

Spontaneous spin polarization in quantum wires

A.D. Klironomos¹, J.S. Meyer², and K.A. Matveev¹

¹ *Materials Science Division, Argonne National Laboratory, Argonne, IL 60439, USA*

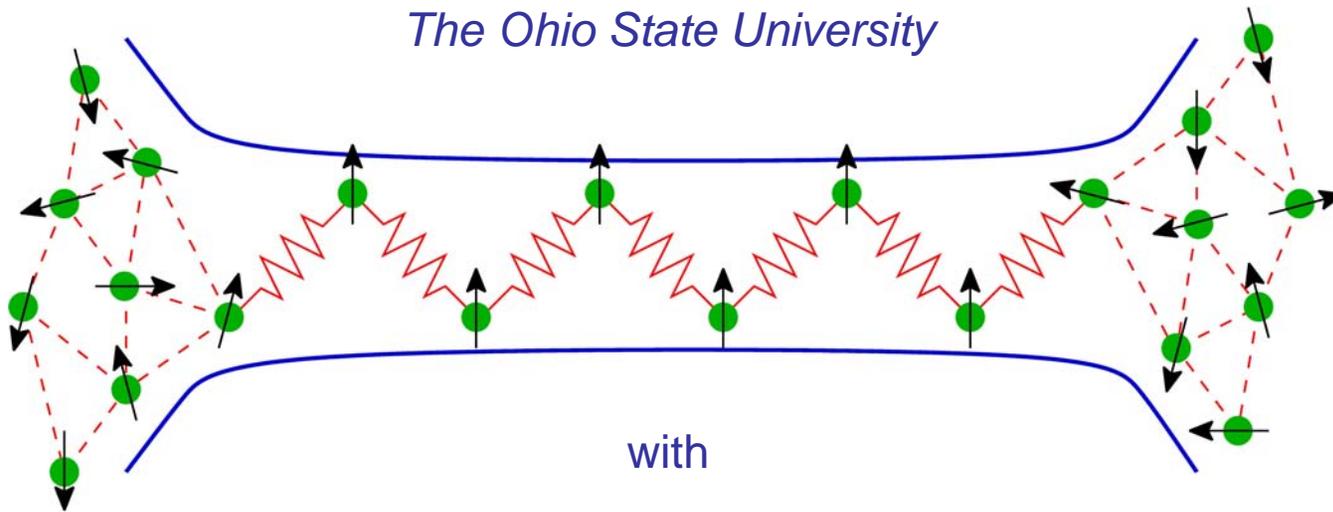
² *Department of Physics, The Ohio State University, Columbus, OH 43210, USA*

A number of recent experiments report spin polarization in quantum wires in the absence of magnetic fields. These observations are in apparent contradiction with the Lieb-Mattis theorem, which forbids spontaneous spin polarization in one dimension. We show that sufficiently strong interactions between electrons induce deviations from the strictly one-dimensional geometry and indeed give rise to a ferromagnetic ground state in a certain range of electron densities. At higher densities, more complicated spin interactions lead to a possibly novel ground state.

Spontaneous Spin Polarization in Quantum Wires

Julia S. Meyer

The Ohio State University



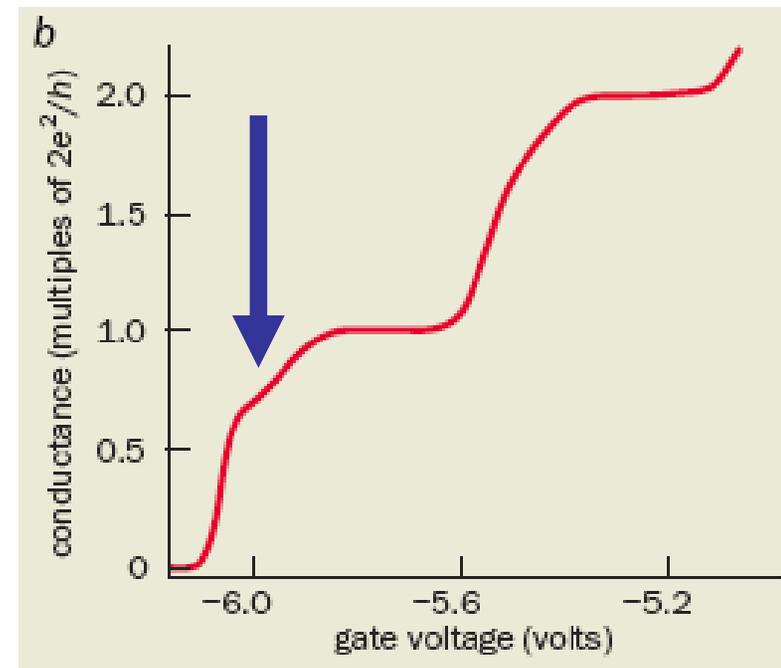
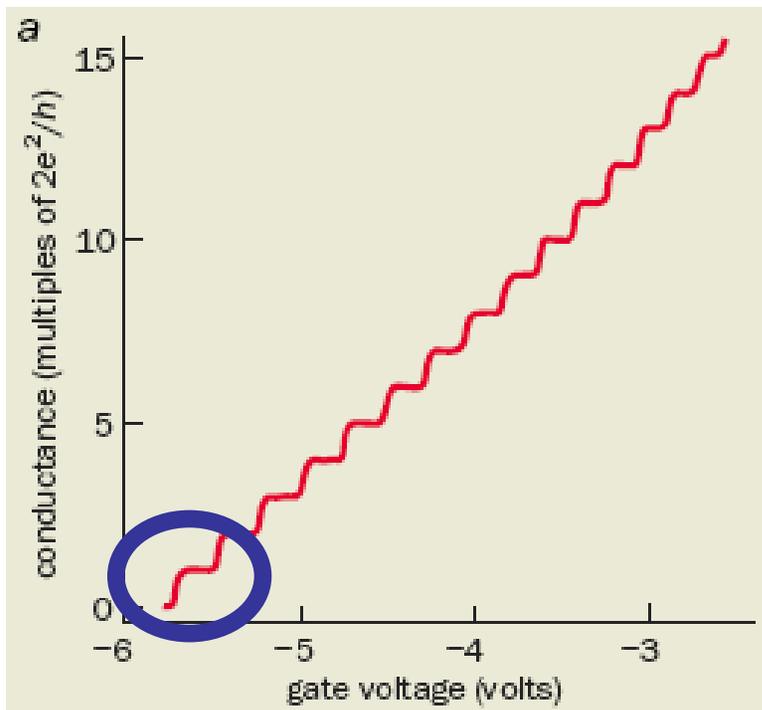
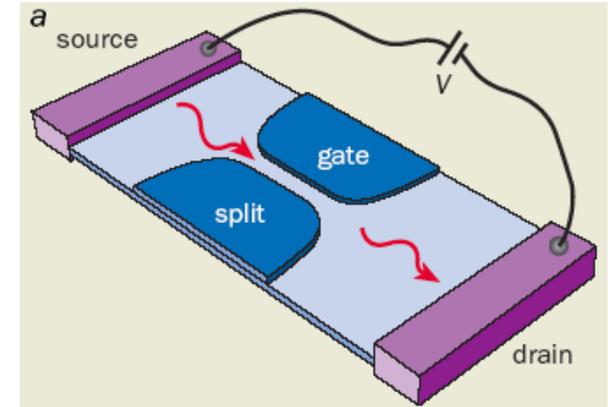
A.D. Klironomos

K.A. Matveev

Why ask this question at all ...

Conductance quantization in Quantum Wires

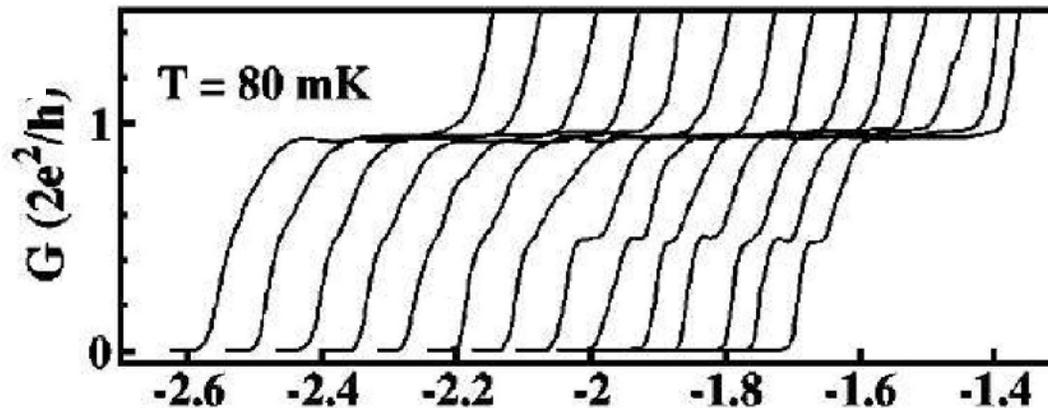
- Theory: $G = k \cdot G_0$ (k integer)
where $G_0 = 2 e^2/h$
↑ spin degeneracy
- Experiment I:



Motivation

Why ask this question at all ...

