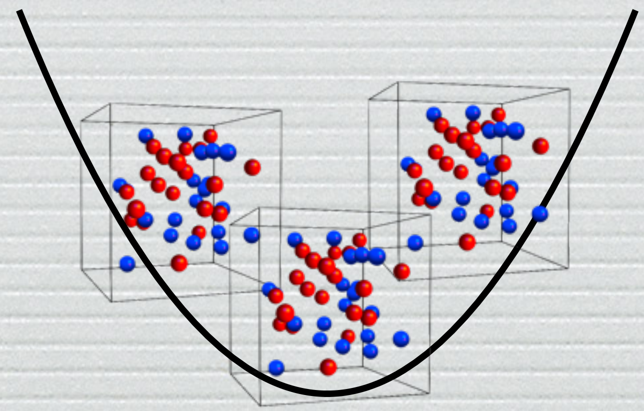
Density functional theory for static and dynamic properties of cold atomic gases



Lei Wang
Theoretische Physik, ETH Zurich

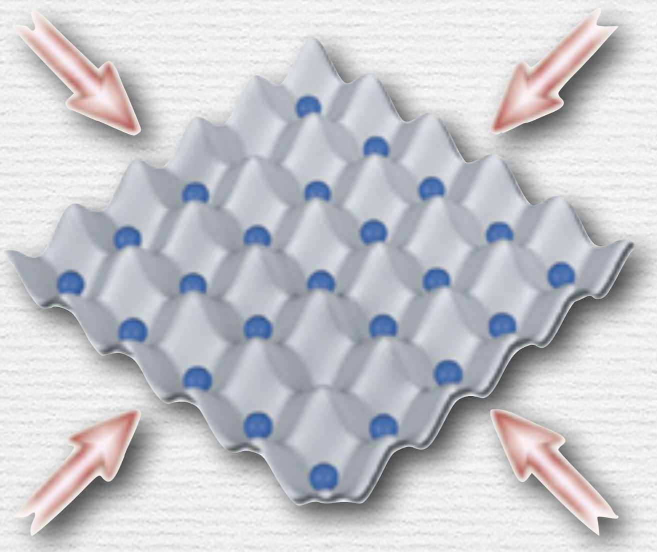
ETH Zürich Ping Nang Ma, Ilia Zintchenko, Matthias Troyer

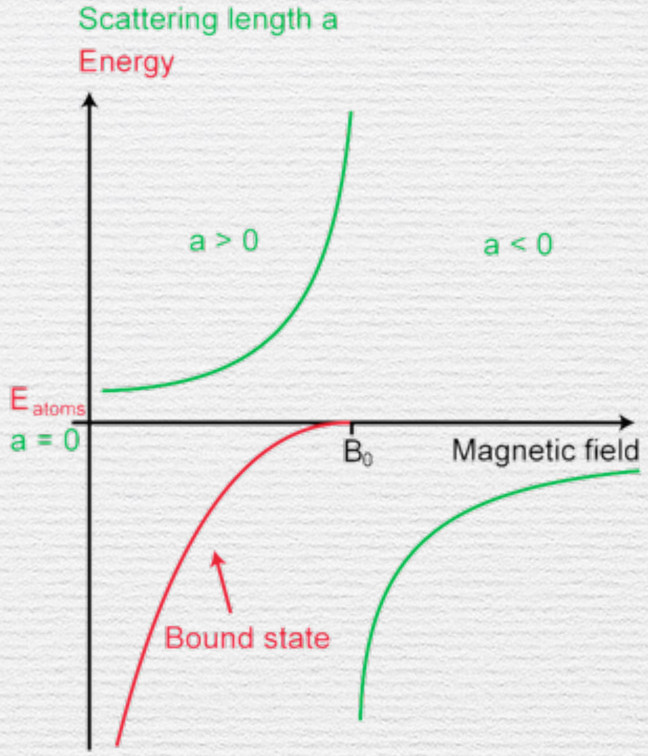
ICTP Sebastiano Pilati

Institute of Physics CAS Xi Dai

Cold atoms: Quantum simulator

- Highly controllable





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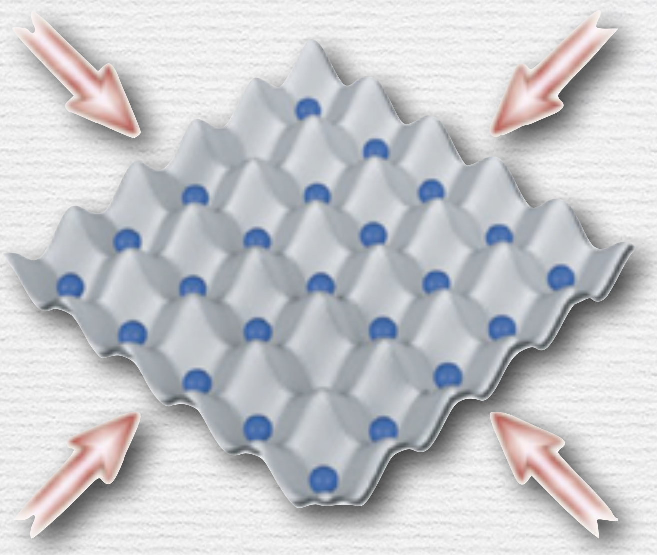

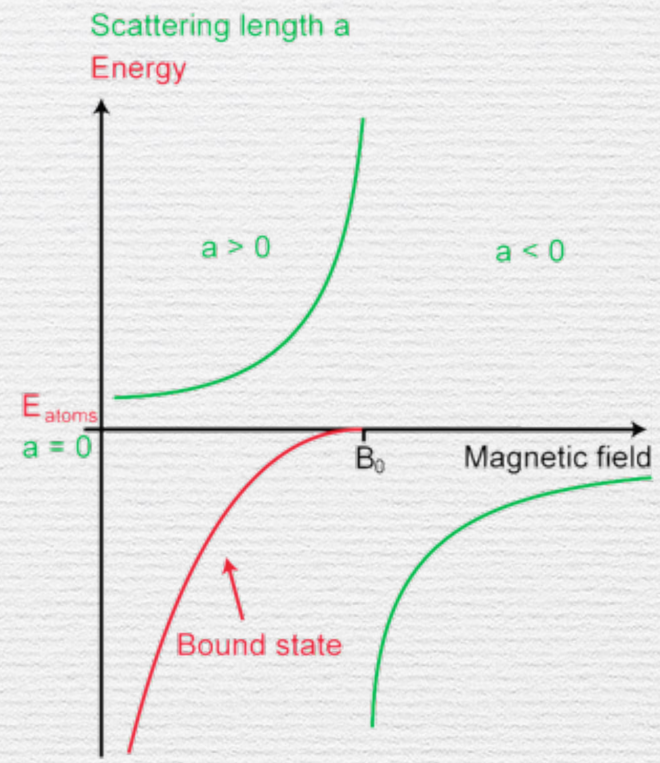

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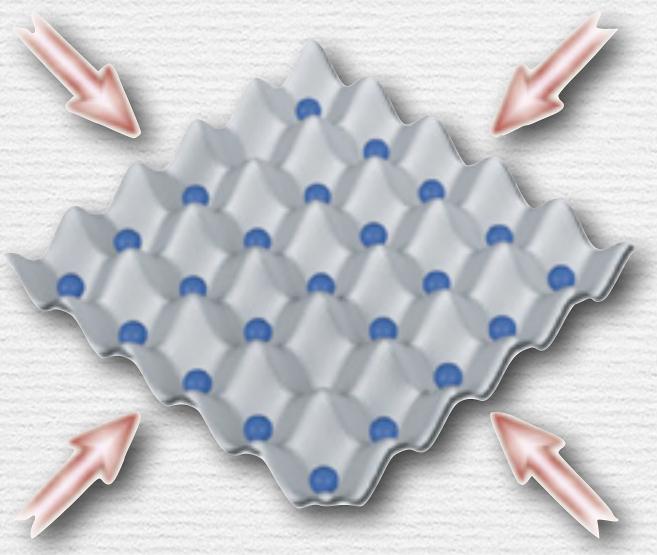
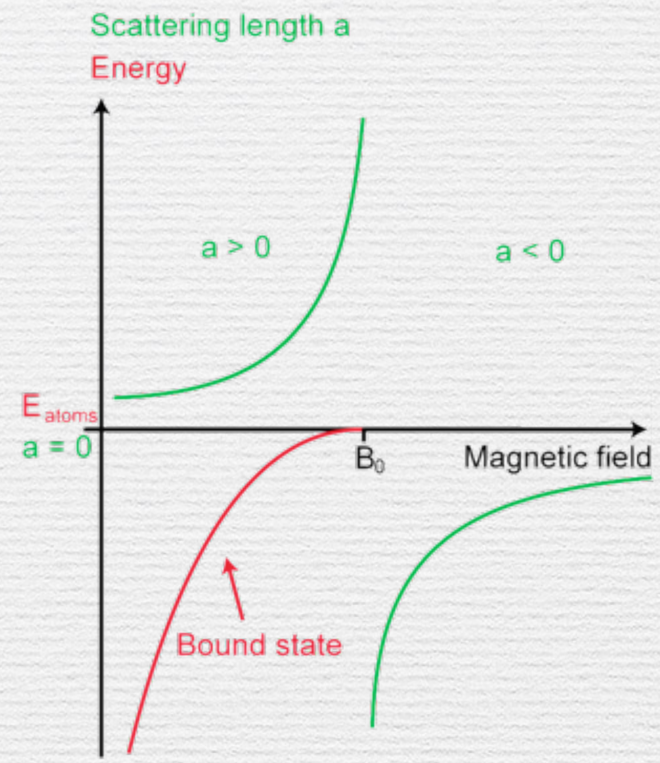




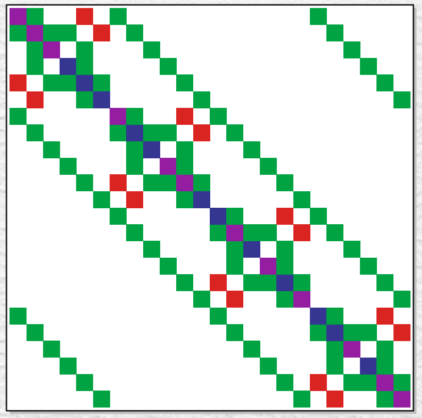
- Quantum simulator for static properties
- Coherent quantum evolution for long time:

ideal playground for quantum dynamics!

OLE
OPTICAL
LATTICE EMULATOR

Exact Diagonalization

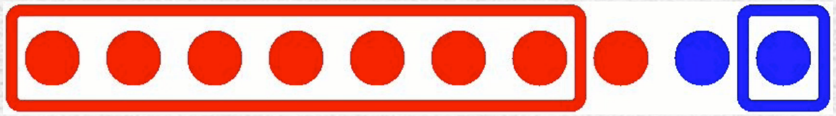
$$H|\Psi\rangle = E|\Psi\rangle$$



- Give exact results
- Limited to small systems
  - 25 site Fermi-Hubbard model with 12 atoms on the Earth Simulator in 2006

DMRG

- Extremely powerful in 1D



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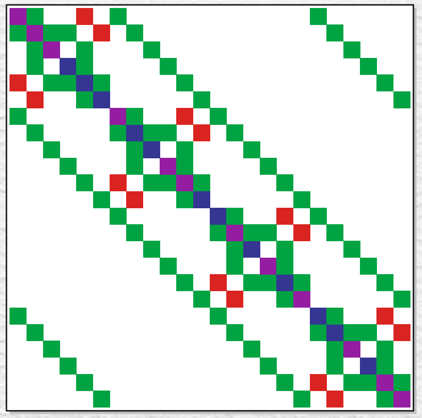

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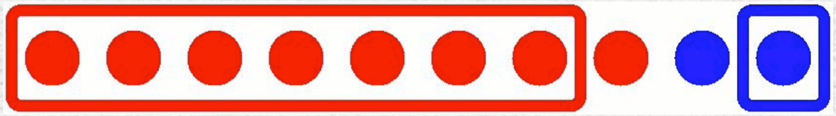

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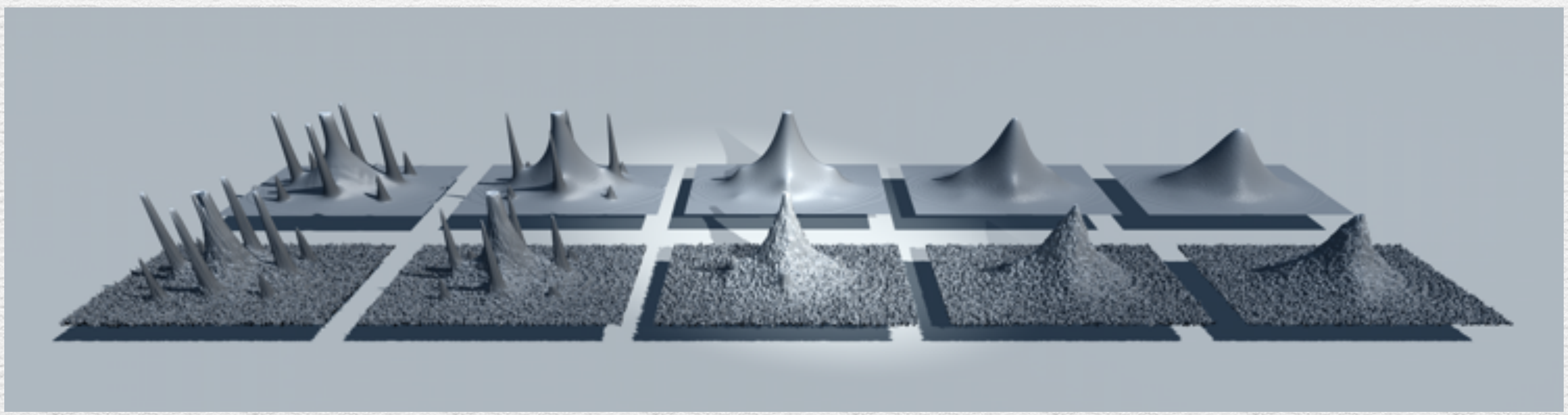
Quantum Monte Carlo

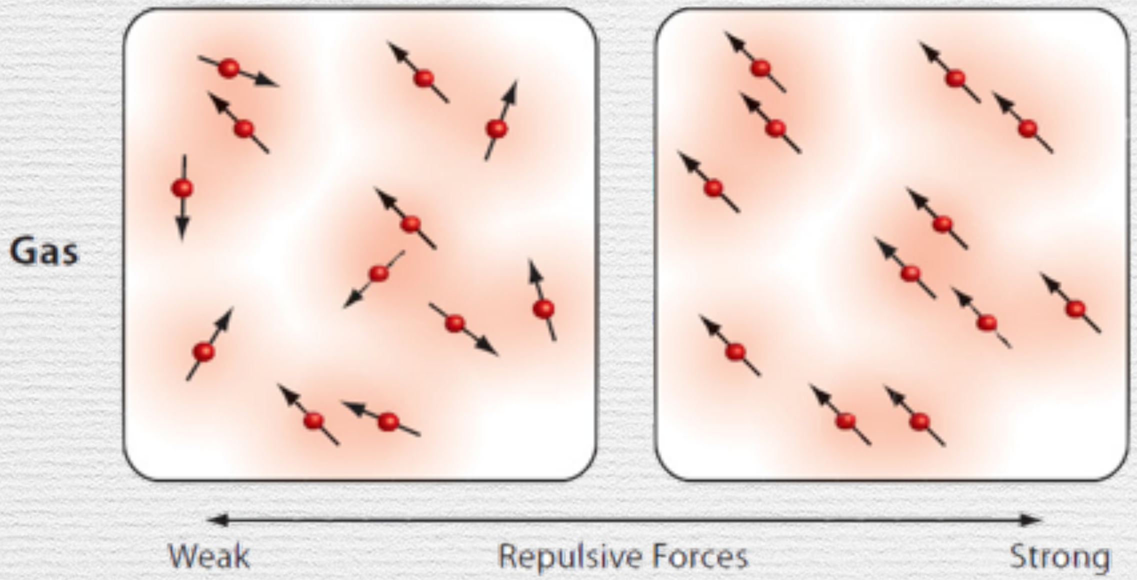
- We can solve static properties of
  - Bosons in any dimensions, Trotzky, Pollet, Nature Physics, 2010

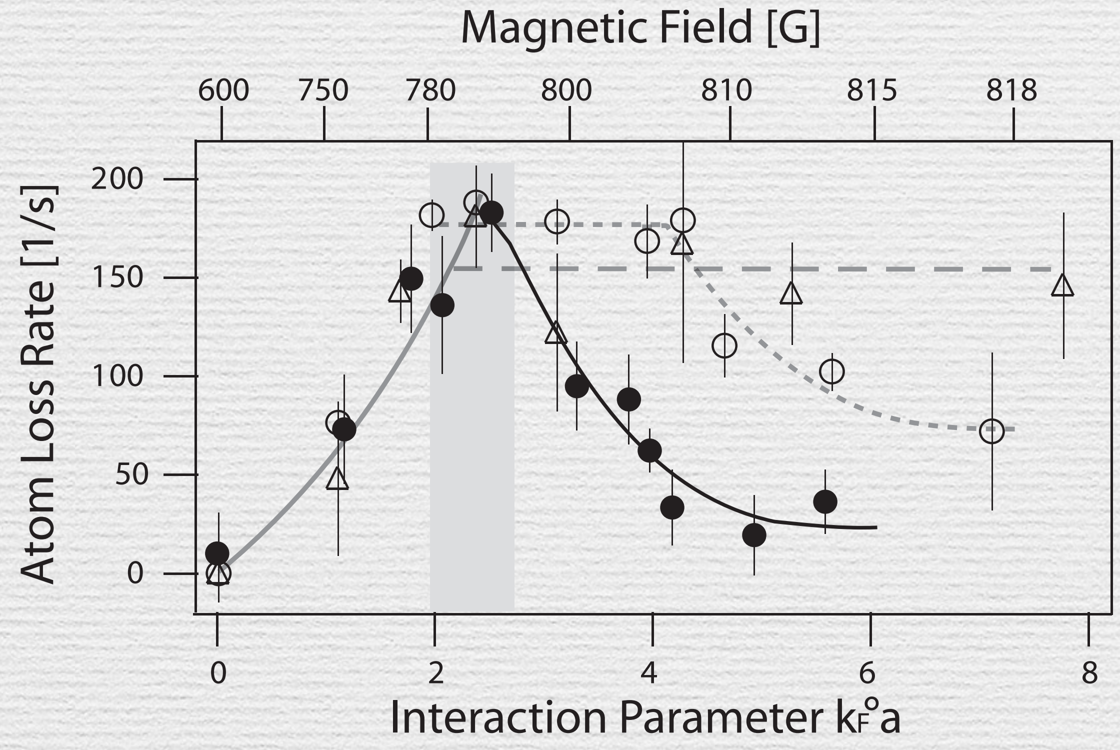


  - Fermions in 1D for all T, 2D and 3D at $T>0.05E_F$

Beyond lattice models

Jo, Science 2009





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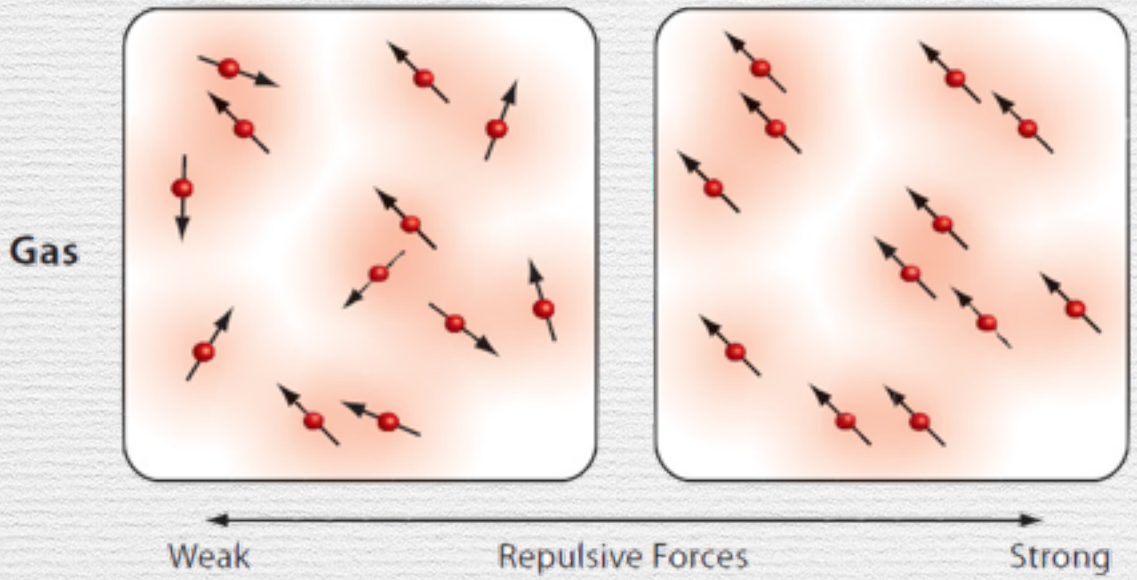
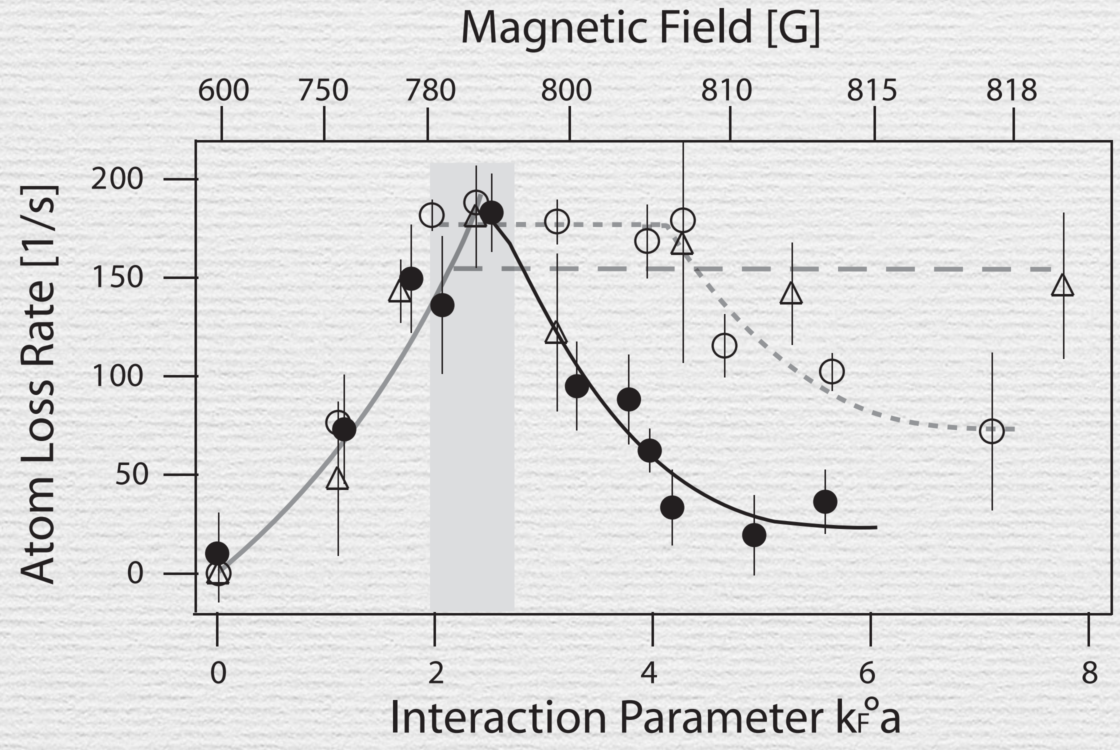
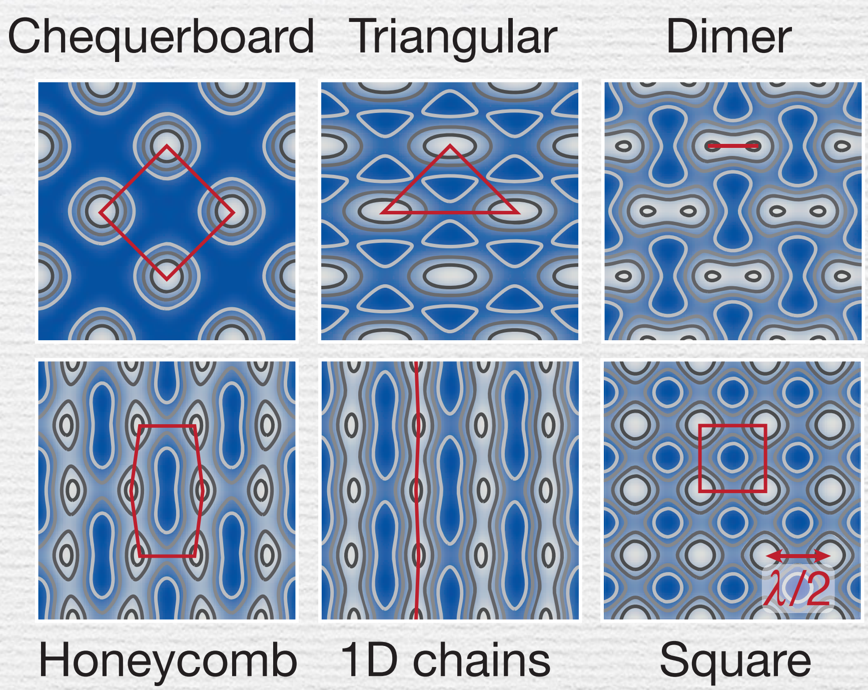




