Ultracold atoms in optical lattices: beyond the Hubbard model

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The Abdus Salam International Centre for Theoretical Physics

"Scientific thought is the common heritage of mankind" –

Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Optical Lattice Emulator (OLE)

Ultracold atoms as:

- Digital quantum computer (Feynman 1982)

- Analog quantum emulator

Main idea:

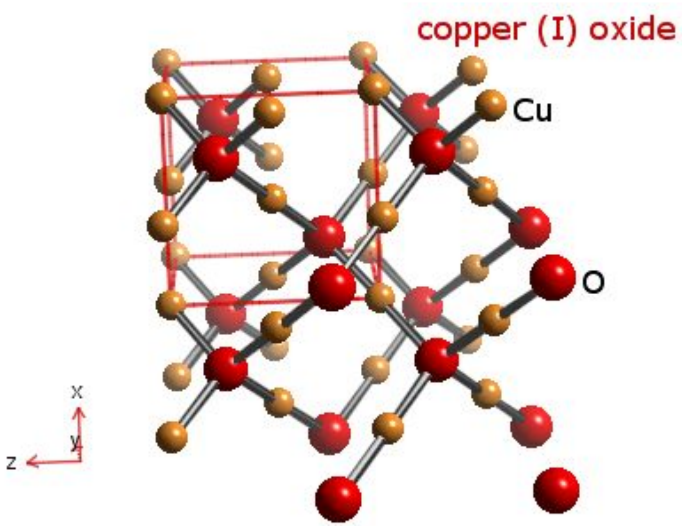
use ultra-cold gases to emulate strongly correlated materials and to test many body theories

Mott insulators

quantum magnetism (ferromagnetism, antif., spin liquids)

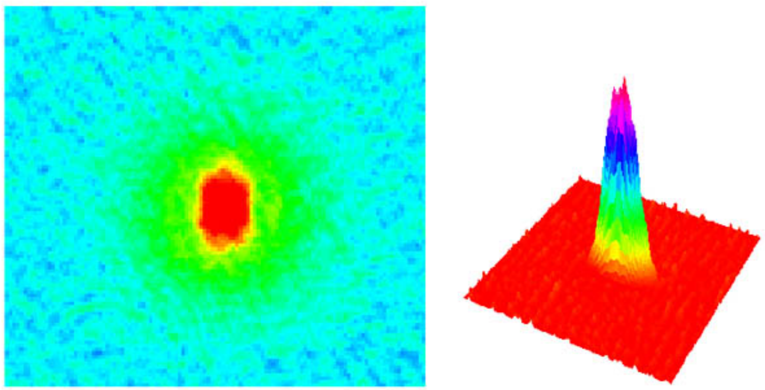
giant magnetoresistance

High-T_C superconductors



Solid state:

Inter-atomic distance ~ 0.1 nm

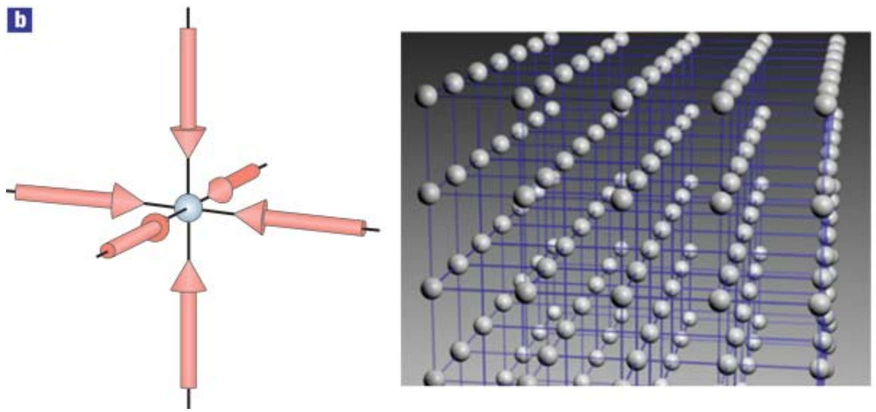


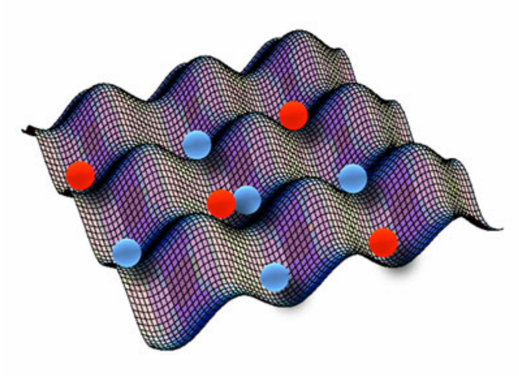
Left: condensate surrounded by thermal cloud; right: a nearly pure Bose-Einstein condensate

Dilute atomic alkali gases:

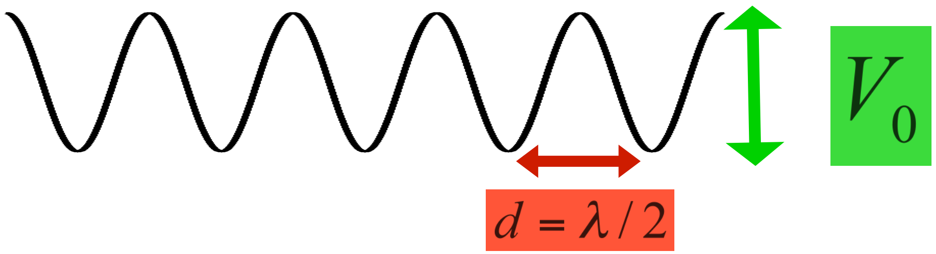
Inter-atomic distance ~ 10^2 - 10^3 nm
Temperature ~ 100 nK

Periodic potentials: optical lattices





$$\mathbf{F} = \tfrac{1}{2}\alpha(\omega_L)\, \boldsymbol{\nabla} \left[|\mathbf{E}(\mathbf{r})|^2 \right]$$



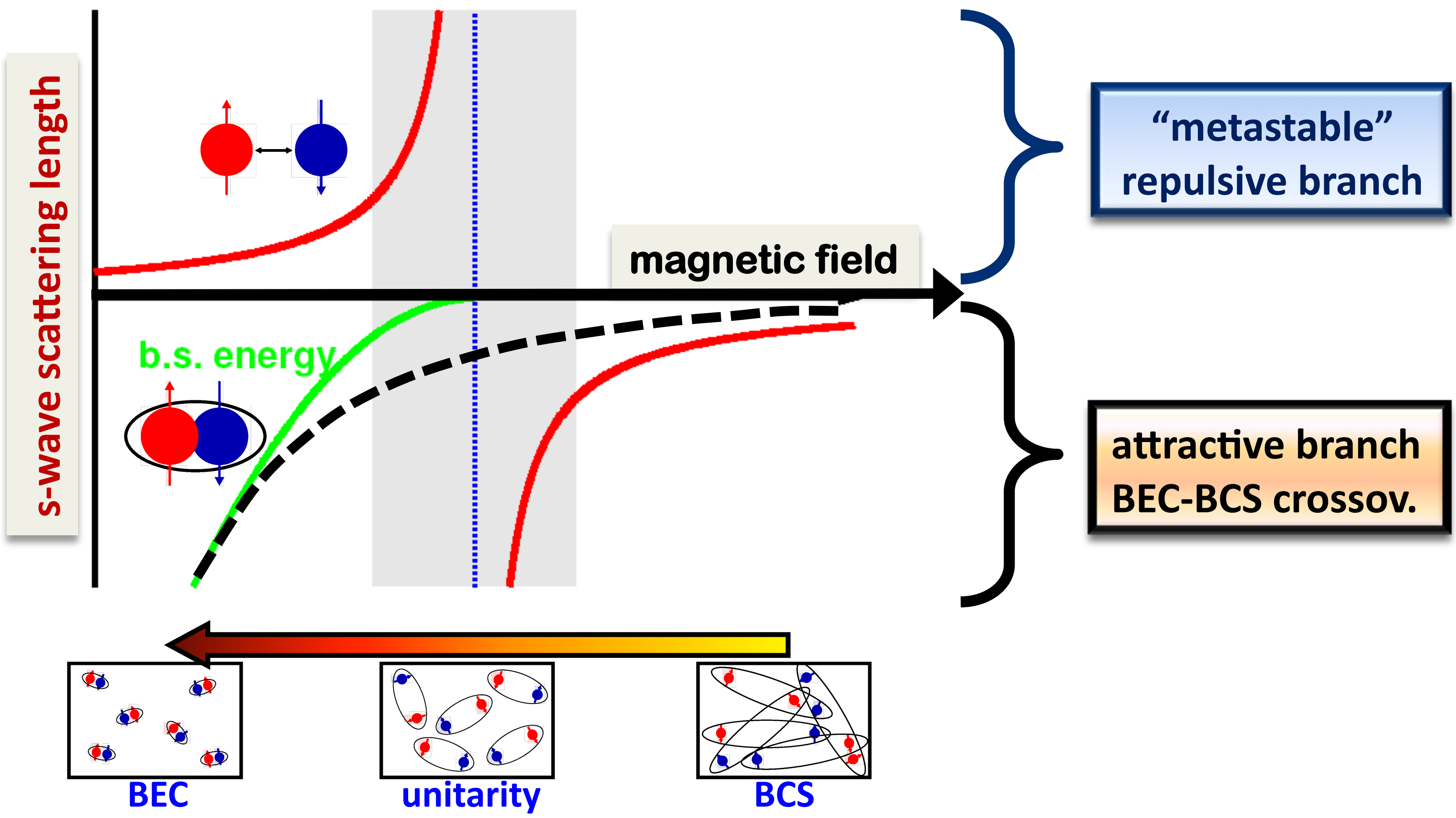
$$V(x) = V_0 \sin^2(\pi x / d)$$
$$+ \; harmonic \;\; terms$$

