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LETTER TO THE EDITOR

On the relation between the Coulomb gas and the lattice XY model†

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Abstract. By using Monte Carlo methods, we study the Coulomb gas in two dimensions. We focus our measurements in the regime in which an area law is expected. Our results confirm such a behaviour. We compare these results with those obtained for the vorticity in the lattice XY model: the comparison shows a sharp contrast in the behaviour of these two models. We conclude that, contrary to the common belief, the topological vortices of the XY model are not correctly described by a dilute Coulomb gas. Our results were obtained using an 8-node concurrent processor built at Caltech.

In this letter we present a Monte Carlo study of the dilute two-dimensional Coulomb gas and we discuss the implications of the results of this study for the two-dimensional XY model (Kosterlitz and Thouless 1974, Villain 1975, Jose *et al* 1977). Because the Coulomb interaction is infinite range, its direct Monte Carlo simulation is very time consuming and we had to use a concurrent processor. The details of the concurrent algorithm will appear elsewhere (Fucito and Solomon 1985).

The XY model is known to present a phase transition between an algebraic ordered phase and a disordered phase. A beautiful intuitive mechanism was proposed for this phase transition: the 'vortex liberation ansatz' (VLA) (Kosterlitz and Thouless 1974, Jose *et al* 1977, Villain 1975). The validity of this ansatz is difficult to check numerically by standard methods (Fox *et al* 1982, van Himbergen 1982, Swendsen 1978, Tobochnik and Chester 1979). Therefore, we proposed (Fucito and Solomon 1984) a measurement which checks more directly the basic elements of the ansatz. These basic elements are:

(i) below the critical temperature (T_c) the topological vortices appear only as pairs or neutral clusters; the density of the free vortices ρ_v is identically zero;

(ii) as the temperature increases above T_c, ρ_c increases in a continuous way from its zero value to finite values;

(iii) the effective interaction between vortices is of Coulomb type.

We reiterate briefly the results of Fucito and Solomon (1984). Let D be a lattice domain (much smaller than the lattice dimensions). Let its area be Aa^2 and its perimeter Pa (a is the lattice spacing). As the temperature increases from T_c toward $+\infty$, the 'VLA' states that the average number of free vortices inside D increases continuously from 0 to a number of the order of (but less than) A. Of course the term 'free vortex' is rather loose. Therefore we devised a quantitative criterion to handle this concept statistically.

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Let us consider the quantity

$$Q_D^2 = \left\langle \left(\sum_{r \in D} q(r) \right)^2 \right\rangle$$

where $q(r)$ is the vorticity on the plaquette r. A vortex pair will contribute to Q_D^2 when the frontier of D passes between the members of the pair. The probability for this to happen is proportional to P. The contribution is $+1$ or -1 depending on which member of the pair falls inside D. Therefore, the contribution of the pairs to Q_D^2 is obtained by considering a one-dimensional random walk with steps ± 1 and a length proportional to P. Accordingly

$$Q_{D_{\text{pairs}}}^2 \sim P.$$

A free charge will contribute to Q^2 when it is situated inside D. The probability for this to happen is proportional to A. Using a random walk reasoning as above one obtains

$$Q_{D_{\text{free}}}^2 \sim A.$$

This argument holds only when one can neglect screening effects, i.e. when the number of free vortices inside D does not exceed a few units, i.e. $\rho_v \leqslant O(1/A)$. However, since in the 'VLA' ρ_v increases continuously from $\rho_v(T_c) = 0$, for every domain D there is always a temperature range $T \in (T_c, T_D)$ for which the condition $\rho_v \leqslant O(1/A)$ is fulfilled. Above T_D, when the domain size becomes bigger than the Debye length (ξ^d), one expects a perimeter law again.

In Fucito and Solomon (1984) we measured Q_D^2 at different temperatures for families of domains D with equal perimeter and different areas. Our data did not show area dependence for any temperature and D range. We concluded that the 'VLA' is not supported by the Monte Carlo data. Accordingly we suggested some alternatives.