Tarruell, Nature 2012



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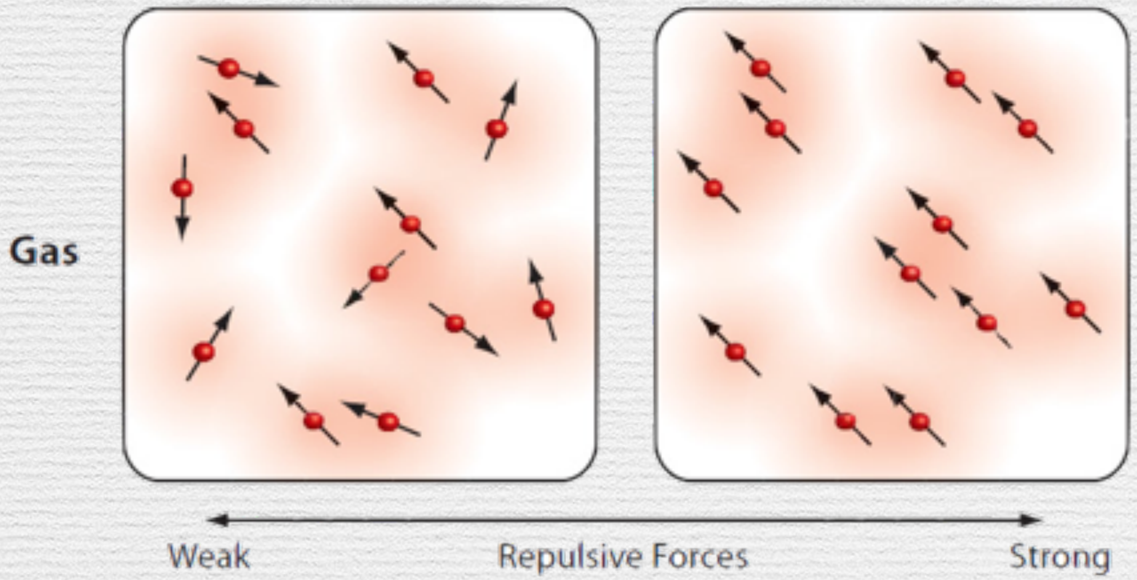

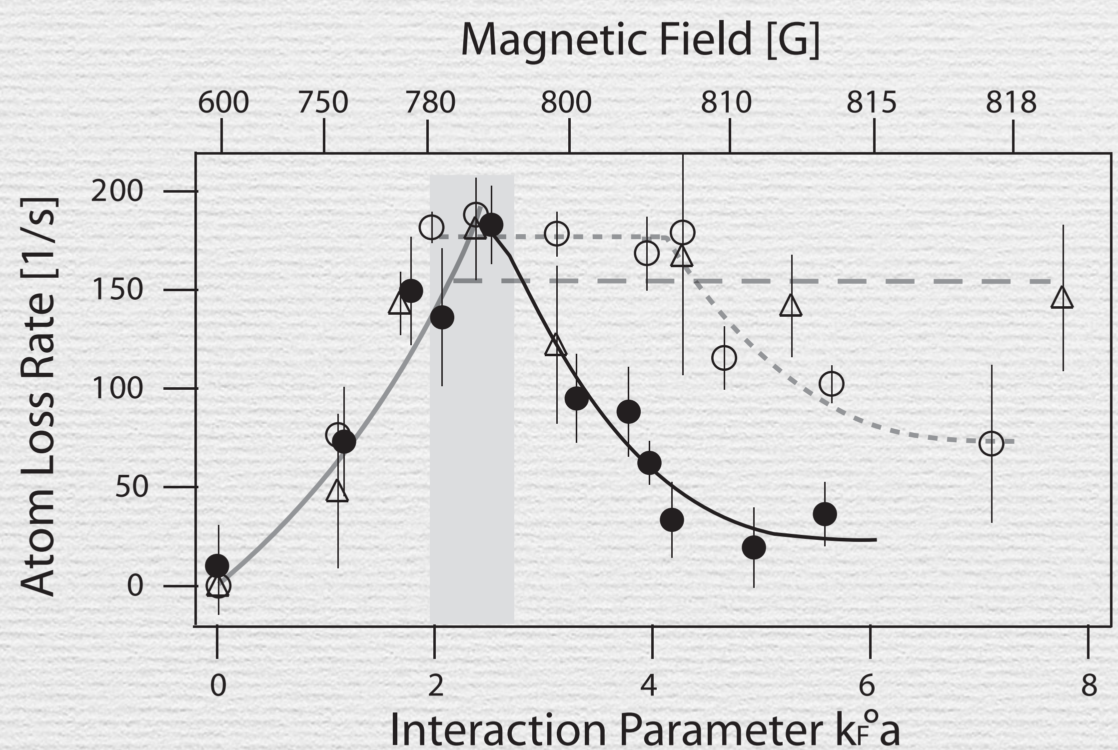

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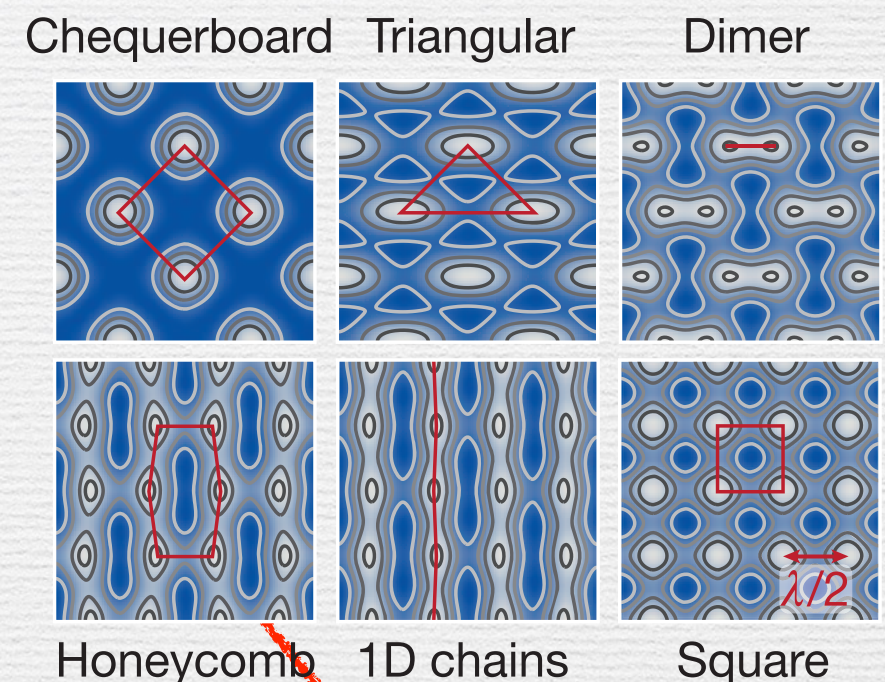
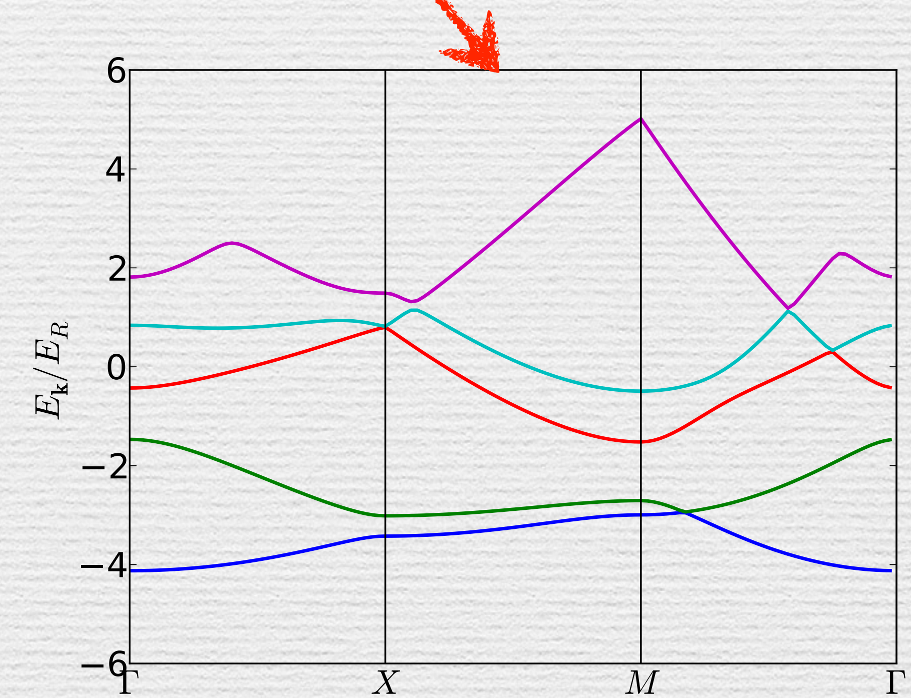
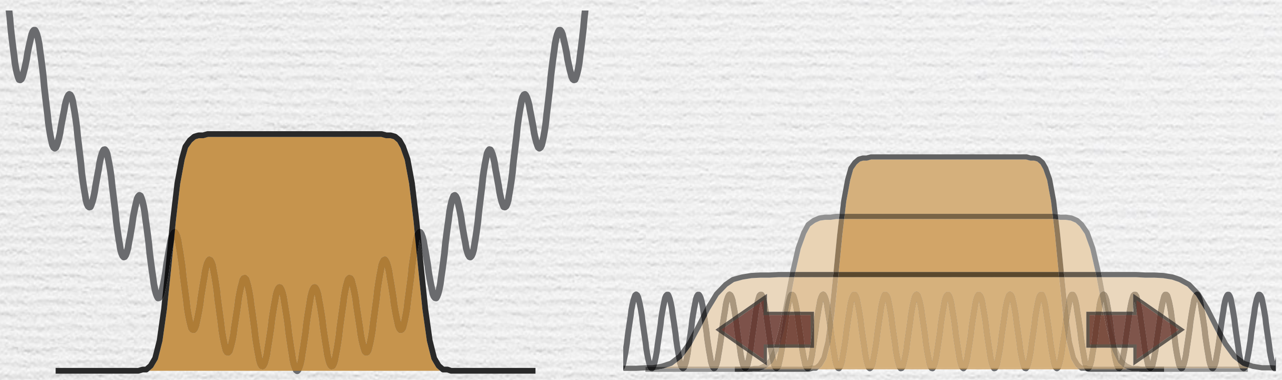
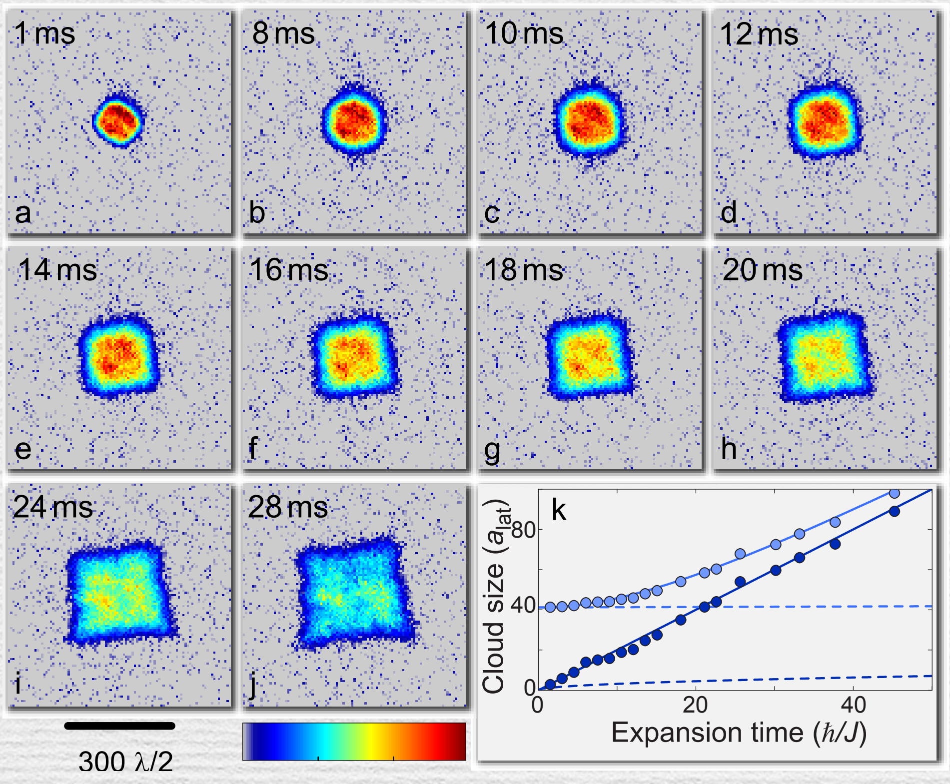




Non-equilibrium dynamics

Schneider, Nature Physics 2012





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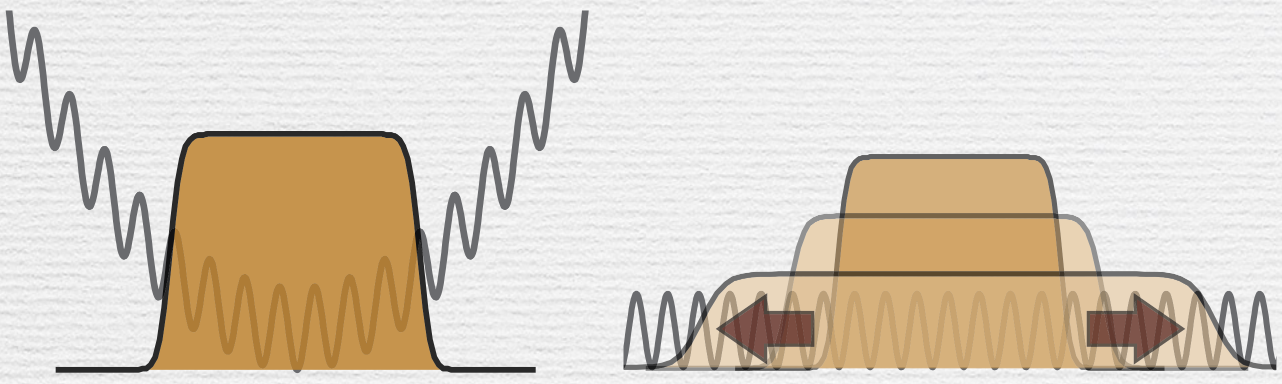
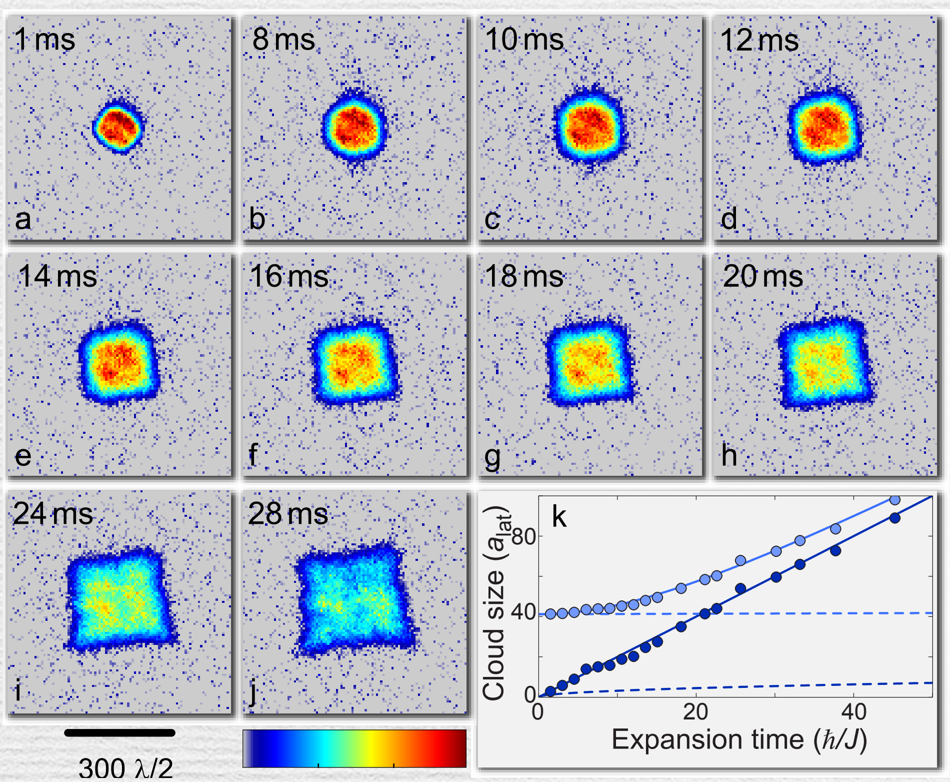
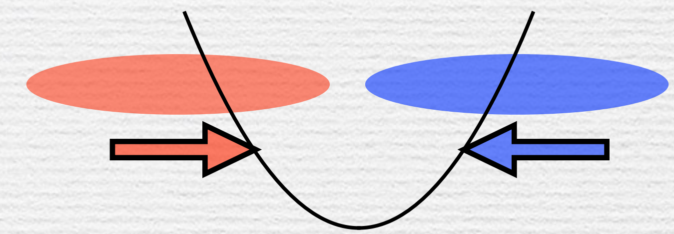
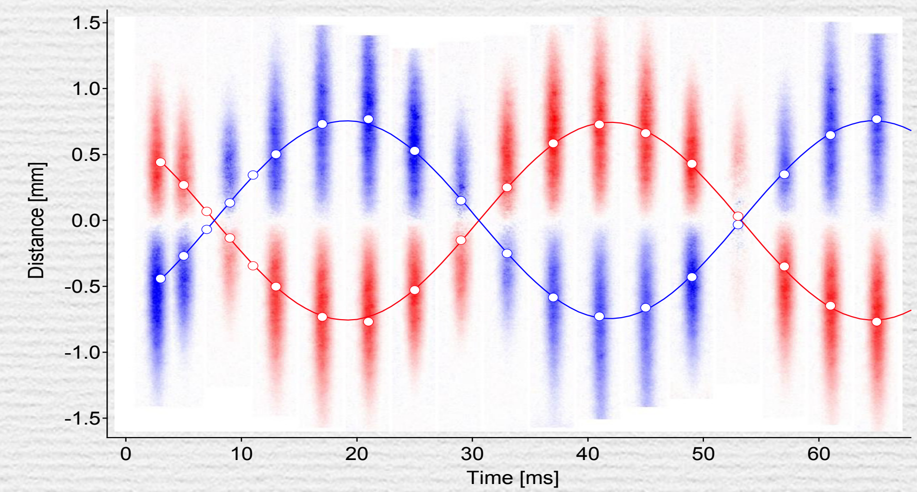
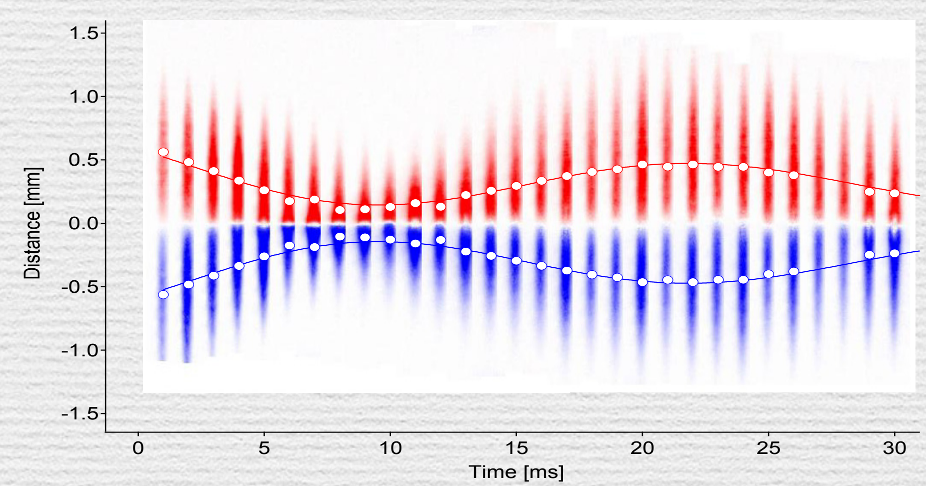




Sommer, Nature 2011







Density functional theory (DFT)

Hohenberg, Kohn 1964

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

$\in \mathbb{R}^{3N}$ → $\in \mathbb{R}^3$

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

Kohn-Sham approach

Kohn, Sham 1965

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

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kinetic
energy

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mean field
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$$(-\frac{\hbar^2\nabla^2}{2m} + V_{\rm ext} + V_{\rm H}[\rho] + \boxed{V_{\rm XC}[\rho]})\psi_j = \varepsilon_j \psi_j$$

Local density approximation

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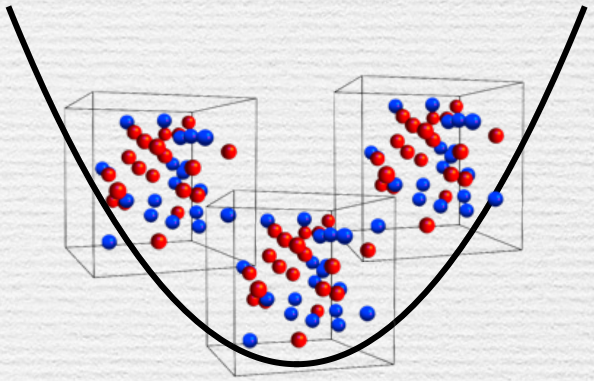
Local density approximation



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  Coulomb gas: Ceperley, Alder 1980, Cold atoms: Pilati 2010

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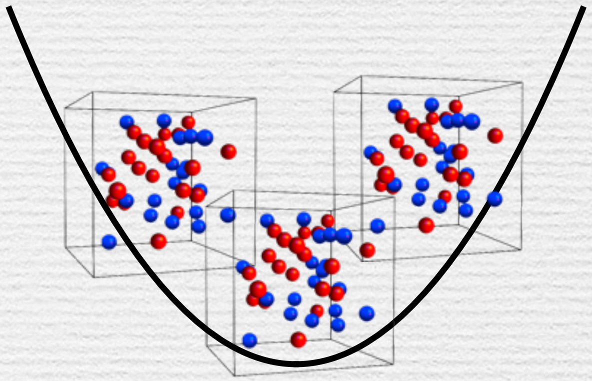
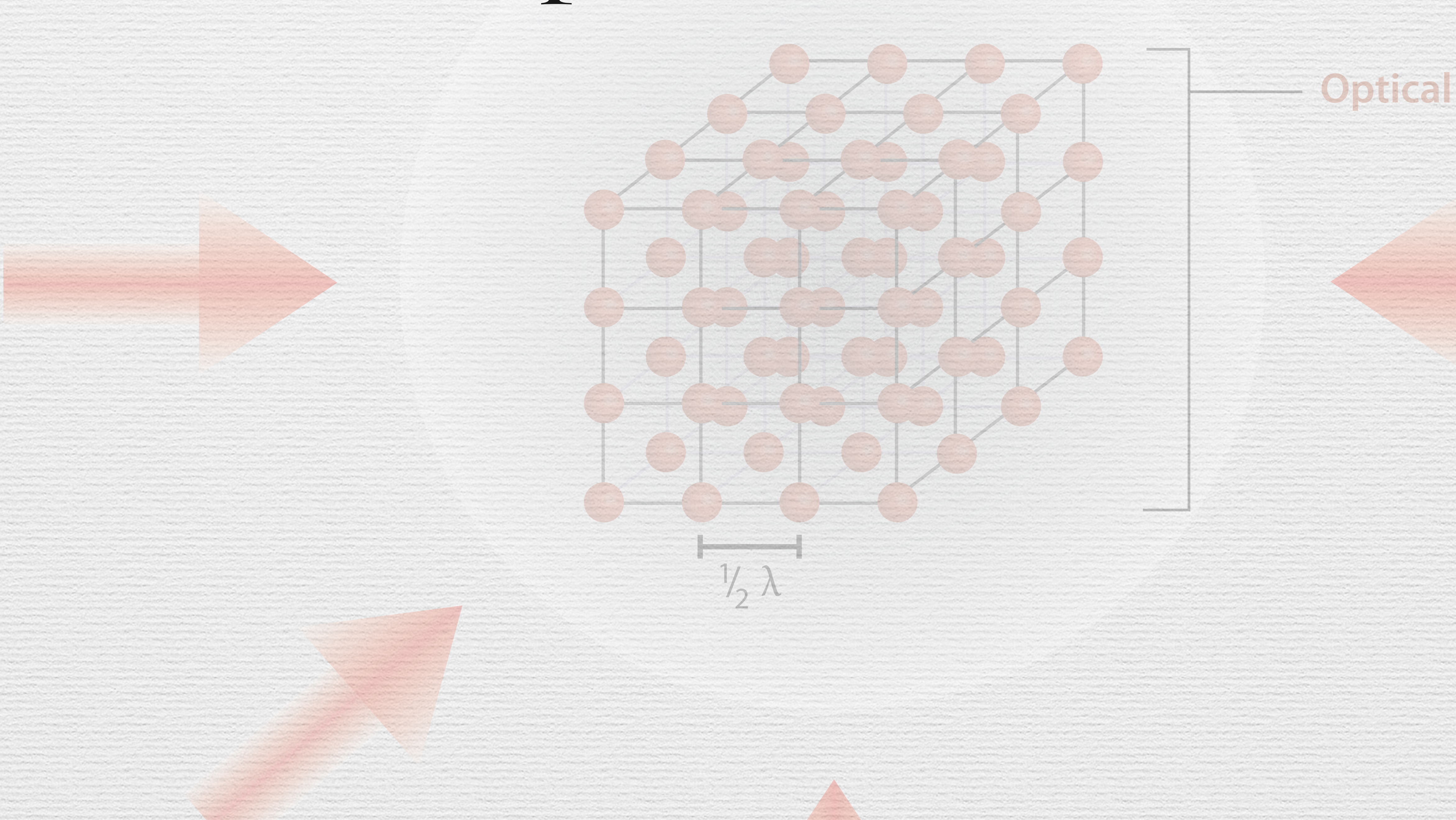


