Localization tensor : Metal-Insulator Transition

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Definitions

Insulator

Zero dc conductivity at 0k

Sustains bulk macroscopic polarization with or without electric field

Metal-insulator transition

Gap opens as a competition between the kinetic energy and potential energy

Types of Insulator

Single-particle

Band

electron interactions with the periodic potential of the ions

Peierls

electron interactions with static lattice deformation

Anderson

electrons interaction with impurities

Many-Particle

Mott

electron-electron interactions

Modern theory of insulating state

[Kohn]:Insulating state arises when the electron many-body wave function is localized

Wave function Ψ breaks into disconnected parts in the configuration space

$$\Psi(x_{1,..}.., x_N) = \Sigma_{x=-\infty}^{\infty} \Psi_M(x_{1,..}.., x_N)$$

The large supercell Ψ_M and Ψ_M'have an exponentially small overlap for M=M'. Kohn proved that dc conductivity vanishes.

Theory of insulating state, W .Kohn, Phys, Rev. 133 A171-A181 1964

Localization tensor

Macroscopic polarization and localization are expectation value of many-body phase operator

$$Z_N^{(\alpha)} = \left\langle \Psi \middle| e^{-i\frac{2\pi}{L_\alpha}\cdot\sum_{i=1}^{n} X_i} \middle| \Psi \right\rangle$$

Phase $\gamma_N^{(\alpha)} = \mathrm{Im}\log z_N^{(\alpha)}$ defines the macroscopic polarization

where $P_\alpha = \frac{eN}{L^3}\langle r_\alpha \rangle_c$

Modulus defines the localization tensor $\langle r_\alpha \rangle_c = \frac{1}{N}\frac{L}{2\pi}\mathrm{Im}\log z_N^{(\alpha)}$

$$\left\langle r_\alpha^2 \right\rangle_c = \frac{-1}{N|G_\alpha|^2}\ln|Z_N^{(\alpha)}|^2$$

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

I. Souza Wilkens T and R. Martin, 2000 Phys. Rev. B 62 1666

Localization tensor

- Localization tensor is related to the conductivity

$$\xi_i^2(N) = \frac{\hbar}{\pi q_e^2 n_0} \int_0^\infty \frac{d\omega}{\omega} \operatorname{Re} \sigma_{ii}(\omega)$$

