Spontaneous Spin Polarization in Quantum Wires

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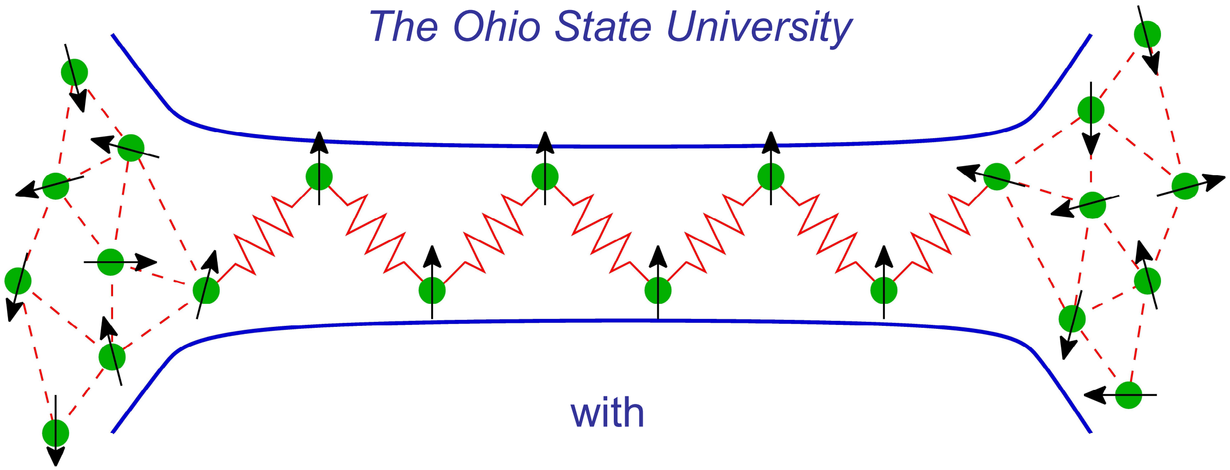


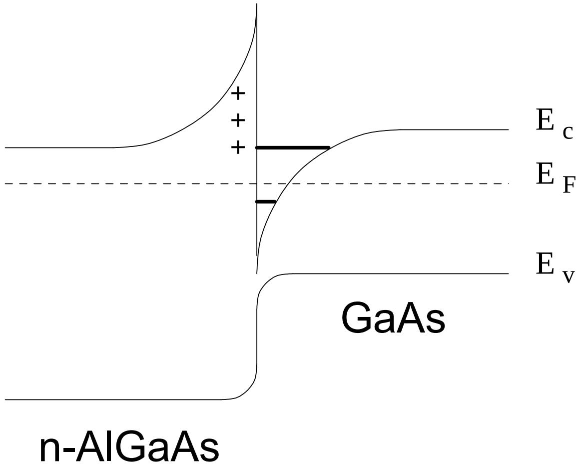
with

A.D. Klironomos

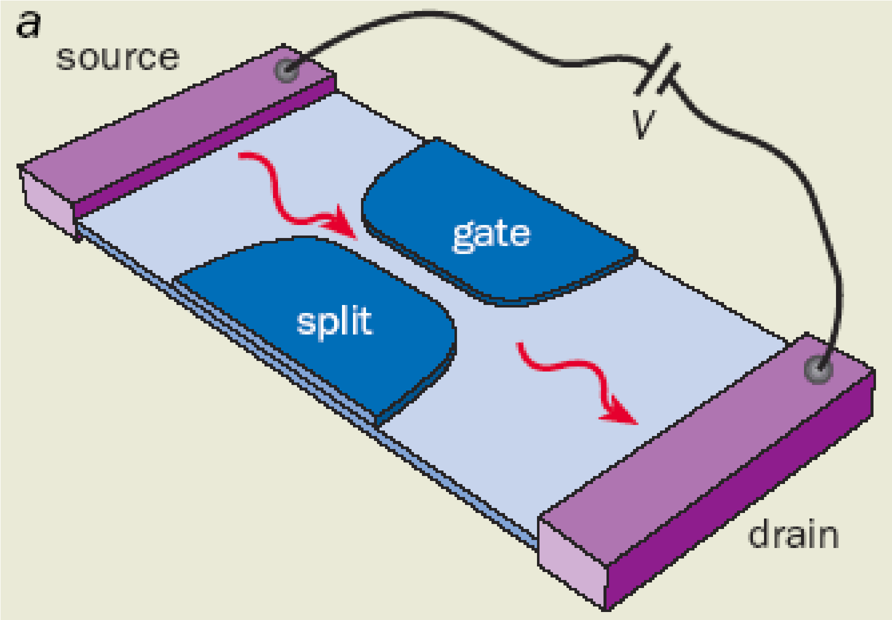
K.A. Matveev

Why ask this question at all …

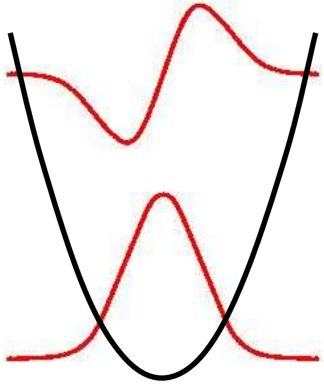
Quantum Wires



- GaAs/AlGaAs heterostucture
  → 2D electron gas
- depletion of the 2D electron gas by gates
  → quasi-1D channel



- parabolic confining potential
  → subband structure



$$\varepsilon_n = \hbar\Omega\,(n+1/2)$$

- change chemical potential with gate voltage

Motivation

Why ask this question at all …

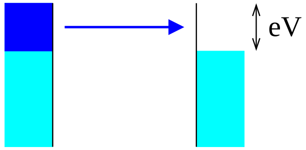
- <u>Theory:</u> conductance quantization $G = k \cdot G_0$ (k integer)

  where $G_0 = 2\, e^2/h$

  spin degeneracy

- current = electron charge × <u>electron density</u> × electron velocity

  = density of states × $(\mu_R - \mu_L)$



$$I = e \times \nu\, eV \times v_F$$

$$= e \times 2\, \frac{1}{h v_F}\, eV \times v_F = 2\, \frac{e^2}{h}\, V$$

- conductance: $G = \partial I / \partial V$

Berggren & Pepper, Physics World 2002

Motivation

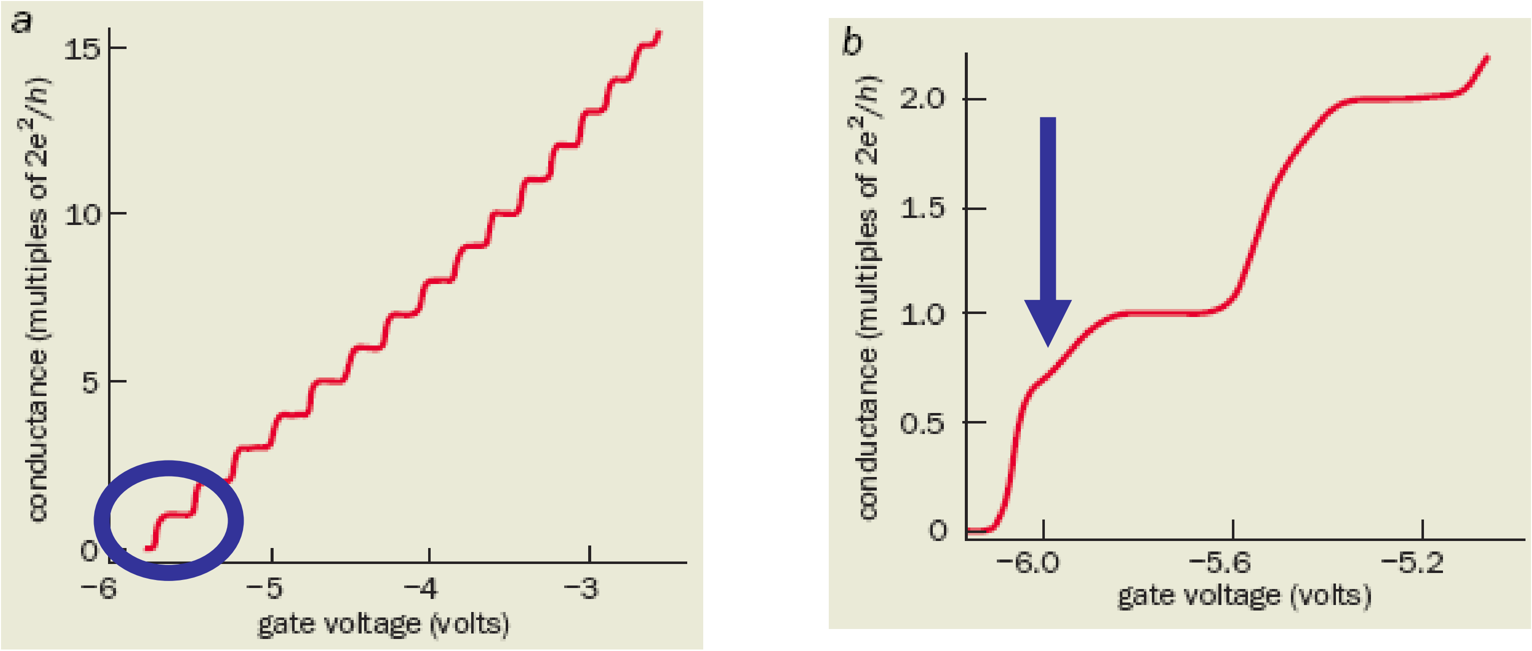
Why ask this question at all …

- Theory: conductance quantization $G = k \cdot G_0$ (k integer)

  where $G_0 = 2\ e^2/h$

  spin degeneracy

- Experiment I:



Berggren & Pepper, Physics World 2002

Motivation

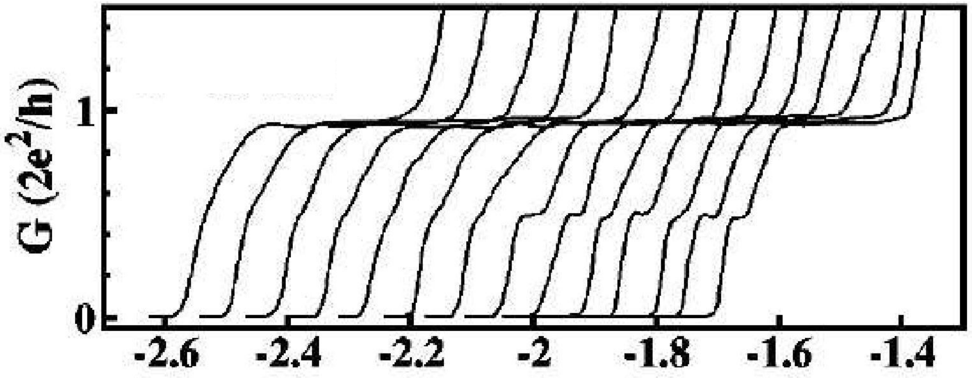
Why ask this question at all …

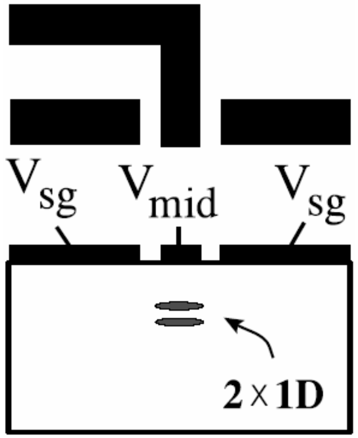
- Experiment II:

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

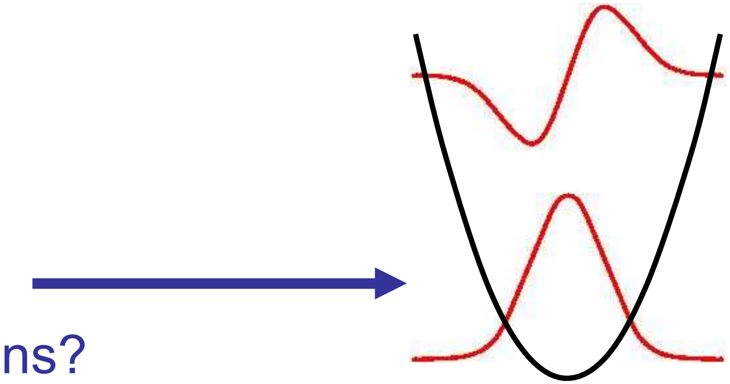
In 1D,
the ground state of an interacting electron system
possesses minimal spin.

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

QUANTUM WIRE:

not a purely one-dimensional system ...

- parabolic confining potential:



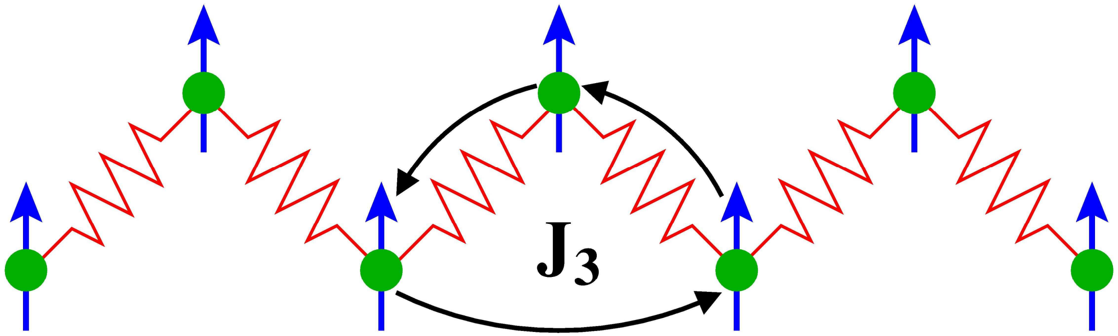
no interactions

strong interactions?

Summary I

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**



Europhys. Lett. **74**, 679 (2006)

Outline

- low density – strong interaction – Wigner crystal

- structure of the crystal in a parabolic confining potential
- spin interactions

- numerical methods & results
- phase diagram → 4-particle ring exchange

- What about experiment?