- Experiment II:
 - conductance anomalies at low density
 - additional structure at $0.7 G_0$ (short wires) or $0.5 G_0$ (long wires)
- see e.g. Thomas *et al.*, Phys. Rev. B **61**, R13365 (2000)



- spontaneous spin polarization?

BUT ...

Lieb-Mattis theorem

In 1D,
the ground state of an interacting electron system
possesses minimal spin.

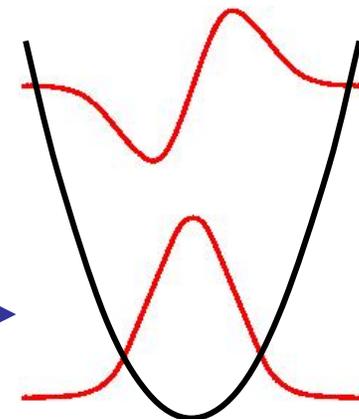
E. Lieb and D. Mattis, Phys. Rev. **125**, 164 (1962).

QUANTUM WIRE:

not a purely one-dimensional system ...

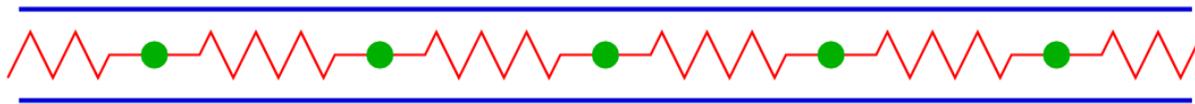
- parabolic confining potential:

no interactions →
strong interactions?



Quantum wires at low density: Wigner crystal

- at low electron densities n_e ,
interaction energy ($\sim n_e$) dominates over kinetic energy ($\sim n_e^2$)
 \Rightarrow formation of (classical) **Wigner crystal**

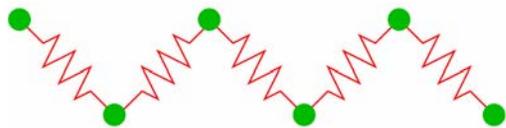


- Coulomb interaction:
- confining potential:

$$V_{\text{int}} = \frac{e^2}{\epsilon} \sum_{i < j} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}$$

$$V_{\text{conf}} = \frac{1}{2} m \Omega^2 \sum_i y_i^2$$

- formation of **zig-zag chain** favorable when V_{int} of order V_{conf}



- minimize $E(d) = \frac{e^2}{\epsilon} \sum_{j=1}^{\infty} \frac{1}{\sqrt{\frac{1}{n_e^2} (2j-1)^2 + d^2}} + \frac{1}{2} m \Omega^2 \left(\frac{d}{2}\right)^2$

with respect to distance d between rows

Zig-zag chain

- $V_{\text{int}}(r_0) = V_{\text{conf}}(r_0) \equiv E_0 \Rightarrow$ characteristic length scale r_0

$$r_0 = \left(\frac{2e^2}{\epsilon m \Omega^2} \right)^{1/3}$$

- dimensionless density $\nu = n_e r_0$

- transition 1D \rightarrow zig-zag

$$\text{at } \nu_c = \left(\frac{4}{7\zeta(3)} \right)^{1/3} \approx 0.78$$

- [crystals with larger number of chains are stable at even higher densities]
Piacente *et al* 04

(a) $\nu < 0.78$



(b) $\nu = 0.80$



(c) $\nu = 1.46$

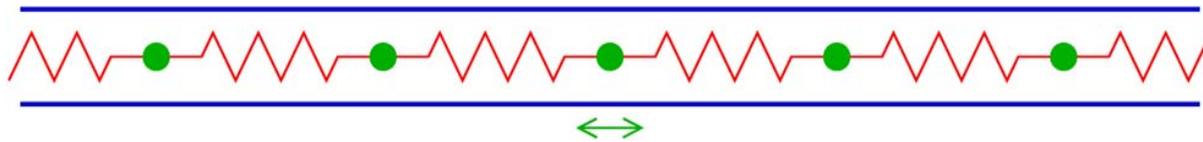


(d) $\nu = 1.75$

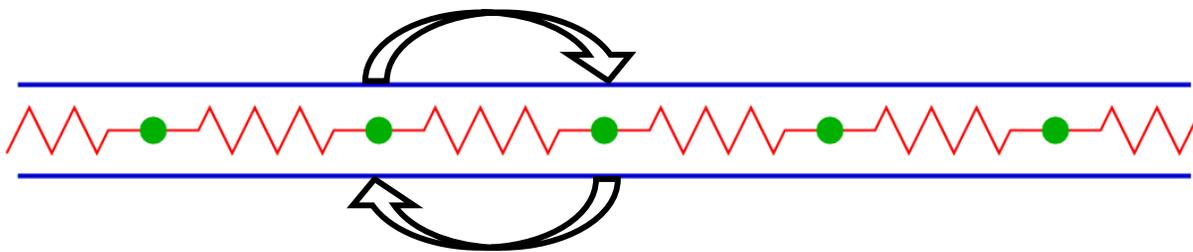


- structure ✓
- spin properties ?

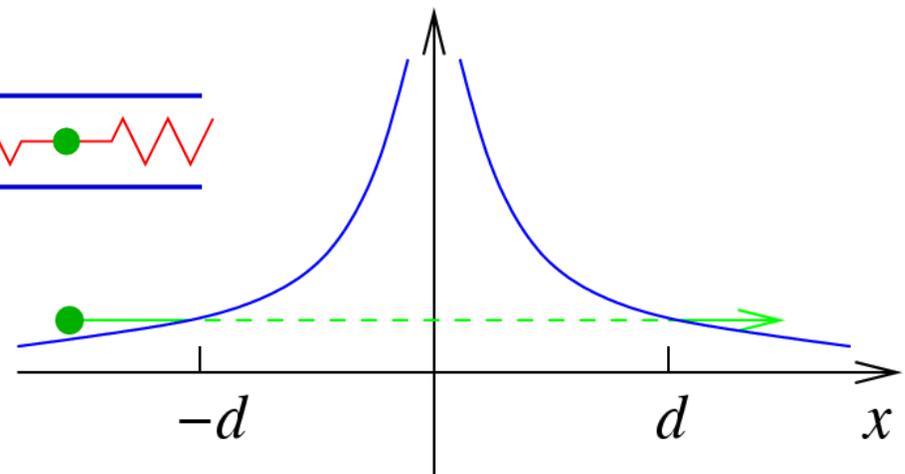
Spin interactions in a Wigner crystal



- to a first approximation, spins do not interact ...
- BUT:
weak tunneling through Coulomb barrier

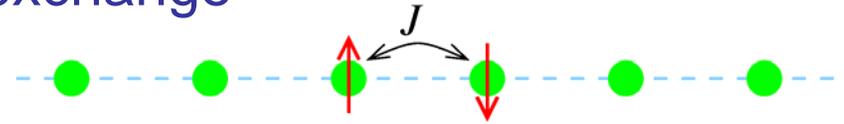


⇒ exponentially small
exchange constants J



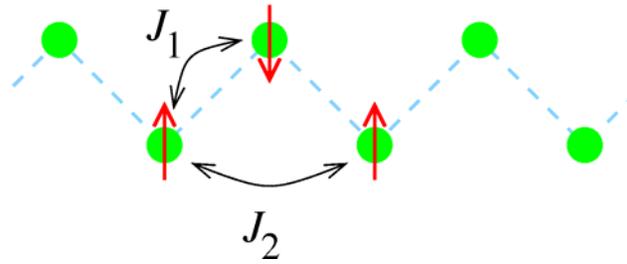
Exchanges in a zig-zag chain

- 1D chain: (AF) nearest-neighbor exchange



- zig-zag chain:

- in addition, next-nearest neighbor exchange



Frustrated Heisenberg spin chain

$$H_P = \frac{1}{2} \sum_j [J_1 P_{j,j+1} + J_2 P_{j,j+2}]$$

use $P_{ij} = \frac{1}{2} + 2\mathbf{S}_i \mathbf{S}_j$

- spin Hamiltonian: $H = \sum_j (J_1 \mathbf{S}_j \mathbf{S}_{j+1} + J_2 \mathbf{S}_j \mathbf{S}_{j+2})$
- next-nearest neighbor exchange J_2 causes **frustration**

