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CONTINUUM QUANTUM MONTE CARLO METHODS

12 - 23 January 2004

EXCHANGE IN QUANTUM CRYSTALS:

MAGNETISM AND MELTING OF THE LOW DENSITY 2D WIGNER CRYSTAL

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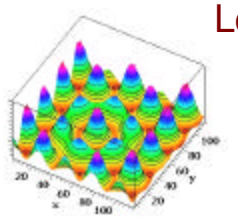
These are preliminary lecture notes, intended only for distribution to participants.

Magnetism and Melting of the Low Density 2D Wigner Crystal



B. Bernu (University of Paris)
L. Candido (University of Goiania, Brazil)
P. Phillips, DMC (UIUC)

- In MOSFETs and above liquid helium, one can make a low density 2D electron gas. $r_s = a/a_B$
- For $r_s > 40$, electrons form 2D Wigner crystal in a triangular lattice. *(unfortunately disorder dominates.)*
- What are defects?
- What is its magnetic order?
- How to go from the microscopic potential to a spin Hamiltonian. $H = -\sum_P (-1)^P J_P P$
  1. Calculate exchange frequencies using PIMC.
  2. Solve exchange Hamiltonian by exact diagonalization of spin Hamiltonian
- How can we understand the properties near melting?
- Relation between magnetism and melting?

2D Electron Phase Diagram at low density.

$$H = -\frac{1}{r_s^2}\sum_i \nabla^2_i + \frac{2}{r_s}\sum_{i<j}\frac{1}{r_{ij}} + cons.$$

Potential energy dominates

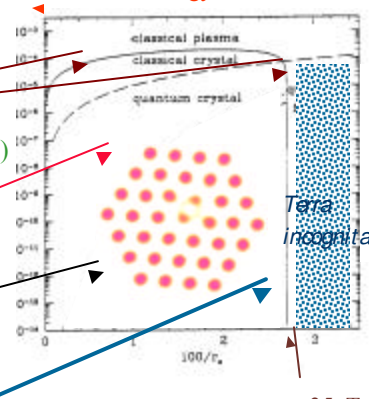
Melting line

T (Ry)

Regime of strong quantum effects

Regime of magnetic effects

$$r_s^2 = \frac{1}{\pi n a_B^2}$$



K

T (K)

mK

Terra incognita

μK

r_s=35 T=0 melting

Fermion sign problem prevents us from definitive calculations in the liquid near freezing!

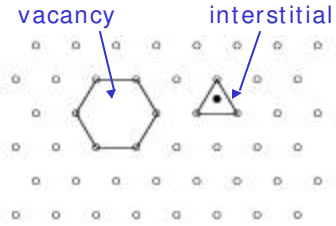
scale does not take into account m^* or ε.

Point defects in the 2d Wigner crystal

- Add and subtract an electron keeping density fixed. (keep same background density)

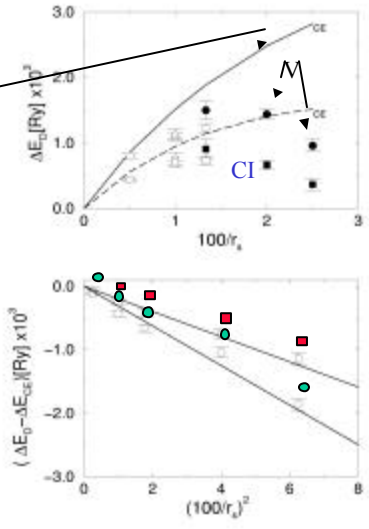
$$E_D = [e(N\pm1,\rho) - e(N,\rho)](N\pm1)$$

- Box rectangular to allow perfect triangular lattice (55,56,57 electrons)
- Calculate total energy using PIMC
- Hexagonal lattice
- Tethers to keep defects from moving around.
- Restricted paths using a localized picture of the nodes and a ferromagnetic spin arrangement.
- Very weak temperature dependence.