V_0 : laser intensity

λ : laser wavelength

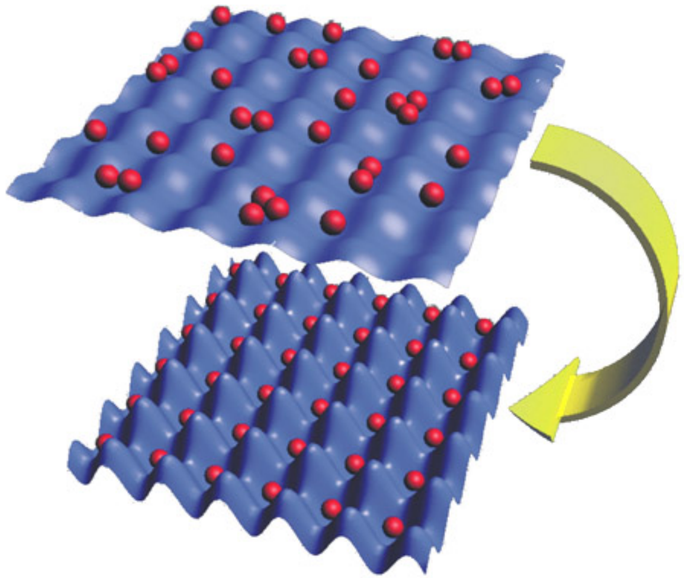
Tuning the interaction strength

Feshbach resonance



INTERACTING BOSONS IN OPTICAL LATTICES

V_0 : laser intensity
λ : laser wavelength
a_s : s-wave scattering length
E_R : recoil energy $E_R = h^2 / 8md^2$



Superfluid phase

Mott insulator

1) Only lowest Bloch band

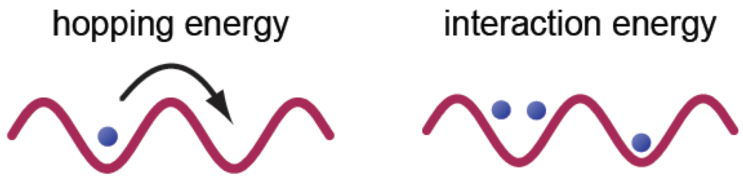
$$V_0 >> E_R$$

2) Born approximation

$$a << d$$

Single-band Bose-Hubbard model:

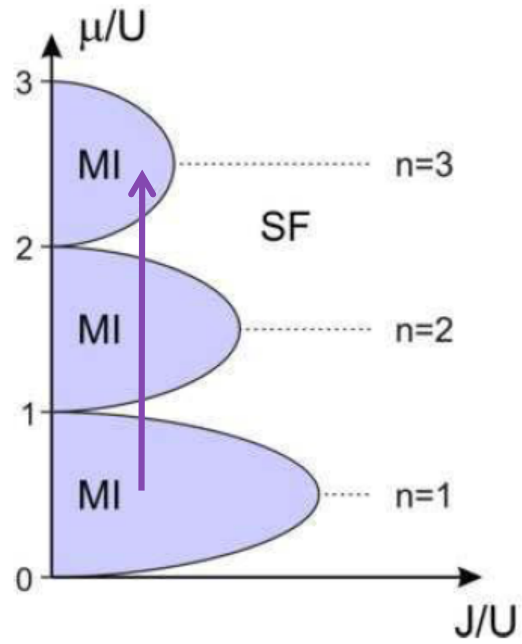
$$\hat{H} = -t \sum_{\langle i,j \rangle} b_i^\dagger b_j + \frac{U}{2} \sum_i b_i^\dagger b_i^\dagger b_i b_i$$



Jaksch et al. PRL (1998)

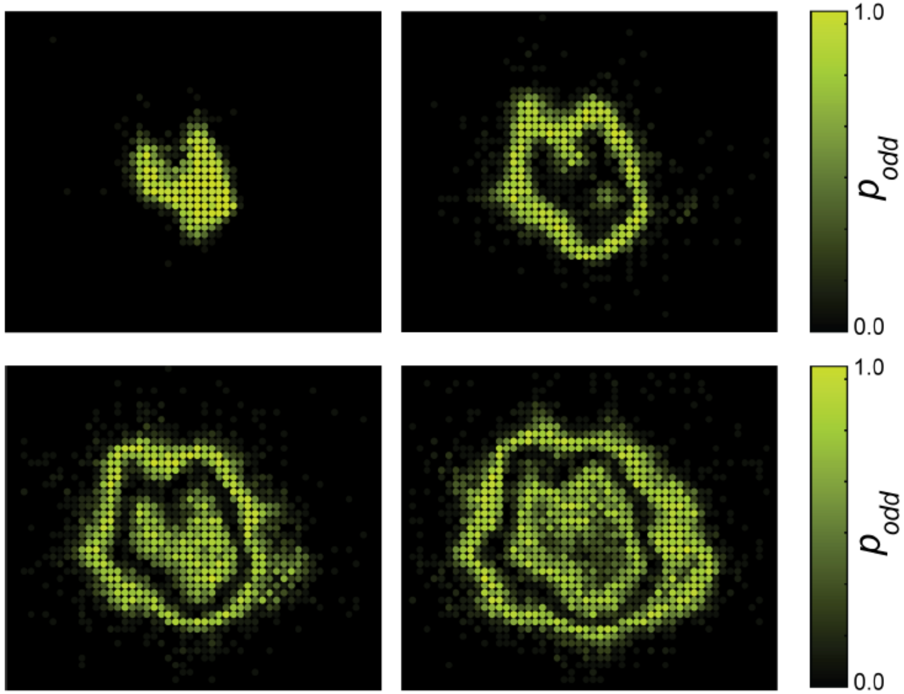
BOSONS IN OPTICAL LATTICES

phase diagram



Fisher *at al.* (1989)

Single-atom (and single-site) microscope

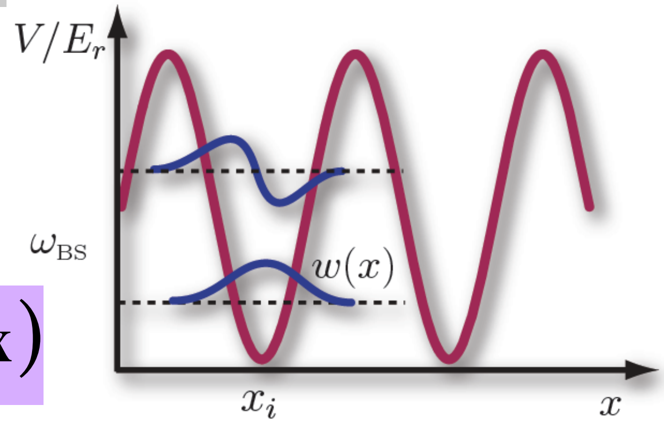


Greiner's group – Harvard (2010)

Bosons: single-band Hubbard model

$$H=\int d\mathbf{x}\,\psi^{+}(\mathbf{x})\left[\frac{-\hbar^2}{2m}\Delta+V_{ext}(\mathbf{x})\right]\psi(\mathbf{x})+\frac{1}{2}\int d\mathbf{x}d\mathbf{y}\,V_{int}(\mathbf{x}-\mathbf{y})\psi^{+}(\mathbf{y})\psi^{+}(\mathbf{y})\psi(\mathbf{x})\psi(\mathbf{x})$$

$$\psi^{+}(\mathbf{x})=\sum_{i,n}b_{i,n}^{+}w_i^n(\mathbf{x})$$



$$U_{n,i;m,j}^{n',i';m',j'}=\int d\mathbf{x}d\mathbf{y}\,V_{\rm int}(\mathbf{x}-\mathbf{y})w_{i'}^{n'}(\mathbf{y})w_{j'}^{m'}(\mathbf{y})w_j^m(\mathbf{x})w_i^n(\mathbf{x})$$

$$V_{int}(\mathbf{r})=\frac{4\pi\hbar^2 a}{m}\delta(\mathbf{r})$$

Jaksch, Bruder, Cirac, Gardiner, Zoller (1998)

