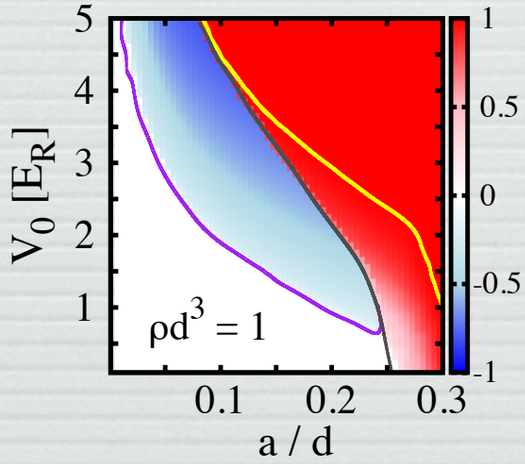
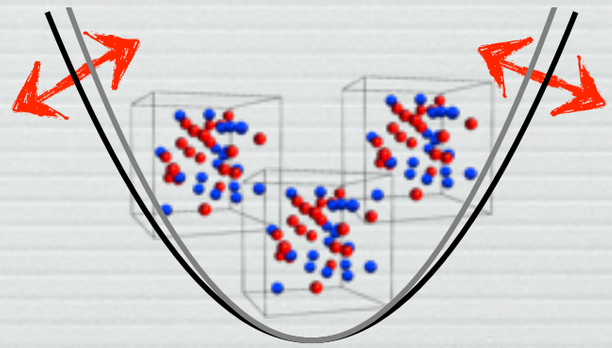
Density functional theory for static and dynamic properties of cold atomic gases





Lei Wang, ETH Zurich

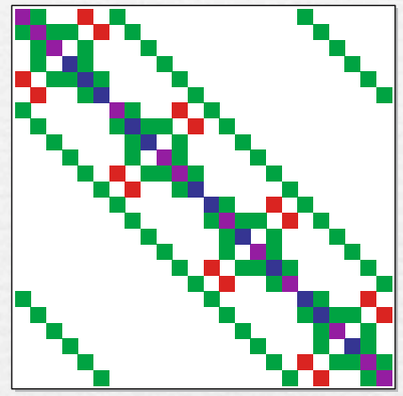
ETH Zürich Ping Nang Ma, Ilia Zintchenko, Matthias Troyer

ICTP Sebastiano Pilati

Institute of Physics CAS Xi Dai

Exact Diagonalization

$$H|\Psi\rangle = E|\Psi\rangle$$



- Gives exact results for static and dynamic properties
- But limited to small systems
  - 25 site Fermi-Hubbard model with 12 atoms on the Earth Simulator in 2006

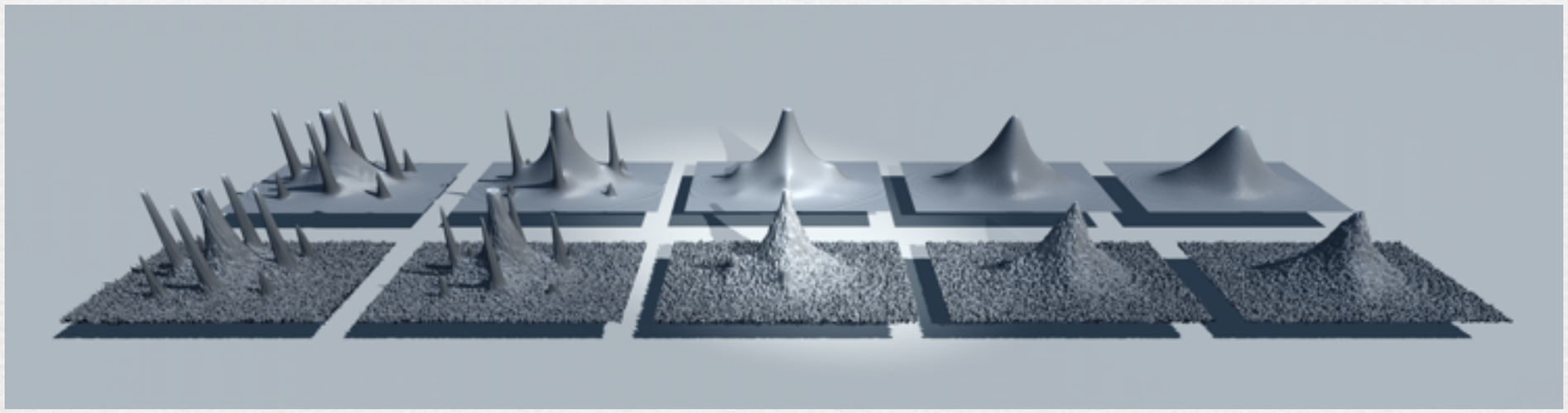
DMRG

- Extremely powerful in 1D

  - Accurate on hundreds of sites
- Higher dimension generalization is possible but very expensive

Quantum Monte Carlo

- Can solve static properties of
  - 1,000,000 bosons in any dimensions,



Trotzky *et al*, Nature Physics, 2010

  - 100 fermions in 2D and 3D at $T>0.05E_F$

ALPS

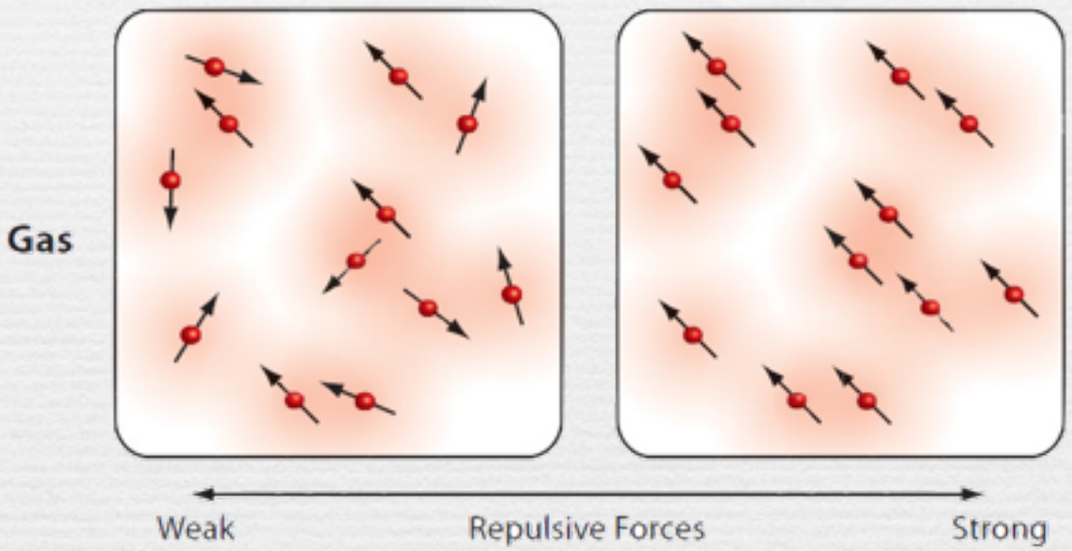
Algorithms and **L**ibraries for **P**hysics **S**imulations

http://alps.comp-phys.org

But limited to single-band Hubbard model

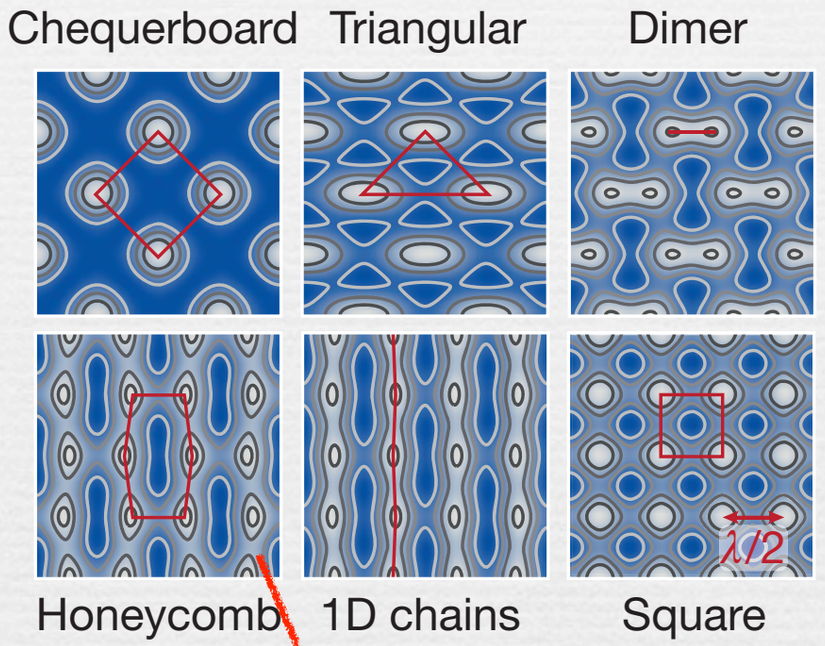
Beyond the Hubbard model

Continuum systems

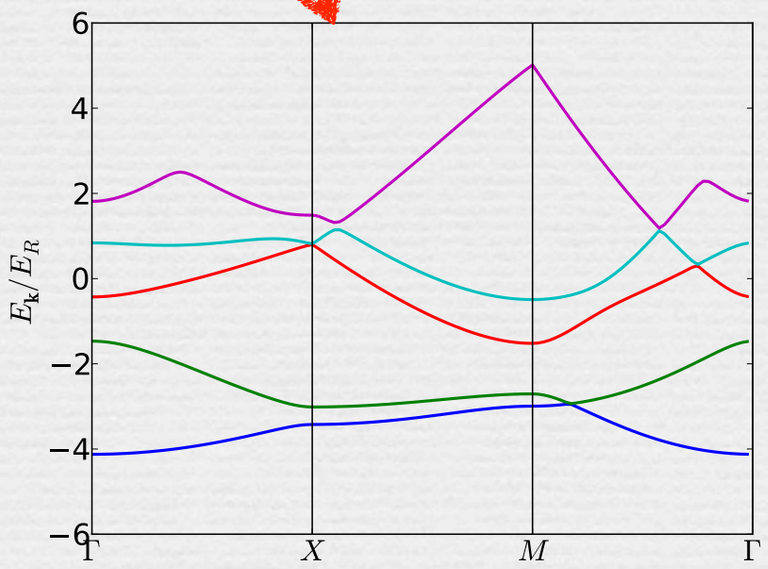


Stoner, 1939, Jo *et al*, Science 2009

Multi-band systems

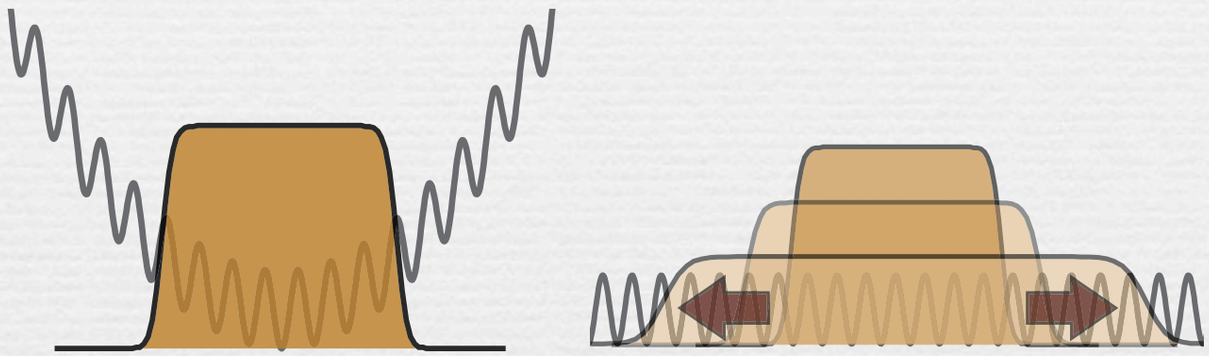


Tarruell *et al*, Nature 2012



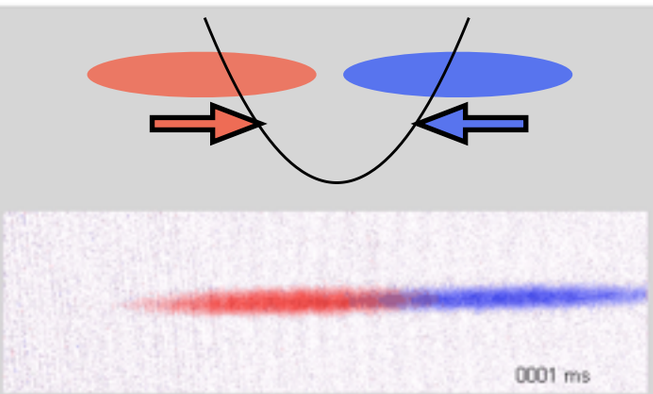
Non-equilibrium dynamics

Expansion in 2D lattice



Schneider *et al*, Nature Physics 2012

Collision of clouds



Sommer *et al*, Nature 2011

Density functional theory

Hohenberg and Kohn 1964

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N) \qquad \rho(\mathbf{r})$$

$$\mathbb{R}^{3N} \mapsto \mathbb{C} \qquad \mathbb{R}^3 \mapsto \mathbb{R}$$

- Hohenberg-Kohn theorem: **All** properties of the system are **completely** determined by the ground state density
- **Exact** ground state density and energy can be obtained by **minimizing** the density functional

$$E[\rho] = F[\rho] + \int d\mathbf{r} V_{\text{ext}}(\mathbf{r})\rho(\mathbf{r})$$

