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2004 J. Phys.: Condens. Matter 16 S701

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# Multi-spin exchange model: the near melting transition of the two-dimensional Wigner crystal

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Received 7 January 2004

Published 4 March 2004

Online at [stacks.iop.org/JPhysCM/16/S701](http://stacks.iop.org/JPhysCM/16/S701) (DOI: 10.1088/0953-8984/16/11/018)

## Abstract

The low temperature properties of fermionic solids are governed by spin exchanges. Near the melting transition, the spin-exchange energy increases as well as the relative contribution of large loops. In this paper, we check the convergence of the multi-spin exchange model and the validity of the Thouless theory near the melting of the Wigner crystal in two dimensions. Exchange energies are computed using a path integral Monte Carlo for loop sizes up to 8, at  $r_s = 40, 50$  and  $75$ . The data are then fitted to a geometric model. Then the exchange energies are extrapolated to larger sizes in order to evaluate their contributions to the leading term of the magnetic susceptibility and the specific heat. These results are used to check the convergence of the multi-spin exchange model.

## 1. Introduction

<sup>3</sup>He atoms as well as electrons carry a spin  $1/2$ . In their solid phases, exchange processes are responsible for the thermodynamics at low temperature. The Thouless theory explains how a multi-spin exchange (MSE) effective Hamiltonian results from these spin exchanges [1]. The applicability of such an approach is based on the very different scales of the exchange energies and the phonon energies (at least three orders of magnitude). In the strong coupling limit ( $r_s \rightarrow \infty$  for the Wigner crystal), a semiclassical calculation (WKB) predicts such very small exchange energies. Moreover, in this limit, only the two or three body exchanges dominate, depending on the dimension and the lattice type, leading to the standard Heisenberg model (for spin  $1/2$ , three body exchanges are equivalent to pair exchanges). Then, at weaker coupling, other loop exchanges arise that may lead to a magnetic phase transition. In general, more and more exchanges are important near the melting transition. The problem we address here is how the MSE Hamiltonian evolves as we approach the melting transition and whether there is a precursor to melting in the magnetic Hamiltonian.

Exchange energies have been obtained for the bulk 3D  $^3\text{He}$  [3] and for  $^3\text{He}$  adsorbed on graphite [4]. The exchange energies have also been obtained for the 2D electron Wigner crystal [5] and [6]. For most densities, from the semiclassical limit to near melting, the WKB and path integral Monte Carlo (PIMC) evaluations assume a stable solid of particles (a triangular lattice in 2D) without taking into account the Fermi statistics. For these densities, only small exchange loops with six or fewer particles have significant energies. These calculations determine the exponential dependence of exchange energies versus the density; the longer loops decreasing more rapidly in the strong coupling limit. The MSE model explains the main features of the magnetic transition of the second solid layer of helium 3 adsorbed on graphite [7].

One problem that has been encountered near melting is that the PIMC calculations become increasingly difficult to converge. This is because the Boltzmann solid melts before the fermion solid. Adding Fermi statistics stabilizes the solid in a wider density region (or, alternatively, imposing antisymmetry increases the energy of the liquid phase into which the crystal melts.) In order to stabilize the crystal, we assume a ferromagnetic spin polarization of ‘spectator’ atoms (non-exchanging atoms) and enforce antisymmetry on those paths. When comparison is possible, only small changes of exchange energies are found with this procedure. The largest differences are seen at  $r_s = 50$  for the system without statistics where the solid is close to melting (melting of the bosonic Wigner crystal occurs at  $r_s \approx 60$ ). The restriction on the path resulting from Fermi statistics does not modify the exchange energies very much. The statistics do not affect the local correlated motions of particles in the vicinity of the exchanging ones, but they have long range effects that stabilize the solid and forestall the melting.

The next question is whether the Thouless theory can be applied near the melting transition. Indeed, a possible scenario could be that the energy difference associated with a given spin-exchange, say  $J_P$ , becomes comparable to the zero-point motion kinetic energy ( $k_e^{(0)}$ ). In that case, a complicated coupling between spin states and phonon excitations could arise. Instead our numerical results demonstrate that all the exchange energies are much smaller than  $k_e^{(0)}$ , even at melting. Even if the exchange energy increases exponentially with the inverse density (WKB predicts  $-\log(J) \propto r_s^{1/2}$ ), each value stays well below  $k_e^{(0)}$ . Thus, up to the melting transition, each exchange can be seen as an independent event.