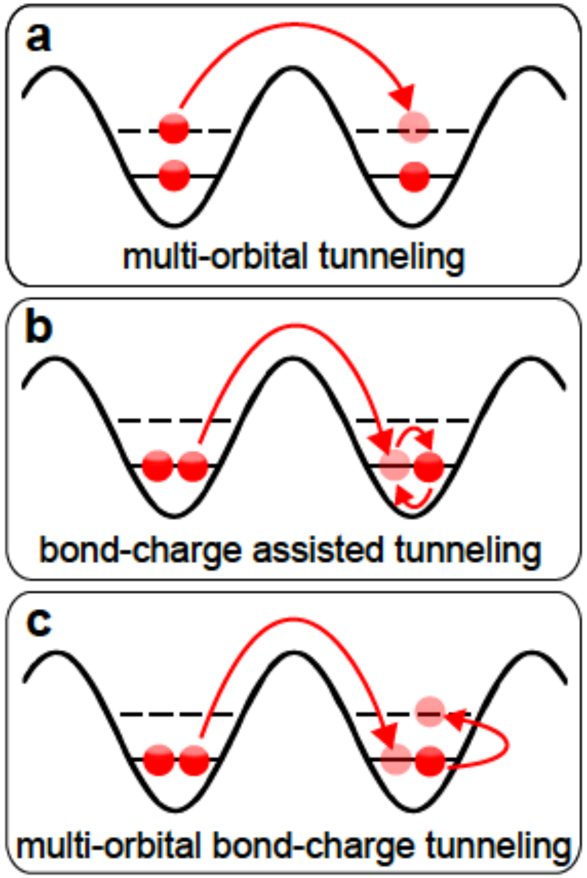
NOTE: not the Fermi-Huang pseudopotential !

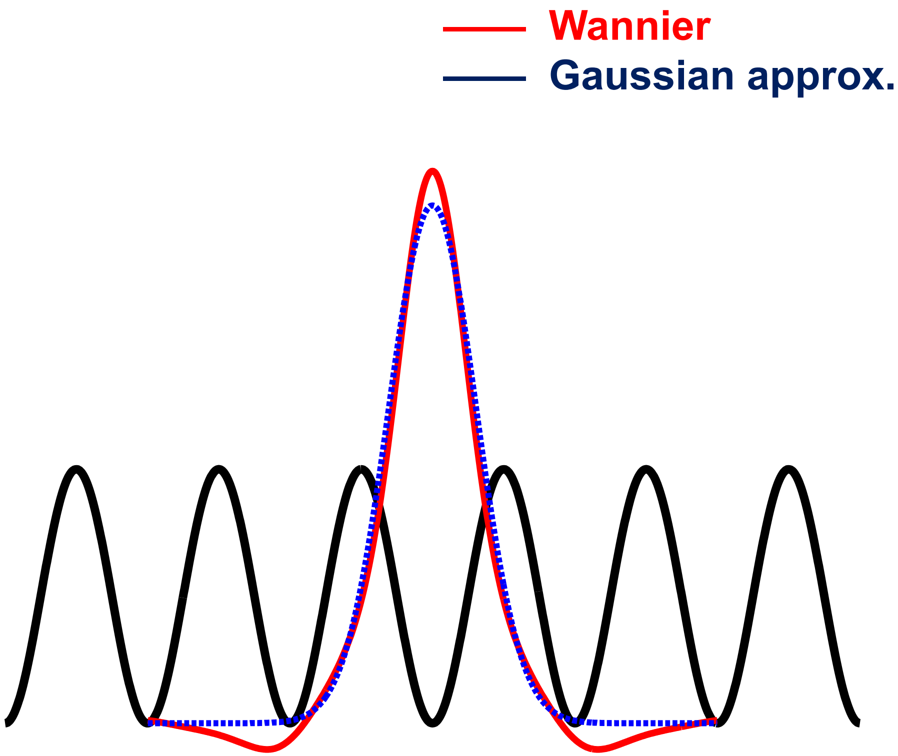
Single-band Bose-Hubbard model:

$$H=-t\sum_{\langle ij\rangle}b_i^{+}b_j^{+}+\frac{U}{2}\sum_i b_j^{+}b_j^{+}b_i b_i$$

Problems with single band Bose - Hubbard model:

- valid only for deep lattices (slow thermalization in experiments)
- neglects virtual excitations to higher bands (strong for short-range interactions)
- No density assisted hopping, nearest neighbour interaction, next nearest neighbour hopping
- No multi orbital tunneling
- Anderson (Science 2009): there is no bosonic Mott insulator!!!



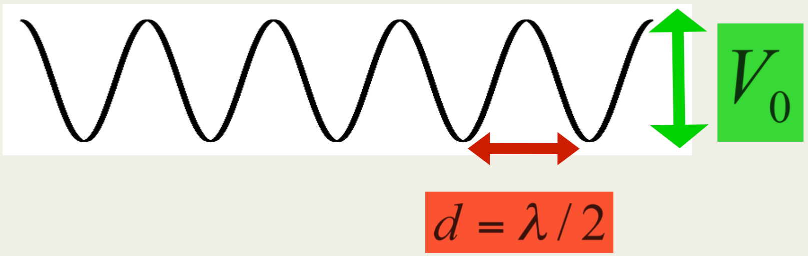


Continuous-space Hamiltonian:

$$\hat{H} = \sum_{i=1}^{N}\left[-\frac{\hbar^2}{2m}\nabla_i^2 + V(\mathbf{r}_i)\right] + \sum_{i<j} v(\mathbf{r}_{ij})$$

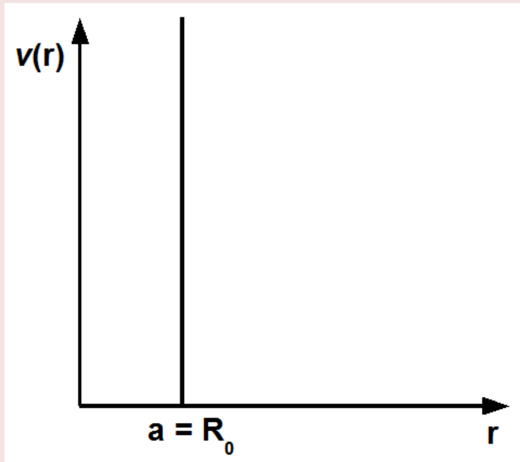
external potential:

$$V(\mathbf{r}) = V_0 \sum_{\alpha=x,y,z} \sin^2(\pi\alpha/d)$$



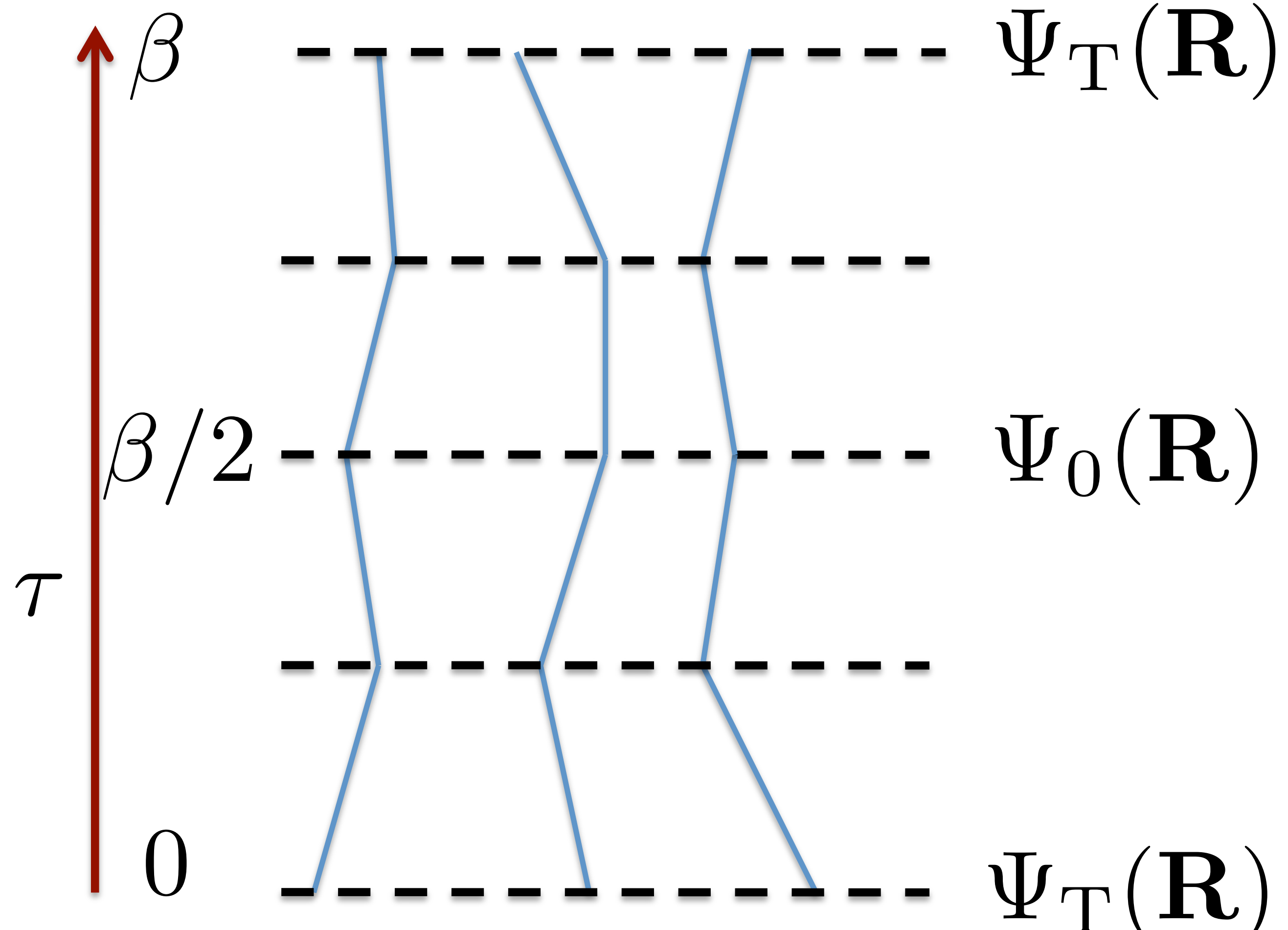
Inter-atomic pseudo potential:

$$v(r) = \begin{cases} \infty & \text{if } r < a \\ 0 & \text{otherwise} \end{cases}$$



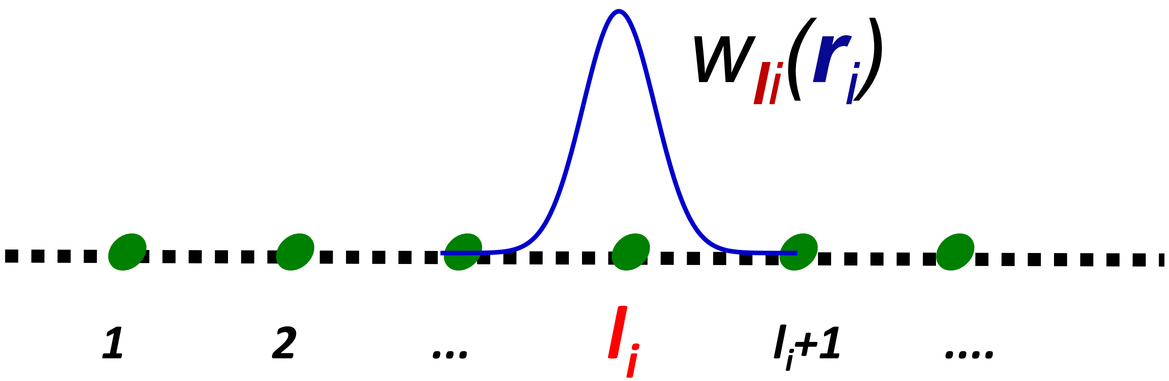
Method: ground state path integral MC (PIGS)

$$\langle \hat{O} \rangle = \frac{\int \mathrm{d}\mathbf{R}\mathrm{d}\mathbf{R}'\Psi_{\mathrm{T}}^{*}(\mathbf{R})\, e^{-\frac{\beta}{2}\hat{H}}\hat{O}e^{-\frac{\beta}{2}\hat{H}}\Psi_{\mathrm{T}}(\mathbf{R}')}{\int \mathrm{d}\mathbf{R}\mathrm{d}\mathbf{R}'\Psi_{\mathrm{T}}^{*}(\mathbf{R})\, e^{-\beta\hat{H}}\Psi_{\mathrm{T}}(\mathbf{R}')}$$



Problems near quantum critical point: $\beta \sim \xi^z$

Hybrid ground-state path integral Monte Carlo (PIGS)



$\mathbf{L} = (\mathbf{l}_1, \ldots, \mathbf{l}_N)$

Bosonic Gutzwiller wave function

$$\phi(\mathbf{l}_1, \ldots, \mathbf{l}_N) = \exp\left[-\gamma \sum_{i<j} \delta_{\mathbf{l}_i \mathbf{l}_j}\right]$$

$\mathbf{R} = (\mathbf{r}_1, \ldots, \mathbf{r}_N)$

$$\psi_{\mathbf{L}}(\mathbf{r}_1, \ldots, \mathbf{r}_N) = \prod_{i=1}^{N} w_{\mathbf{l}_i}(\mathbf{r}_i)$$

$$\Psi_T(\mathbf{R}) = \sum_{\mathbf{L}} \phi(\mathbf{L})\, \psi_{\mathbf{L}}(\mathbf{R})$$

$$\int \mathrm{d}\mathbf{R} \;\rightarrow\; \sum_{\mathbf{L}} \int \mathrm{d}\mathbf{R} \qquad \mathbf{R} \;\rightarrow\; (\mathbf{R}, \mathbf{L})$$

$\gamma = 0$

$$\Psi_{\mathrm{T}}\left(\mathbf{R}\right) \simeq \prod_{i,j} b_{\mathbf{k}=\mathbf{0}}\left(\mathbf{r}_i\right) \prod_{i} f\left(r_{ij}\right)$$

Bloch function

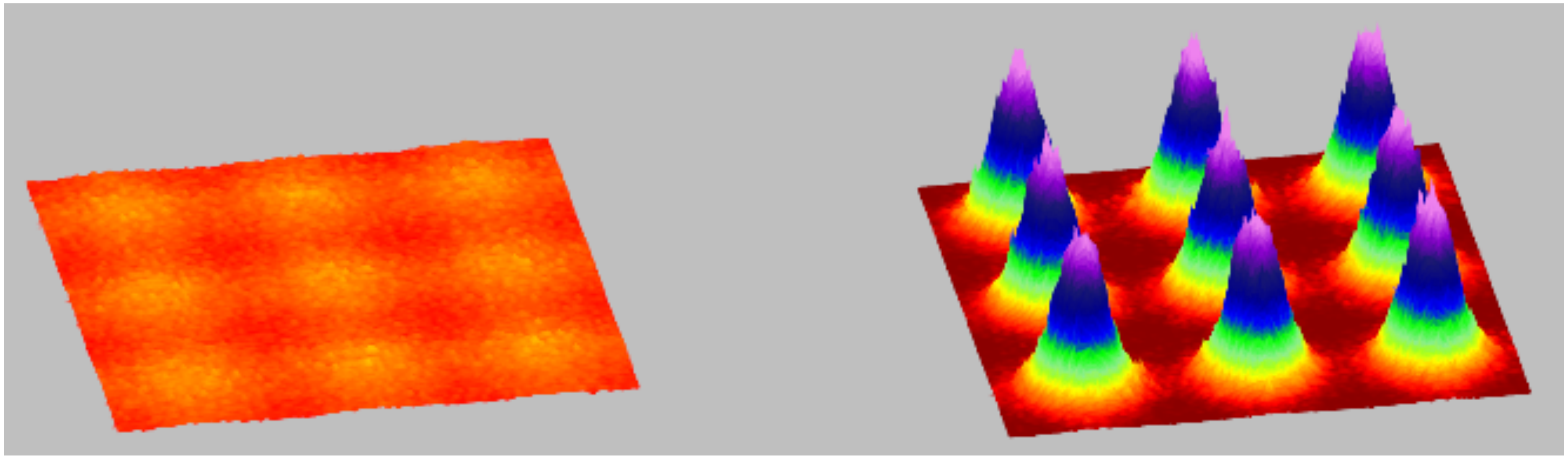
$$b_{\mathbf{k}}(\mathbf{r}) = M^{-1/2} \sum_{\mathbf{l}} \exp\left(i\mathbf{k}\cdot\mathbf{l}\right) w_{\mathbf{l}}(\mathbf{r})$$

$\gamma = \infty$

$$\Psi_{\mathrm{T}}(\mathbf{R}) = \mathrm{Perm}\left[w_{\mathrm{l}}(\mathrm{r}_i)\right] \prod_{i,j} f(r_{i,j})$$

