Phase transition of a Coulomb system on a lattice

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Abstract

A lattice half-filled with localised particles interacting via the long-range Coulomb potential is studied by numerical simulations. The temperature dependences of the specific heat and of the susceptibility related to the staggered occupation indicate the presence of a phase transition in two- and three-dimensional systems. The critical behaviour, obtained by a finite-size analysis, resembles that of the short-range Ising model.

Key words: phase transition; Coulomb glass; specific heat

The possible existence of a phase transition in the Coulomb glass has been under controversial debate for many years [1–4].

We approach this problem considering in a first step a lattice half-filled with localised particles which interact via the long-range Coulomb potential (without static disorder),

$$H = \frac{1}{2} \sum_{\alpha \neq \beta} \frac{(n_\alpha - 1/2)\,(n_\beta - 1/2)}{|\mathbf{x}_\alpha - \mathbf{x}_\beta|} \qquad (1)$$

where $n_\alpha \in \{0,1\}$ denote the occupation numbers of states localized at sites $\mathbf{x}_\alpha$. We simulate the behaviour of d-dimensional hypercubes of size L^d. To reduce finite size-effects, we impose periodic boundary conditions using the minimum image convention for $d = 1$ as well as for $d = 2$, and consider the sample to be surrounded by eight equally occupied samples for $d = 3$. Elementary charge, lattice spacing, dielectric and Boltzmann constants are all taken to be 1.

We have numerically investigated this model by means of the Metropolis procedure [5,6]. To reduce the problems arising from long correlation times we consider the following processes: one-electron exchange with the surroundings (corresponding to flipping a single spin in the Ising model), one-electron hops over resticted distance (two-spin flips), and two-electron hops modifying the occupation of four neighbouring sites (flips of clusters of four spins). At high temperature T, we use the original Metropolis procedure [5], whereas the calculations for low T are accelerated by utilizing the hybrid-Metropolis algorithm presented in Ref. [6].

The specific heat was determined according to $c(T) = (\langle H^2\rangle - \langle H\rangle^2)/(T^2\ L^3)$. Fig. 1 shows that sharp peaks evolve as L increases for the two- and three-dimensional cases. This points to the possible existence of a phase transition as it was observed in lattice gas simulations by Dickmann and Stell [7]. Such peaks are not observed for $d = 1$.

For the model considered here, the order can naturally be characterized by the staggered occupation in analogy to the description of an antiferromagnet. In the case $d = 3$, the staggered occupation is defined by

$$\sigma = (2n_\alpha - 1) \cdot (-1)^{x_\alpha + y_\alpha + z_\alpha} \qquad (2)$$

where x_α, y_α, and z_α denote the (integer) components of the site vector $\mathbf{x}_\alpha$. Again in analogy to the Ising model of a ferromagnet, the related susceptibility is given by

$$\chi = L^d(\langle\sigma^2\rangle - \langle|\sigma|\rangle^2)/T\ . \qquad (3)$$

Fig. 2 shows that also $\chi(T)$ exhibits sharp peaks increasing rapidly with L. This corroborates the presence of a phase transition.

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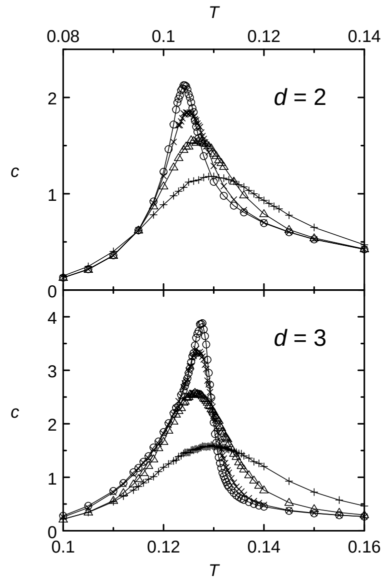

Fig. 1. Temperature dependence of the specific heat, $c(T)$, for samples of various size. $d = 2$: $L = 8$ (+), 14 (△), 24 (×), and 40 (○); $d = 3$: $L = 4$ (+), 6 (△), 10 (×), and 14 (○).

