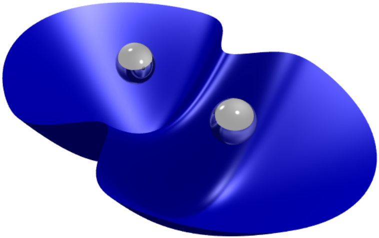
Cold Atoms:
A quantum test bed for magnetism?

Pascal Bugnion and Gareth Conduit



Why cold atoms?

They are useful to simulate complex many-body systems.

Simulating electronic systems

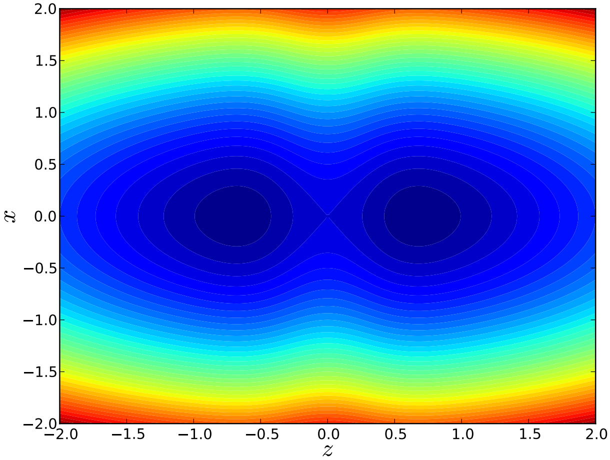
Prepare a mixture of ^{6}Li atoms, such that the total angular momentum for each atom is $F = 1/2$.
This gives two hyperfine states: $m_F = +1/2$ and $m_F = -1/2$.

Simulating electronic systems

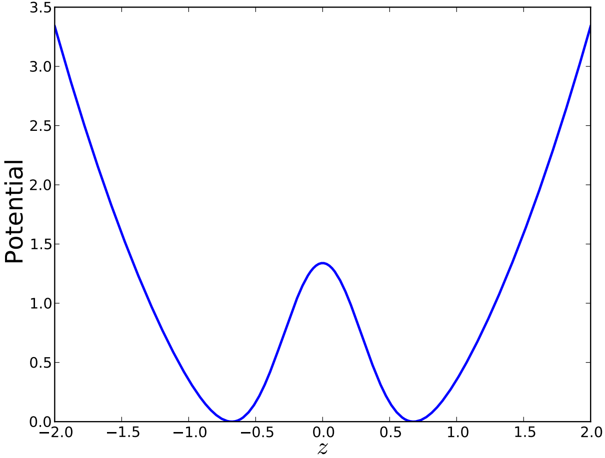
Prepare a mixture of ^{6}Li atoms, such that the total angular momentum for each atom is $F = 1/2$.
This gives two hyperfine states: $m_F = +1/2$ and $m_F = -1/2$.

The interaction between different atoms can be tuned by changing the underlying magnetic field.