Wannier function

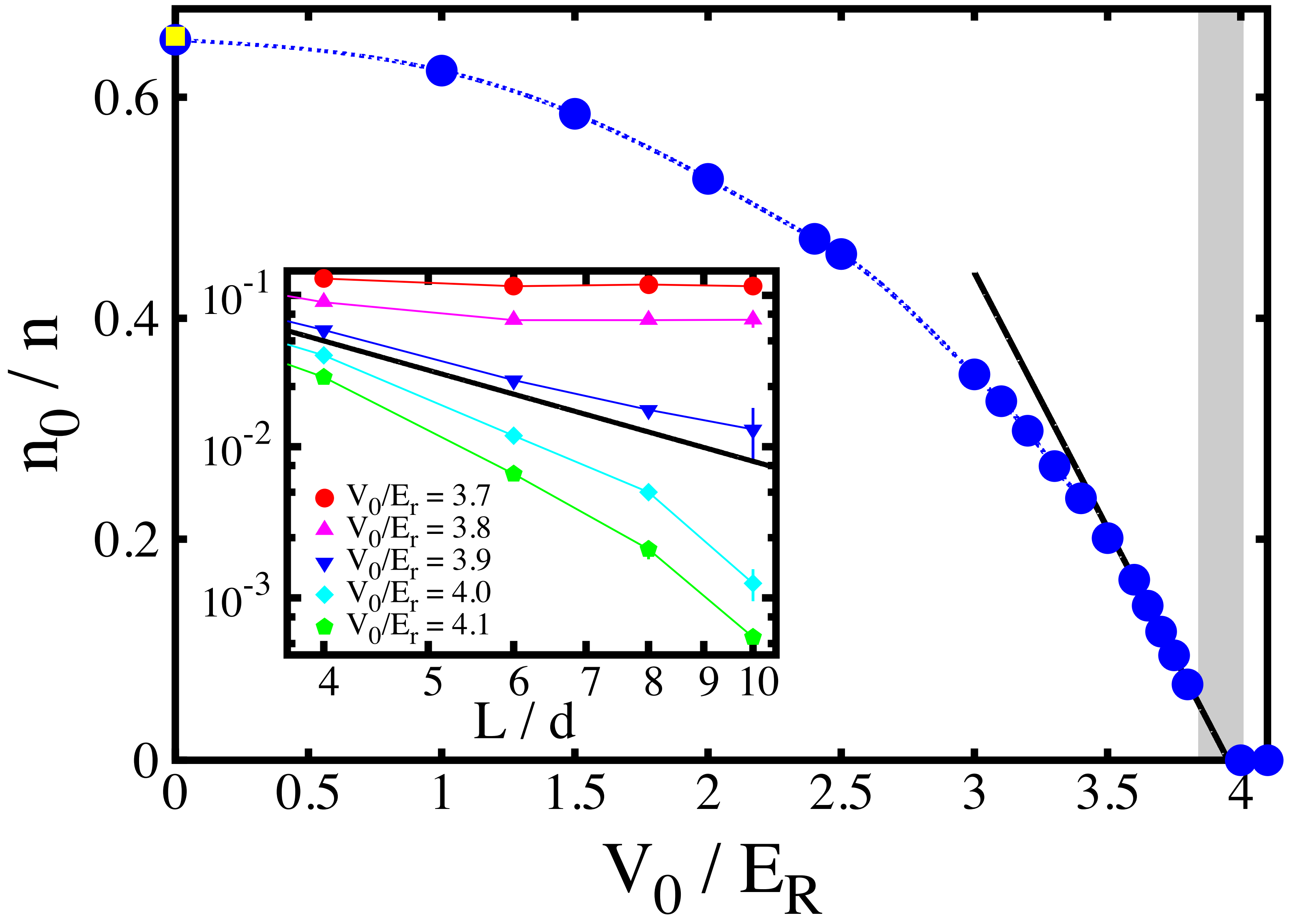
$$w_{\mathbf{l}}(\mathbf{r}) = M^{-1/2} \sum_{\mathbf{k}} \exp\left(-i\mathbf{k}\cdot\mathbf{l}\right) b_{\mathbf{k}}(\mathbf{r})$$