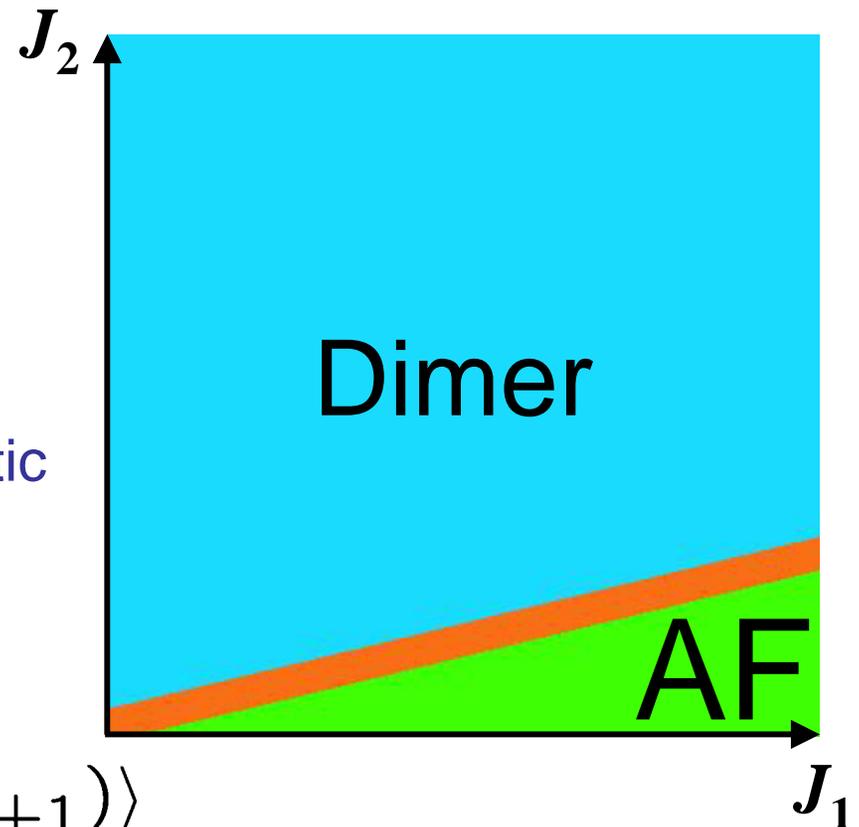
- **phase diagram**

[Majumdar & Ghosh, Haldane, Eggert,
White & Affleck, Hamada *et al.*, Allen *et al.*,
Itoi & Qin, ...]

$J_2 < 0.24... J_1$: weak frustration
→ the groundstate is antiferromagnetic

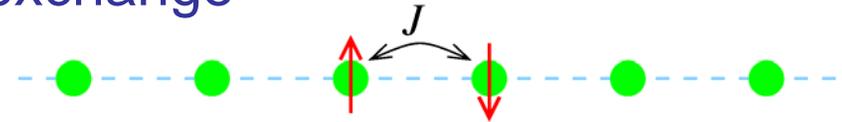
$J_2 > 0.24... J_1$: strong frustration
→ the ground state is dimerized

dimerization $d = \langle \mathbf{S}_j (\mathbf{S}_{j-1} - \mathbf{S}_{j+1}) \rangle$



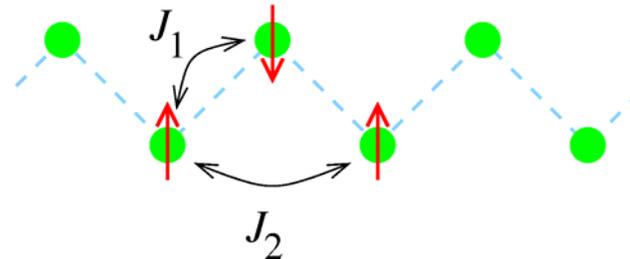
Exchanges in a zig-zag chain

- 1D chain: (AF) nearest-neighbor exchange

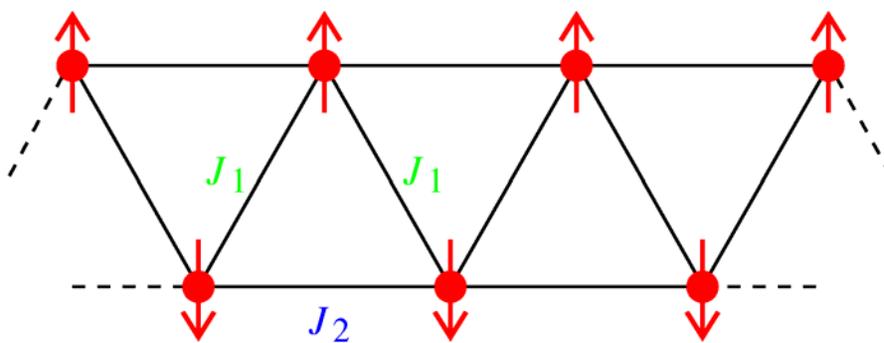


- zig-zag chain:

- in addition, next-nearest neighbor exchange

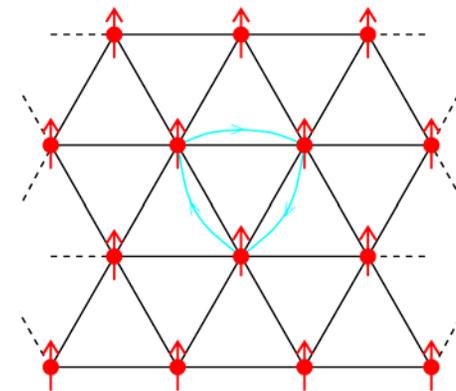


- increase distance between rows \rightarrow equilateral configuration



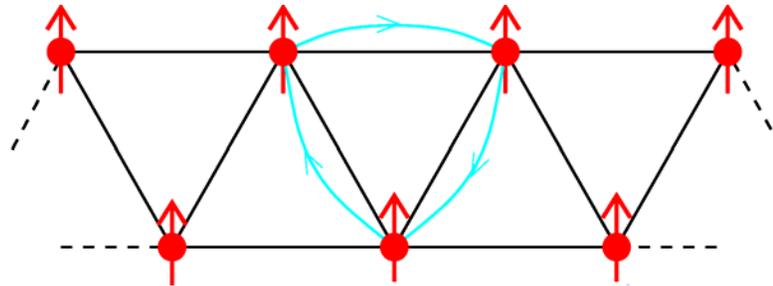
\rightarrow **RING EXCHANGES**

cf. 2D Wigner crystal:

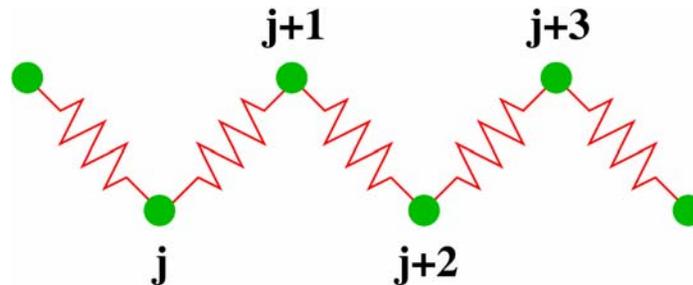


(Roger 84, Bernu, Candido & Ceperley 01, Voelker & Chakravarty 01, ...)

Ring exchanges



- cyclic exchange of l particles: $P_{j_1 \dots j_l} = P_{j_1 j_2} P_{j_2 j_3} \dots P_{j_{l-1} j_l}$
 - ring exchange of **even** number of particles: **antiferromagnetic**
 - ring exchange of **odd** number of particles: **ferromagnetic**
- (Thouless 1965)



- Hamiltonian:

$$H_P = \frac{1}{2} \sum_j [J_1 P_{j j+1} + J_2 P_{j j+2} - J_3 (P_{j j+1 j+2} + P_{j+2 j+1 j}) + J_4 (P_{j j+1 j+3 j+2} + P_{j+2 j+3 j+1 j}) - \dots]$$

Frustrated Heisenberg spin chain + 3-particle ring exchange

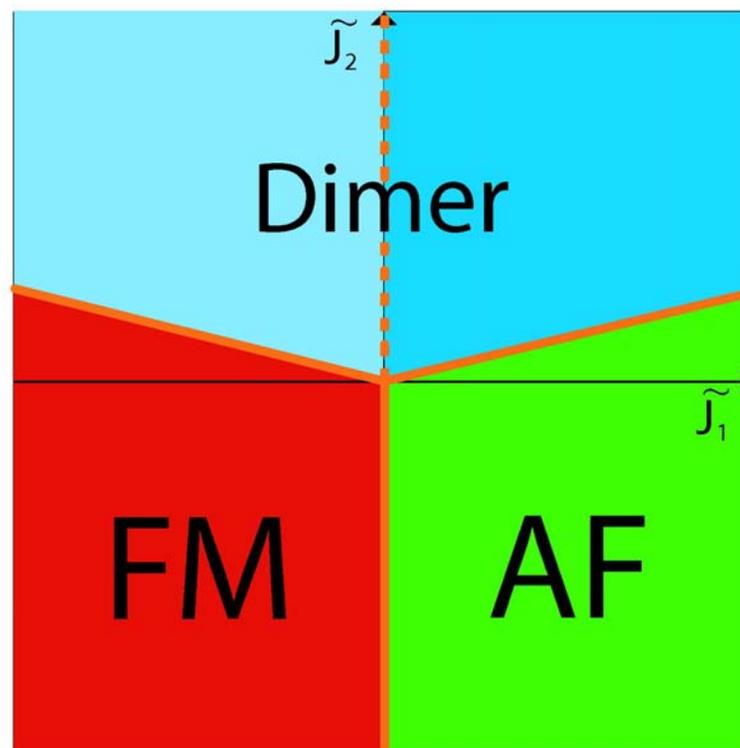
$$H_P = \frac{1}{2} \sum_j [J_1 P_{j,j+1} + J_2 P_{j,j+2} - J_3 (P_{j,j+1} P_{j+1,j+2} + P_{j+2,j+1} P_{j+1,j})]$$