Now, near the melting transition, the number of important exchanges increases considerably. In this paper, we address the question of the convergence of this MSE model versus the number of exchanges. Indeed, if the exchange energies decrease roughly exponentially with the loop size  $n$ , the number of loops of size  $n$  does increase exponentially. The convergence of the MSE model is thus questionable. Does the total spin-exchange energy diverge when the crystal melts? Is the existence of long-exchanges a mechanism for the melting transition or a by-product? We try to answer these questions from the analysis of the two-dimensional Wigner crystal exchange data. In section 2, we present the results of path integral Monte Carlo (PIMC) simulations and we give the formula to test the convergence of the MSE model. In section 3, different models are used to fit PIMC results in order to extrapolate to larger loop sizes.

## 2. PIMC results and thermodynamics

For a given permutation  $P$ , the exchange energy  $J_P$  calculated from PIMC needs to be monitored carefully with respect to several parameters such as the number of particles and the time step  $\tau$ . There are additional parameters associated with the Bennett method. Fortunately, those parameters change smoothly with the density or the type of exchange or even the system

**Table 1.** Exchanges energies (in  $10^{-9}$  Ryd) obtained by PIMC simulations for the fully polarized 2D Wigner crystal. Results are for 64 electrons, and  $\beta = 1/T = 10\,000, 16\,600, 20\,000$  Ryd $^{-1}$ , time step  $\tau = 40, 66, 100$  Ryd $^{-1}$  for  $r_s = 40, 50, 75$ , respectively. The multiplicity is the number permutation  $P$  of the same shape per site, including  $P^{-1}$  symmetry. All exchanges are for nearest neighbour on the triangular lattice. For 2–6 particle exchange there is only one sort of diagram, but for larger exchanges there are multiple possibilities which we have labelled arbitrarily with an index. The authors can be contacted for further details.

$J$	Multiplicity	$r_s = 40$		$r_s = 50$		$r_s = 75$	
2	3	1402	2%	323	3%	13.4	3%
3	4	1184	3%	281	3%	14.2	2%
4	6	809	3%	165	5%	6.2	3%
5	12	295	6%	42	7%	1.1	6%
6 <sub>1</sub>	2	476	5%	88	9%	2.3	11%
6 <sub>2</sub>	12	143	7%	17.1	8%	0.24	8%
6 <sub>3</sub>	12	92	8%	9	9%	0.116	9%
6 <sub>4</sub>	4	40	13%	3.2	8%	0.021	8%
7 <sub>1</sub>	12	105	9%	14.4	6%	0.16	18%
7 <sub>2</sub>	12	72	11%	7.8	9%	0.076	21%
7 <sub>3</sub>	24	43	11%	3.6	9%	0.018	13%
7 <sub>4</sub>	12	37	21%	2.8	16%	0.0037	19%
7 <sub>5</sub>	24	20	15%	0.97	11%	0.004	17%
8 <sub>1</sub>	6	130	11%	15.3	7%		
8 <sub>2</sub>	6	29	13%	1.74	9%		
8 <sub>3</sub>	12	19	12%	1.19	10%		
8 <sub>4</sub>	12	23	10%	1.72	7%		
8 <sub>5</sub>	24	40	13%	3.1	9%		
8 <sub>6</sub>	12	44	12%	3.5	11%		
8 <sub>7</sub>	6	1.3	21%	0.058	17%		
8 <sub>8</sub>	12	4.3	26%	0.32	26%		
8 <sub>9</sub>	24	6.4	24%	0.25	21%		
8 <sub>10</sub>	12	23	11%	1.5	14%		
8 <sub>11</sub>	24	7.6	14%	0.25	20%		
8 <sub>12</sub>	24	18	18%	0.97	11%		
8 <sub>13</sub>	12	8.8	16%	0.24	15%		
8 <sub>14</sub>	24	22	10%	2.5	8%		
8 <sub>15</sub>	24	9.8	14%	0.51	10%		
8 <sub>16</sub>	12	14	12%	1.08	8%		
9 <sub>1</sub>	4	75	15%	5.2	10%		

(helium atoms or electrons). The most important effect is the  $\beta = 1/T$  dependence of the results. Indeed, the calculations are done at a temperature sufficiently low so that the phonon excitations are non-existent but sufficiently high that the spins have not magnetically ordered. In these conditions, the exchange energy should be independent of the temperature. However, near melting (the precise density depends on the statistics) results show a linear increase versus  $\beta$  (note that each independent run at a given temperature is well converged). This is in fact interpreted as a signature of melting that would most probably occur for larger systems. The following tables contain only exchange values converged and independent of  $\beta$ .

