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TOWARDS A PRECISE DETERMINATION OF THE ORDER OF THE PHASE TRANSITION IN COMPACT PURE GAUGE QED

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We present results obtained with a new numerical method, which in principle allows to determine the partition function of a lattice gauge theory, and its derivatives, with an accuracy dictated only by statistical fluctuations. We have used this method in order to determine the order of the phase transition of pure gauge, compact QED and we have found that the height of the peak in the specific heat grows with the lattice size not faster than $L^{2.4\pm0.3}$ for $L \leqslant 10$.

The knowledge of the phase structure of lattice (gauge) theories is an essential ingredient for the understanding of their continuum limit, if it exists. This is why a large amount of human and computer time has been devoted to this subject.

In the case of non-abelian, asymptotically free gauge theories, which have an ultraviolet fixed point (like QCD), the renormalization group equations can be solved in perturbation theory, and in principle it is possible to check how the quantum continuum limit is approached on the lattice.

On the contrary, the abelian case, i.e. the prototype of QED, in spite of the enormous success of perturbative calculations in the continuum, is completely different, since perturbation theory breaks down at short distances, indicating that the continuum limit of compact QED on the lattice, if it exists, must correspond to some finite value of the coupling constant. As a consequence, perturbation theory is of no help in solving the RG equations, making evident the necessity of resorting to non-perturbative methods.

The phase structure of compact quantum electrodynamics has been studied both in the quenched [1–3] and unquenched [4,5] cases by means of Monte Carlo simulations. In the quenched case, a phase transition at $\beta = 1/g^2 \approx 1$ was found and the application of finite size scaling analysis to the results gave evidence of a second order character [1]. Later, a more extensive high statistics Monte Carlo calculation was performed and evidence was found for metastability in the vicinity of the phase transition [2]. This result was taken as an indication of the first order nature of the transition.

At present, however, it is generally accepted that metastability does not, by itself, signal the first order nature of the phase transition, since examples of second order transitions, with metastability near the critical point, have been produced [6]. Thus other methods, such as the study of the dependence of physical quantities on the lattice size, combined with finite size scaling arguments, have to be used in order to distinguish a (possibly) weak first order from a second order phase transition.

In this letter we report results for the mean plaquette energy and specific heat of numerical simulations of compact quenched QED with the standard Wilson action on 4^4, 6^4, 8^4 and 10^4 lattices. This simulation has been performed using a new method for computing physical quantities around transition points, which is in the same spirit of that used firstly by Falcioni et al. [7] to study the nature of the crossover phenomenon in the pure SU(2) model.

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The main advantage of this approach is that it takes into account all the (Monte Carlo) informations concerning the partition function at some fixed value of $\beta_0 = 1/g_0^2$ in order to reconstruct the vacuum expectation values of physical quantities in a $(\beta_0 - \epsilon) - (\beta_0 + \epsilon)$ interval, without performing any additional numerical simulation. This method is described in the following.

The lattice action for the compact U(1) gauge model is (p stands for plaquette)

$$S = -\beta \sum_{\mathrm{p}} \cos \theta_{\mathrm{p}}. \tag{1}$$

From this one can build the partition function

$$\mathscr{Z} = \int [\mathrm{d}\theta] \exp\left(\beta \sum_{\mathrm{p}} \cos \theta_{\mathrm{p}}\right), \tag{2}$$

where $[\mathrm{d}\theta]$ is the Haar measure for the gauge group U(1). The knowledge of the dependence of the partition function $\mathscr{Z}$ on β allows one to compute the vacuum expectation value of any physical quantity by performing the appropriate logarithmic derivative. For instance, the mean energy per plaquette can be written as

$$\bar{E}(\beta) = \langle \cos \theta_{\mathrm{p}} \rangle = \frac{\mathrm{d}}{\mathrm{d}\beta} (\ln \mathscr{Z}^{1/6V}) = \frac{1}{6V} \frac{\int [\mathrm{d}\theta] \sum_{\mathrm{p}} \cos \theta_{\mathrm{p}} \exp(\beta \sum_{\mathrm{p}} \cos \theta_{\mathrm{p}})}{\int [\mathrm{d}\theta] \exp(\beta \sum_{\mathrm{p}} \cos \theta_{\mathrm{p}})} \tag{3}$$

with V the hypercube lattice volume.

