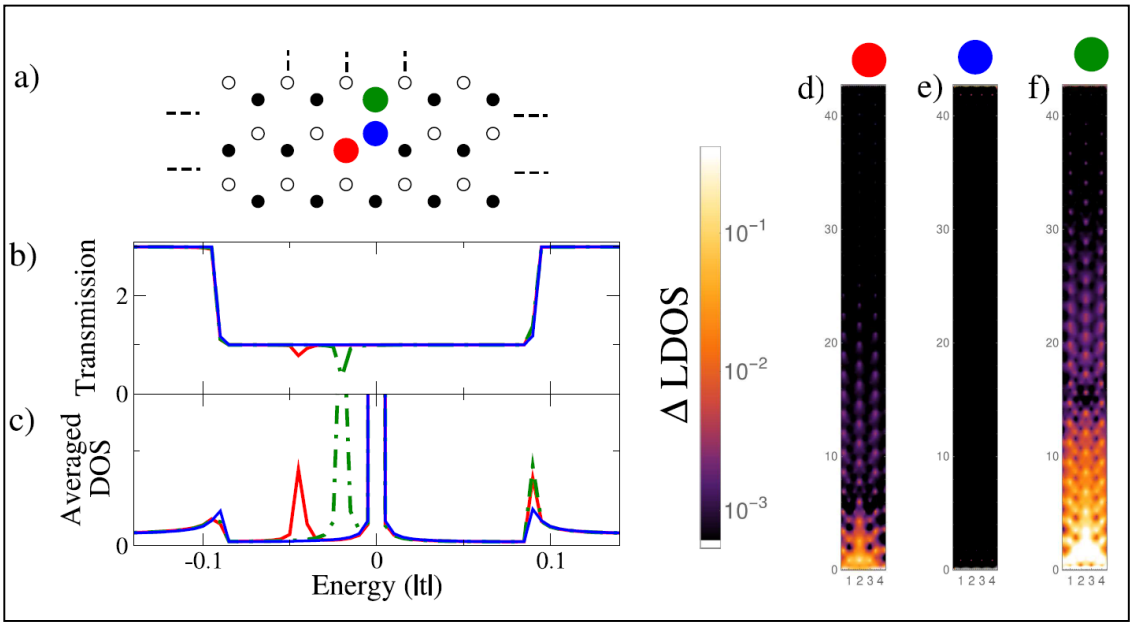
Center for Nanostructured Graphene

Graphene nanoribbons with sublattice-asymmetric doping

Thomas Aktor, Antti-Pekka Jauho and Stephen R. Power

Aktor et al. (2016) Phys. Rev. B., Vol. 93, 035446.

- Effects of breaking sublattice symmertry in graphene with doping.
- Interaction with edges in graphene nanoribbons.
- Density of states and transport.
- Interfaces and channels.



DTU Nanotech
Department of Micro- and Nanotechnology

Center for Nanostructured Graphene (CNG), DTU Nanotech,
Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark

Danmarks Grundforskningsfond
Danish National Research Foundation

DTU Danmarks Tekniske Universitet

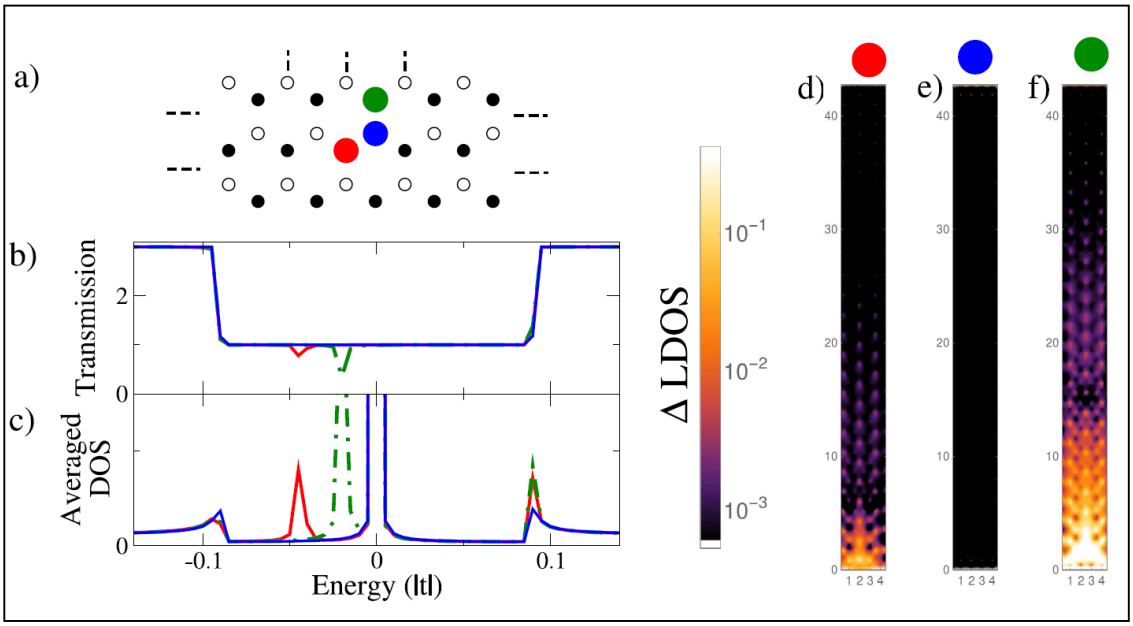
Center for Nanostructured Graphene

Graphene nanoribbons with sublattice-asymmetric doping

Thomas Aktor, Antti-Pekka Jauho and Stephen R. Power

Aktor et al. (2016) Phys. Rev. B., Vol. 93, 035446.

- Effects of breaking sublattice symmertry in graphene with doping.
- Interaction with edges in graphene nanoribbons.
- Density of states and transport.
- Interfaces and channels.



DTU Nanotech
Department of Micro- and Nanotechnology

Center for Nanostructured Graphene (CNG), DTU Nanotech,
Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark

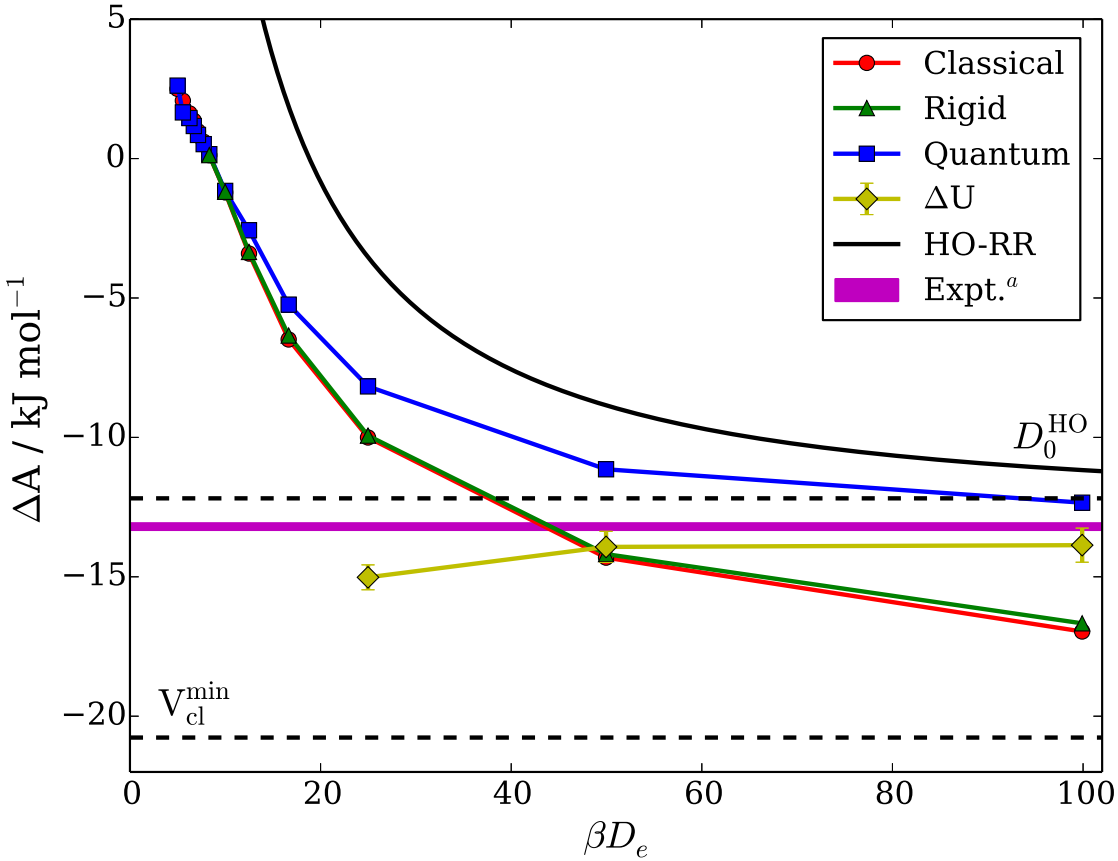
Danmarks Grundforskningsfond
Danish National Research Foundation

DTU Danmarks Tekniske Universitet

Quantum free energy calculations of the water dimer

Kevin Bishop*, Matthew Schmidt, Pierre-Nicholas Roy
University of Waterloo

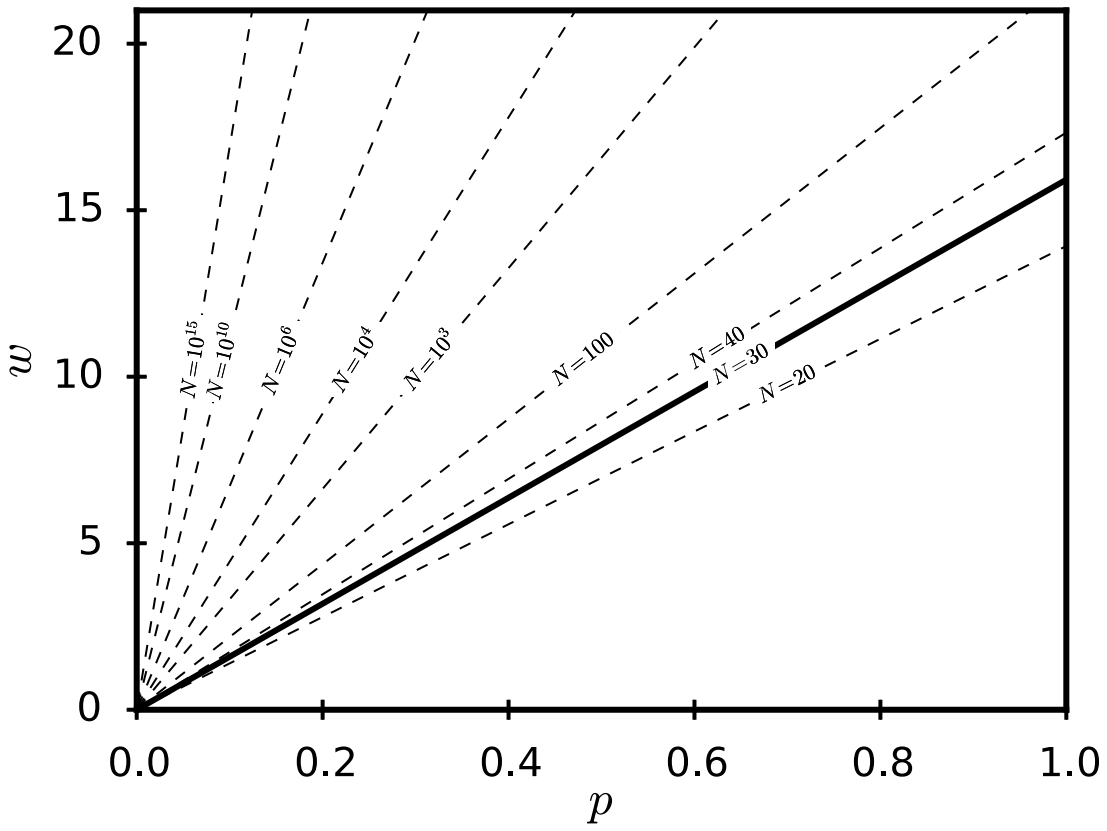
- Utilize path integral molecular dynamics and umbrella sampling methods to obtain free energy as a function of temperature
- Test classical and ground state limits against known methods and experiments



