MŰEGYETEM 1782

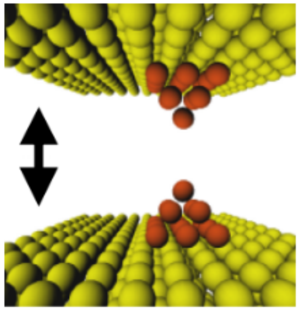
Study of a cobalt nanocontact

**László Balogh, Krisztián Palotás, Bence Lazarovits,
László Udvardi, László Szunyogh**

Budapest, November 11—12, 2010.

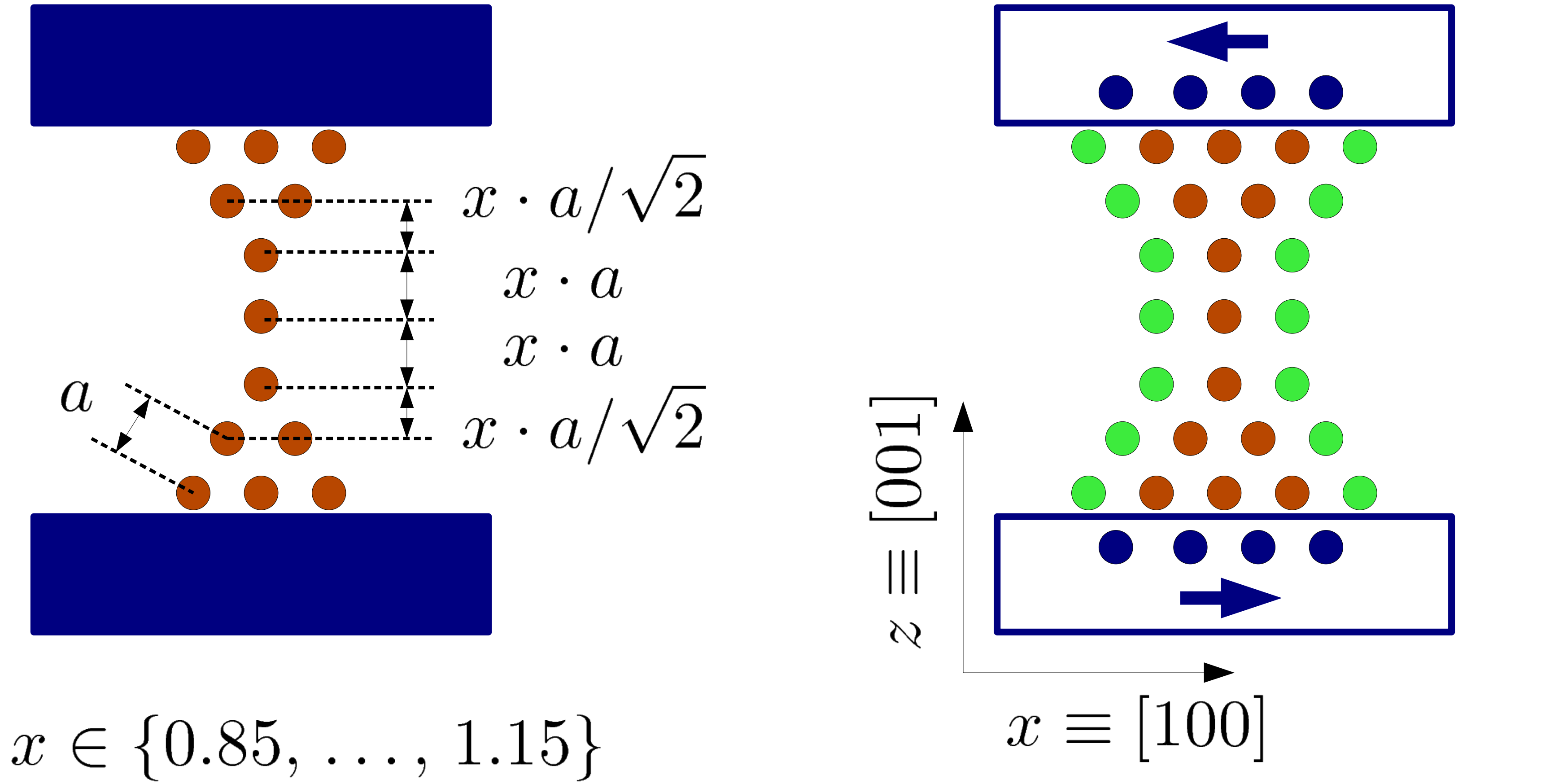
Review: last slide from Uppsala

- Future plans
  - STM structure ground state: simulated annealing



Physical system:

Co[001] + 3 x 3 + 2 x 2 + 1 + 1 + 1 + 2 x 2 + 3 x 3 + Co[001]



Questions

- What is the (magnetic) ground state?
  - Bloch ↔ Néel wall
  - versus *x*
- What spin model describes the system?
  - Isotropic Heisenberg
  - *Ab initio* energy function
  - Anisotropy

Methods

Screened Korringa–Kohn–Rostoker / embedded cluster method [1]

Infinitesimal rotations method: [2]
► parameters of isotropic Heisenberg model

Monte Carlo: simulated annealing / Metropolis algorithm
► ≈ ground state

Minimization of the band energy by Newton−Raphson method
- frozen potential approximation