- F is a **universal** functional independent of the external potential

Kohn-Sham approach

Kohn and Sham 1965

$$F[\rho] = K[\rho] + E_{\mathrm{H}}[\rho] + E_{\mathrm{XC}}[\rho]$$

kinetic energy

mean field energy

exchange-correlation energy

$$\frac{\delta E}{\delta \rho} = 0$$

$$\frac{\delta K_{\mathrm{S}}}{\delta \rho} + \frac{\delta E_{\mathrm{H}}[\rho]}{\delta \rho} + \frac{\delta E_{\mathrm{XC}}[\rho]}{\delta \rho} + V_{\mathrm{ext}} = 0$$

$$V_{\mathrm{H}}[\rho] \quad V_{\mathrm{XC}}[\rho]$$

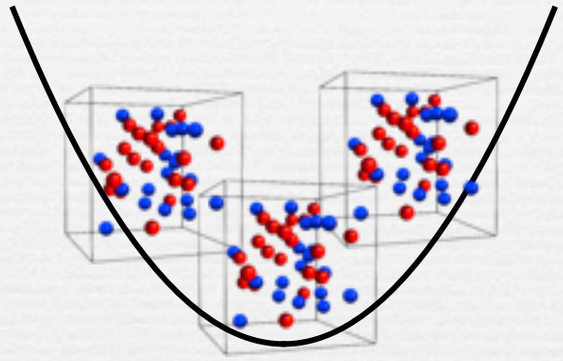
$$\rho = 2\sum_{j=1}^{N/2} |\psi_j|^2$$

$$\left(-\frac{\hbar^2\nabla^2}{2m} + V_{\mathrm{ext}} + V_{\mathrm{H}}[\rho] + V_{\mathrm{XC}}[\rho]\right)\psi_j = \varepsilon_j \psi_j$$

Self-consistently solve single-particle Schrödinger equation
to solve the many-body problem

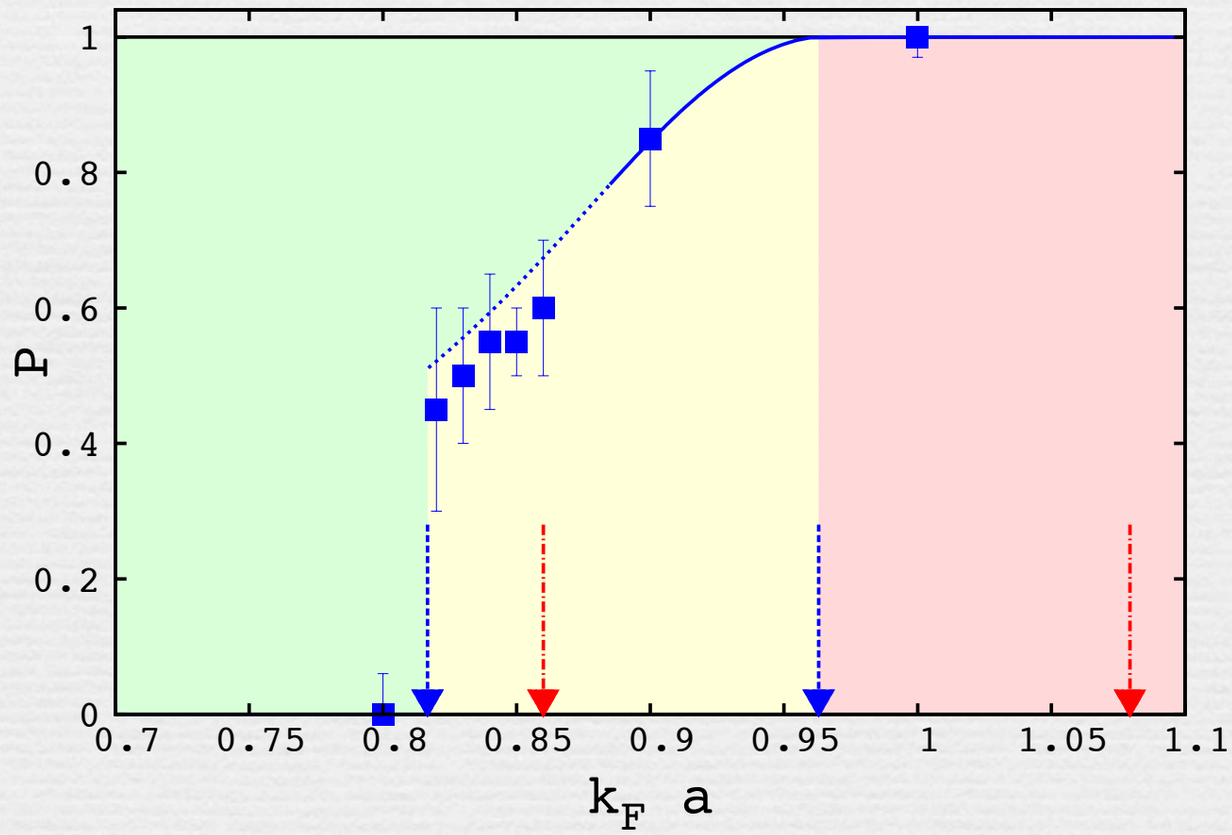
Local density approximation

Use E_{XC} of a uniform system with same local density



Coulomb gas: Ceperley and Alder 1980, Cold atoms: Pilati *et al* 2010

Repulsive fermions show ferromagnetism for high density and large interactions



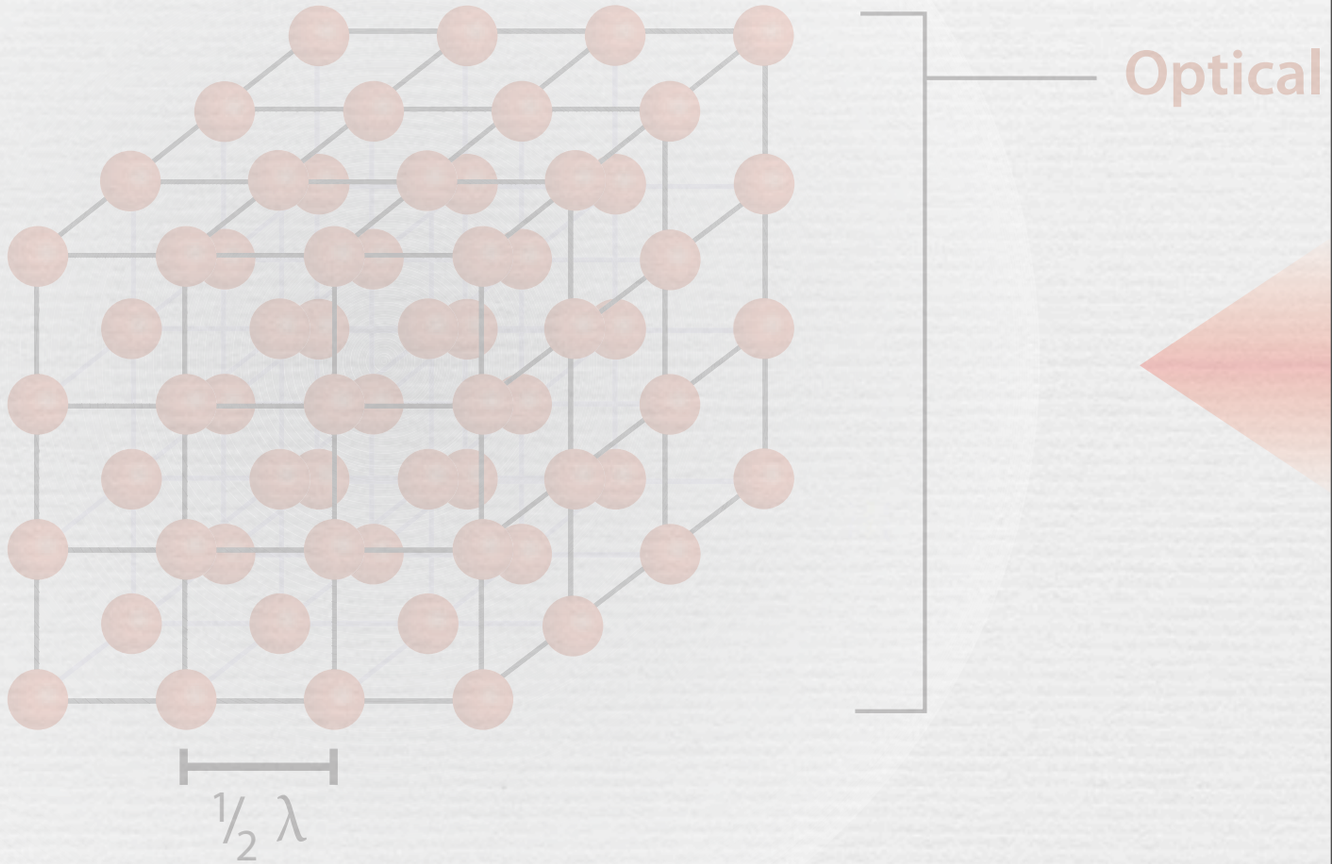
We extract E_{XC} from ground state energy $e_{\rm xc}(k_F a, P) = \frac{3}{5} E_F (1 + \ldots)$

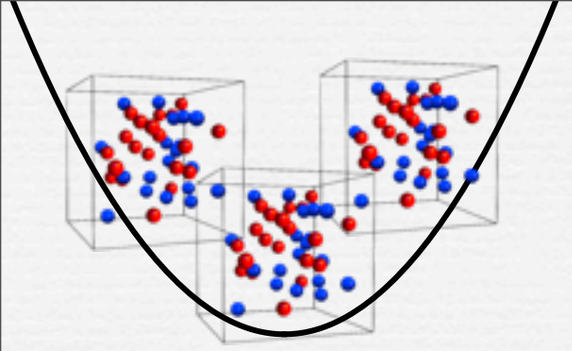
20 most cited papers in APS journals

http://mml.materials.ox.ac.uk/Main/Top10

c	Publication	# cites	Title	Author(s)
1	PHYSICAL REVIEW B, 37 (2): 785-789 *(JAN 15 1988)*	30198	Development of the Colle-Salvetti Correlation-Energy Formula into a Functional of the Electron-Density	Lee, CT; Yang, WT; Parr, RG
2	PHYSICAL REVIEW A, 38 (6): 3098-3100 *(SEP 15 1988)*	18610	Density-Functional Exchange-Energy Approximation with Correct Asymptotic-Behavior	Becke, AD
3	PHYSICAL REVIEW, 140 (4A): 1133-1138 *(1965)*	17196	Self-Consistent Equations Including Exchange and Correlation Effects	Kohn, W; Sham, LJ
4	PHYSICAL REVIEW LETTERS, 77 (18): 3865-3868	15663	Generalized Gradient Approximation Made Simple	Perdew, JP; Burke, K; Ernzerhof, M
5	PHYSICAL REVIEW B, 13 (12): 5188-5192 *(1976)*	9063	Special Points for Brillouin-Zone Integrations	Monkhorst HJ; Pack JD
6	PHYSICAL REVIEW B, 54 (16): 11169-11186 *(OCT 15 1996)*	8652	Efficient Iterative Schemes for Ab Initio Total-Energy Calculations Using a Plane-Wave Basis Set	Kresse, G; Furthmuller, J
7	PHYSICAL REVIEW B, 45 (23): 13244-13249 *(JUN 15*	8421	Accurate and Simple Analytic Representation of the Electron-Gas Correlation-Energy	Perdew, JP; Wang, Y
8	PHYSICAL REVIEW B, 23 (10): 5048-5079 *(1981)*	8307	Self-Interaction Correction to Density-Functional Approximations for Many-Electron Systems	Perdew, JP; Zunger, A
9	PHYSICAL REVIEW, 46 (7): 0618-0622 *(OCT 1934)*	8272	Note on an Approximation Treatment for Many-Electron Systems	Moller, C; Plesset, MS
10	PHYSICAL REVIEW B, 33 (12): 8822-8824 Part 2 *(JUN 15*	8013	Density-Functional Approximation for the Correlation-Energy of the Inhomogeneous Electron-Gas	Perdew, JP
11	PHYSICAL REVIEW B, 46 (11): 6671-6687 *(SEP 15 1992)*	7819	Atoms, Molecules, Solids, and Surfaces-Applications of the Generalized Gradient Approximation for Exchange and Correlation	Perdew, JP; Chevary, JA; Vosko, SH; Jackson, KA; Pederson, MR; Singh, DJ;
12	PHYSICAL REVIEW B, 41 (11): 7892-7895 *(APR 15 1990)*	7768	Soft Self-Consistent Pseudopotentials in a Generalized Eigenvalue Formalism	Vanderbilt, D
13	PHYSICAL REVIEW B, 136 (3B): B864-871 *(1964)*	7594	Inhomogeneous Electron Gas	Hohenberg, P; Kohn, W
14	PHYSICAL REVIEW LETTERS, 45 (7): 566-569	6645	Ground-State of the Electron-Gas by a Stochastic Method	Ceperley, DM; Alder, BJ
15	PHYSICAL REVIEW LETTERS, 56 (9): 930-933	6517	Atomic Force Microscope	Binnig, G; Quate, CF; Gerber, C
16	PHYSICAL REVIEW LETTERS, 58 (20): 2059-2062	6457	Inhibited Spontaneous Emission in Solid-State Physics and Electronics	Yablonovitch, E
17	PHYSICAL REVIEW B, 43 (3): 1993-2006 *(JAN 15 1991)*	5887	Efficient Pseudopotentials for Plane-Wave Calculations	Troullier, N; Martins, JL
18	PHYSICAL REVIEW B, 59 (3): 1758-1775 *(JAN 15 1999)*	5868	From Ultrasoft Pseudopotentials to the Projector Augmented-Wave Method	Kresse, G; Joubert, D
19	PHYSICAL REVIEW, 124 (6): 1866-1878 *(1961)*	5816	Effects of Configuration Interaction on Intensities and Phase Shifts	Fano, U
20	PHYSICAL REVIEW, 108 (5): 1175-1204 *(1957)*	5760	Theory of Superconductivity	Bardeen, J; Cooper, LN; Schrieffer, JR