Redner, Physics Today, 2005

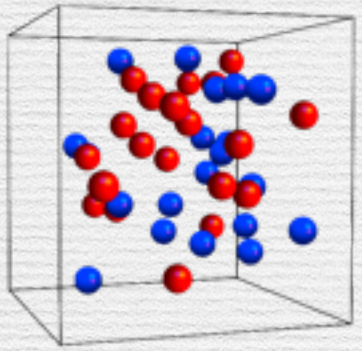
Table 1. *Physical Review* Articles with more than 1000 Citations Through June 2003

Publication	# cites	Av. age	Title	Author(s)
PR **140**, A1133 (1965)	3227	26.7	Self-Consistent Equations Including Exchange and Correlation Effects	W. Kohn, L. J. Sham
PR **136**, B864 (1964)	2460	28.7	Inhomogeneous Electron Gas	P. Hohenberg, W. Kohn
PRB **23**, 5048 (1981)	2079	14.4	Self-Interaction Correction to Density-Functional Approximations for Many-Electron Systems	J. P. Perdew, A. Zunger
PRL **45**, 566 (1980)	1781	15.4	Ground State of the Electron Gas by a Stochastic Method	D. M. Ceperley, B. J. Alder
PR **108**, 1175 (1957)	1364	20.2	Theory of Superconductivity	J. Bardeen, L. N. Cooper, J. R. Schrieffer
PRL **19**, 1264 (1967)	1306	15.5	A Model of Leptons	S. Weinberg
PRB **12**, 3060 (1975)	1259	18.4	Linear Methods in Band Theory	O. K. Anderson
PR **124**, 1866 (1961)	1178	28.0	Effects of Configuration Interaction of Intensities and Phase Shifts	U. Fano
RMP **57**, 287 (1985)	1055	9.2	Disordered Electronic Systems	P. A. Lee, T. V. Ramakrishnan
RMP **54**, 437 (1982)	1045	10.8	Electronic Properties of Two-Dimensional Systems	T. Ando, A. B. Fowler, F. Stern
PRB **13**, 5188 (1976)	1023	20.8	Special Points for Brillouin-Zone Integrations	H. J. Monkhorst, J. D. Pack

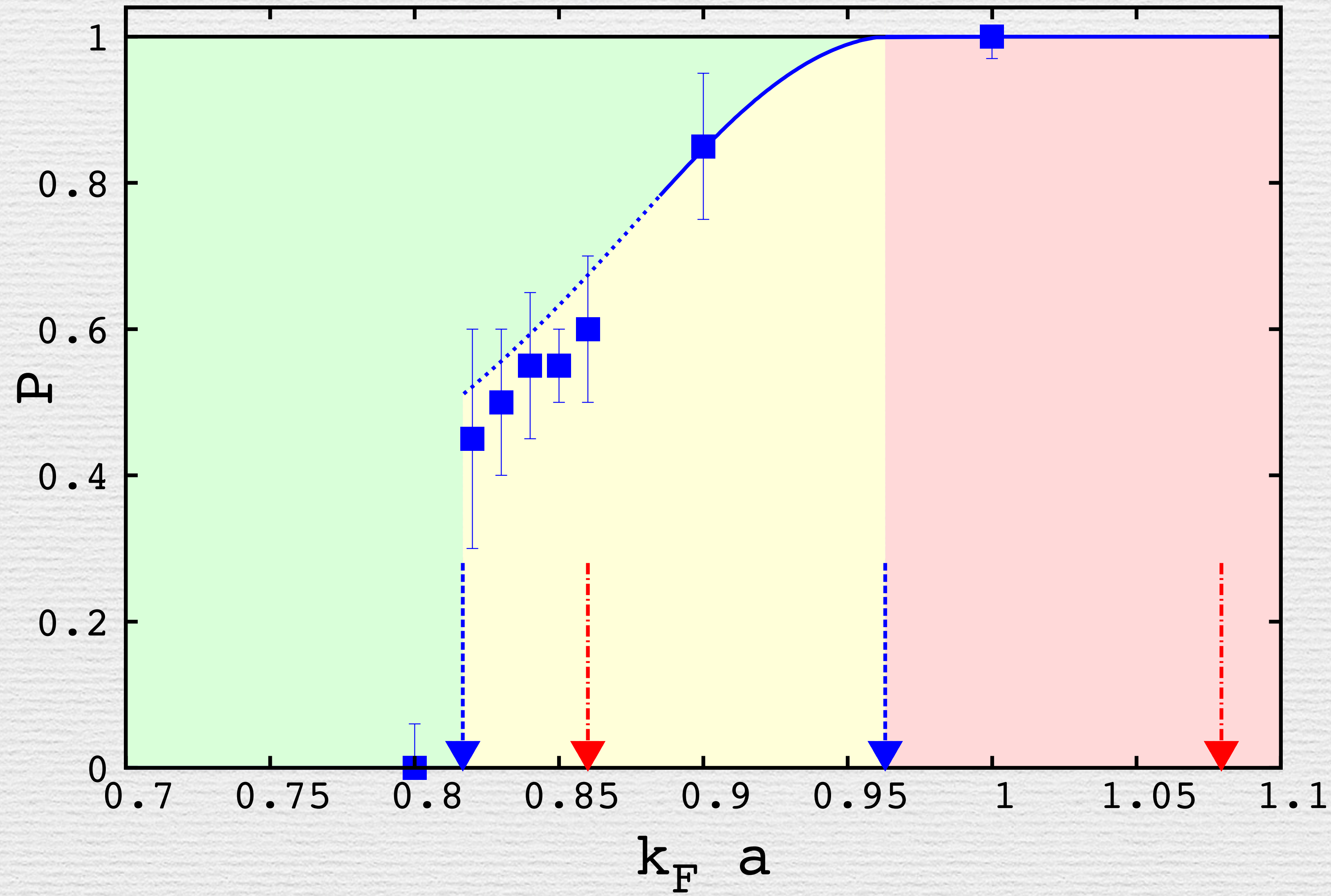
Magnetism in harmonic trap and shallow optical lattice



Uniform system: QMC

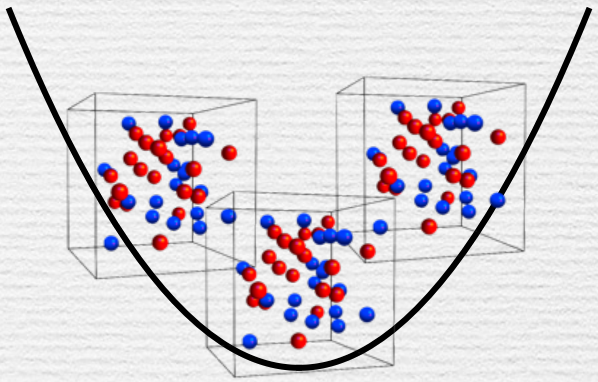


Uniform system shows ferromagnetism for high density and large interactions



Pilati 2010

Harmonic Trap: DFT



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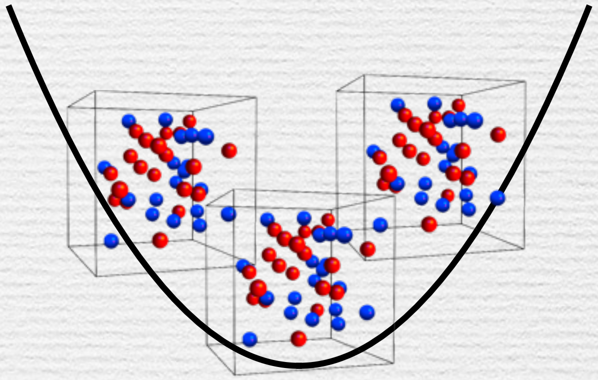

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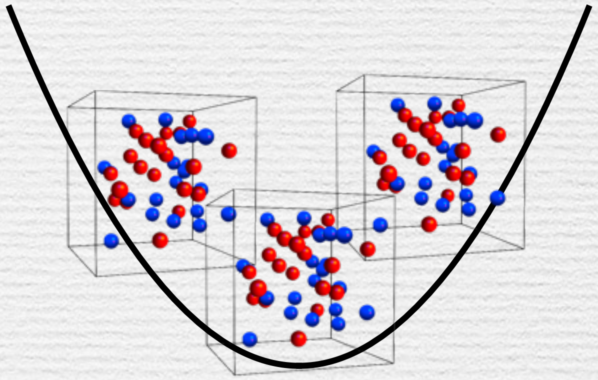
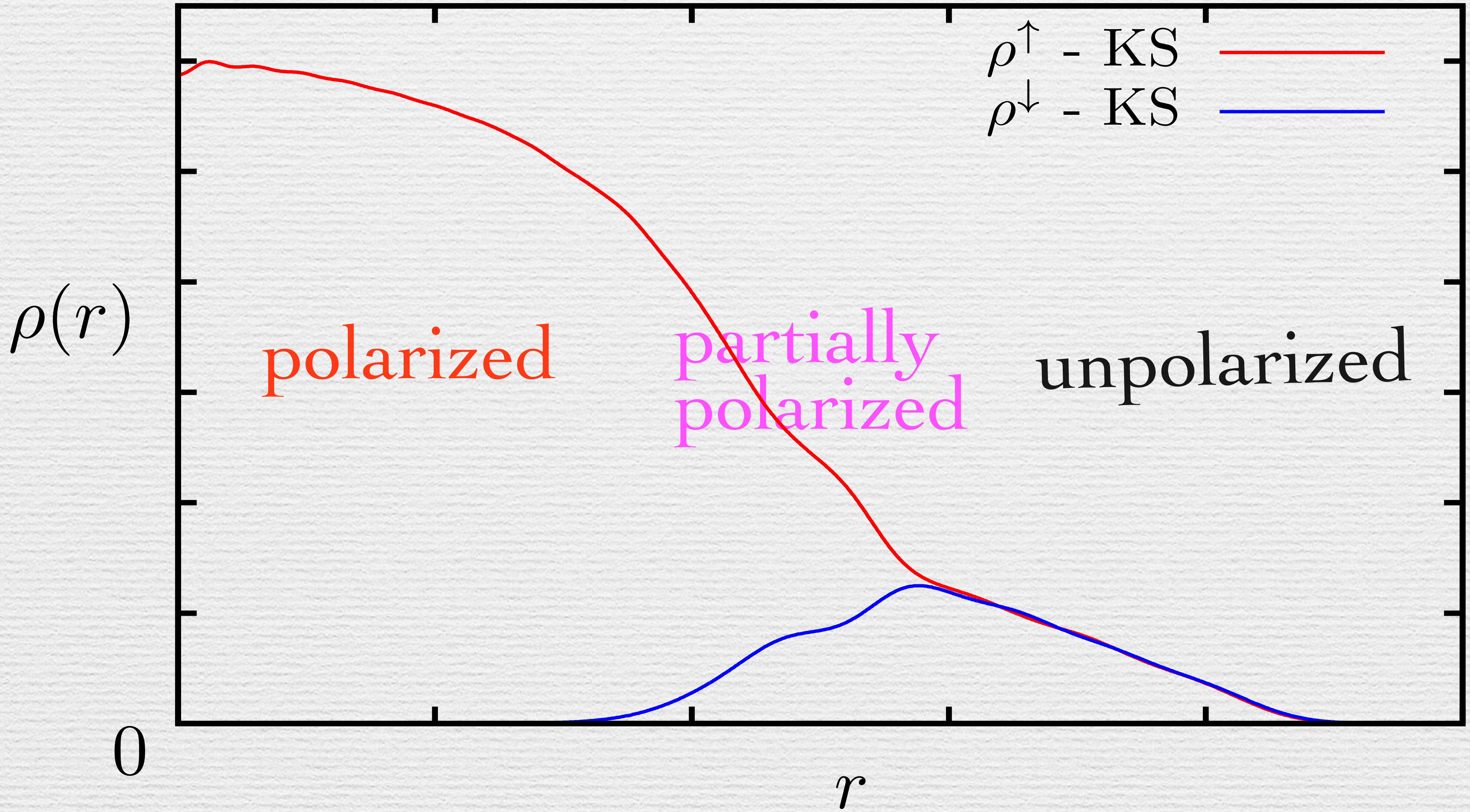


Radial density profile



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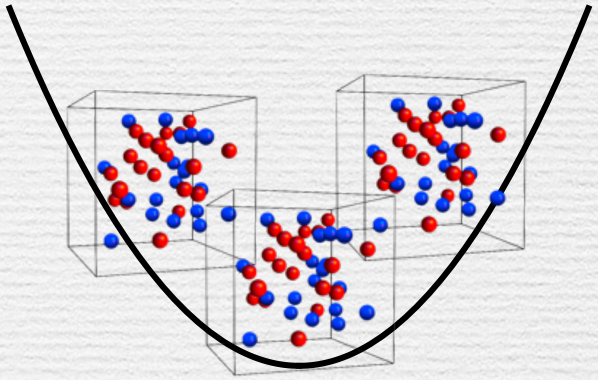

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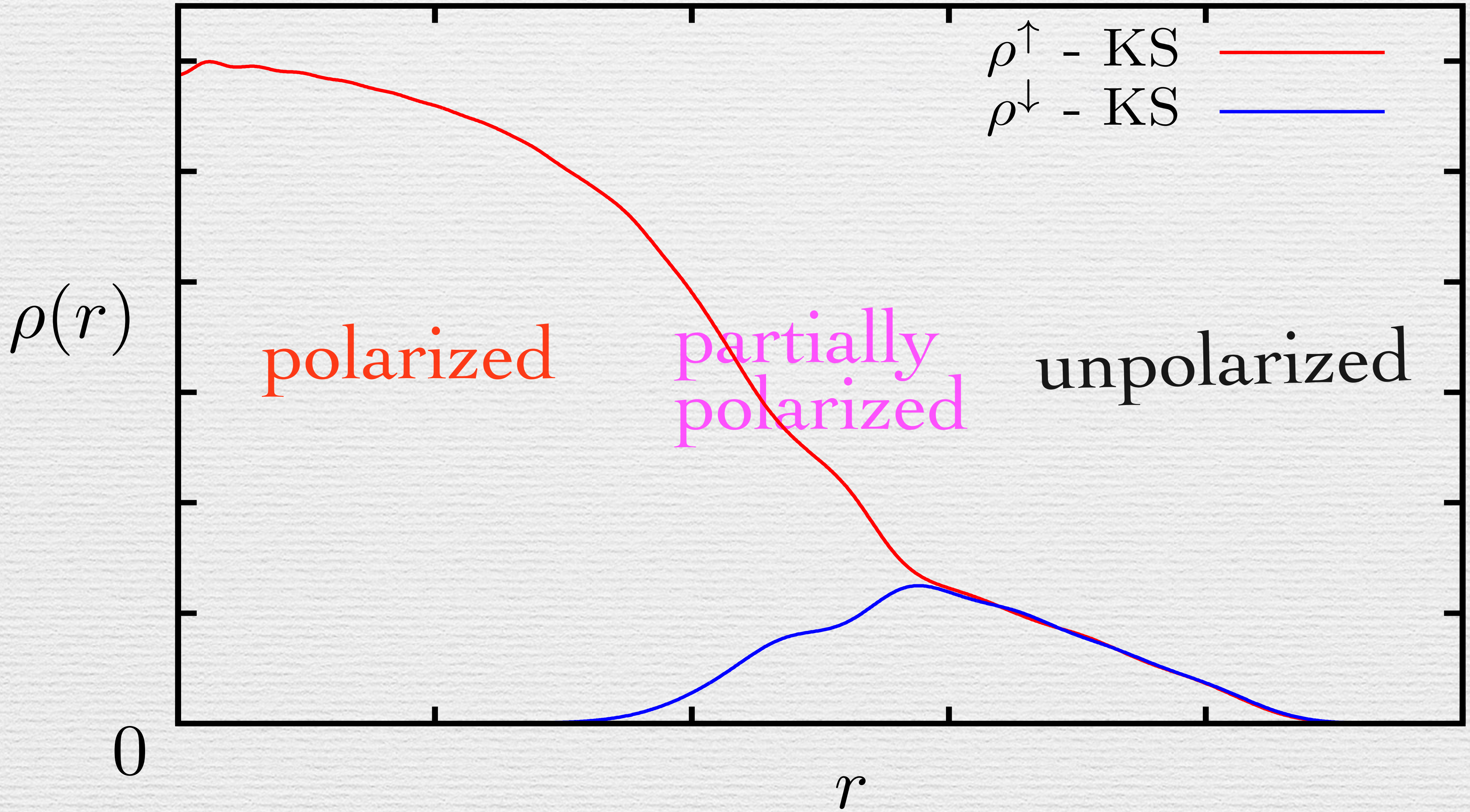

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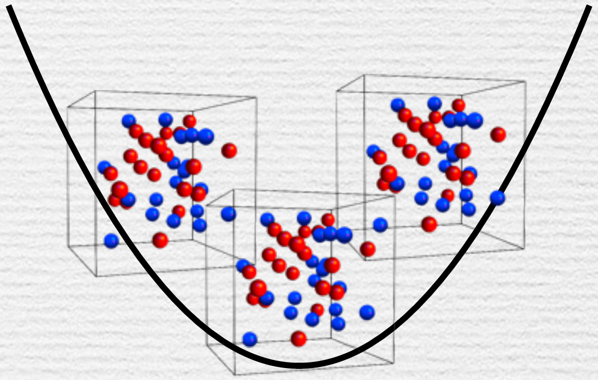

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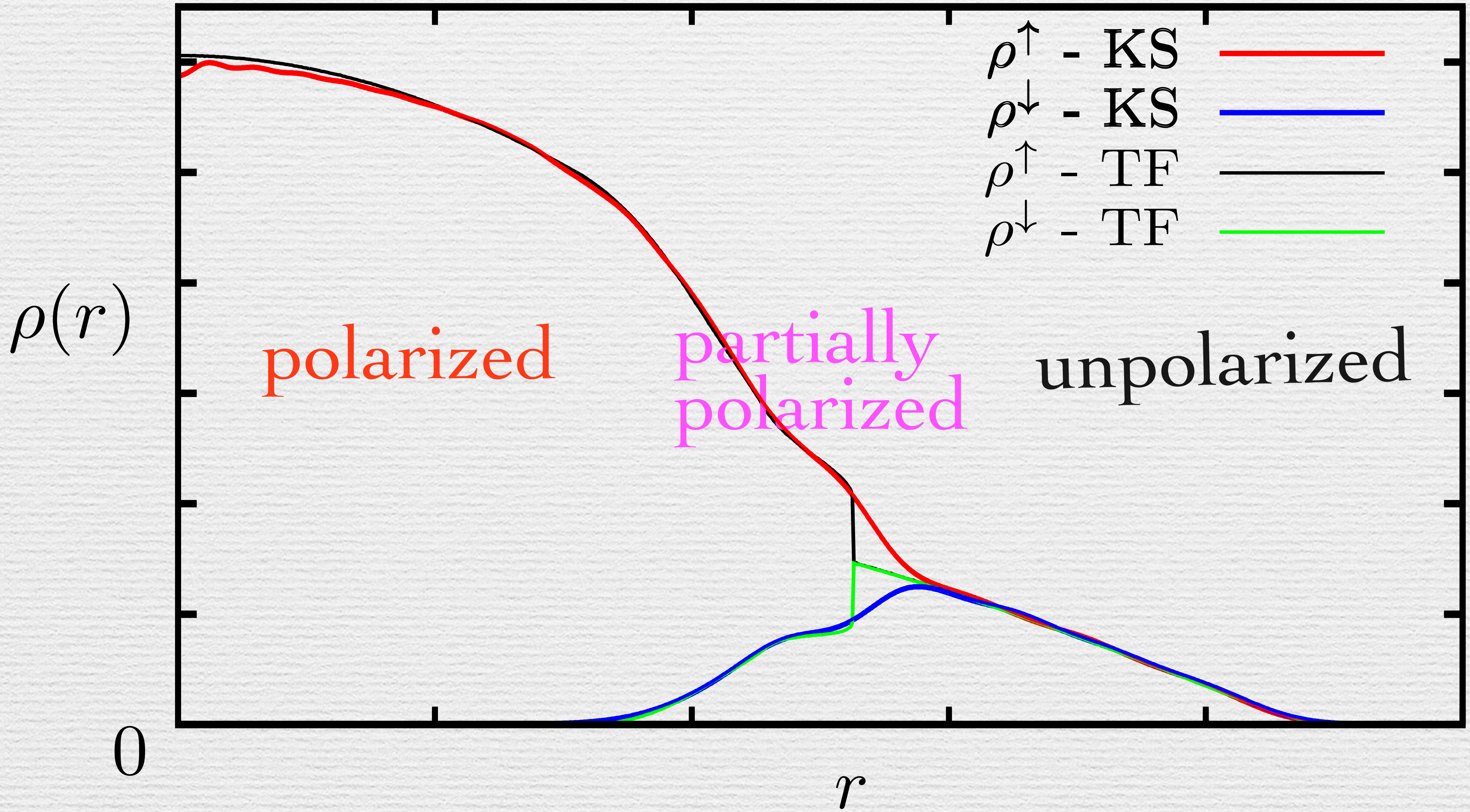

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Ferromagnetism in shallow optical lattices