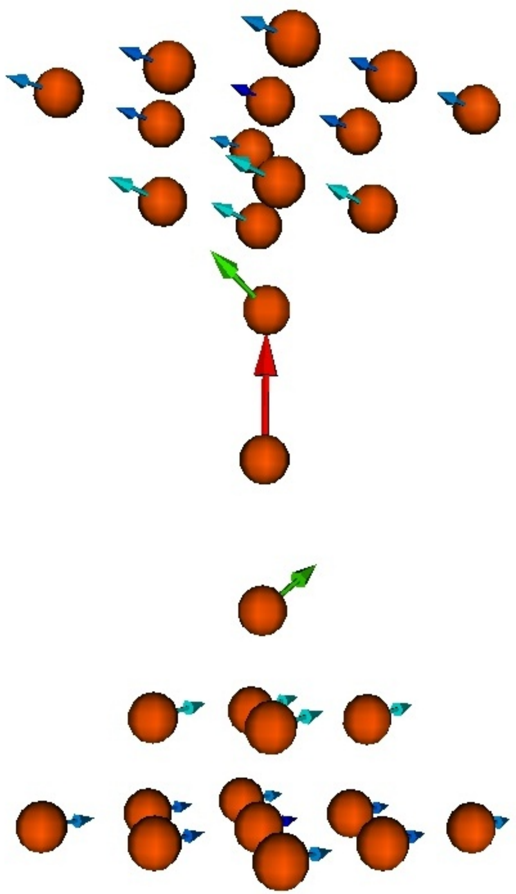
► ground state
► local quantities

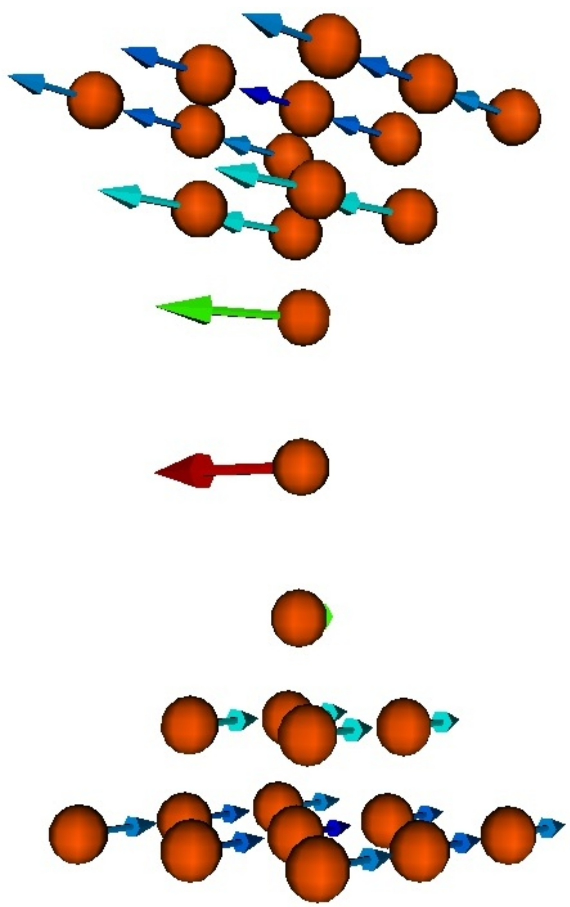
Self-consistent energy calculation [1]
► GS energy, local quantities

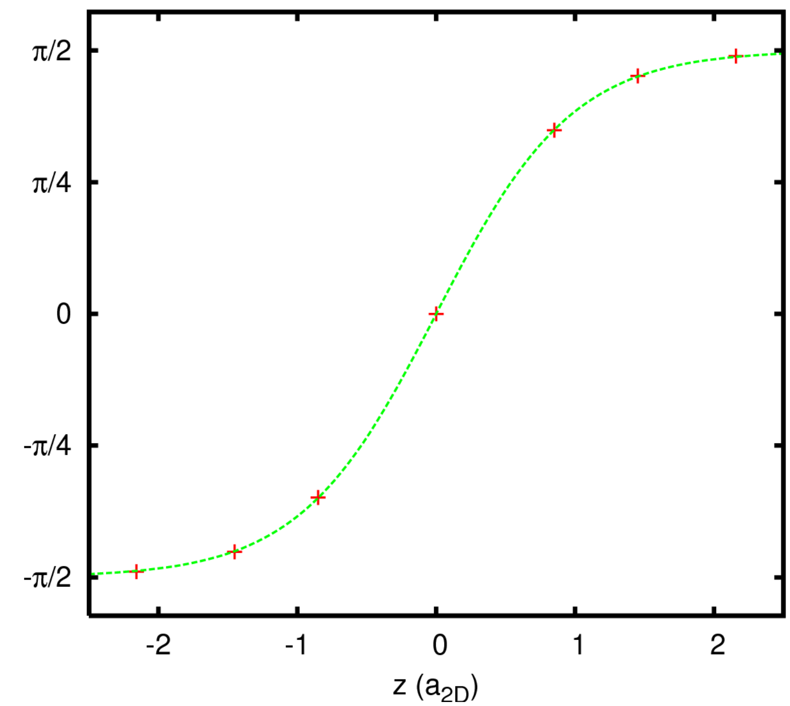
[1] B. Lazarovits, *et. al.* PRB **65**, 104441 (2002)

[2] A.I. Liechtenstein *et al.* JMMM **67**, 65 (1987)
[2] L. Udvardi *et al.* PRB **68**, 104436 (2003)