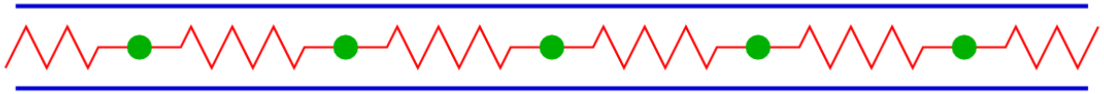
- conclusions & outlook

Quantum wires at low density: Wigner crystal

- at low electron densities n_e ,

  interaction energy ($\sim n_\mathrm{e}$) dominates over kinetic energy ($\sim n_\mathrm{e}^2$)

  $\Rightarrow$ formation of (classical) Wigner crystal



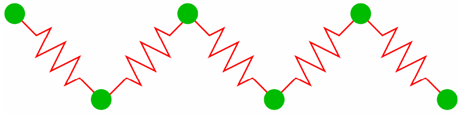
- Coulomb interaction:

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

- confining potential:

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

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



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

  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

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

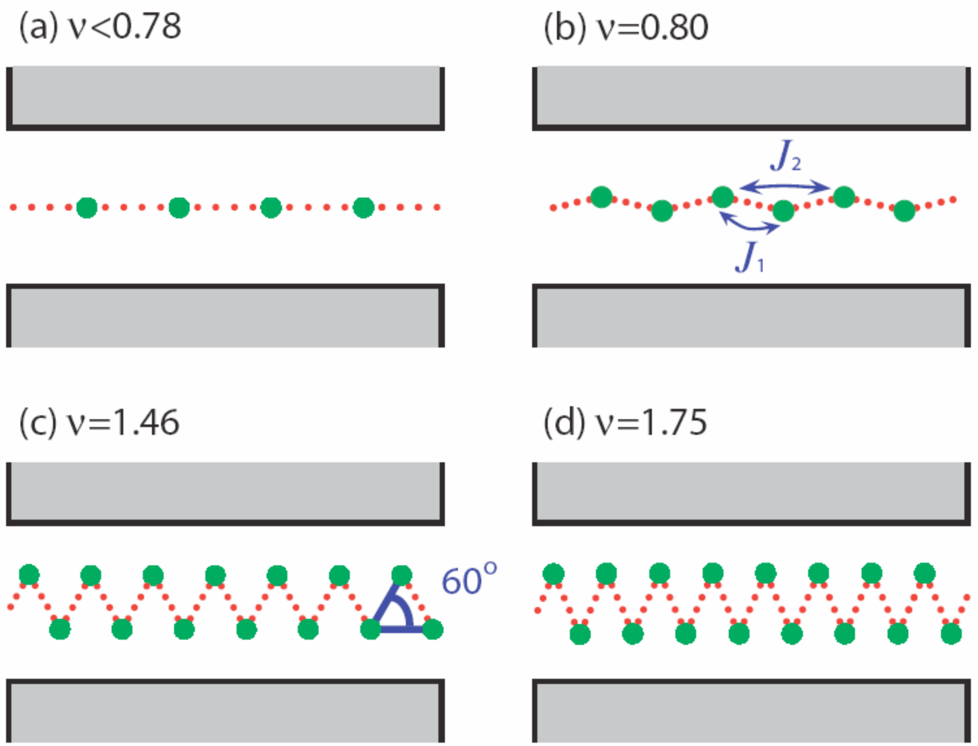
- dimensionless density $\nu = n_e r_0$

- transition 1D → zig-zag

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

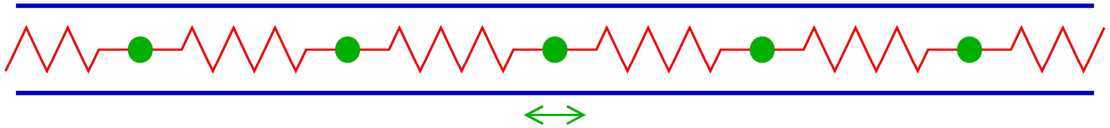
≈ 0.78

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

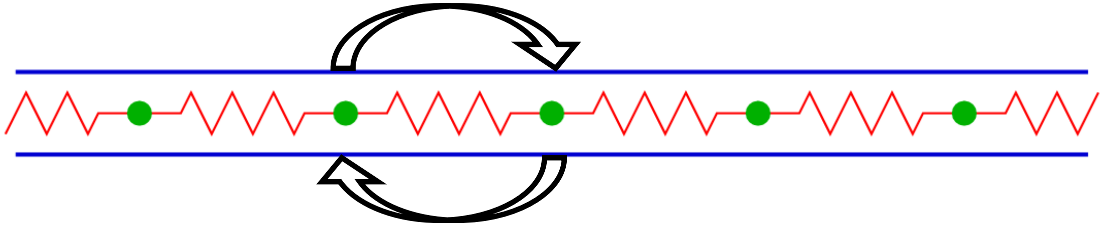


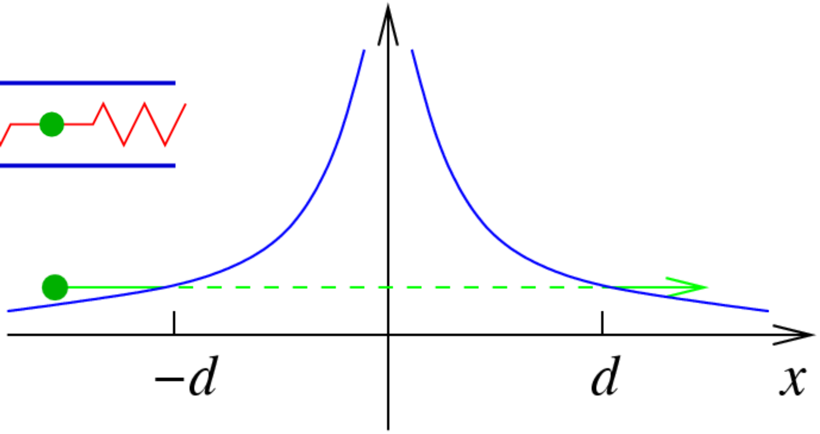
- **structure** ✓
- **spin properties ?**

Spin interactions in a Wigner crystal



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

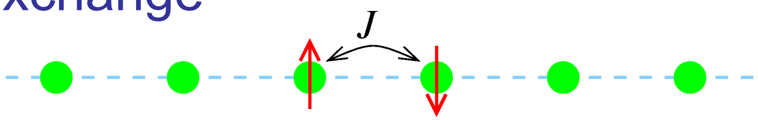




$\Rightarrow$ exponentially small
exchange constants J

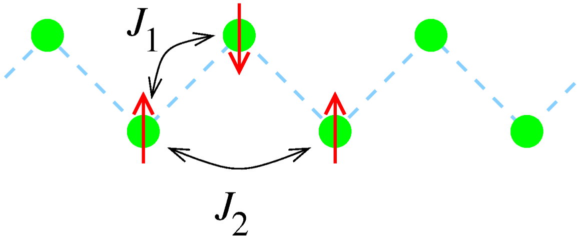
Exchanges in a zig-zag chain I

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



see poster of **Revaz Ramazashvili**:
Exchange coupling in a one-dimensional Wigner crystal

- **zig-zag chain**:
  - in addition, next-nearest neighbor exchange



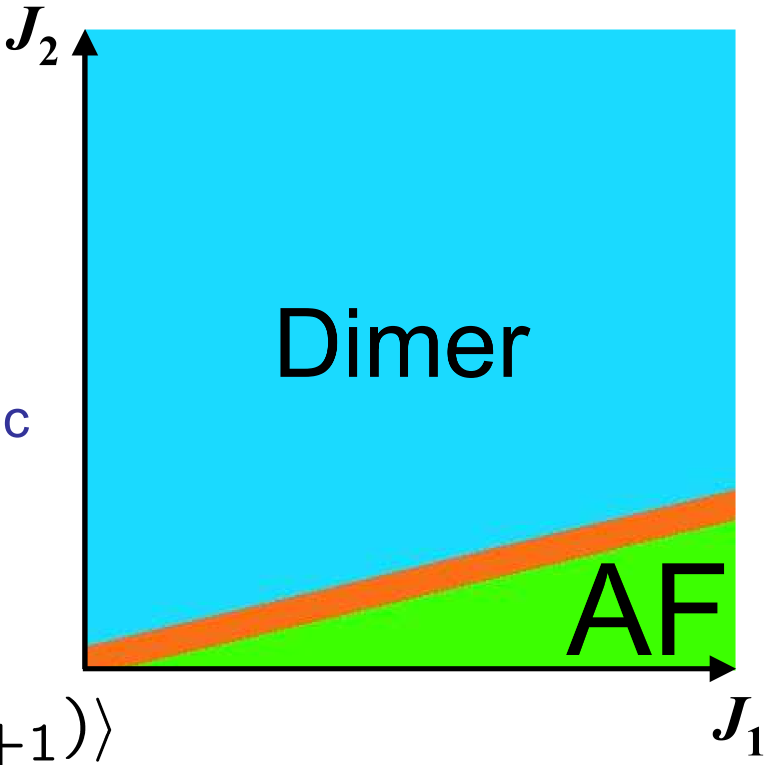
Frustrated Heisenberg spin chain

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

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

- spin Hamiltonian: $H = \sum_j \left(J_1 \, \mathbf{S}_j \mathbf{S}_{j+1} + J_2 \, \mathbf{S}_j \mathbf{S}_{j+2} \right)$
- 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

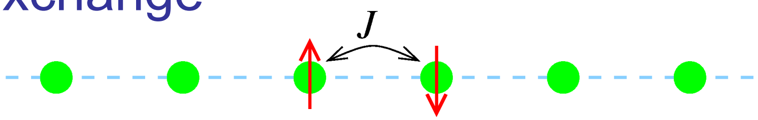
$J_2 > 0.24...\, J_1$: strong frustration

→ the ground state is dimerized

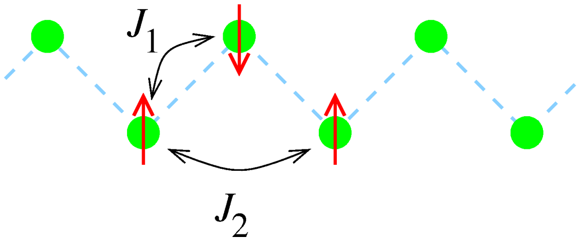
dimerization $d = \langle \mathbf{S}_j (\mathbf{S}_{j-1} - \mathbf{S}_{j+1}) \rangle$

Exchanges in a zig-zag chain II

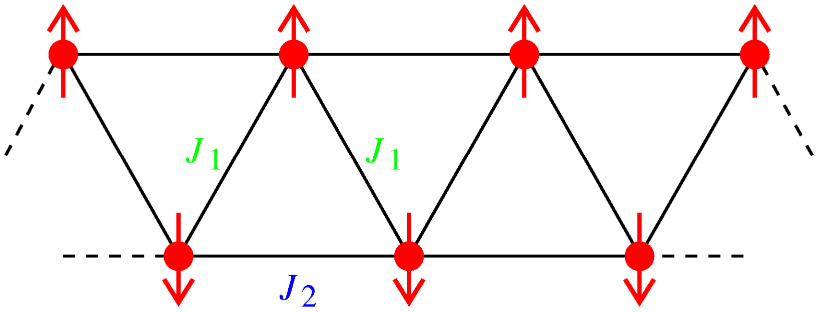
- **1D chain**: (AF) nearest-neighbor exchange



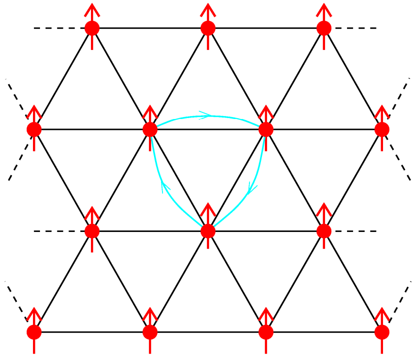
- **zig-zag chain**:
  - in addition, next-nearest neighbor exchange



  - increase distance between rows → equilateral configuration



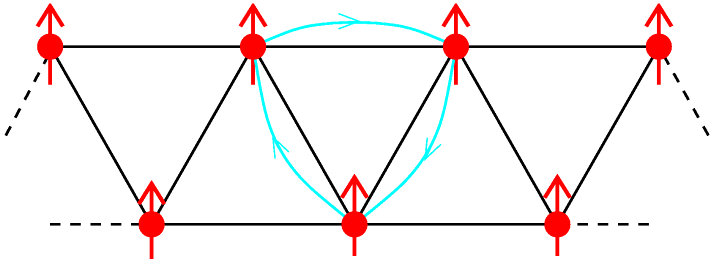
cf. 2D Wigner crystal:



$\longrightarrow$ **RING EXCHANGES**

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

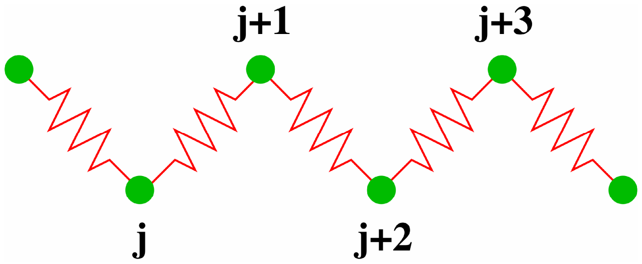
Ring exchanges



- cyclic exchange of l particles: $P_{j_1 \ldots j_l} = P_{j_1 j_2} P_{j_2 j_3} \ldots P_{j_{l-1} j_l}$

- ring exchange of even number of particles: antiferromagnetic
  ring exchange of odd number of particles: ferromagnetic
  (Thouless 1965)

- Hamiltonian:



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

Frustrated Heisenberg spin chain
+ 3-particle ring exchange

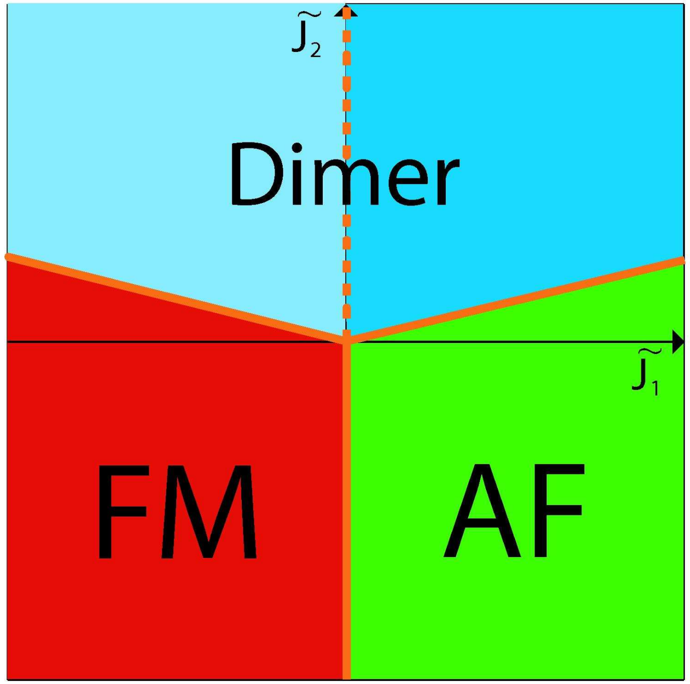
$$H_P = \frac{1}{2}\sum_j [J_1 P_{j\,j+1} + J_2 P_{j\,j+2} - J_3(P_{j\,j+1}P_{j+1\,j+2} + P_{j+2\,j+1}P_{j+1\,j})]$$

- 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

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

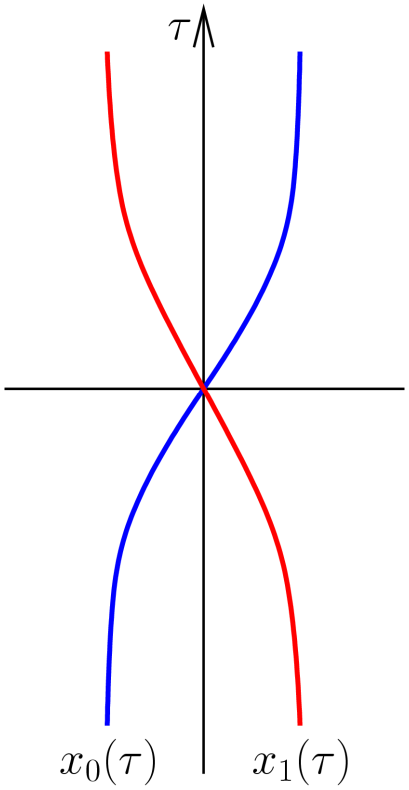
(where a_B Bohr's radius ≈ 100 Å in GaAs)