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

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

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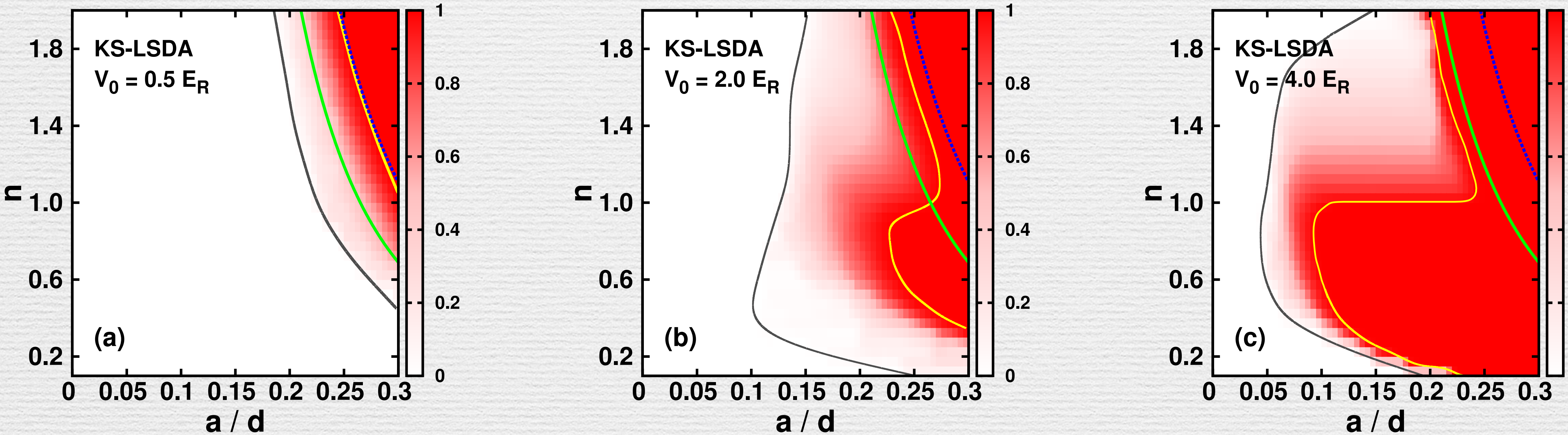
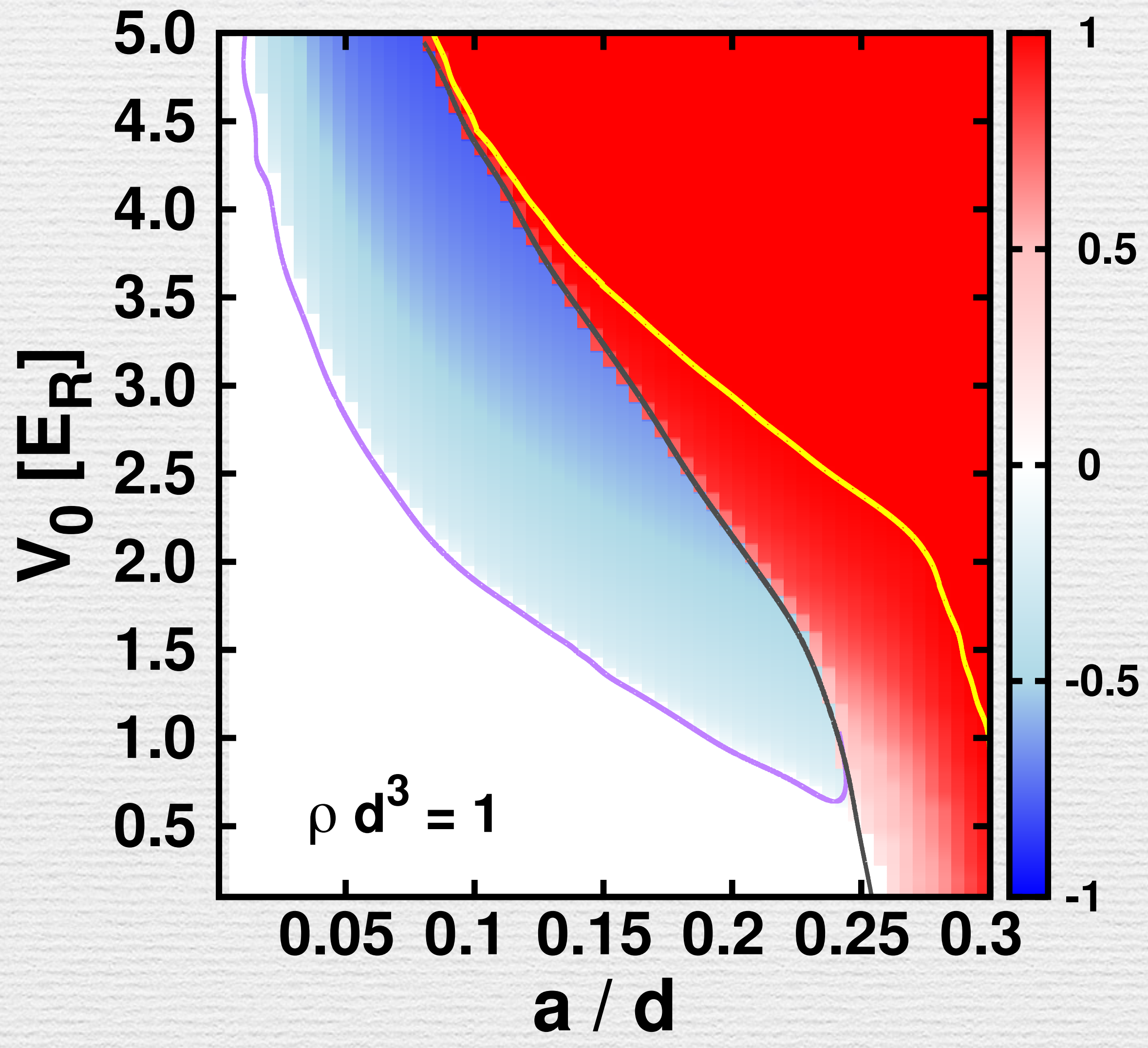


Green and Blue: partially and fully polarized in free-space

Black and Yellow: partially and fully polarized with optical lattice

Antiferromagnetism

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



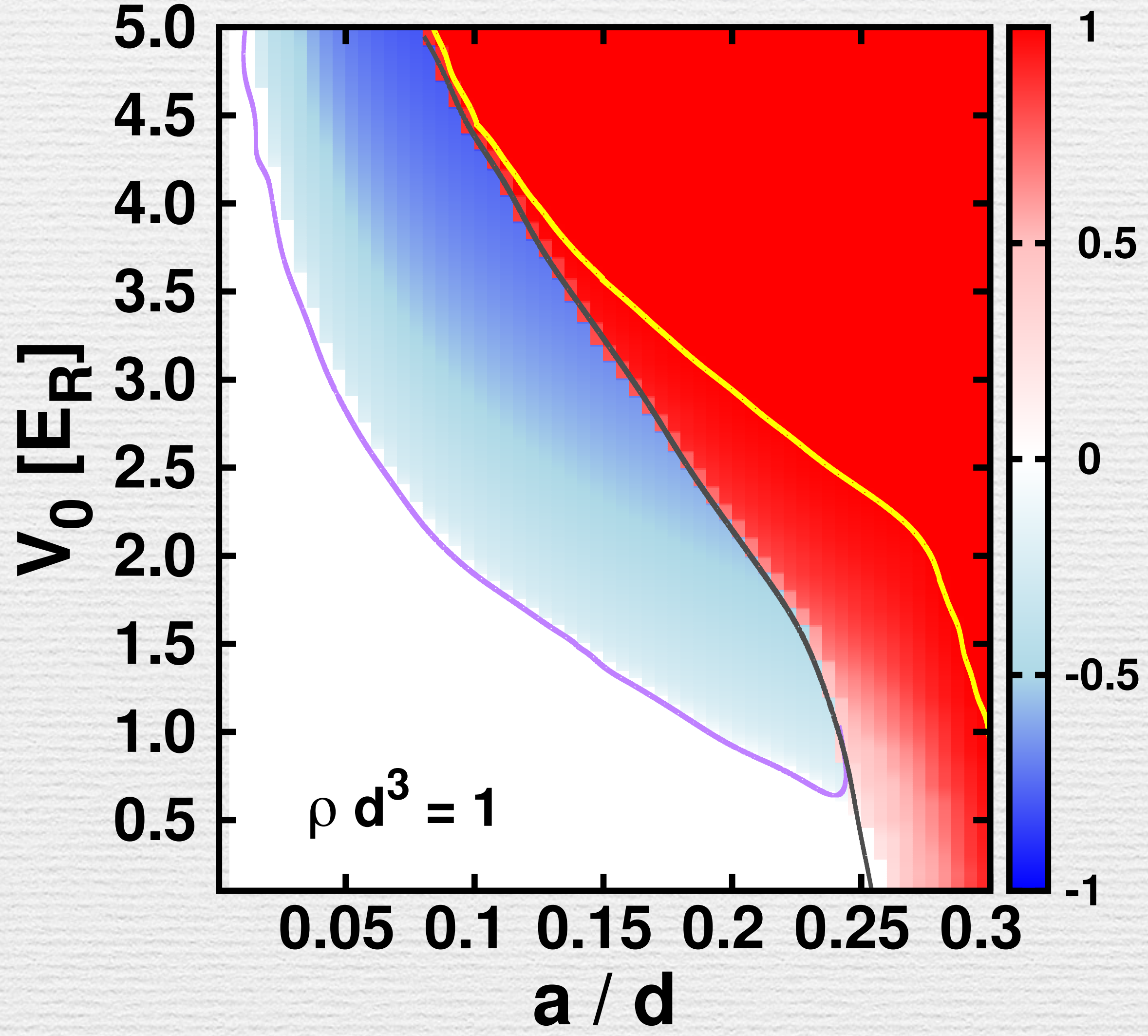
Blue: staggered magnetization

Red: uniform magnetization

Antiferromagnetism

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

One Band
Hubbard model
Here



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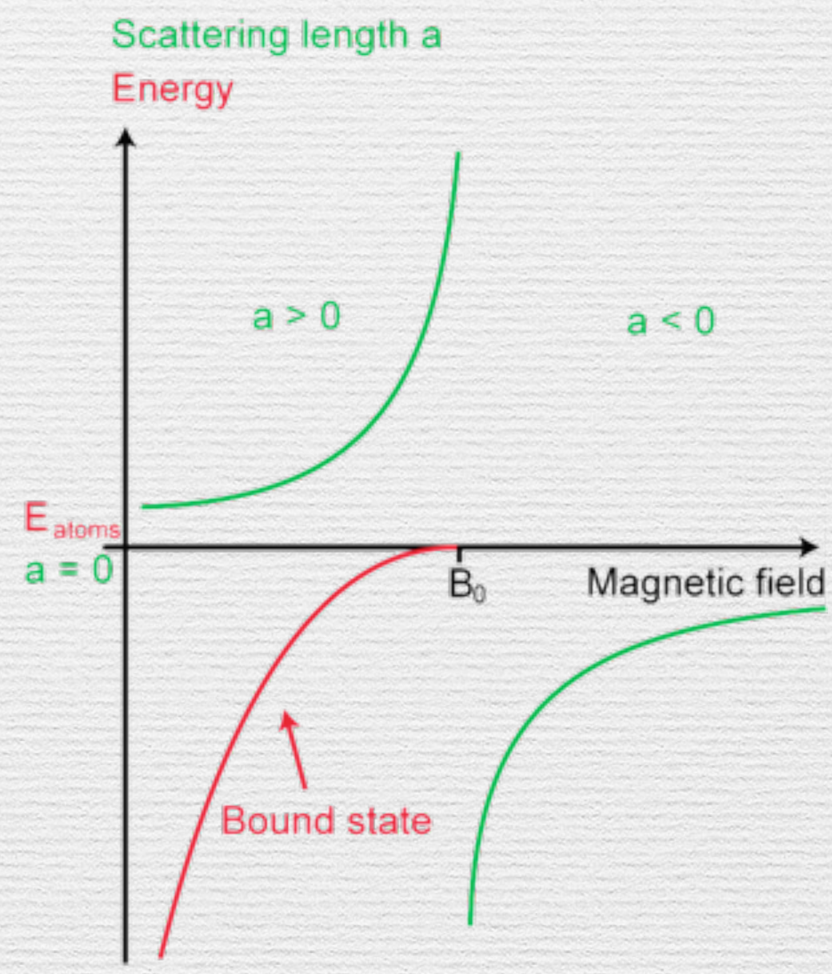

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- 2012: Pair formation in repulsive Fermi gas (Sanner, PRL, Lee, PRA)

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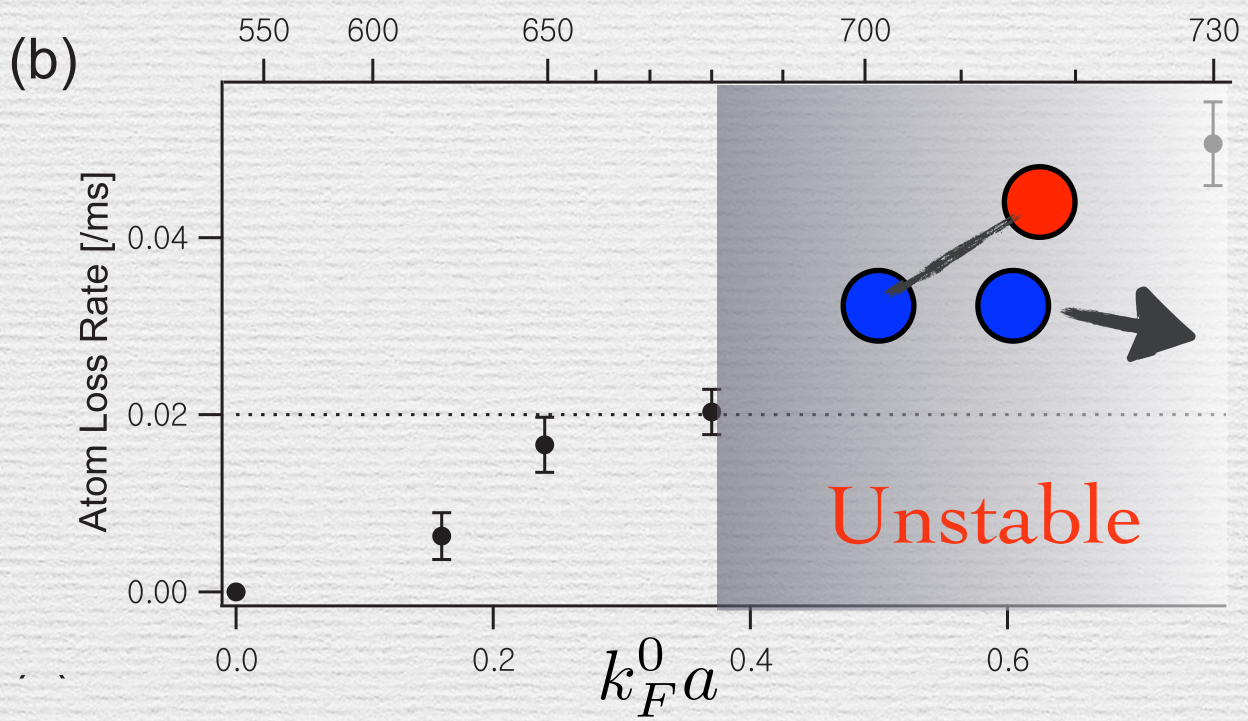
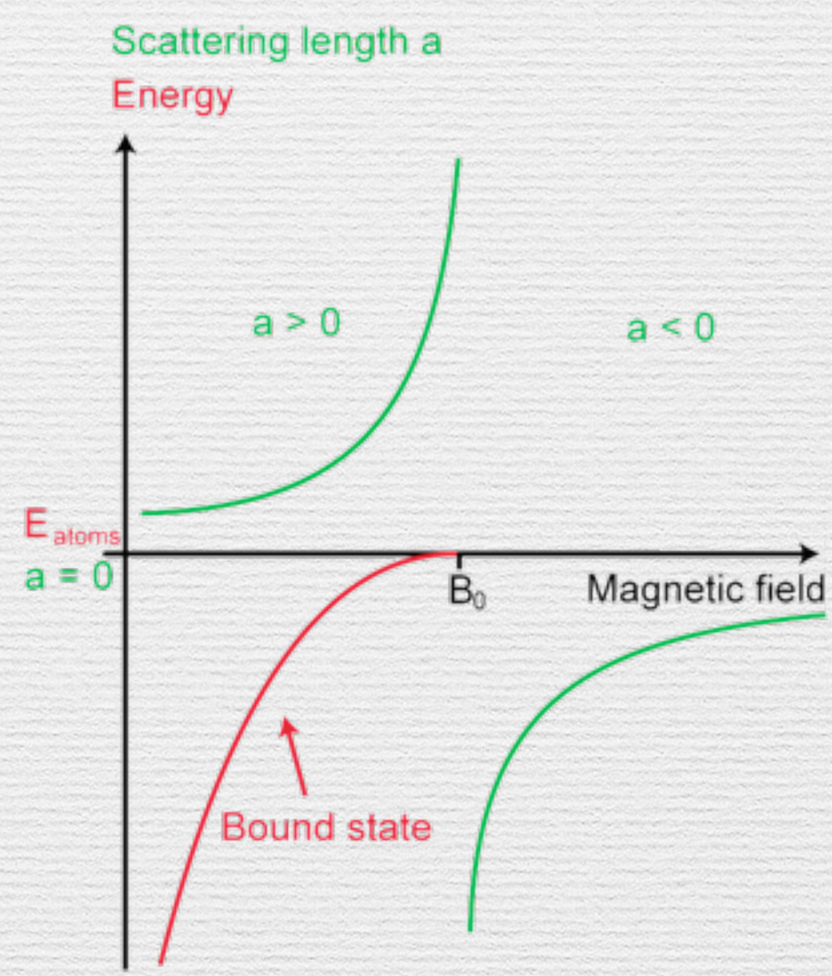
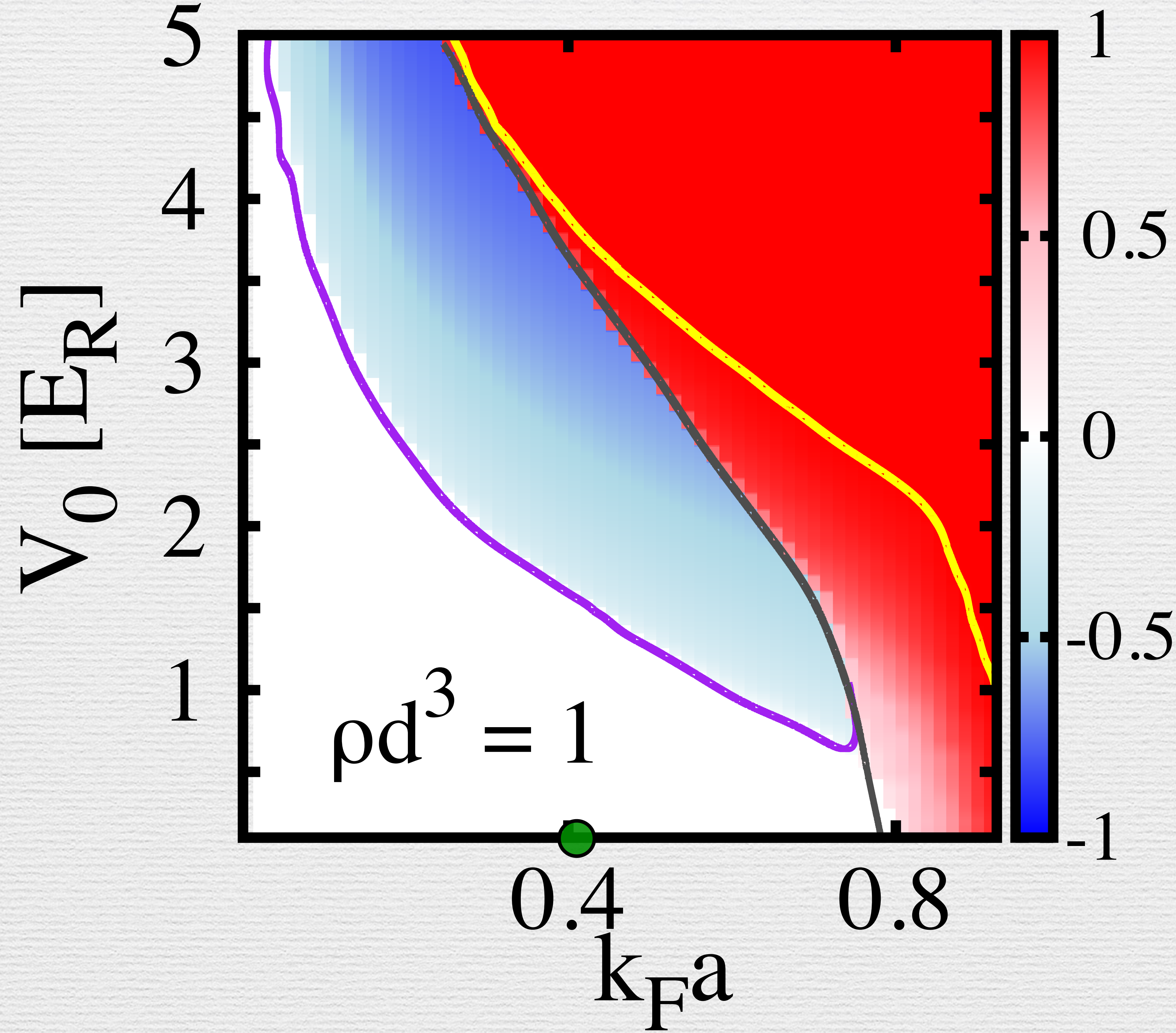




Can a lattice help ?



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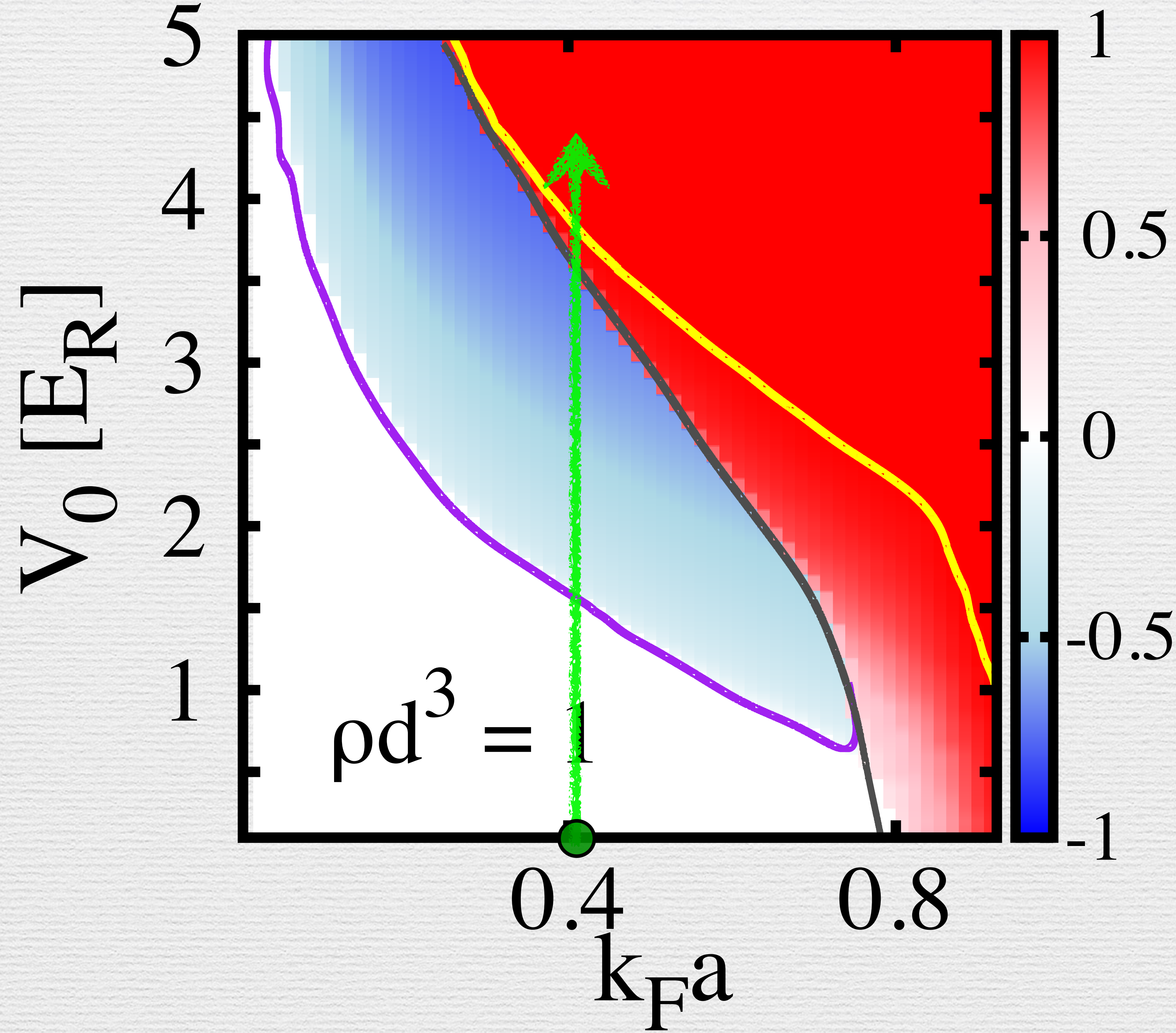
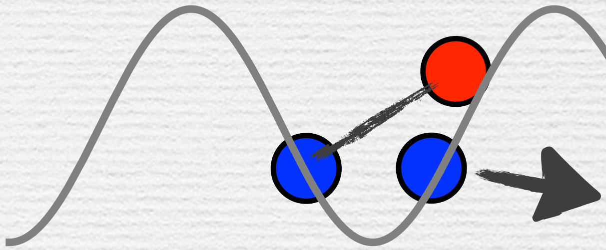
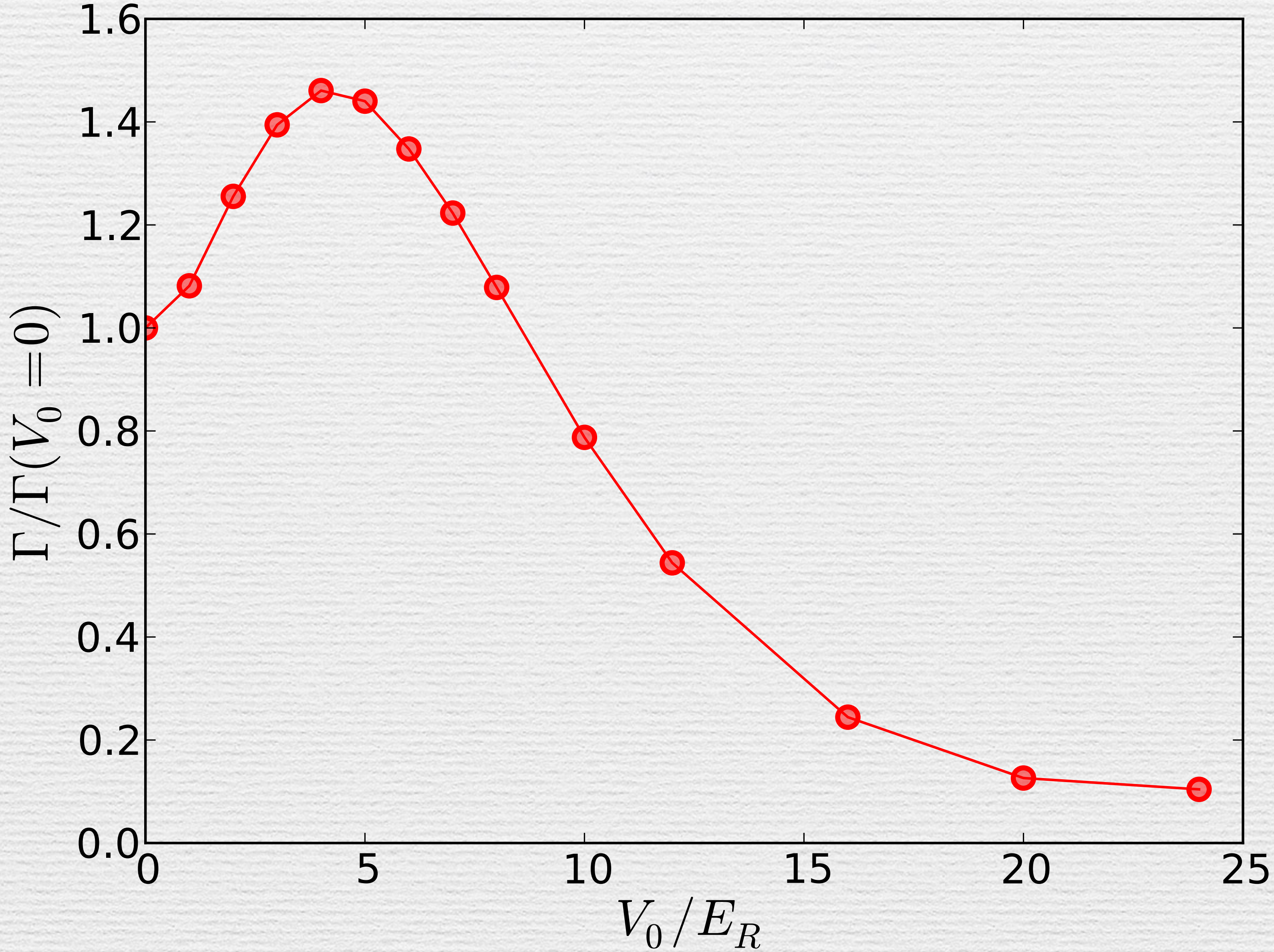


