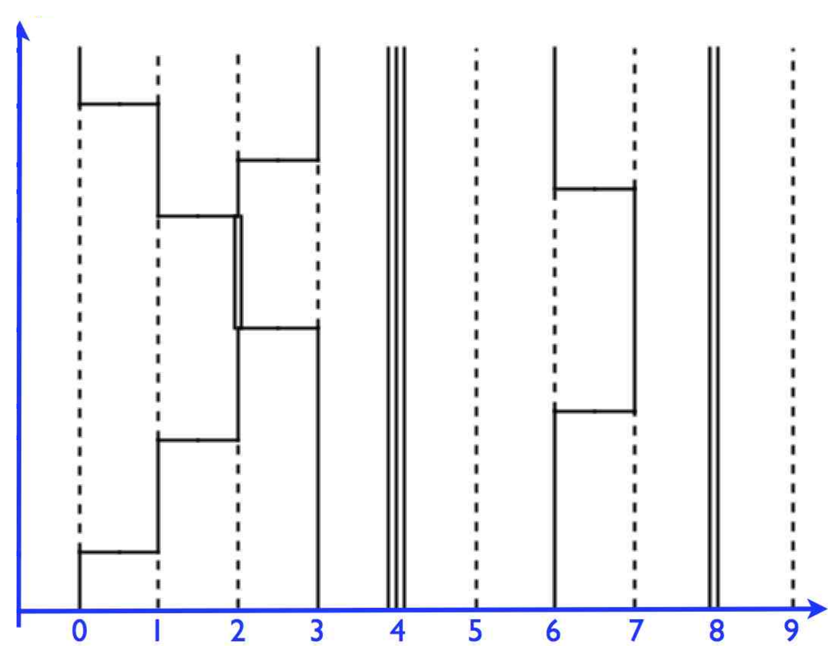
Feynmann perturbation (boson Hubbard model):

$$Z = \sum_{m=0}^{\infty} \sum_{i_1\cdots i_m} e^{-\beta\epsilon_1} \int_0^\beta d\tau_1 \cdots \int_0^{\tau_{m-1}} d\tau_m \ \underline{\left(e^{-\tau_1\epsilon_1} V_{i_1 i_2} e^{\tau_1\epsilon_2}\right) \cdots \left(e^{-\tau_m\epsilon_m} V_{i_m i_1} e^{\tau_m\epsilon_1}\right)}$$

or simply:

$$Z = \sum_{\mathcal{C}} Z(\mathcal{C})$$

Worldlines configuration



In this example:

$$|i_1\rangle = |0,1,0,1,3,0,1,0,2,0\rangle$$
$$|i_2\rangle = |0,0,1,1,3,0,1,0,2,0\rangle$$
$$|i_3\rangle = |0,0,1,1,3,0,0,1,2,0\rangle$$
$$|i_4\rangle = |0,0,2,0,3,0,0,1,2,0\rangle$$
$$|i_5\rangle = |0,1,1,0,3,0,0,1,2,0\rangle$$
$$|i_6\rangle = |0,1,1,0,3,0,1,0,2,0\rangle$$
$$|i_7\rangle = |0,1,0,1,3,0,1,0,2,0\rangle$$
$$|i_8\rangle = |1,0,0,1,3,0,1,0,2,0\rangle$$

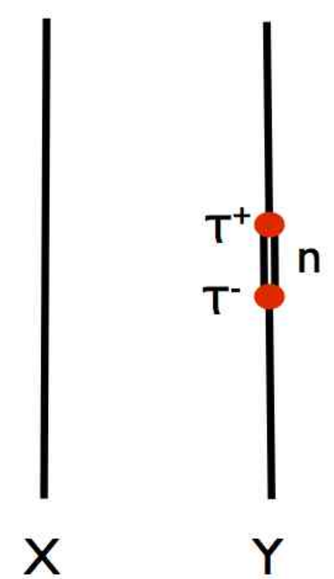
$$V_{i_1i_2} = 1 \ , \ V_{i_2i_3} = 1 \ , \ V_{i_3i_4} = 1 \ , \ V_{i_4i_5} = \sqrt{2}$$
$$V_{i_5i_6} = \sqrt{2} \ , \ V_{i_6i_7} = 1 \ , \ V_{i_7i_8} = 1 \ , \ V_{i_8i_1} = 1$$