Magnetism in harmonic trap and shallow optical lattice



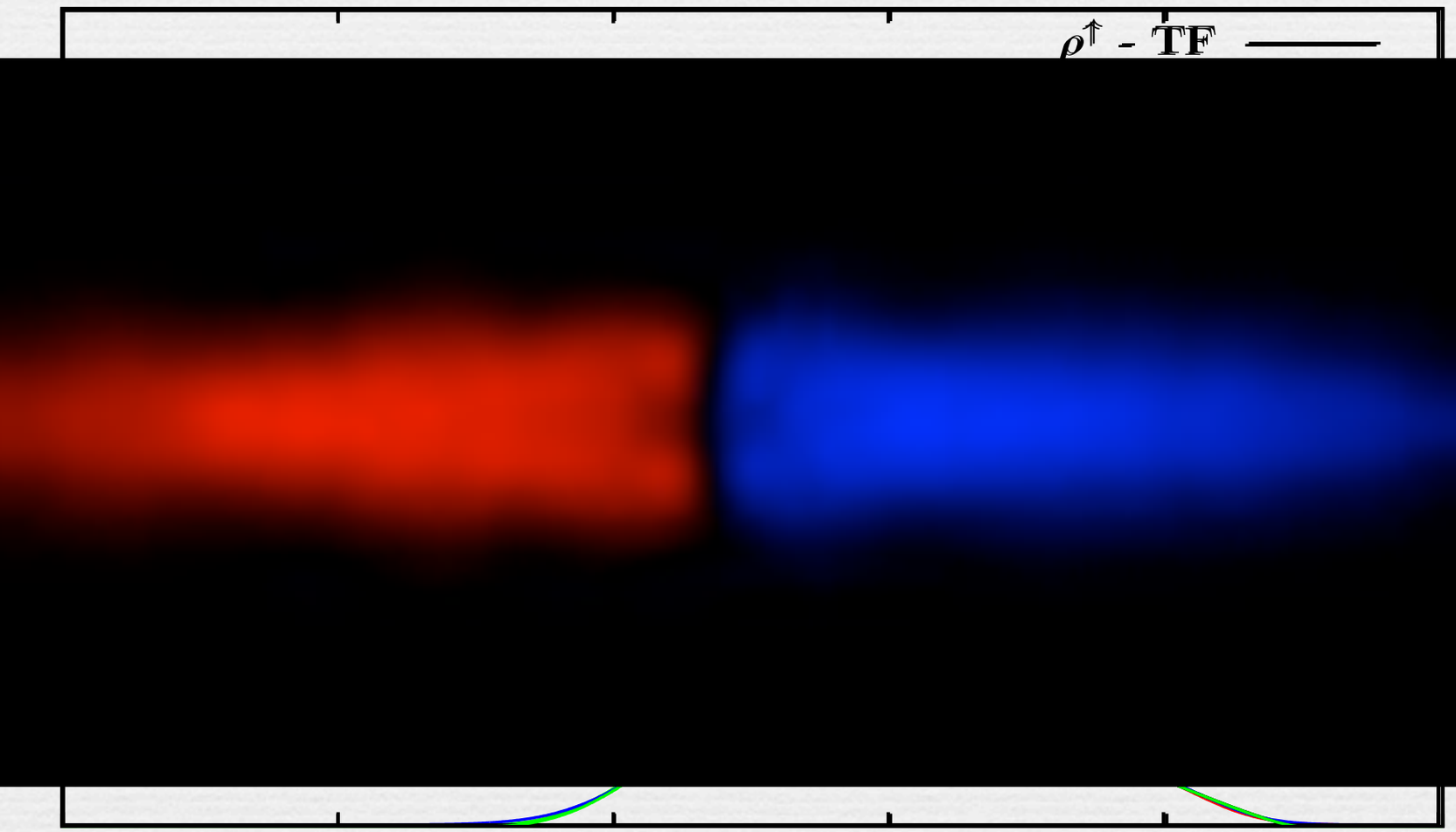


Ferromagnetism in a trap

$$E^{\mathrm{KS}}[\rho] = T[\rho] + \int V_{\mathrm{ext}}(\mathbf{r})\,\rho(\mathbf{r})\,d\mathbf{r} + E_{\mathrm{H}}[\rho] + E_{\mathrm{xc}}[\rho]$$

$$E^{\mathrm{TFA}}[\rho] = T_{\mathrm{unif}}[\rho] + \int V_{\mathrm{ext}}(\mathbf{r})\,\rho(\mathbf{r})\,d\mathbf{r} + E_{\mathrm{H}}[\rho] + \int e_{\mathrm{xc}}^{\mathrm{unif}}(\rho(\mathbf{r}))\,\rho(\mathbf{r})\,d\mathbf{r}$$

Radial density

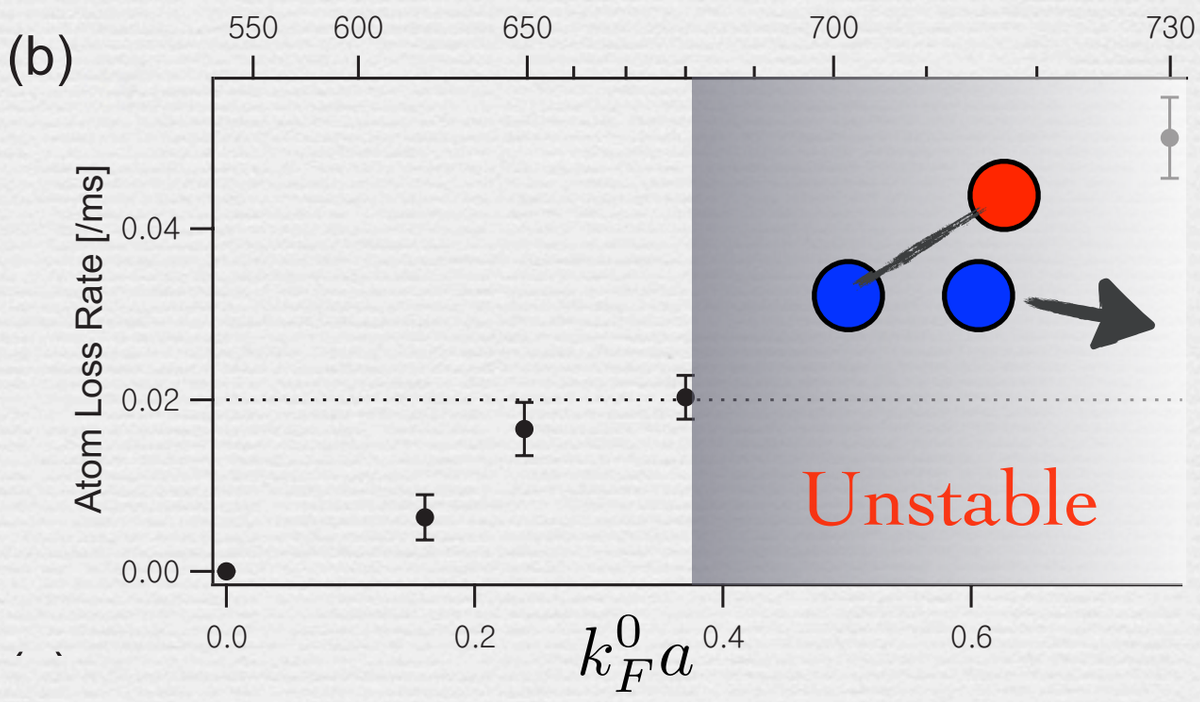


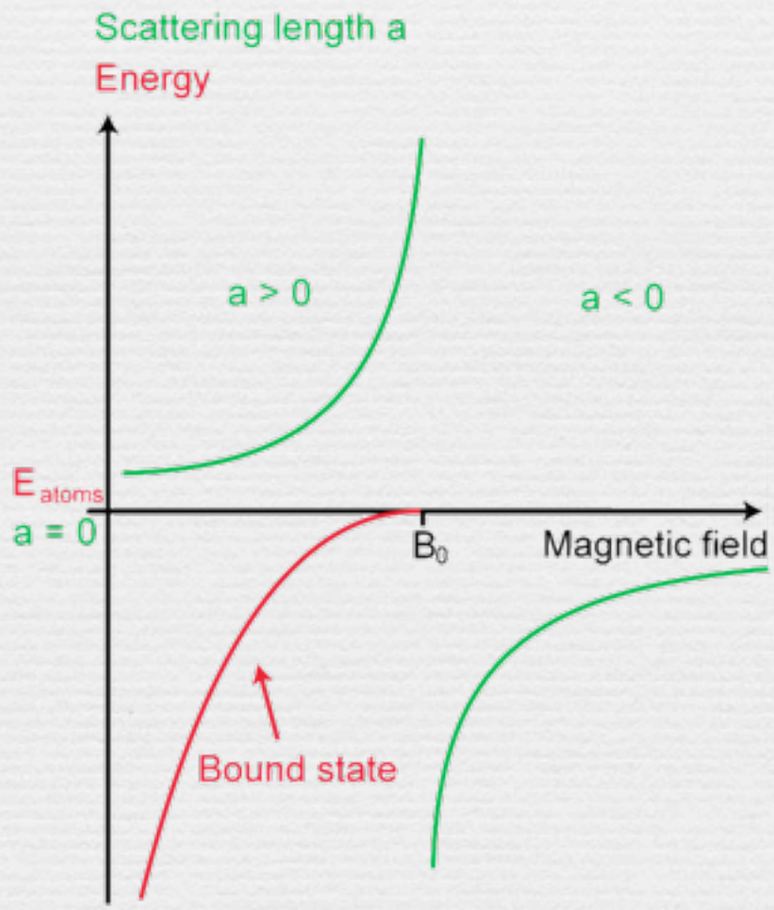
Zintchenko 2011

Ferromagnetism in the lab?

- 2009: Indirect evidences for itinerant ferromagnetism Jo *et al*, Science 2009
- 2012: Pair formation in repulsive Fermi gas Sanner *et al*, PRL, Lee *et al*, PRA

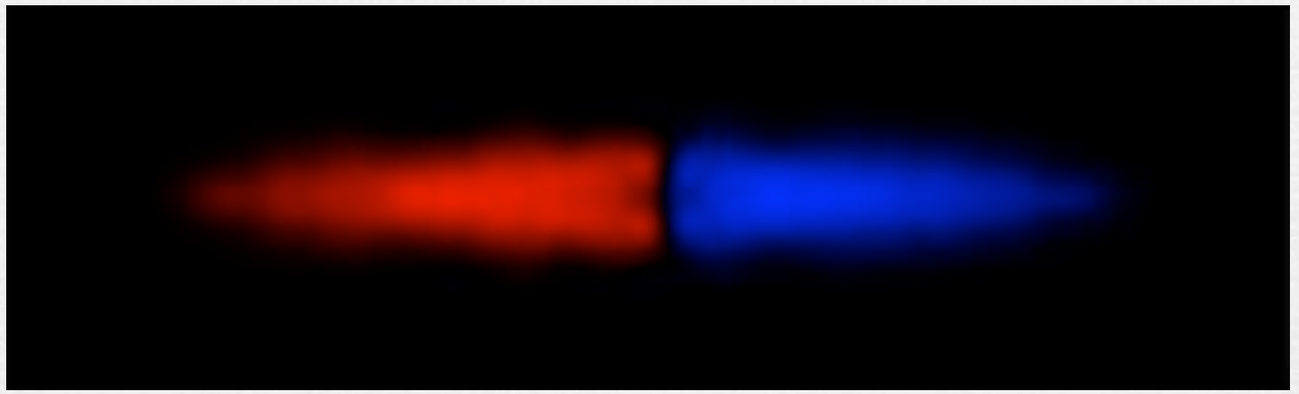
Our conclusion is that an ultracold gas with strong short range repulsive interactions near a Feshbach resonance remains in the paramagnetic phase. The fast formation of molecules and the accompanying heating makes it impossible to study such a gas in equilibrium, confirming predictions of a rapid conversion of the atomic gas to pairs