3-body loss rate

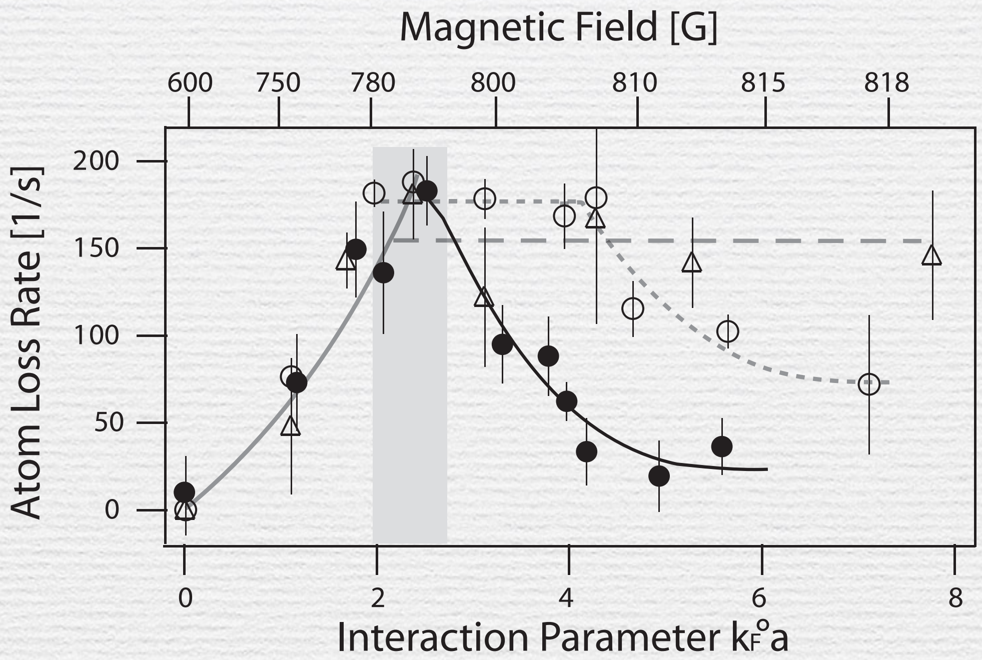


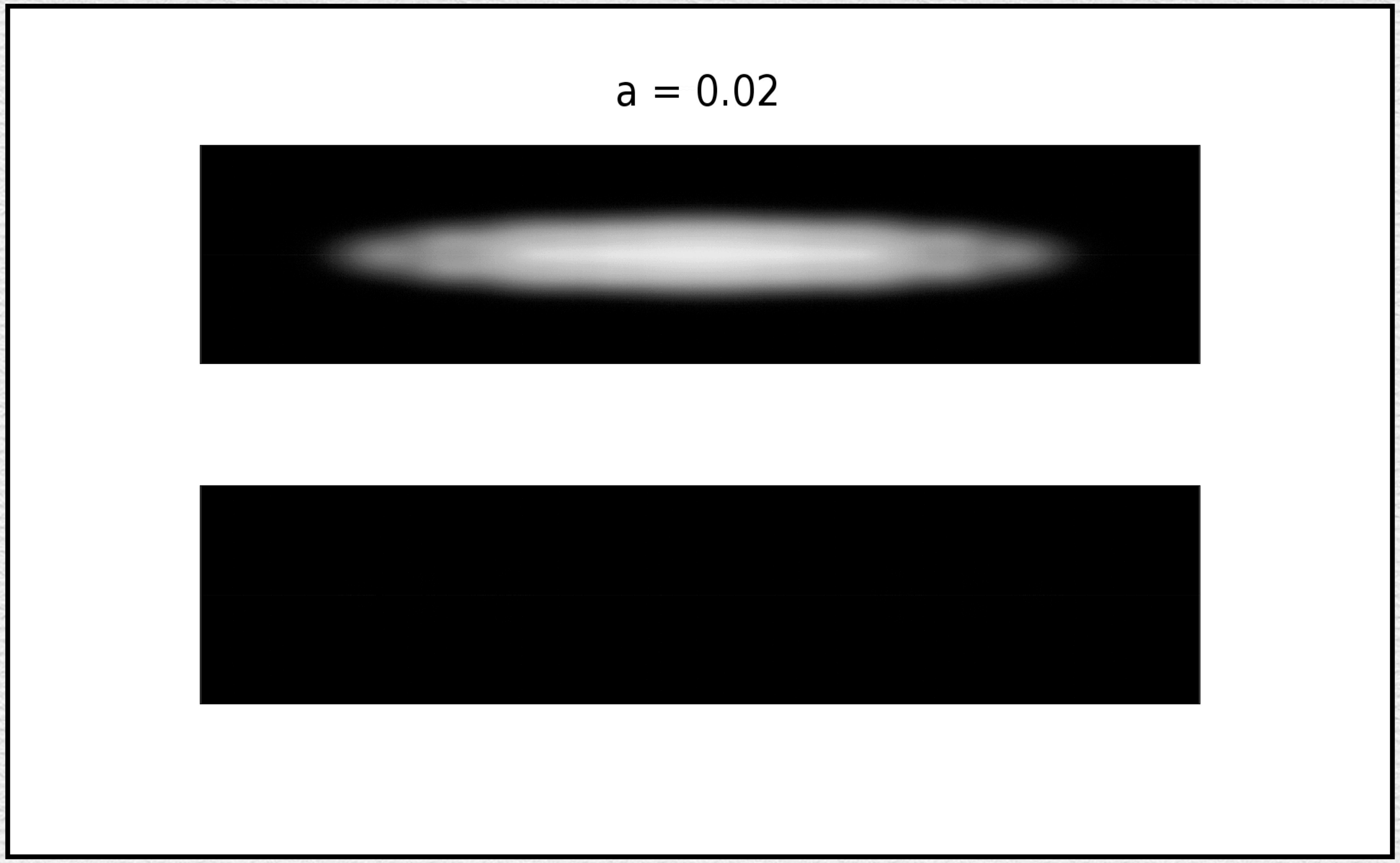
$$\Gamma = \int_{\Omega} d\mathbf{x} \int_{|\mathbf{x}'-\mathbf{x}|<a} d\mathbf{x}' \, n_{\uparrow}(\mathbf{x}) g_{\downarrow\downarrow}(\mathbf{x}, \mathbf{x}')$$



Back to Trap

Jo, Science 2009





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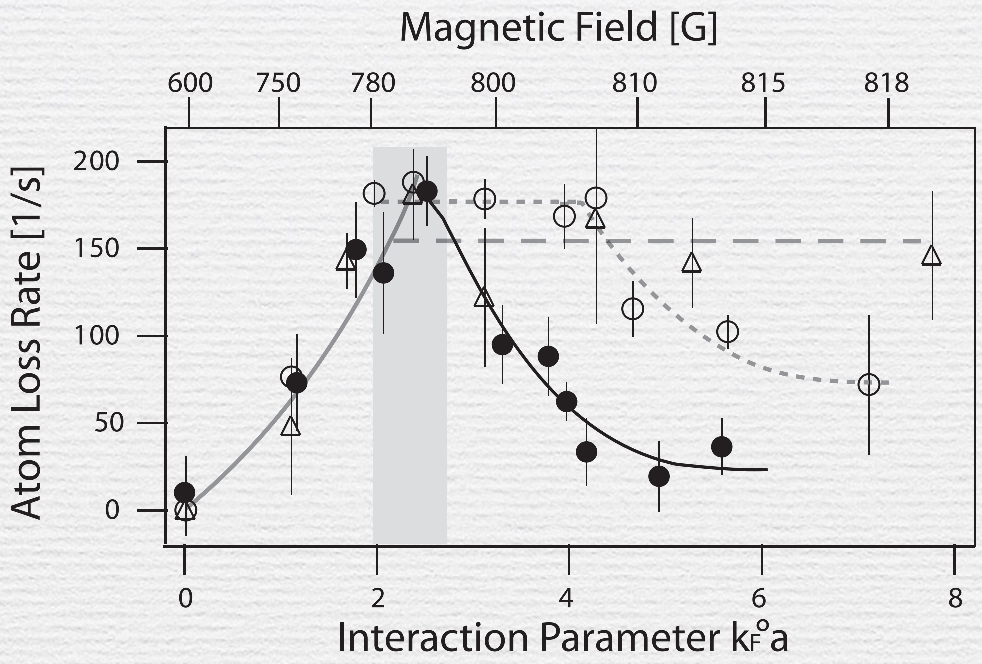
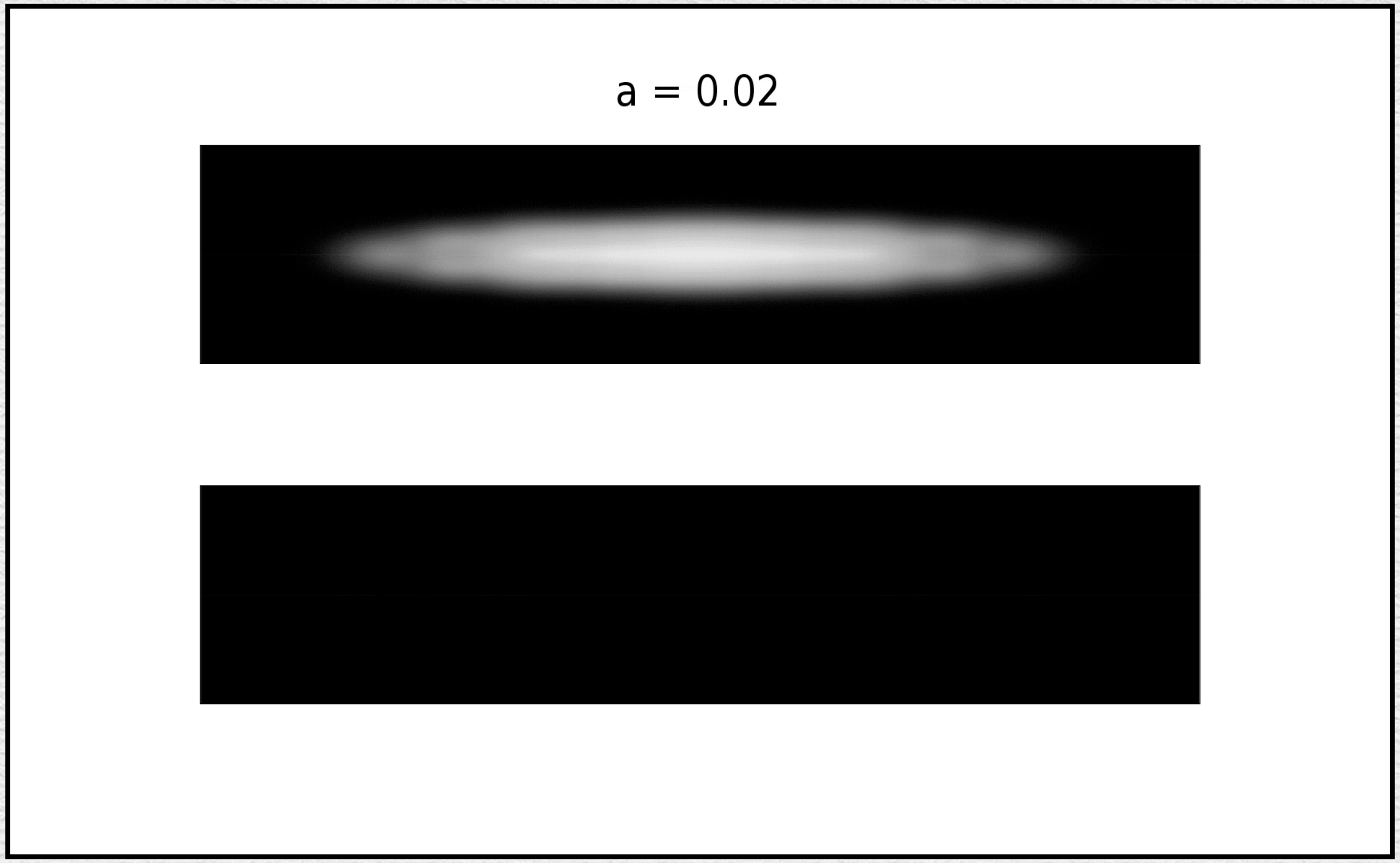
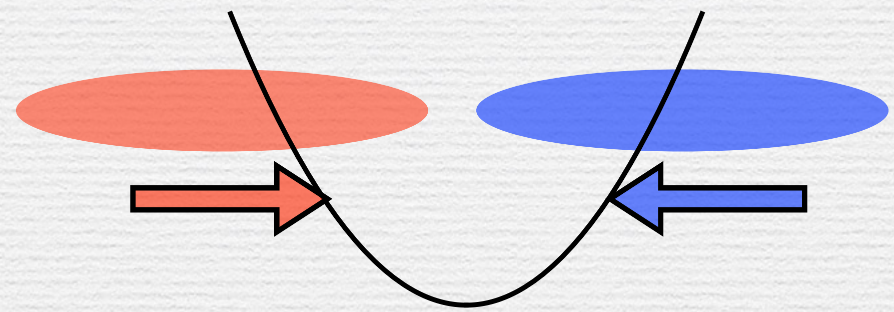
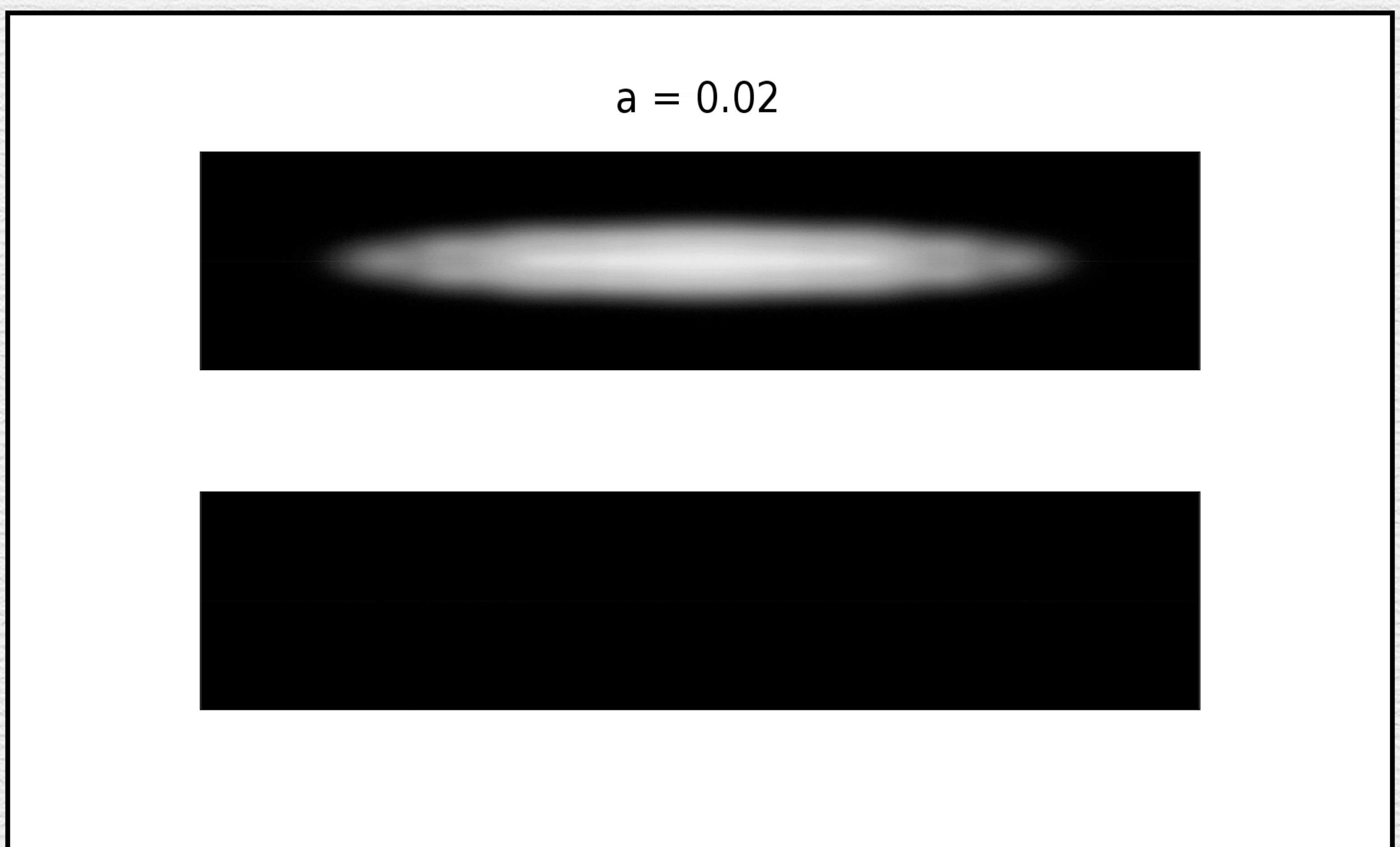




Back to Trap

Sommer, Nature 2011





Time-dependent DFT

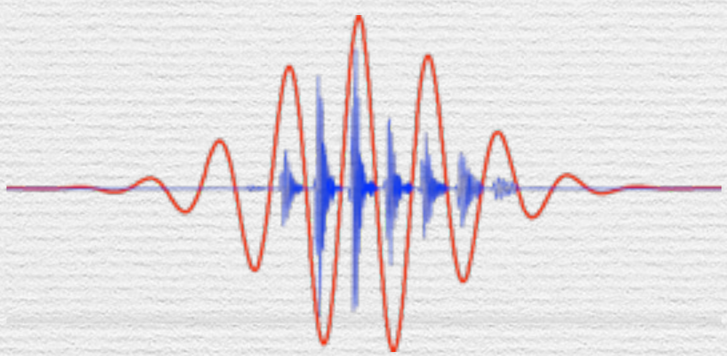
Runge, Gross 1984

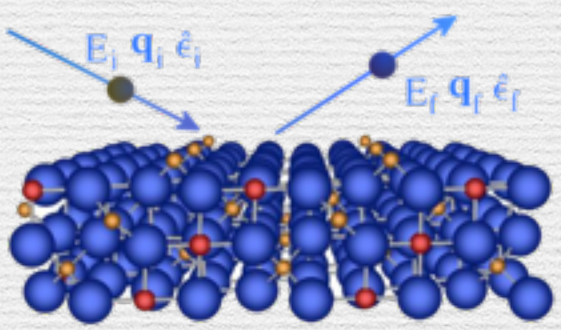
- Time-dependent density obtained from

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

- TDDFT is exact with exact exchange-correlation potential-> adiabatic local-density approximation

- Widely applied to dynamics in chemistry, biophysics and solid-state physics, see http://www.tddft.org/