- We will actually use

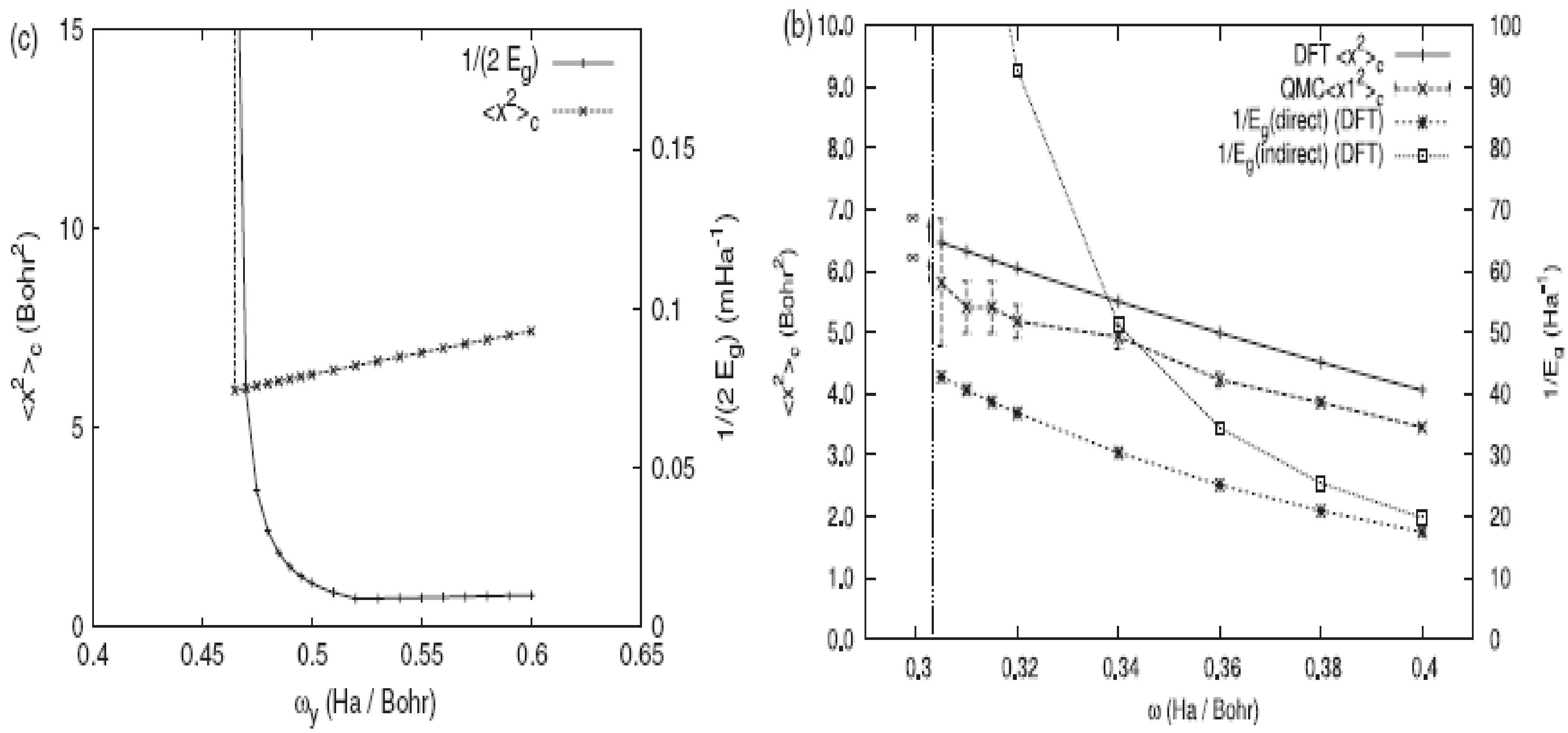
$$\langle r_\alpha r_\beta \rangle_c = \frac{L^2}{4\pi^2 N} \ln \frac{\langle \Psi_0(\boldsymbol{\kappa}_\alpha) | \Psi_0(\boldsymbol{\kappa}_\beta) \rangle}{\langle \Psi_0(\boldsymbol{\kappa}_\alpha) | \Psi_0(0) \rangle \langle \Psi_0(0) | \Psi_0(\boldsymbol{\kappa}_\beta) \rangle},$$

in CASINO

Numerical implementation

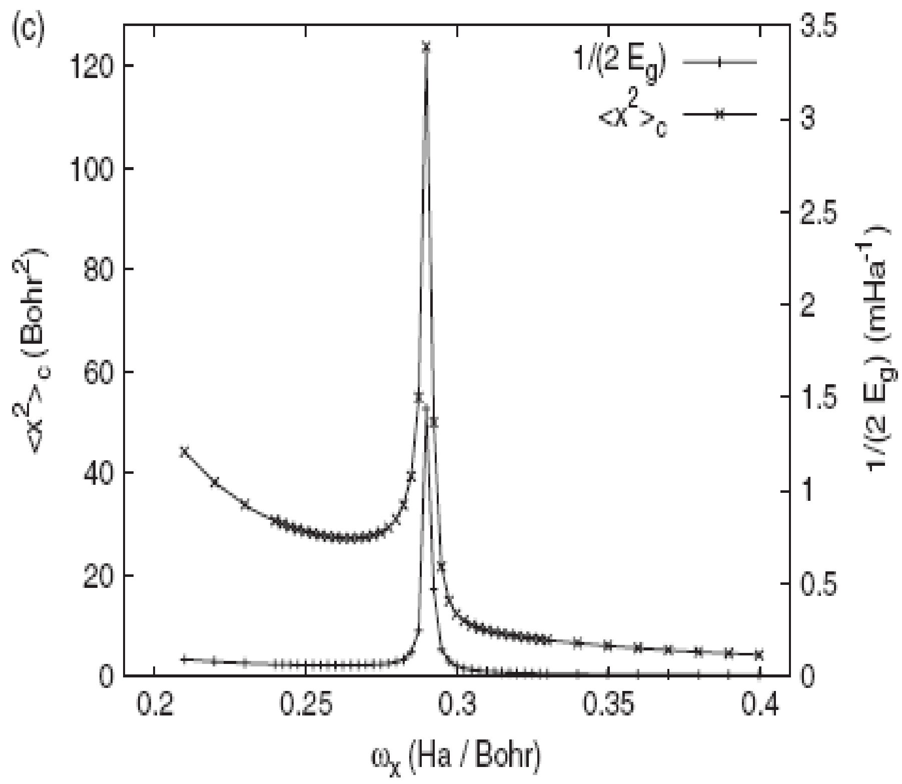
1. Sum over the electron positions
2. Add up the $e^{(i.k.x)}$ for each configurations then average over the weight to get Zn
3. Evaluate localization tensor and polarization tensor