Superfluid to insulator transition

$nd^3 = 1$

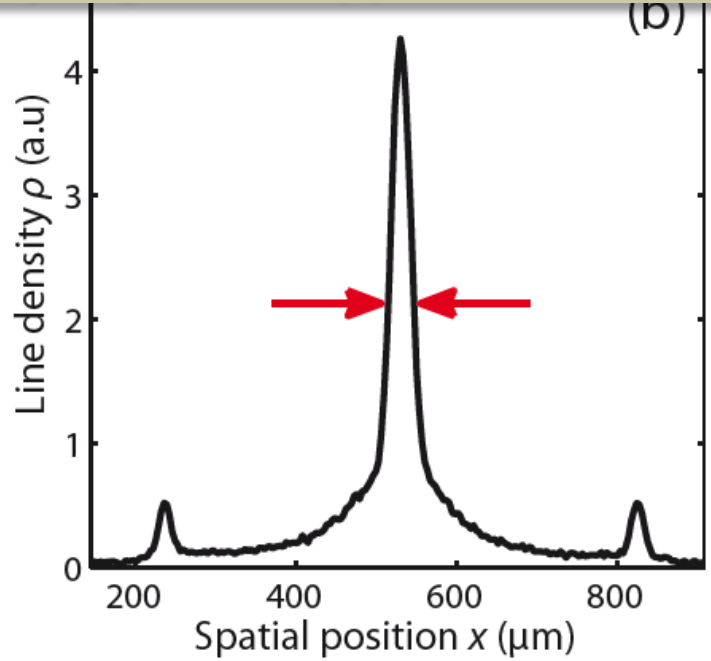
$a / d = 0.3$

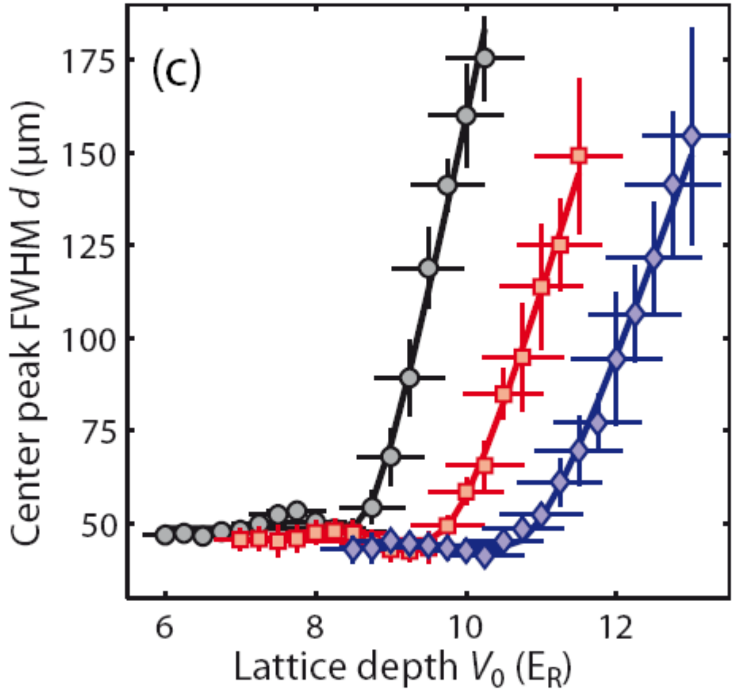


Superfluid to Mott insulator transition: experiment in Innsbruck

Mark, Haller, Lauber, Danzl, Daley, Nägerl Phys. Rev. Lett. 2011

Doubly integrated density profile after time-of-flight



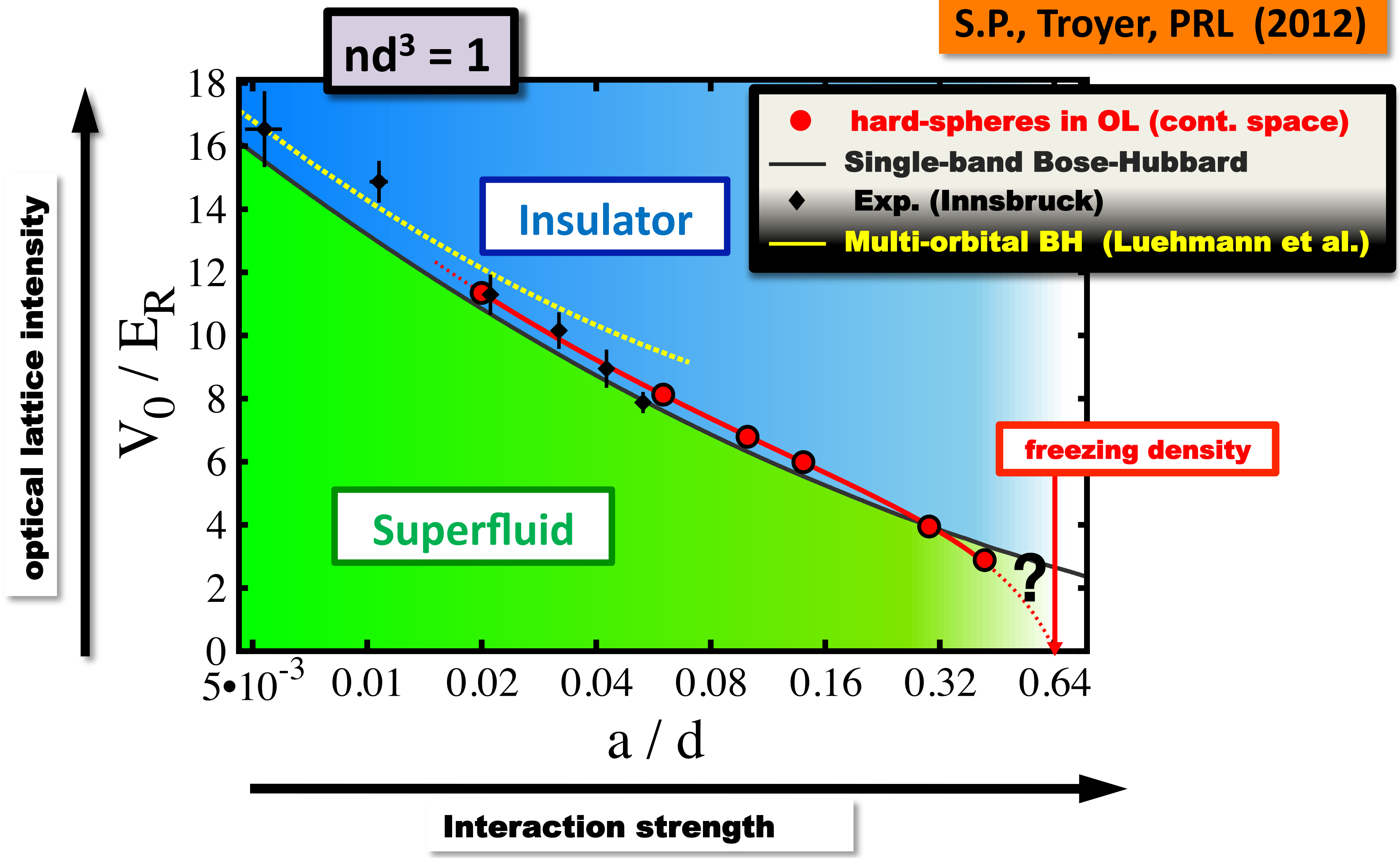


→ obtain V_C *vs* (a_S)

The critical depth V_C is identified as the intersection point of two linear functions that we add quadratically and fit to the data.

Hard Spheres in OL (cont. space) *vs.* single-band Bose-Hubbard

S.P., Troyer, PRL (2012)

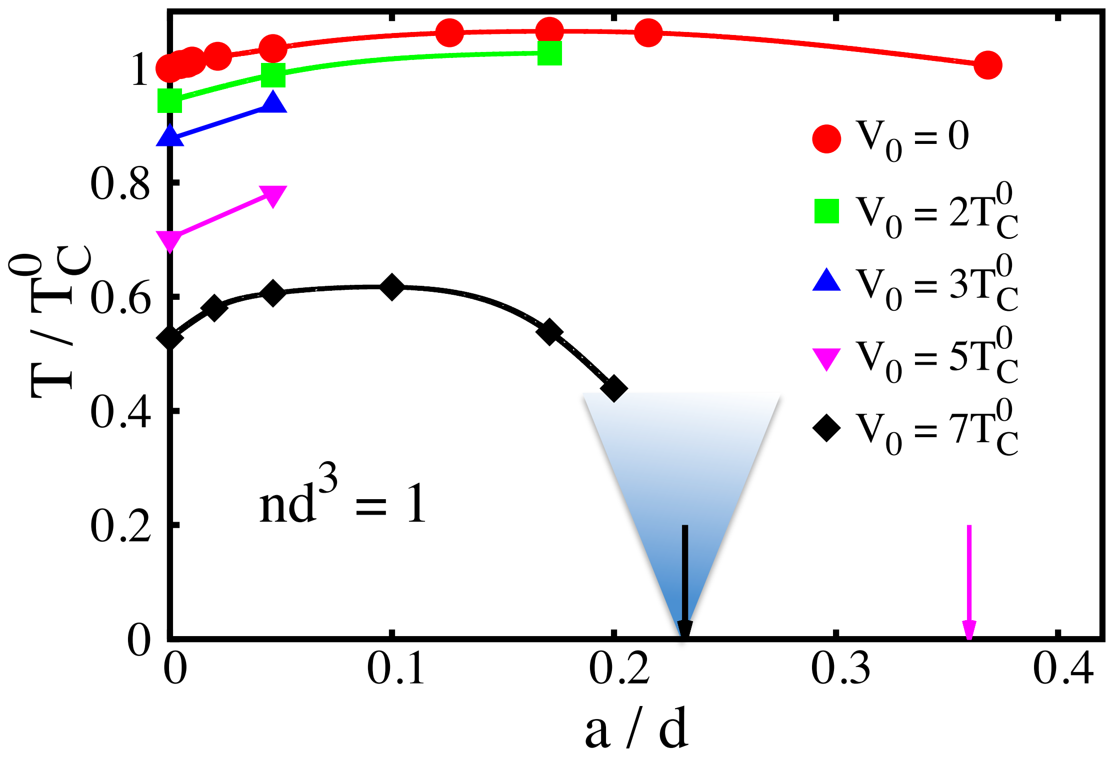


- single-band Bose-Hubbard model: Capogrosso-Sansone *et al.* PRB 75 134302 (2007)
- Hard-sphere freezing: $na^3 = 0.265(1)$ Rota, Giorgini (Private Communications)

  $na^3 \approx 0.25$ Kalos *et al.* PRA (1974)

Critical temperature for interacting Bose gases in optical lattices

S.P., Nguyen, Herrmann, Troyer, *in preparation*



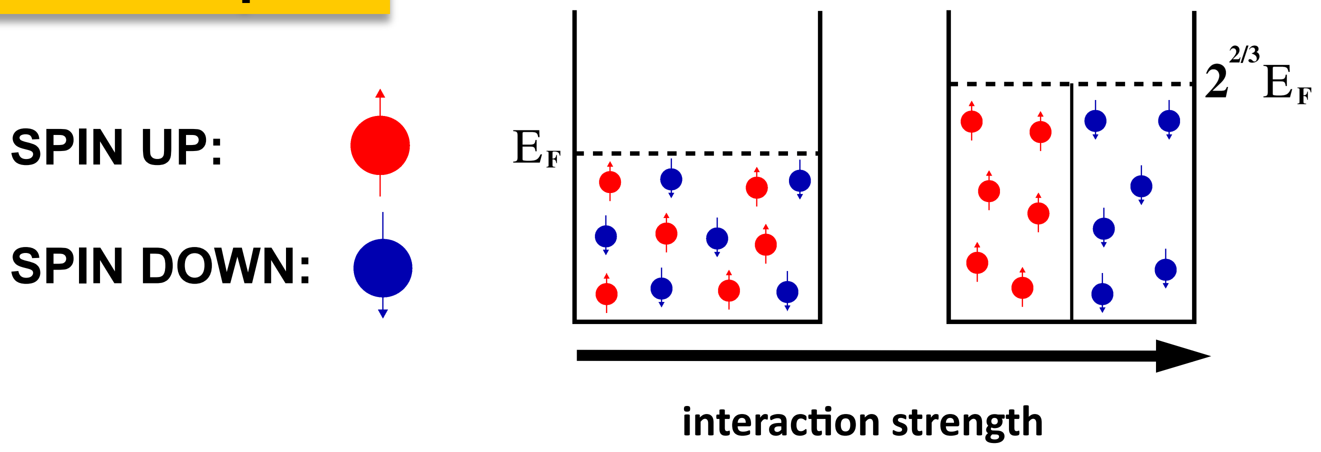
<u>Critical temperature of homogeneous Bos gas</u>

-) Grüter, Ceperley, Laloë PRL 1997

-) S.P. Giorgini, Prokof'ev PRL 2008

Two-component repulsive Fermi gas

Fermions in free space → STONER INSTABILITY

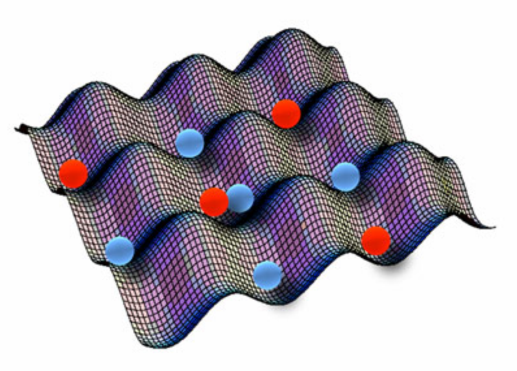


Mean-field theory:	$k_F a_s = 1.57$	(Stoner model)
2^{nd} order pert. Th.:	$k_F a_s = 1.054$	Duine, MacDonald PRL 2009
QMC:	$k_F a_s \approx 0.8$	Chang *et al.* PNAS 2011 S. P., Bertaina, Giorgini, Troyer PRL 2010 Conduit *et al.* PRL 2009

<ins>However</ins> : instability against molecule formation

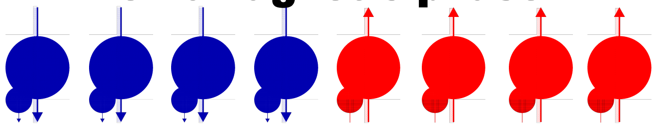
Pekker *et al.* PRL(2011)
Lee *et al.*, PRA 85 063615 (exp @ MIT 2012) → maximum $k_F a_s \approx 0.25$