Domain wall: Néel- or Bloch



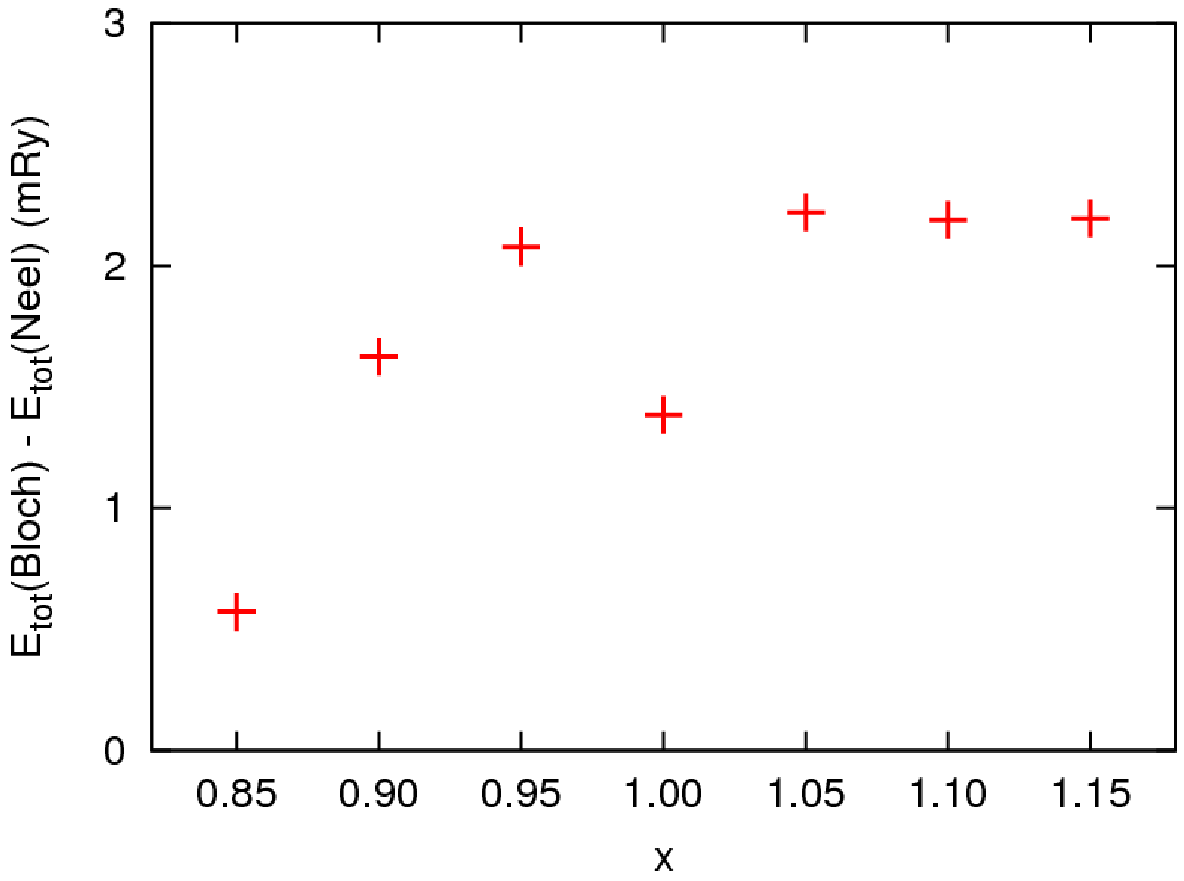




$$\varphi(z) = \frac{\pi}{2}\mathrm{th}\left(\frac{z}{z_0}\right)$$

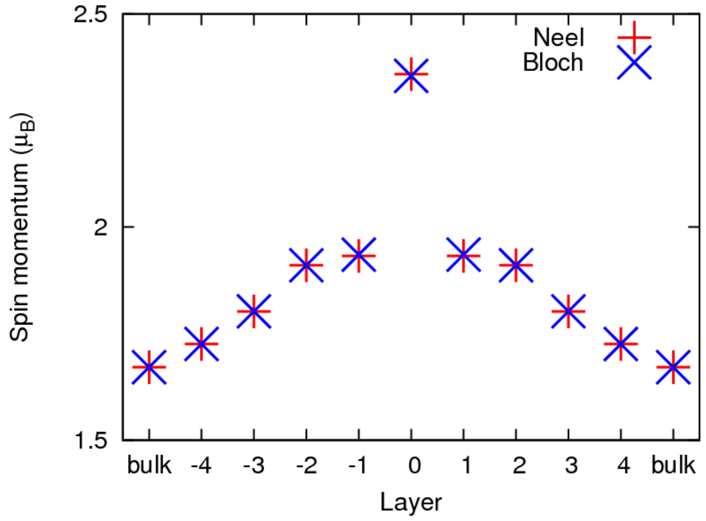
Self-consistent energies

E_{tot}(Bloch) – E_{tot}(Néel) > 0

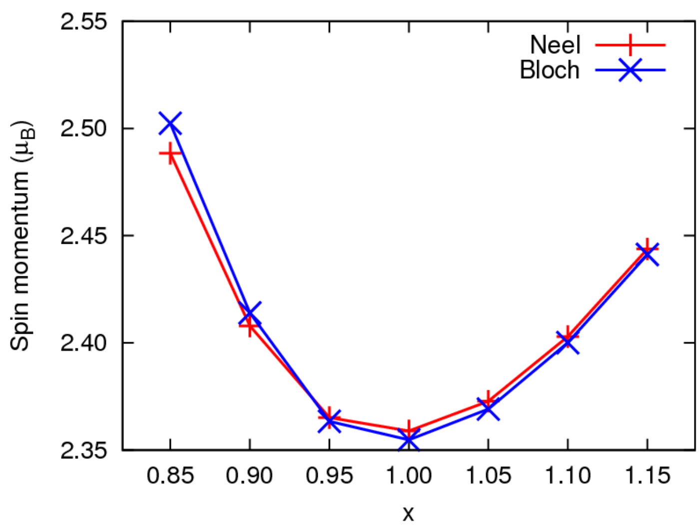


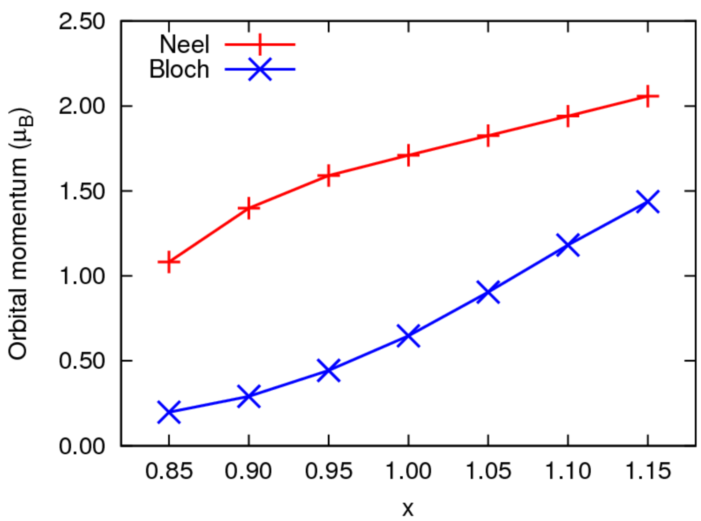
Local quantities

- Spin momentum vs. layer (x = 1.00)

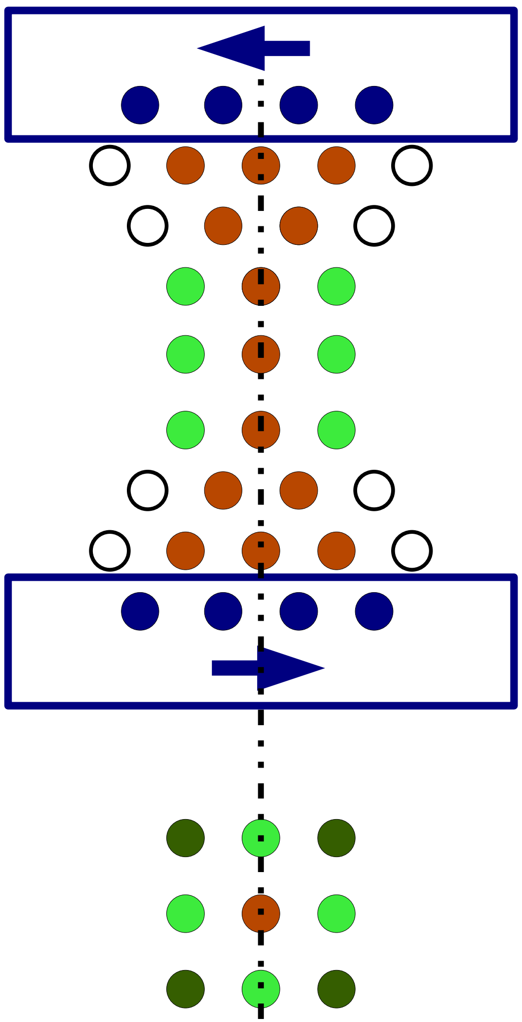


- Spin-, orbital momentum vs. x (cental atom)