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

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

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

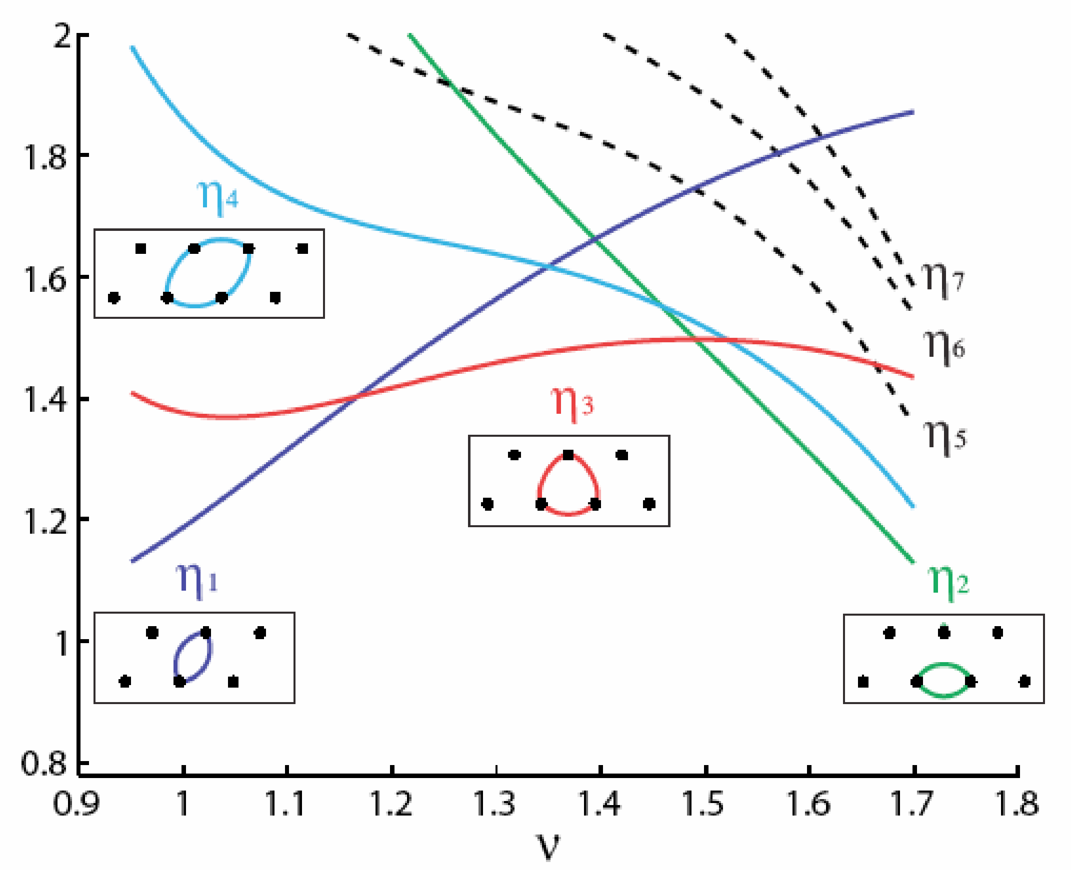
confinement interaction



instanton exchange path

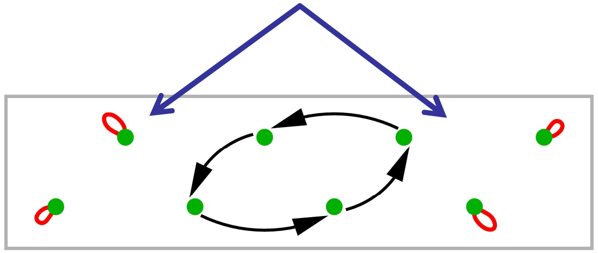
Numerical results I

- exchange constants: $$\boxed{J_l = J_l^* \, \text{exp}\left[-\eta_l \sqrt{r_\Omega}\right]}$$
- 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

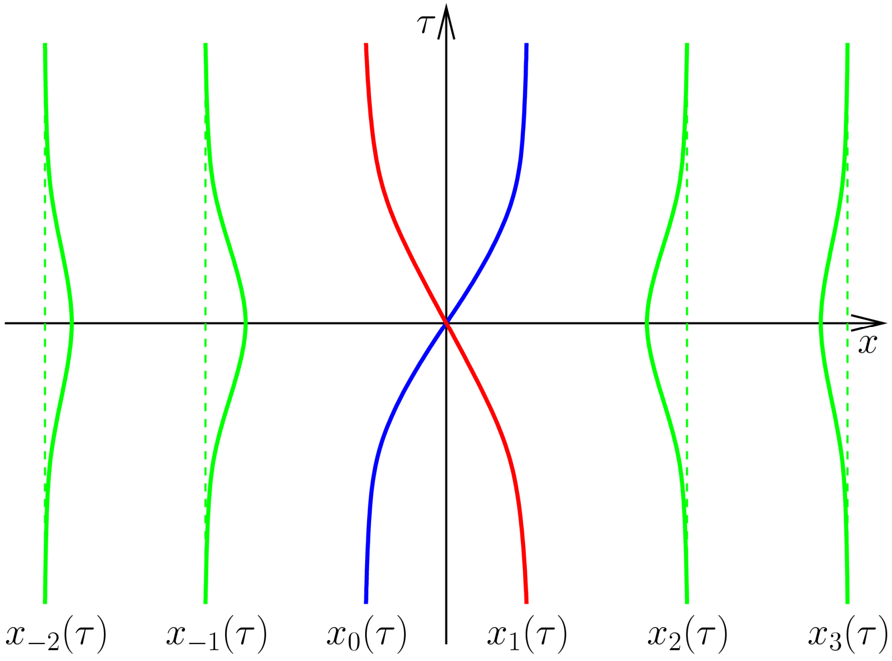


Numerical results II

- "spectators" participate in exchange process



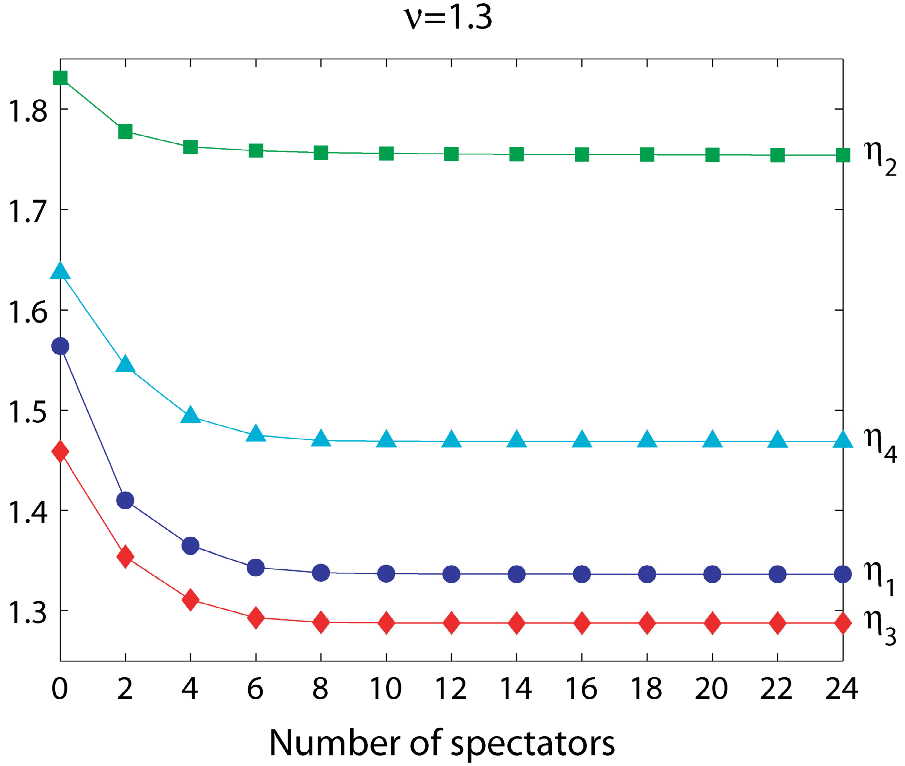
- 12 spectators included
  on either side
  of the exchanging particles

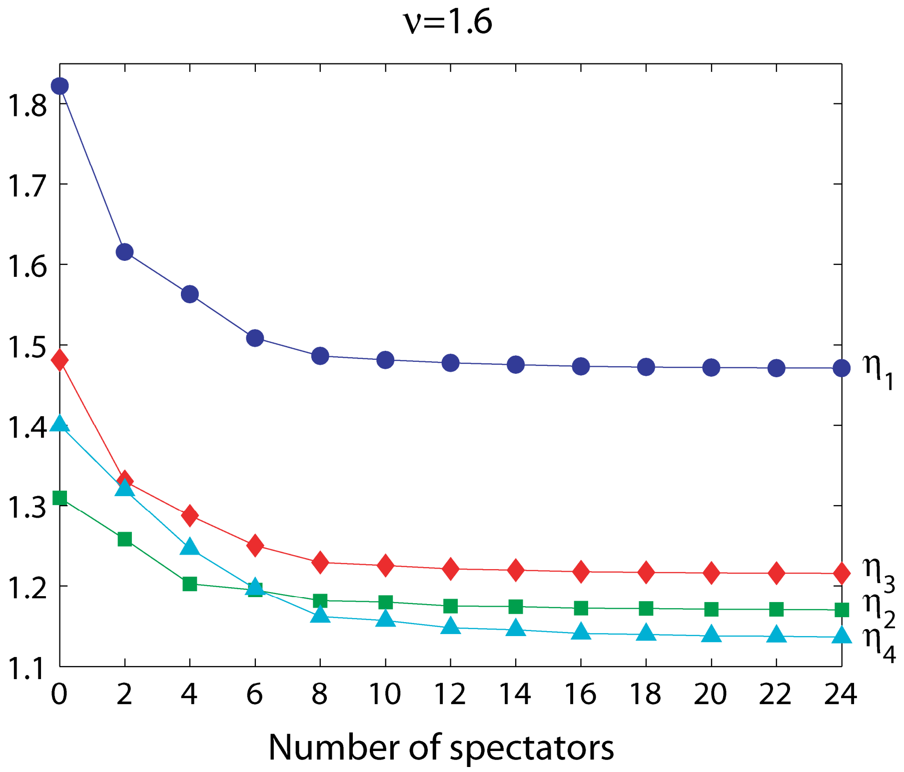


⇒ • smaller values η_l

Numerical results II

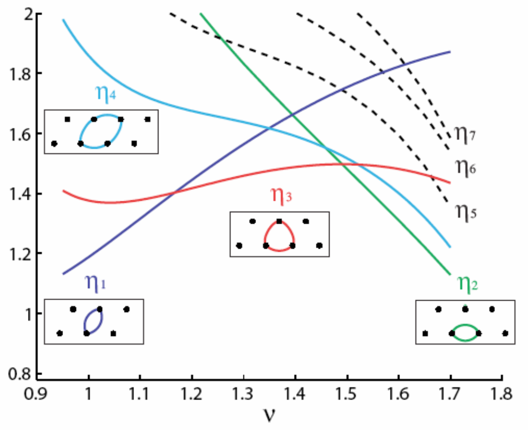
e.g.:

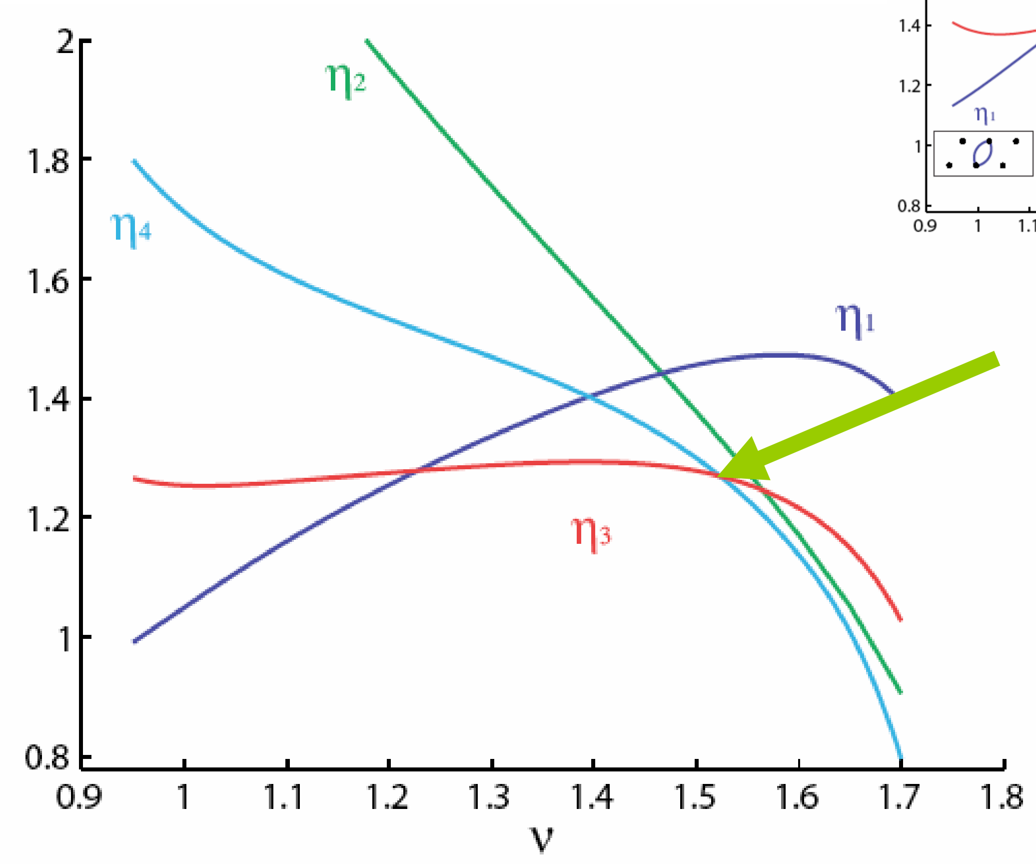




Numerical results II

⇨ • J_4 wins over J_2 at large densities!