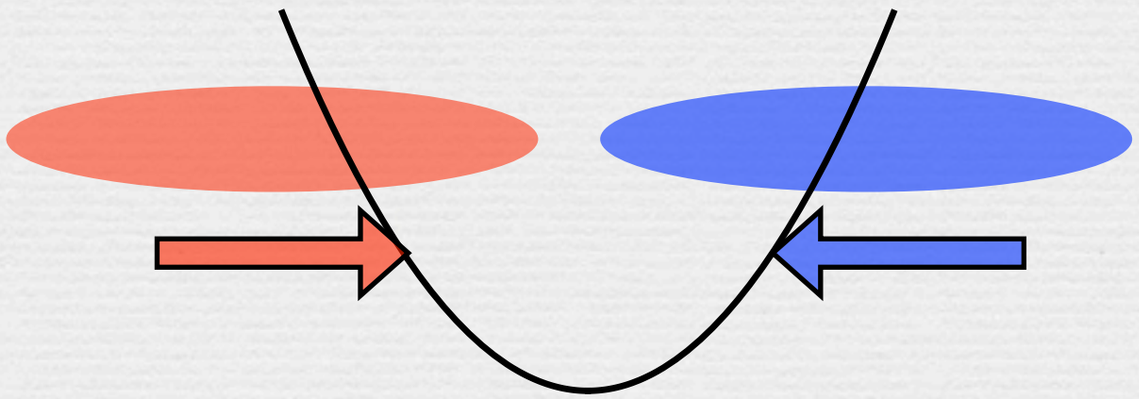


Prepare clouds separately

- Start with **mixtures**: Redistribution time >> Local loss time



- Start with **separated** clouds



Sommer *et al.*, Nature 2011

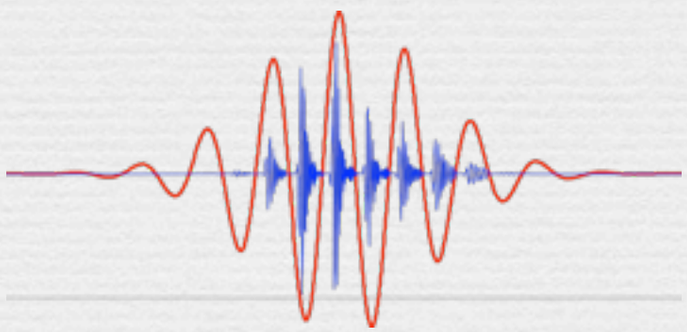
Time-dependent DFT

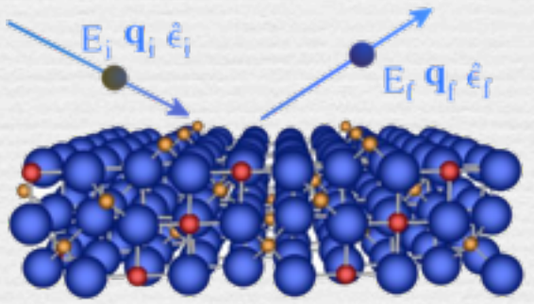
Runge and Gross, 1984

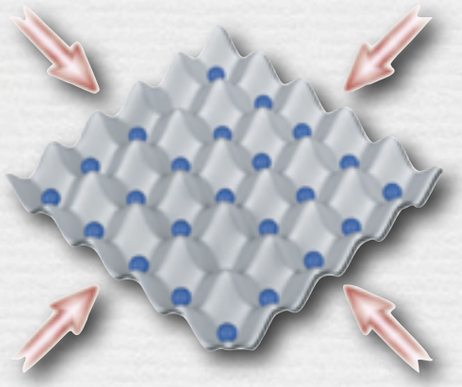
- Time-dependent density obtained from

$$i\frac{\partial}{\partial t}\psi_j(\mathbf{r},t) = \left[-\frac{\hbar^2\nabla^2}{2m} + V_{\text{ext}}(\mathbf{r},t) + V_{\text{H}}(\mathbf{r},t) + V_{\text{xc}}[\rho(\mathbf{r}',t')](\mathbf{r},t)\right]\psi_j(\mathbf{r},t)$$

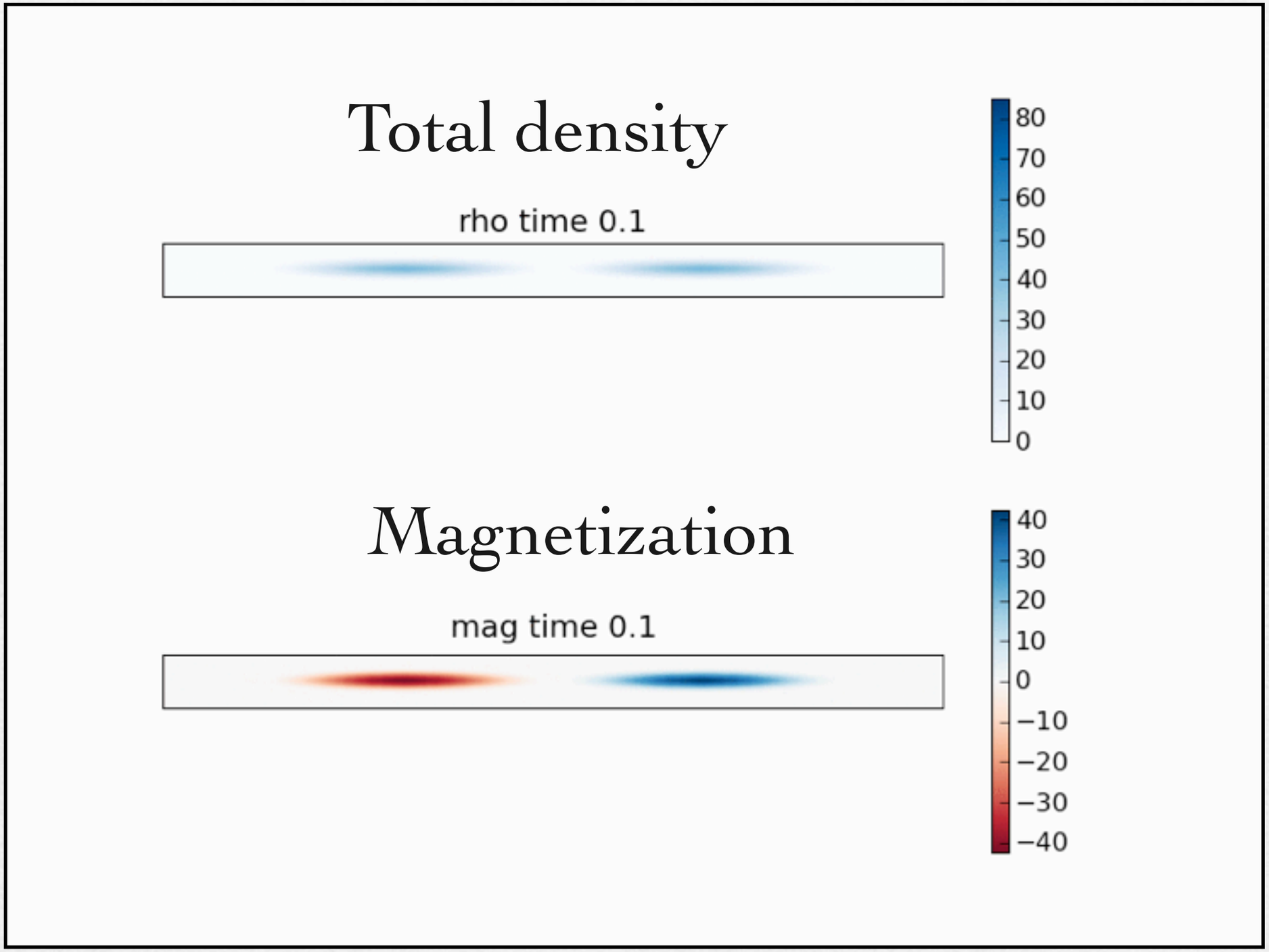
- We use the adiabatic local-density approximation







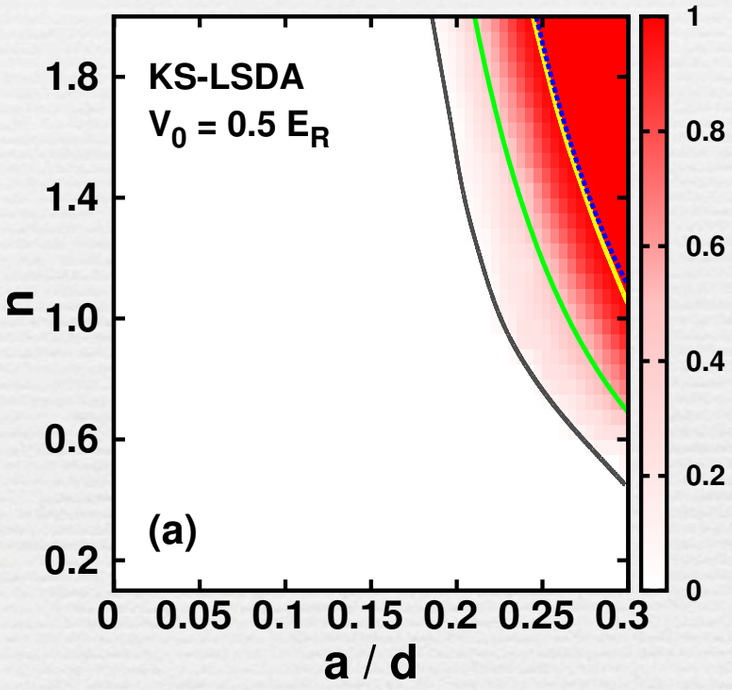
Simulation of collision

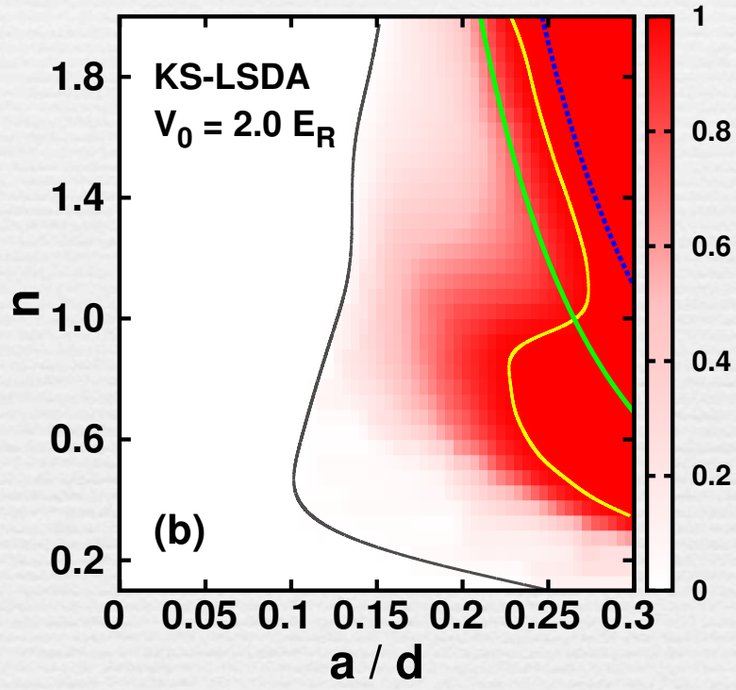


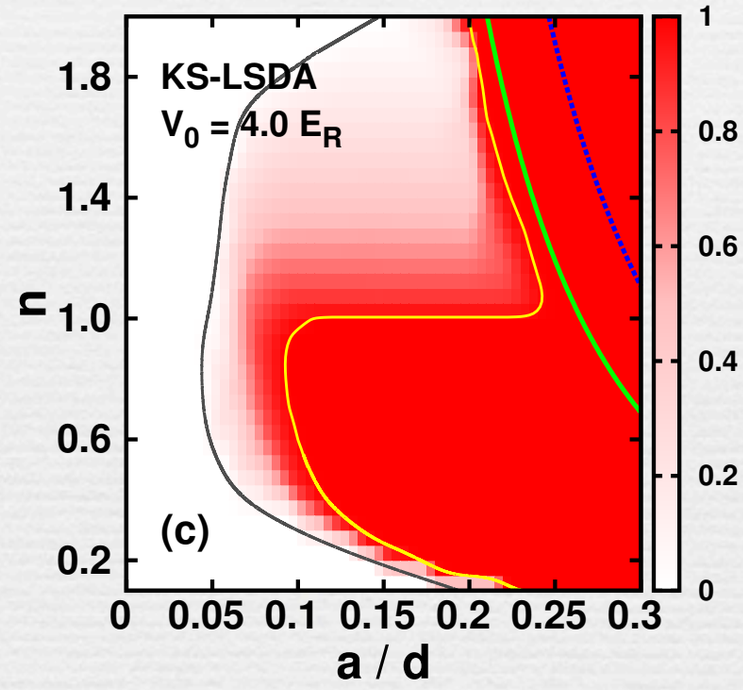
Ferromagnetism in shallow optical lattices

Ma, Pilati, Troyer and Dai, Nature Physics, 2012

$$V_{\mathrm{OL}}(\mathbf{r}) = V_0 \left[\sin^2(\frac{\pi}{d}x) + \sin^2(\frac{\pi}{d}y) + \sin^2(\frac{\pi}{d}z)\right]$$







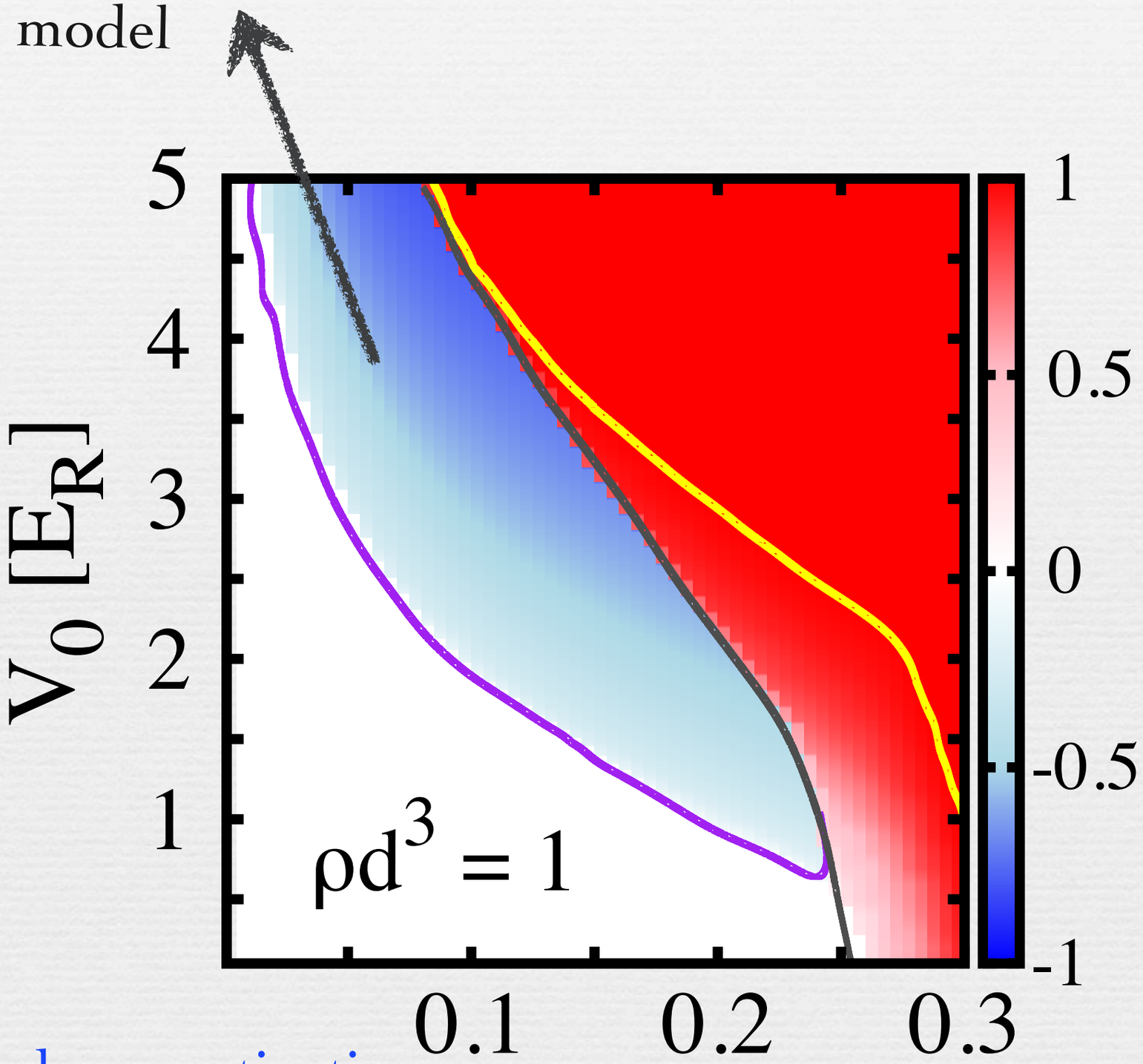
Green and Blue: partially and fully polarized in free-space