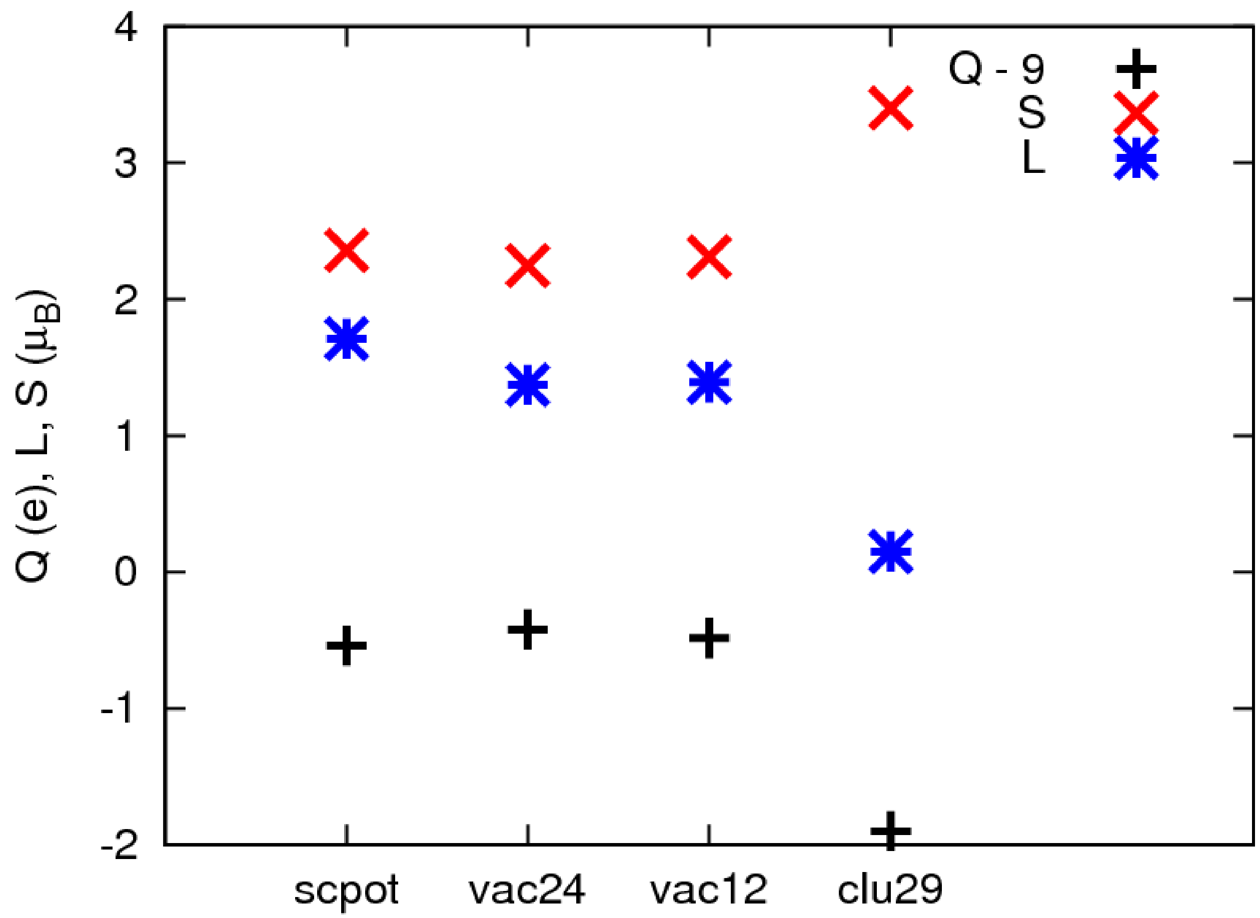




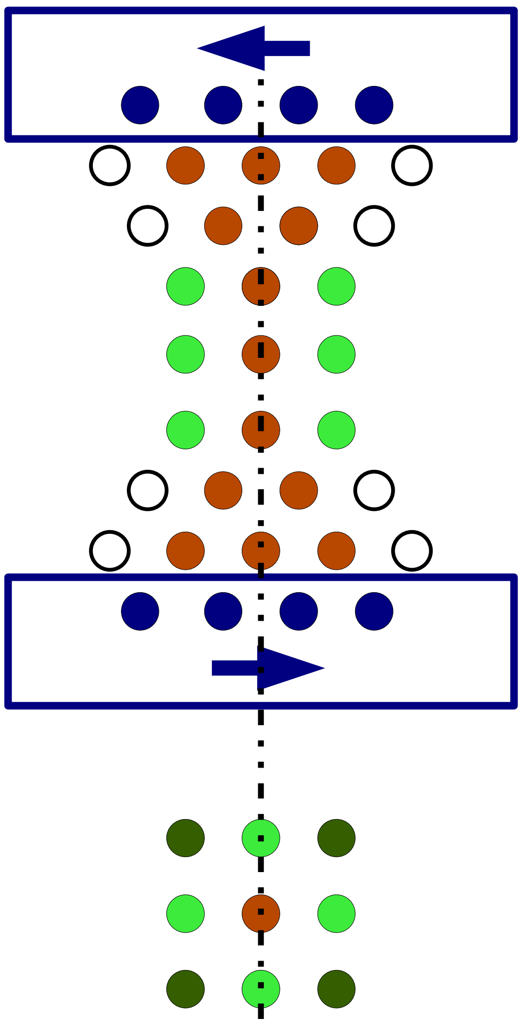
Effect of the vacuum “envelop”