Energy of Defect

- Interstitials have a lower energy than vacancies!
- Cockayne-Elser determined exact harmonic energy
- Anharmonic terms reduce the defect energy for $r_s \sim 100$
- The creation energy for an interstitial vanishes for $r_s \sim 35$ (for a ferromagnetic crystal)
- This is very close to the melting density $r_s \sim 39$
- Interstitials and vacancies may be responsible for melting at T=0 in 2D.



2D SUPERSOLID?

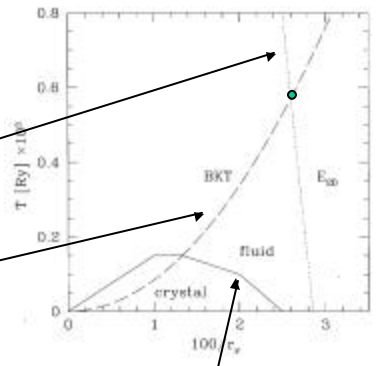
- Most defects are paired interstitials which could obey bose statistics
- Are there enough to Bose condense?
- Density of pairs is thermally activated

$$?_{2D} = ?_0 e^{-E_{2D}/k_B T}$$

- BKT transition T_C when:

$$k_B T_c = 1.8 \frac{\hbar^2}{m} \rho_{2D}$$

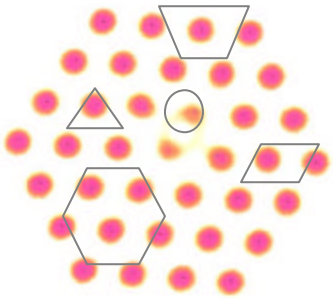
- Supersolid transition does not happen in the density regime where the crystal is stable.



Estimated melting line

Thouless theory of magnetic order

- At low temperature there are **very** few defects, phonons, etc.
- The many body wavefunction has N! peaks, corresponding to possible electron relabelings.
- Expand exact wavefunction in terms of localized wavefunctions.
- System remains in one peak, then tunnels to another.
- Dominant tunneling rates are few particle cyclic exchanges.
- Exchange frequencies (J_P) determine the magnetic order.
- The resulting Hamiltonian is:

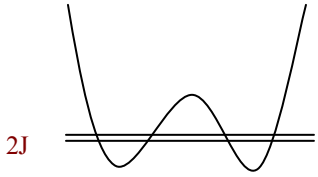


$$H = H_{phonon} - \sum_p (-1)^p J_p \hat{P}$$

Unimportant at low temperatures

Double well example

- Consider a particle in a double well potential
- The ground state is symmetric. The first excited state is anti-symmetric
- We can expand in left and right localized states:

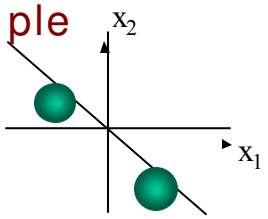


$$\left.\begin{matrix}|\mathrm{L}\rangle \\ |\mathrm{R}\rangle\end{matrix}\right\} = \frac{1}{\sqrt{2}}\left[|\mathrm{S}\rangle \pm |\mathrm{A}\rangle\right]$$

- $J = \frac{1}{2}(E_a - E_s)$ is the frequency with which the system oscillates from left to right.

$$\langle \mathrm{L}(t) \mid \mathrm{L}(0)\rangle = \cos(\mathrm{J}t)e^{-iE_0 t}$$

Two particle example



Now consider two electrons in a double well

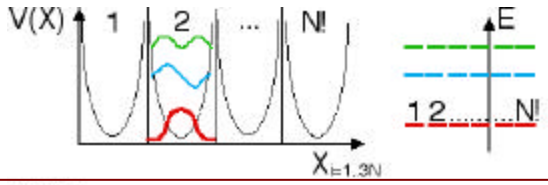
- The ground state is symmetric⇒anti symmetric spin state (singlet)
- The first excited state is anti-symmetric ⇒ symmetric spin state (triplet)
- J_2 is the frequency with which the spin oscillates.
- The system gets spin ordered in the antisymmetric spin state when the temperature goes below J_2.
- We can replace continuum problem with a spins on a lattice:

  $H_{spin} = 2 J_2 \sigma_1 \cdot \sigma_2$
- For more spins

$$H_{spin} = -\sum_p (-1)^p J_p \hat{P}$$

Odd exchanges $J_3, J_5 \ldots$⇒ferromagnetism
Even exchanges $J_2, J_4 \ldots$⇒antiferromagnetism

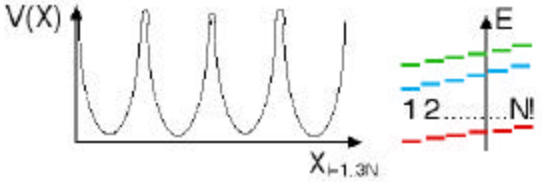
N! wells in configuration space



Infinite barriers

No exchange

Degenerate levels



Finite barriers

Exchange

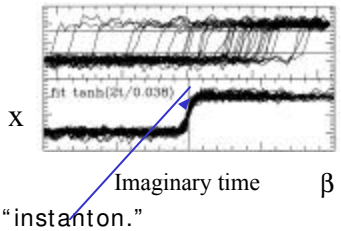
Energy bands

Path Integral Method to determine exchange frequency

- We make a path extending from Z to PZ and evaluate the change in the action. Z= perfect lattice.
- We estimate the ratio:

$$f_P(\beta) = \frac{Q_P(\beta)}{Q_I(\beta)} = \tanh(J_P(\beta - \beta_0))$$

$$Q_P(\beta) = \left\langle Z \left| e^{-\beta \hat{H}} \right| PZ \right\rangle$$



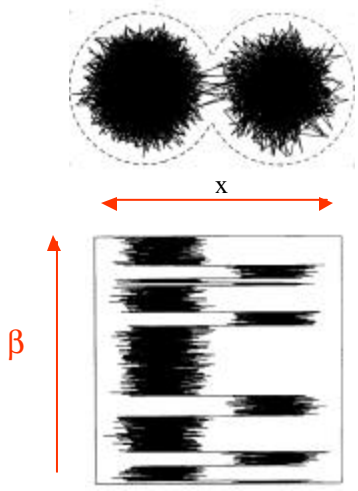
- J_P is the imaginary time tunneling rate.
- β_0 is the width in imaginary time of the "instanton."

- We can calculate the Q's using Path Integral MC by mapping paths from exchange to non-exchange (Bennett's method) and estimate the slope to get J.
- Note that we use distinguishable particle statistics.

(see Ceperley & Jacucci: PRL 58, 1648, 1987)

Symmetric double well in imaginary time

- Consider a single particle inside of a double sphere
- Localization is caused by kinetic energy not potential, as happens in solid helium.
- Exchange happens rarely but very fast (an instanton is confined in imaginary time).
- Frequency in imaginary time (used in Path Intgerals) is proportional to that in real time.

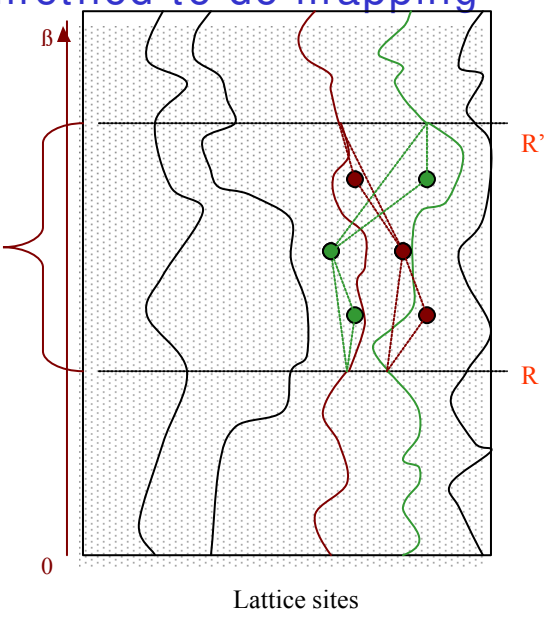


Use Bisection method to do mapping

1. Select time slices
2. Select desired exchange.
3. Sample midpoints
4. Bisect again, until lowest level
5. Determine change in action caused by exchange.