- nearest neighbor exchange: $\tilde{J}_1 = J_1 - 2J_3$
- next-nearest neighbor exchange: $\tilde{J}_2 = J_2 - J_3$
- spin Hamiltonian:

$$H = \sum_j (\tilde{J}_1 \mathbf{S}_j \mathbf{S}_{j+1} + \tilde{J}_2 \mathbf{S}_j \mathbf{S}_{j+2})$$

- **phase diagram** 

[Majumdar & Ghosh, Haldane, Eggert,
White & Affleck, Hamada *et al.*, Allen *et al.*,
Itoi & Qin, ...]



Computation of exchange constants

- strength of interactions is characterized by

$$r_{\Omega} = \frac{r_0}{a_B} = 2 \left(\frac{me^4}{2\hbar^2\epsilon^2} \frac{1}{\hbar\Omega} \right)^{2/3}$$

(where a_B Bohr's radius $\approx 100\text{\AA}$ in GaAs)

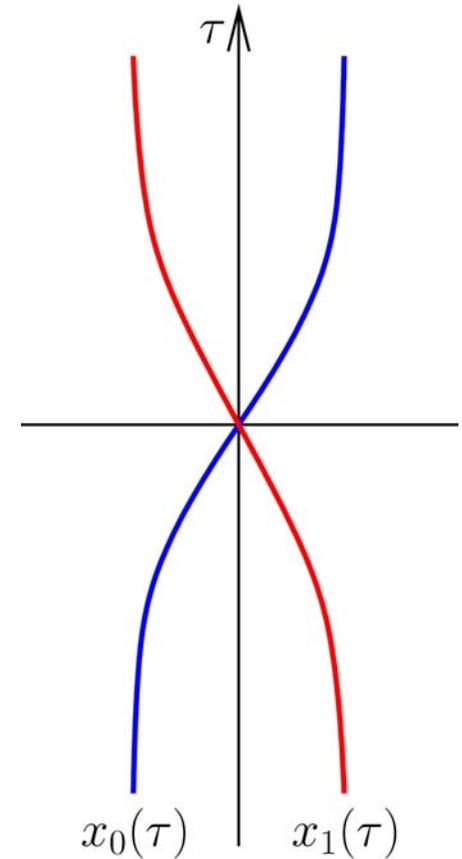
- use WKB at $r_{\Omega} \gg 1$ [note: $r_s \sim r_{\Omega}/v$]

- imaginary-time action $S = \hbar\eta\sqrt{r_{\Omega}}$ with

$$\eta[\{\mathbf{r}_j(\tau)\}] = \int_{-\infty}^{\infty} d\tau \left[\sum_j \left(\frac{\dot{\mathbf{r}}_j^2}{2} + y_j^2 \right) + \sum_{j<i} \frac{1}{|\mathbf{r}_j - \mathbf{r}_i|} \right]$$

confinement

interaction

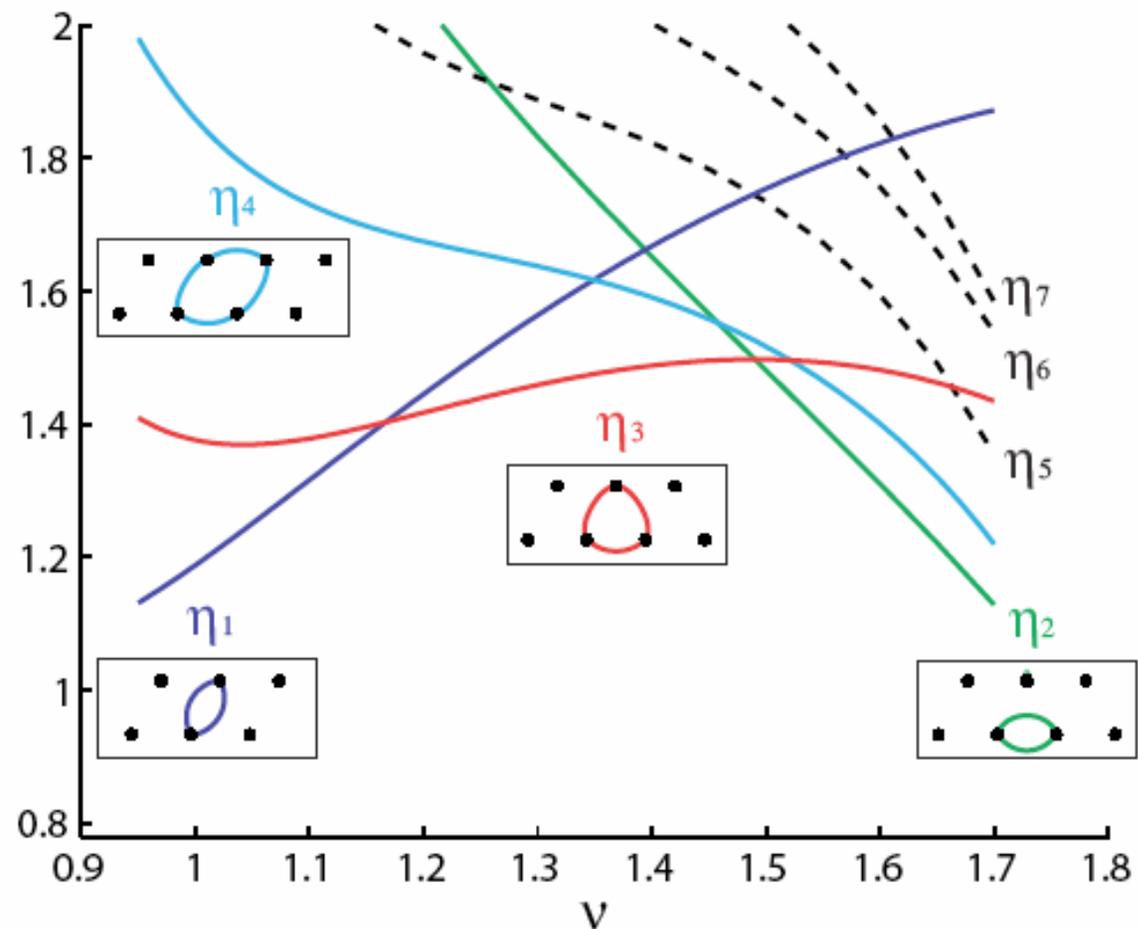


instanton
exchange
path

Numerical results I

- exchange constants: $J_l = J_l^* \exp[-\eta_l \sqrt{r\Omega}]$
- solve equations of motion for various exchange processes numerically

- nearest and next-nearest neighbor as well as 3-, 4-, 5-, 6-, and 7-particle ring exchanges



- dominant exchange: $J_1 \rightarrow J_3 \rightarrow J_2$

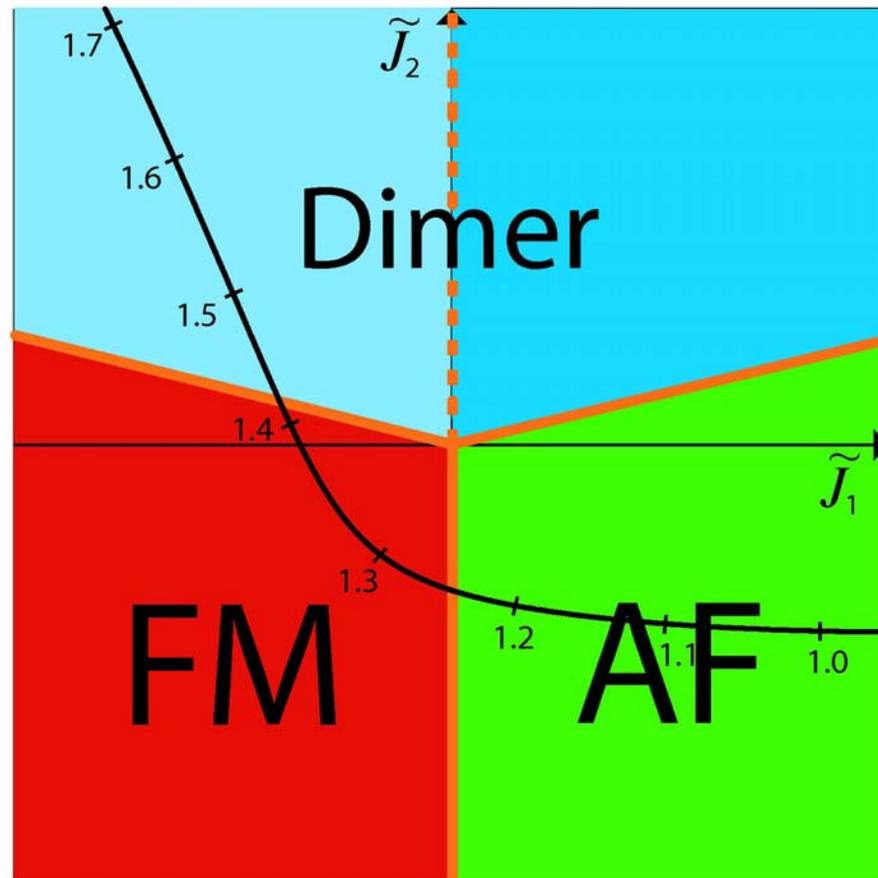
Heisenberg spin chain with nearest and next-nearest neighbor exchange