Quantum localization of particles with dipolar hopping in three-dimensional lattices of finite size

Joshua T. Cantin, Tianrui Xu, Roman V. Krems

University of British Columbia
Vancouver, BC



- Dipolar hopping has no localization transition for *infinite* 3D systems
- The localization transition exists for **FINITE** 3D systems
  - Even macroscopically large, but finite, systems
  - Caused by a finite number of resonances
- The location of the localization transition line changes logarithmically with the system size

Electronic Band Structure of $MgZn_2$ using first principle approach

Adwait Mevada, N.Y. Pandya, and **P. N. Gajjar**

Department of Physics, University School of Sciences, Gujarat University, Ahmedabad, 380009, Gujarat, India
Email: *pngajjar@rediffmail.com*

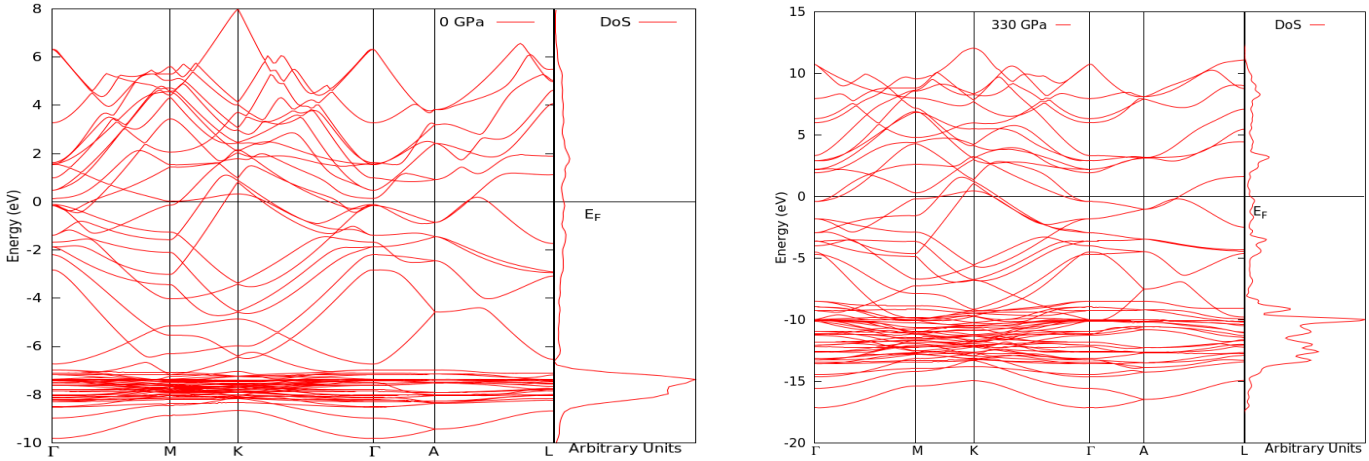
$MgZn_2$ is c14 type Laves phase having hexagonal lattice with a=5.15Å and b=8.48 Å [1]. The space group is *P63/mmc (No. 194)* and pearson symbol is *hP12*. It has 12 atoms in primitive unit cell.

In this paper we study the electronic properties of $MgZn_2$ at different pressures using DFT as applied within Quantum ESPRESSO package [2].

Ultrasoft pseudopotential along with GGA using PBE scheme was used to describe the electron-ion and electron exchange and correlation energies.

Kinetic energy and charge density cutoffs were set at 100 Ry and 800 Ry respectively to ensure convergence within 1mRy limit.

Brillouin zone sampling with a k-point mesh of 8x8x8 for the unit cell and smearing of thickness 0.02 Ry.



- There is no band gap in band structure at 0 or 330 Gpa.
- E_F = 9.1628 eV at 0 GPa and E_F =24.075 eV at 330 GPa.
- The dense collection of bands below Fermi level is due to 3d orbitals of Zn.
- The 3d orbitals are main contributors to tdos.
- In absence of pressure 3d orbitals are flat and dense.
- The band structure at 330 Gpa is more spaced and less dense compared to 0 Gpa state.
- On application of pressure the single peak in tdos becomes roughly a plateau of half the initial peak height.

Acknowledgements

Support under DST-FIST Level-I program from Department of Science and Technology, Government of India, New Delhi and DRS-SAP-I from University Grants Commission, New Delhi is highly acknowledged.

References

[1] J. B. Friauf, The crystal structure of Magnesium di-Zincide, Phys. Rev., **29**, 34 (1927)
[2] P. Giannozzi et al., http://www.quantum-espresso.org

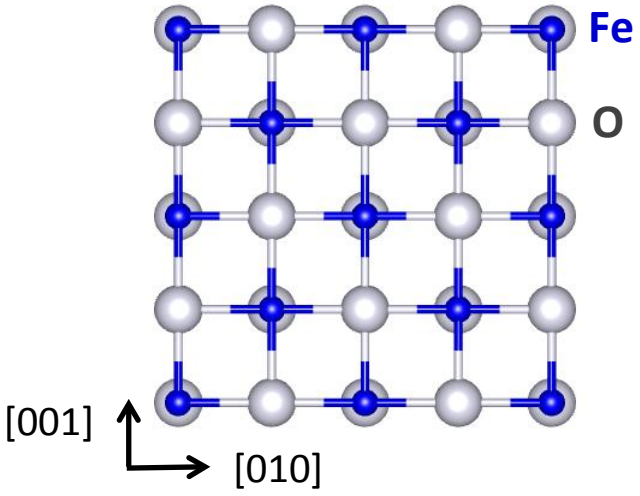
Magnetically induced distortion of the O sublattice in FeO

I. Bernal-Villamil, S. Gallego

Instituto de Ciencia de Materiales de Madrid, CSIC. 28049 Madrid, Spain

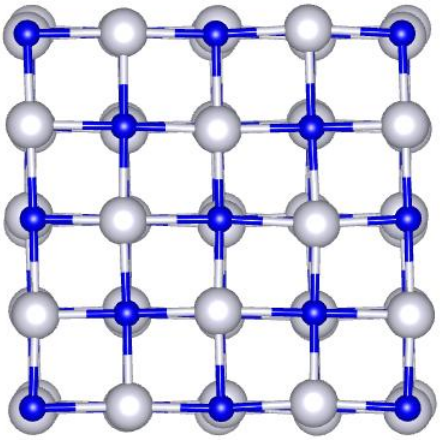
Non-magnetic

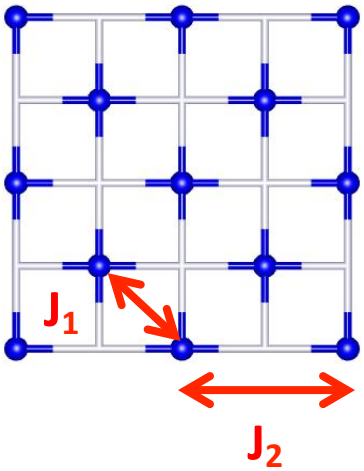
Cubic



Magnetic (AF-II)

Rhombohedral
+
O Sublattice distortion





The O sublattice distortion arises to equilibrate the balance between exchange constants and preserve the AF-II order.

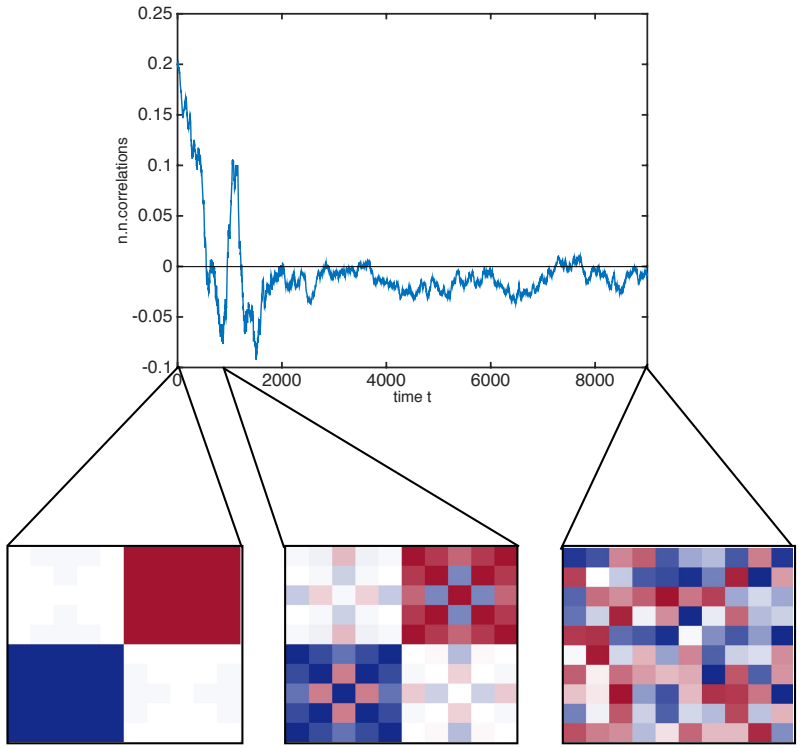
Method: DFT+U, mapping to Heisenberg

Universität Hamburg
DER FORSCHUNG | DER LEHRE | DER BILDUNG

I. Institut für Theoretische Physik
Universität Hamburg

Real-time dynamics in the Kondo lattice model with classical spins

Lena-Marie Gebauer, Mohammad Sayad and Michael Potthoff



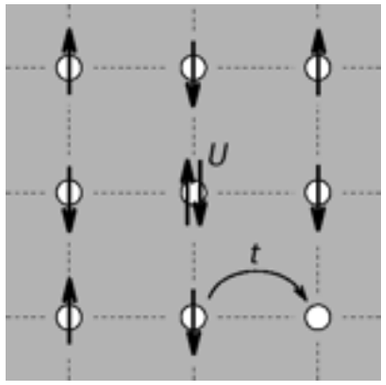
- Kondo lattice model with classical spins
  → **CMR-Manganites**
- real-time dynamics of classical spins can be calculated **exactly** for **large 2D systems** and on **long time scales**
- Kondo impurity model → dynamics beyond the **LLG equation**