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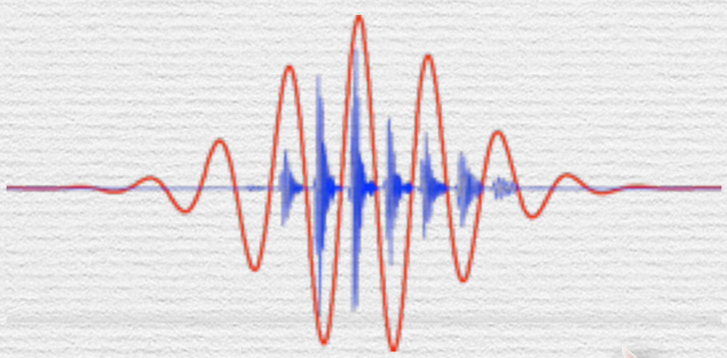
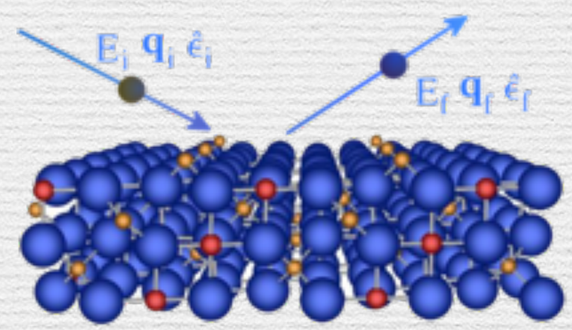
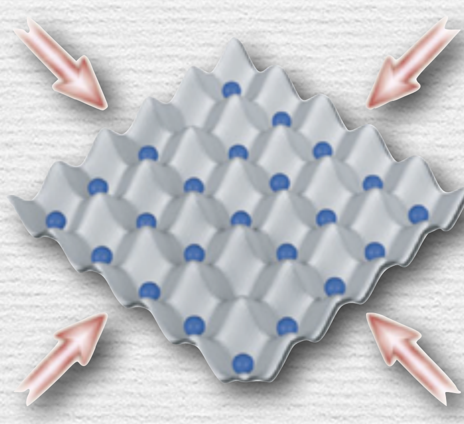
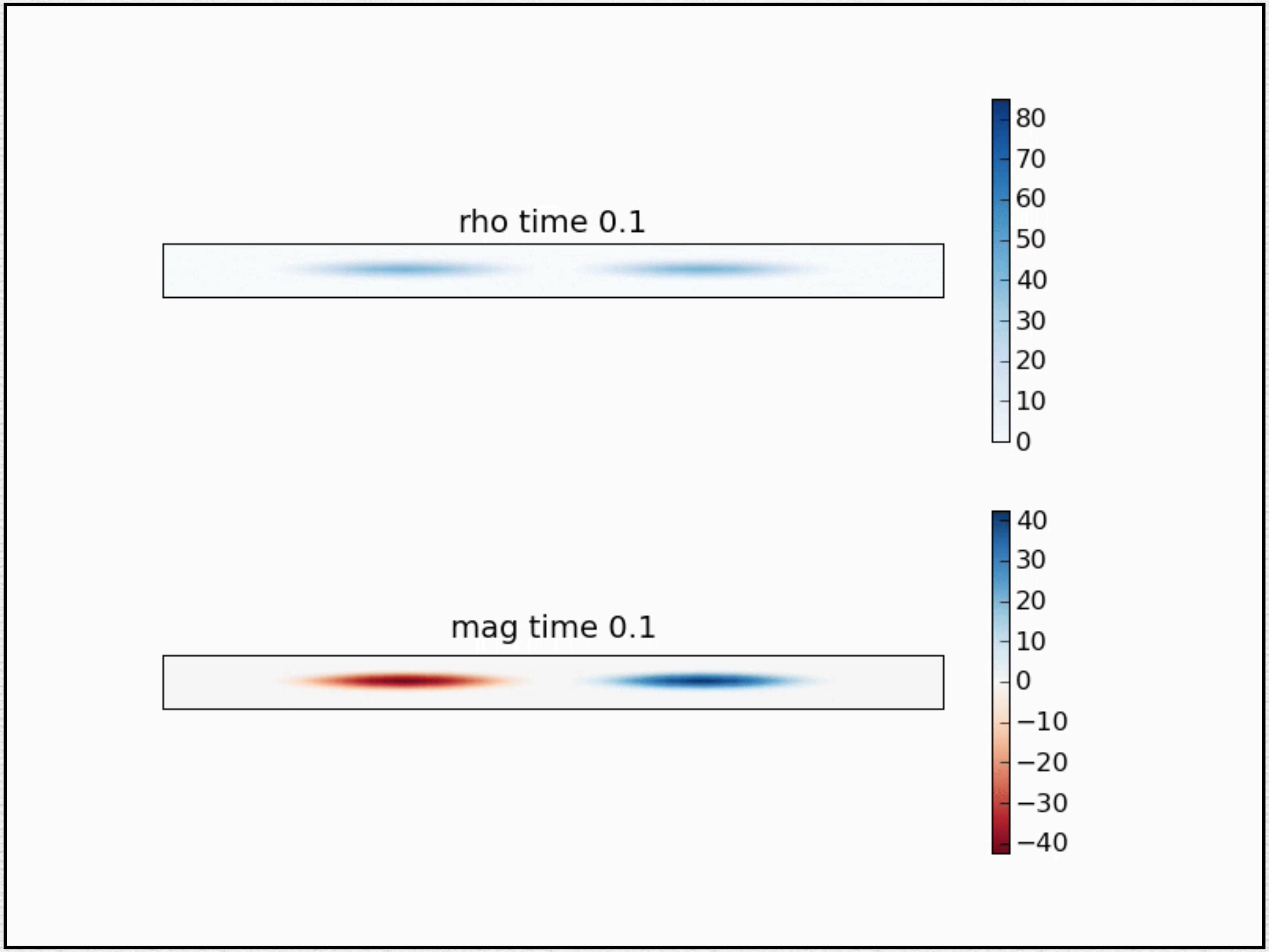






Strongly interacting: Bounce



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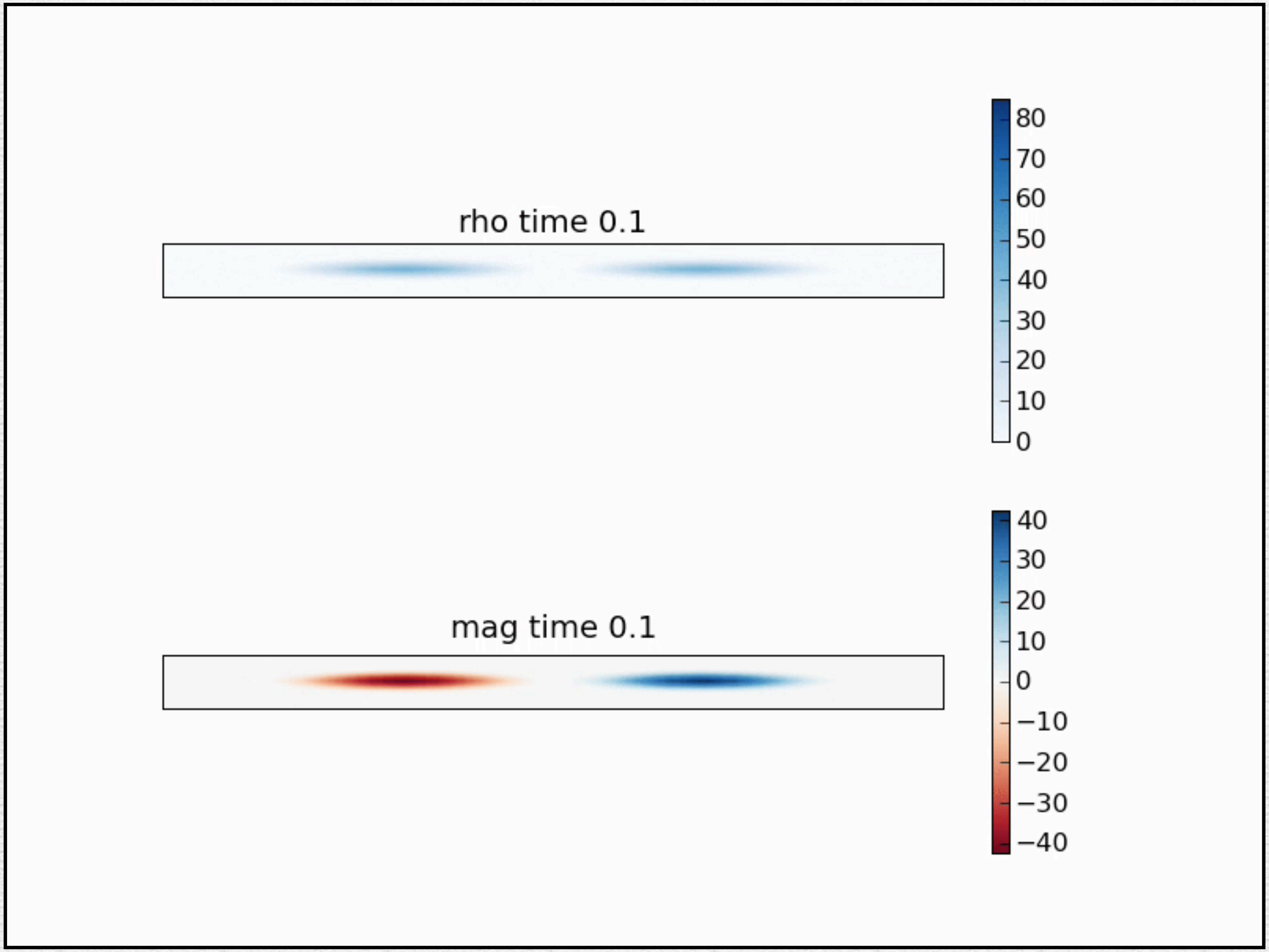
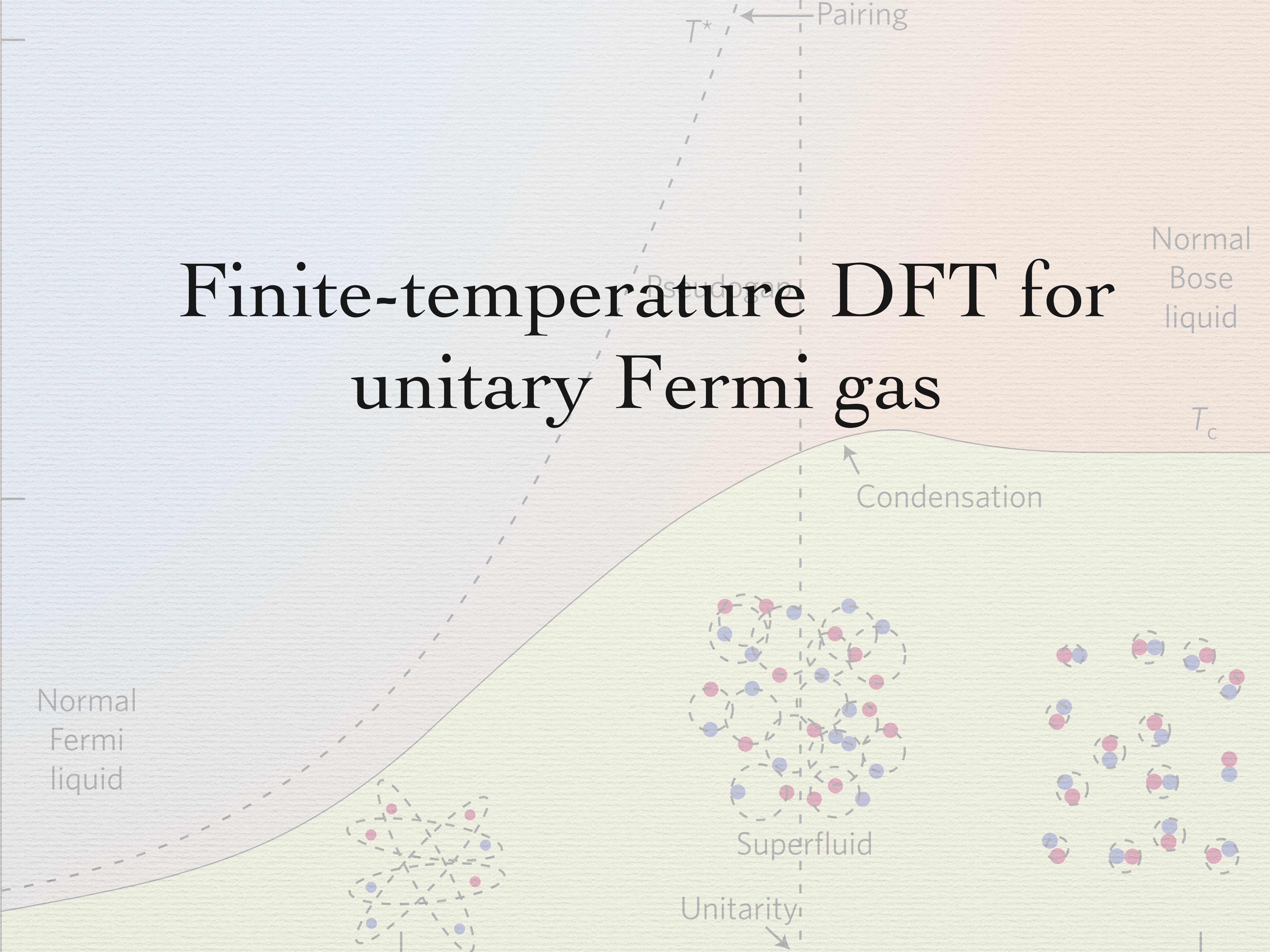
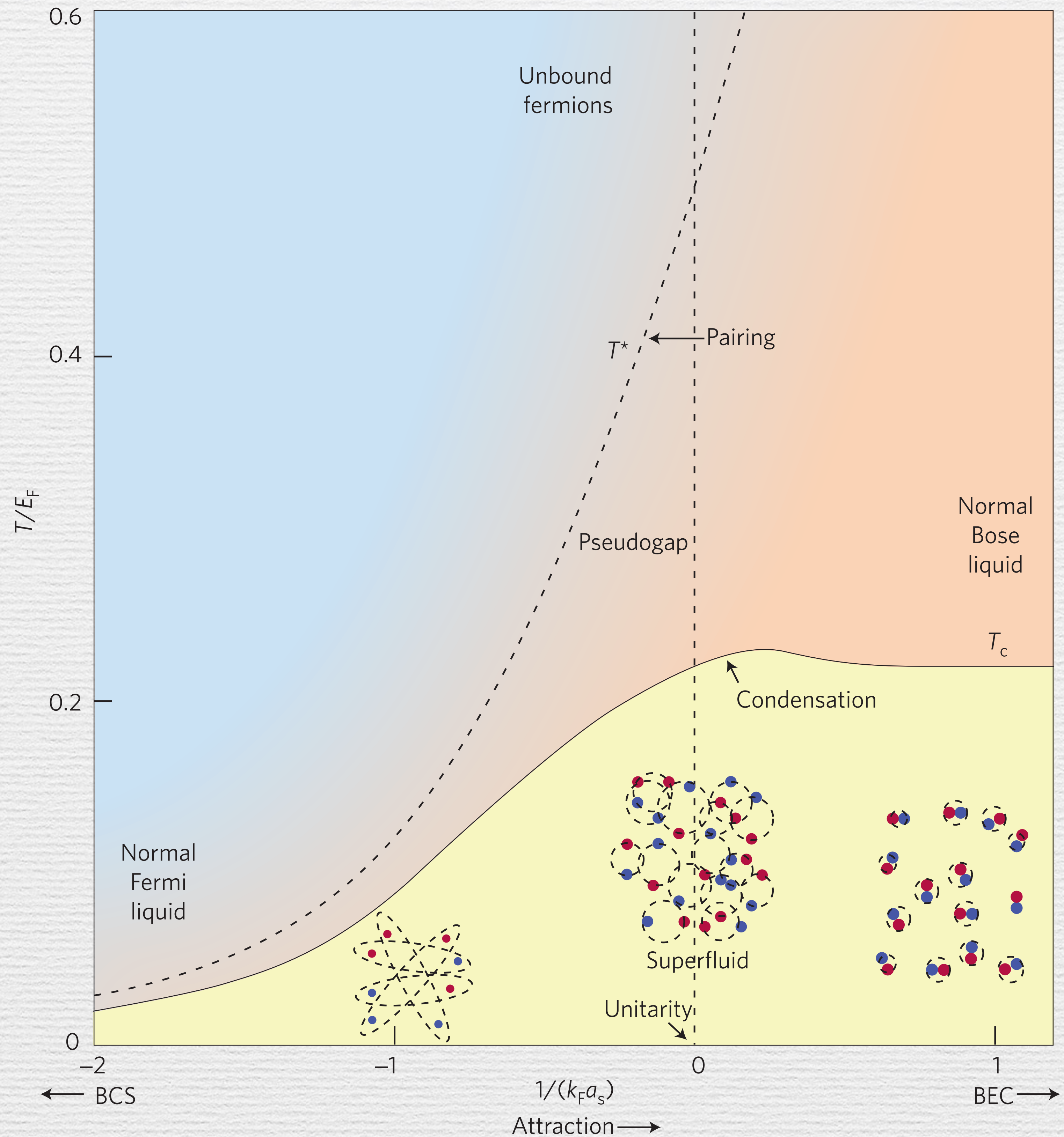


Finite-temperature DFT for unitary Fermi gas



Unitary Fermi gas

Randeria 2010



Unitary Fermi gas

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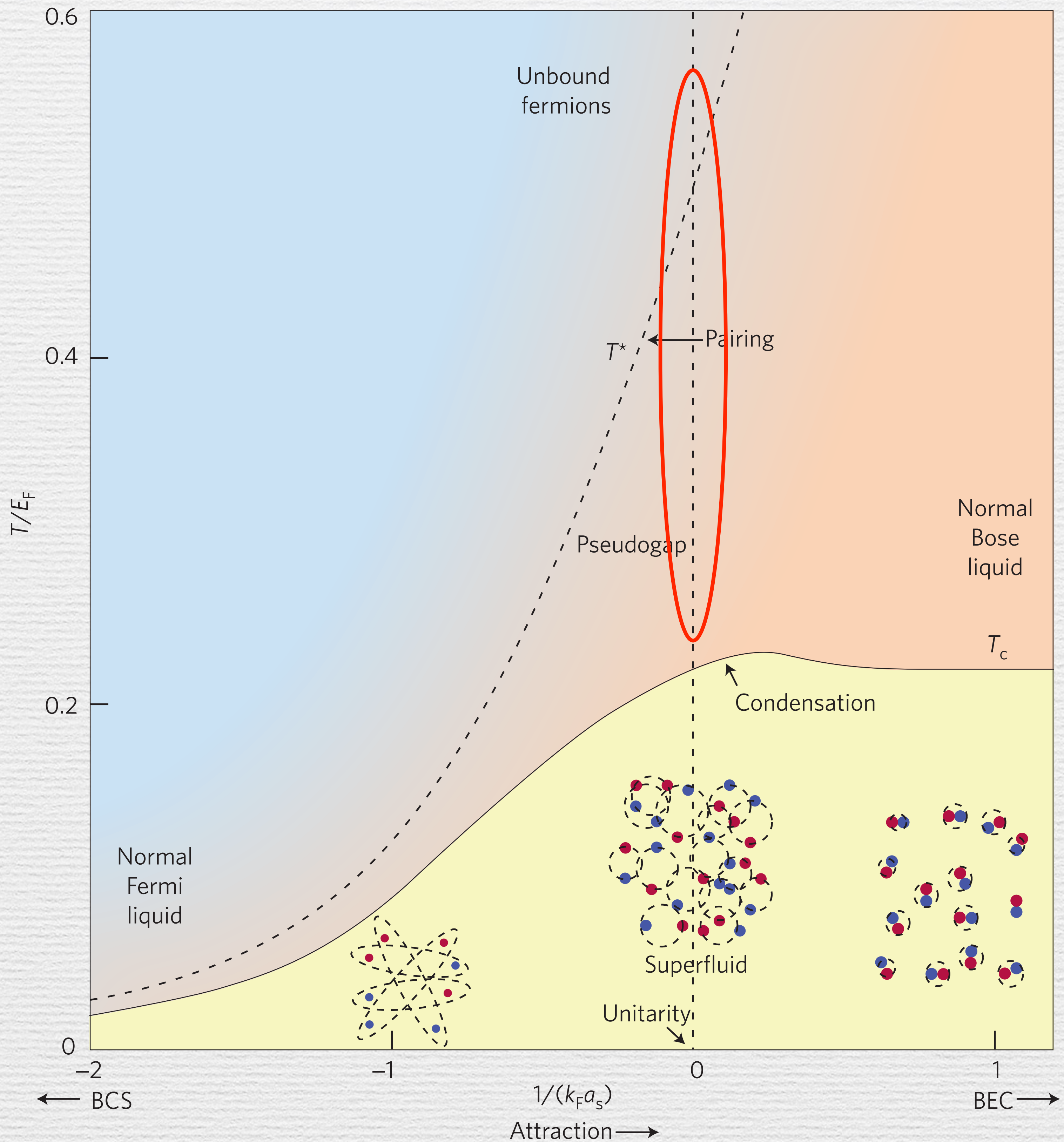

Finite-T DFT

Mermin 1965

Kohn,Sham 1965

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

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$$\downarrow$$

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

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LDA

$$V^T_{\mathrm{HXC}} = \frac{F^T_{\mathrm{HXC}}[\rho]}{\delta\rho} \approx \mu^T(\rho) - \mu^T_0(\rho)$$

Finite-T V_{HXC}

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- Lack of finite-T energy functional

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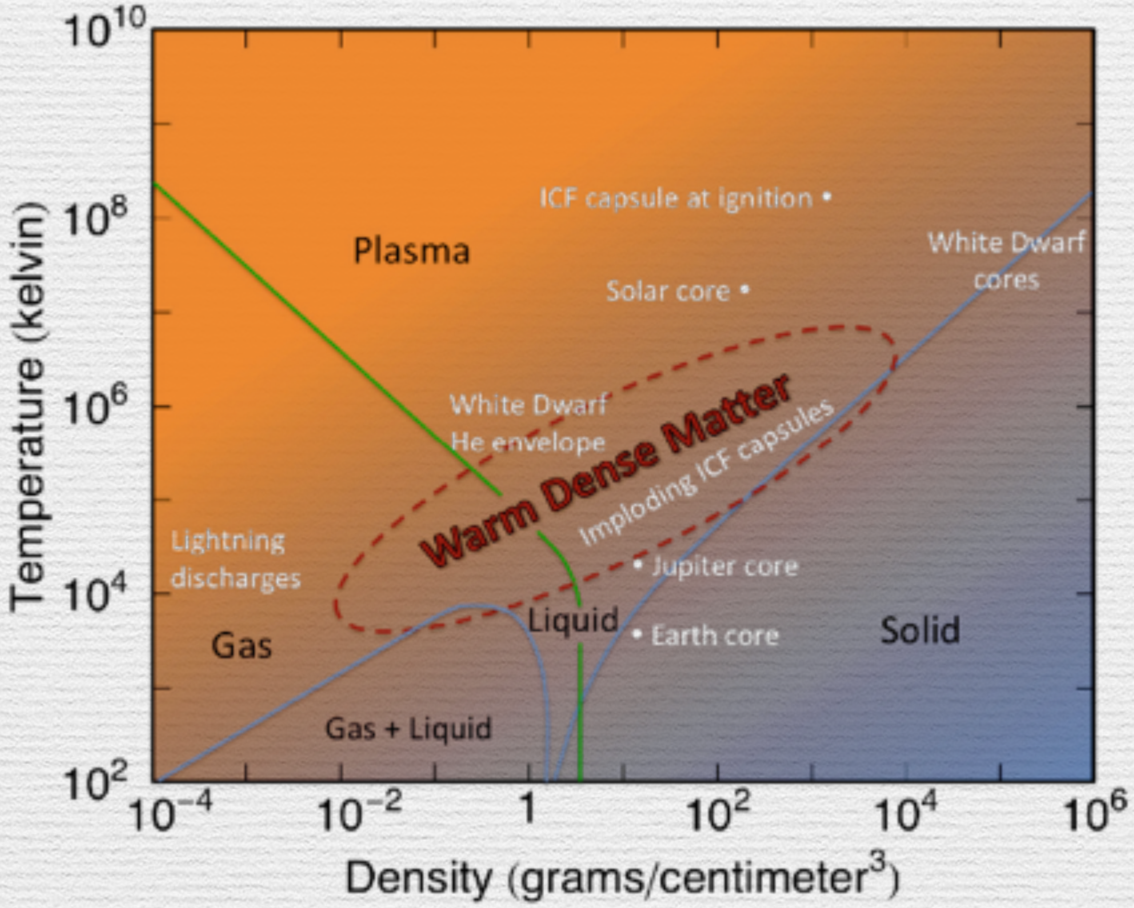