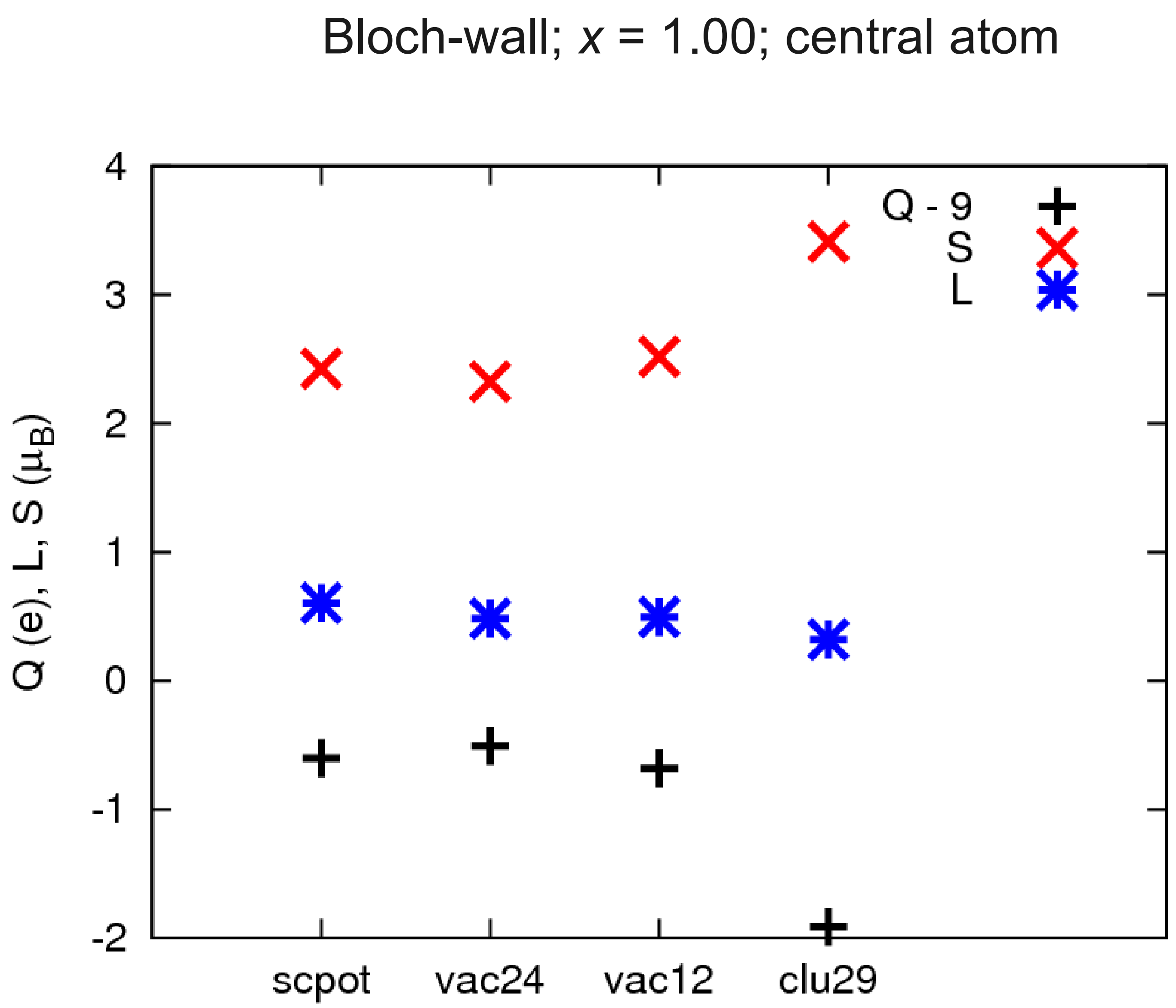


Néel-wall; *x* = 1.00; central atom



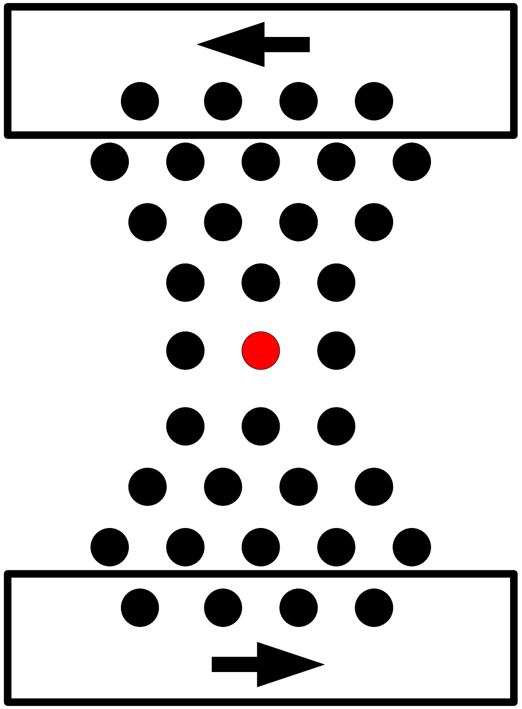
Effect of the vacuum "envelop"





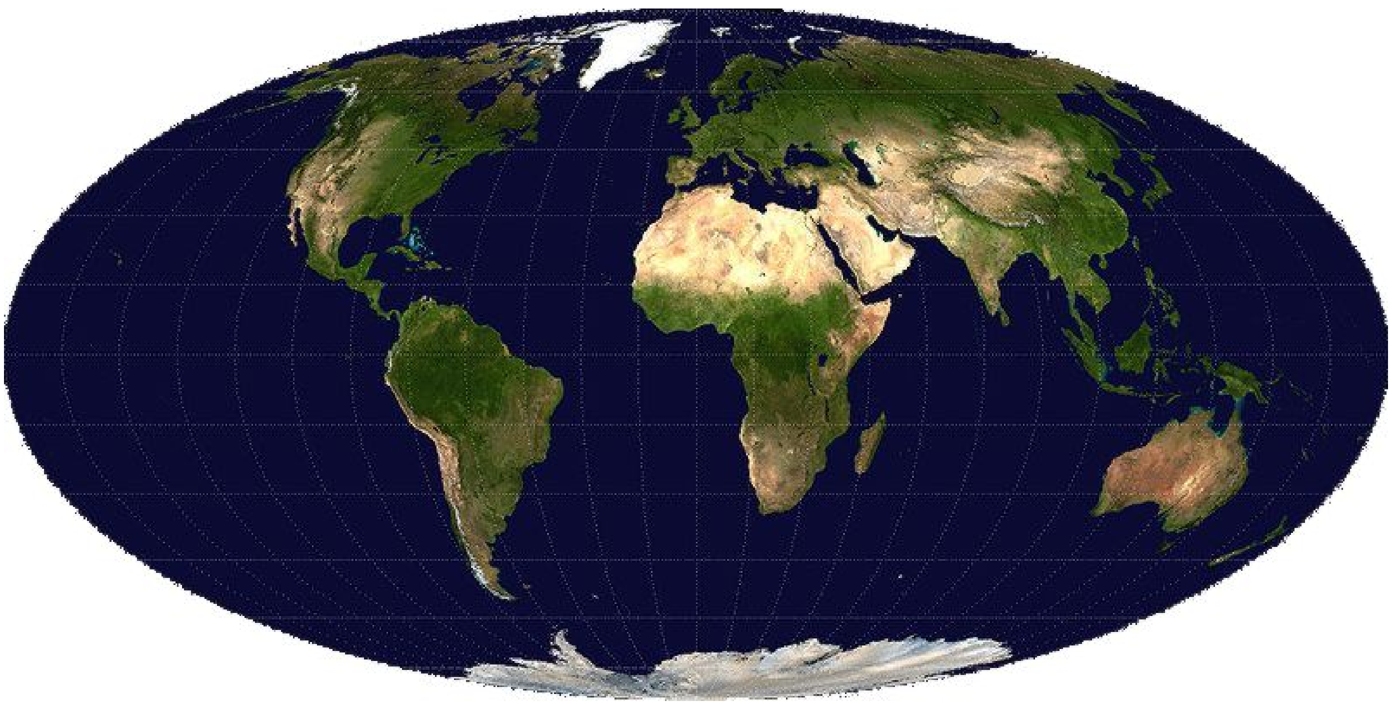
Model of the energy function

$$E_{\text{band}}(\underbrace{\ldots}_{\text{fixed}},\ \vartheta,\ \varphi,\ \underbrace{\ldots}_{\text{fixed}}) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} E_{lm}Y_{lm}(\vartheta,\varphi)$$



Mollweide-projection

How to plot an $E(\vartheta, \varphi)$ function?