$$H = \sum_j (\tilde{J}_1 \mathbf{S}_j \mathbf{S}_{j+1} + \tilde{J}_2 \mathbf{S}_j \mathbf{S}_{j+2})$$

with nearest neighbor exchange: $\tilde{J}_1 = J_1 - 2J_3$
 next-nearest neighbor exchange: $\tilde{J}_2 = J_2 - J_3$

$\tilde{J}_2 > 0$: frustration

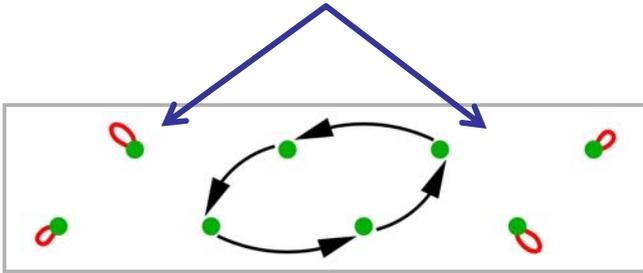
$\tilde{J}_2 < 0$: ✓



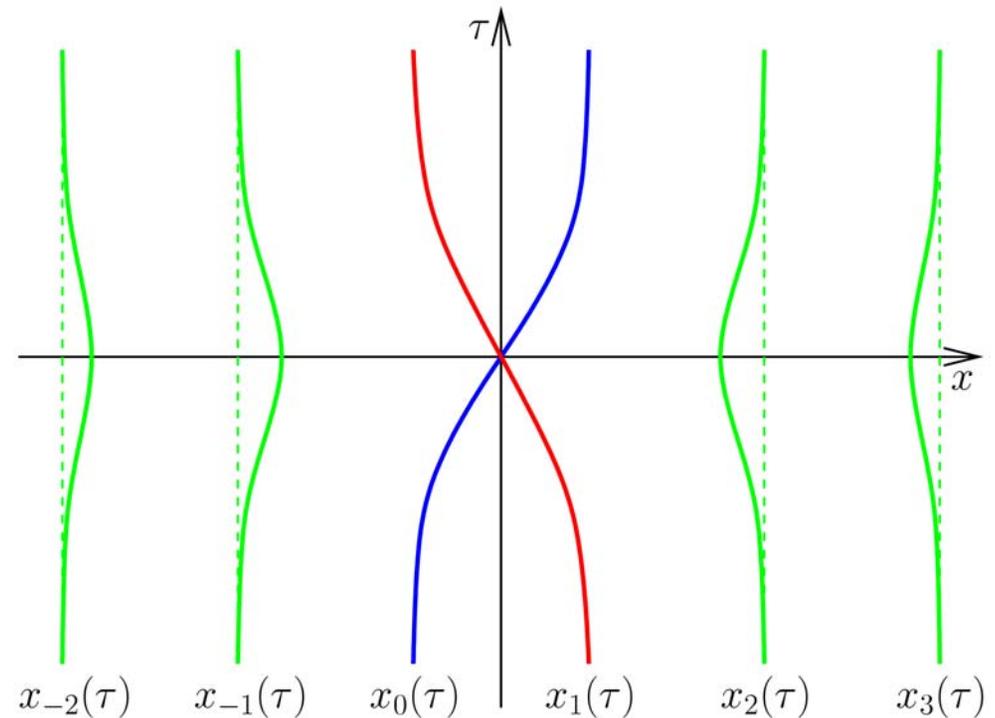
← $\tilde{J}_2 \approx 0.24 \tilde{J}_1$

Numerical results II

- “spectators” participate in exchange process



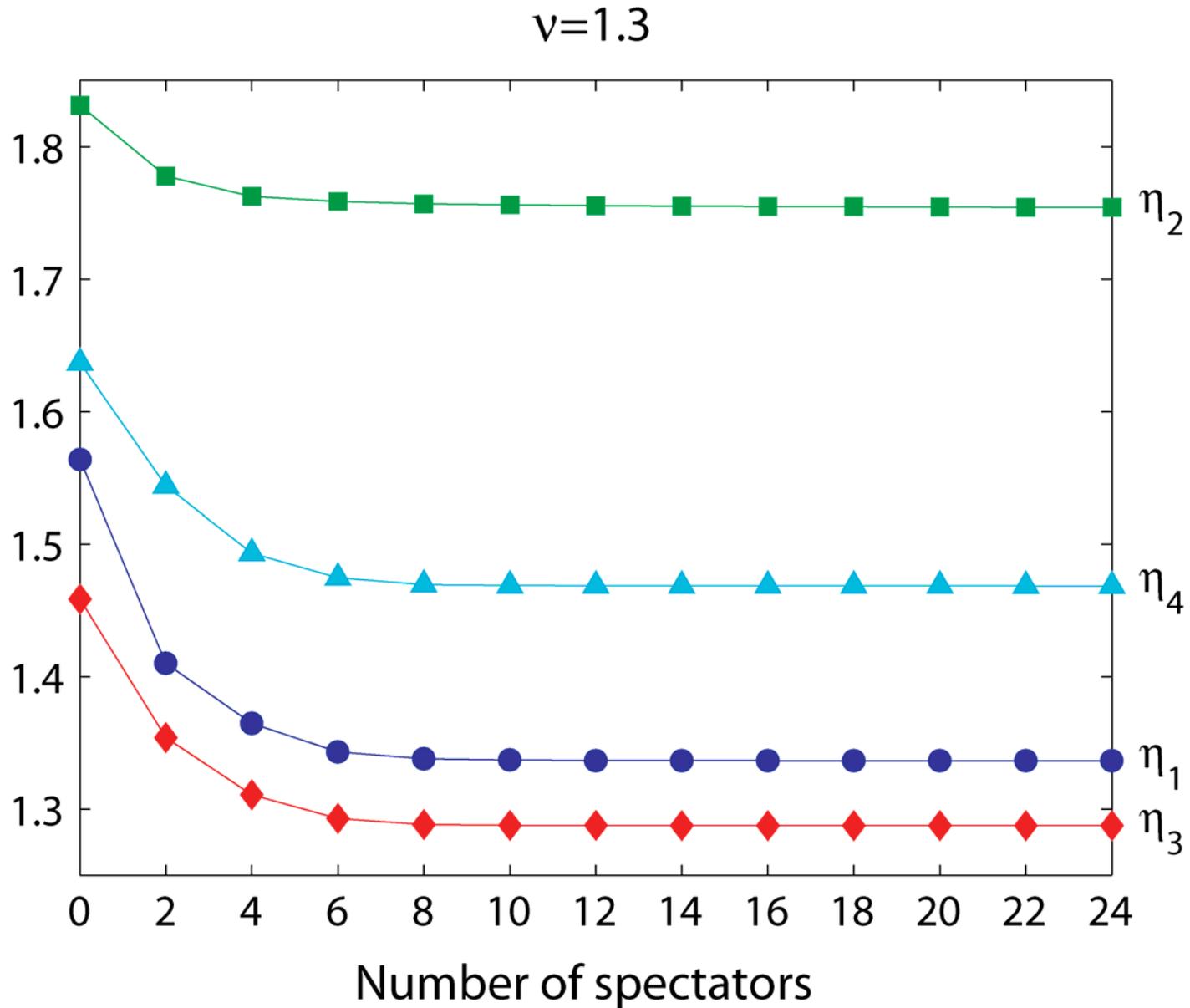
- 12 spectators included on either side of the exchanging particles