Let us consider some fixed $\beta = \beta_0$ value of the bare coupling constant. Then (3) can be written as

$$\bar{E}(\beta) = \langle \cos \theta_{\mathrm{p}} \rangle = \frac{\bar{E}_0(\beta)}{\mathscr{Z}_0(\beta)}, \tag{4}$$

where

$$\bar{E}_0(\beta) = \frac{1}{6V} \frac{\int [\mathrm{d}\theta] \sum_{\mathrm{p}} \cos \theta_{\mathrm{p}} \exp(\beta_0 \sum_{\mathrm{p}} \cos \theta_{\mathrm{p}}) \exp\{(\beta - \beta_0) \sum_{\mathrm{p}} [\cos \theta_{\mathrm{p}} - \bar{E}(\beta_0)]\}}{\int [\mathrm{d}\theta] \exp(\beta_0 \sum_{\mathrm{p}} \cos \theta_{\mathrm{p}})}, \tag{5}$$

$$\mathscr{Z}_0(\beta) = \frac{\int [\mathrm{d}\theta] \exp(\beta_0 \sum_{\mathrm{p}} \cos \theta_{\mathrm{p}}) \exp\{(\beta - \beta_0) \sum_{\mathrm{p}} [\cos \theta_{\mathrm{p}} - \bar{E}(\beta_0)]\}}{\int [\mathrm{d}\theta] \exp(\beta_0 \sum_{\mathrm{p}} \cos \theta_{\mathrm{p}})}. \tag{6}$$

Notice that thermodynamical functions, as functions of beta, can be expressed as logarithmic derivatives of $\mathscr{Z}_0(\beta)$, apart from a known additive constant.

A similar expression can be written for the specific heat.

Our numerical method consists in performing a numerical simulation of the model at a fixed value $\beta = \beta_0$, storing the plaquette energy of each equilibrium configuration, and finally computing the quantities (4)–(6) for in principle arbitrarily many values of β around β_0.

In the above expressions we have inserted the mean plaquette energy mainly to give an idea of the efficiency of the method. In fact one can expect good efficiency when the product $(\beta - \beta_0) \sum_{\mathrm{p}} [\cos \theta_0 - \bar{E}(\beta_0)]$ is not much larger than 1, which in turn implies $(\beta - \beta_0) \approx \alpha/\sqrt{V}$. The coefficient α is difficult to estimate, since it depends on β_0 and, near the transition, also on the lattice volume.

In practice, the method works as follows: first we estimate the position of the transition point (typically from standard numerical computations); next, we choose $\beta = \beta_0$ from the above estimate, thermalize the system starting from a cold initial configuration to avoid problems related to the presence of Dirac sheets, and compute, for instance, the average plaquette and specific heat in order to find a new value for β_0. We repeat this procedure until it becomes stable: typically we needed only two or three iterations on the lattices we have used. At the end, we have the behaviour (in β) of the thermodynamical quantities in the vicinity of the critical point β_0. Notice that no fitting of the thermodynamical functions is involved in this procedure, so that the only error in the determination e.g. of the phase transition point is due to statistical fluctuations.

To give an idea of the goodness of the method, let us consider the results on the average plaquette and specific heat in a 4^4 lattice. The transition point has been located around $\beta=0.98$ [1]. We have performed a simulation at $\beta_0=0.982$ using 38 000 configurations for evaluating $\mathscr{Z}_0$; for this lattice size we have also results from a long simulation, in which, following the method of ref. [8], but using also weighting functions, the partition function was computed and from it the thermodynamical functions. In figs. 1a and 1b the results ($\langle E_p \rangle$ and C_s) of these two different numerical methods are compared: we can see that in this β range the agreement is very good, especially noting that the results with our present method have been obtained in 2 hours of VAX 8650 CPU time, to be compared with 365 hours for the longer simulation.