Table 1 shows the PIMC results. Also shown are the energies versus exchange for the three densities considered. It is seen that exchange energies decrease as  $r_s$  increase or at fixed  $r_s$ , when the loop size increases. The strong dependence on the shape of the exchange we examine next.

The overall importance of the exchange processes can be measured by the leading term of the high temperature (HT) expansion of the magnetic susceptibility (the Curie–Weiss temperature  $\theta$ ) and the specific heat:

$$\theta = - \sum_{n=2}^{n_{\max}} (-1)^n \frac{n(n-1)}{2^{n-1}} J_n^{(T)} \quad (1)$$

where

$$J_n^{(T)} = \sum_{\text{shape of } n \text{ sites}} n_{\text{shape}} J_n^{(\text{shape})} \quad (2)$$

$n_{\text{shape}}$  is the number of loops per site of a given shape and  $J_n^{(\text{shape})}$  the associated exchange value.

The leading HT term of the specific heat is defined as

$$\lim_{T \rightarrow \infty} \frac{C_V(T)}{Nk_B} \sim \frac{9}{4} \left( \frac{J_{C_V}}{T} \right)^2 \quad (3)$$

where  $J_{C_V}$  is given by a positive quadratic form of the exchange values:

$$J_{C_V}^2 = \sum_{ij} J_i M_{ij} J_j. \quad (4)$$

Unfortunately, no simple formula exists for the matrix  $M$ . At very large  $r_s$  (WKB limit) only  $J_2$  and mainly  $J_3$  dominate in a ferromagnetic phase and  $|\theta| = J_{C_V} = J_2 - 2J_3$ . At  $r_s \sim 200$ ,  $J_4$  is large enough and the system becomes antiferromagnetic.

### 3. Fits of exchange energies to analytic formula

In order to determine the contribution of larger exchanges to the magnetic susceptibility and specific heat in equations (1) and (3), we want to understand how exchange energies vary with the loop size and shape.

Exchange energies depend mainly on the loop size  $n$ . Then, for a given loop size  $n$ , the exchange is much larger if the exchange contains only smooth angles, that is when its area  $\mathcal{A}$  is maximum ( $\mathcal{A} = (n-2+2p)\mathcal{A}_0$ , where  $\mathcal{A}_0$  is the area of the enclosed triangles and  $p$  is the number of lattice sites inside the loop). In order to quantify this shape dependence we assume that each local section of the exchange contributes to the exchange probability and use the following formula:

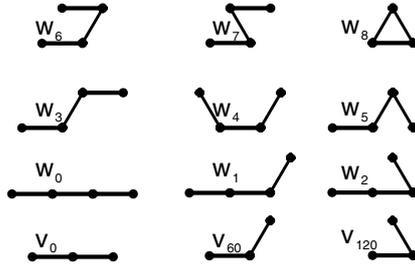
$$\log(J_{n,s}^{\text{fit}}) = \alpha_0 + \alpha_n n + \alpha_p p_s + \sum_v \alpha_v N_{s,v}. \quad (5)$$

Here  $p_s$  is the number of non-exchanging sites contained inside the loop of shape  $s$  and  $N_{s,v}$  is the number of patterns of type  $v$  encountered in the loop of shape  $s$ . The  $\alpha$  s are parameters determined from a least-squares fit minimizing:

$$\chi^2 = \frac{1}{N_J} \sum_{n,s} \left( \frac{\log(J_{n,s}/J_{n,s}^{\text{fit}})}{\sigma_{n,s}} \right)^2, \quad (6)$$

where  $N_J$  are the number of degrees of freedom (the number of exchanges minus the number of fitting parameters) and  $\sigma_{n,s}$  is the Monte Carlo error of  $\log(J_{n,s})$ . We now discuss the results for the fit allowing for three successively more detailed patterns.

*Fitting without patterns.* Without using any of the parameters that depend on the shape of the exchange ( $\alpha_v = 0$ ), only three parameters remain:  $\alpha_0$ ,  $\alpha_n$  and  $\alpha_p$ . The results are given in table 2 (top). Such a fit is not accurate as can be seen by the large value of  $\chi^2$ . As an interpretation of the parameters,  $\exp(\alpha_0)$  is the prefactor for the initiation of an exchange,