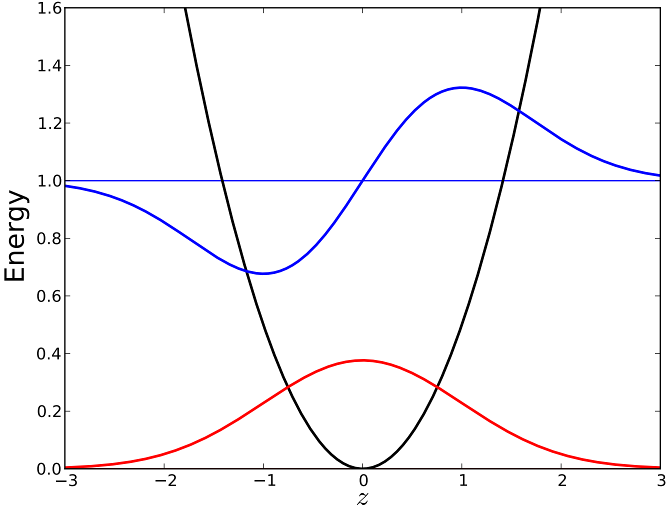
Experimental setup



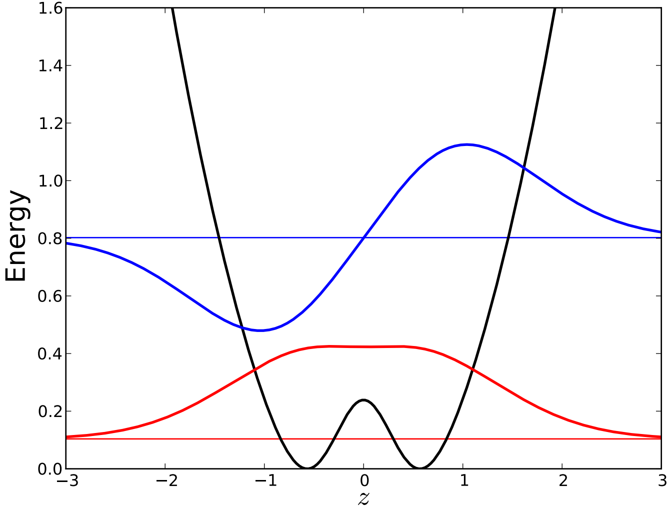
Experimental setup



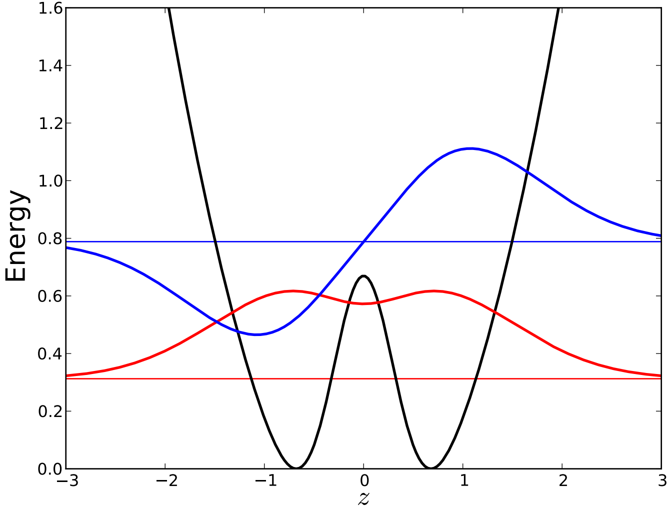
Low-barrier limit



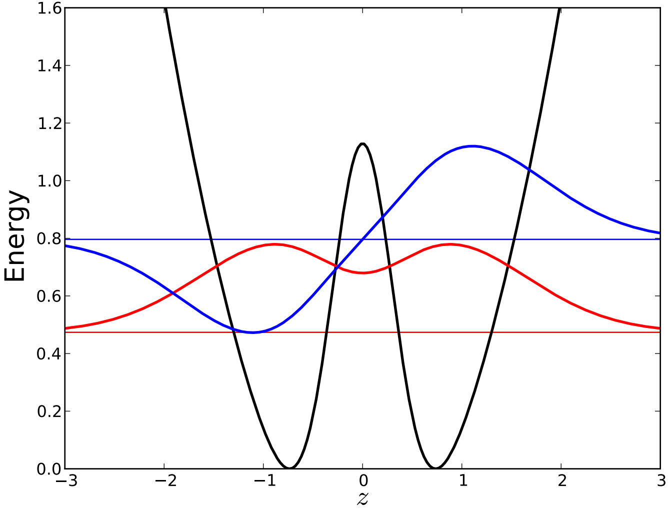
Increasing barrier height



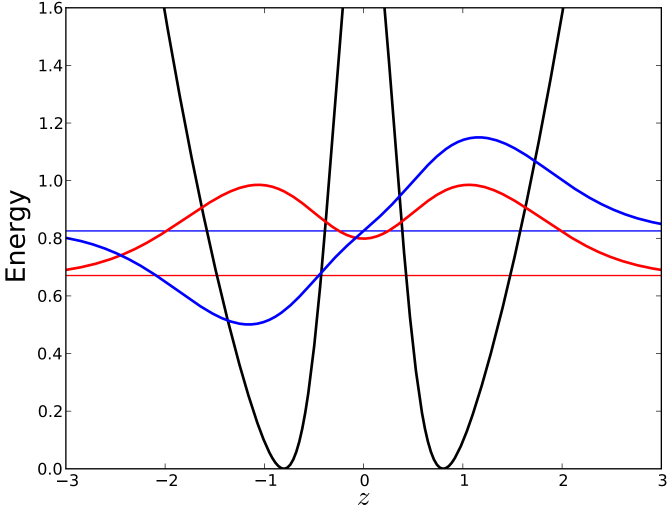
Increasing barrier height



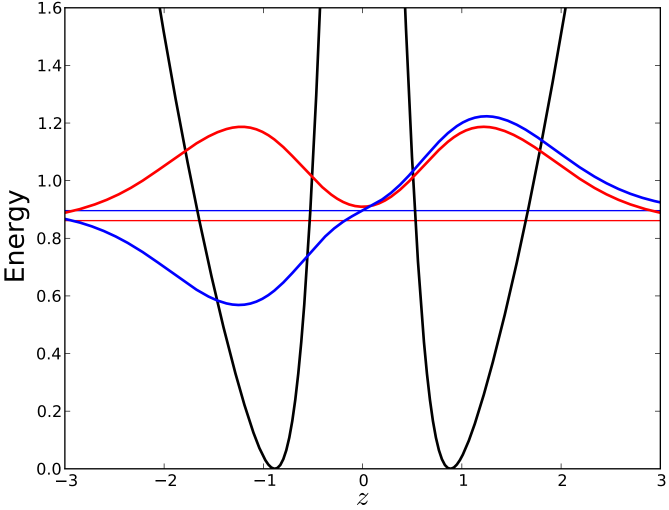
Increasing barrier height



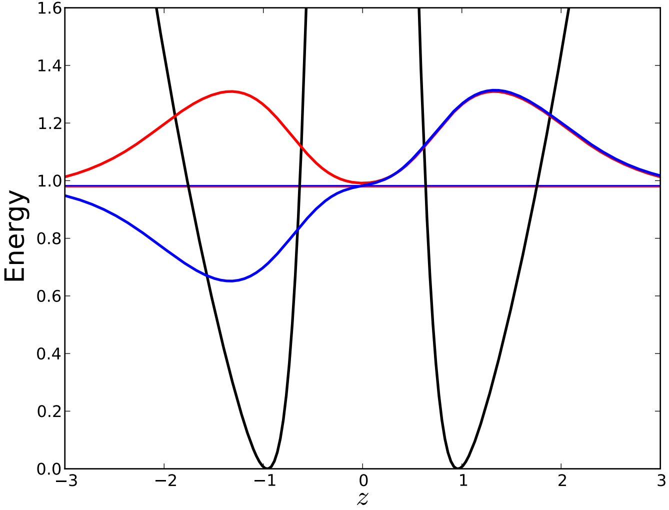
Increasing barrier height



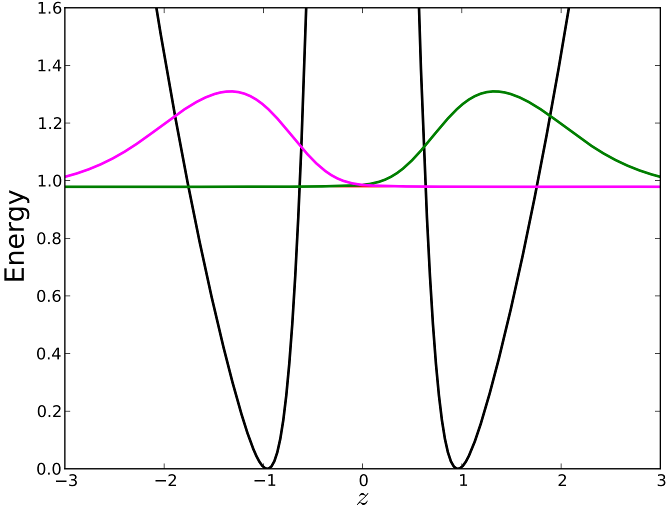
Increasing barrier height



High barrier



High barrier

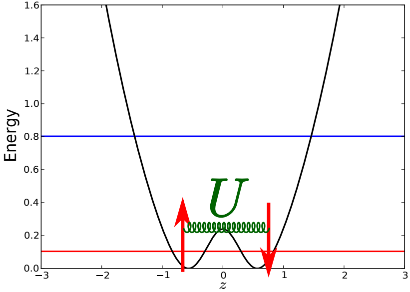


Simulating magnetism

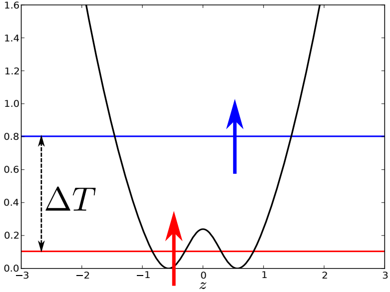
Ashcroft and Mermin on magnetism:

> “*The development of a tractable model of a magnetic material, capable of describing both the characteristic electron spin correlations as well as the electronic transport properties [. . .] remains one of the major unsolved problems of modern solid state theory.*”