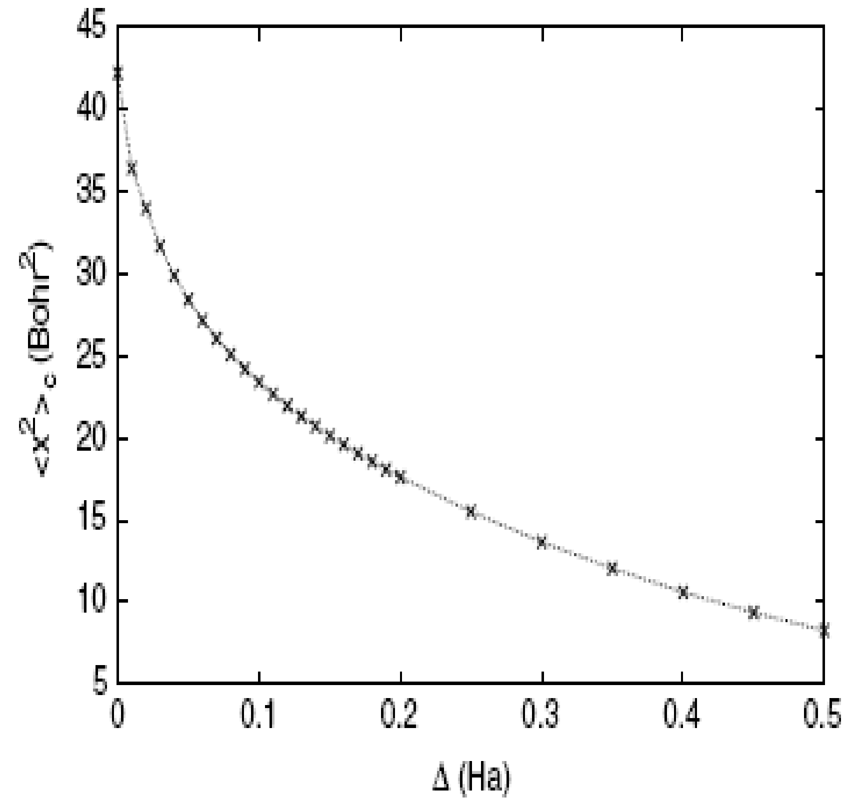
Localization tensor over metal to band insulator