Then:

$$J_p \sim \left\langle \frac{1}{\beta} e^{-\Delta S_P} \right\rangle$$



Aspects of PIMC Method for J

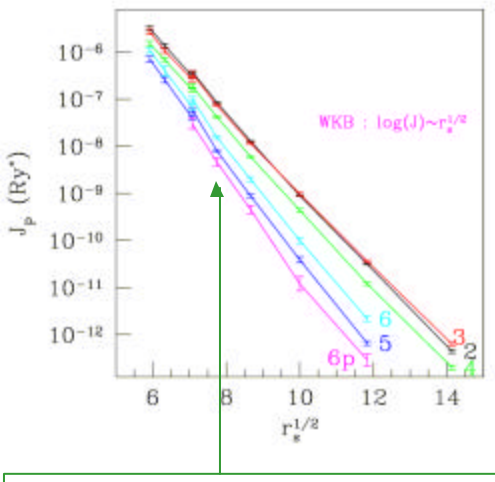
- State space is path space and permutation space
- We bias distribution so the system spends roughly the same time in the two states (I and P).
- Note that $\beta_0 < \beta << 1/J$
- We only need one value of β to get rate since effect of β_0 can be determined by confining exchange in center of world line.
- J is computed as a ratio of rates not as a difference between two numbers
- As sampling is improved the error of J goes to zero. **(zero variance principle)**
- Computational effort can be concentrated around the exchange. **O(N) method.**

Solid ^{3}He

- We have calculated *(Ceperley & Jacucci PRL 58, 1648, 1987)* exchange frequencies in bcc and hcp ^{3}He for 2 thru 6 particle exchanges.
- PIMC gives convincing support for the empirical multiple exchange model.
- Exchanges of 2,3,4,5 and 6 particles are important *(Roger, Delrieu and Hetherington)* because of Metro effect.
- Large cancellation of effects of various exchanges $\Rightarrow$ frustrated broken symmetry ground state (u2d2).
- Agrees with experiment measurements on magnetic susceptibility, specific heat, magnetic field effects, ...
- System of 2d ^{3}He on graphite is more difficult because of exchange outside the layers. It has a ferromagnetic-antiferromagnetic transition as a function of coverage and is rather similar to 2D Wigner crystal.

Dependence of J on density

- 2 and 3 particle exchange have about the same frequency and partly cancel.
- 4 particle exchange is of the same order.
- Higher ring exchanges, though smaller cannot be neglected
- Ground state is frustrated because of competition of multiple exchanges.



Breakdown of Thouless model because of melting of "boltzmannon WC". Need to antisymmetrize to keep stable.

WKB theory

- Calculate the ratio f_P by taking the most probable path, that which minimizes the action:

$$S_P = \int_Z^{PZ} dx \sqrt{V(R(x))}$$

- $J_p = A_p \omega B_p^{1/2} \exp(-B_p)$
  $B_p = b_p r_s^{1/2}$
  $\omega = 1/r_s^{3/2}$ is the attempt frequency.

P	b_p^*	A_p
2	1.66	5.6
3	1.52	1.5
4	1.67	2.9
5	1.91	2.8
6	1.77	2.0

- At low density, exchange rate with the smallest b_p will dominate.
- Roger *(PRB 30, 6432, 1984)* showed that P= 3 dominates, implying that as $r_s \to \infty$ system is ferromagnetic.
- However experiments will not be in the low density limit.

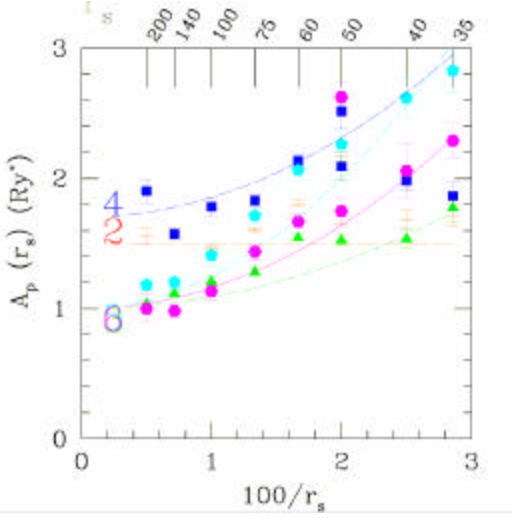
Chakravarty, cond-mat/9805383

Voelker, cond-mat/0107151

Katano, PRB 62, 2573 (2000).