Two-component Fermi gases in optical lattices

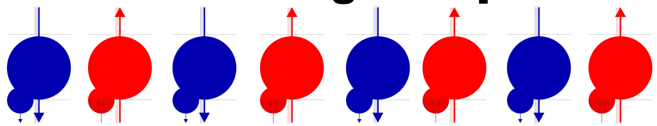


→ **QUANTUM MAGNETISM**

ferromagnetic phase



anti-ferromagnetic phase



Note:
in atomic gases the number of spin-up and spin-down particles are fixed

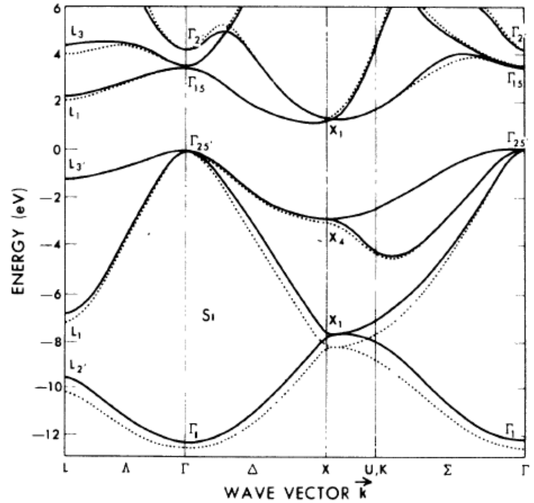
Kohn-Sham Density Functional Theory

<u>the standard computational method in material science</u>

1998 Nobel prize in chemistry

Walter Kohn

Es.: band structure of silicon



Chelikowsky and Cohen, PRB (1974)

successful in calculating properties of many metals, insulators, semiconductors

reduces the N-body problem to an effective single-particle problem

$$E = \left\langle \Psi \middle| \hat{H} \middle| \Psi \right\rangle$$

find $\Psi(\mathrm{R})$

$$E = \min\left\{E\left[n(\mathbf{r})\right]\right\}$$

find $n(\mathbf{r})$

Use of DFT in quantum chemistry and materials science

Perspective on density functional theory

Kieron Burke[1]

Department of Chemistry, 1102 Natural Sciences 2, UC Irvine, CA 92697, USA

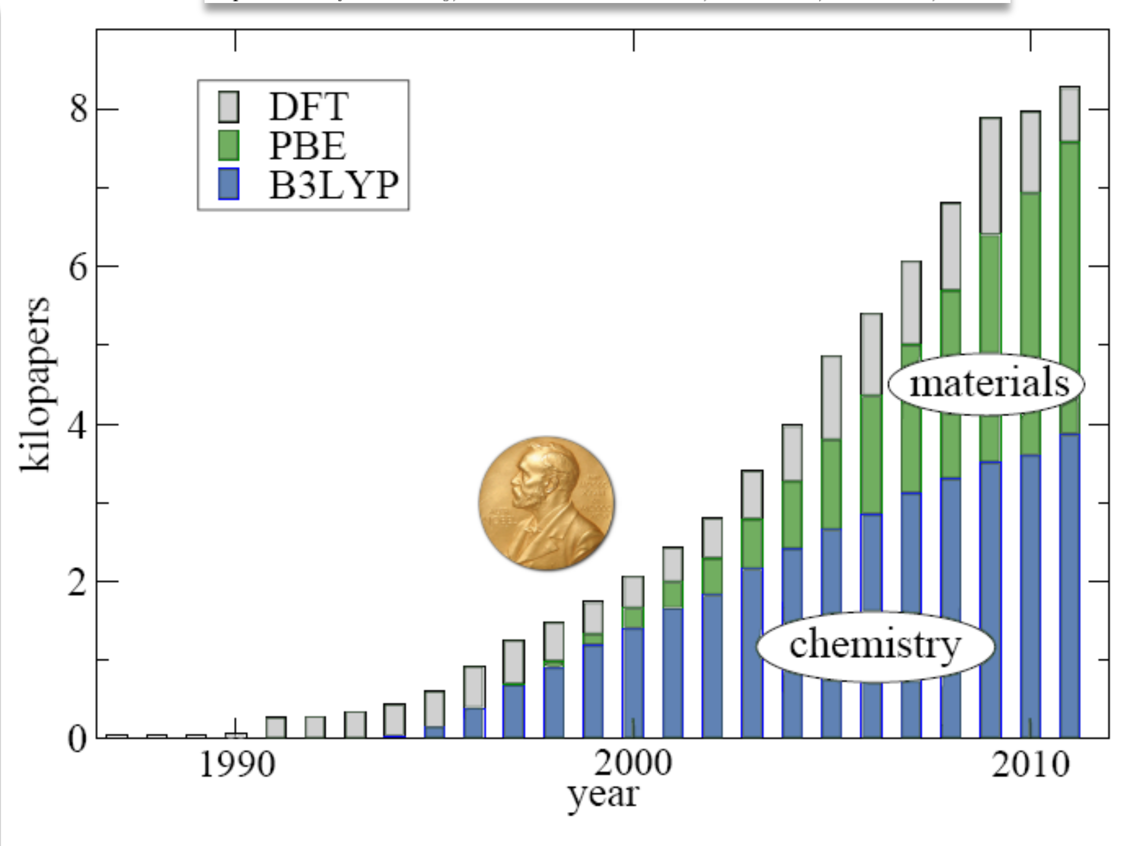


FIG. 1. Numbers of papers when DFT is searched as a topic in Web of Knowledge (grey), B3LYP citations (blue), and PBE citations (green, on top of blue).

Energy-density functional:

$$E[\rho] = E_{\mathrm{KIN}}[\rho] + \int d\mathbf{r} V(\mathbf{r})\rho(\mathbf{r}) + \iint d\mathbf{r} d\mathbf{r}' V_{\mathrm{INT}}(|\mathbf{r}-\mathbf{r}'|)\rho(\mathbf{r})\rho(\mathbf{r}') + E_{\mathrm{XC}}[\rho]$$

kinetic energy

external potential

mean-field/classical interaction

eXchange and Correlation (unknown!)

Basic approx. → Local Spin-Density Approximation:

note: not the AMO LDA!!

$$E_{\mathrm{XC}}\left[\rho^{\uparrow}(\mathbf{r}),\rho^{\downarrow}(\mathbf{r})\right] = \int d\mathbf{r}\,\varepsilon_{\mathrm{XC}}^{\mathrm{homo}}\left(\rho^{\uparrow}(\mathbf{r}),\rho^{\downarrow}(\mathbf{r})\right)$$