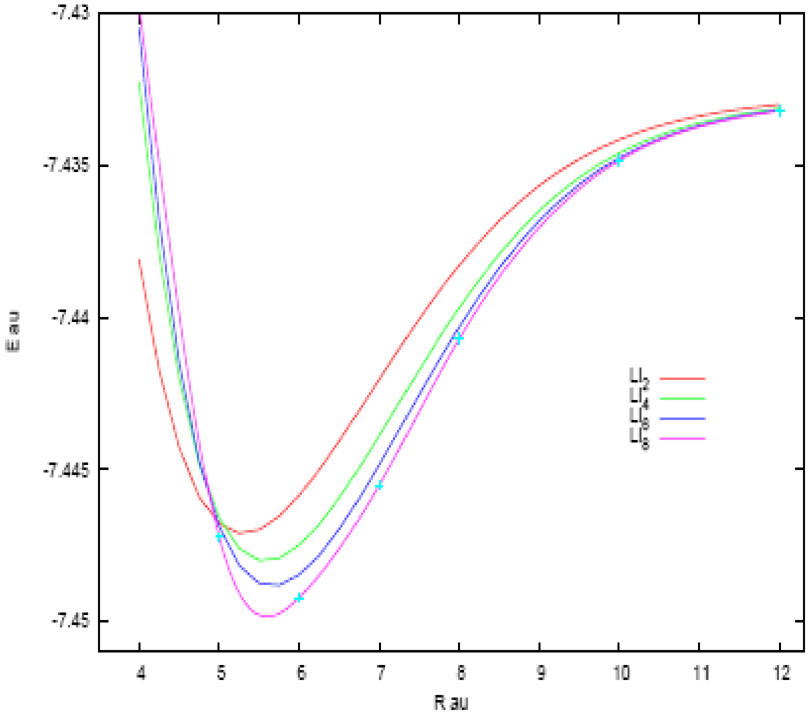
N D M Hine, W M C Foulkes, J Phy Condens. Matter 19 (2007) 506212

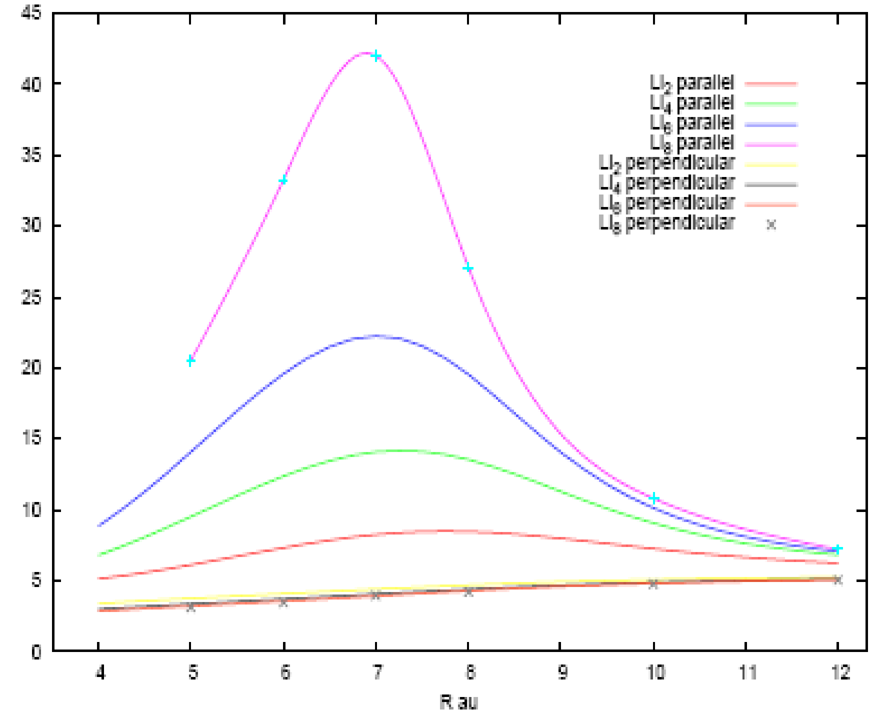
Localization tensor over metal to band insulator





