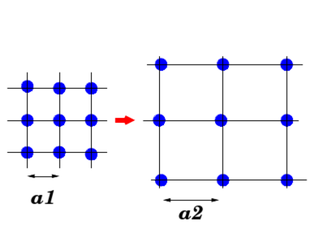
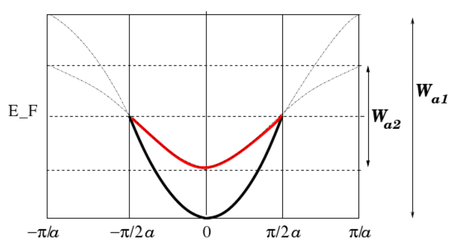
Mott-Hubbard transition in a hydrogen chain: a Quantum Monte Carlo study

L. Stella[1], C. Attaccalite[2] and A. Rubio[1]
1) European Theoretical Spectroscopy Facilities ETSF San Sebastian (Spain)
2) Institute Neel, CNRS/UJF, Grenoble (France)

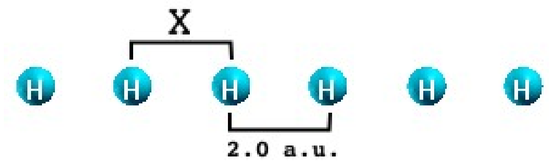
In this work we consider the variational approach as a possible route to describe the Mott transition in a realistic system. Our goal is to find a realistic description of Mott insulators, which allows for charge fluctuations without breaking any symmetry and makes it possible to connect the strong-coupling insulating state to the weak-coupling region. Our approach is based on an approximate form for the ground-state wavefunction which contains the physically relevant terms for the correct description of the Mott insulating state.

The Mott-Hubbard transition





A Schematic representation of the Mott *Gedankenexperiment*: a lattice of Hydrogen atoms with lattice constant a_1 and $a_2 > a_1$ and related band-theory picture. W_{a1} (W_{a2}) is the bandwidth associated to the lattice constant a_1 (a_2). By increasing the lattice constant, the bandwidth decreases, but the band is always half filled, i.e., the system is predicted to be metallic for any lattice constant a.

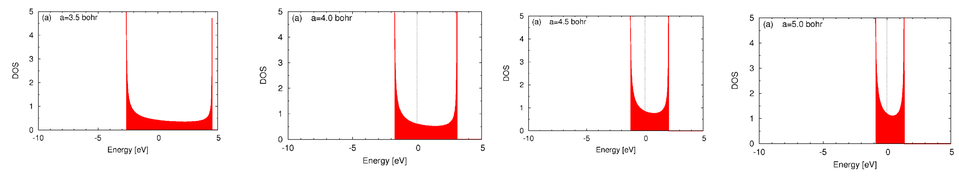


We decide to study an hydrogen chain because it is the simplest realistic system where one has a genuine Mott-Hubbard metal-insulator transition

The hydrogen chain in DFT

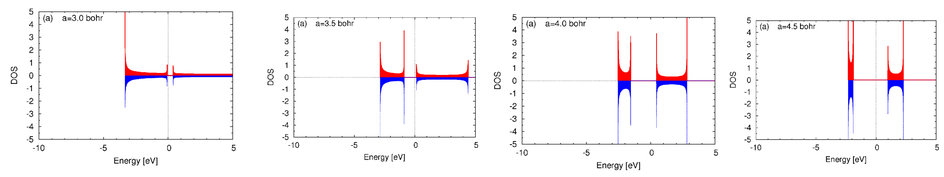
Band theory says that the hydrogen chain will remain always a metal because the energy difference between the HOMO and LUMO remains vanishingly small. And this is true also in DFT for any functional that does not contain a discontinuity as a function of the number of electrons.

Density of States:



Metal-insulator transition can be obtained using a cell with two atoms and LSDA, in this case the system becomes an anti-ferromagnet for large separation.
But in a real Mott transition the spin symmetry is not broken

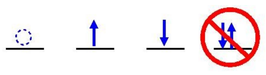
Density of States:



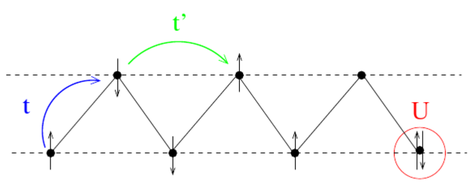
An exchange correlation functional with discontinuity could describe a Mott insulator:
N. A. Lima - L. N. Oliveira - K. Capelle Europhys. Lett., **60** (4), p. 601 (2002)

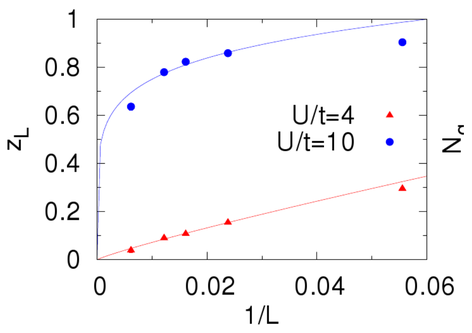
Lattice Models

The Mott transition in a one-dimensional Hubbard model with t'/t=0.75



$$\mathcal{P} = \prod_i \left(1 - n_{i\uparrow} n_{i\downarrow}\right)$$





The **Gutzwiller** wave-function is not an insulator!!!!!
Long-range correlations are necessary to generate an insulator