Our arguments in Fucito and Solomon (1984) about the existence of an area dependence region for the dilute Coulomb gas were not rigorous. Moreover, they were contrary to the pre-existing intuition acquired at scales larger than ξ^d. Therefore, in principle, the following alternative was still open: there is a Coulomb gas of free vortices in the neighbourhood above T_c such that for some domains $\rho_v \leqslant O(1/A)$, but a Coulomb gas does not contribute an area dependence of Q_D^2 in any range of temperatures and/or domains (this would presumably be due to the fact that in all practical computations ξ^d is much smaller than the considered domain).

In order to dismiss such a possibility, we performed the present Monte Carlo simulation of a two-dimensional Coulomb system. Because of the computer limitations we limited our objective to proving the existence of a range of parameters in which the Coulomb gas exhibits the area law: therefore all our results are for $T > T_c$ (we are presently collecting data in all the regions of the phase diagram). Our runs were performed on a 64×64 lattice (we have performed some short runs with 128×128 sites which indicate that the measurement of Q_D^2 is insensitive to finite volume effects).

We simulated a system with Boltzman weight:

$$\exp(-JE\{q(r)\}) = \exp\left[-J\left(\sum_r q^2(r) \ln \frac{L}{\varepsilon} - \sum_{r,r' \neq r} q(r) q(r') \ln \frac{d}{L} \right) \right] \tag{1}$$

where L is the linear dimension of the lattice, ε is related to the charge core energy, $J = 1/T$ is the inverse of the physical temperature and $d = |r - r'|$ is the distance between

the points r and r'. The variable q takes the value 0, ± 1. The action of (1) contains infinite range forces. If in equation (1) we define $v(r) = \Sigma_{r' \neq r} q(r') \ln(d/L)$, it can easily be realised that each time a charge $q(r)$ is updated, all the potentials $v(r')$ with $r' \neq r$ have to be updated too. Therefore on a sequential computer, the CPU time needed to perform the updating of a charge with an action like (1) grows linearly with the lattice volume. However, on a parallel machine (composed of many processors, each one residing at one corner of a hypercube) the CPU time grows like the volume of the sublattice contained in each processor (for more details see Fucito and Solomon (1985)): this makes the collection of good statistics more feasible than on sequential computers. All the processors run the same code and perform the same operations: a site r is addressed and (1) is computed for the three different values that $q(r)$ can assume. Using these values a new value for $q(r)$ is chosen by means of a heat bath algorithm: if $q^{\text{new}}(r) \neq q(r)$ (we cannot upgrade more than one charge at the same time, otherwise we would infringe the detailed balance prescription: the details of our upgrading procedure are discussed at length in Fucito and Solomon (1985)) all the $v(r')$ are updated simultaneously in each processor (this parallel updating of the $v(r')$ is what makes the parallel procedure extremely advantageous with respect to the sequential algorithm).

In order to have a dilute gas our parameters must be carefully chosen: for $\varepsilon/a \sim 100$ the density of pairs around T_c is much smaller than $1/a^2$. Therefore, the lattice artefacts are not important and the system is imitating correctly a continuous system. The area law for a family of domains of perimeter $64a$ and different areas is displayed in figure 1. The area dependence holds as long as the domains have dimensions smaller than ξ^d. As the domain dimensions increase beyond ξ^d, the dependence of Q_D^2 on the area decreases. For domains of size bigger than ξ^d the Q_D^2 graph saturates and approaches asymptotically a constant.

For $\varepsilon \sim a$ the system is a Coulomb crystal rather than a Coulomb gas and the lattice artefacts dominate the physics.

In order to achieve a desired statistical accuracy err we had to perform $O(\text{err}^{-2})$ measurements on independent configurations. We call the number of measurements between two independent configurations the autocorrelation time τ. τ characterises the speed with which our Monte Carlo procedure spans the configuration space, not the static thermodynamic properties of the system. Given a sequence $\{x_i\}_{i=1,N}$ of N measurements of a quantity x (total energy, domain charge, etc) we estimated the autocorrelation time by constructing the function

$$S(n) = \frac{\langle x_i x_{i+n} \rangle - \langle x \rangle^2}{\langle x^2 \rangle - \langle x \rangle^2}. \tag{2}$$

τ is then the biggest value of n for which

$$S(n) < (N - n - 1)^{-1/2}. \tag{3}$$

The bars in figure 1 represent only the statistical errors: τ was estimated to be around 20 (for total energy, τ was smaller).