Black and Yellow: partially and fully polarized with optical lattice

Half-filled system

Ma, Pilati, Troyer and Dai, Nature Physics, 2012

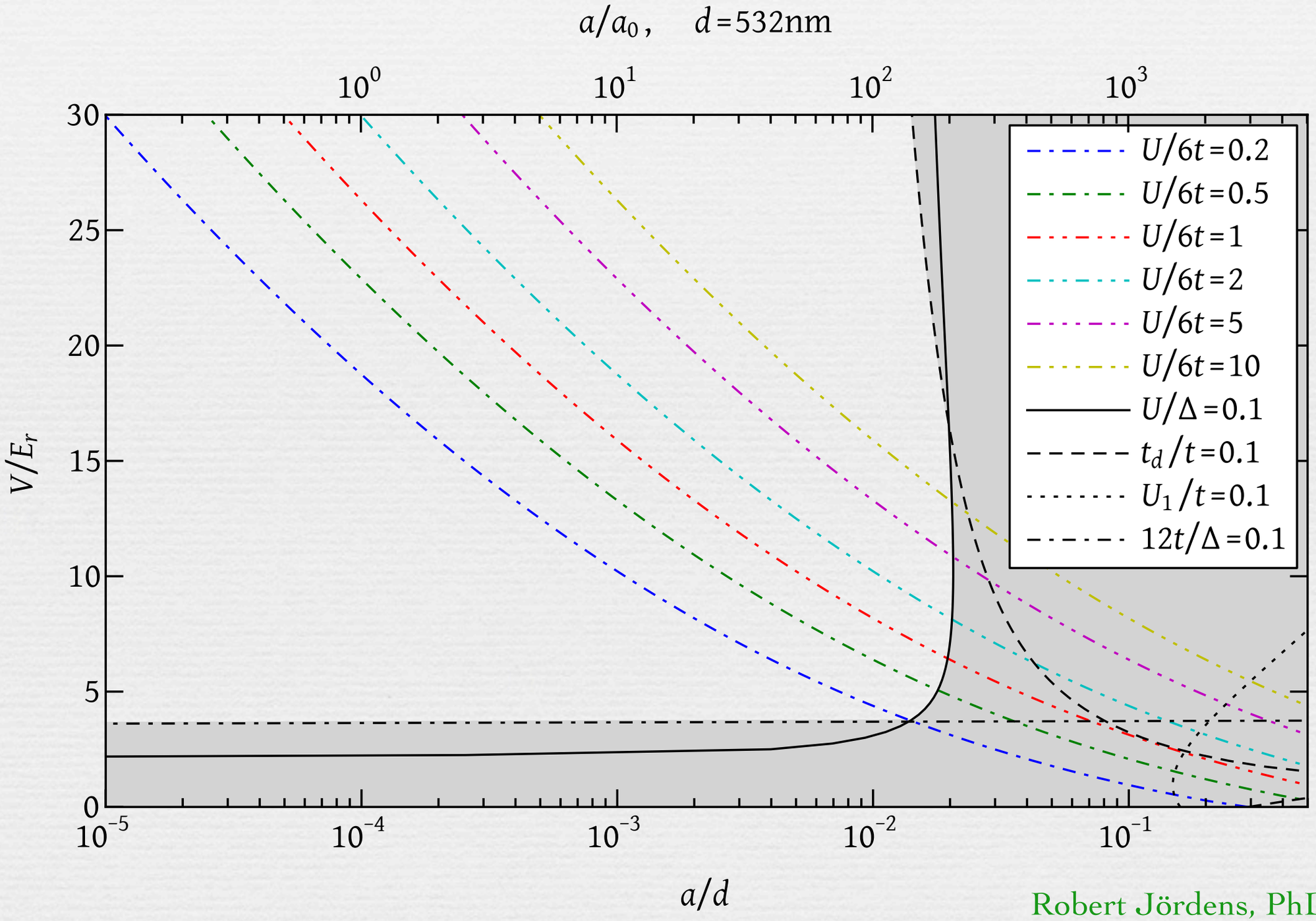
Hubbard model



Blue: staggered magnetization

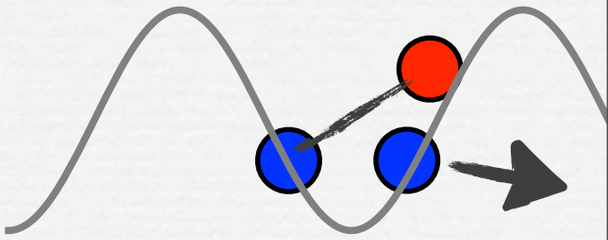
Red: uniform magnetization

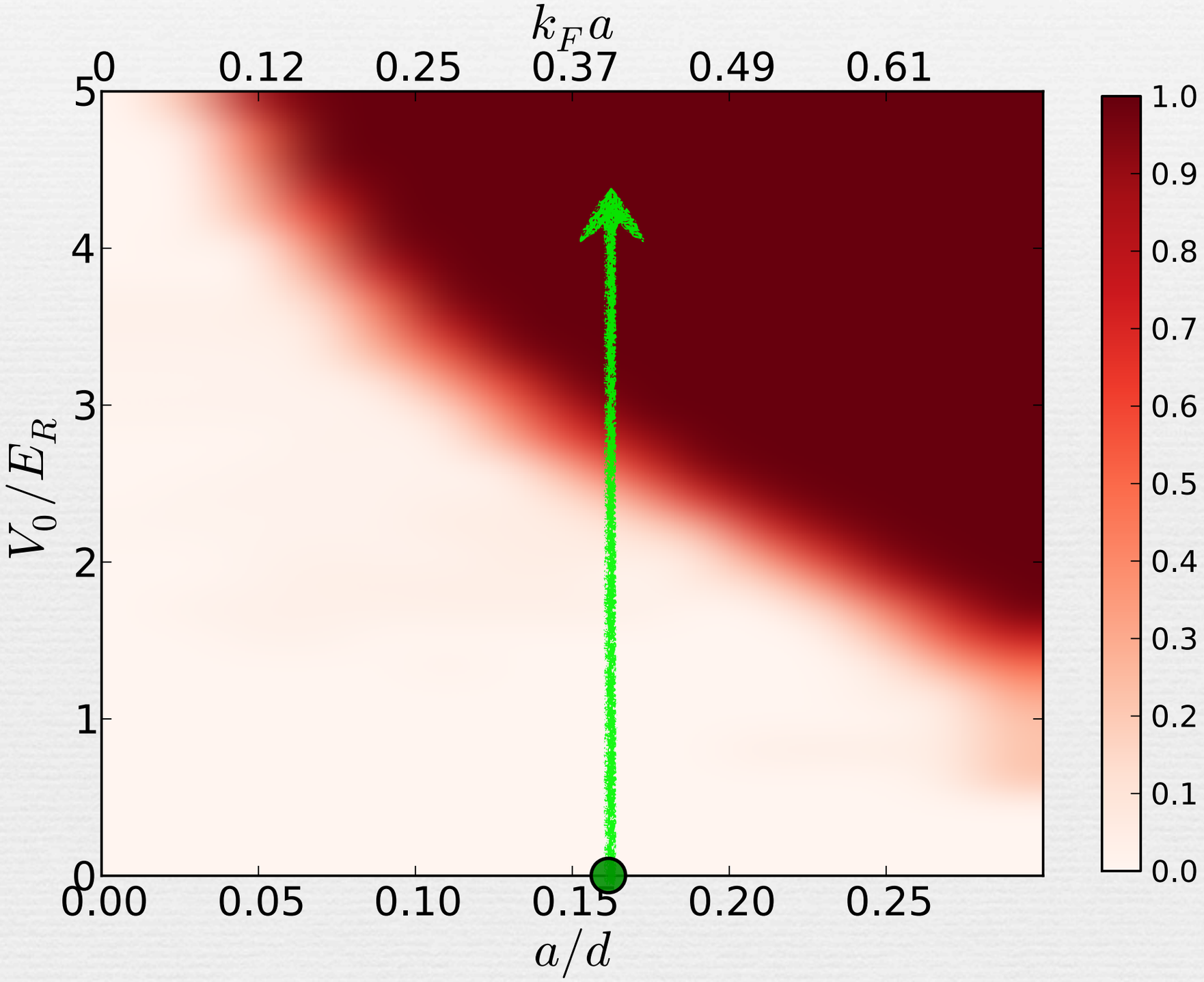
Validity of single-band Hubbard model



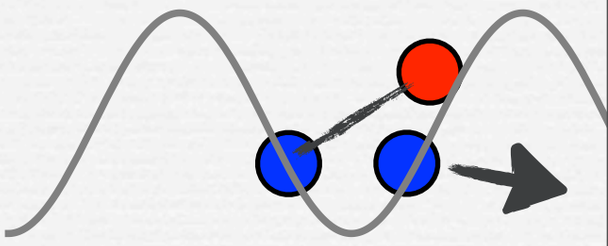
Robert Jördens, PhD thesis, 2010

Can a lattice help ?