Now let us consider the results for 6^4, 8^4 and 10^4 lattices. For these and larger lattice sizes, successive configurations are strongly correlated, especially in the vicinity of the transition. Notice that in this, as well as any other numerical methods, the efficiency depends critically on how well the physical fluctuations of the integration measure are reproduced; with long correlations any method becomes very inefficient.

In order to overcome this problem, we have used in our numerical calculations at $\beta=\beta_0$ the standard Metropolis algorithms, combined with a modified overrelaxation procedure.

This procedure is as follows: for each link, we change the link variable in such a way as to leave invariant its contribution to the action, while maximizing the distance from the original link in the group manifold. This is the standard procedure for continuous gauge groups. We however have discretized U(1) to Z(256); in this case the above procedure moves outside the group. We then choose for the new link the nearest Z(256) element and use a standard Metropolis algorithm to accept or reject the change. Obviously the acceptance rate is quite high (99%); notice also that this procedure never leads outside the U(1) in which Z(256) is embedded. In figs. 2a and 2b we present the plaquette energy as function of number of iterations for a 6^4 lattice at $\beta=1.00$, respectively without and with overrelaxation: it is quite evident the decrease of the period of the correlations.

We have used this method for the 6^4, 8^4 and 10^4 lattices, with 5 overrelaxation sweeps per Metropolis iteration. The histogram of the average plaquette in the 10^4 lattice is presented in fig. 3; the two peak structure clearly indicates that the system is fluctuating enough to allow the evaluation of the partition function and related quantities.

In fig. 4 we present our results for the specific heat. The transition points are located at $\beta_c=0.9794(5)$ (4^4), $\beta_c=1.0021(2)$ (6^4), $\beta_c=1.0072(2)$ (8^4), $\beta_c=1.0095(2)$ (10^4).

The above determinations of the specific heat in the lattices considered allows the study of the dependence of the height and location of the maximum on lattice size.

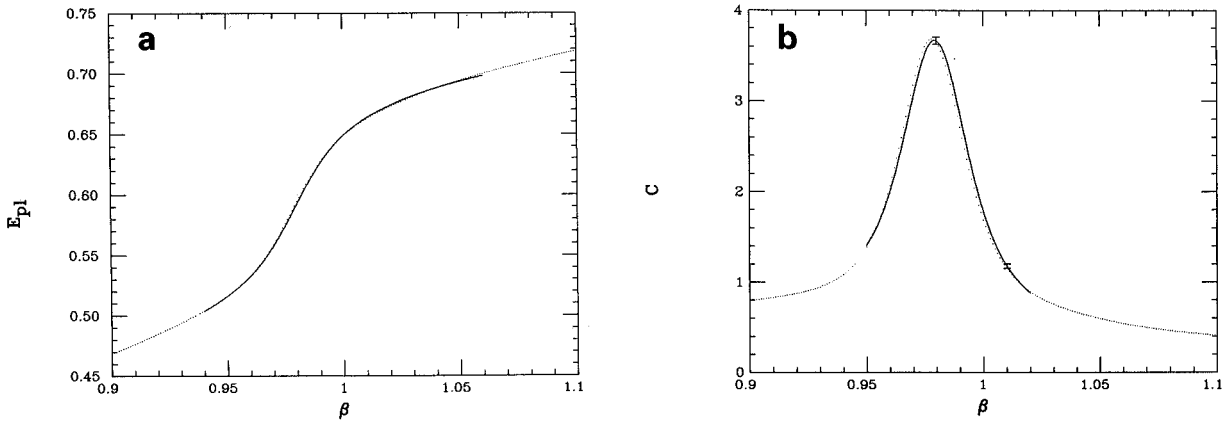

Fig. 1. Results for a 4^4 lattice. Continuous line: the present method; dotted line: results from a long standard simulation. (a) Average plaquette energy versus β (error bars are not visible at this scale). (b) Specific heat versus β.