⇒ • smaller values η_l

Numerical results II

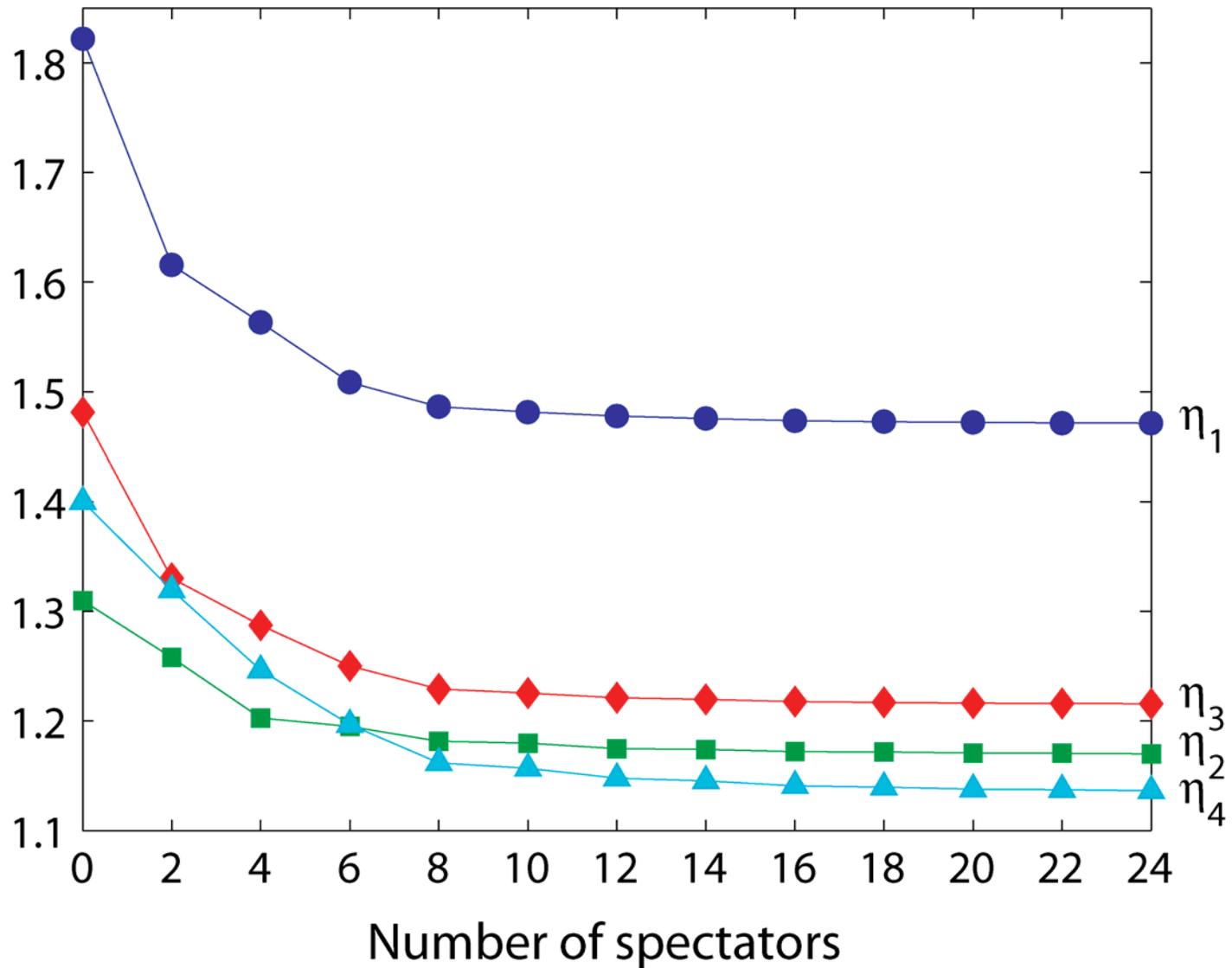
e.g.:



Numerical results II

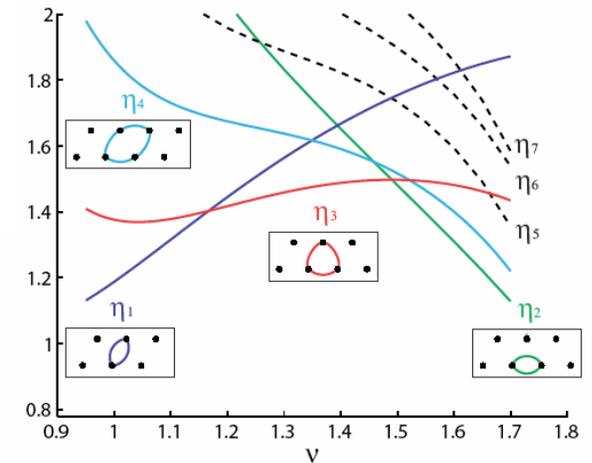
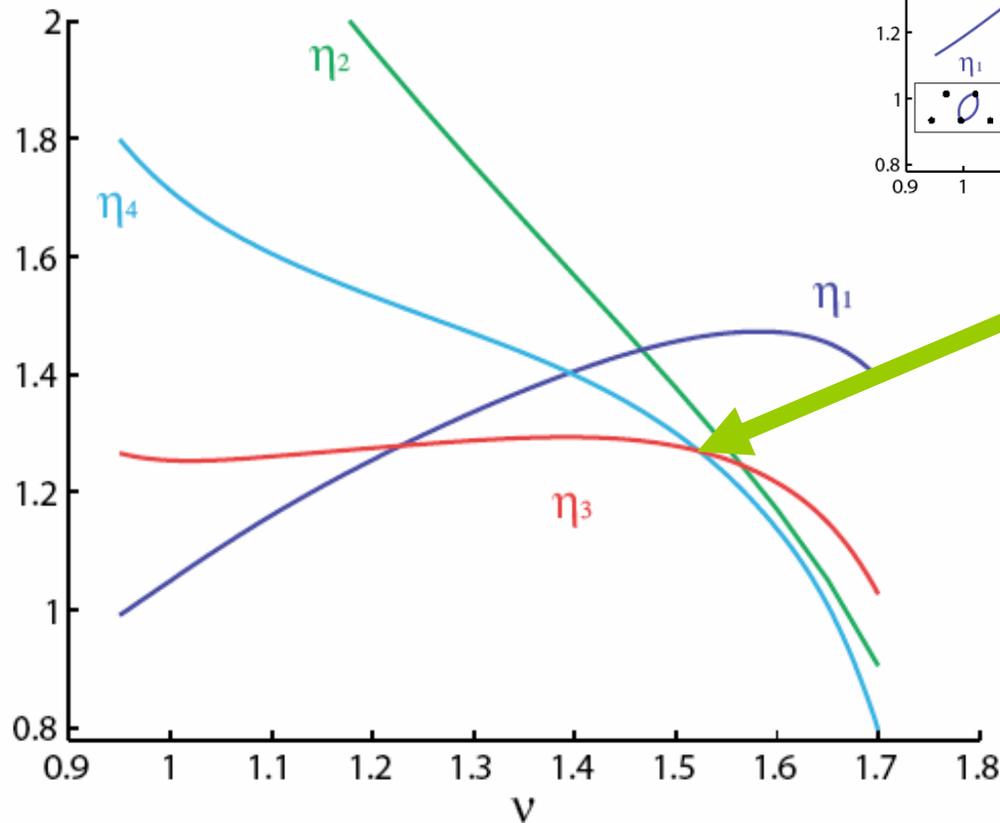
e.g.:

$v=1.6$



Numerical results II

- ⇒ • J_4 wins over J_2 at large densities!



