Phase transition in 2-d system of quadrupoles on square lattice with anisotropic field

A K Sallabi and M Alkhttab
Department of Physics, Faculty of Science, Misurata University, Libya
sallabiabdulwahab@yahoo.ca

Abstract. Monte Carlo method is used to study a simple model of two-dimensional interacting quadrupoles on ionic square lattice with anisotropic strength provided by the ionic lattice. Order parameter, susceptibility and correlation function data, show that this system form an ordered structure with $p(2 \times 1)$ symmetry at low temperature. The $p(2 \times 1)$ structure undergoes an order–disorder phase transition into disordered $(1 \times 1)$ phase at 8.3K. The two-point correlation function show exponential dependence on distance both above and below the transition temperature. At $T_c$ the two-point correlation function shows a power law dependence on distance, e.g. $C(r) \sim r^{-\eta}$. The value of the exponent $\eta$ at $T_c$ shows small deviation from the Ising value and indicates that this system falls into the same universality class as the XY model with cubic anisotropy. This model can be applied to prototypical quadrupoles physisorbed systems as $N_2$ on NaCl(100).

1. Introduction
The research on two-dimensional (2-d) continuous phase transition has a long history and continues to inspire basic theoretical work [1-10] as well as computational and experimental research on diverse phenomena such as magnetic reorientation in ultrathin metal films [5] and phase transitions at solid surfaces, e.g. the $N_2$/NaCl(001) [11,12]. Monte Carlo simulation [11], using pairwise additive potential with adjustable parameters and distributed point dipoles on atomic sites, predicted that a monolayer of nitrogen molecules adsorbed on a NaCl surface will, like the CO/NaCl system[13], undergoes an order-disorder transition at 25K from $p(2 \times 1)$ phase to $p(1 \times 1)$ phase, and that the phase transition is predicted to be fallen in the same universality class as the XY model with cubic anisotropy. This class is of considerable interest because it is predicted to exhibit nonuniversal critical exponents [3], i.e. exponents whose values depend on the relative strengths of an anisotropic external potential (provided by the NaCl substrate in this case) and the molecule-molecule interactions. The XY model with cubic anisotropy will exhibit Ising behaviour in the limit of infinite anisotropy, whereas Kosterlitz-Thouless (K-T) behaviour occurs at zero anisotropy. In recent article, Vogt [12] reported experimental work about $N_2$/NaCl(001) at temperatures between 20K and 40K, and provides experimental evidence that nitrogen molecules form a phase with $p(1 \times 1)$ symmetry at the NaCl(100) surface but found no hints for a disorder-order phase transition from a $p(1 \times 1)$ to $p(2 \times 1)$ structure above 20K (the experiment was performed at temperatures above 20K), as predicted by MC simulations [11]. It is worth noting that Vogt [12] does not exclude the existence of a phase transition from a $p(1 \times 1)$ to $p(2 \times 1)$ phases below 20K. In this article we present the results of Monte Carlo
methods of a simple model of two-dimensional interacting quadrupoles on square lattice with anisotropic strength provided by the ionic lattice and pure quadrupole–quadrupole potential. Order parameter, susceptibility and correlation function data results are presented. This model can be applied to prototypical quadrupoles physisorbed systems as N$_2$ on NaCl(100).

2. Method of simulation

The discrepancy between Monte Carlo simulation [11] and the experimental work [12] regarding the existence of phase transition of N$_2$ on NaCl(001) above 20K reflects the need to use a model potential with less or no adjustable parameters. In the Monte Carlo simulation [11] the potential parameters in the repulsion part of Tang-Toennies and Buckingham atom-atom/ion potentials have been adjusted to reproduce the elastic constants and the lattice properties of N$_2$ and NaCl crystals. Nitrogen on graphite was well described by the electric quadrupole–quadrupole (EQQ) interaction only [14]. It is well known that most of the contribution to the interaction potential comes from the electrostatic potential.

In our present work, instead of using a full pairwise potential, we use pure quadrupole–quadrupole potential between fixed point quadrupoles on square lattice and the field is provided by the lattice with no adjustable parameters.

Details of the Monte Carlo methods used in this work can be found in our previous work to simulate N$_2$/NaCl [11] system. The coordinate system used to describe the positions of the quadruples on the (001) face of a square lattice has an arbitrary origin in the plane of the lattice. The $x$ axis runs along the [1,−1, 0] and the $y$ axis runs along the [1,1,0] crystallographic directions, while the $z$ axis was set perpendicular to the plane of the lattice. The orientation of the quadrupoles is described by a polar angle $\theta$ (tilt with respect to the surface normal) and an azimuthal angle $\phi$ (angle between the $x$ axis and the projection of the quadrupole axis onto the plane of the lattice). These angles may be used to define an order parameter $\Phi = \langle \Phi^2_x + \Phi^2_y \rangle^{1/2}$ through the relations

$$\Phi_x = N^{-1} \sum_{i=1}^{N} (-1)^{n_{xi}} \cos(\phi_i)$$

and

$$\Phi_y = N^{-1} \sum_{i=1}^{N} (-1)^{n_{yi}} \sin(\phi_i),$$

where the indices $n_{xi}$ and $n_{yi}$ are integers with values from 1 to L which label the $x$ and $y$ positions of the site $i$ on a square lattice. The summations are with respect to index $i$ and run over all of the localized sites $(n_{xi}, n_{yi})$ from 1 to N=L$^2$. The phase factors $(-1)^{n_{xi}}$ and $(-1)^{n_{yi}}$ are used for systems with antiferro-like ground states. The angled brackets denote an ensemble average over the configurations generated from the MC simulations. The susceptibility is constructed from fluctuations in the order parameter, viz.

$$\chi = \langle \Phi^2_x + \Phi^2_y - 2 \Phi_x \Phi_y \rangle / N k_B T.$$  

Similarly, the two point correlation function as a function of distance is defined as

$$C_2(\mathbf{r}) = \langle \cdot \cdot \cdot \rangle - \langle \cdot \cdot \cdot \rangle \langle \cdot \cdot \cdot \rangle,$$

where $\hat{S}$ is the transformed spins and $\hat{r}$ is the position vector of the quadrupoles.