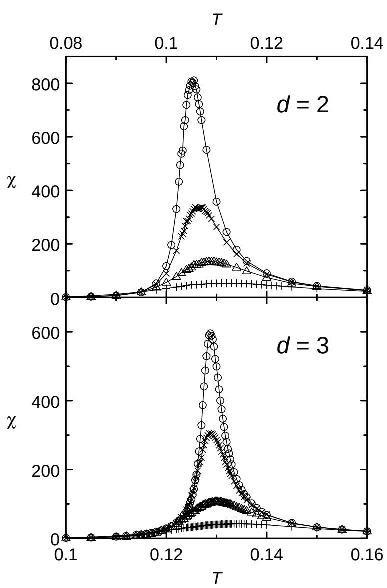

Fig. 2. Temperature dependence of the susceptibility, $\chi(T)$, for samples of various size. The symbols have the same meaning as in Fig. 1.

The critical temperature T_C of the phase transition is given by the limes $L \to \infty$ of the positions of the maxima of $c(T)$ and $\chi(T)$. It can be determined also by analysing the size dependence of the Binder cumulant [8]. Using both methods, we obtained $T_\mathrm{C} = 0.1032 \pm 0.0002$ for $d = 2$, and $T_\mathrm{C} = 0.1287 \pm 0.0004$ for $d = 3$.

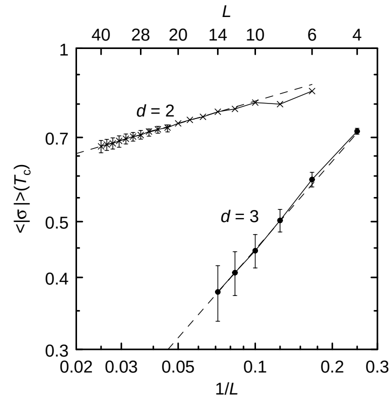

Fig. 3. Finite-size scaling of the order parameter at the critical temperature.

The finite-size scaling analysis of the value of the order parameter at the critical temperature, $\langle|\sigma|\rangle(T_\mathrm{C}, L)$, represented in Fig. 3, yields the ratio of the critical exponents β and ν, related to order parameter and correlation length, respectively. We have obtained the following values of this quotient: $\beta/\nu = 0.130 \pm 0.018$ for $d = 2$ and $\beta/\nu = 0.51 \pm 0.13$ for $d = 3$. These results coincide with the exponent ratios of the short-range Ising model, $1/8$ and 0.52 for $d = 2$ and 3, respectively; they differ clearly from the mean-field result $\beta/\nu = 1$ [9].

It is a surprising finding that, in spite of the long-range interaction, model (1) may belong to the same universality class as the short-range Ising model. This is supported by our detailed analysis of the critical properties which will be published elsewhere.

We thank T. Vojta for a valuable literature hint and critical discussions.

References

[1] E.R. Grannan, C.C. Yu, Phys. Rev. Lett. **71** (1993) 3335.

[2] T. Vojta, M. Schreiber, Phys. Rev. Lett. **73** (1994) 2933.

[3] F.G. Pikus. A.L. Efros, Solid State Commun. **92** (1994) 485.

[4] A. Díaz-Sánchez, M. Ortuño, A. Pérez-Garrido, E. Cuevas, phys. stat. sol. (b) **218** (2000) 11.

[5] N. Metropolis, A.W. Rosenbluth, M.N. Rosenbluth, A.H. Teller, E. Teller, J. Chem. Phys. **21** (1953) 1087.

[6] A. Möbius, P. Thomas, Phys. Rev. B **55** (1997) 7460.

[7] R. Dickman, G. Stell, cond-mat/9906364.

[8] *Applications of the Monte Carlo Method in Statistical Physics*, edited by K. Binder, in Topics in Current Physics, Vol. 36, (Springer-Verlag, Berlin, 1984).

[9] N. Goldenfeld, *Lectures on Phase Transitions and the Renormalization Group*, Frontiers in Physics, Vol. 85, (Wesley, Reading, 1992).