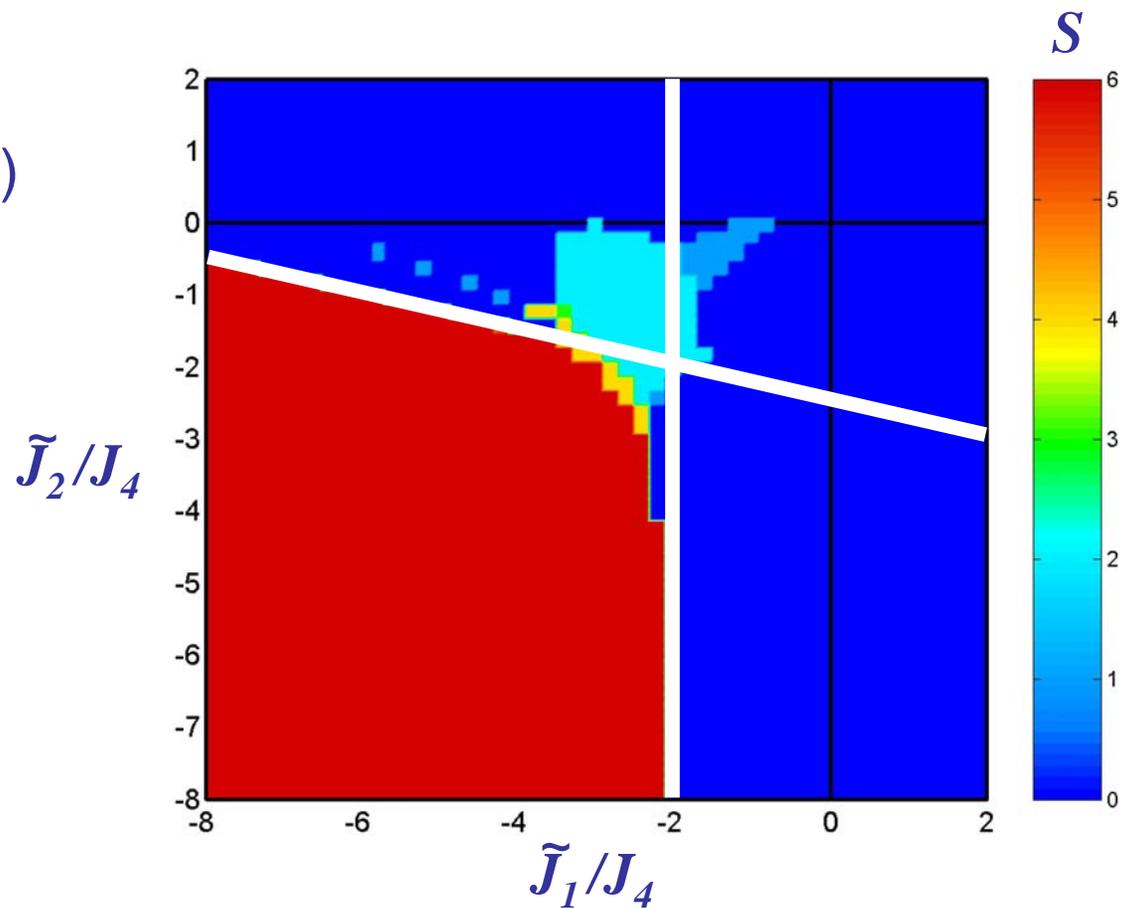
- 4-particle ring exchange generates 4-spin interaction:

$$H_4 \sim (\mathbf{S}_j \mathbf{S}_{j+1})(\mathbf{S}_{j+2} \mathbf{S}_{j+3}) + (\mathbf{S}_j \mathbf{S}_{j+2})(\mathbf{S}_{j+1} \mathbf{S}_{j+3}) - (\mathbf{S}_j \mathbf{S}_{j+3})(\mathbf{S}_{j+1} \mathbf{S}_{j+2})$$

4-particle ring exchange

PRELIMINARY RESULTS:
exact diagonalization

spin
of the ground state
for 12 spins
(periodic boundary conditions)



What about experiment? ...

... Are quantum wires ferromagnetic?

- Are interactions in realistic quantum wires strong enough?
- ``strength of interaction`` controlled by confining potential:

$$r_{\Omega} \propto \Omega^{-2/3}$$

2 types of quantum wires:

- cleaved-edge overgrowth:

steep confining potential – $r_{\Omega} < 1$

- split gate:

shallow confining potential – $r_{\Omega} > 1$

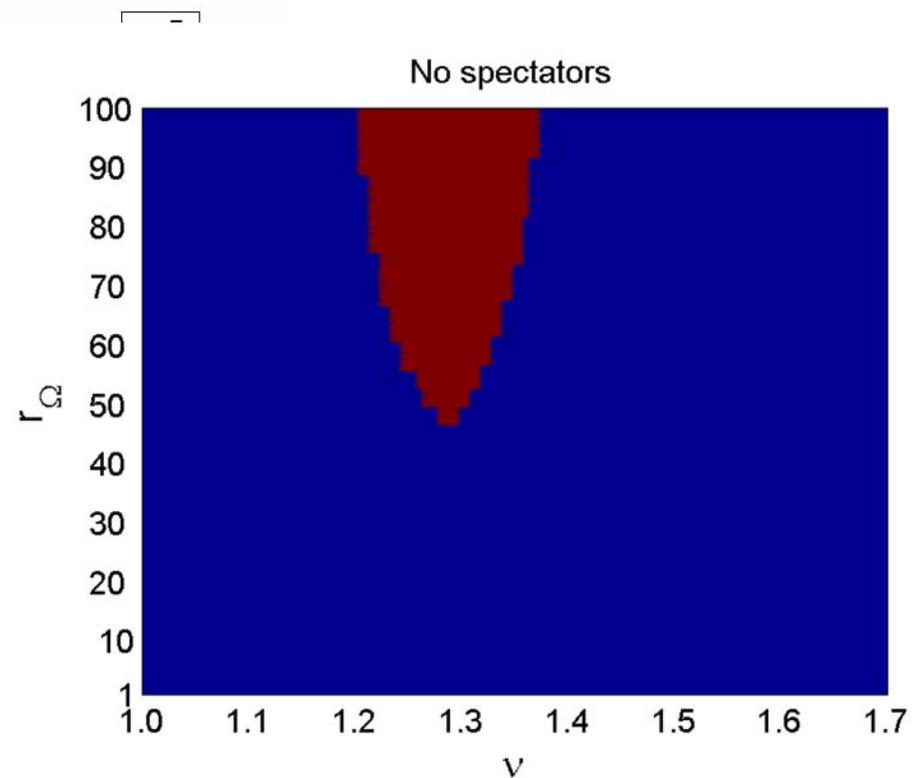
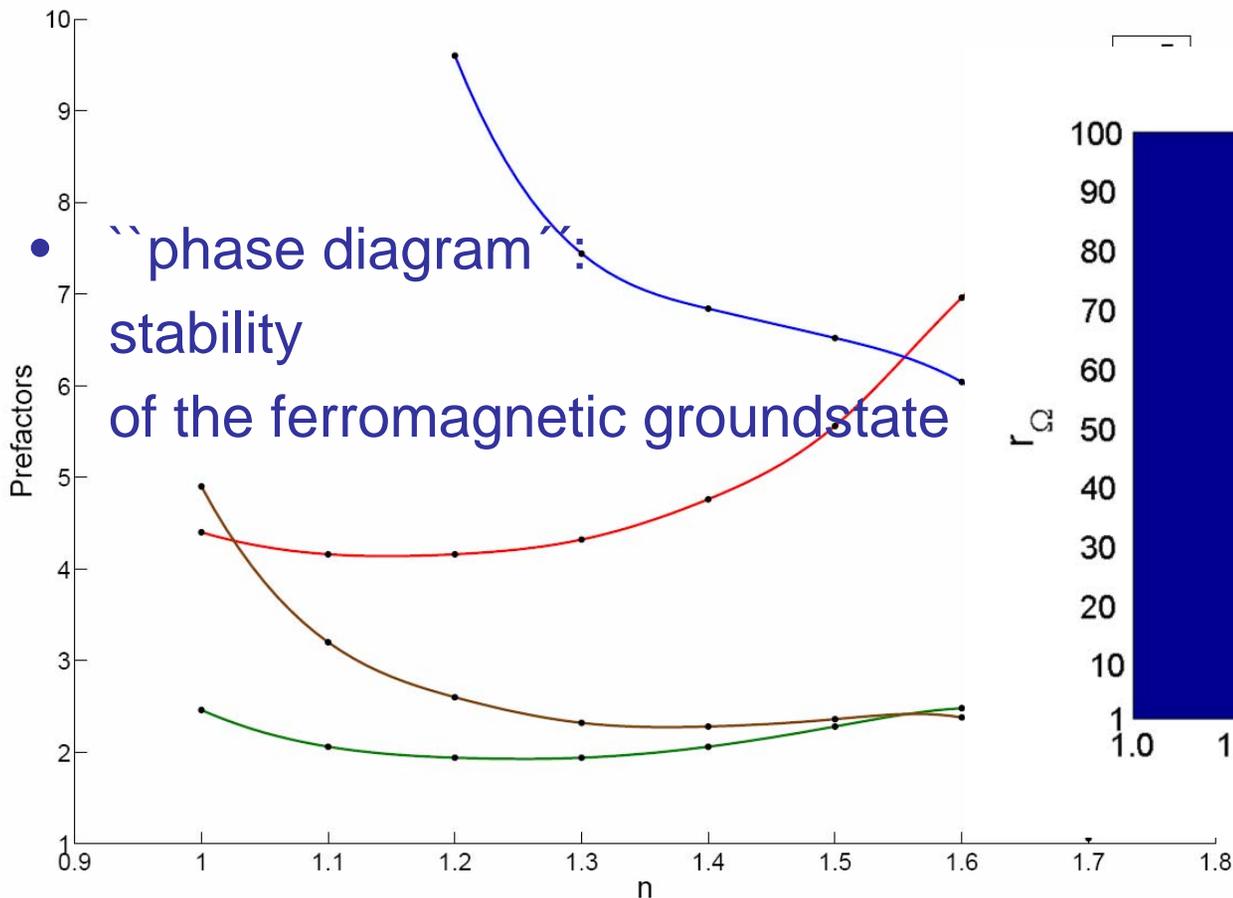
(e.g. Thomas *et al.*, Phys. Rev. B **61**, R13365 (2000): $r_{\Omega} = 3 - 6$)