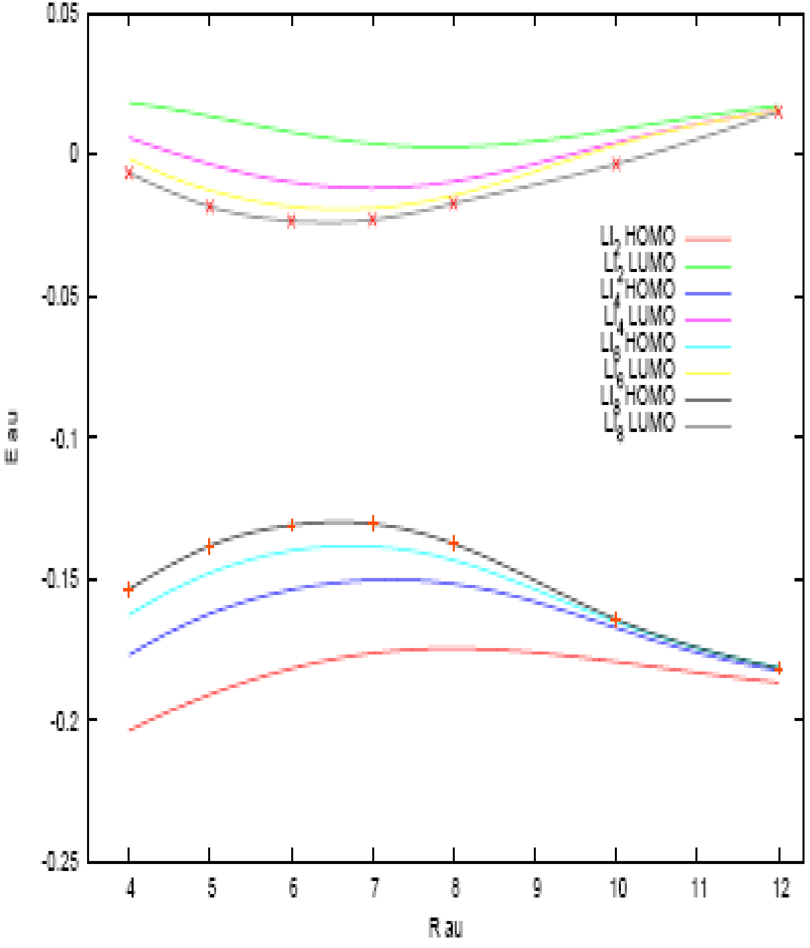
Metal-insulator transition of Lithium linear chain (n=2,4,6,8)