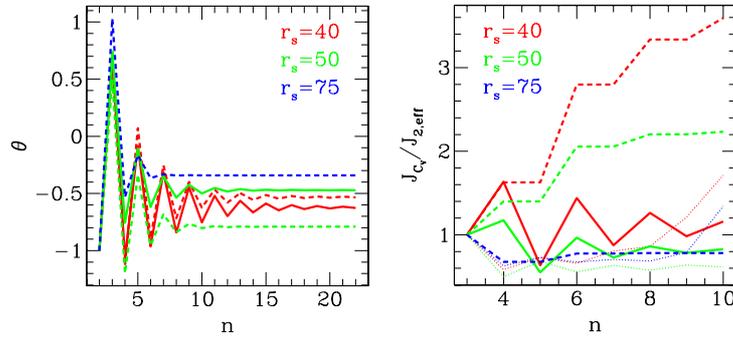
**Figure 1.** List of the three possible patterns made of two links (last line) and the eight patterns made of three links.

**Table 2.** Top table: fit of exchange energies according to equations (5) and (6).  $\alpha_n$  is the main varying parameter. Uncertainties are in parenthesis. Middle table: same for fits with the two-link patterns. For each  $r_s$ , the third column is the ratio  $v_i/v_0$ : within error bars, they are independent of  $r_s$  for this model. Bottom table: same for the three-link patterns. For each  $r_s$ , the third column is the ratio  $w_i/w_0$ , the ratio depends on  $r_s$  for patterns with smooth angles, and not for patterns with sharp angles.

$r_s$	40	50	75			
$\alpha_0$	8.99(4)	8.34(5)	6.79(6)			
$\alpha_p$	0.91(3)	1.09(3)	2.52(1)			
$\alpha_n$	-0.752(9)	-1.038(9)	-1.466(14)			
$\chi$	8.5	9.5	16.0			
$\alpha_0$	12.1(1)	12.32(1)	12.9(2)			
$\alpha_p$	0.19(4)	0.14(4)	0.39(12)			
$\alpha_{v_0}$	-0.883(14)	-1.185(12)	-1.954(2)			
$\alpha_{v_{60}}$	-1.009(14)	1.14	-1.28(12)	1.08	-2.05(3)	1.04
$\alpha_{v_{120}}$	-1.69(3)	1.91	-2.28(3)	1.92	-3.43(7)	1.75
$\chi$	2.5	4.5	5.0			
$\alpha_0$	11.3(7)	8.8(5)				
$\alpha_p$	0.03(8)	-0.07(7)				
$\alpha_{w_0}$	-0.63(5)	-0.8(4)				
$\alpha_{w_1}$	-0.76(4)	1.20	-0.8(4)	1.0		
$\alpha_{w_2}$	-1.27(11)	2.01	-1.25(9)	1.56		
$\alpha_{w_3}$	-0.93(4)	1.47	-1.15(3)	1.43		
$\alpha_{w_4}$	-0.87(1)	1.38	-0.69(8)	0.86		
$\alpha_{w_5}$	-1.37(6)	2.17	-1.65(5)	2.06		
$\alpha_{w_6}$	-1.15(16)	1.82	-0.92(13)	1.15		
$\alpha_{w_7}$	-1.44(7)	2.28	-1.94(5)	2.42		
$\chi$	1.3	1.3				

$\alpha_n$  is the action needed for adding a link onto the exchange, and  $\alpha_p$  is a term which favours non-compact exchanges.

*Fitting with two-link patterns.* The simplest patterns  $v$  consist of the angles subtended by two adjacent links. On a triangular lattice there are three possible cases, since two adjacent links can have angles of  $0^\circ$ ,  $60^\circ$ ,  $120^\circ$  or  $180^\circ$  (see figure 1), but the parameter  $v_{180}$  only occurs in  $J_2$ . Also  $\alpha_n$  becomes redundant because it can be determined from the angles:  $\sum_v N_{s,v} = n$ , the number of angles equals the number of sites in the loop. Thus we are left with five parameters. The results for this fit are shown in table 2 (middle).



**Figure 2.** Left: contribution of loops of length  $n$  to the Curie–Weiss temperature versus  $n$  (see equation (1)). Right: contribution of loops of length  $n$  to  $J_{C_V}$  versus  $n$  (see equations (3) and (4)). The full lines stand for the model with three-link patterns, dashed lines for the model with two-link patterns, and the dotted line for the model without patterns (see text).

(This figure is in colour only in the electronic version)

The mean error is significantly reduced by including the angles in the fit. We find that  $\alpha_0$  depends weakly on density,  $\alpha_p$  is not very significant. Note that the ratio  $v_i/v_0$  is almost independent of  $r_s$ .