Solving the Hubbard Model Using DMFT with CTQMC

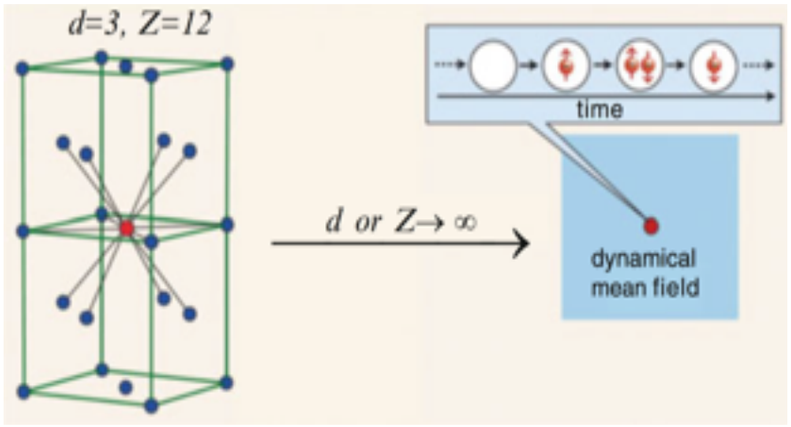
Beomjoon Goh[1] and Ji Hoon Shim[1,2]

[1]*Dept. of Chem., POSTECH, Pohang 790-784, Korea*
[2] *Dept. of Chem. and Div. of Adv. Nuc. Eng., POSTECH, Pohang 790-784, Korea*

- Hubbard model
  - $H = \sum_{ij\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$
  - 3D cubic lattice
  - Half filled, fixed temp.
  - U/W = 0.6 ~ 1.3 (W = 6)

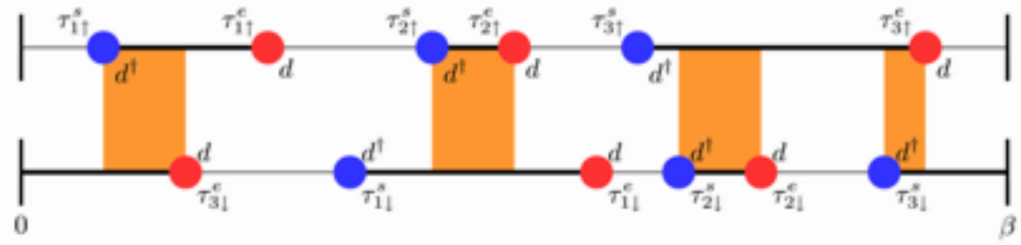


- Dynamical Mean Field Theory (DMFT)[1)]

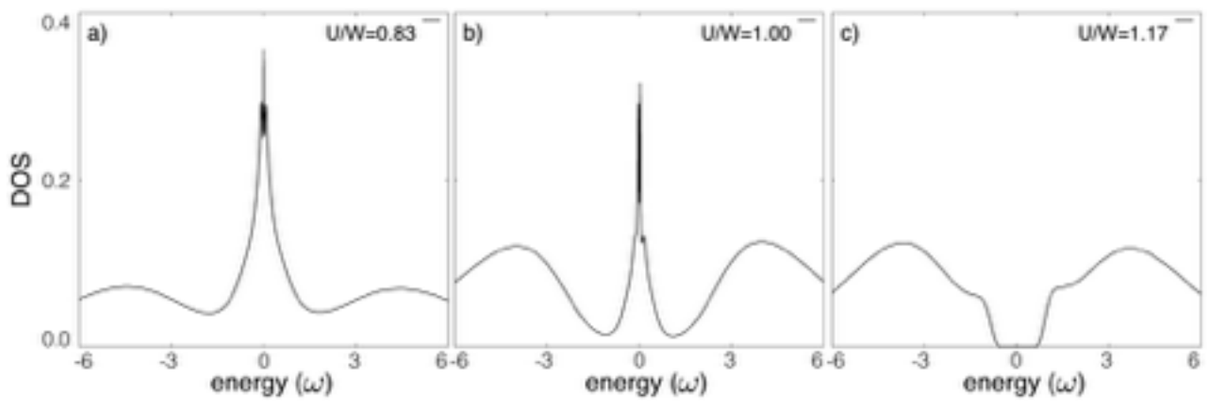


  - Replacement of a lattice problem to an impurity embedded in an effective field determined self consistently.

- Continuous-Time Quantum Monte Carlo (CTQMC)[2)]
  - Hybridization expansion, segment representation



- Density of states



  - Reproduced the famous three peak structure.
  - With a slight variation of U/W around 1, the middle peak abruptly disappears and the system behaves as a metal or an insulator.

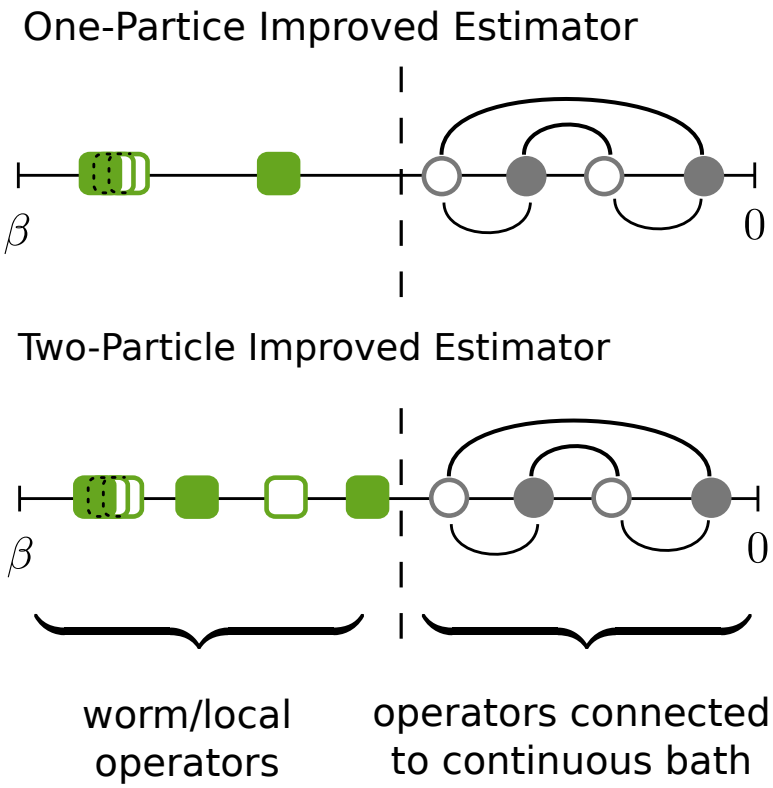
1) D.Vollhardt, Ch. 7, “Strongly Correlated Systems” Springer, 2012
2) E. Gull *et al.*, Rev. Mod. Phys. **83**, 349 (2011)

Worm Improved Estimators in Continuous-time Quantum Monte Carlo

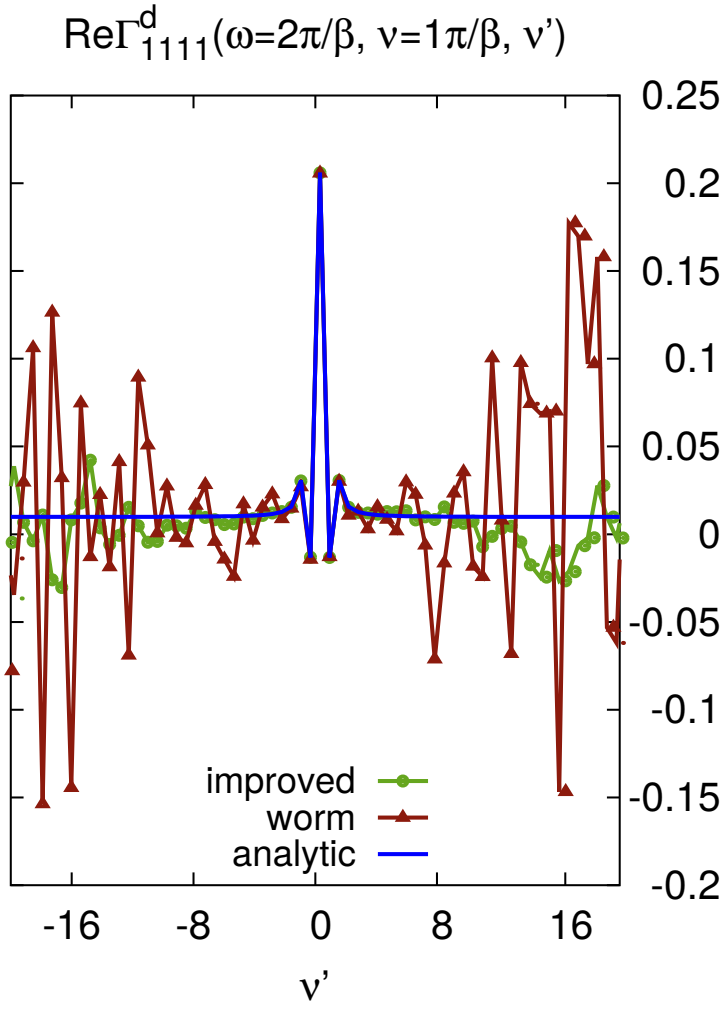
P. Gunacker[1], M. Wallerberger[1], T. Ribic[1], A. Hausoel[2], G. Sangiovanni[2], K. Held[1]

[1] Institut für Festkörperphysik, Technische Universiät Wien, Austria
[2] Theoretische Physik I, Julius-Maximilians-Universität Würzburg, Germany

CT-HYB Trace Pictures



Two-Particle Irreducible Vertex



Continuous-time quantum Monte Carlo algorithm for the Anderson impurity model of a multi-orbital system with general (local) interaction[1]

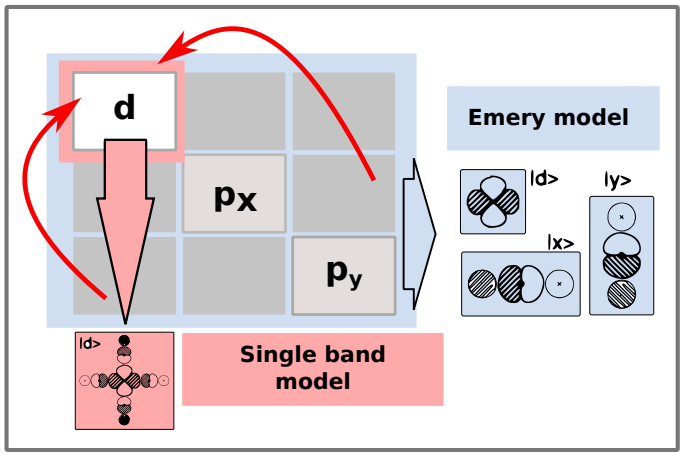
Improved measurement of irreducible quantities (self-energy, vertex) in CT-HYB[2]