$$N \ : \ N(\mathcal{C}) = 8$$
$$E_0 \ : \ E_0(\mathcal{C}) = 16$$

Directed worm algorithm

L. Pollet, K.V. Houcke, S. M.A. Rombouts, Engineering local optimality in QMC algorithms, J. Comp. Phys. **225/2**, 2249-2266 (2007)

Creation/ Annihilation of worms



$$\begin{aligned} Z(X) &= 4\beta L \\ Z(Y) &= n \\ P(X \to Y) &= \frac{1}{4\beta L} \\ P(Y \to X) &= \frac{1}{n} \,. \end{aligned}$$

$P_{\text{acceptance}}(X \to Y) = 1$

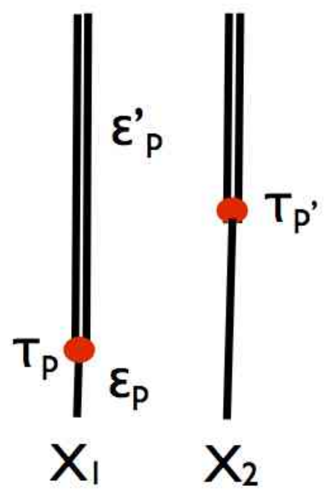
$P_{\text{acceptance}}(Y \to X) = 1$

Move is globally balanced.

Directed worm algorithm

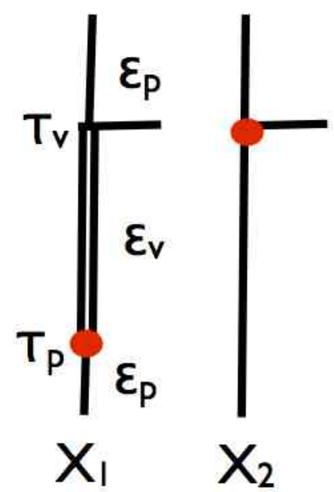
L. Pollet, K.V. Houcke, S. M.A. Rombouts,
Engineering local optimality in QMC algorithms,
J. Comp. Phys. **225/2**, 2249-2266 (2007)

Movement of worms:



1. not halted

$$P(X_1 \to X_2) = \epsilon_p e^{-\epsilon_p \tau_{p'p}}$$



2. halted

$$P(X_1 \to X_2) = \int_{\tau_{vp}}^{\infty} \epsilon_p \, e^{-\epsilon_p \tau_{p'p}} \, d\tau_{p'p}$$

$$P(X_1 \to X_2) = e^{-\epsilon_p \tau_{vp}}$$

1. QMC-DWA assigns:

   $\tau_{p'p} \sim \mathrm{Exp}(\varepsilon_p)$

   ⇒ Choose a exponential random number.