The quadrupoles (each one is similar to the quadrupole of a nitrogen molecule and has a value of -1.41D·Å) were simulated by placing an L×L (L=20, 60) array of quadrupoles in an anisotropic strength provided by the ionic lattice similar to the lattice of NaCl(001) with lateral periodic boundary conditions. The quadrupoles are constrained to the lattice sites at a definite polar angle $\theta$=29$^\circ$ to the plane lattice normal, the projections of the quadrupoles lie in the lattice plane and are allowed to azimuthally rotate within the plane of the lattice. The potentials consists of the potential U(\(\phi\)) provided by square lattice of the NaCl(001), which has a fourth-order symmetry and can be approximated by the hindered-rotation potential U(\(\phi\))=-2.4939-0.01096cos(4\(\phi\)). This equation is obtained by fitting the surface potential of N$_2$ molecule adsorbed on NaCl(001) surface as a function of $\phi$. The quadrupole–quadrupole interactions are performed in the similar way as discussed in reference [15].
3. Results

Our focus is to check the existence of an order–disorder phase transition and to investigate whether this phase transition belongs to XY- with cubic anisotropic universality class. The results of our Monte Carlo simulation show that the system of quadrupoles on ionic square lattice form an ordered structure with p(2×1) symmetry at low temperatures as shown in figure 1. As shown in figure 2, this structure undergoes an order–disorder phase transition into disorder (1×1) phase around 8.3K. In figure 3 the order parameter is plotted as a function of temperature for systems ranging from L=20 to L=60. The associated susceptibility, χ, is plotted in figure 4 as a function of temperature. The peak at 8.3K in the susceptibility coincides with a sharp drop in the order parameter and has features consistent with a continuous order- disorder phase transition at 8.3K.
In order to shed some light on the nature of the transition, we have analyzed the dependence of the correlation function on distance below $T_c$. If the transition is as that observed in the four-state clock model, the correlation function will have an exponential dependence on distance as described. However if the system is isotropic, the correlation function will have a power law dependence on distance. The two point correlation functions as function of distance at several values of temperature are obtained. Semi-log and log-log plots of the correlation function as a function of distance below and above the critical temperature are shown in figure 5 and figure 6 respectively. In the case of semi-log plots a reasonable straight line fit can be obtained for distances greater than 5 lattice spacing and less than half the system size (15 lattice spacing). It is obvious in the log-log plots of the correlation function that the data deviates from a straight line fit. At $T_c$ (8.3K), as shown in figure 6 the two-point correlation function show power law dependence on distance $C(r) \sim r^\eta$ where $\eta$ is calculated by fitting the log-log plot to straight line and is found to have a values ranged between 0.22 (for 5 spacing to 15 lattice spacing) and 0.255 (for one lattice spacing to 20 lattice spacing) depending on the number of lattice spacings considered in the fitting. The exponent $\eta$ at the critical temperature shows deviation from the Ising value of 0.25 [16] and indicate that this system may falls into the same universality class as the XY model with cubic anisotropy.
4. Conclusion
The two-point correlation functions show exponential dependence on distance both above and below the critical temperature \(T_c\), \(C(r) \sim \exp(-r/\xi)\) where \(\xi\) is the correlation length. This result is consistent with an ordering transition in a system with rotational anisotropy. At \(T_c\) (8.3K) the exponent \(\eta\) shows small deviation from the Ising value [15] of 0.25 and indicate that this system may falls into the same universality class as the XY model with cubic anisotropy. This model is applied to prototypical quadrupoles physisorbed systems as \(N_2\) on \(NaCl(100)\) [11,12].

References
[1] Kosterlitz J M and Thouless D J 1973 J. Phys. C: Solid State Phys. 6 1181
[2] Kosterlitz J M 1974 J. Phys. C: Solid State Phys. 7 1046
[3] Jose J V, Kadanoff L P, Kirkpatrick S and Nelson D R 1977 Phys. Rev. B 16 1217
[4] Abraham D B and Upton P J 2000 Phys. Rev. Lett. 85 2541
[5] De’Bell, MacIsaac, and Whitehead J 2000 Rev. Mod. Phys. 72 225
[6] Géza Ódor 2004 Rev. Mod. Phys. 76 663
[7] Lapilli C M, Pfeifer P and Wexler C 2006 Phys. Rev. Lett. 96 140603
[8] Park J H, Onoda S, Nagaos N, and Han J H 2008 Phys. Rev. Lett. 101 167202
[9] Yuri M 2011 arXiv preprint arXiv 1102 1085
[10] Poderoso F C, Arenzon J J and Levin Y 2011 Phys. Rev. Lett. 106 067202
[11] Sallabi A K and Jack D B 2000 Phys. Rev. B 62 4841
[12] Vogt J 2012 J. Chem. Phys. 137 174705
[13] Vu N -T, Jakalian A, and Jack D B 1997 J. Chem. Phys. 106 2551
[14] O. G. Mouritsen and A. J. Berlinsky, 1982 Phys. Rev. Lett. 48, 181
[15] O’Shea S F, Dubey G S and Rasaiah J C 1997 J. Chem. Phys. 107 237
[16] Back D H, Chung J W and Han W K 1993 Phys. Rev. B 47 8461