Worm algorithm for non-density-density (local) interaction[3]

[1] P. Werner, A.J. Millis - Phys. Rev. B 74, 155107 (2006)
[2] H. Hafermann, K.P. Patton, P. Werner. - Phys. Rev. B 85, 205106 (2012)
[3] P Gunacker et al. - Phys. Rev. B 92, 155102 (2015)

Construction of effective low-energy interactions for three-orbital cuprate models with electronic correlation

Cornelia Hille[1], X. Cao[2], C. Honerkamp[3], P. Hansmann[2], S. Andergassen[1]
[1] *University of Tübingen,* [2] *MPI Stuttgart,* [3] *RWTH Aachen*



many-orbital problem
$\rightarrow$ **effective few-orbital problem**
new hopping parameters
new interaction parameters

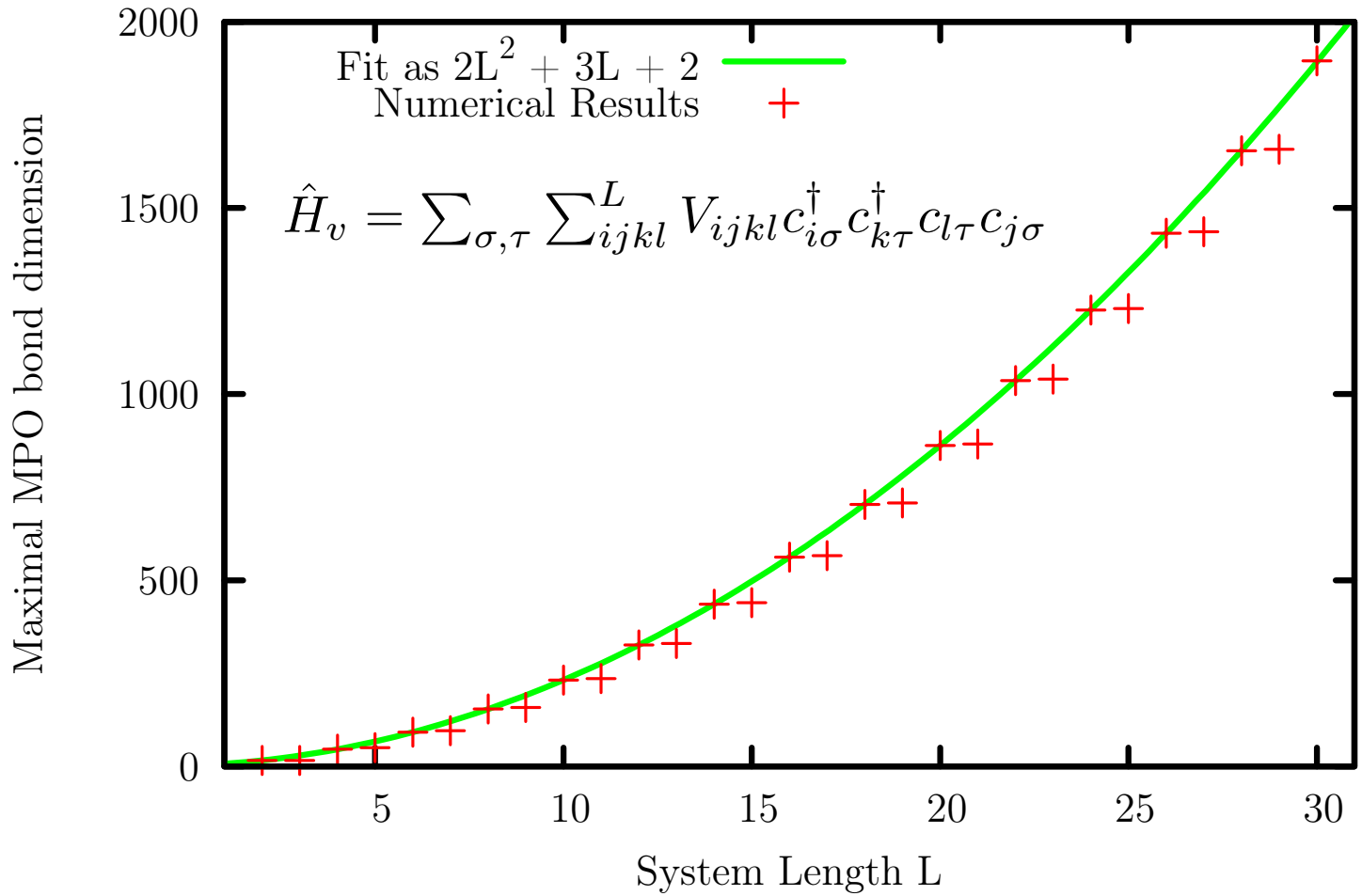
Effective interaction parameters:
constrained Random Phase Approximation (cRPA)

Further: different basis sets for Emery-model (dp, ligand)
effective interactions for EDMFT input

Generic Algorithm for the Construction of Efficient Matrix Product Operators

Claudius Hubig and Uli Schollwöck, LMU München

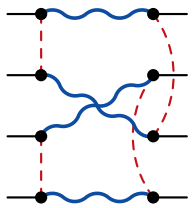
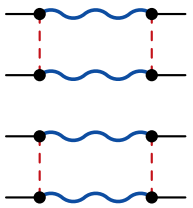
c.hubig@physik.uni-muenchen.de

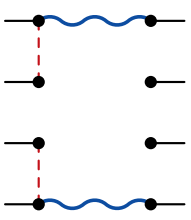


Estimating ground state entanglement entropy using path integral molecular dynamics

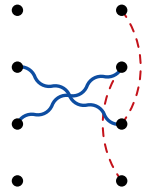
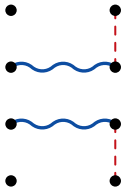
Dmitri Iouchtchenko and Pierre-Nicholas Roy

Department of Chemistry, University of Waterloo, Ontario, Canada

$$\operatorname{Tr} \varrho_A^2 = \int \mathrm{d}\mathbf{q}$$  $$\Big/ \int \mathrm{d}\mathbf{q}$$ 

sample from 

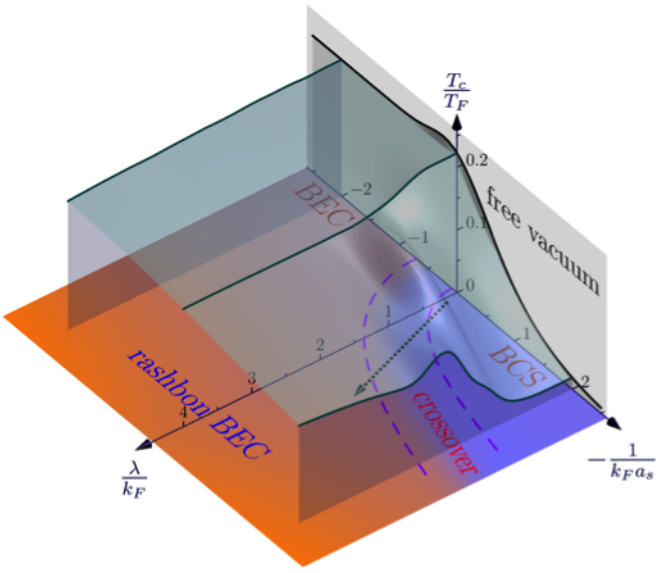
- Arbitrary path connectivity.
- Force field scaling.
- Adjustable dynamically during simulation.

$$\operatorname{Tr} \varrho_A^2 = \left\langle \right.$$  $$\left. \right\rangle \Big/ \left\langle \right.$$  $$\left. \right\rangle$$

Thermodynamics of Interacting Cold Atomic Fermi Gases with Spin-Orbit Coupling

Scott S. Jensen, Yoram Alhassid, Chris N. Gilbreth
Yale University

May 22, 2016



[Figure taken from J. P. Vyasanakere and V. B. Shenoy, Phys. Rev. B 92, (2015)]

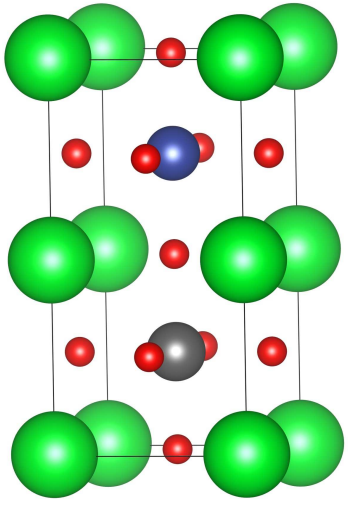
In this work we explore the phase diagram of the two-species interacting Fermi gas in the presence of spherical Rashba spin-orbit coupling in three dimensions using finite-temperature auxiliary-field quantum Monte Carlo methods. Our studies focus on the crossover from BCS behavior to Rashbon-BEC behavior in this system.

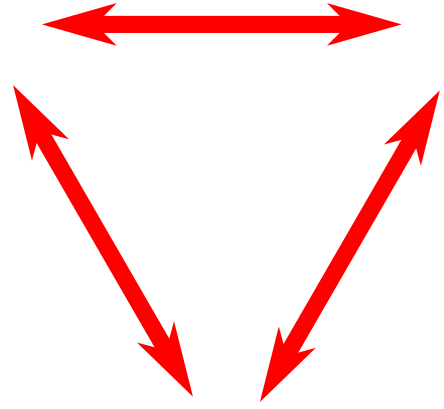
Correlated Electronic Properties of Different $SrIrO_3/SrTiO_3$ Heterostructures

Gernot J. Kraberger and Markus Aichhorn

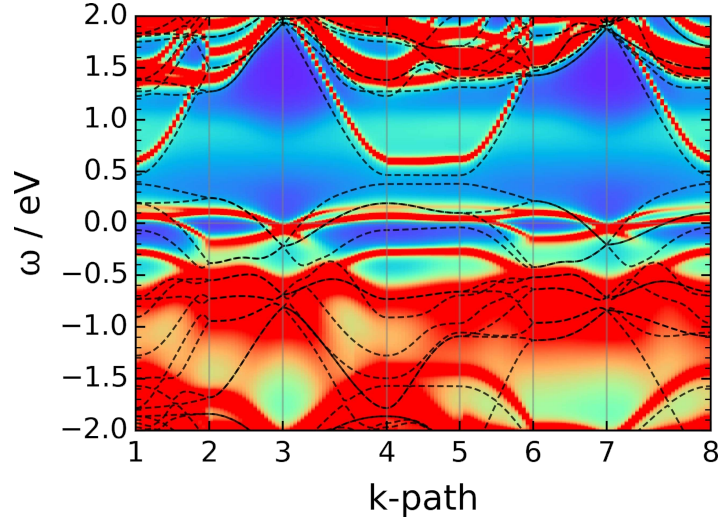
Institute of Theoretical and Computational Physics, NAWI Graz, Graz University of Technology