- dominant exchange: $J_1 \rightarrow J_3 \rightarrow J_4$

Heisenberg spin chain with nearest and next-nearest neighbor exchange

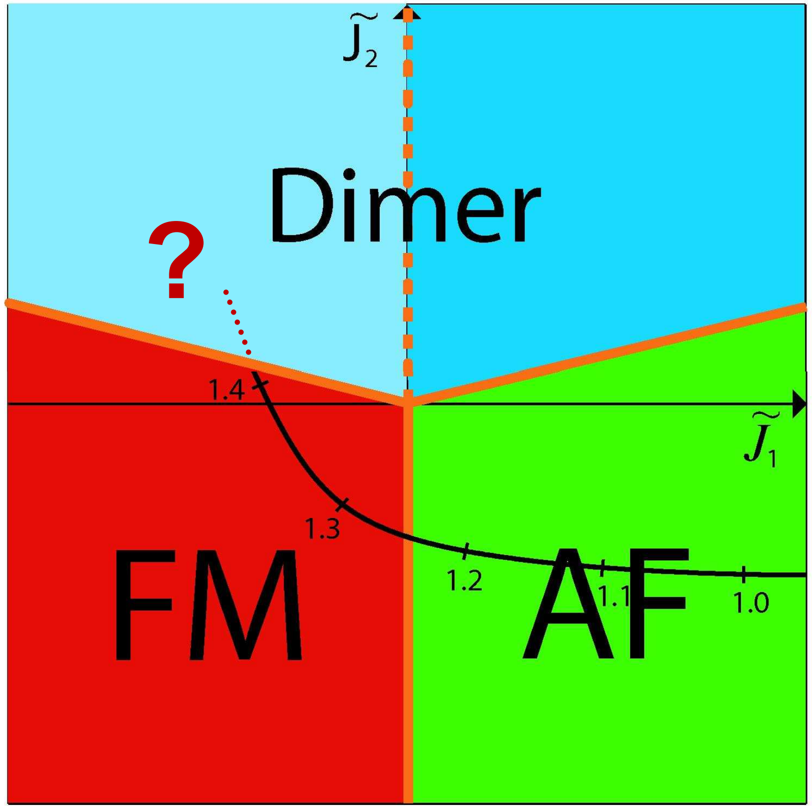
$$H = \sum_j (\tilde{J}_1\, \mathbf{S}_j\mathbf{S}_{j+1} + \tilde{J}_2\, \mathbf{S}_j\mathbf{S}_{j+2})$$

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

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

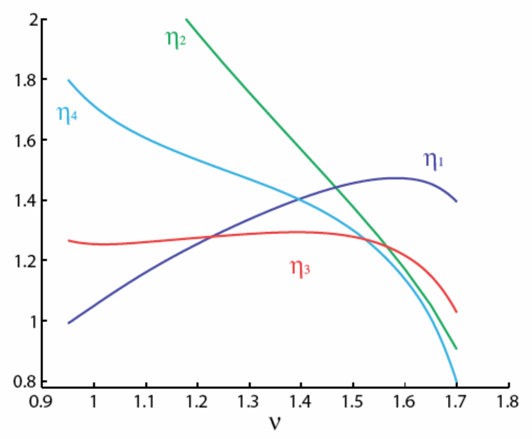
$\tilde{J}_2 > 0$: **frustration**

$\tilde{J}_2 < 0$: ✓



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

4-particle ring exchange



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

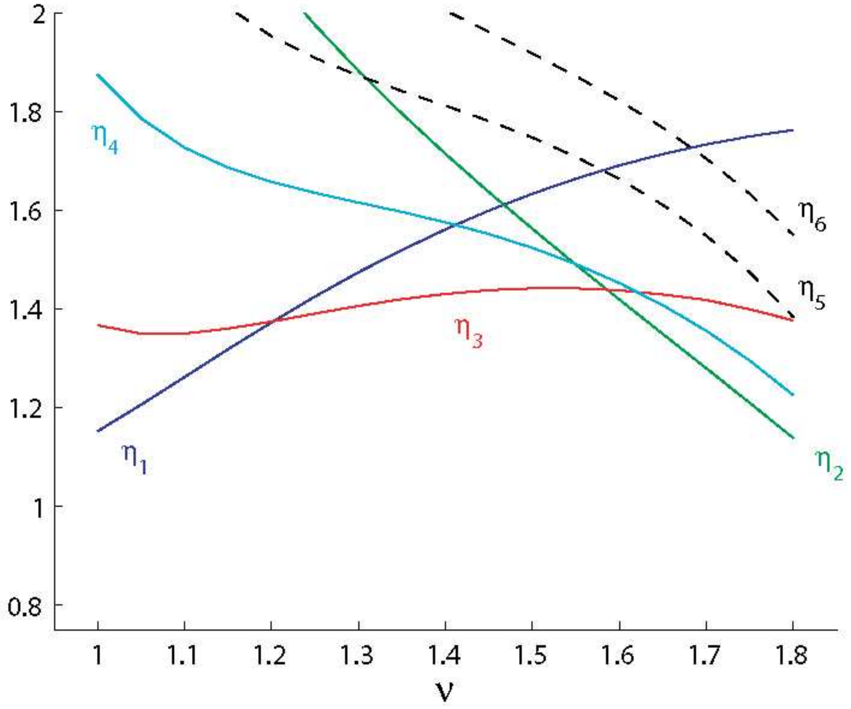
$$H_4 \sim (\mathbf{S}_j\mathbf{S}_{j+1})(\mathbf{S}_{j+2}\mathbf{S}_{j+3}) + (\mathbf{S}_j\mathbf{S}_{j+2})(\mathbf{S}_{j+1}\mathbf{S}_{j+3}) - (\mathbf{S}_j\mathbf{S}_{j+3})(\mathbf{S}_{j+1}\mathbf{S}_{j+2})$$

Screened interaction

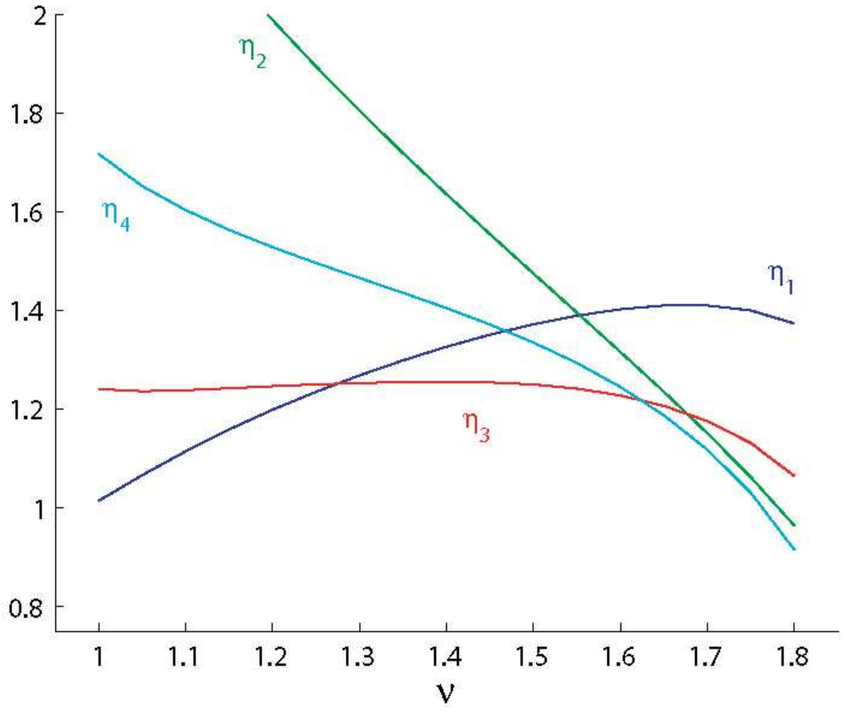
$$V(r) \sim \frac{1}{r} - \frac{1}{\sqrt{r^2 + (2d)^2}}$$

d distance to gate

$\sim$ inter-particle distance



no spectators

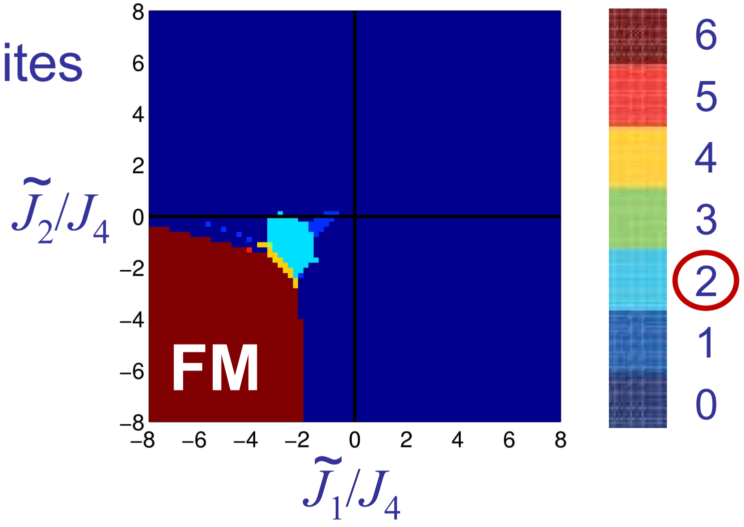


14 spectators

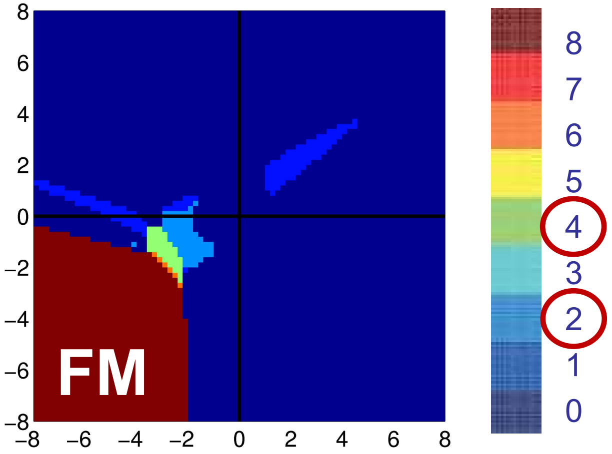
4-particle ring exchange I

- exact diagonalization of short chains: total spin of the ground state

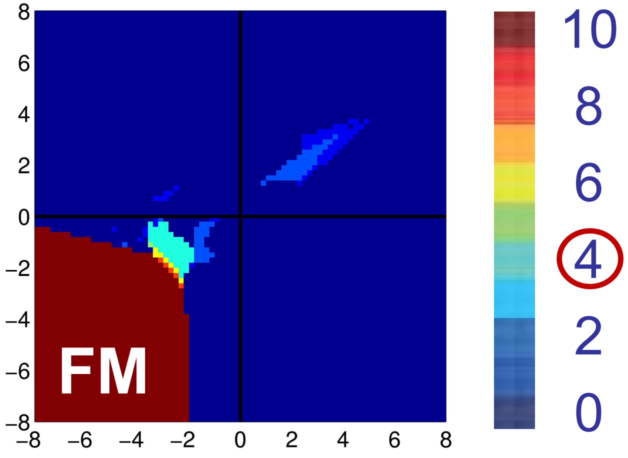
12 sites



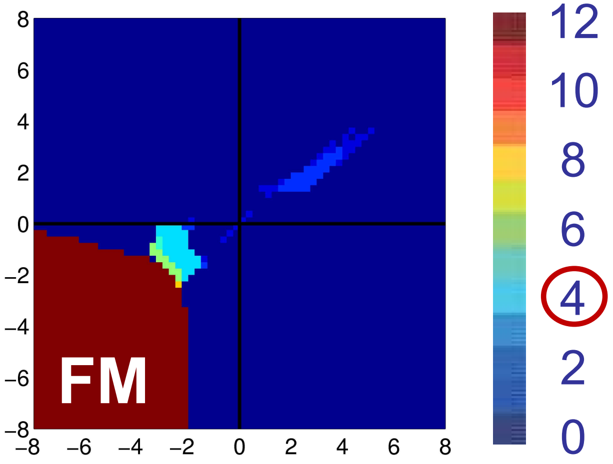
16 sites



20 sites



24 sites



4-particle ring exchange II

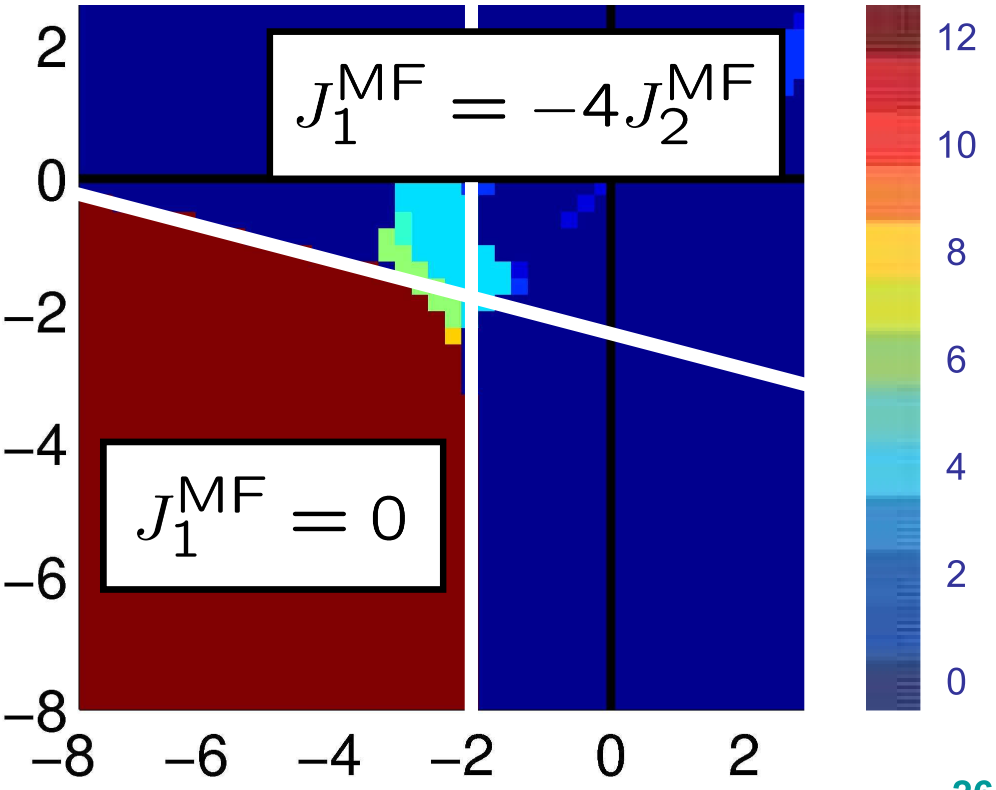
- **MEAN FIELD:**

$$
\begin{aligned}
& (\mathbf{S}_k\mathbf{S}_l)(\mathbf{S}_m\mathbf{S}_n) \\
\rightarrow\ & \frac{1}{2}\left(\langle \mathbf{S}_k\mathbf{S}_l\rangle \mathbf{S}_m\mathbf{S}_n + \mathbf{S}_k\mathbf{S}_l\langle \mathbf{S}_m\mathbf{S}_n\rangle\right) \\
\rightarrow\ & \frac{1}{4}\left(\mathbf{S}_k\mathbf{S}_l + \mathbf{S}_m\mathbf{S}_n\right)
\end{aligned}
$$