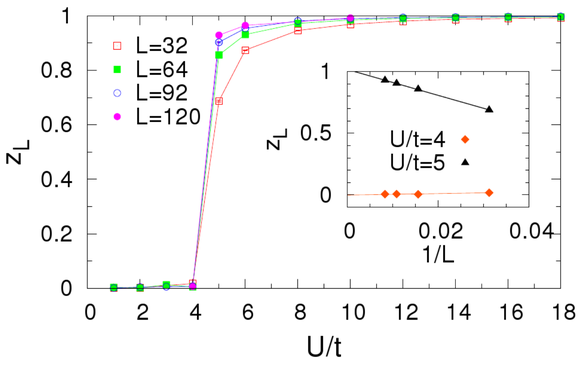


Figure 4.15: Berry phase as a function of U/t for $t'/t = 0.75$ and different sizes. Inset: size scaling of z_L for $U/t = 4$ and $U/t = 5$. Lines are two parameters fits.

W. F. Brinkman and T. M. Rice, Phys. Rev. B **2**, 4302(1970)

M. Capello, F. Becca, M. Fabrizio, S. Sorella, and E. Tosatti Phys. Rev. Lett. **94**, 026406 (2005)

Quantum Monte Carlo approach

Variational Monte Carlo

- each operator is calculate on the trial-wave function
- the wave-function is optimized in order to minimize the energy

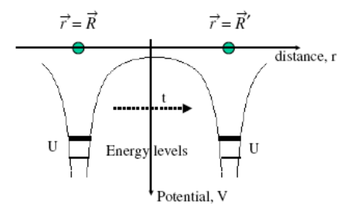
$$\langle A \rangle_{var} = \frac{\int \Psi_T^*(R) \hat{A} \Psi_T(R) dR}{\int \Psi_T^*(R), \Psi_T(R) dR}$$

The trial-wave function : RVB+Jastrow

$$\Psi = J\,\Phi_{RVB}$$

The **RVB** for two atoms:

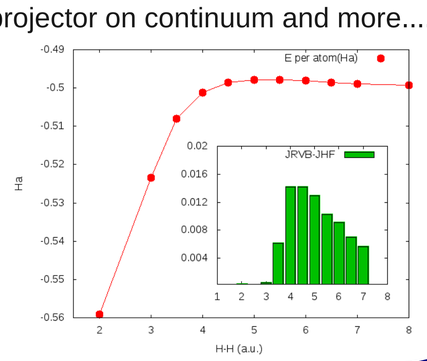
$$\begin{aligned}\Psi_{H_2} &= \lambda_{11}\phi_{1s}^A(r_1)\phi_{1s}^A(r_2) + \lambda_{22}\phi_{1s}^B(r_1)\phi_{1s}^B(r_2) \\ &+ \lambda_{12}\phi_{1s}^A(r_1)\phi_{1s}^B(r_2) + \lambda_{21}\phi_{1s}^B(r_1)\phi_{1s}^A(r_2)\end{aligned}$$



The **Jastrow** plays the role of the **Gutzwiller** projector on continuum and more.....

$$\Delta E = E[J\Phi_{HF}] - E[J\Phi_{RVB}]$$

....from single to multi-determinant....



Berry-phase and localization

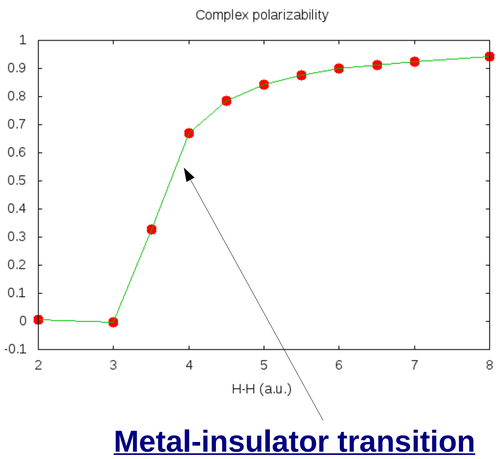
$$z[\Psi] = \langle \Psi | e^{iG\hat{X}} | \Psi \rangle$$

$$G = 2\pi / L$$

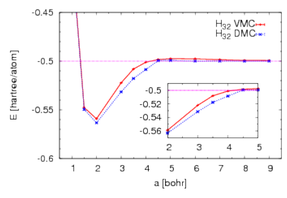
In thermodynamic limit:

z $\rightarrow$ 1 if the system is localized: *insulator*

z $\rightarrow$ 0 if the system is delocalized: *metallic*



Metal-insulator transition



We checked the quality of our WF comparing with DMC results

P. Umari, and Nicola Marzari, J. Chem. Phys. **131**, 094104(2009)

P. Umari, A. J. Williamson, G. Galli, and N. Marzari, Phys. Rev. Lett. **95**, 207602 (2005)

R. Resta and S. Sorella, Phys. Rev. Lett. **82**, 370 (1999)

Conclusions:

- We present the first simulation of a Mott-insulator in a realistic system
- Multi-determinant wave-function (and/or RVB) are important to carefully describe correlated systems
- Quantum Monte Carlo could be applied to study the phase-diagram of more complex systems (oxides etc..)

To do:

- To compute other observables
- Larger systems and thermodynamic limit
- May we construct an exchange-correlation functional from the QMC results?