2. It either gets halted or not.

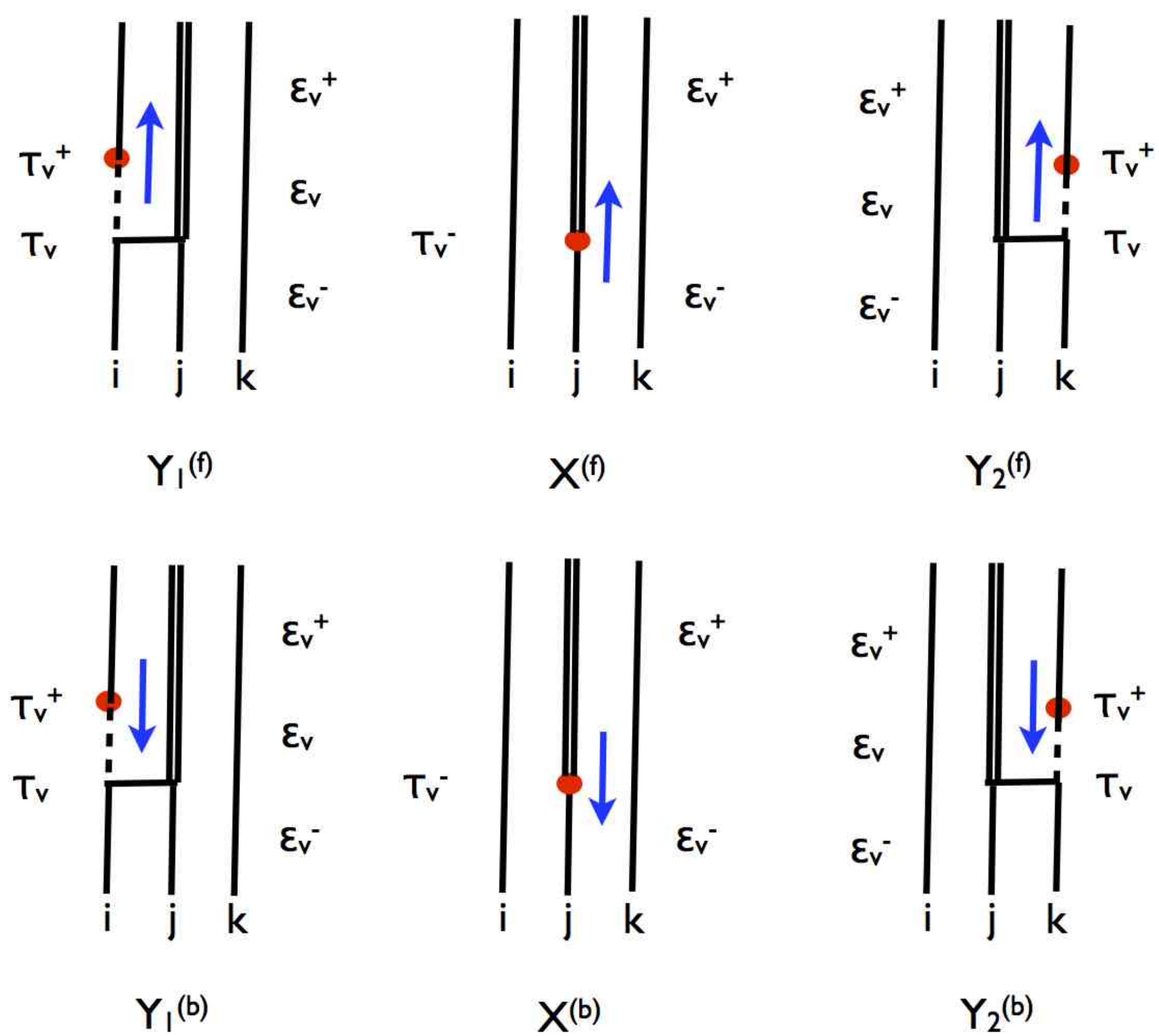
3. Memoryless

Move is **NOT** globally balanced.

Directed worm algorithm

L. Pollet, K.V. Houcke, S. M.A. Rombouts,
Engineering local optimality in QMC algorithms,
J. Comp. Phys. **225/2**, 2249-2266 (2007)

1) Inserting vertex, 2) deleting vertex, 3) relinking vertex, or 4) worm bounce:



1. QMC-DWA assigns:

$$
\begin{aligned}
P(X, Y_1, Y_2 \to X) &= \epsilon_{v-} \langle i_{v+} | \hat{b}_j^\dagger | i_{v-} \rangle \\
P(X, Y_1, Y_2 \to Y_1) &= t \langle i_{v+} | \hat{b}_i^\dagger | i_v \rangle \langle i_v | \hat{b}_i \hat{b}_j^\dagger | i_{v-} \rangle \\
P(X, Y_1, Y_2 \to Y_2) &= t \langle i_{v+} | \hat{b}_k^\dagger | i_v \rangle \langle i_v | \hat{b}_k \hat{b}_j^\dagger | i_{v-} \rangle
\end{aligned}
$$