near the ferromagnetic phase

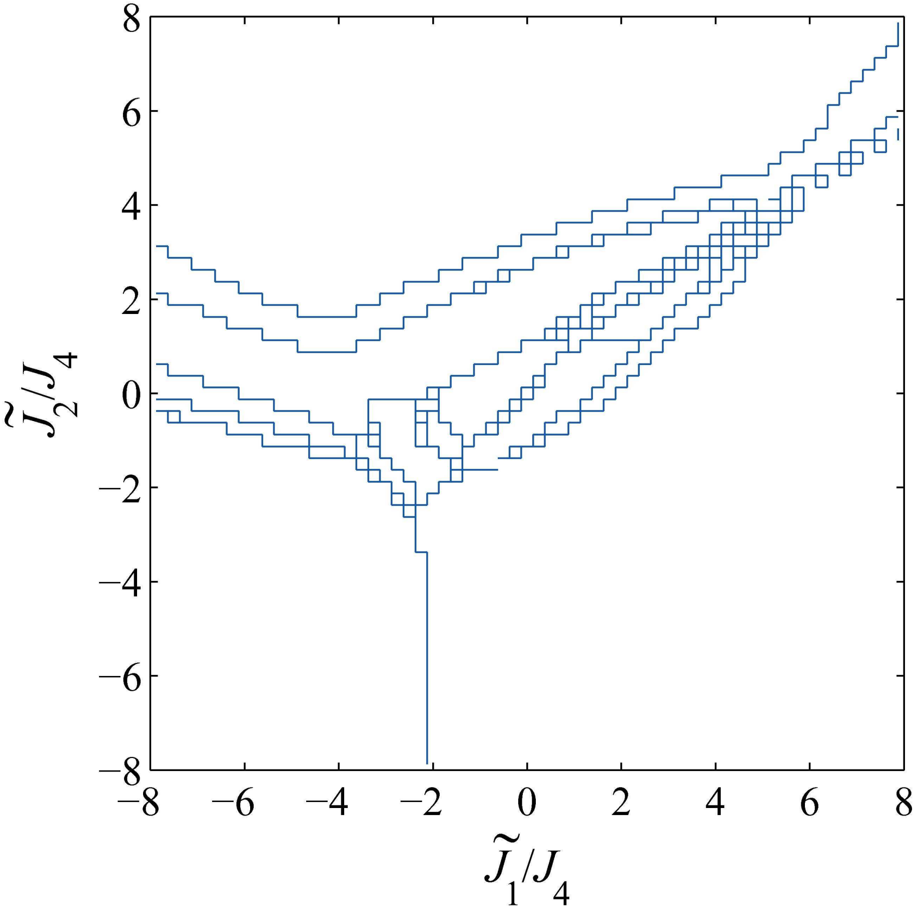
MF exchange constants:

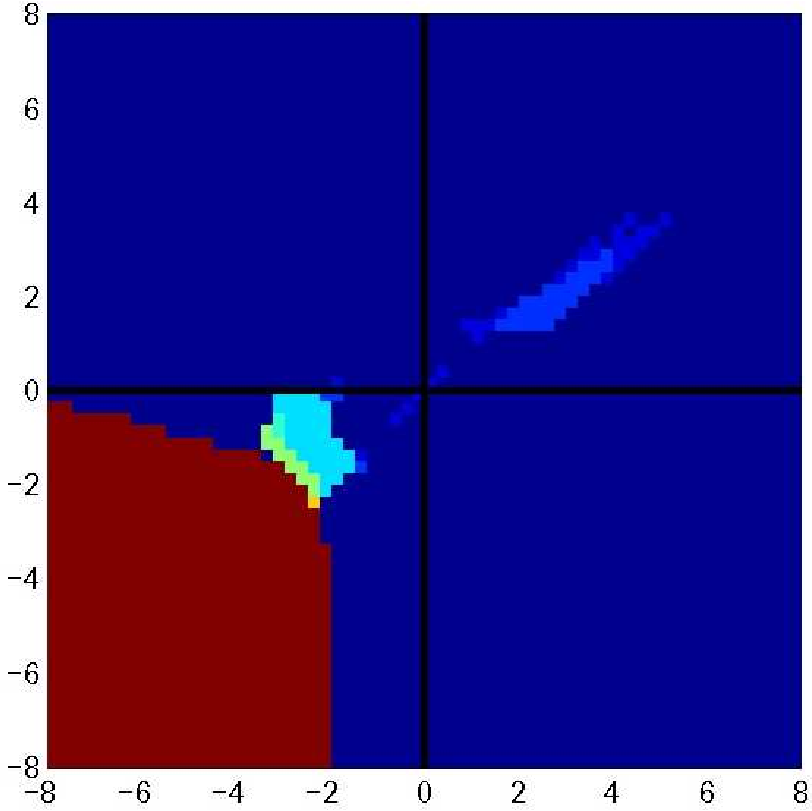
$$
\begin{aligned}
J_1^{\mathrm{MF}} &= J_1 - 2J_3 + 2J_4 \\
J_2^{\mathrm{MF}} &= J_2 - J_3 + 2J_4
\end{aligned}
$$



4-particle ring exchange III

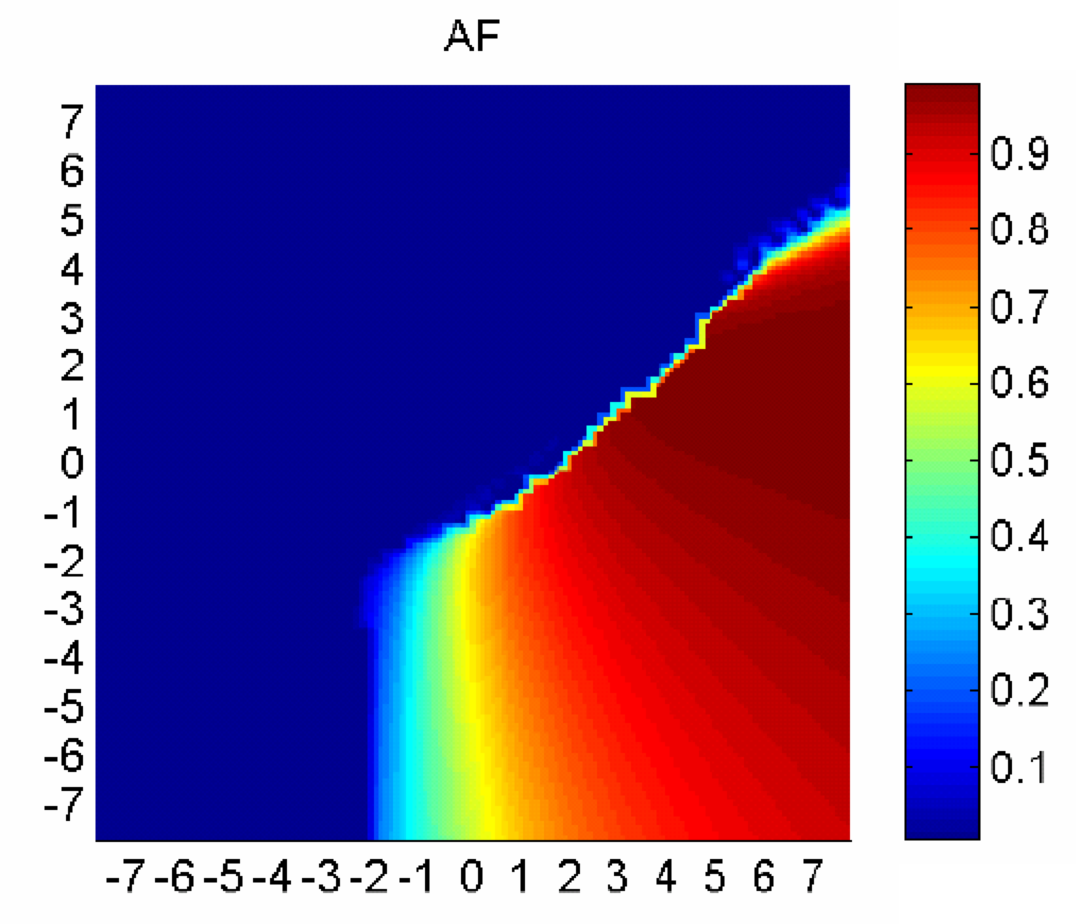
- wave function overlaps

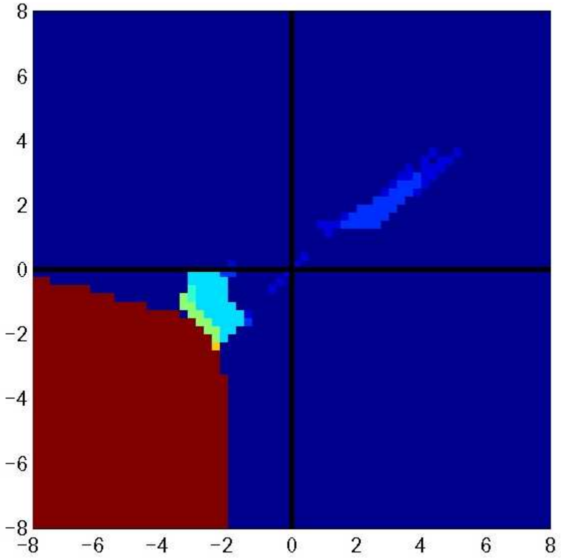


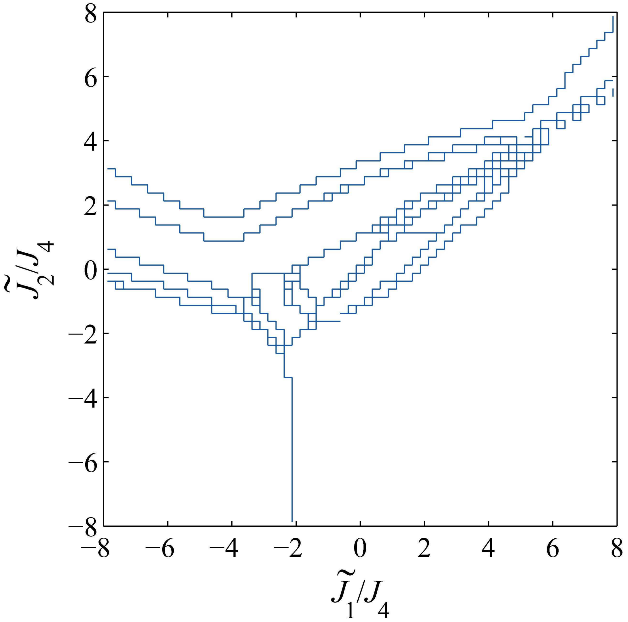


4-particle ring exchange IV

- wave function overlaps:
  identify different phases
  by comparing with known results for $J_4 = 0$



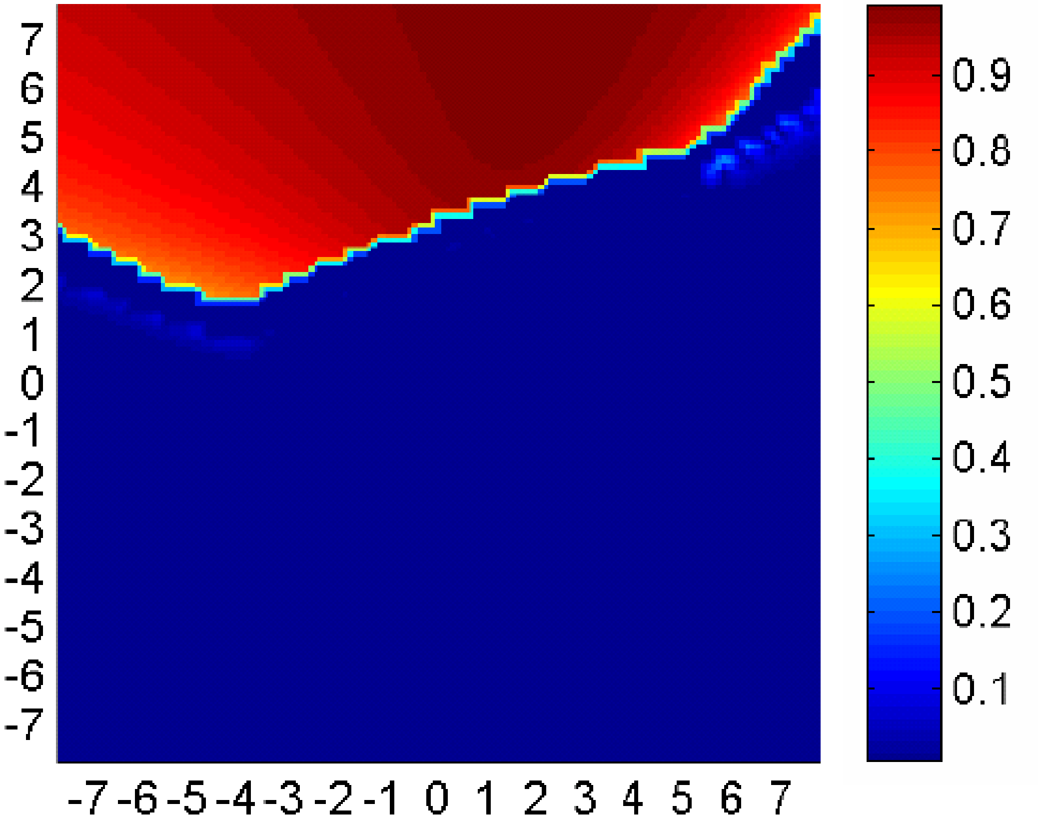


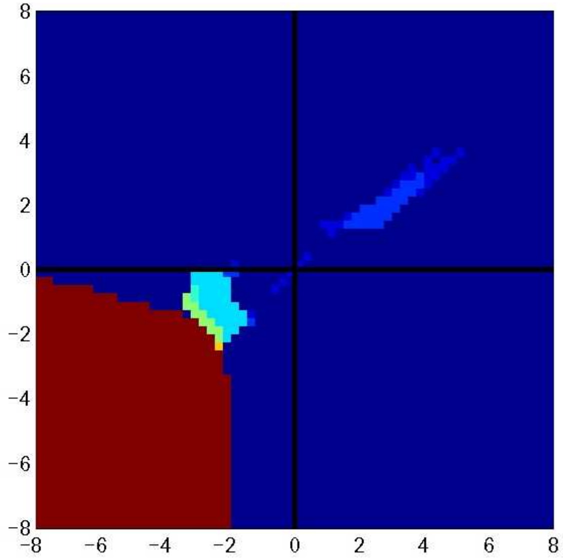


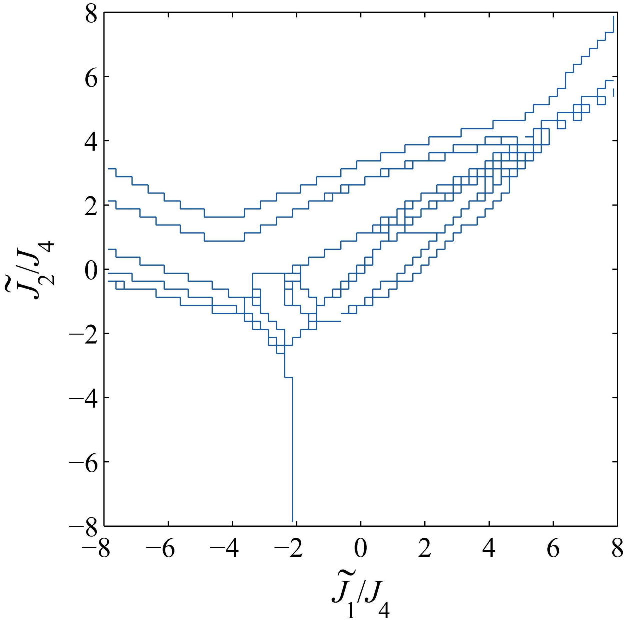
4-particle ring exchange IV

- wave function overlaps:
  identify different phases
  by comparing with known results for $J_4 = 0$