Heterostructuring

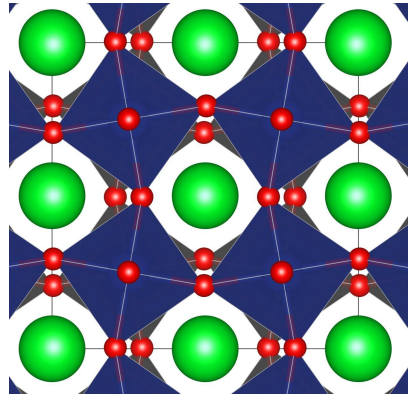




Electronic Correlations



Structural distortions



Resonant inelastic X-ray scattering study at oxygen K-edge of corner-shared Sr_2CuO_3 cuprate

U. Kumar[1], J. Schlappa[2], K.J. Zhou[2], S. Singh, V.N. Strocov[2], A. Revcolevschi, H. M. Ronnow, S. Johnston[1], and T. Schmitt[2]

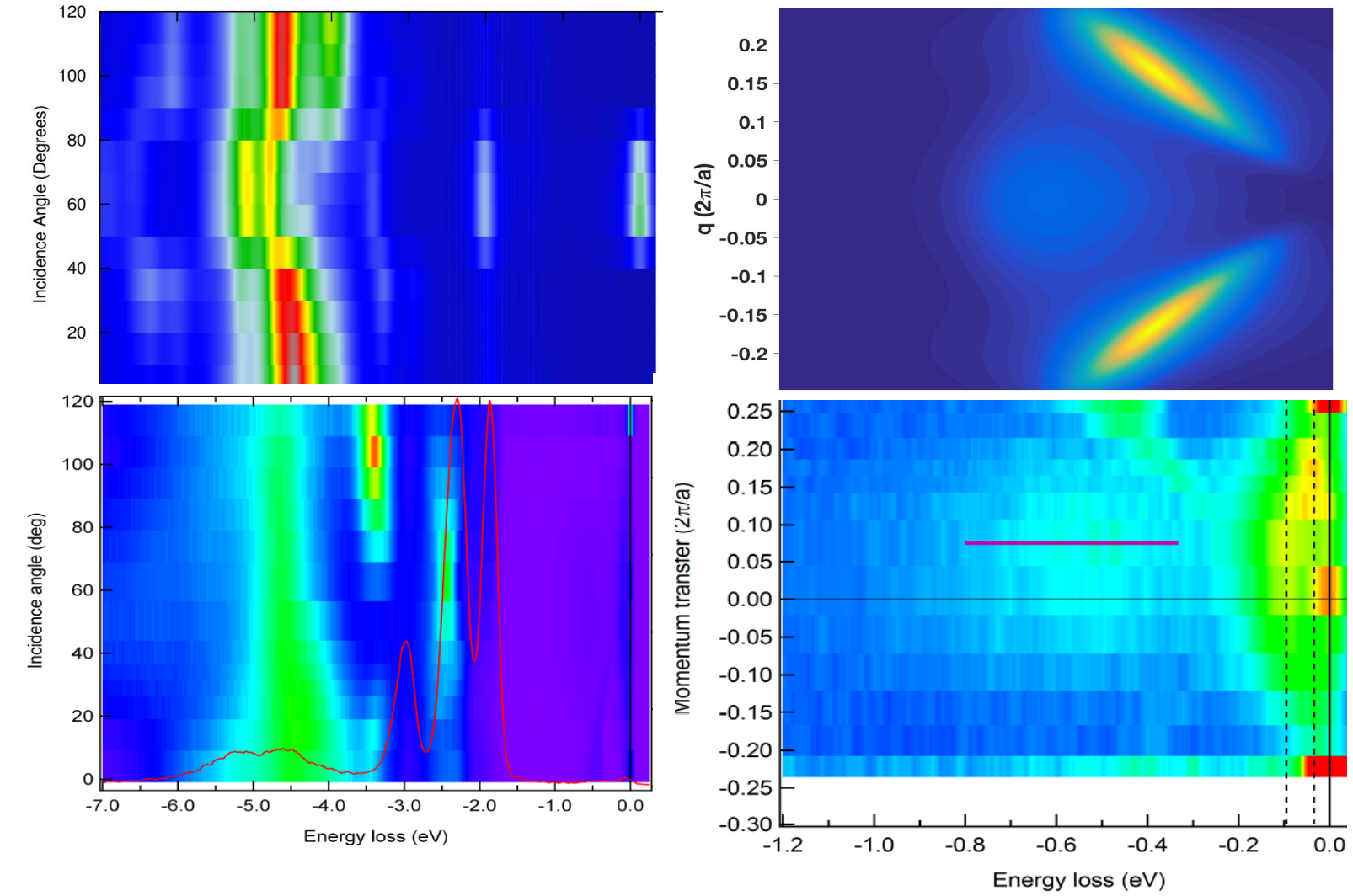
[1]*University of Tennessee, Knoxville, USA,* [2]*Swiss Light Source, Paul Scherrer Institut, Villigen, Switzerland*

Orbital Excitations

Bimagnon Excitation

Calculated

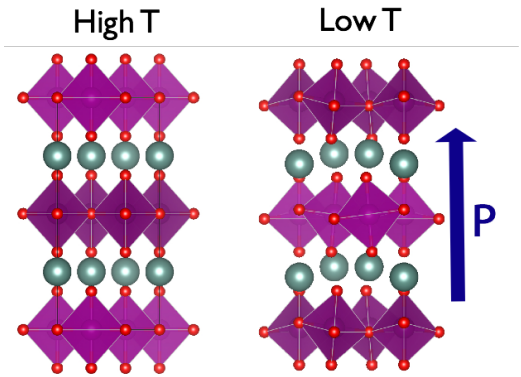
Experiment



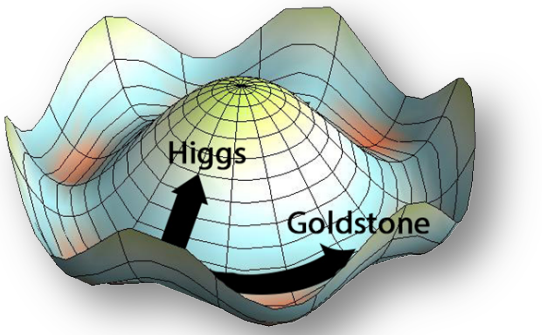
- Studied **Multi-orbitals** excitations using Exact Diagonalization for a small cluster.
- Excellent corroboration of ***dd*** and **Charge Transfer excitation** observed at *O* K-edge RIXS.
- Studied **Bimagnon excitation** at O K-edge using 1-D Heisenberg model for infinite chain.
- Bimagnon excitation with a **dispersive and bound state** observed.

Higgs and Goldstone modes in the hexagonal manganites

A. Stucky[1] & Q. Meier[2], F. Lichtenberg[2], M. Fiebig[2], N. Spaldin[2] and D. van der Marel[1]
[1]*University of Geneva, Department of Quantum Matter Physics, Geneva*
[2]*Department of Materials, ETH Zürich*



Crystal Structure of h-RMnO3



Landau free energy surface
from first principles

- 6-fold degenerate ferroelectric ground state
- Spontaneous symmetry breaking at around 1000 K.
- Breaking of a quasi U(1) symmetry
- Existence of Higgs- and Goldstone modes
- Studied using Raman spectroscopy and first principles calculations

UNIVERSITÉ DE GENÈVE
FACULTY OF SCIENCE
Departement of Quantum Matter Physics
ETH zürich

Non-equilibrium Kondo effect in nanoscale quantum dots using NCA and beyond

Chang Woo Myung[1], Geunsik Lee[2] & Kwang S. Kim[1]

[1] *Center for Superfunctional Materials, Department of Chemistry, School of Natural Science, Ulsan National Institute of Science and Technology (UNIST), Ulsan 44919, Korea*

[2] *Department of Chemistry, School of Natural Science, Ulsan National Institute of Science and Technology (UNIST), Ulsan 44919, Korea*

Nanoscale quantum dots exhibit the zero-bias resonant tunnelling known as the non-equilibrium Kondo effect. This has been observed in several experiments of various quantum dots such as single-electron transistor, carbon nanotube and molecular quantum dots. However, there still exist some puzzlings in understanding the nature of Kondo effect out of equilibrium.

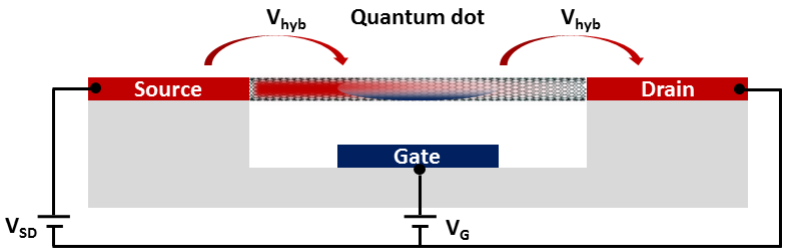


Figure 1. Schematic for nanoscale quantum dot system with source-drain voltage V_{DS}, gate voltage V_G and hybridization V_{hyb}.

We investigate different kinds of quantum dot systems exhibiting the Kondo behaviour by controlling the degeneracy at the first principles level. We use the impurity solver for the Anderson impurity model such as Non-Crossing Approximation (NCA) or One-Crossing Approximation that includes vertex correction [1] (or crossing term) using auxiliary particle approach to treat low temperature limit.

To evaluate the real time green's functions and the steady state observables, we use the Keldysh formalism and Landauer-Buttinker formula. We expect that the implementation of the impurity solver with the finite Coulomb interactions U and with the cluster expansion in NEGF-DFT methods can deal with many realistic systems [2, 3].