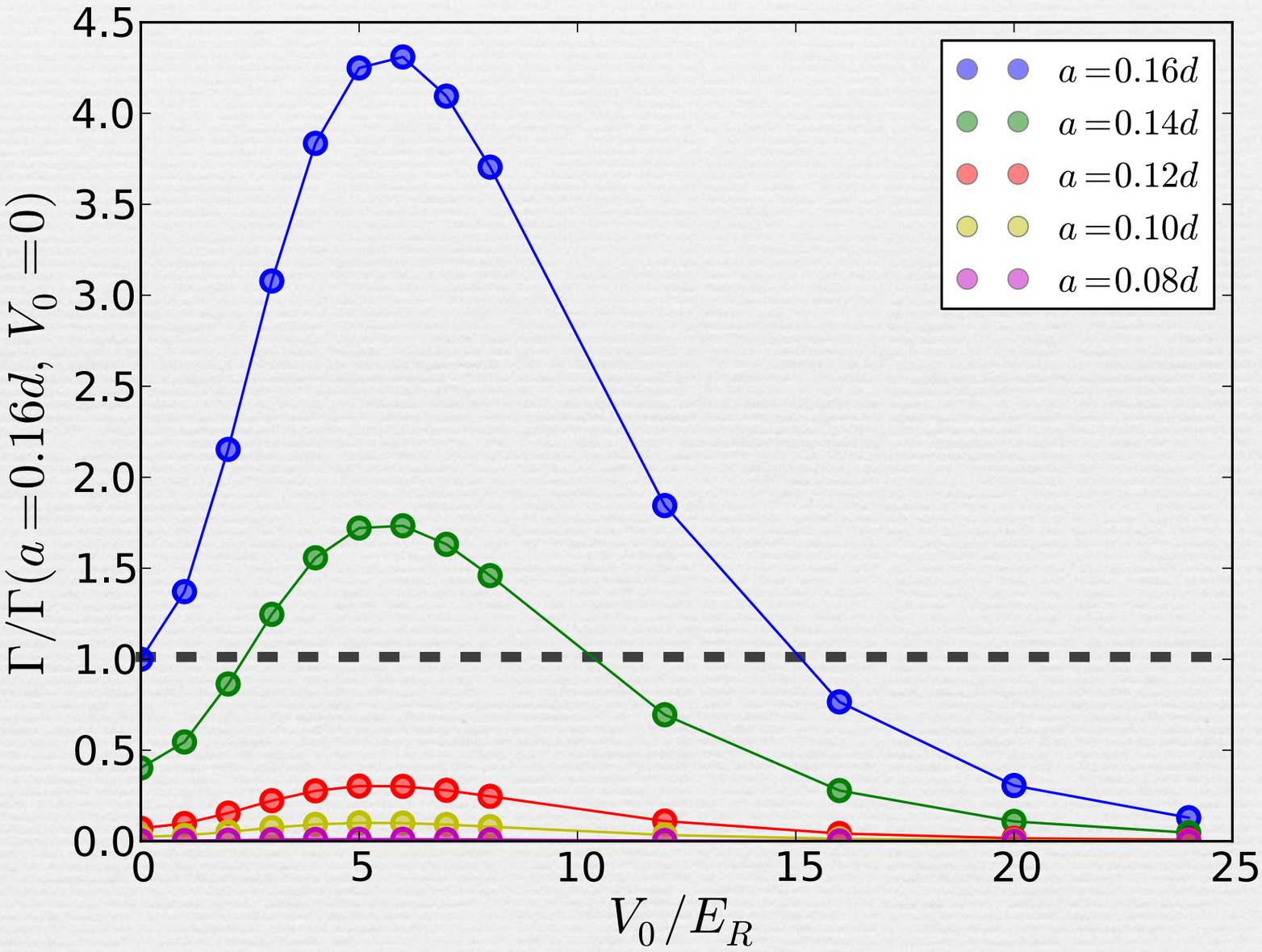




3-body loss rate

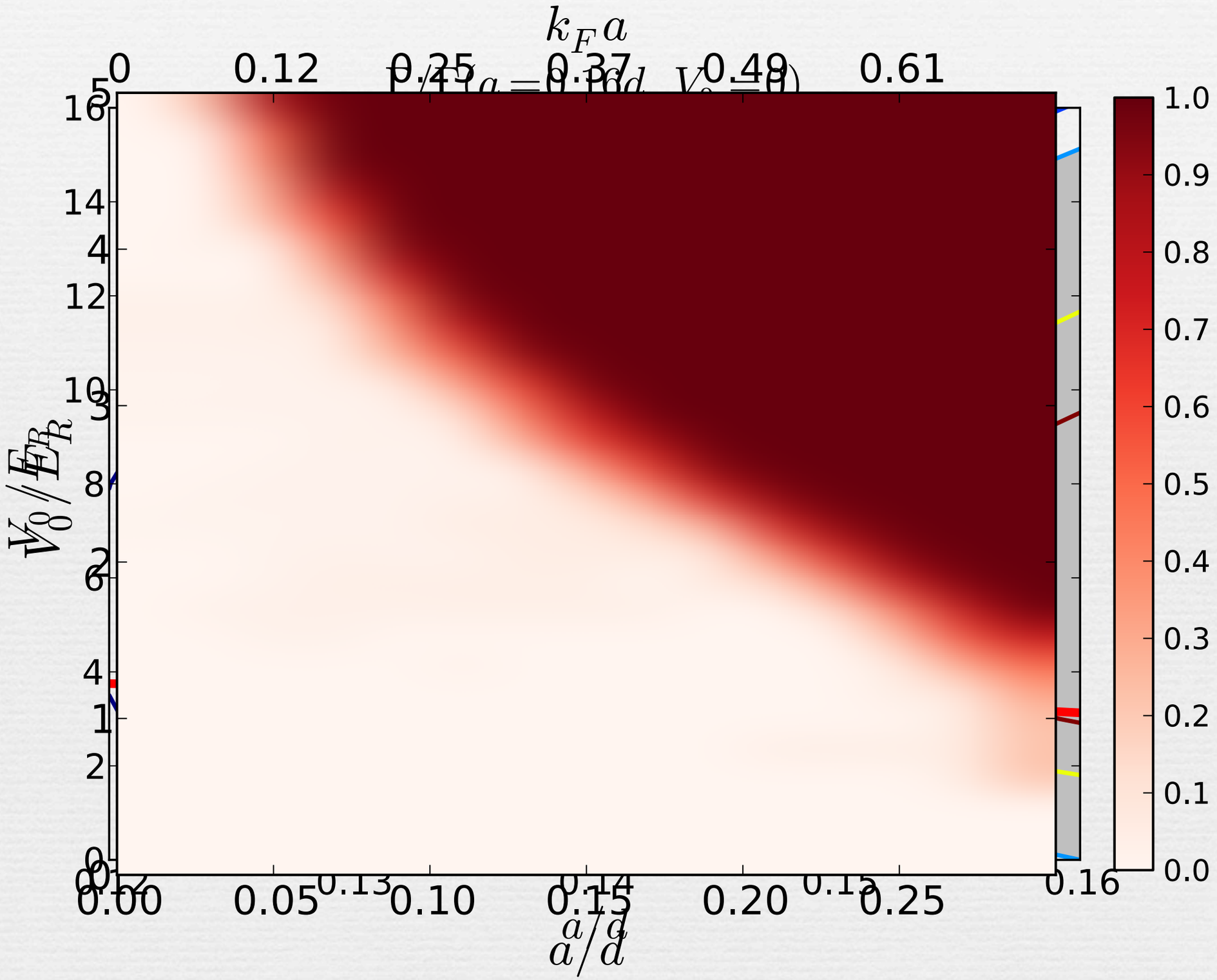


$$\Gamma = a^3 \sum_{\sigma} \int_{\Omega} d\mathbf{r} \int_{|\mathbf{r}'-\mathbf{r}|<a} d\mathbf{r}' \varepsilon_F(\mathbf{r}) n_{\bar{\sigma}}(\mathbf{r}) g_{\sigma\sigma}(\mathbf{r},\mathbf{r}')$$



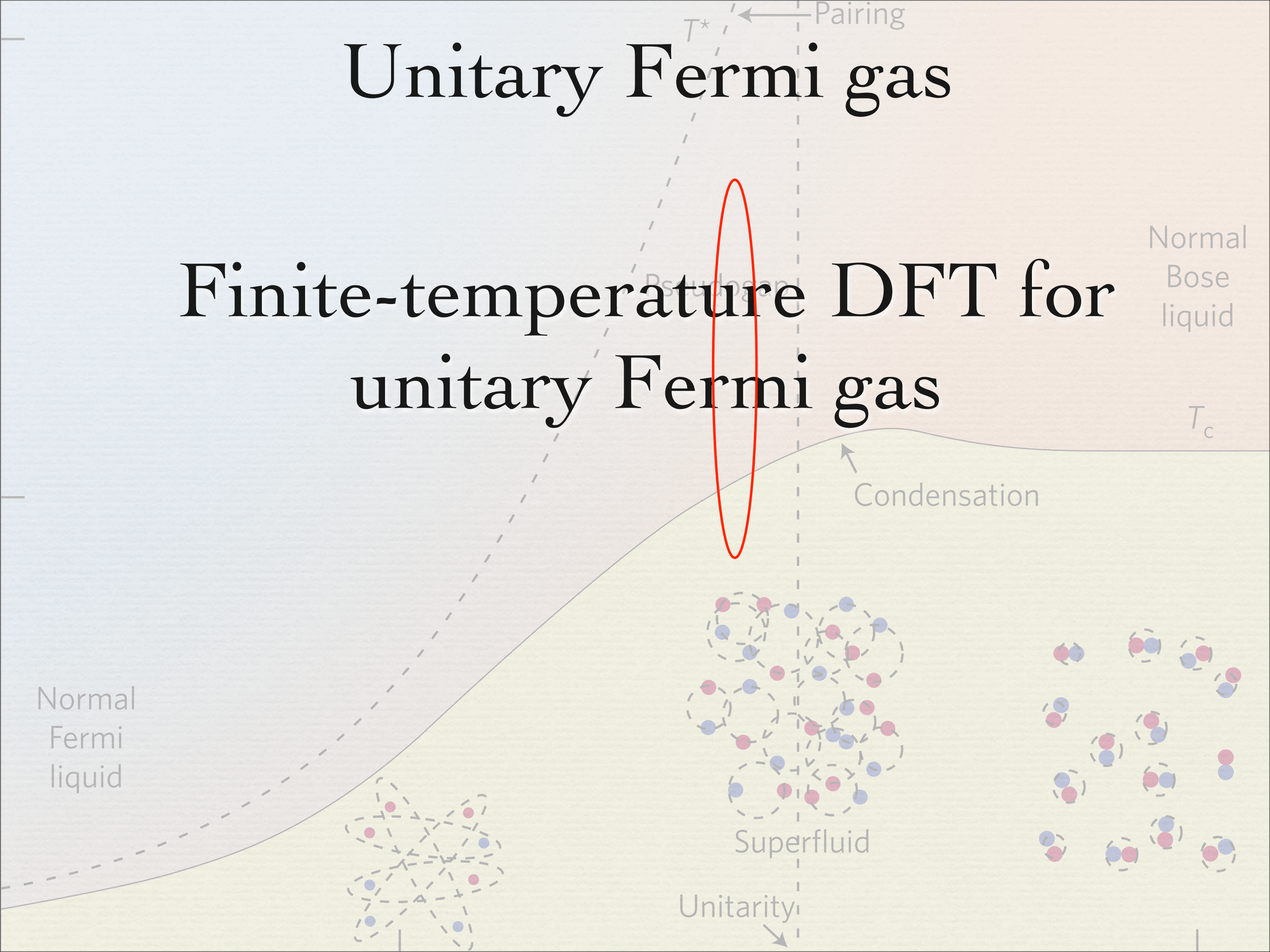
Still more favorable than increasing the scattering length in free space

Contour plot of Gamma

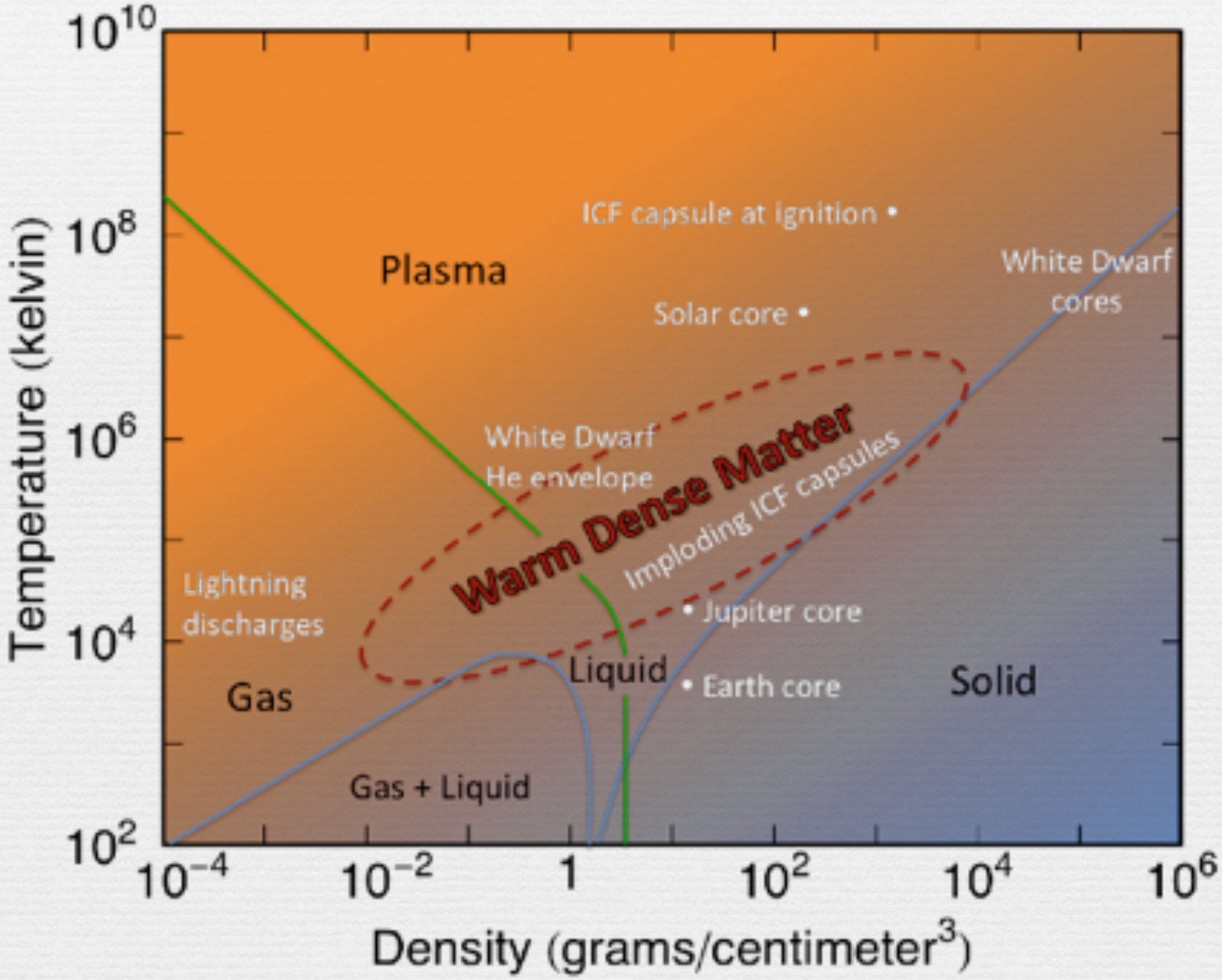


Unitary Fermi gas

Finite-temperature DFT for unitary Fermi gas



Finite-Temperature DFT Applications



Finite-Temperature DFT Formalism

Mermin 1965

Kohn and Sham 1965

$$\Omega^T[\rho] = K^T[\rho] + \boxed{F^T_{\mathrm{HXC}}[\rho]} + \int \mathrm{d}\mathbf{r}(V_{\mathrm{ext}}(\mathbf{r}) - \mu)\rho(\mathbf{r})$$

$$\left(-\frac{\hbar^2\nabla^2}{2m} + V_{\mathrm{ext}} + \boxed{V^T_{\mathrm{HXC}}[\rho]}\right)\psi_j = \varepsilon_j\psi_j \qquad \rho = 2\sum_j \frac{|\psi_j|^2}{e^{(\varepsilon_j-\mu)/k_BT}+1}$$