2. The following moves are globally balanced:

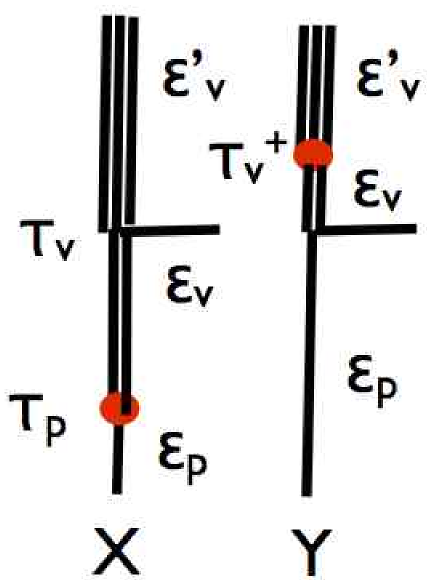
   a. unhalted move +
      insert vertex/ bounce worm

   b. halted move +
      delete/relink vertex/ bounce worm

Directed worm algorithm

L. Pollet, K.V. Houcke, S. M.A. Rombouts,
Engineering local optimality in QMC algorithms,
J. Comp. Phys. **225/2**, 2249-2266 (2007)

Crossing vertex:



1. It gets halted by like-vertex.
2. It crosses the vertex with acceptance probability 1

$$
\begin{aligned}
Z(X) &= e^{-\epsilon_p \tau_p} \langle i_v | \hat{b}^\dagger | i_p \rangle e^{\epsilon_v \tau_p} \times e^{-\epsilon_v \tau_v} \langle i'_v | \hat{b}^\dagger | i_v \rangle e^{\epsilon'_v \tau_v} \\
Z(Y) &= e^{-\epsilon_p \tau_v} \langle i_v | \hat{b}^\dagger | i_p \rangle e^{\epsilon_v \tau_v} \times e^{-\epsilon_v \tau_v^+} \langle i'_v | \hat{b}^\dagger | i_v \rangle e^{\epsilon'_v \tau_v^+}
\end{aligned}
$$

$$
\frac{Z(Y)}{Z(X)} = \frac{e^{-\epsilon_p \tau_{vp}}}{e^{-\epsilon_v \tau_{vp}}}
$$

$$
\begin{aligned}
P(X \to Y) &= e^{-\epsilon_p \tau_{vp}} \\
P(Y \to X) &= e^{-\epsilon_v \tau_{vp}}
\end{aligned}
$$

Move is globally balanced.

ALPS-2.2: QMC-DWA

Implementing QMC-DWA is easy and convenient within ALPS Python!

1. Setup the parameters:

```
import pyalps

parms = [
  {
    'LATTICE' : 'inhomogeneous simple cubic lattice' ,
    'L'       : 60 ,

    'MODEL'   : 'boson Hubbard' ,
    'Nmax'    : 20 ,

    't'  : 1. ,
    'U'  : 60. ,
    'mu' : '40. - (0.09416*(x-(L-1)/2.)*(x-(L-1)/2.) + 0.12955*(y-(L-1)/2.)*(y-(L-1)/2.) + 0.11496*(z-(L-1)/2.)*(z-(L-1)/2.))' ,

    'T'  : 1. ,

    'THERMALIZATION' : 1000000 ,
    'SWEEPS'         : 3000000 ,
    'SKIP'           : 1000 ,

    'MEASURE[Local Density]': 1
  }
]
```

