Phase transition of a Coulomb system on a lattice

Arnulf Möbius \textsuperscript{a,1}, Ulrich K. Rößler \textsuperscript{a}

\textsuperscript{a}Leibniz Institute for Solid State and Materials Research Dresden, PF 27 01 16, D-01171 Dresden, Germany

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 \cite{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),

\begin{equation}
H = \frac{1}{2} \sum_{\alpha \neq \beta} \frac{(n_\alpha - 1/2)(n_\beta - 1/2)}{|x_\alpha - x_\beta|} \tag{1}
\end{equation}

where \( n_\alpha \in \{0, 1\} \) denote the occupation numbers of states localized at sites \( x_\alpha \). 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 \cite{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 restricted 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 \cite{5}, whereas the calculations for low \( T \) are accelerated by utilizing the hybrid-Metropolis algorithm presented in Ref. \cite{6}.

The specific heat was determined according to

\begin{equation}
c(T) = \frac{\langle H^2 \rangle - \langle H \rangle^2}{T^2 L^3} \tag{2}
\end{equation}

where \( x_\alpha, y_\alpha, \) and \( z_\alpha \) denote the (integer) components of the site vector \( x_\alpha \). Again in analogy to the Ising model of a ferromagnet, the related susceptibility is given by

\begin{equation}
\chi = L^d (\langle \sigma^2 \rangle - \langle |\sigma| \rangle^2) / T \tag{3}
\end{equation}

Fig. 2 shows that also \( \chi(T) \) exhibits sharp peaks increasing rapidly with \( L \). This corroborates the presence of a phase transition.
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 $T_c = 0.1032 \pm 0.0002$ for $d = 2$, and $T_c = 0.1287 \pm 0.0004$ for $d = 3$.

The finite-size scaling analysis of the value of the order parameter at the critical temperature, $\langle |\sigma| \rangle(T_c/L)$, represented in Fig. 3, yields the ratio of the critical exponents $\beta$ and $\nu$, 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