Mollweide-projection

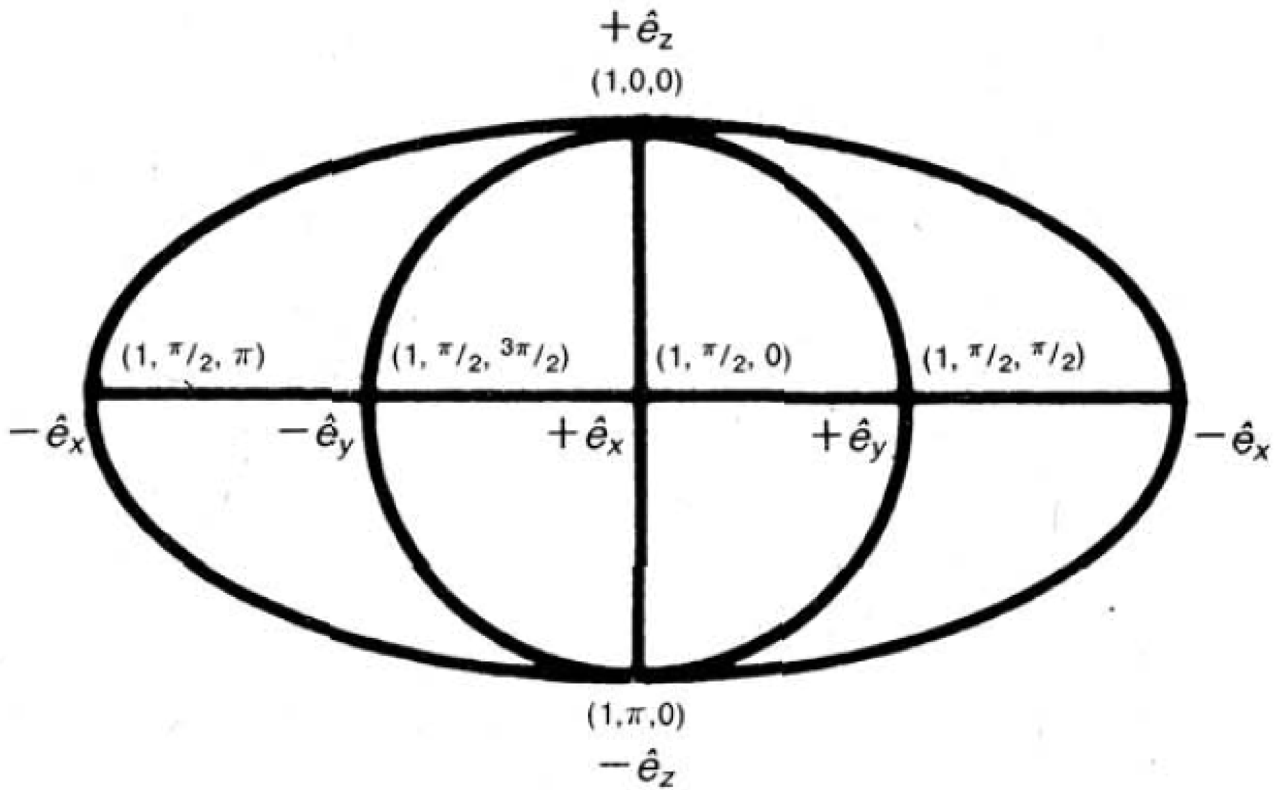


Figure 1. Mollweide's elliptical projection of the unit sphere based on the normal right-handed Cartesian coordinate system viewed towards the coordinate origin from along the $+x$ axis.

$$x = 2\sqrt{2}\,\frac{\varphi}{\pi}\cos(\xi)$$

$$y = \sqrt{2}\sin(\xi)$$

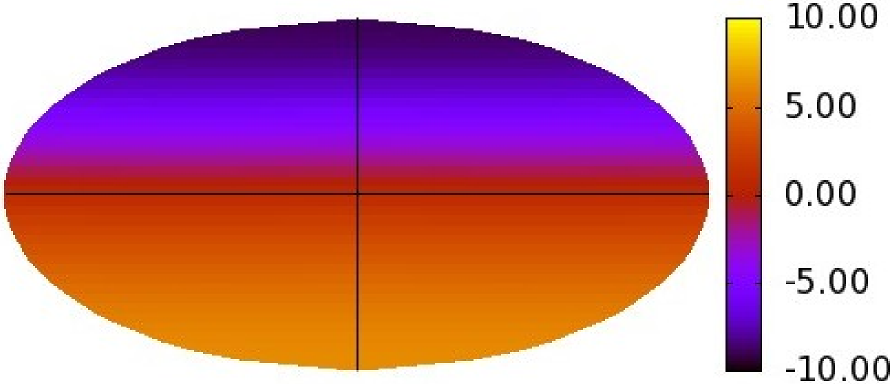
$$2\xi + \sin(2\xi) = \pi\cos(\vartheta)$$

C. M. Quinn *et al.*, J. Chem. Edu., **61,** 569, (1984)

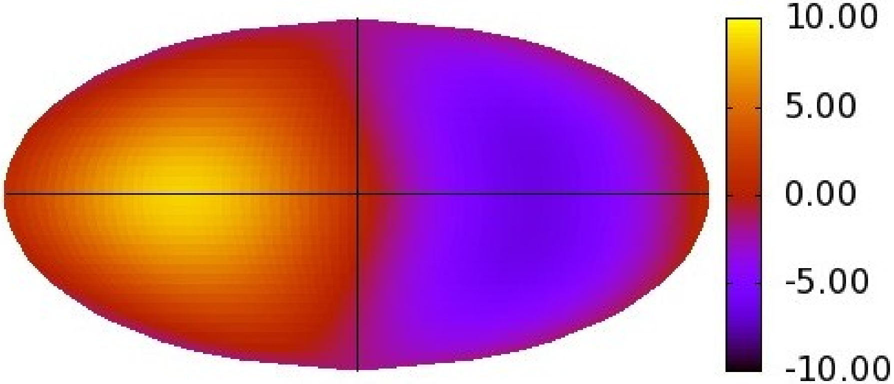
http://en.wikipedia.org/wiki/Mollweide_projection

Energy function (mRyd)

Néel (x = 1.00)