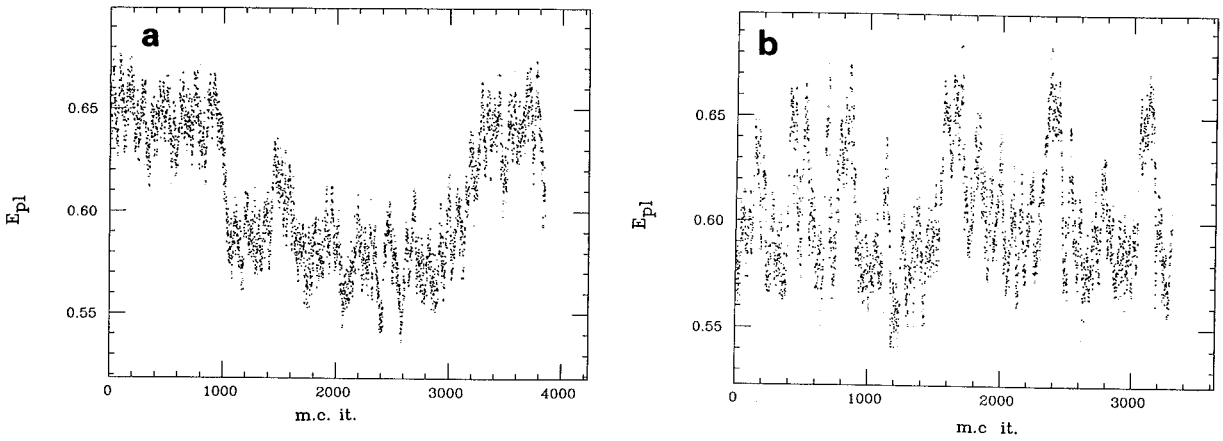

Fig. 2. Plaquette energy versus MC time in a 6^4 lattice. (a) Standard Metropolis algorithm. (b) Metropolis plus overrelaxation.

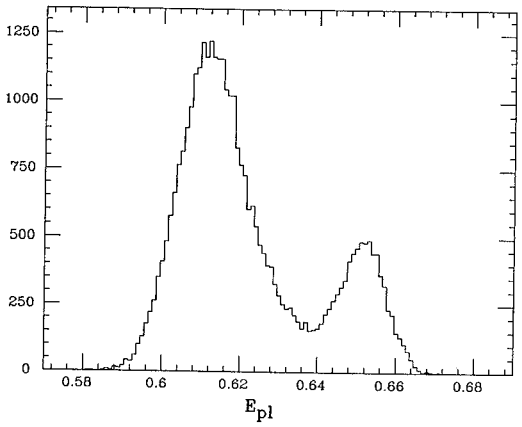

Fig. 3. Plaquette energy distribution in a 10^4 lattice at $\beta_0 = 1.009$.

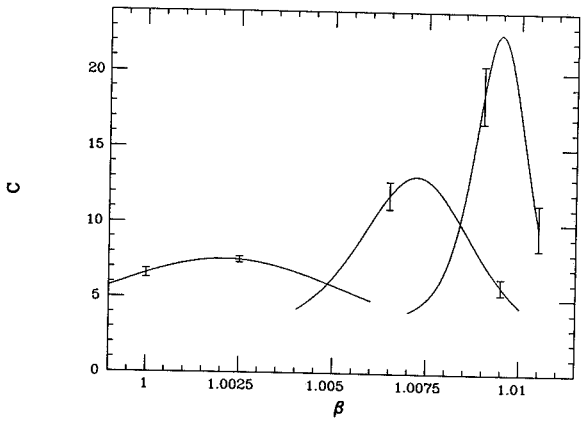

Fig. 4. Specific heat versus β in 6^4 (40 000 iterations, each consisting in 1 Metropolis plus 5 overrelaxations), 8^4 (33 500 iterations) and 10^4 (36 500 iterations) lattices.