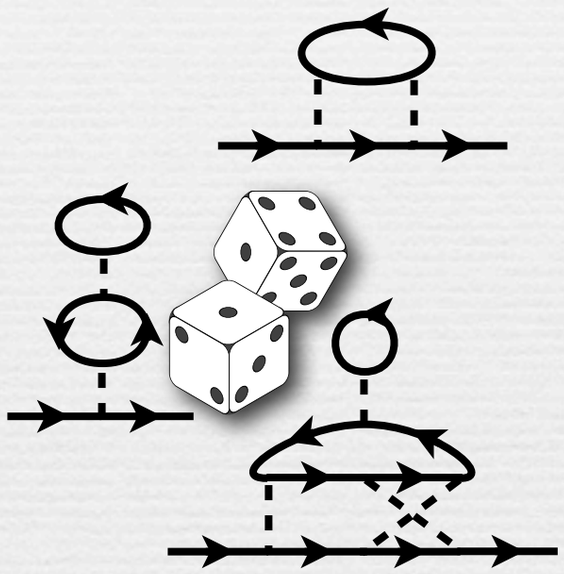
Approx. 1 $\quad \boxed{V^T_{\mathrm{HXC}}} = \dfrac{\delta F^T_{\mathrm{HXC}}[\rho]}{\delta\rho} \approx \mu^T(\rho) - \mu^T_0(\rho)$

Approx. 2 $\quad \boxed{V^T_{\mathrm{HXC}}} \approx V^{T=0}_{\mathrm{HXC}}$

Feynman diagrams vs Feynman emulator

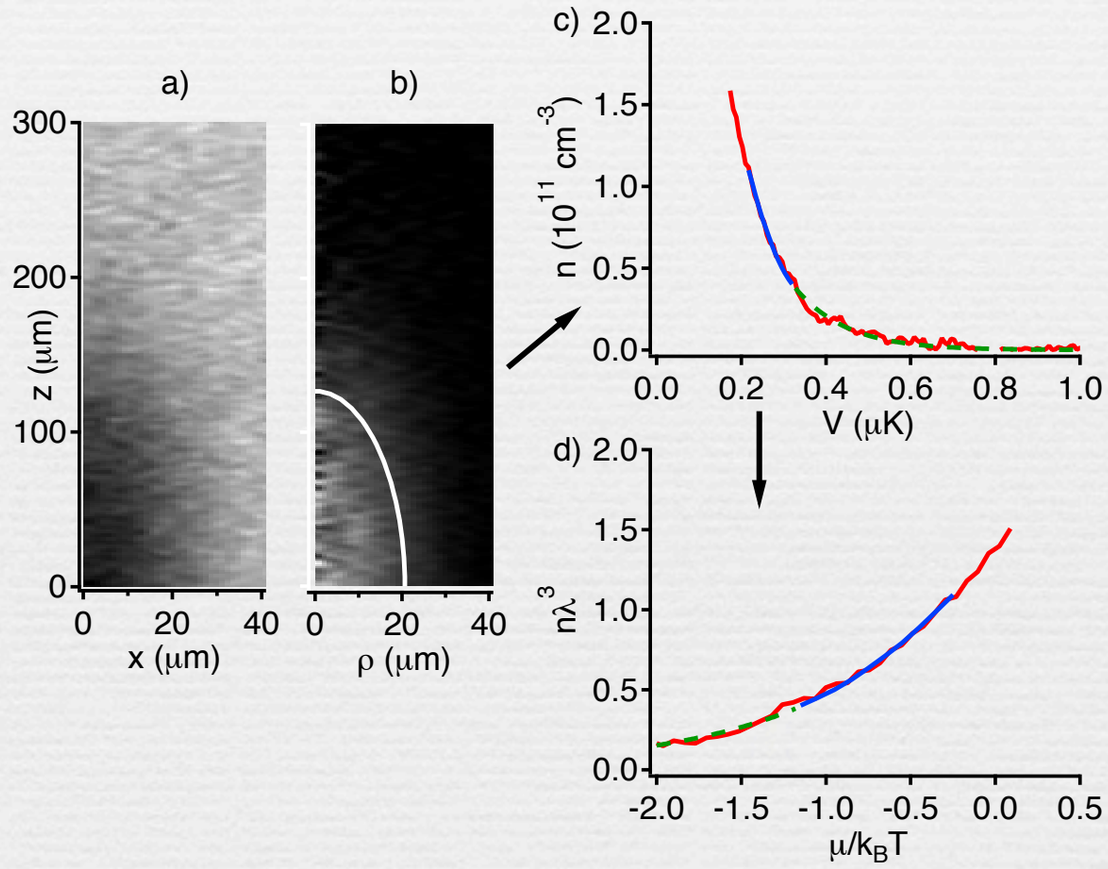
Bold Diagrammatic Monte Carlo

Van Houcke *et al*, Nature Physics, 2012



MIT Experiment

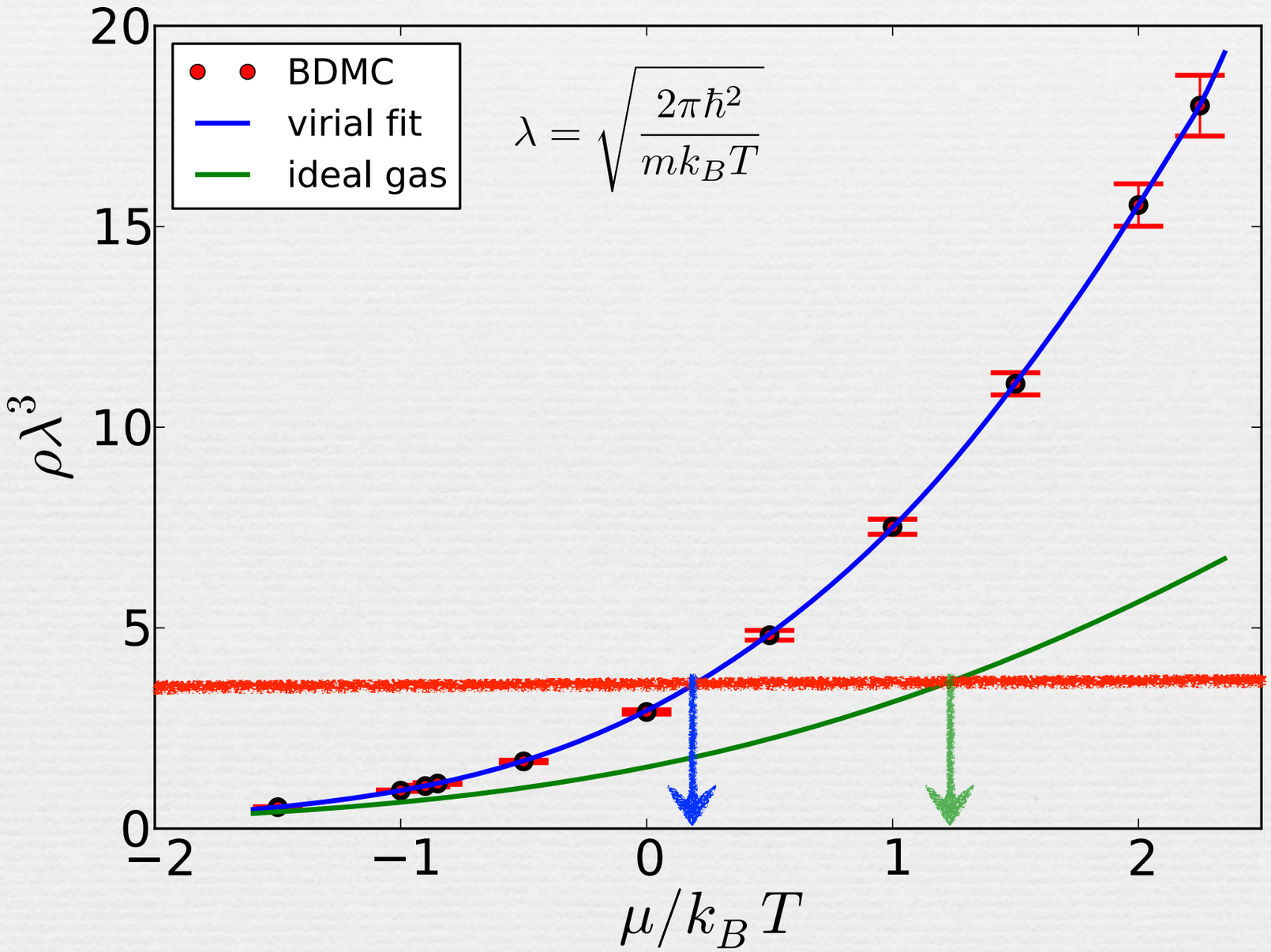
Ku *et al*, Science, 2012



Unprecedented agreement between experiment and theory for strong interacting Fermions!