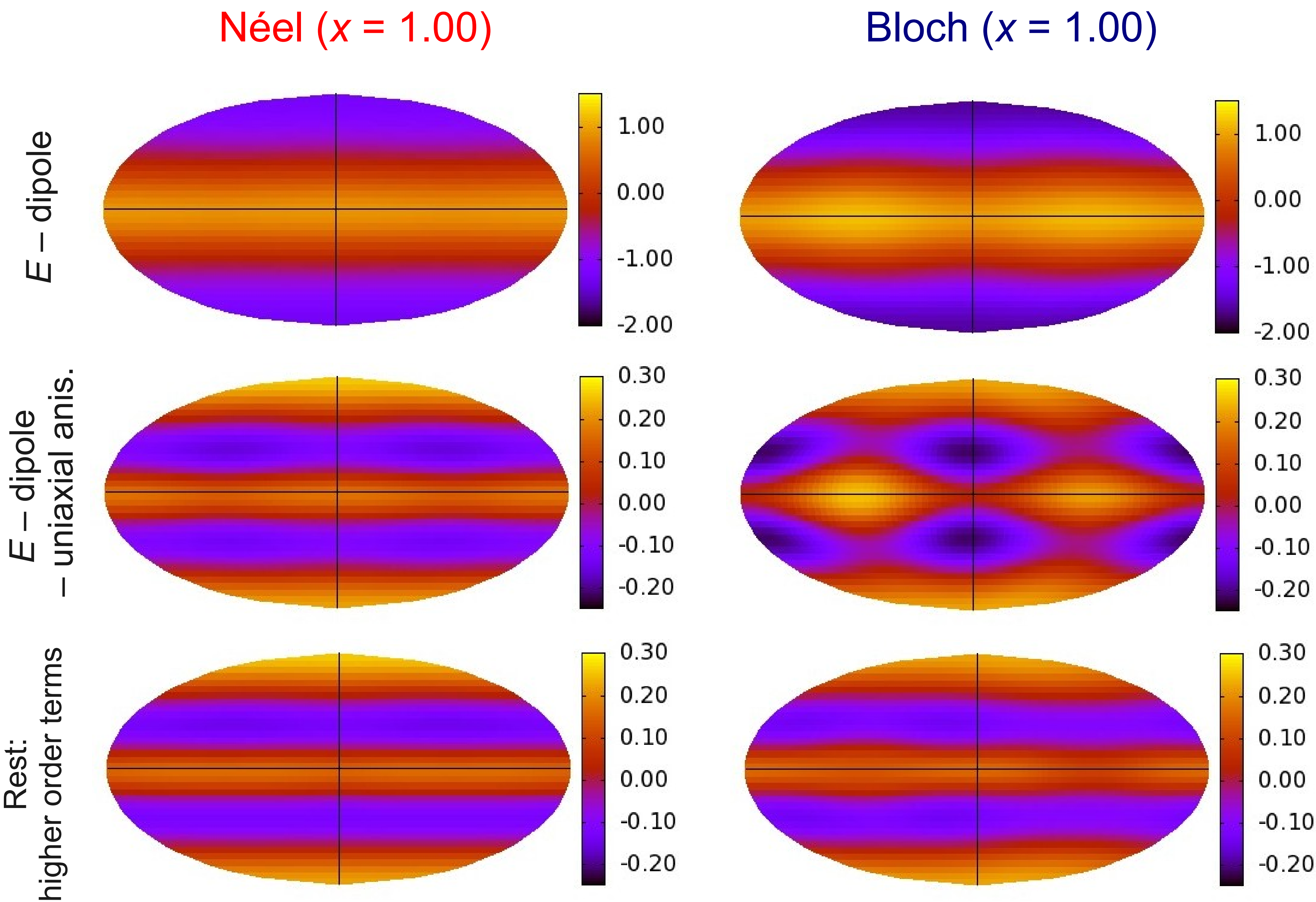


Bloch (x = 1.00)

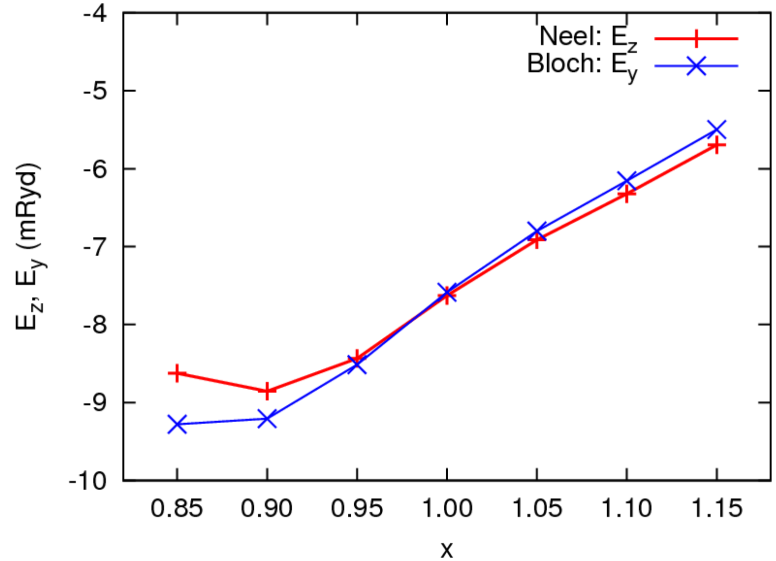


(1 mRyd = 13.6 meV)