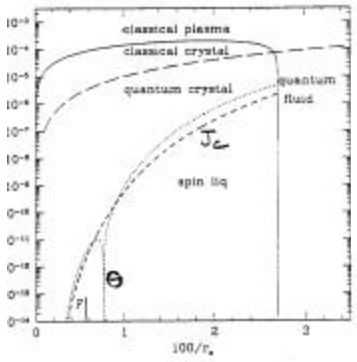
Exchange frequencies

- Plotted are ratios to WKB calculation
- 2-body prefactor is double since there are 2 types of exchanges
- Smaller effects for higher exchanges
- Ratios increase at high density because of more quantum fluctuations--perhaps diverging at melting.
- Our calculations become difficult near melting because fermi statistics are needed to stabilize the crystal.



2D Electron high T magnetic Phase Diagram

- The magnetic susceptibility and specific heat coefficients set temperature scale for magnetic interactions.
- Exchange frequencies are 1,000 times smaller than the melting temperature (except for r_s= 40).
- Justifies that defects and phonons are not important for magnetic ordering.
- We can determine high temperature behavior with simple calculations.
- The magnetic susceptibility changes sign at r_s~ 120.



$$\chi^{-1} = \frac{T}{C_0}\left[1 - \frac{?}{T} + \frac{a}{T^2} + \ldots\right]$$

$$\theta = -3\,J_2 + 6\,J_3 - 9\,J_4 + 15\,J_5 - 2\,J_6 + \ldots$$

[does not take into account m* or ε.]

How to solve the Lattice Model?

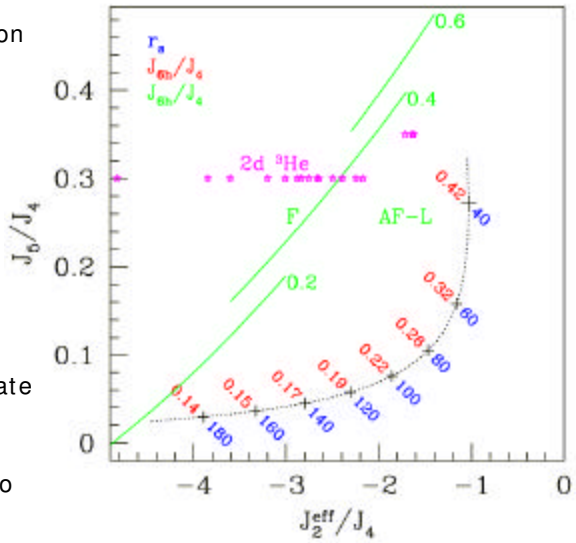
- If only 2 and 3 electron exchanges⇒Heisenberg model
- We cannot neglect the other exchanges! (non Heisenberg)
- High temperature expansions of the free energy involve lattice combinatorics:

  Magnetic susceptibility $\theta = -3J_2 + 6J_3 - 9J_4 + 15J_5 - 2J_6$

  Specific heat = (quadratic in the J's)
- We see big cancellation of various exchanges.
- At zero temperature: mean field theory + spin waves but only in ordered phases!
- But one can exactly diagonalize the Hamiltonian with up to 36 sites by using all the symmetries.
- Misguich, Bernu, Lhuillier, *(PRL 81, 1098, 1998)* mapped out phase diagram (3 parameter model!)