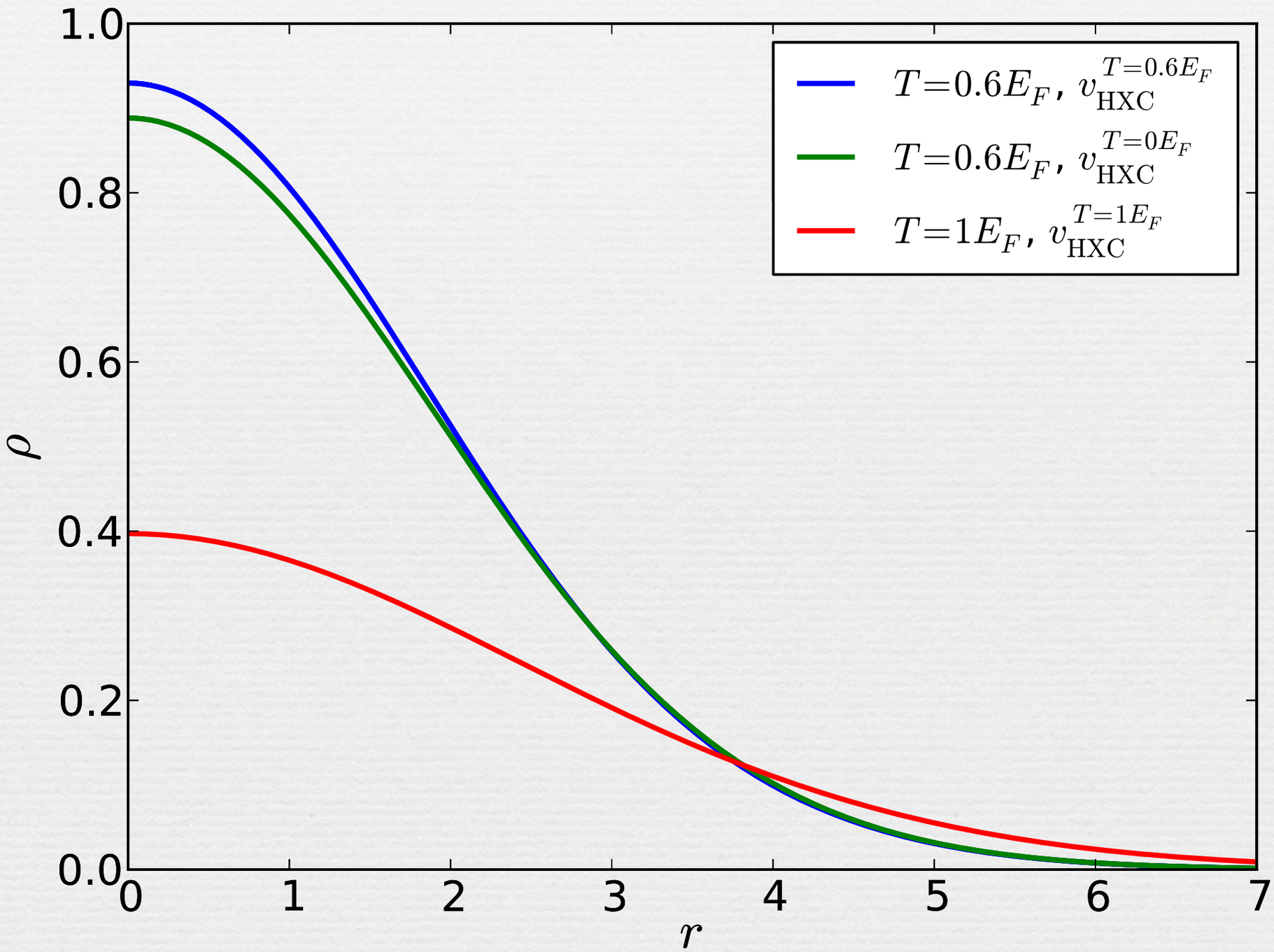
V_{HXC} for unitary Fermi gas

Fit Bold Diagrammatic Monte Carlo EOS and get V_{HXC}

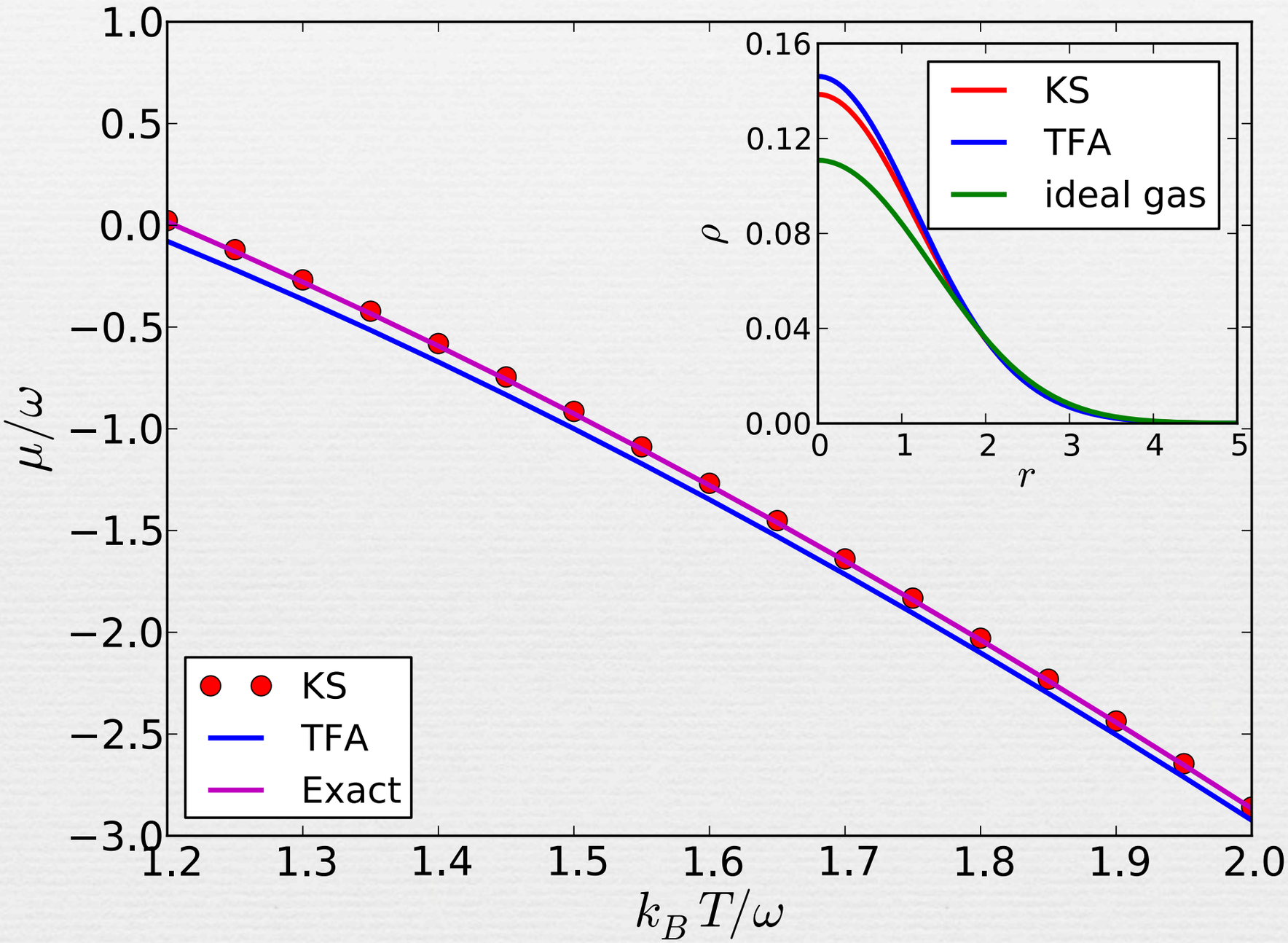


$$V^T_{\mathrm{HXC}} = \mu^T(\rho) - \mu^T_0(\rho)$$

Temperature dependence of v_{HXC}



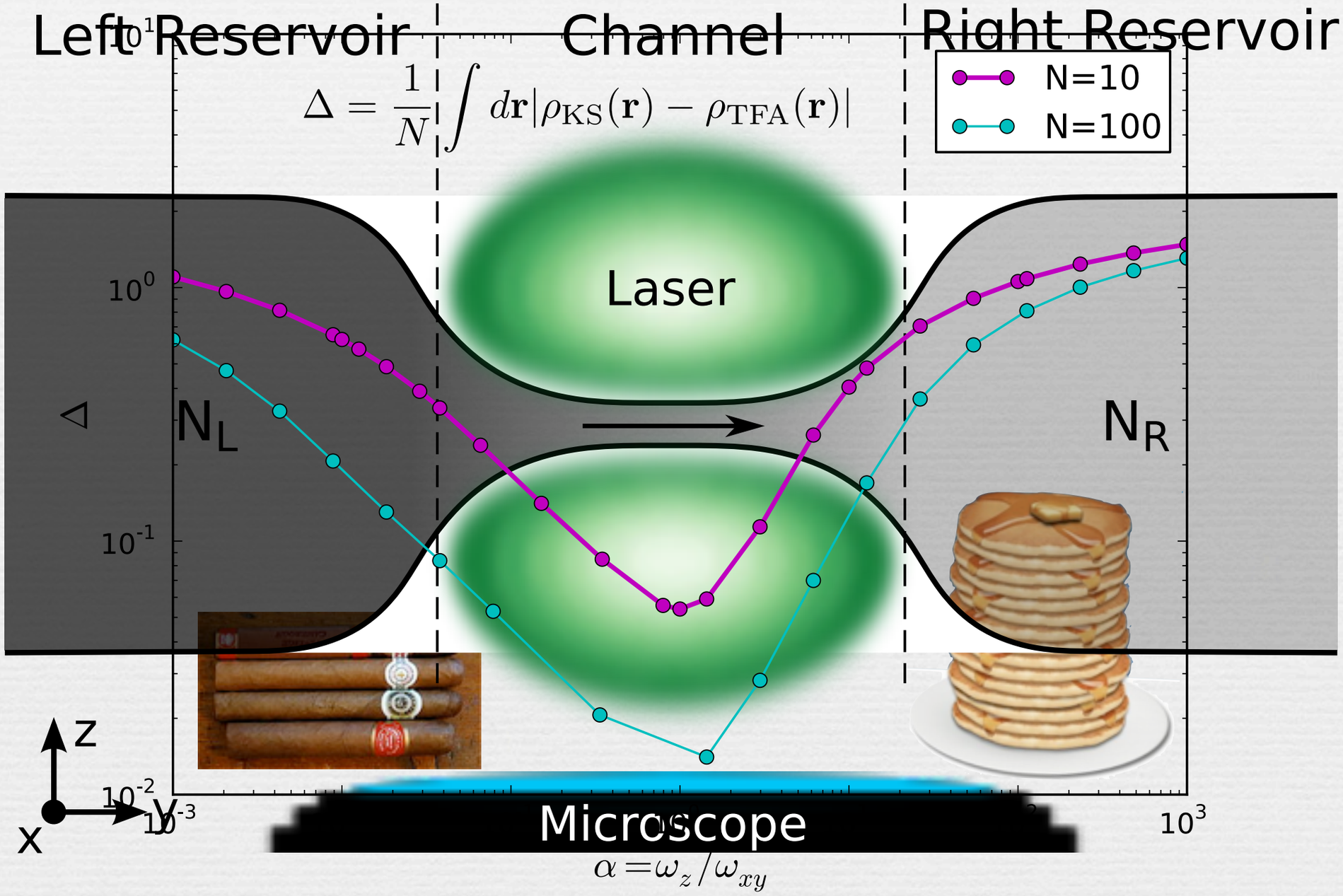
Benchmark: 4 atoms in a trap



$$N = \frac{2e^{-3\omega/2k_BT}}{(1-e^{-\omega/k_BT})^3}(z + 2b_2^\omega z^2 + 3b_3^\omega z^3 + ...) \qquad z = e^{\mu/k_BT}$$

KS vs TFA

Advantage of KS is more pronounced for constrained systems

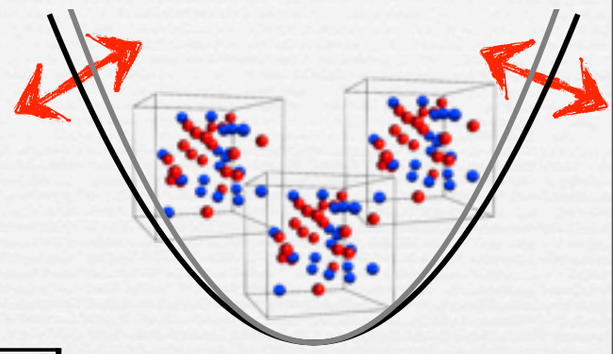


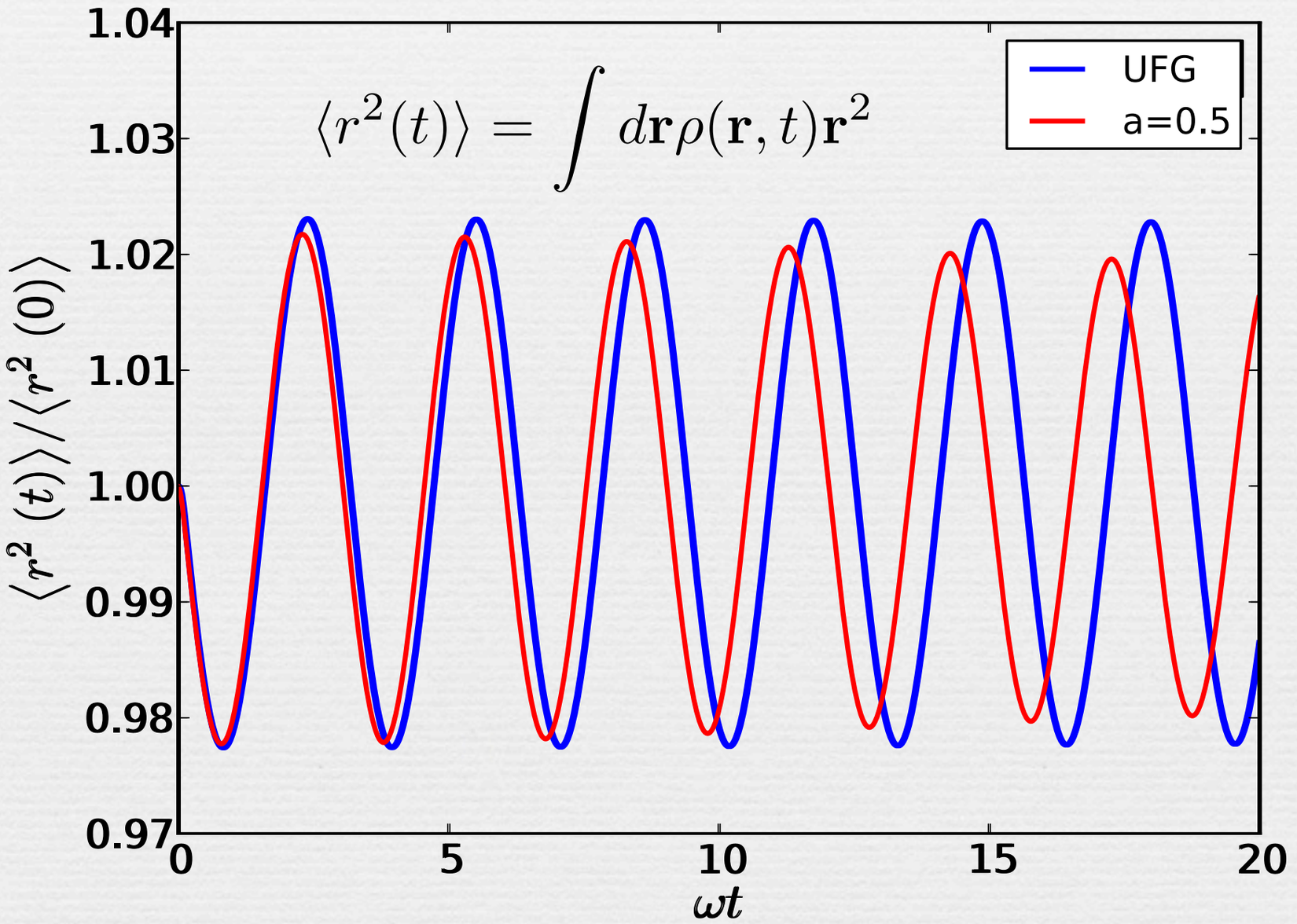
Brantut *et al* 2012

Finite-Temperature TDDFT

$$i\frac{\partial}{\partial t}\psi_j = \left(-\frac{\hbar^2\nabla^2}{2m} + \frac{m\omega(t)^2 r^2}{2} + V_{\mathrm{HXC}}\right)\psi_j$$

Breathing mode

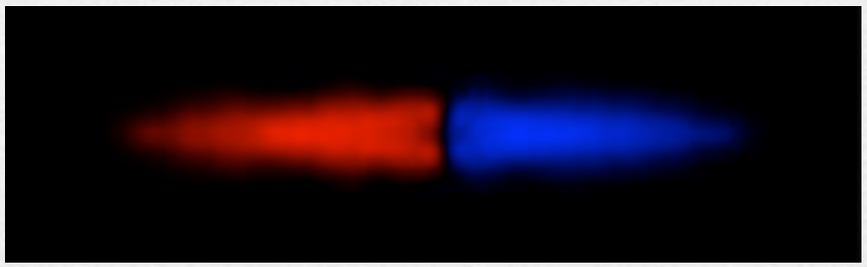


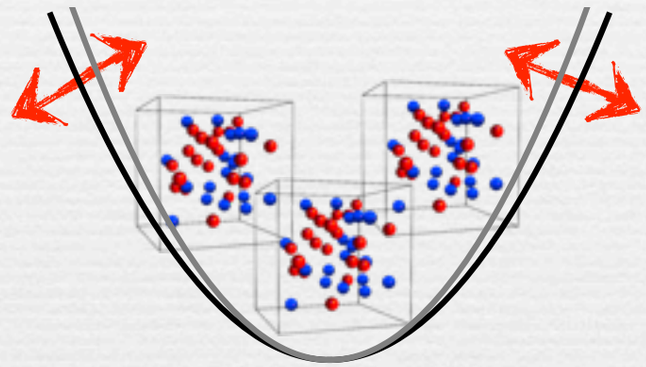


cf vanishing bulk viscosity of UFG
Castin 2004, Son 2007

Summary & Outlook

- DFT is a useful tool for statics and dynamics of cold atom systems





Optical lattice loading,
Free expansion,
Lattice modulation,
Bloch oscillation,
...

- Moreover...
  - Bosons, superfluidity, open systems ...
  - Well controllable cold atom experiments can be used to calibrate and improve DFT itself

Thank you!