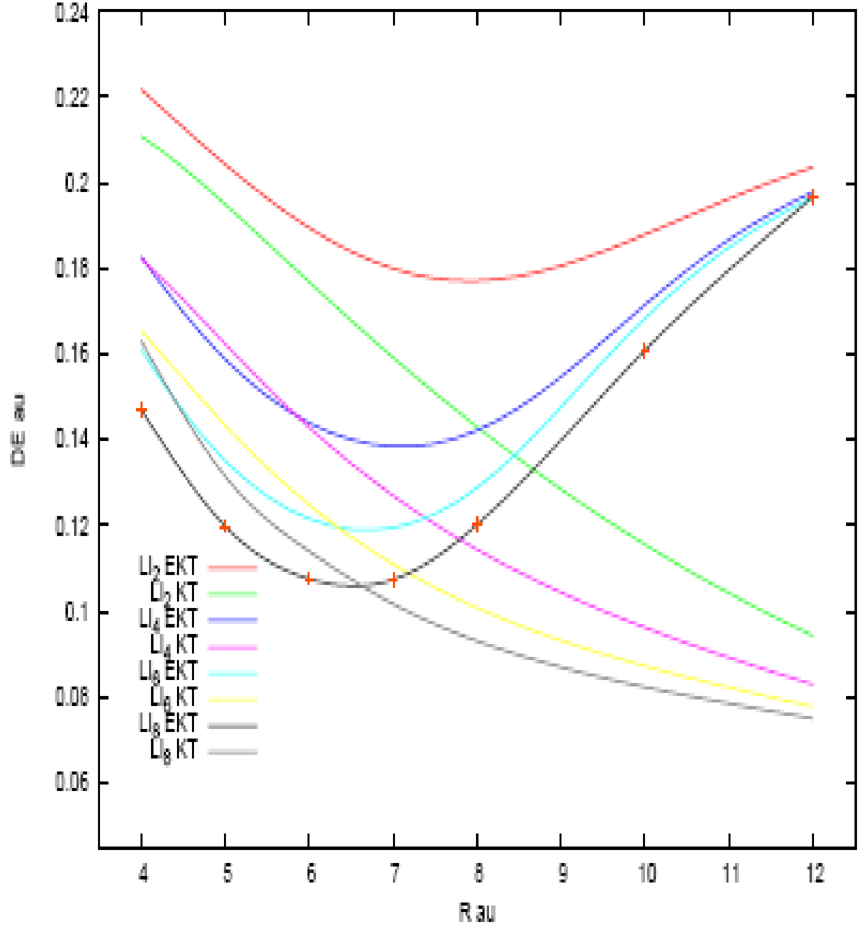




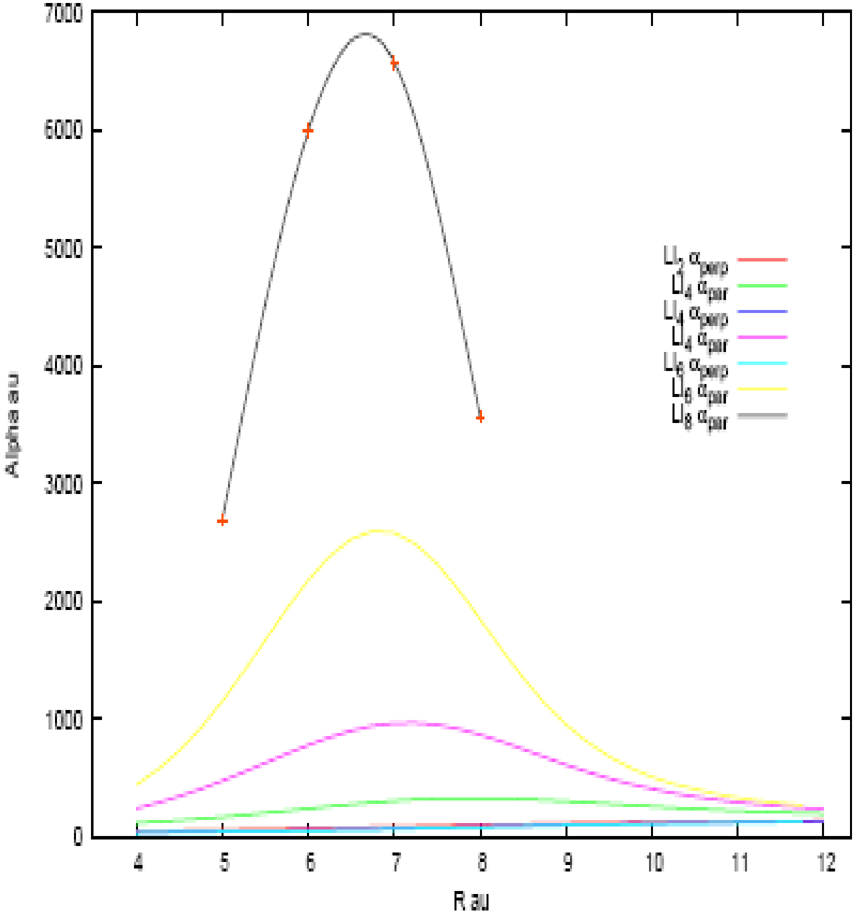
Full configuration-interaction study of the metal-insulator transition in model systems, G L Bendazzoli, S Evangelisti, A Monari, B Paulus, V Vetere, IOP Publishing, 17 (2008) 012005

Metal-Insulator transition of Lithium Linear Chain





Metal-Insulator transition of lithium linear chain



Plan

- Use Gaussian basis set with Jastrow factor
- K-point sampling of the expectation value
- Calculate linear hydrogen chain of atoms with larger system size ($n>8$)
- See if we can locate a maximum

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