Dimer$_3$







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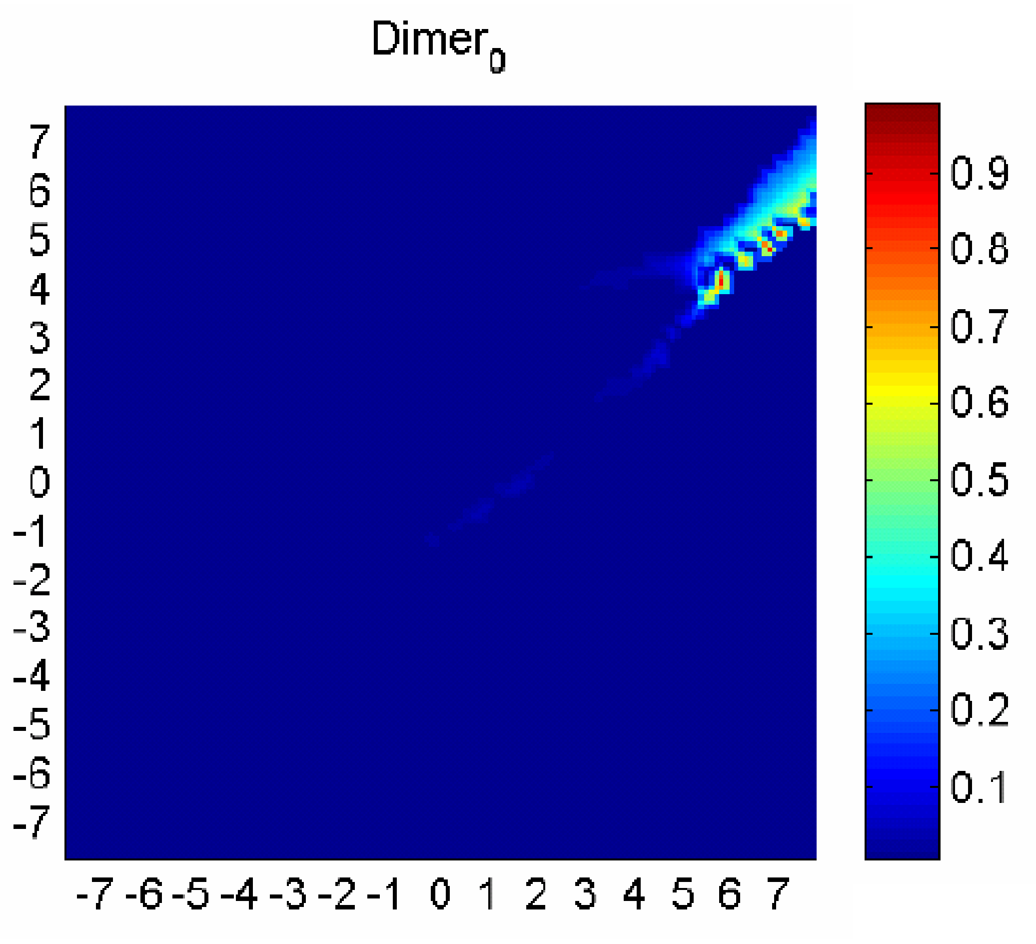

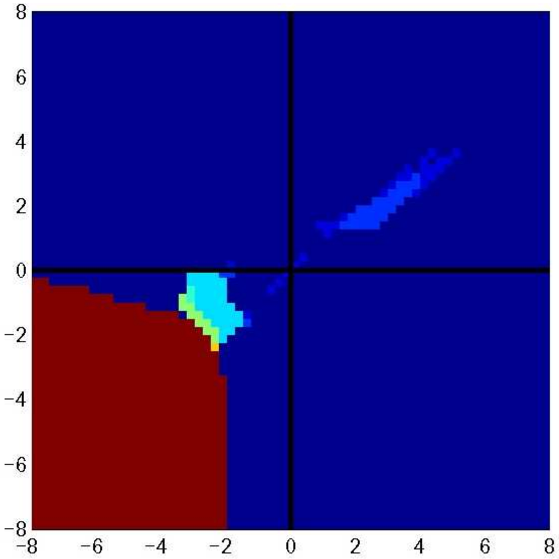

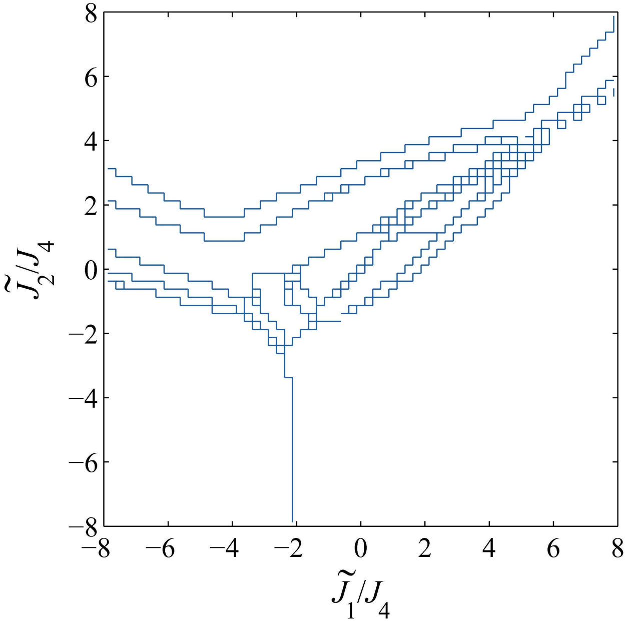

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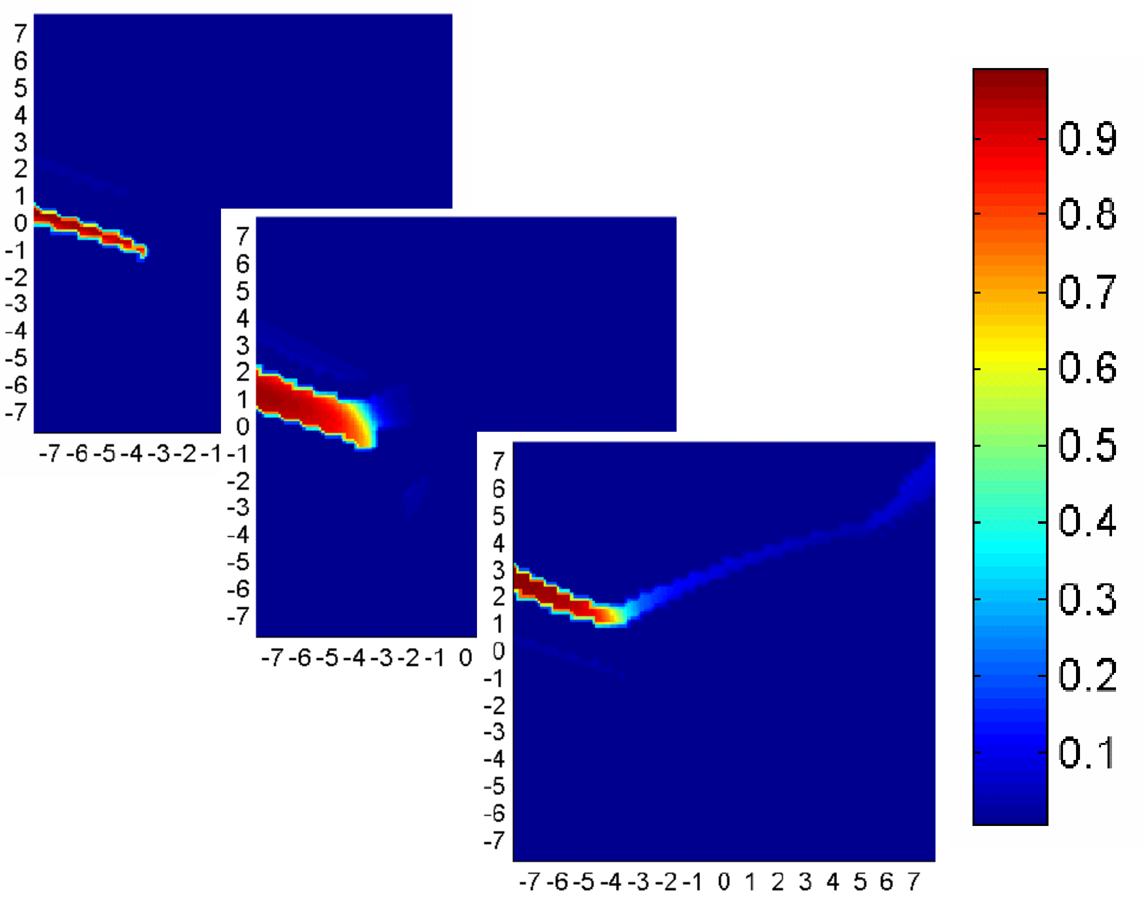
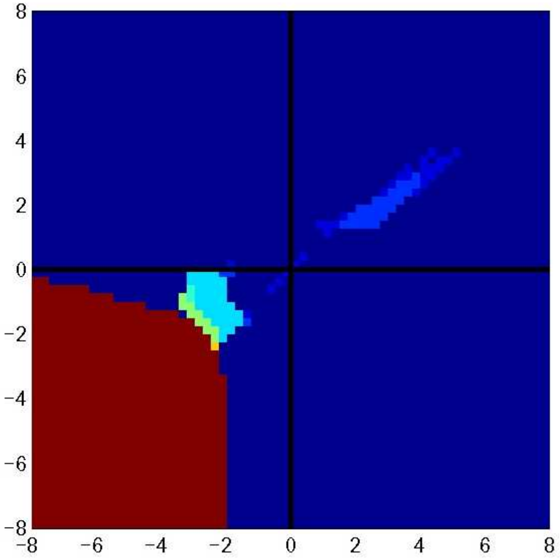
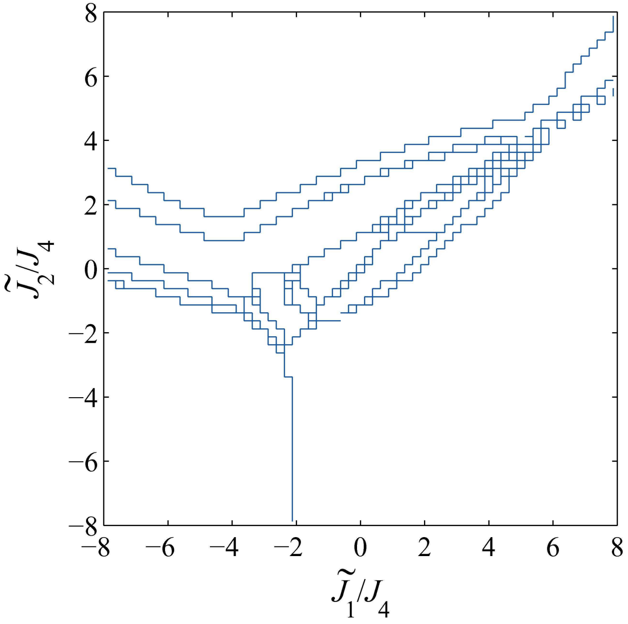
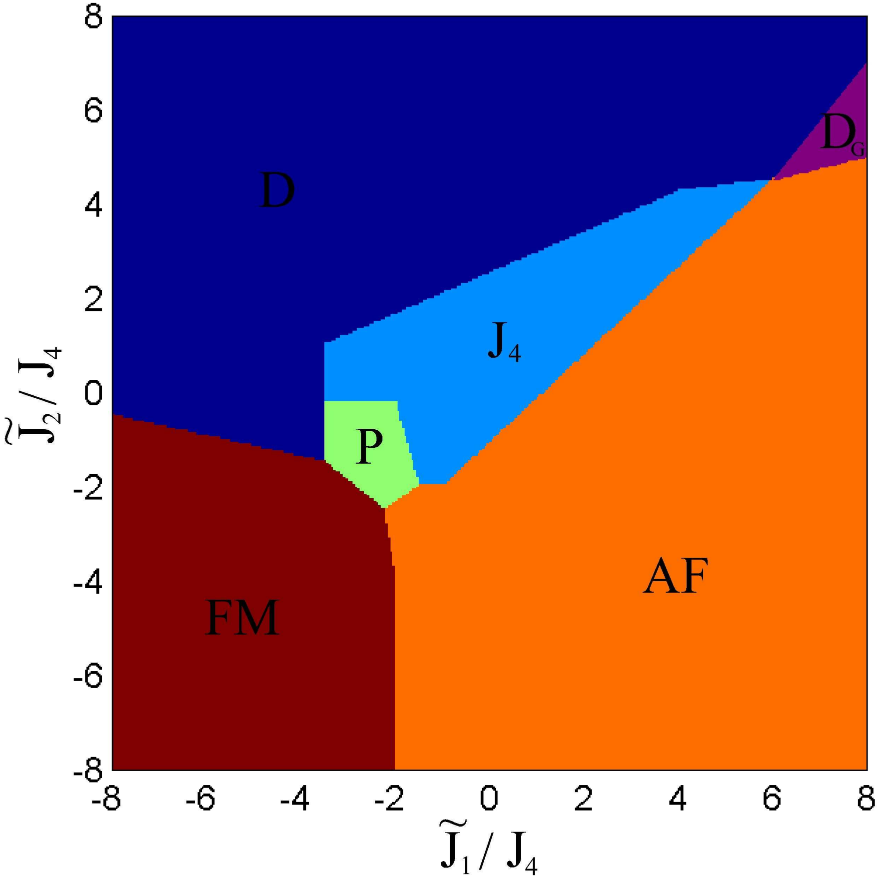