Fig. 5 reports our data for the value of the maximum of specific heat h_c as a function of lattice size; the solid line is an interpolation with

$$h_c \sim L^{\alpha} \tag{7}$$

with $\alpha = 1.96$.

If we compute the exponent α using only the data from the two larger lattices [remember that eq. (7) holds in the large volume limit] we get $\alpha = 2.4(3)$.

On the other hand, from standard finite size scaling analysis we expect that the transition point shifts with increasing lattice size as

$$(\beta_c^{\infty} - \beta_c^{L}) \sim L^{-\gamma}. \tag{8}$$

From the results of the (6^4), (8^4) and (10^4) lattices we get $\beta_c^{\infty} = 1.0134(6)$ and $\gamma = 2.1(3)$.

These results have to be compared with the theoretical expectations for a first order transition ($\alpha = 4 = \gamma$).

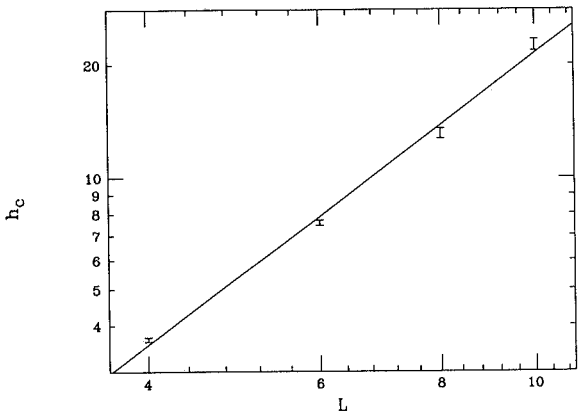

Fig. 5. h_c versus lattice size. The solid line is an interpolation of our data using eq. (7).

Our α and γ values suggest that we are not dealing with a first order phase transition. However, in principle we cannot exclude strong changes in the α and γ exponents when the lattice size increases.

A final remark is in order about the calculation of the errors. Error bars in the figures and in the β_c and h_c values reported here have been computed in the following way. We have typically run, after thermalization, 30 000–40 000 gauge sweeps with 5 overrelaxations per sweep and obtained the thermodynamical functions. Next we have grouped the Monte Carlo data at each β_0 in 8 sets computing for each set the same functions as before and checking that the content of the sets is large enough to give $\langle E \rangle$, β_c, h_c, $C(\beta)$ within statistical fluctuations (notice the nonlinearity of this approach). Then the reported errors are the standard deviation in these sets.

In conclusion, we have presented a method which in principle allows the determination of the functional form of the partition function of the theory on the coupling constant with an arbitrary precision. This will permit a precise analysis of the structure of abelian and nonabelian gauge models. We are running simulations on 14^4 and 18^4 lattices, and results will be published elsewhere.

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References

[1] B. Lautrup and M. Nauemberg, Phys. Lett. B 95 (1980) 63.
[2] J. Jersak, T. Neuhaus and P.M. Zerwas, Phys. Lett. B 133 (1983) 103.
[3] J. Bartholomew, J. Kogut, S. Shenker, J. Sloan, M. Stone, H. Wyld, J. Shigemitsu and D. Sinclair, Nucl. Phys. B 230 (1985) 149.
[4] V. Azcoiti, A. Cruz, E. Dagotto, A. Moreo and A. Lugo, Phys. Lett. B 175 (1986) 202.
[5] J.B. Kogut and E. Dagotto, Phys. Rev. Lett. 59 (1987) 617.
[6] Ape Collab., P. Bacilieri et al., Nucl. Phys. B 318 (1989) 553;
J.F. McCarthy, Indiana preprint IUHET 164 (1989).
[7] M. Falcioni, E. Marinari, M.L. Paciello, G. Parisi and B. Taglienti, Phys. Lett. B 108 (1982) 331.
[8] G. Bhanot, K.M. Bitar and R. Salvador, Phys. Lett. B 188 (1987) 246.