Diamagnetic-Ferromagnetic transition

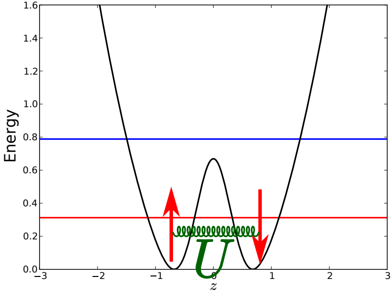


$$E_{\uparrow\downarrow} = U$$

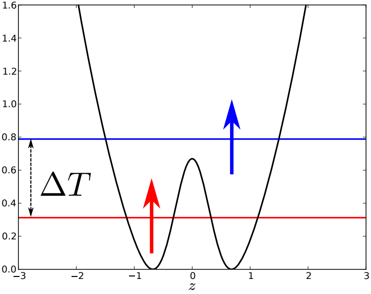


$$E_{\uparrow\uparrow} = \Delta T$$

Diamagnetic-Ferromagnetic transition

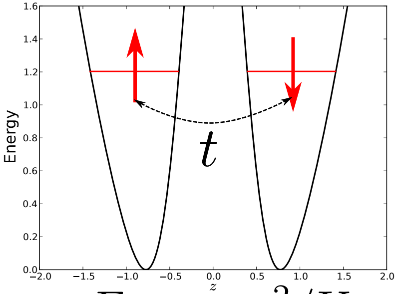


$$E_{\uparrow\downarrow} = U$$

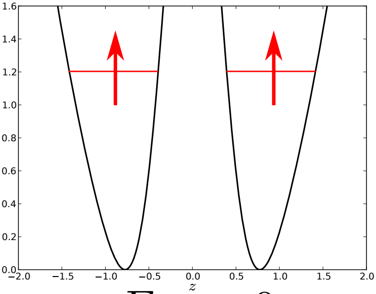


$$E_{\uparrow\uparrow} = \Delta T$$

Ferromagnetic-Antiferromagnetic transition



$$E_{\uparrow\downarrow} = -t^2/U$$



$$E_{\uparrow\uparrow} = 0$$

Full Configuration Interaction

We want to find the stationary states of the time-independent Schrödinger equation, that is, all $E, |\Psi\rangle$ pairs such that

$$\hat{H}\,|\Psi\rangle = E\,|\Psi\rangle$$

Full Configuration Interaction

We want to find the stationary states of the time-independent Schrödinger equation, that is, all $E, |\Psi\rangle$ pairs such that

$$\hat{H}\,|\Psi\rangle = E\,|\Psi\rangle$$

where

$$\hat{H} = \sum_i \hat{h}(\mathbf{r}_i) + \sum_{i>j} \hat{V}(\mathbf{r}_i, \mathbf{r}_j)$$

Full Configuration Interaction (2)

The Hamiltonian eigenvalue equation $\hat{H}|\Psi\rangle = E|\Psi\rangle$ can always be solved by expanding $|\Psi\rangle$ in a basis with the correct symmetry.

Let the basis functions be called $\{|i\rangle\}$. The method proceeds as follows:

1. Write the Hamiltonian matrix in the $\{|i\rangle\}$ basis: $\left\langle i \middle| \hat{H} \middle| j \right\rangle$.
2. Diagonalise this matrix. The eigenvalues are the energies and the eigenvectors are the stationary states $|\Psi\rangle$ expressed in the $\{|i\rangle\}$ basis.

Full Configuration Interaction (3)

1. Define a set of one-electron orbitals $\{\phi_i\}$.
2. Build all n-electron Slater determinants:

$$|D_\alpha\rangle = |\phi_{\alpha_1}\phi_{\alpha_2}\dots\phi_{\alpha_n}\rangle$$

   that you can in this basis.
3. Construct all matrix elements $\left\langle D_\alpha \middle| \hat{H} \middle| D_\beta \right\rangle$.
4. Diagonalise the resultant matrix.

Full Configuration Interaction (4)

Pros

- Arbitrarily improvable. Gives the right answer in the limit of complete basis set.
- Variational.
- Gives excited states.
- Conceptually simple (and easy enough to implement).

Full Configuration Interaction (4)

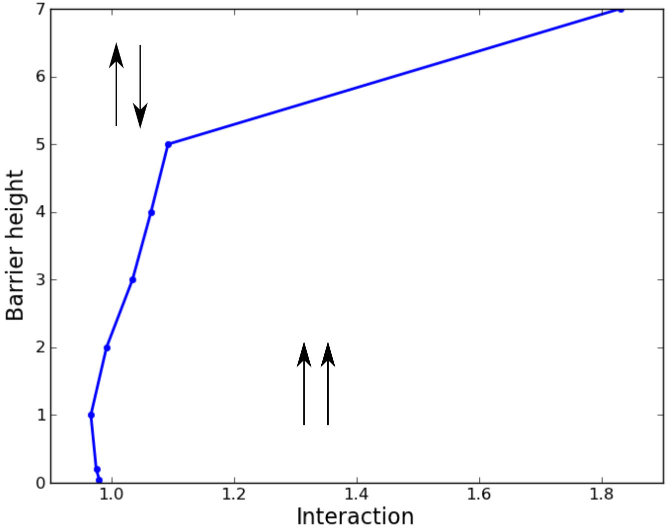
Pros

- Arbitrarily improvable. Gives the right answer in the limit of complete basis set.
- Variational.
- Gives excited states.
- Conceptually simple (and easy enough to implement).

Cons

Very expensive: for N orbitals and n electrons, there are ${}^{N}C_{n}$ Slater determinants. This gives a cost of $O(n!^3)$.

Phase diagram



Thank you for your attention!