Magnetic Phase Diagram

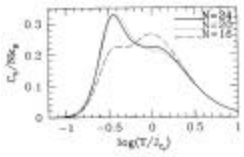
- For $r_s < 120$ inside anti-ferromagnetic phase region (singlet ground state)
- Perhaps a transition at $r_s = 160$ to ferromagnetic (maximal spin)
- AF is a "spin liquid".
  - NOT a state with Neel order.
  - All excitations are gapped.
  - short range order
  - Topological ground state degeneracy (4-fold)
  - Maybe RVB state.
- Spin parameters similar to 2d ^{3}He



Frustrated Spin Model

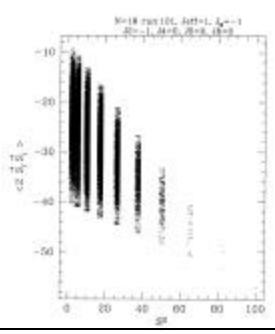
Specific heat

Shows peak at local ordering temperature

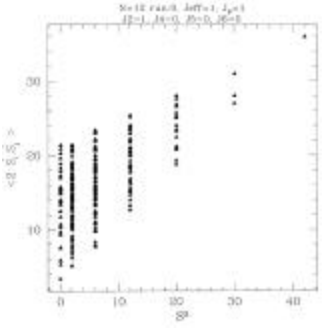


Energy versus spin spectrum

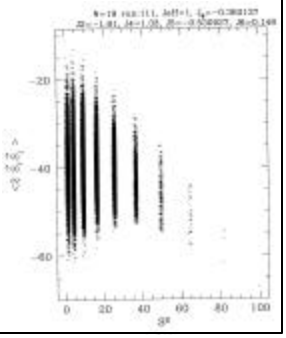
Ferro-magnetic



Anti-ferromagnetic

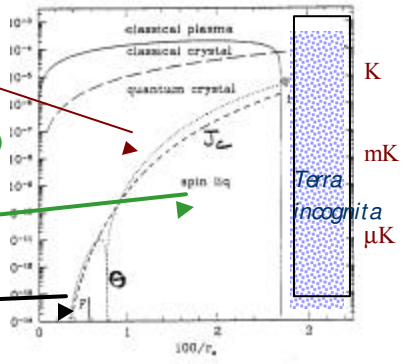


Frustrated



2D Electron high T magnetic Phase Diagram

- temperature scale for magnetic interactions.
- Spin liquid at intermediate densities
- Ferromagnetic phase at very low density



Mysteries

- Is melting transition second order because of point defects? Relation to hexatic transition?
- Do exchange cycles explode at melting? Relation to energy of point defects
- Why are exchange parameters for solid ^{3}He so similar at melting? (caused by similar vacancy-interstitial model?)
- Why are the magnetic properties of the liquid so similar?

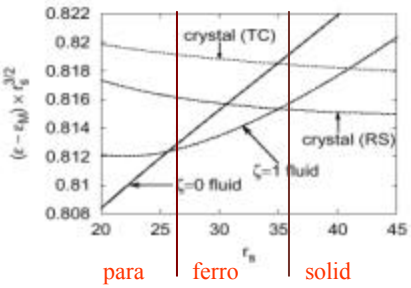
T=0 fixed-node calculation:

Used high quality backflow wave functions to compute energy vs spin polarization.

Energies are nearly identical →

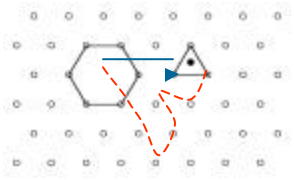
Magnetic susceptibility diverges

Attaccalite et al. PRL 88,256601 (02).



Vacancy-Interstitial Model

1. Form a vacancy-interstitial pair
2. One of the pair diffuses.
3. The pair is attracted by crystal stress fields
4. Bound state implies eventual recombination.
5. Result is a spin exchange.