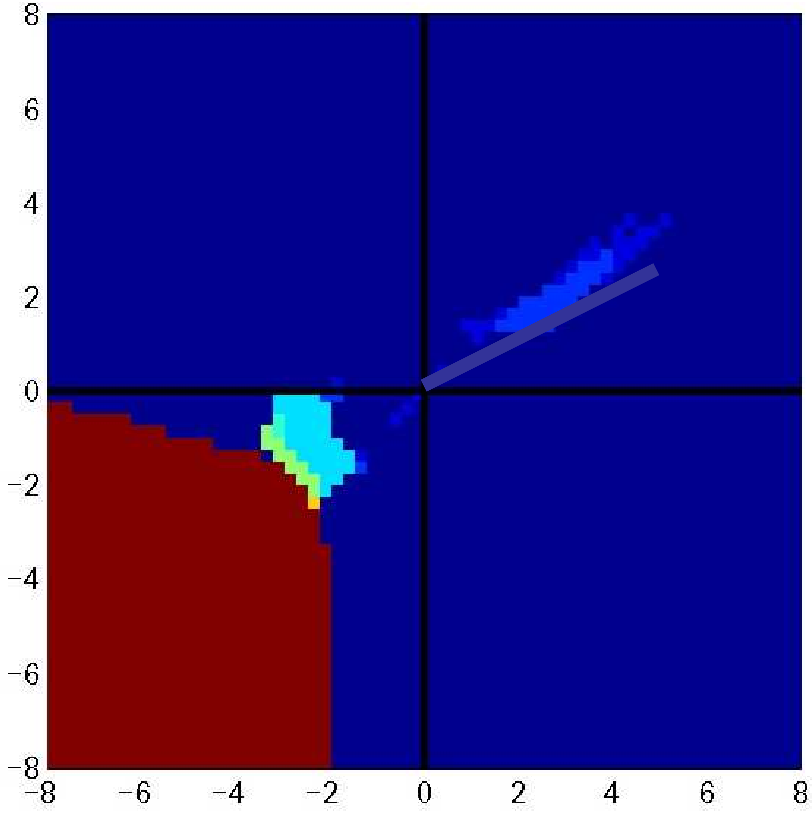




4-particle ring exchange IV

- phase diagram **(PRELIMINARY)**





4-particle ring exchange IV

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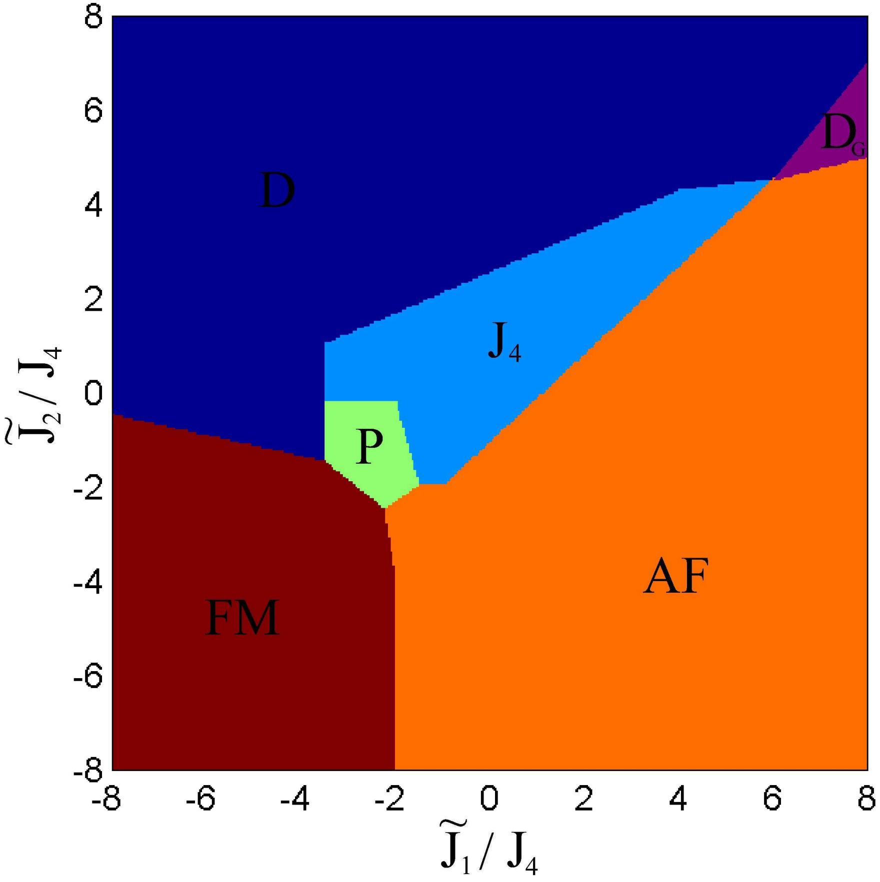
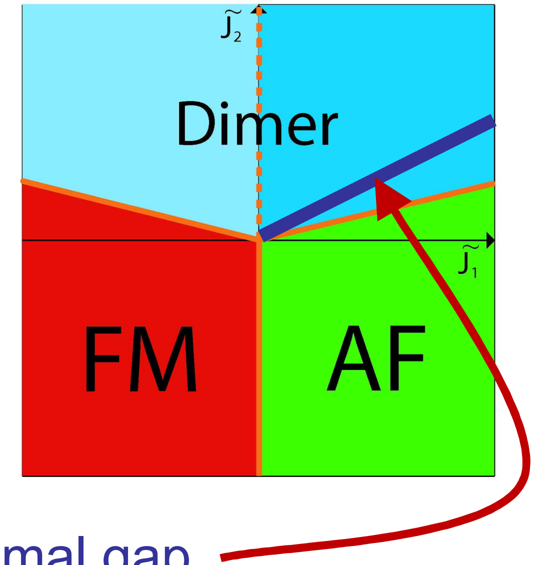




maximal gap
(close to Majumdar-Gosh line,
$J_2 = 0.5\, J_1$)

What about experiment? ...
... Are quantum wires ferromagnetic?

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

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

2 types of quantum wires:

- cleaved-edge overgrowth:

  steep confining potential – $r_\Omega < 1$

- split gate:

  shallow confining potential – $r_\Omega > 1$

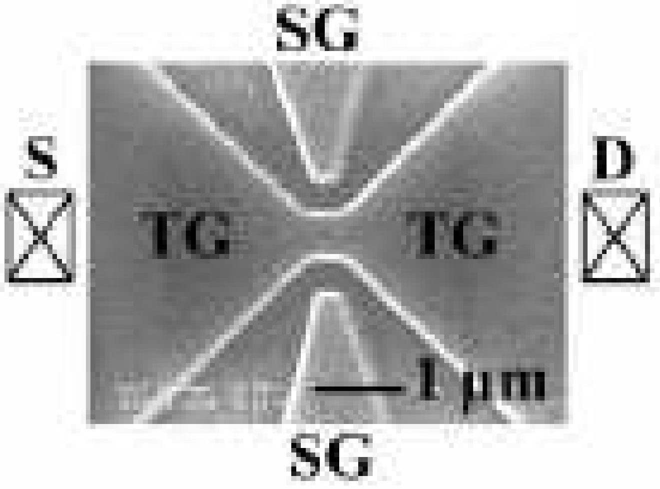
  (e.g. Thomas *et al.*, Phys. Rev. B **61**, R13365 (2000): $r_\Omega = 3 - 6$)

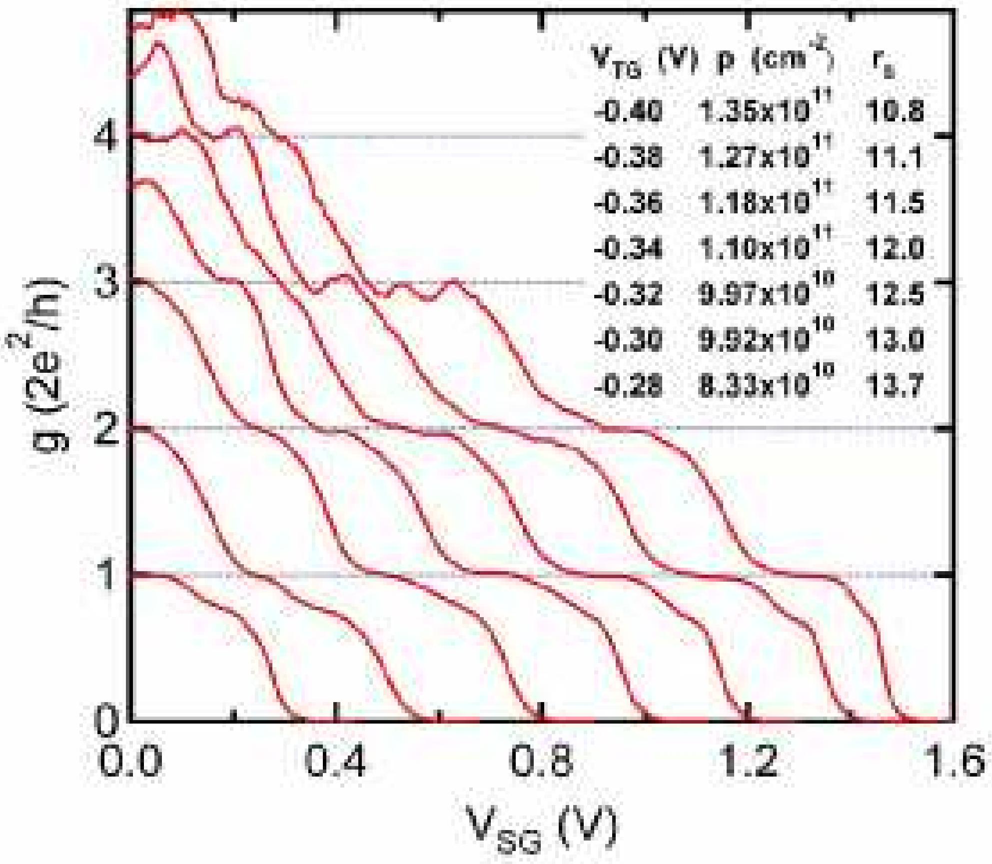
2D hole gas in GaAs:

$\mathbf{r_\Omega > 40}$ **!**

(Klochan *et al.*,
cond-mat/0607509)

Experiment: 1D holes





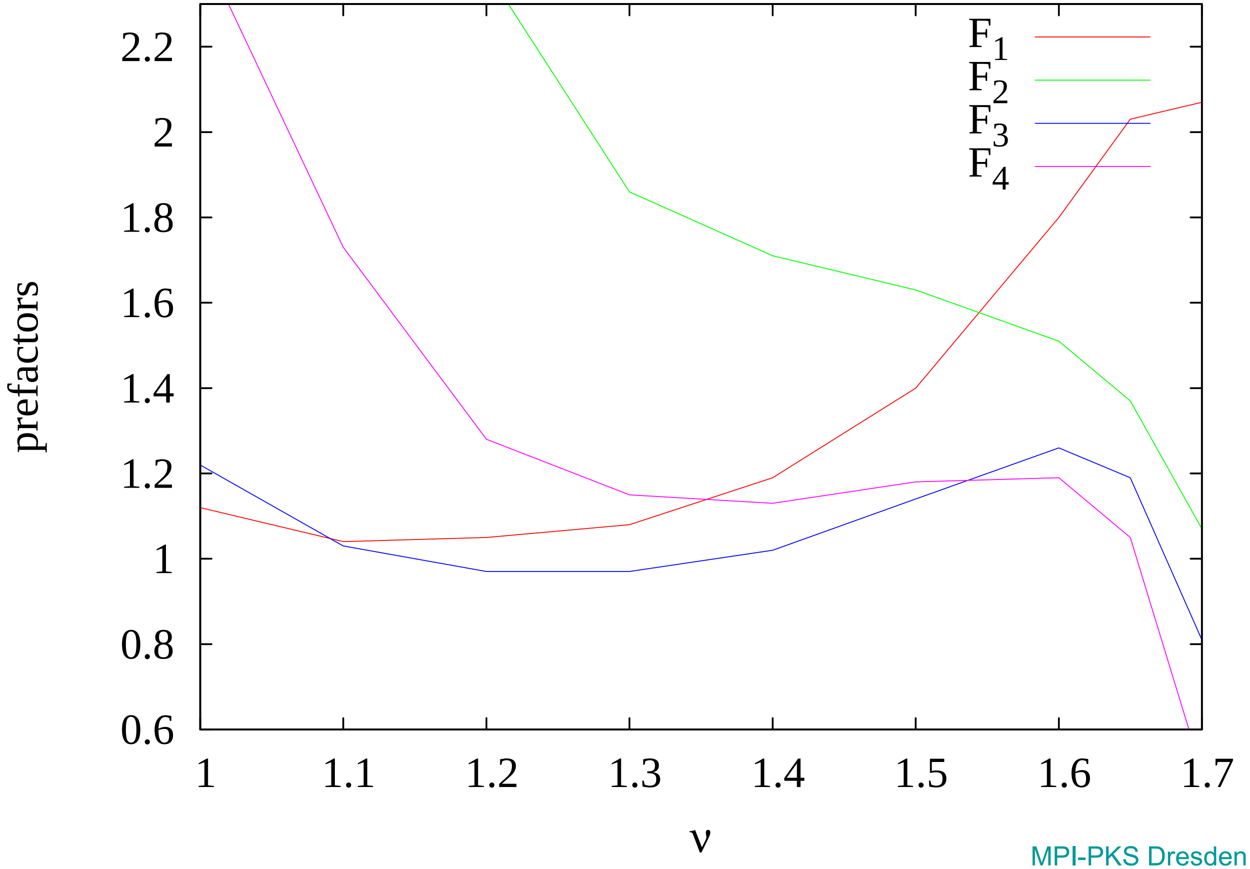
V_{TG} (V)	p (cm^{-2})	r_s
-0.40	1.35×10^{11}	10.8
-0.38	1.27×10^{11}	11.1
-0.36	1.18×10^{11}	11.5
-0.34	1.10×10^{11}	12.0
-0.32	9.97×10^{10}	12.5
-0.30	9.52×10^{10}	13.0
-0.28	8.33×10^{10}	13.7

Prefactors

- exchange constants:

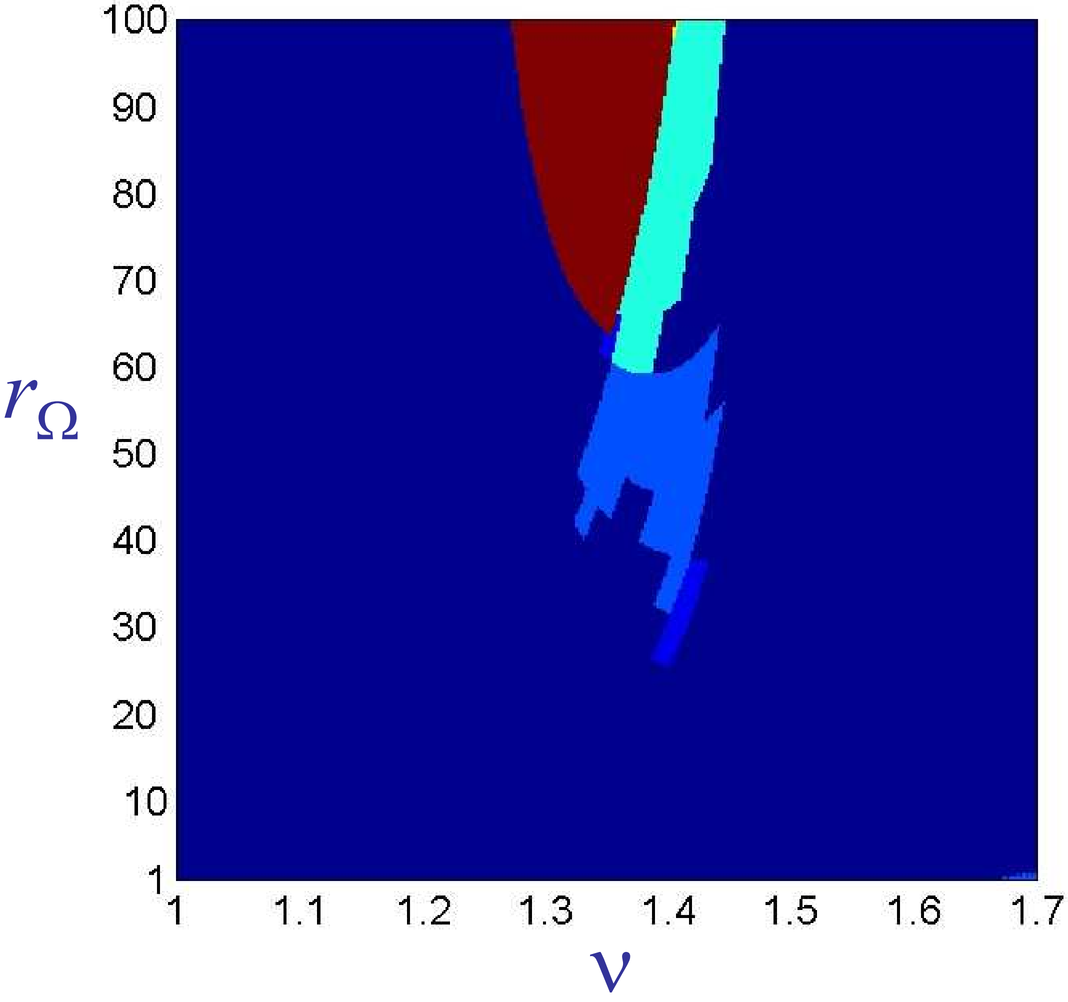
$$J_l = J_l^* \exp\left[-\eta_l \sqrt{r_\Omega}\right] \text{ where } J_l^* = \frac{e^2}{\epsilon a_B} m_l F_l \left(\frac{\eta_l}{2\pi}\right)^{1/2} r_\Omega^{-5/4}$$

(Gaussian fluctuations around classical exchange path)

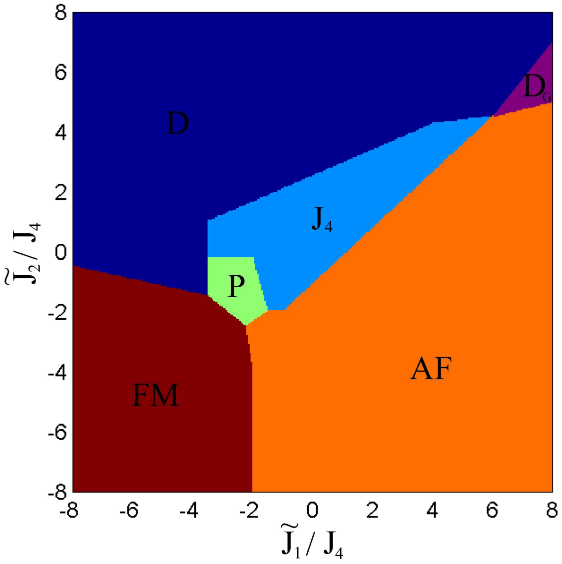


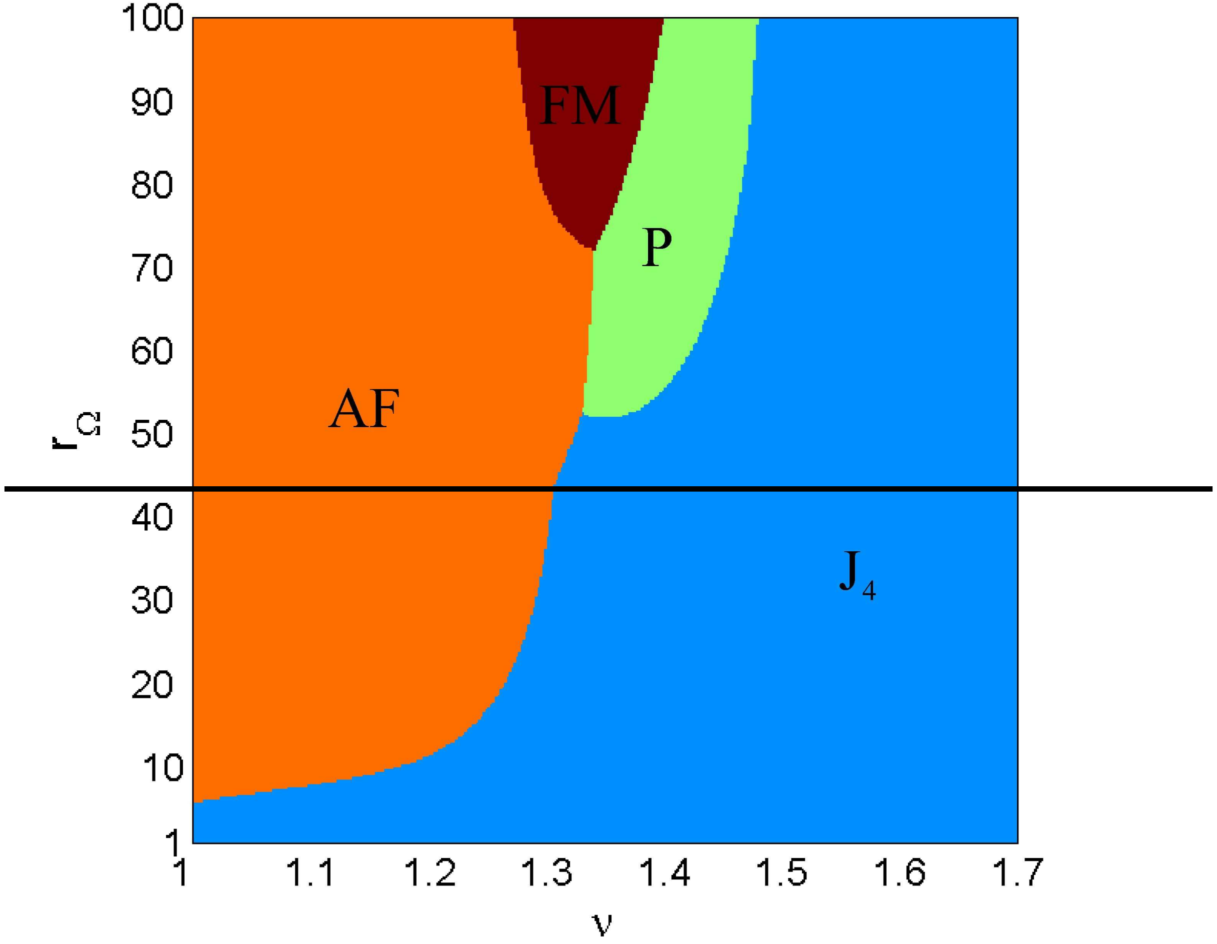
“Phase diagram” I

- ground state spin using the results for the 24-site chain

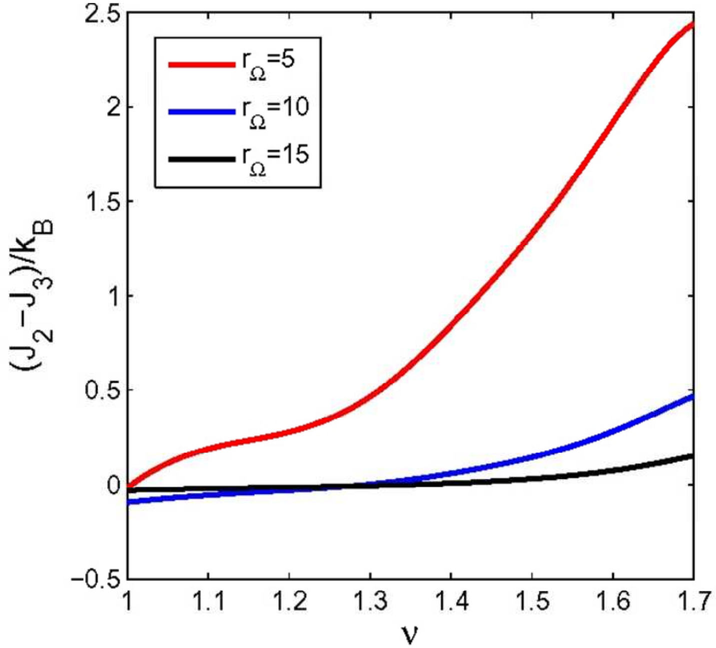


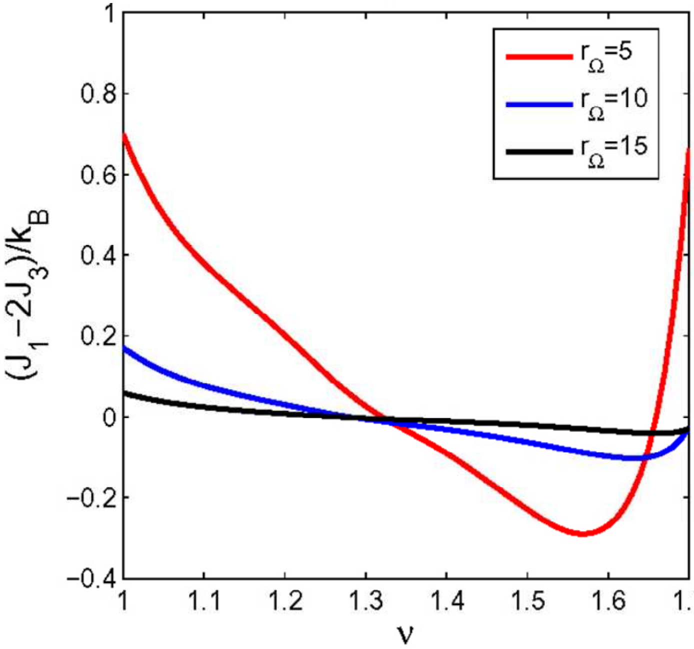
"Phase diagram" II

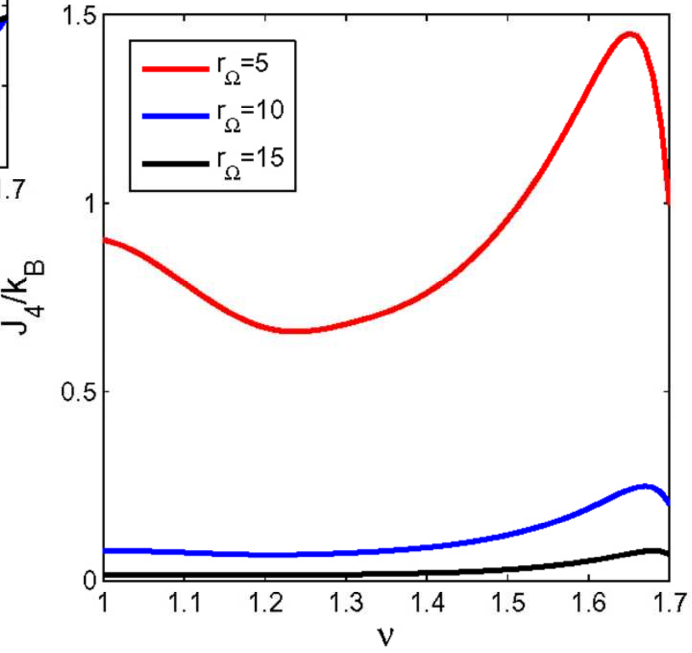




Magnitude of the exchange constants



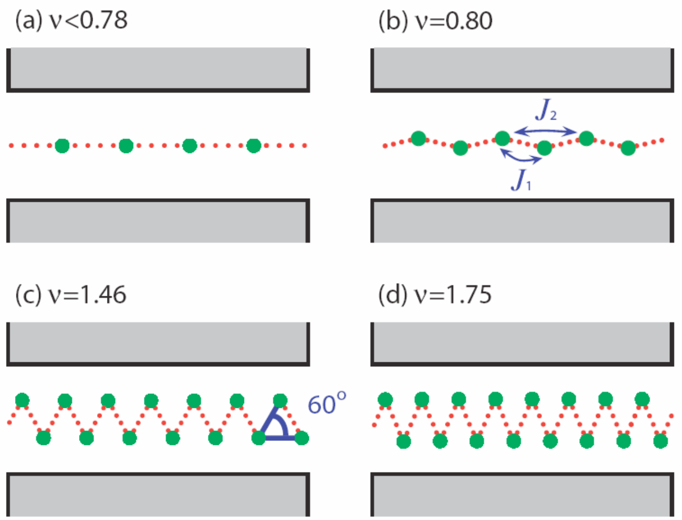


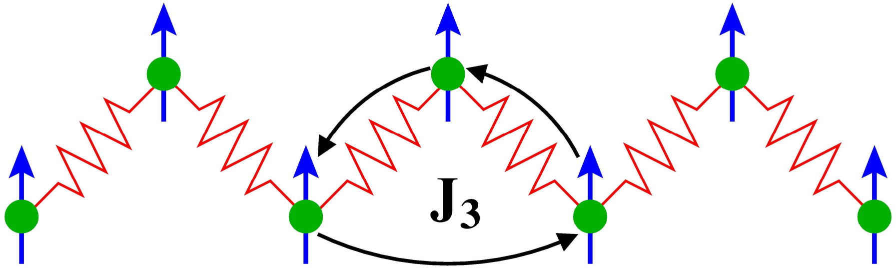


… for electrons

for holes: × $m_h/m_e \sim 5.5$

Conclusions & Outlook

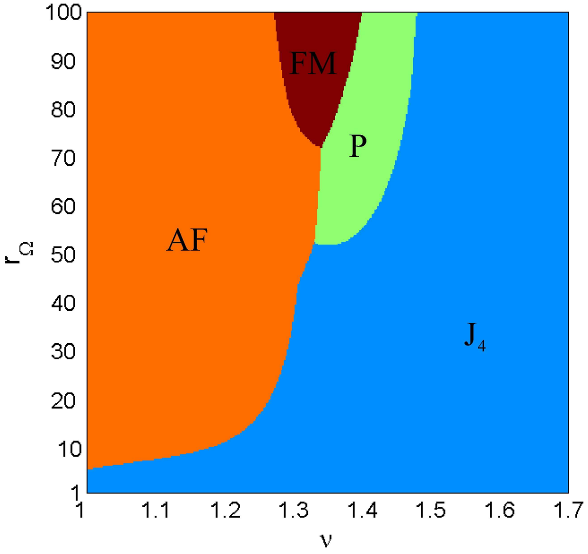




A ferromagnetic ground state in quantum wires is possible at strong enough interactions.
The interactions induce deviations from one-dimensionality and lead to ferromagnetism in a certain range of electron densities.

Conclusions & Outlook

- **4-particle ring exchange dominant at large densities**



TO DO ...

EXPERIMENT:

- ideal devices to observe spontaneous spin polarization: split-gate wires with widely separated gates
  $\Rightarrow$ shallow confining potential $\Rightarrow$ large r_Ω … holes?

THEORY:

- further explore zig-zag chains with 4-particle ring exchange
- conductance? **(Does ferromagnetism lead to $G = 0.5\ G_0$?)**