Since we are not sweeping through the lattice but accessing the sites at random we measure the length of our runs by the number of individual site updatings. In general, performing 10^6 individual site updatings was enough for most values of ε and J. About a fifth of each run was allowed for equilibration and was discarded from the statistics. We checked that the rest of the run did not present any drift trend. In the region

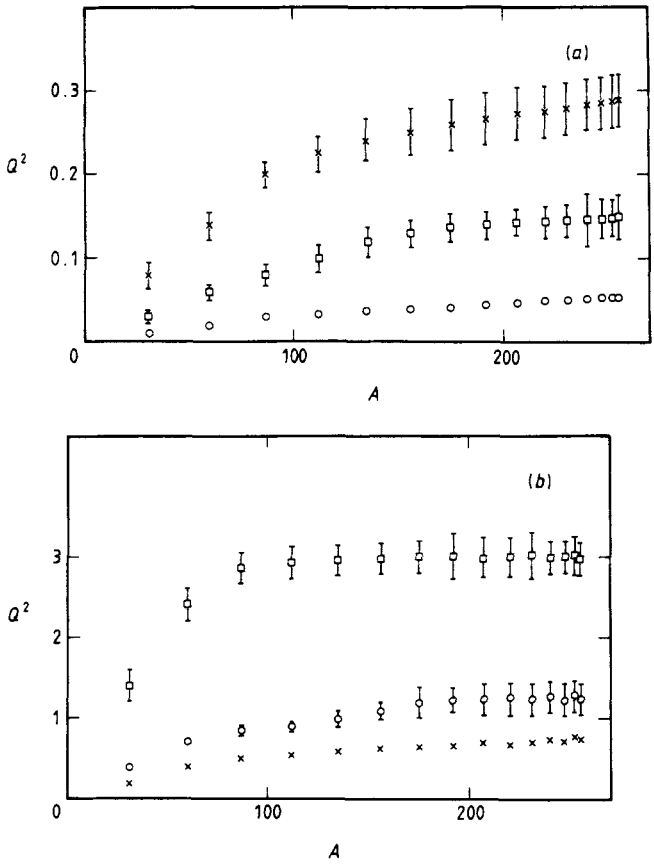

Figure 1. The dependence of Q^2 on the area for domains of perimeter 64*a*. (*a*) ○, $J = 1.2$, $\varepsilon = 0.01$; □, $J = 1.1$, $\varepsilon = 0.01$; ×, $J = 1.0$, $\varepsilon = 0.01$. (*b*) ×, $J = 0.9$, $\varepsilon = 0.01$; ○, $J = 0.8$, $\varepsilon = 0.01$; □, $J = 0.7$, $\varepsilon = 0.02$.

$\varepsilon/a \sim 1$ and large J one produces crystals of vortices and antivortices and much longer runs are necessary. Luckily this region of parameters is outside our present interest.

We performed one measurement every 1000 individual site updatings. In addition to Q_D^2 we measured the energy and the correlation between the values of the charges on different sites as a function of the distance between the sites. Unfortunately both the energy and the correlation function were too noisy to extract any conclusions. The data for Q_D^2, however, were quite nicely behaved. Q_D^2 was measured for few families of fixed perimeter domains. In figure 1 we have presented results for the family with the largest perimeter (64*a*). Similar plots hold for families of different perimeters.

Comparing figure 1 of this work with figure 1 of Fucito and Solomon (1984) we see that the topological charges of the XY model do not behave as a dilute gas of Coulomb charges. Indeed, the area dependence is present in the dilute Coulomb gas and absent in the XY case. This result may look surprising at first glance: in Jose *et al* (1977) and in many other works, it is rigorously proven that a type of XY model ('Villain') and the Coulomb gas are mathematically equivalent, i.e. their partition sums can be mapped one unto the other. There is a caveat though: the topological vortices of the Villain model (expressed in terms of periodic variables) are not mapped rigorously

onto the charges of the Coulomb gas formulation. The correspondence is only approximate and holds only in the low temperature region ($T \ll T_c$). At higher temperatures the topological vortices are not connected to the Coulomb charges anymore; therefore their interaction does not have to be Coulomb. Thus the fact that the topological vortices of the XY model do not behave as a dilute gas of Coulomb charges does not contradict any previously established rigorous result.

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