1. Haule, K., Kirchner, S., Kroha, J., Wolfle, P. *Anderson impurity model at finite Coulomb interaction U : Generalized noncrossing approximation*, Phys. Rev. B 64, 155111, 2001

2. Paaske, J., Rosch, A., Wolfle, P., Mason, N., Marcus, C.M., Nygard, J. *Non-equilibrium singlet-triplet Kondo effect in carbon nanotubes*, Nature Physics 2, 460, 2006

3. Kim, W.Y., Kim, K.S. *Prediction of very large values of magnetoresistance in a graphene nanoribbon device*, Nature Nanotechnology 6, 162, 2008

Robustness of the Haldane phase under strong charge fluctuations on a three-legged ladder at two-thirds filling

H. L. Nourse,[1,*] C. Janani,[1,2] I. P. McCulloch,[1,2] and B. J. Powell[1]

[1] *School of Mathematics and Physics, The University of Queensland, Brisbane, Queensland 4072, Australia*
[2] *Centre for Engineered Quantum Systems, School of Mathematics and Physics, The University of Queensland, Brisbane, Queensland 4072, Australia*

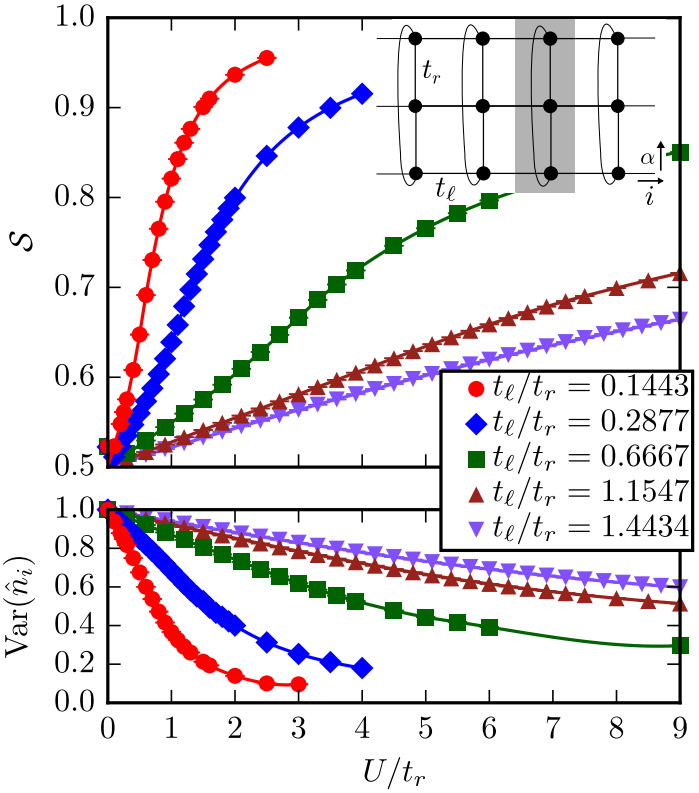


FIG. 1: Effective spin per unit cell (top), charge fluctuations (bottom) and three-legged ladder where shaded region indicates the unit cell (inset).

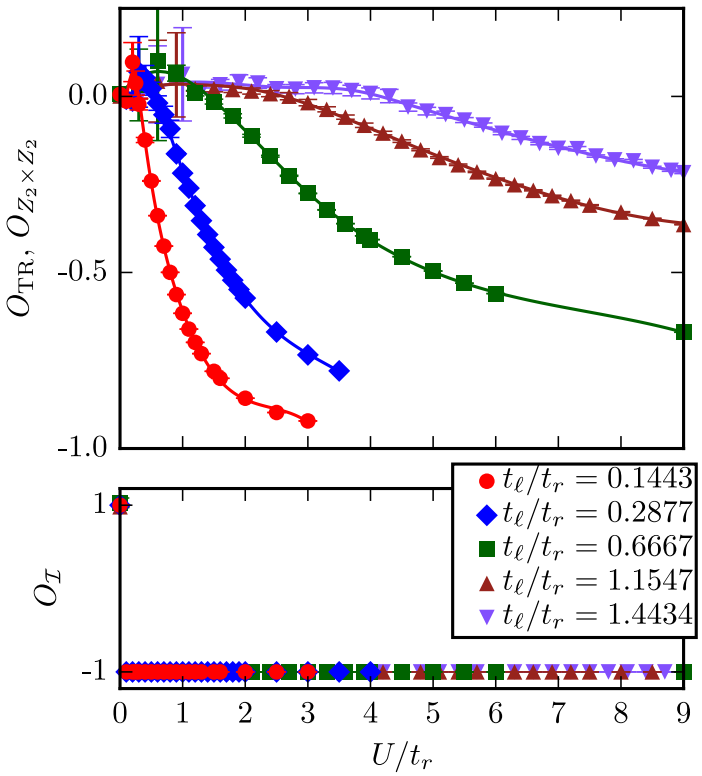


FIG. 2: Order parameters where $O = 1$ in the trivial SPT phase and $O = -1$ in the non-trivial SPT phase. $|O| < 1$ if the symmetry is not protective.

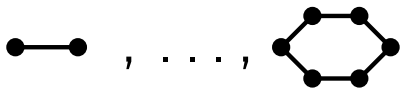
Interactions cause an insulating state that is not the usual Mott type as have two-thirds electron filling. Additionally, interactions give the Haldane phase as the ground state, a non-trivial symmetry protected (SPT) topological phase, even though the spin-one moment is heavily suppressed from charge fluctuations. Unlike in spin-one chains, in fermionic models and real materials only inversion ($\mathcal{I}$) is protective, while time reversal (TR) and $Z_2 \times Z_2$ are not protective due to charge fluctuations.

* hnourse@gmail.com

Extended Hubbard model – Full parquet solution within dynamical vertex approximation

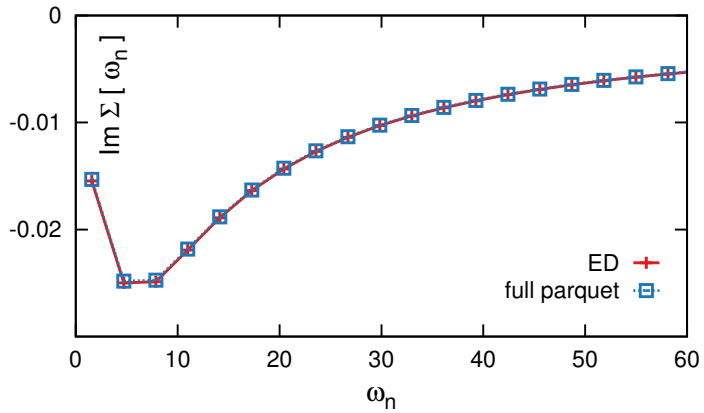
TECHNISCHE UNIVERSITÄT WIEN
Vienna | Austria

simulation of small nanoscopic molecules (Hubbard rings)



Output:

benchmark with *exact diagonalization (ED)* for 2-site system



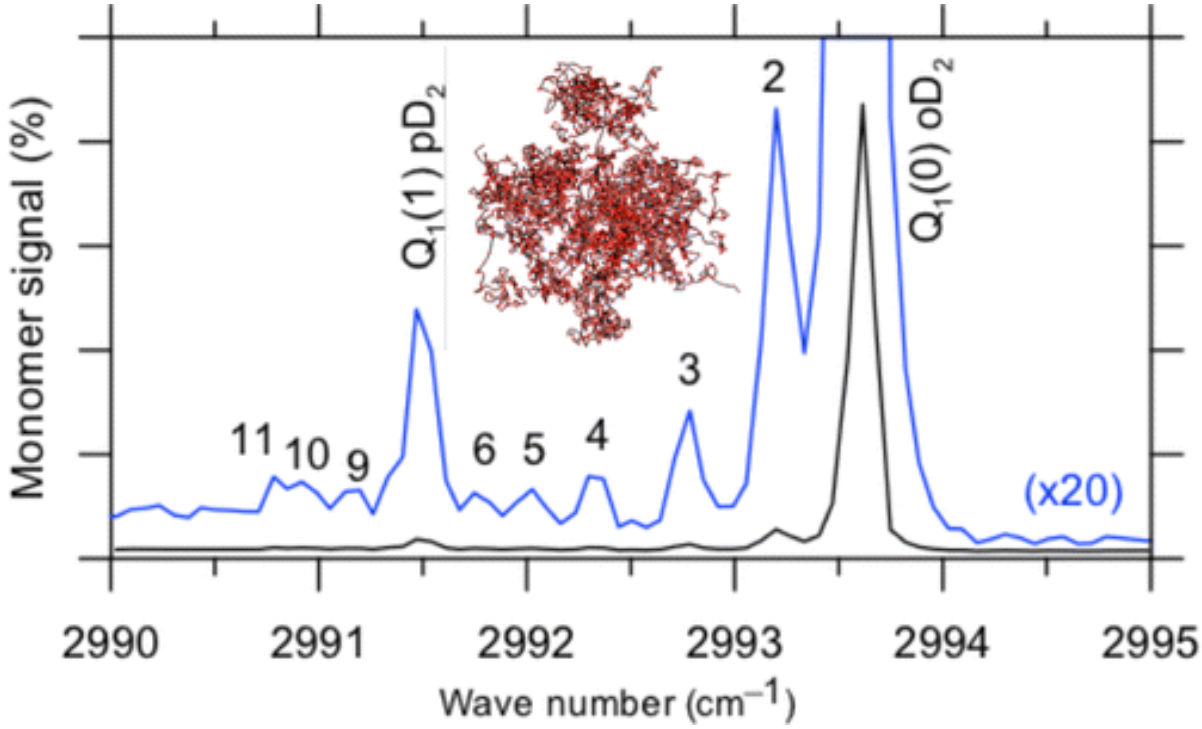
Method:

- approximation influences 2-particle vertex
- hence, includes long- & short-range correlations
- "*extending DMFT*"
- details in *G. Li et al. PRB 93 (2016)*

by: Petra Pudleiner, Gang Li, and, Karsten Held

Methodological Advances in Low (and Zero) Temperature Path Integral Molecular Dynamics

Matthew Schmidt, Dmitri Iouchtchenko, Kevin Bishop, and Pierre-Nicholas Roy
Department of Chemistry, University of Waterloo, Waterloo, Ontario



Raman spectra of $(oD_2)_N$ and path integral representation of a oD_2 cluster
Ref: *J. Phys. Chem. A*, **2015**, *119* (50), pp 12551–12561

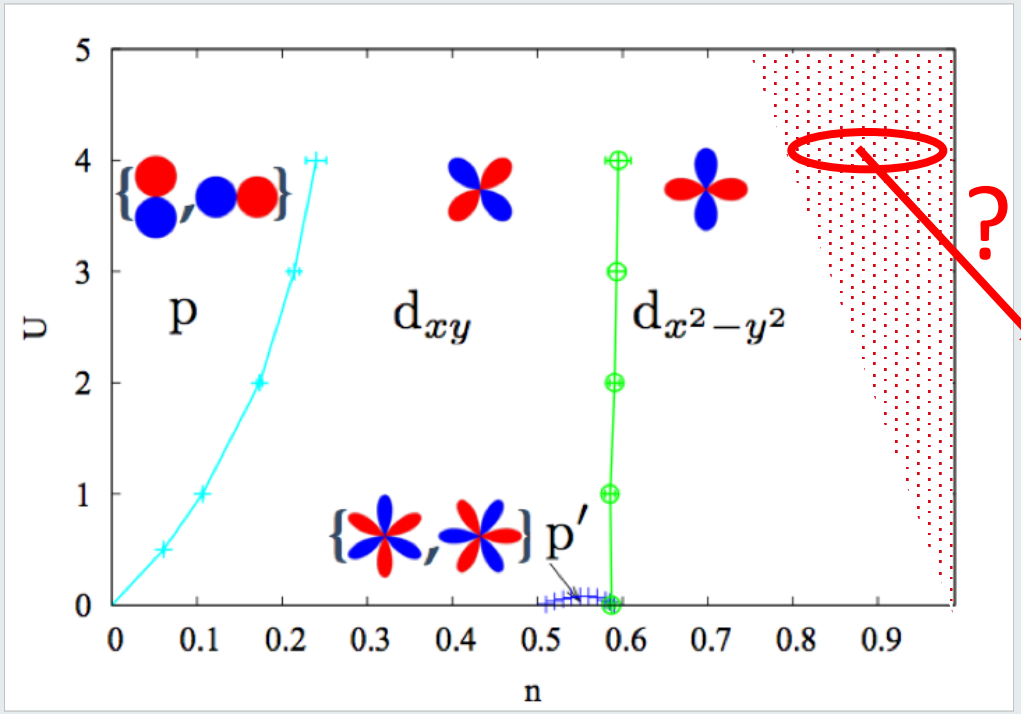
Molecular dynamics simulations are often used to calculate properties of classical chemical systems. However, we apply molecular dynamics to quantum systems using Feynman path integrals, in which quantum particles are represented as a necklace of classical particles. Using this Path Integral Molecular Dynamics technique, we calculate energetic and structural properties of water and hydrogen systems at finite temperature and in the limit of zero temperature where a separate formulation is required. Of note, we examine hydrogens encapsulated in water "cages" known as clathrates which has important clean energy storage implications and we theoretically calculate Raman vibrational shifts and compare to experiment (see above figure). We also introduce the WORM algorithm of nuclear exchange into molecular dynamics for the first time.