Components of the energy function

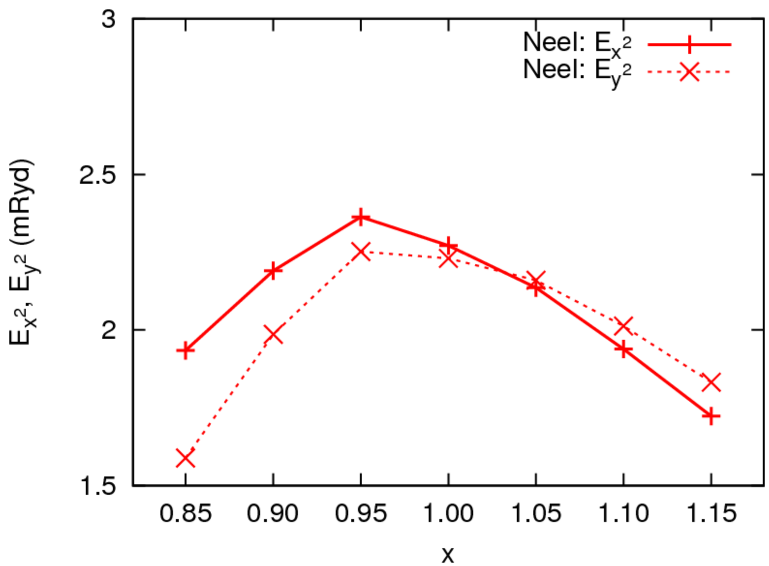


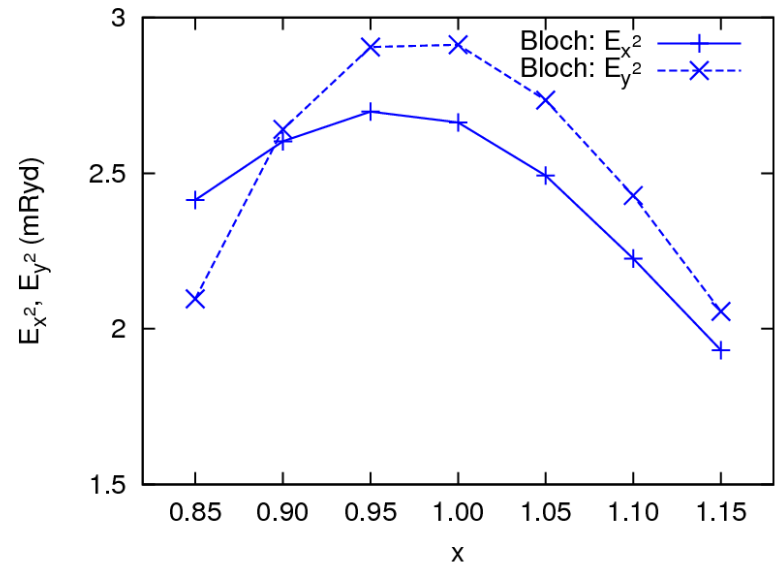
Anisotropy vs. deformation



Néel

Bloch





Summary

Screened Korringa–Kohn–Rostoker /
embedded cluster method

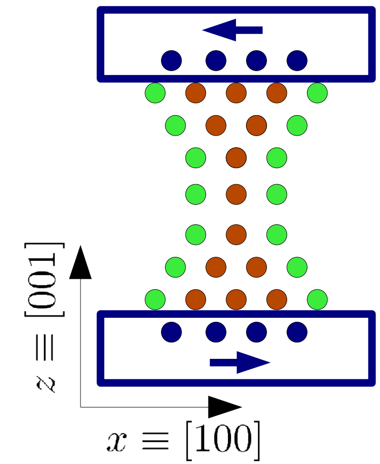
Infinitesimal rotations method:
▶ parameters of isotropic Heisenberg model

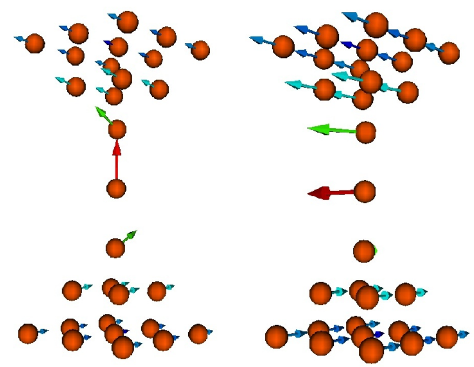
Monte Carlo: simulated annealing /
Metropolis algorithm
▶ ≈ ground state

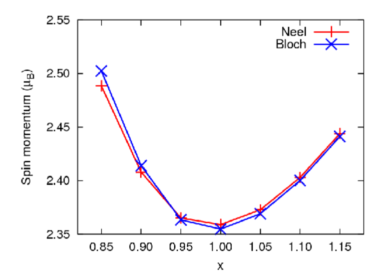
Minimization of the band energy by Newton−Raphson method
- frozen potential approximation

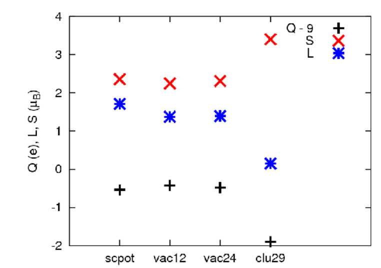
▶ ground state
▶ local quantities

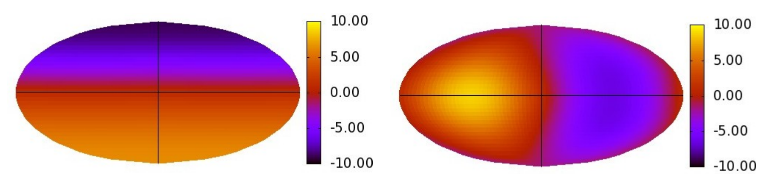
Self-consistent energy calculation
▶ GS energy, local quantities







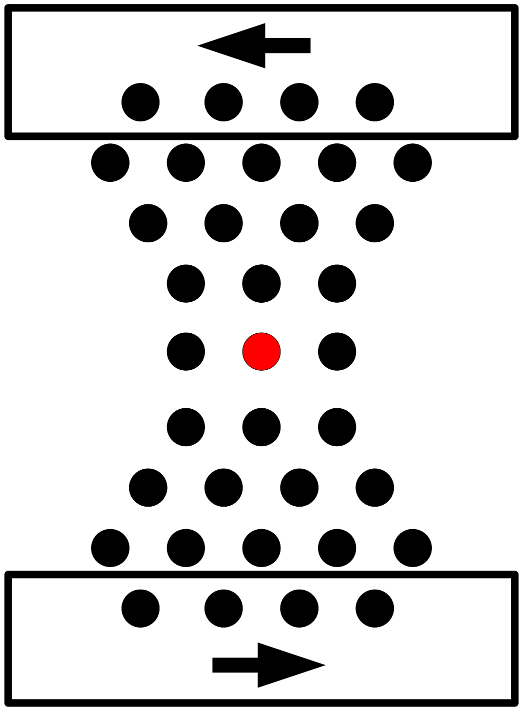




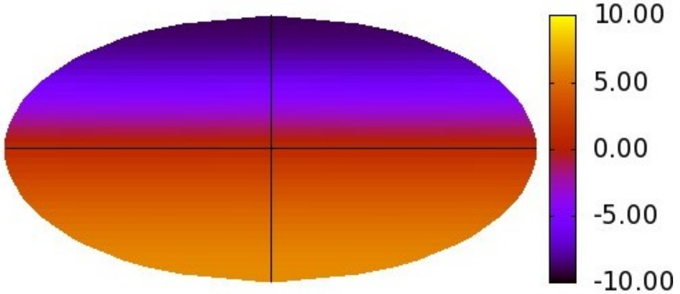
Thank you for your attention

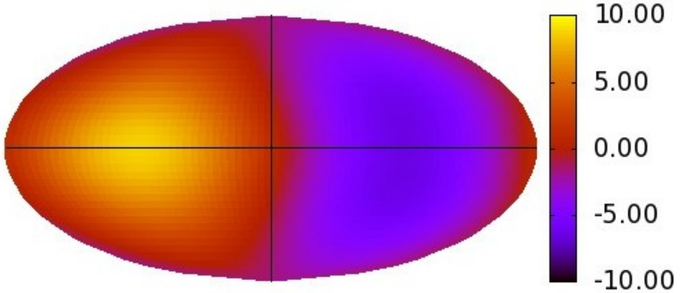
László Balogh, Krisztián Palotás, Bence Lazarovits,
László Udvardi, László Szunyogh

Bonus slide: quantize the spin model



$$E_{\text{band}}(\underbrace{\ldots}_{\text{fixed}}, \vartheta, \varphi, \underbrace{\ldots}_{\text{fixed}}) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} E_{lm} Y_{lm}(\vartheta, \varphi)$$





$$\mathcal{H} = \alpha\,\hat{\mathrm{S}}_{y/z} + \beta\,\hat{\mathrm{S}}_x^2 + \gamma\,\hat{\mathrm{S}}_y^2$$

- ▶ Eigenenergies (*x*) ?
- ▶ Degenerations (*x*) ?