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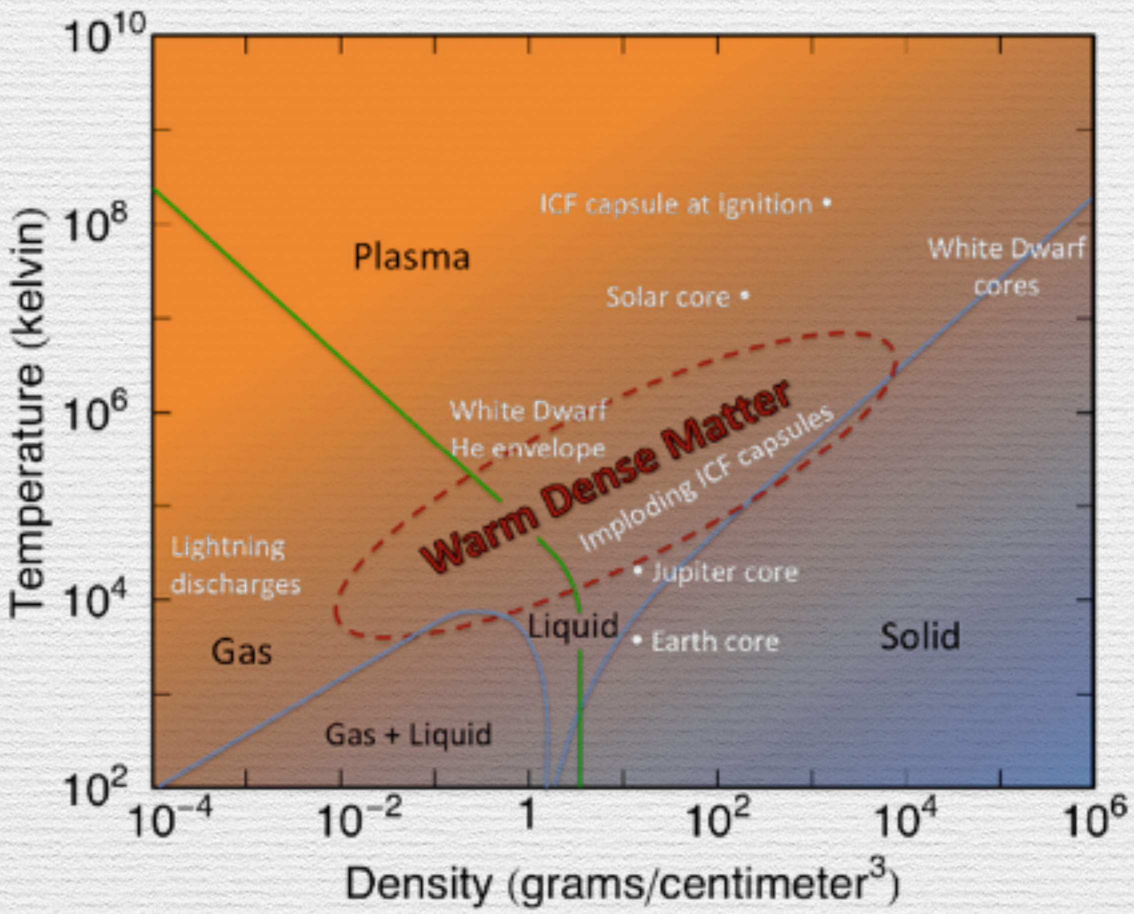

$$T \sim E_F$$

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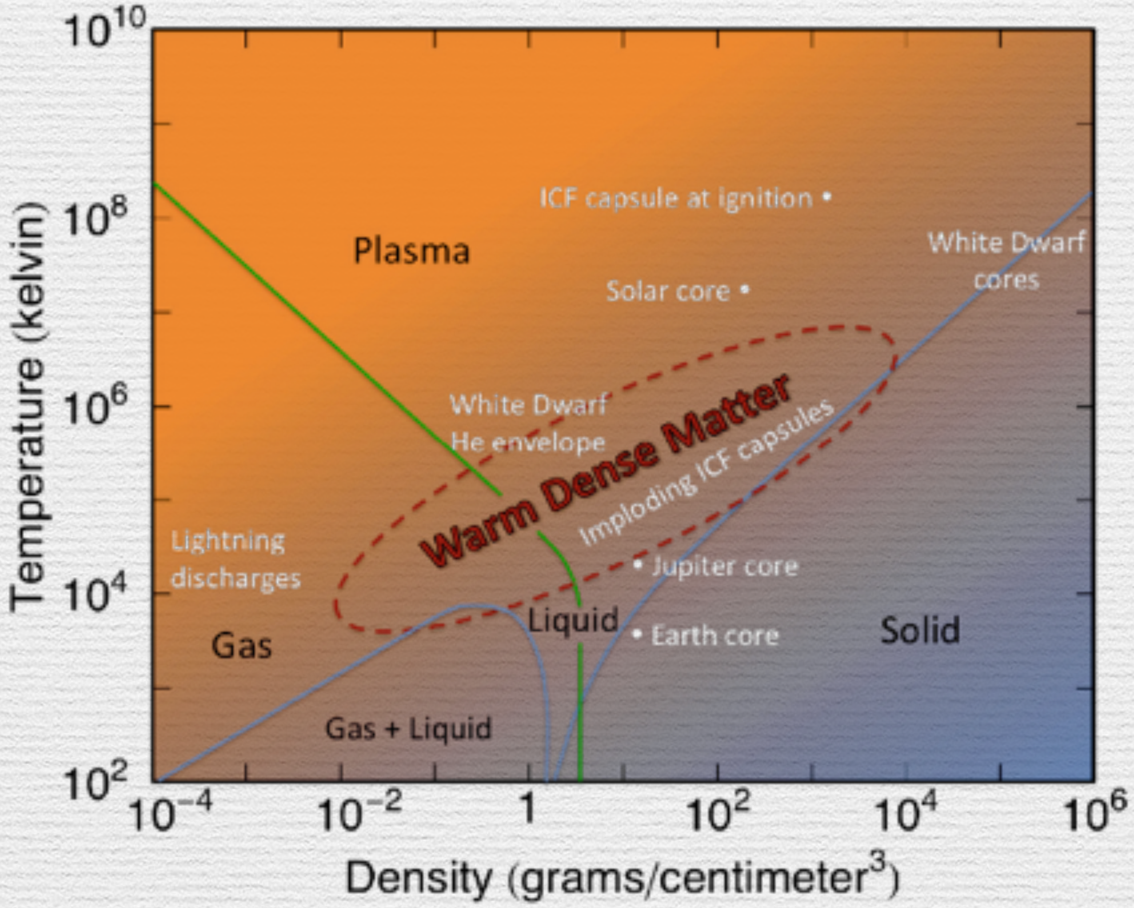
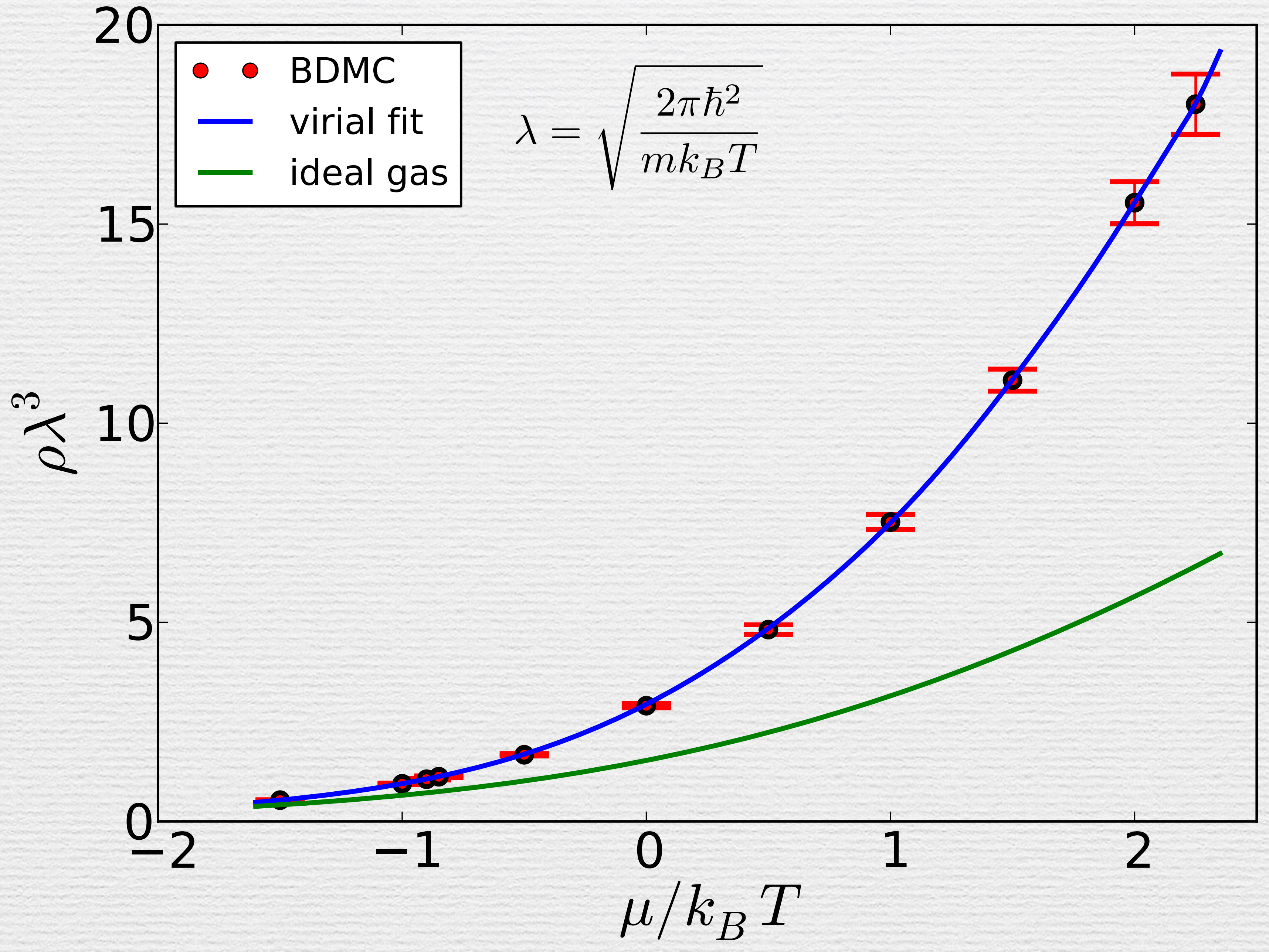


$T \sim E_F$

So does UFG!

V_{HXC} from Bold Diagrammatic MC

Van Houcke 2012 Nature Physics



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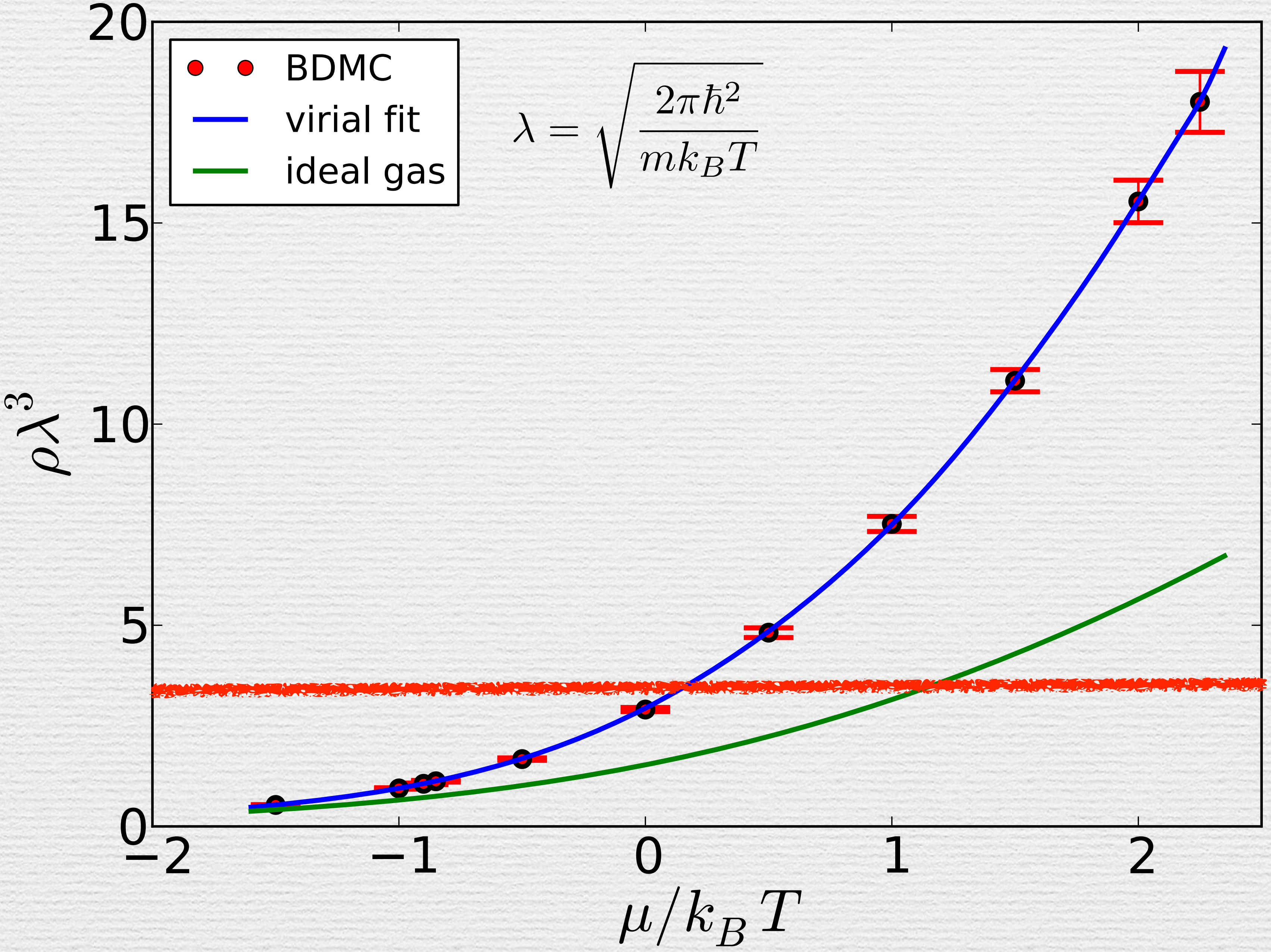

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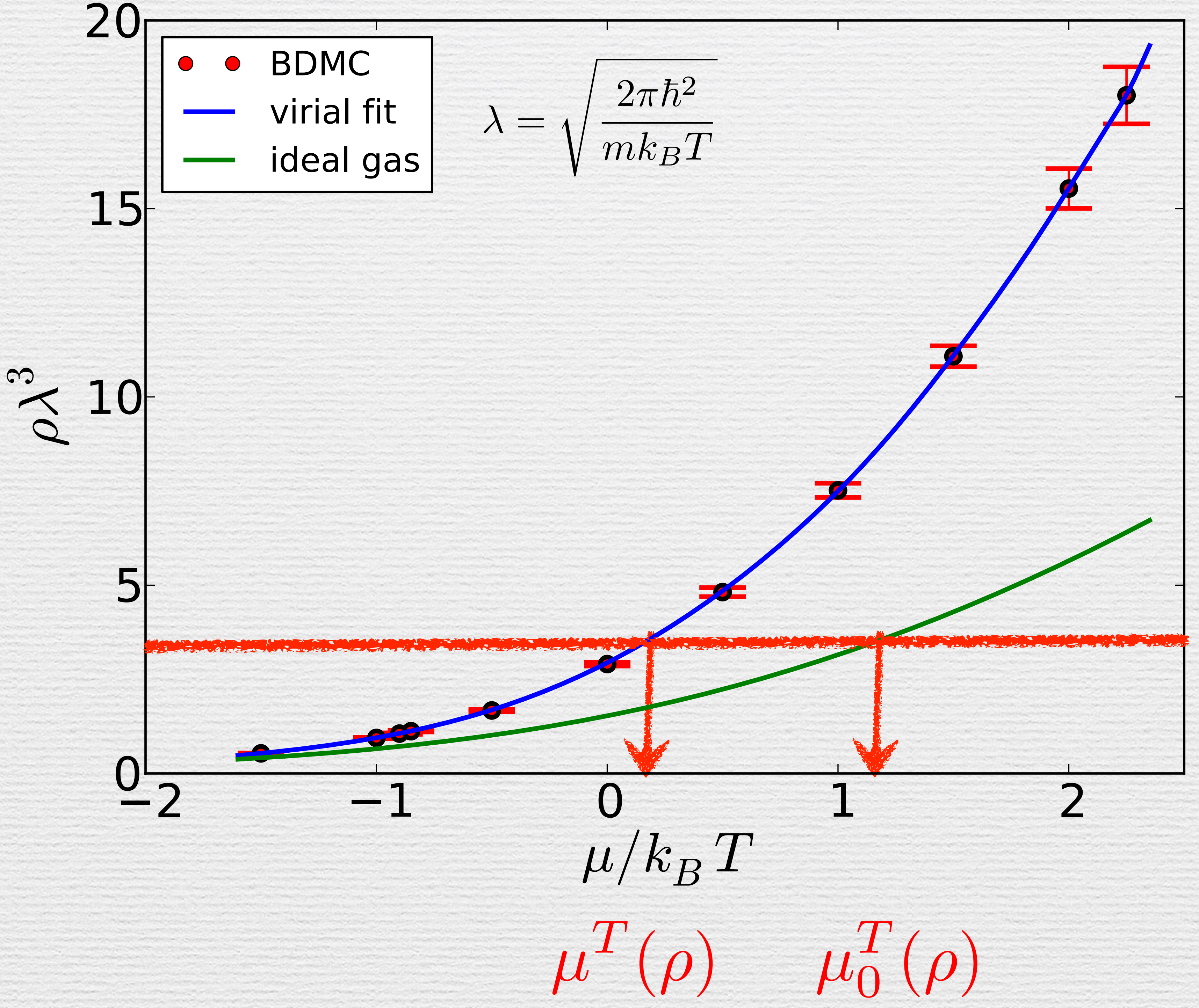

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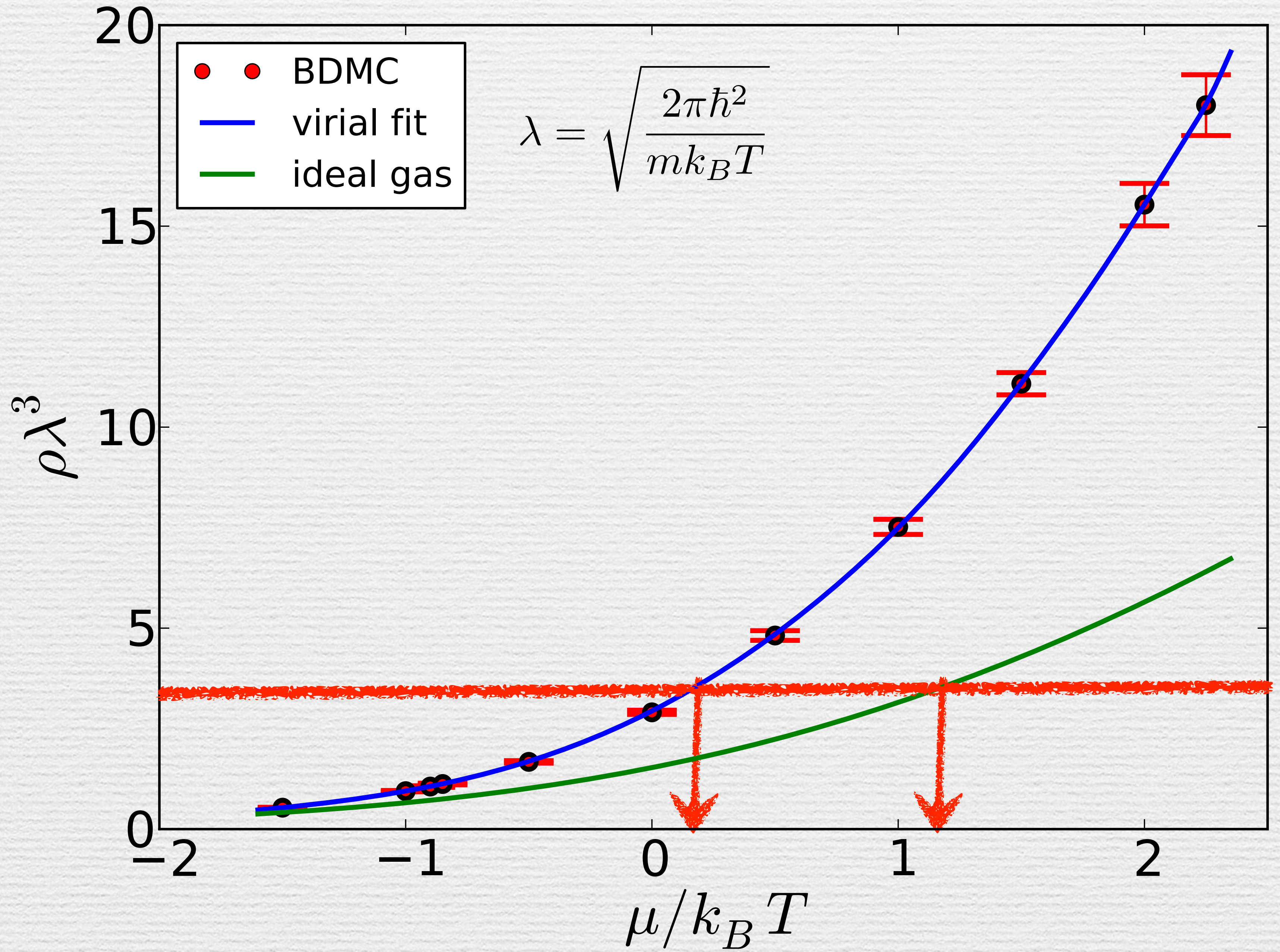
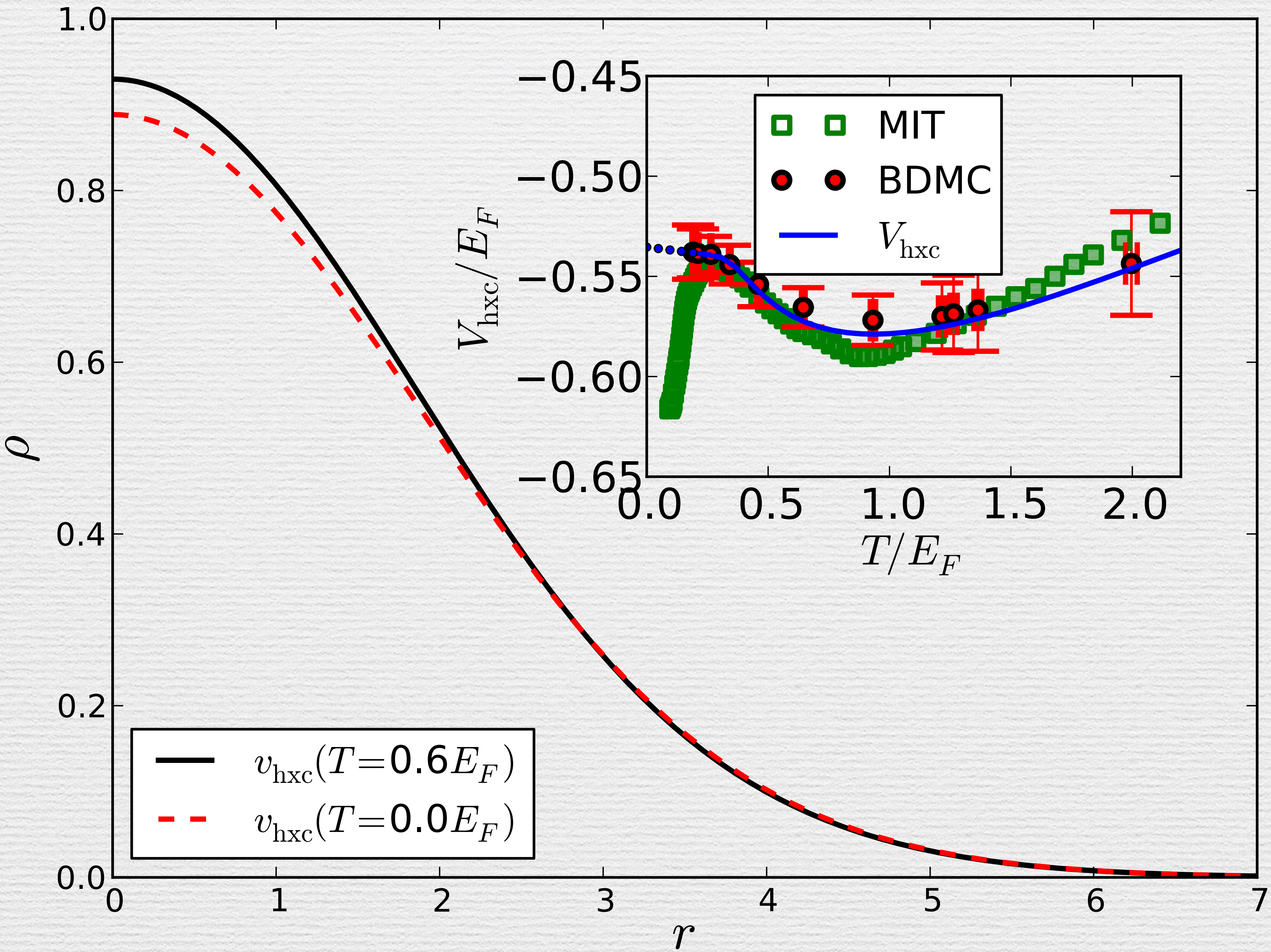
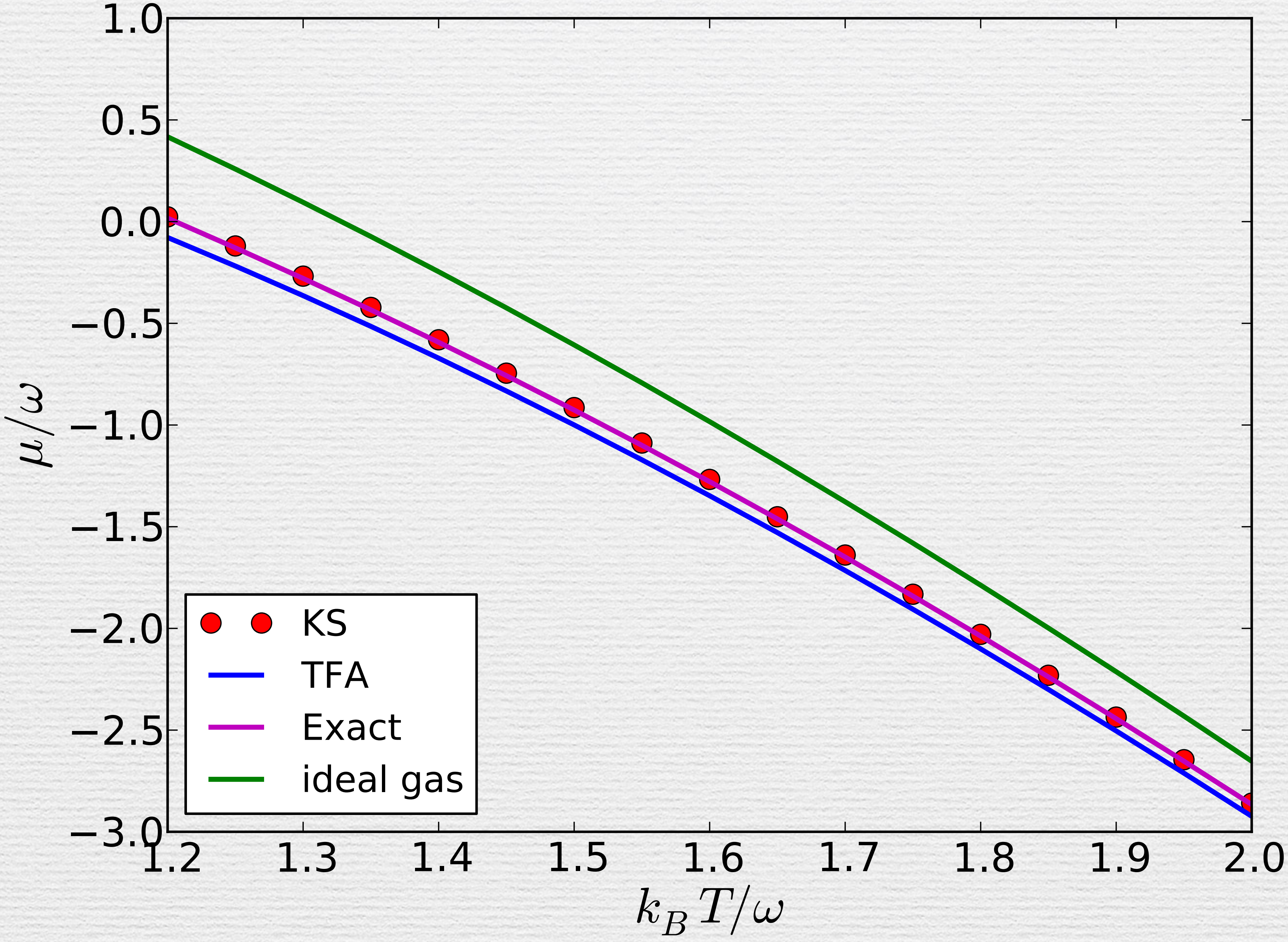