EVIDENCE FOR PHASE SEPARATION IN THE FERMIONIC HUBBARD MODEL

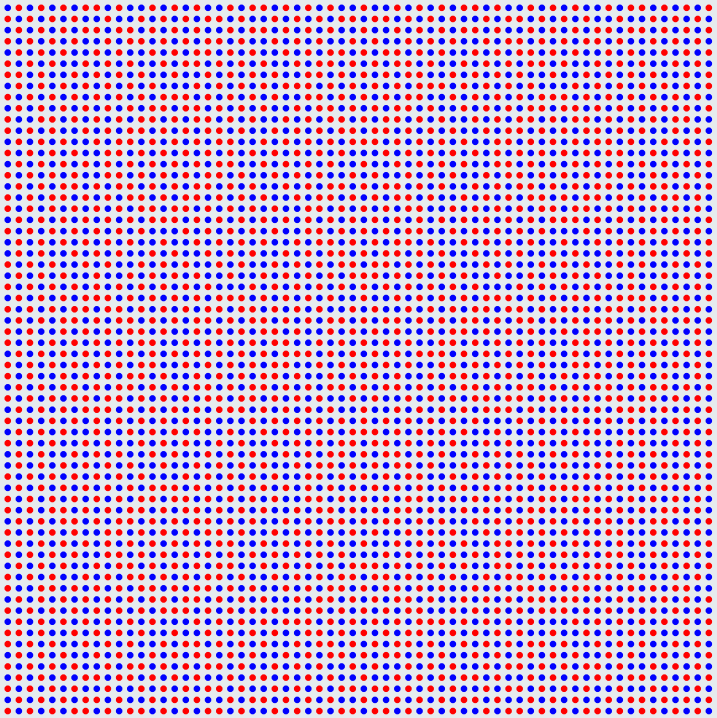
Fedor Šimkovic

In collaboration with: Y. Deng, E. Kozik, N. Prokofiev, B. Svistunov

KING'S College LONDON



Deng et al., EPL 2015



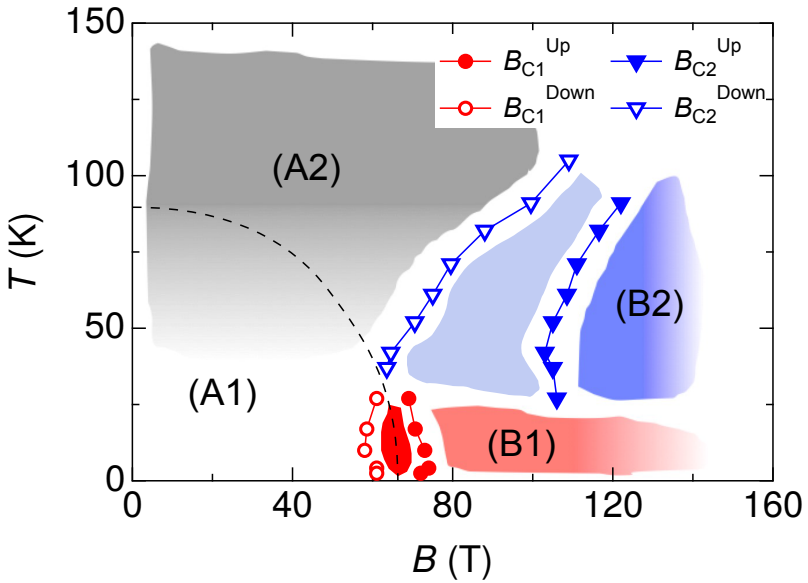
diagonally striped phase

Field-induced exciton condensation in $LaCoO_3$

Andrii Sotnikov and Jan Kuneš
– Institute of Physics, Prague, Czech Republic

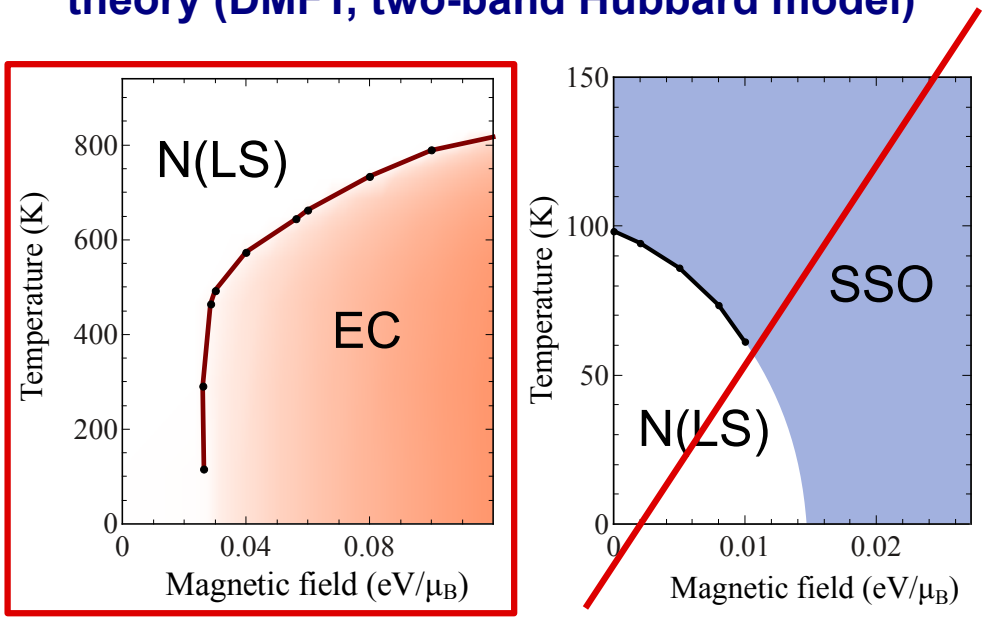
From the comparison of experimental observations with our theoretical analysis, the transition in $LaCoO_3$ happens according to the exciton condensation scenario.

experimental data ($LaCoO_3$)



A. Ikeda et al., arXiv: 1512.00535

theory (DMFT, two-band Hubbard model)



A. Sotnikov and J. Kuneš, arXiv: 1604.01997

MAGNETO-OPTICAL PROPERTIES OF MASSIVE DIRAC FERMIONS.

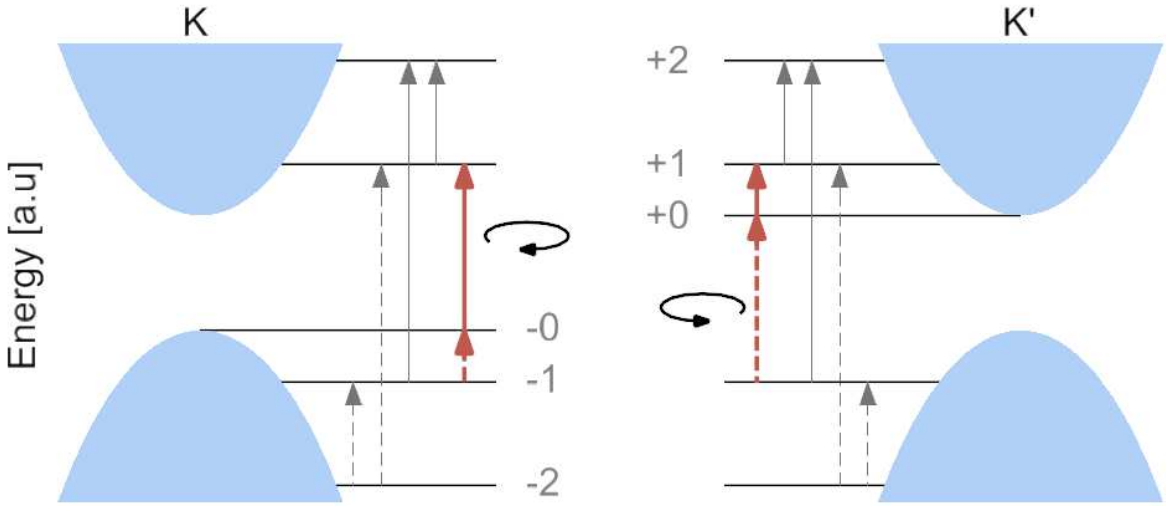
Ludmiła Szulakowska[2], Paweł Potasz[1], Paweł Hawrylak[2]

[1]Wrocław University of Science and Technology, Wrocław, Poland
[2]Advanced Research Complex, University of Ottawa, Ottawa, Ontario, Canada

The low-energy carriers in atomically-thin **transition metal dichalcogenides** (here MoS2) are described as massive Dirac fermions (MDF) [1-3].

Analogically to graphene, their energy structure exhibits **two non-equivalent valleys, K and K'** with two parabolic bands separated by a gap (see fig.). They **couple to oppositely circularly polarised light** [2-3], which allows to address them independently.

When subjected to external magnetic field, each valley splits into a **peculiar sequence of Landau levels** (LLs) with contributions from valence and conduction bands.



Here, we study the **effect of electron-electron interactions on the optical properties of massive Dirac fermions in strong magnetic fields**, studied in refs. [4,5].

We use the massive Dirac equation to construct a single-electron picture. We form excitations from occupied LLs and then calculate the excitonic spectrum for both valleys with the **configuration interaction method**. We use selection rules to obtain the **absorption and emission spectra**.