2. Run simulation:

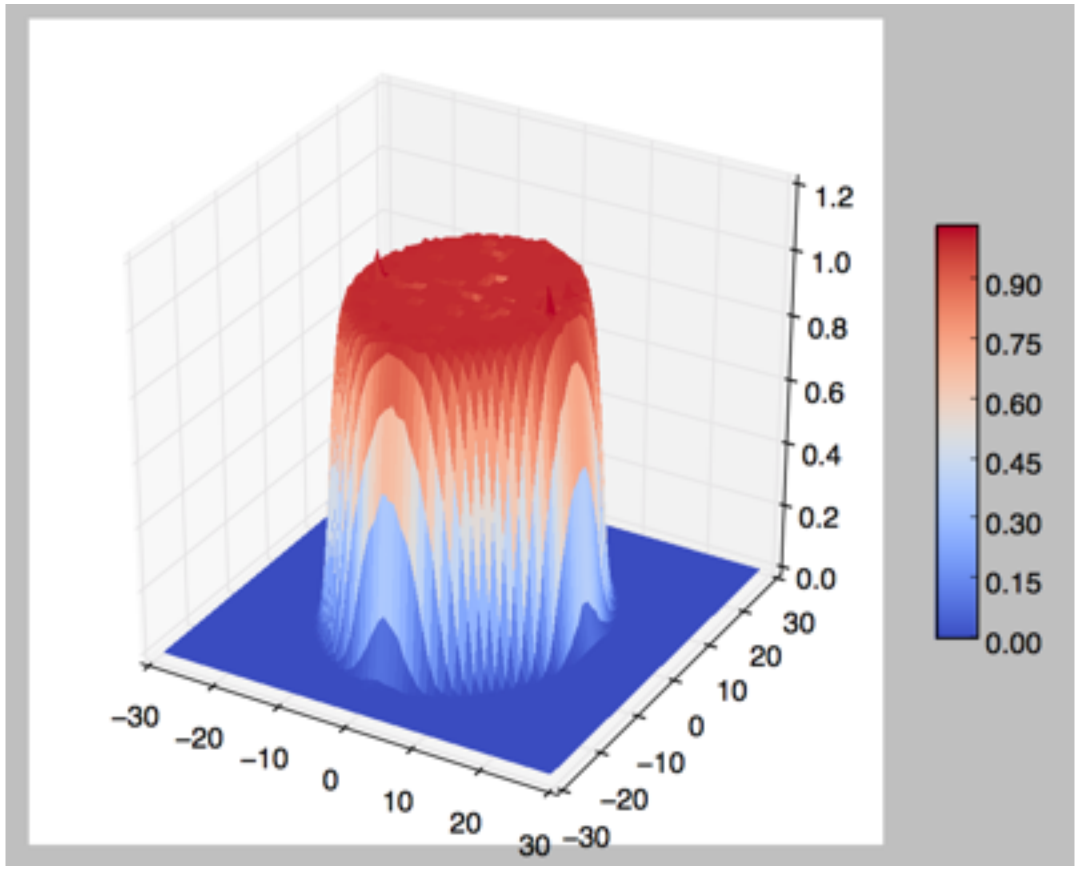
```
input_file = pyalps.writeInputFiles('parm2b', parms)
res = pyalps.runApplication('dwa', input_file)
```

3. Evaluate results:

```
import pyalps
data = pyalps.loadMeasurements(pyalps.getResultFiles(prefix='parm2b'), 'Local Density');
```

4. Visualize:

```
import pyalps.plot as aplt;
aplt.plot3D(data, centeredAtOrigin=True, layer="center")
```



Tutorial example: https://alps.comp-phys.org/mediawiki/index.php/ALPS_2_Tutorials:DWA-02_Density_Profile

Conclusion/Outlook

P. N. Ma, S. Pilati, M. Troyer, and X. Dai,
Density functional theory for atomic Fermi gases,
Nature Phys. **8**, 601 (2012)

1. **Magnetism in optical lattices**
   - **Density Functional Theory (for shallow fermionic optical lattices)**
   - **Magnetism is stabilized by lattice bandstructure effects**
   - **Phase diagram, ferromagnetism/ antiferromagnetism, SDW gap as indirect probe**

P. N. Ma, L. Pollet, and M. Troyer,
Measuring the equation of state of trapped ultracold bosonic systems in an optical lattice with in-situ density imaging ,
Phys. Rev. A. **82**, 033627 (2010)

2. **Thermometry in optical lattices**
   - **Fluctuation-dissipation thermometry -- feasible via window sizing**
   - **Wing thermometry -- HTE2 valid entirely in normal region.**

3. **QMC-DWA implementation in ALPS-2.2**
   - **easy and convenient within ALPS Python**