*Fitting with three-link patterns.* In our most elaborate fit, the possible configurations of three adjacent links are used (see figure 1). The triangular pattern  $w_8$  occurs only in the three-body loop, and thus is removed from the fitting procedure. Note that if the patterns for three links are used, those of two links are redundant. Here again  $\alpha_n$  is a redundant parameter. Hence, we are left with 10 parameters for 28 exchanges for which we have computed exchange frequencies. At  $r_s = 75$  we have not computed enough different exchanges to do this fit, so we only discuss it at smaller values of  $r_s$ .

The results are shown in table 2 (bottom). This fit is now reasonable as the mean standard deviation is of the order of one, i.e. within statistical error bars of the PIMC results. Clearly the parameter  $\alpha_p$  can be removed. In this fit, the ratios  $w_i/w_0$  depend on  $r_s$  except for  $w_3$ ,  $w_5$  and  $w_7$ .

#### 4. Expanding to larger loop cycles

From the fits of the previous section, it is now possible to evaluate, at high temperature, the leading term  $\theta$  of the magnetic susceptibility (see equation (1)) and  $J_{C_V}$  of the specific heat (see equation (3)) by including much larger loops. Those terms give an estimate of the temperature as the spins begin to become correlated (note that the expected ground state is a spin liquid). We test here if the MSE model still converges when more and more exchanges are involved as appears near the melting transition.

We have calculated all self-avoiding walks of lengths up to  $n = 22$  on the triangular lattice with their shape properties ( $p$ , angles  $v$  and  $w$ ).

Figure 2 (left) shows the sum  $J_n^T$  of all energies of loops of size  $n$ .  $J_n^T$  decreases at large  $r_s$ , but clearly increases exponentially at  $r_s = 40$ . Nevertheless the Curie–Weiss temperature seems to converge at all densities (figure 2 (middle)) even if strong oscillations appear at  $r_s = 40$ .

The leading term of the specific heat  $J_{C_V}$  (equation (3)) can be used to scale energies/temperatures. A divergence of this term means a huge energy associated with

exchanges, and likely the melting of the solid. Figure 2 (right) shows a good convergence of  $J_{C_V}$ , again at large  $r_s$ . The two-link and three-link models provide rather different results. This means that  $J_{C_V}$  is a rather subtle combination of exchange energies. Still, all models seem to converge at  $r_s = 50$ . At the smallest  $r_s = 40$ , the two-link model diverges, whereas the three-link model seems to converge, though with strong oscillations.

## 5. Conclusion

Exchange energies can be computed with a path integral Monte Carlo up to the melting transition. Use of Fermi statistics is necessary to stabilize the solid (non-local effect), but it does not change the exchange energies (local contribution). As one approaches the melting transition, an increasing number of different exchanges becomes important. The Thouless theory allows one to write a multi-spin exchange model to describe the low energy physics. But the convergence of this model is not guaranteed and must be verified. We have checked that for the 2D Wigner crystal, the Curie–Weiss temperature  $\theta$  and the first-order contribution to the specific heat ( $\text{Tr}(H - \langle H \rangle)^2$ ) converge for the lowest densities. The large oscillations seen in both these quantities at  $r_s = 40$  hint at a possible divergence in the thermodynamic properties at higher densities. Though the MSE model converges at lower densities, a divergence of the model is possible at the critical melting density, consistent with the picture that multi-spin exchange is itself a mechanism for melting.

## References

- [1] Thouless D J 1965 *Proc. Phys. Lond.* **86** 893
- [2] Ceperley D M 1995 *Rev. Mod. Phys.* **67** 279
- [3] Ceperley D M and Jacucci G 1987 *Phys. Rev. Lett.* **58** 1648
- [4] Bernu B and Ceperley D M 1999 *Quantum Monte Carlo Methods in Physics and Chemistry* ed M P Nightingale and C J Umrigar (Dordrecht: Kluwer)
- [5] Bernu B, Candido L and Ceperley D M 2001 *Phys. Rev. Lett.* **86** 870
- [6] Bernu B, Candido L and Ceperley D M 2002 *Proc. Rolduc School on Quantum Simulations of Complex Many Body Systems*  
Bernu B and Ceperley D M 2002 Exchange frequencies in 2d solids *J. Phys.: Condens. Matter* **14** 9099
- [7] Misguich G, Bernu B, Lhuillier C and Waldtmann C 1998 *Phys. Rev. Lett.* **81** 1098  
Misguich G, Bernu B, Lhuillier C and Waldtmann C 1999 *Phys. Rev. B* **60** 1064