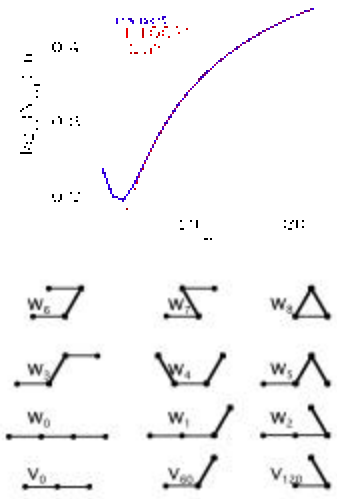
- Explains similarity of J's since they have a common prefactor.
- Common density dependence of step # 1
- Explains universality of spin Hamiltonian at melting as due to crystal field.
- Relation of melting to exchanges

- the J_P increases with density but no divergence in individual exchanges.
- exponential growing number of large loops contribute:

$$n \to \infty : N_{loop} \sim \frac{4.1557^n}{n^{3/2}}$$

- need to extrapolate exchange data but without doing too many calculations.
- fit $\ln(J_P)$ to number of patterns in the calculated loops

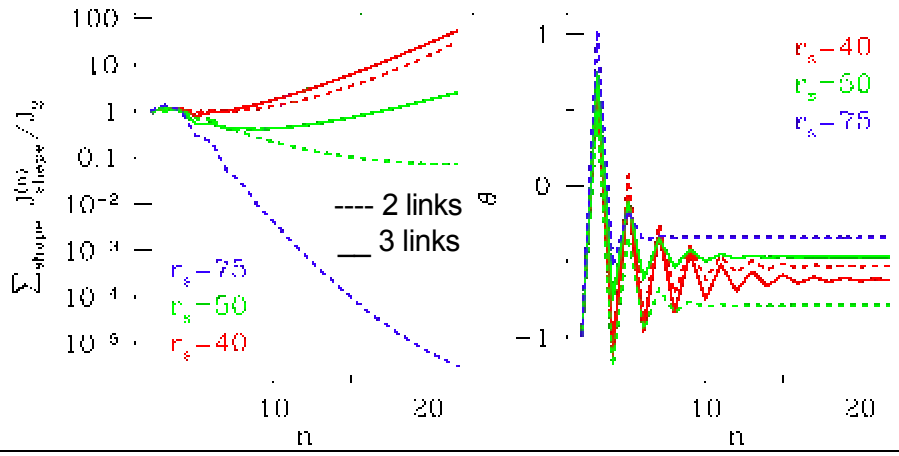
$$J_{ring} = e^{a_0 n + a_1 n^{1/2} + a_2 N_2 + a_3 N_3}$$



Patterns with 2 and 3 links

Look at the convergence in the magnetic susceptibility vs N.

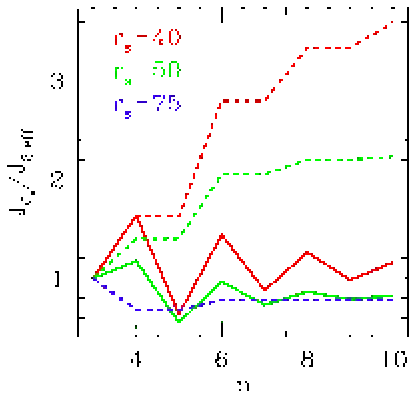
$$\theta = -\sum_{n=2}^{n_{max}} \left[(-1)^n \frac{n(n-1)}{2^{n-1}} \sum_{shape\ of\ n\ sites} n_{shape} J_n^{(shape)} \right]$$



Or the convergence of the specific heat coefficient vs N:

$$\lim_{T\to\infty}\frac{C_V(T)}{Nk_B}\sim\frac{9}{4}\left(\frac{J_{C_V}}{T}\right)^2$$

$$J_{C_V}^2=\sum_{ij}J_iM_{ij}J_j.$$



---- 2 links model
___ 3 links model

Summary

- We can do accurate calculations of the exchange frequencies in Wigner crystal.
- Magnetic order in 2D Wigner crystal is likely to be density dependent and frustrated, probably an RVB-like spin liquid.
- Remarkable similarity to 2D ^{3}He.
- Thouless theory applicable up to melting
  - No divergence of individual exchange energies
  - An increasing number of exchanges contribute
  - Simple models allow to extrapolate the data to larger loops
  - $\theta_{J_{C_V}}$ are nearly divergent at melting
- Do exchanges melt the solid?
- Is the vacancy-interstitial model of exchange is correct?
- Are the magnetic properties related to unusual properties of the higher density 2DEG?