- 3D electron gas : Ceperley, Alder 1980
- 3D repulsive Fermi gas: this work

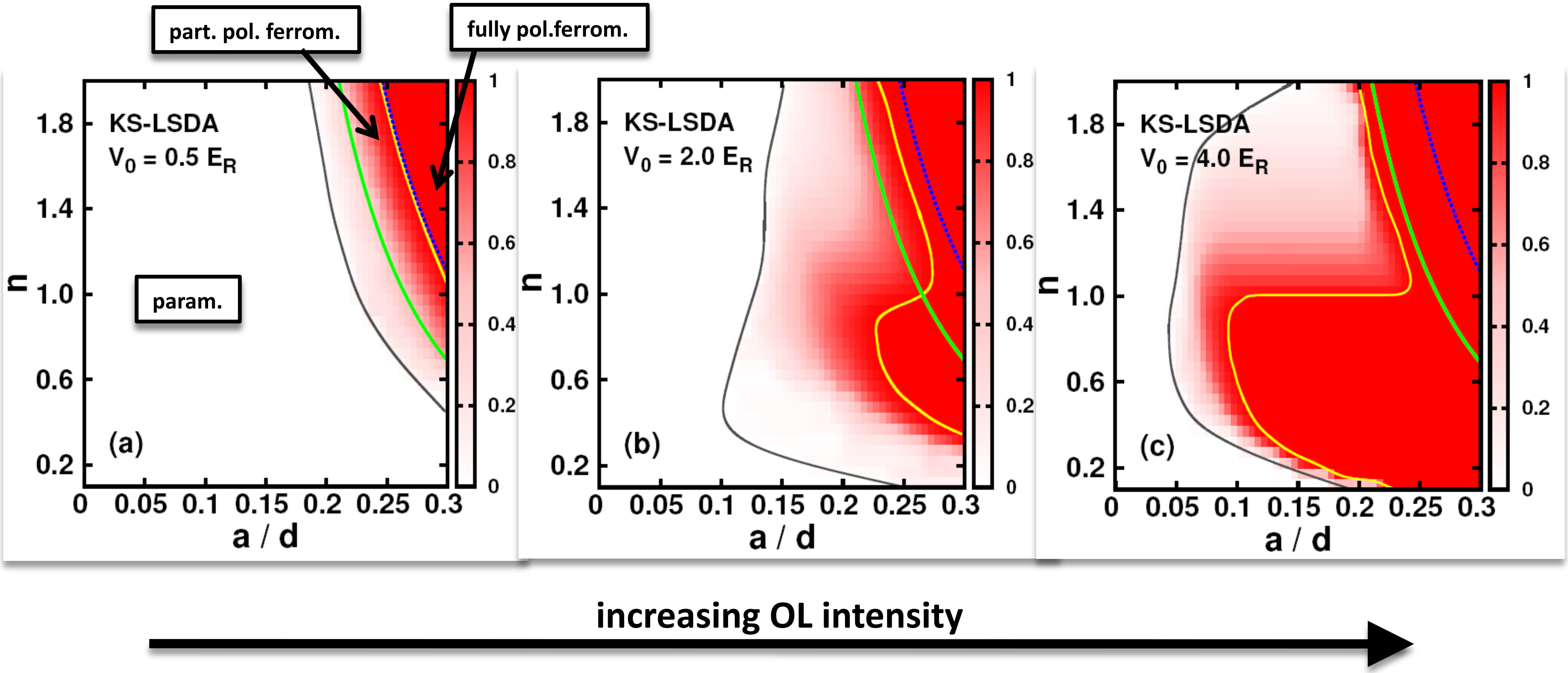
From Fixed-Node Diffusion Monte Carlo

DFT for unitary Fermi gas: Bulgac et al, SCIENCE **332**, 1288 (2011)

Beyond LDA:
GGA, meta GGA, hybrid functionals, LDA + U, LDA + DMFT, GW, LDA +Gutzwiller...

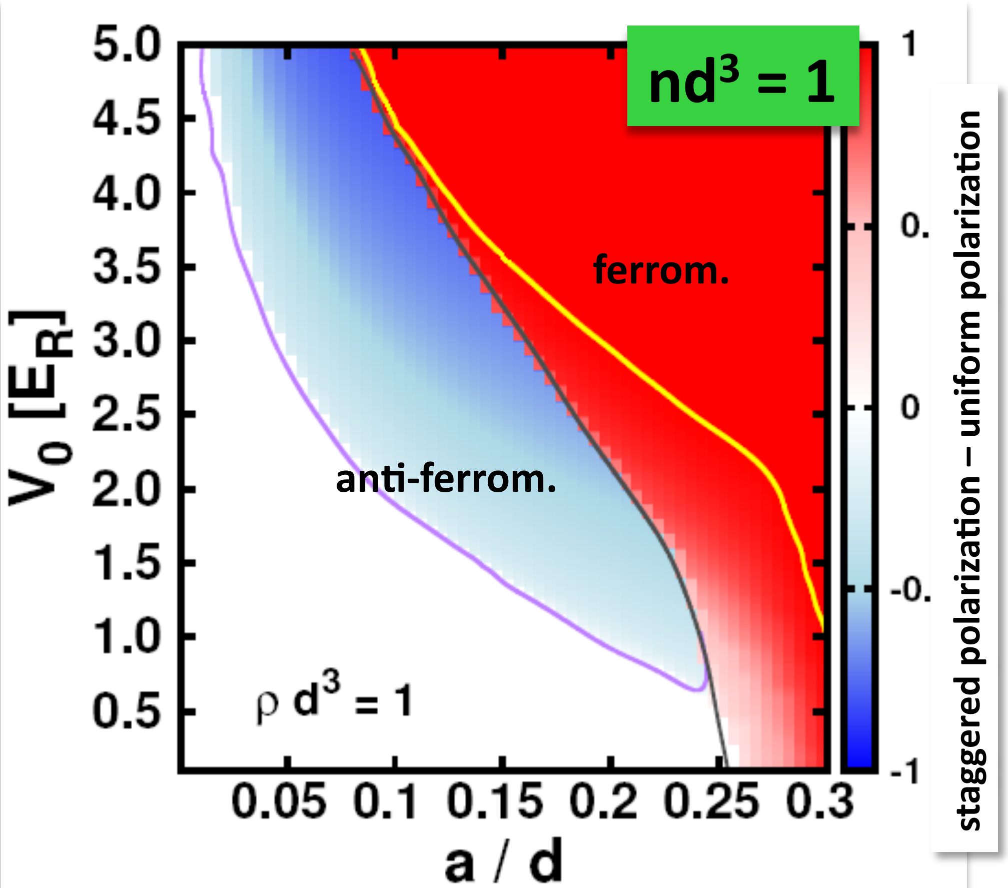
Kohn Sham-DFT with LSDA for a repulsive Fermi gas in OL

GROUND-STATE PHASE DIAGRAM



Ma, SP, Xi, Troyer, Nature Physics 2012

Phase diagram at half-filling



Ma, SP, Xi, Troyer, Nature Physics 2012

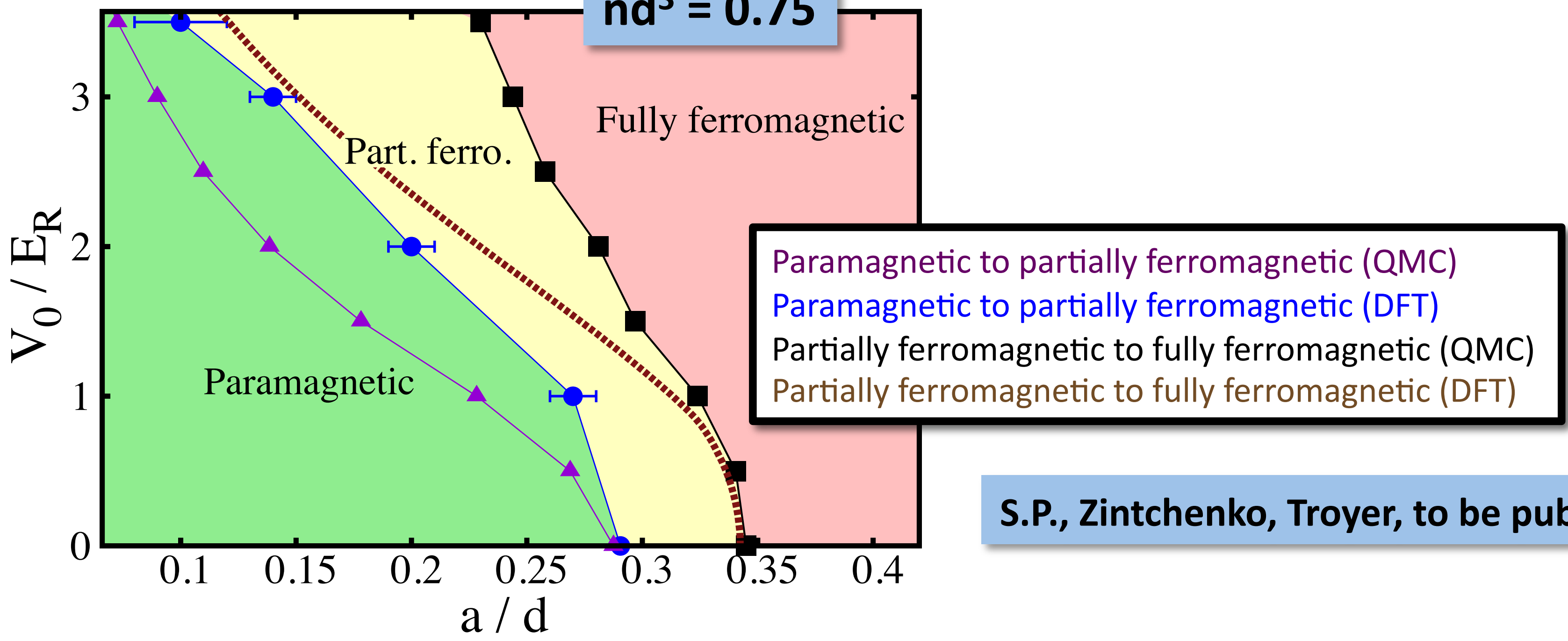
short range anti-ferromagnetic order observed @ ETH

Science 340, 1307-1310 (2013)

DFT *vs* Fixed-Node DMC: phase diagram

FN-DMC: Slater determinant with Bloch functions

$nd^3 = 0.75$



S.P., Zintchenko, Troyer, to be published

<u>Repulsive Hubbard model:</u>

infinite U -> Ferromagnetism at $nd^3 \approx 0.75$
Becca Sorella 2001, Park Haule Marianetti Kotliar 2008,
Liu Yao Berg White Kivelson 2012

finite U -> no ferromagnetism for $nd^3 <= 0.5$
Chang Zhang Ceperley 2010

SUMMARY:

- ultracold atoms in optical lattices:

IDEAL TOOL TO PLAY WITH STRONG CORRELATIONS

- simulations for (shallow) optical lattices can be done in continuous space

- QMC methods for discrete lattice models and continuous-space Hamiltonians can be combined

- we could use experiments with cold atoms and QMC to develop energy functionals for DFT

- Challenges for QMC (beyond sign problem): strong correlations in realistic Hamiltonians, disorder (many-body localization), combining DFT and QMC