Prefactors (preliminary)

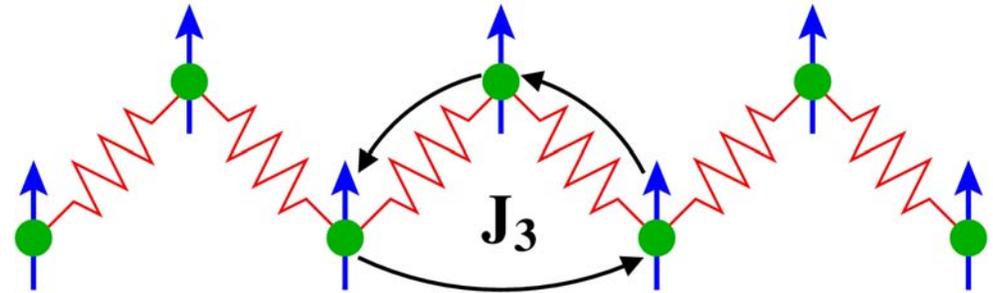
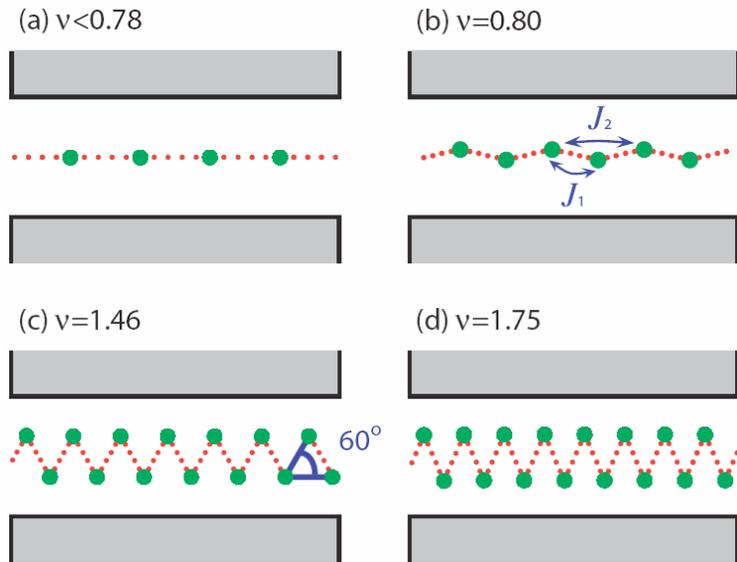
- exchange constants:

$$J_l = J_l^* \exp[-\eta_l \sqrt{r\Omega}] \quad \text{where} \quad J_l^* = \frac{e^2}{\epsilon a_B} m_l F_l \left(\frac{\eta_l}{2\pi}\right)^{1/2} r_{\Omega}^{-5/4}$$

(Gaussian fluctuations around classical exchange path)



Conclusions & Outlook



A ferromagnetic ground state in quantum wires is possible at strong enough interactions. The interactions induce deviations from one-dimensionality and lead to ferromagnetism in a certain range of electron densities.

Conclusions & Outlook

TO DO ...

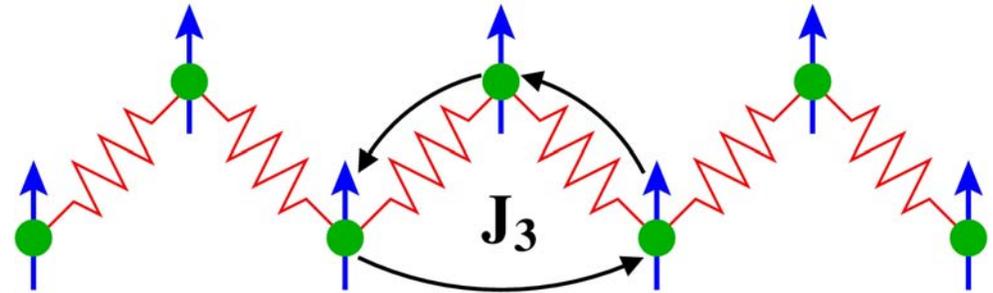
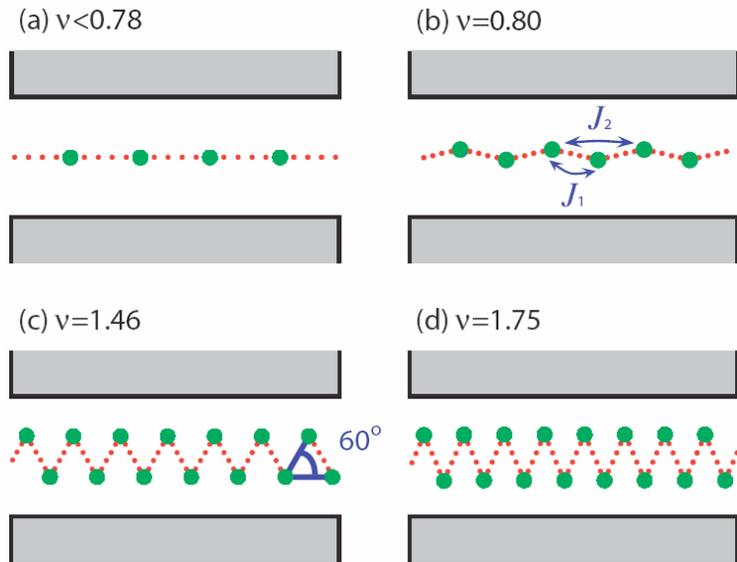
EXPERIMENT:

- ideal devices to observe spontaneous spin polarization:
split-gate wires with widely separated gates
⇒ shallow confining potential ⇒ large r_{Ω}

THEORY:

- compute prefactors (under way)
- explore zig-zag chains with 4-particle ring exchange
- conductance?

Conclusions & Outlook



A ferromagnetic ground state in quantum wires is possible at strong enough interactions. The interactions induce deviations from one-dimensionality and lead to ferromagnetism in a certain range of electron densities.

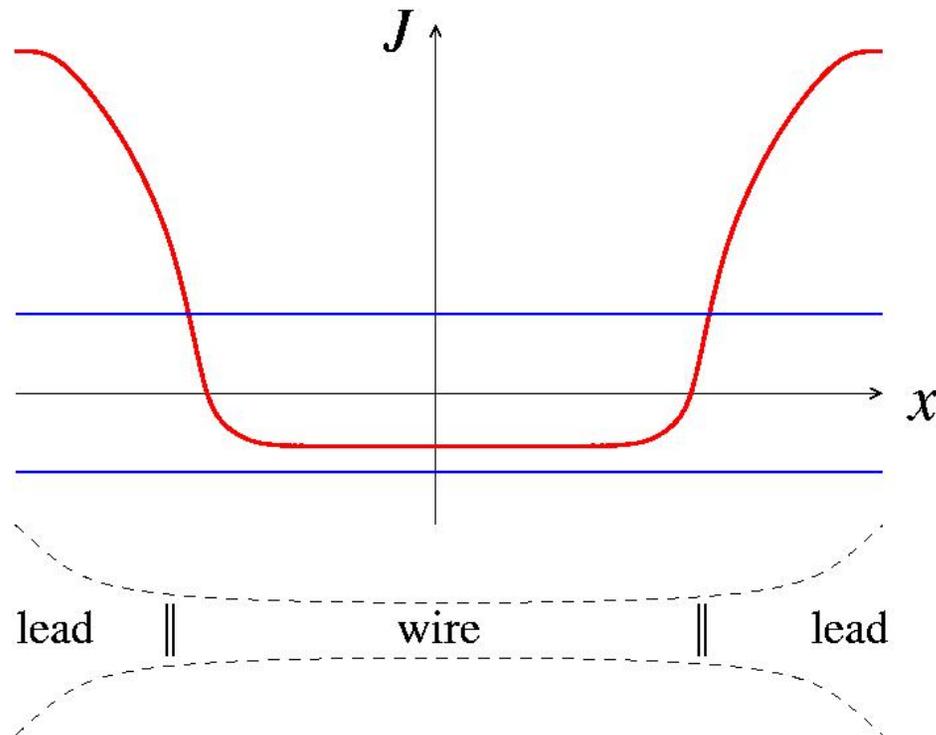
What about experiment? ...

... Does ferromagnetism lead to $G = 0.5 G_0$?

- coupling of spin and charge excitations due to leads

$$\mathcal{H}_s = \sum_{k=1,2} \left[\sum_j J_k(j + q(t)) \mathbf{S}_j \mathbf{S}_{j+k} \right]$$

- reflection of spin excitations



Summary

*Can the ground state of the electron system
in a quantum wire be ferromagnetic?*

- YES** - for sufficiently strong interactions, there is a range of electron densities, where the electrons form a **zig-zag Wigner crystal** and the spin interactions due to **3-particle ring exchange** make the system **ferromagnetic**