[1] E. Kadantsev, P. Hawrylak , *Solid St. Com,* **152,** (2012).
[2] T. Scrace, Y. Tsai, B. Barman, L. Schweidenback, A. Petrou, G. Kioseoglou, I. Ozfidan, M. Korkusinski, P. Hawrylak, *Nature Nanotechnology*, **10**, (2015).
[3] D. MacNeill, C. Heikes, K. F. Mak, Z. Anderson, A. Kormányos, *Phys. Rev. Lett*, **114**, (2015).
[4] F. Rose, M. O. Goerbig, F. Piechon, *Phys. Rev. B*, **88**, (2013).
[5] P. Hawrylak, M. Potemski, *Phys. Rev. B*, **56**, (1997).

Computational analysis of Many Body Localized phases beyond 1D

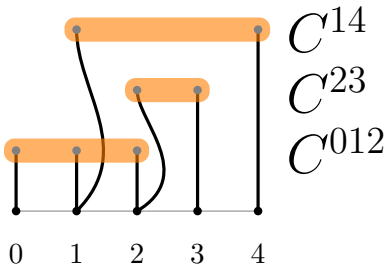
Benjamín Villalonga Correa[1], Bryan K. Clark[1], and David Pekker[2]

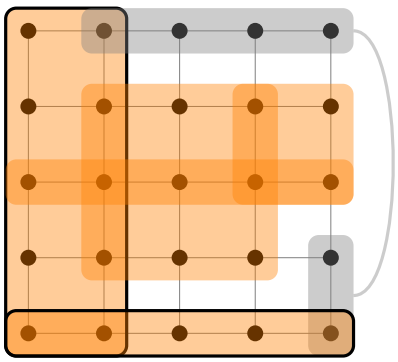
[1]Department of Physics, University of Illinois at Urbana-Champaign, IL 61801, USA
[2]Department of Physics and Astronomy, University of Pittsburgh, PA 15260, USA

PROBLEM: The **Many Body Localized** problem is one concerned with excited levels of energy of many-body models with disorder that localize after the so-called mobility edge. Many difficulties arise when studying this problem beyond 1D:

- Accessing interior eigenstates is hard.
- ED has a limit (22 sites) [*Luitz 2014*].
- MPS restricted to 1D [*Yu 2015*, *Khemani 2015*].

PROPOSAL: We propose the use of **Correlator Product States** ([*Huse-Elser 1988*, *Mezzacapo 2009*, *Changlani 2009*, *Marti 2010*]) as a class of tensor network, variational wavefunctions:



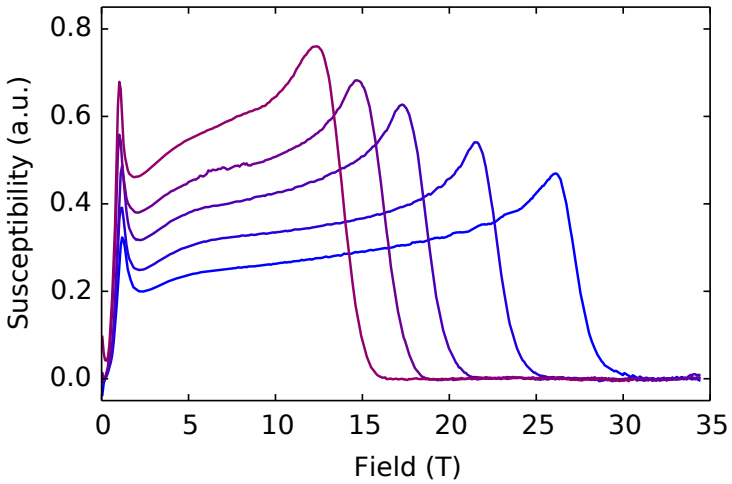


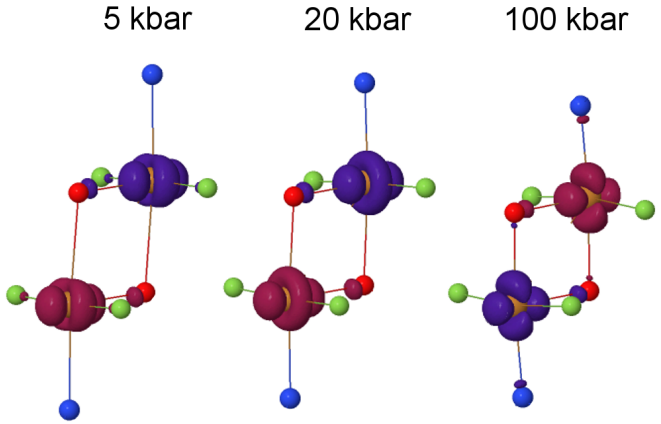
- Straighforward to use beyond 1D.
- Capture local entanglement naturally.

OUTCOME: For the localized phase, our method finds eigenstates at different energy densities with **overlaps** with *ED* eigenstates of above **98%**.

Dimensional crossover in a metal-organic Heisenberg antiferromagnet.

Björn Wehinger





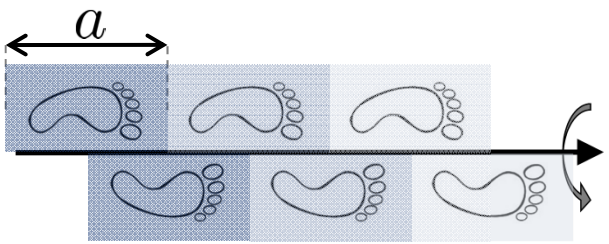
FACULTY OF SCIENCE
Department of Quantum Matter Physics
UNIVERSITÉ DE GENÈVE

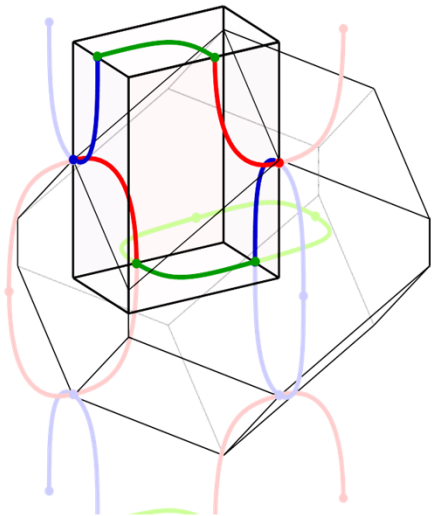
ETH zürich

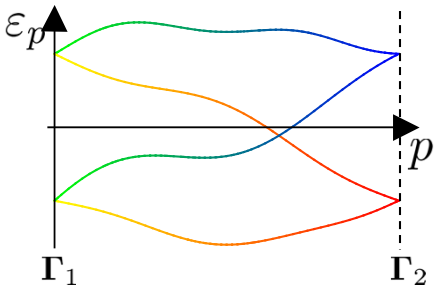
Nodal chain metals

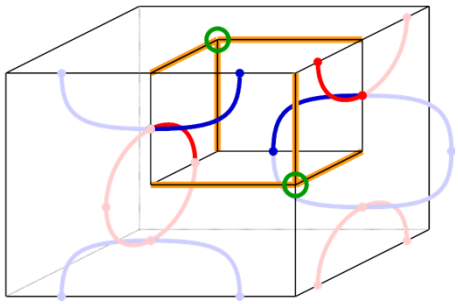
QuanSheng Wu

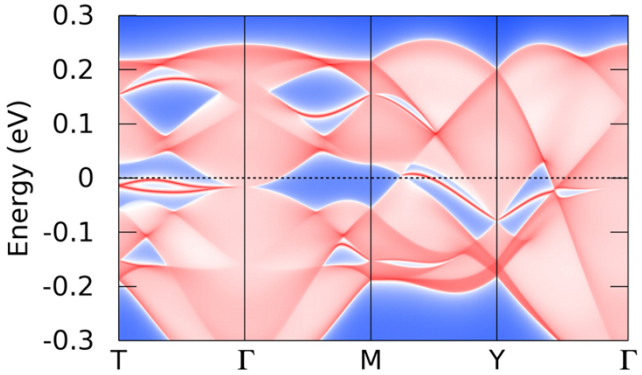
ETH Zürich











Co-authors

Tomáš Bzdušek

Alexey Soluyanov

Andreas Rüegg

Manfred Sigrist

Importance of effective dimensionality in manganese pnictides

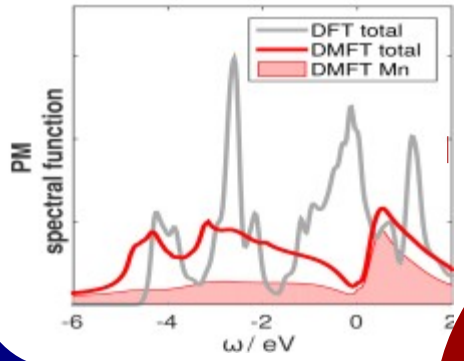
M. Zingl,[1*] E. Assmann,[1] P. Seth,[2] I. Krivenko,[3] and M. Aichhorn[1]

[1] Institute of Theoretical and Computational Physics, Graz University of Technology, Austria
[2] Institut de Physique Théorique (IPhT), CEA, CNRS, UMR CNRS 3681, 91191 Gif-sur-Yvette, France
[3] Institut für Theoretische Physik, Uni. Hamburg, Jungiusstraße 9, 20355 Hamburg, Germany

arXiv:1603.02115

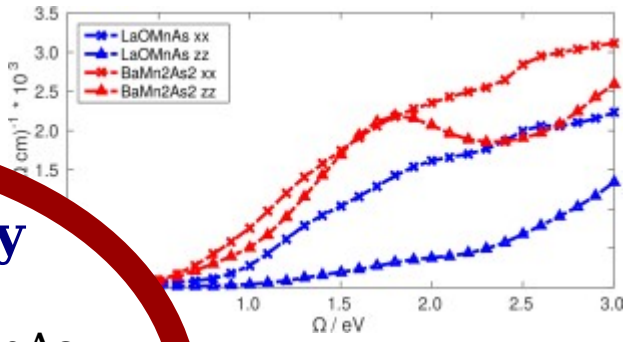
***manuel.zingl@tugraz.at**

DFT+DMFT



triqs

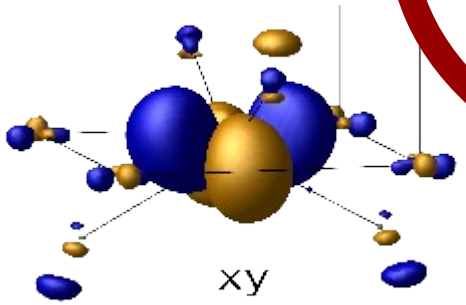
Optical conductivity



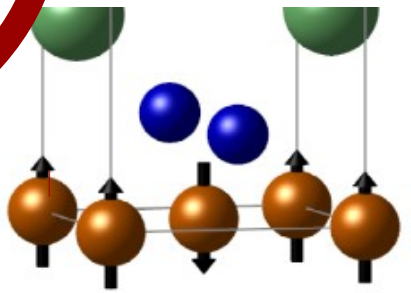
Dimensionality

LaMnAsO: quasi-2D MnAs layers

$BaMn_2As_2$: 3D with strong interlayer coupling



Wannier orbitals



Néel temperature