$$V_{\mathrm{HXC}}^{T} = \mu^{T}(\rho) - \mu_0^{T}(\rho)$$

Temperature dependence of V_{HXC}



Four atoms in a trap



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

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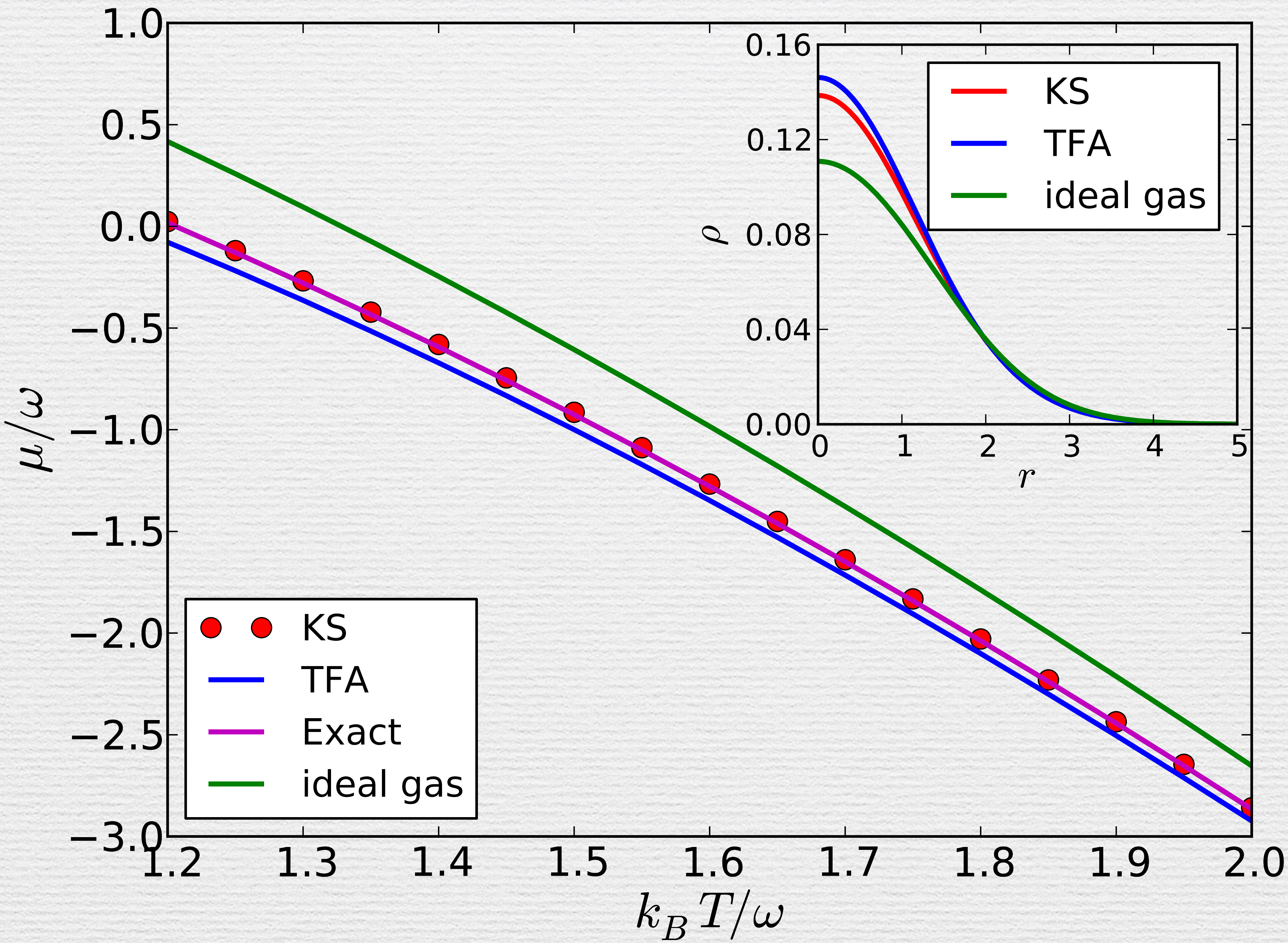

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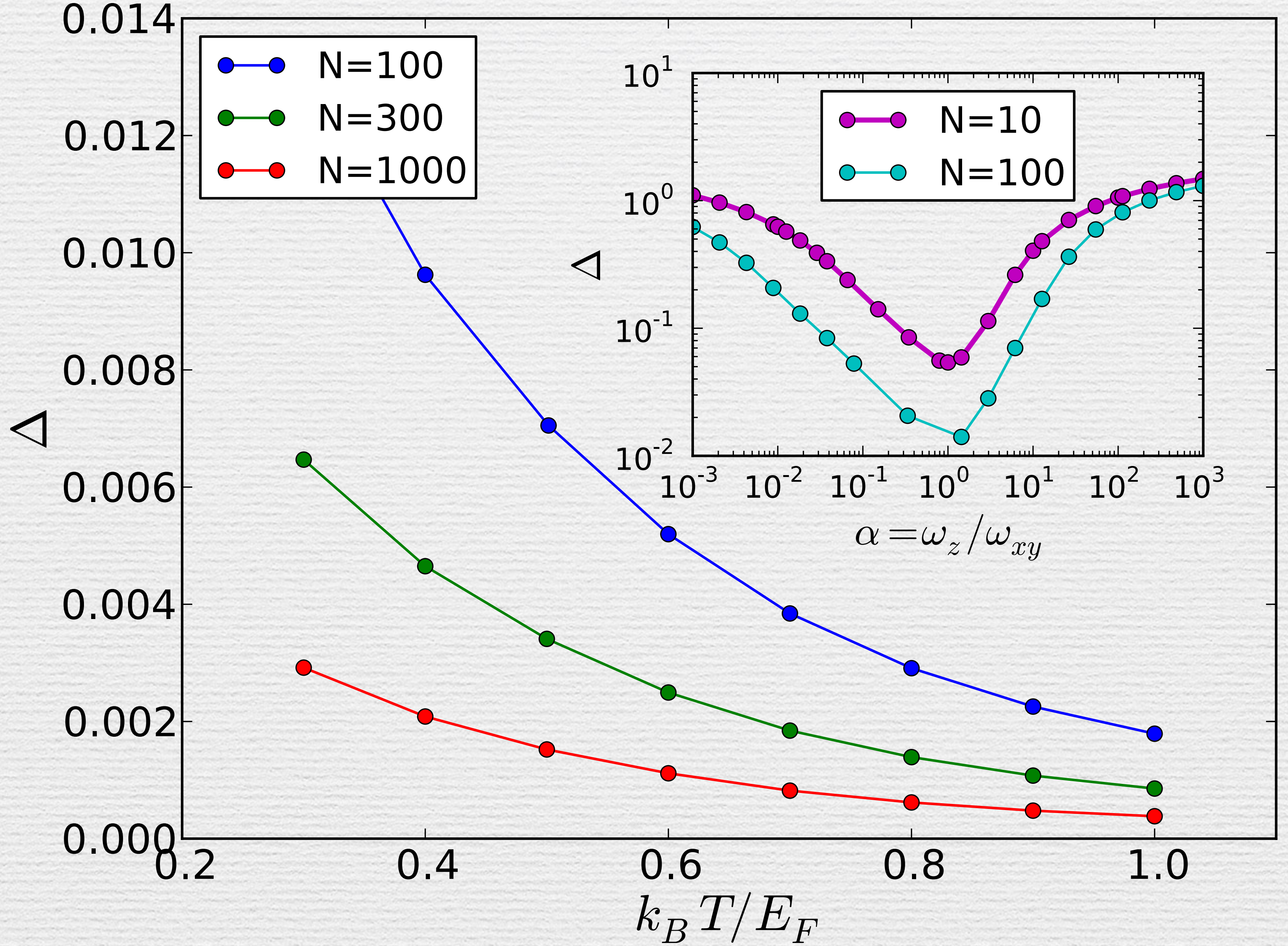
KS vs TFA

$$\Delta = \frac{1}{N}\int d\mathbf{r}|\rho_{\mathrm{KS}}(\mathbf{r}) - \rho_{\mathrm{TFA}}(\mathbf{r})|$$



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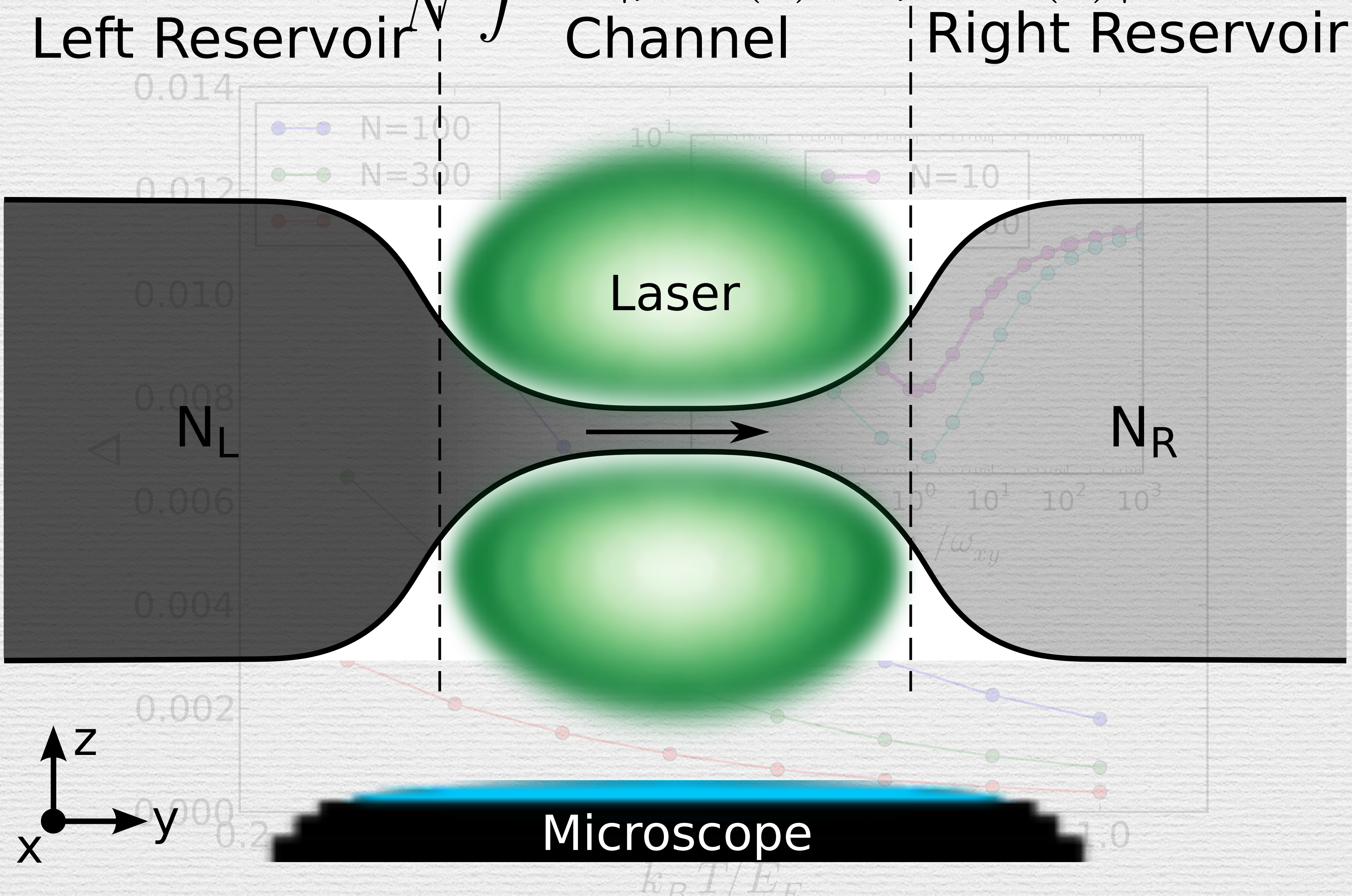
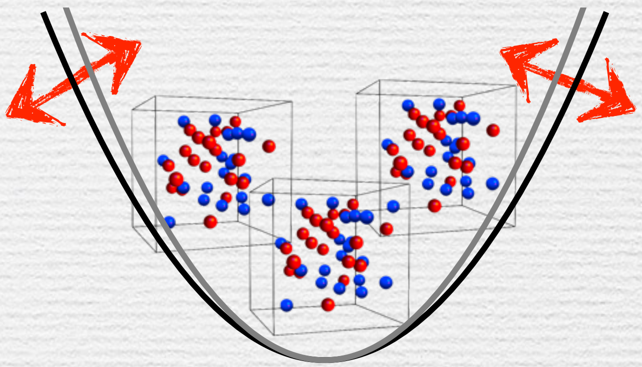
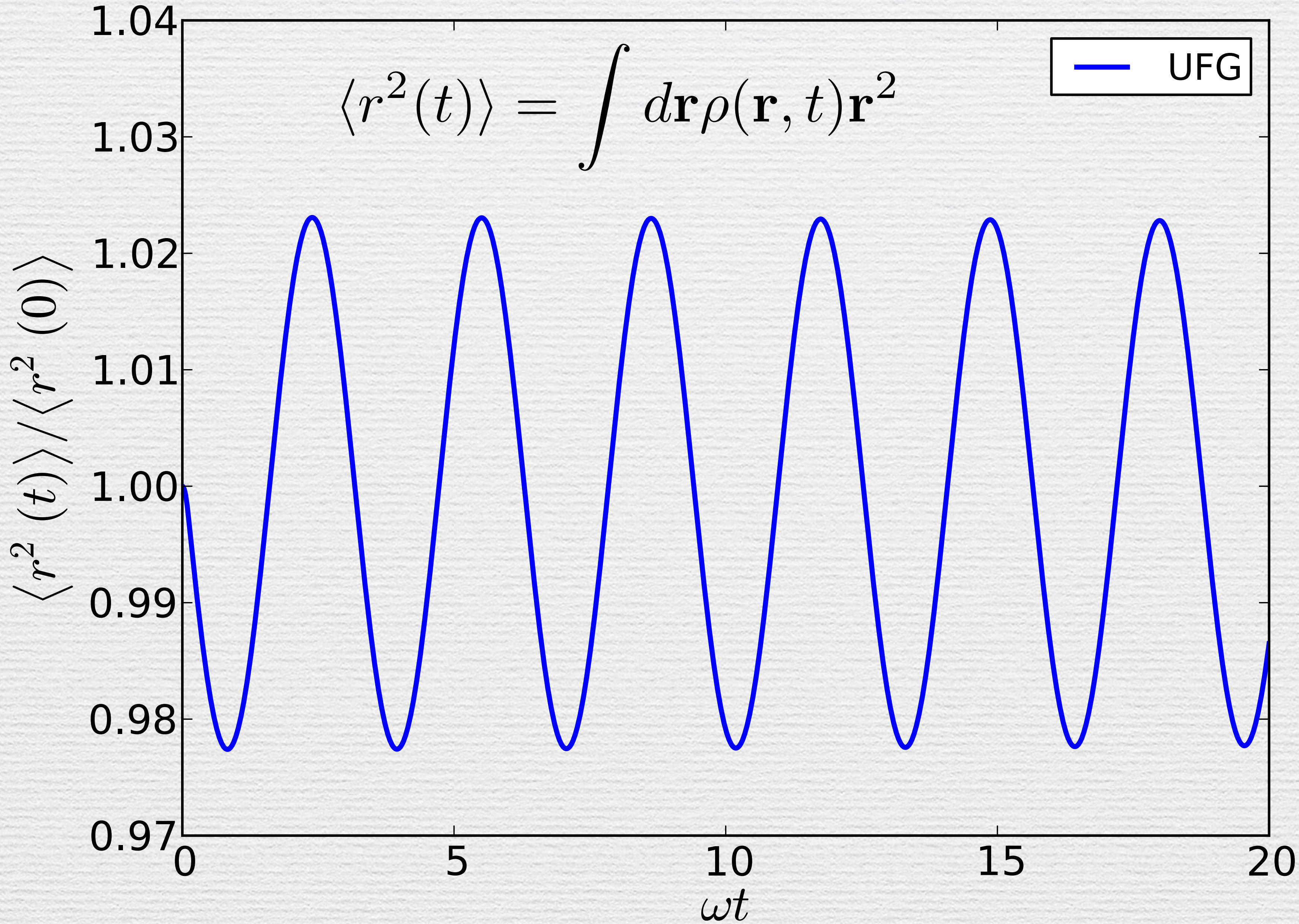


Brantut 2012
Talk on Thursday

Breathing mode

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





cf vanishing bulk viscosity of UFG
Castin 2004, Son 2007

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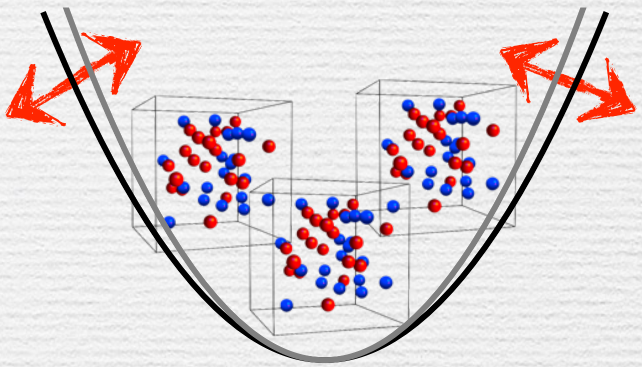

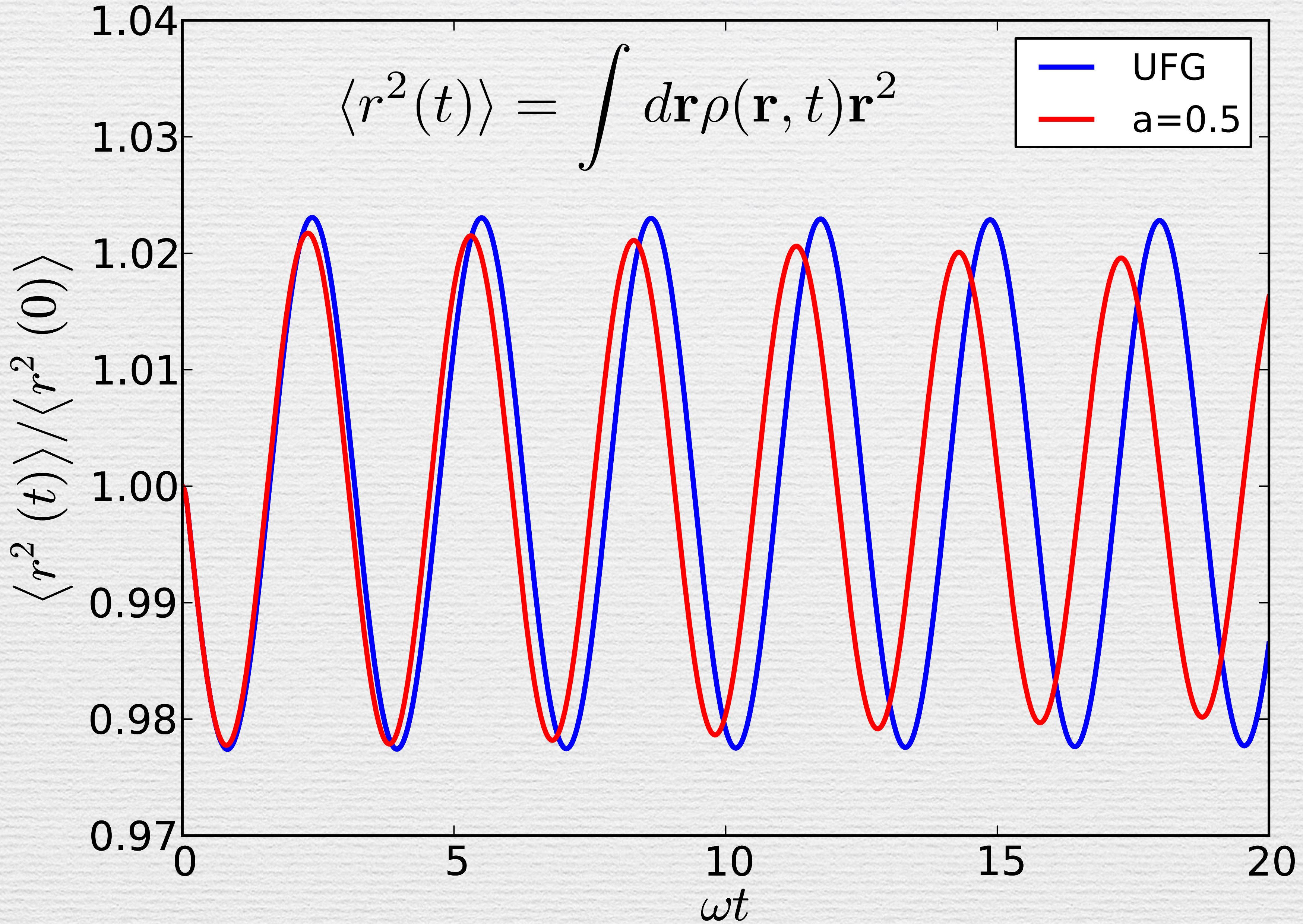

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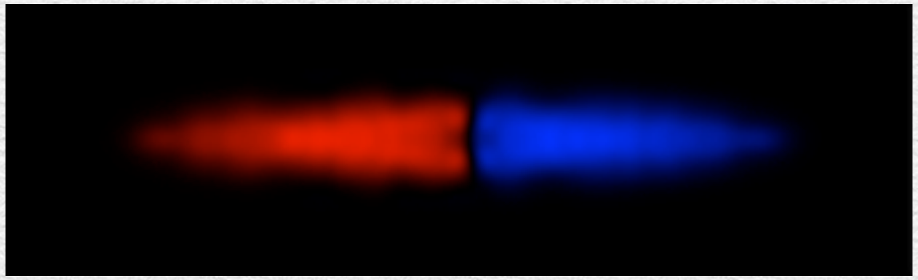
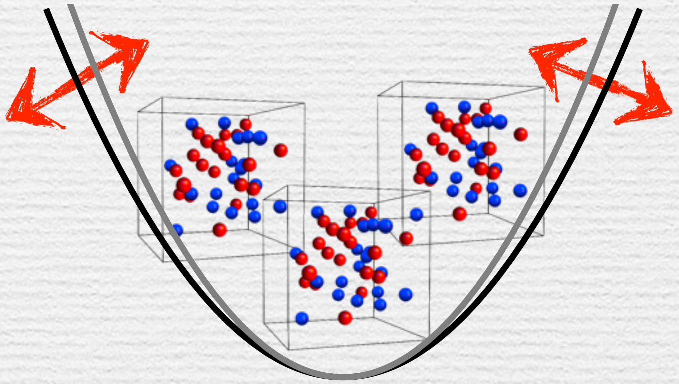
Summary & Outlook

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





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

Thank you!