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G. Parisi: CORRELATIONS FUNCTIONS AND COMPUTER SIMULATIONS II

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ABSTRACT.

In this paper we show some efficient methods to compute correlations functions from computer simulations. Results are presented for the two-dimensional σ-model.

1. - INTRODUCTION.

In a previous paper of the same title[1] it was shown that in the framework of the Langevin equation[2] it is possible to compute the correlations functions in an indirect way using the fluctuation-dissipation theorem and a subtraction technique. Indeed if one consider a field theory characterized by an Euclidean action $A(\Phi)$ it is possible to construct the associated Langevin equation[2]:

$$\dot{\Phi}(x,t) = -\frac{\partial A}{\partial \Phi} + \eta(x,t) \,, \qquad \overline{\eta(x,t)\,\eta(x',t')} = 2\,\delta(x-x')\delta(t-t') \qquad (1)$$

where η is a white noise. The statistical correlations functions can be computed by a time average of the solution of the Langevin equation:

$$\langle \Phi(x)\,\Phi(y)\rangle = \lim_{\tau \to \infty} \frac{1}{\tau} \int_0^{\tau} \Phi(x,t)\,\Phi(y,t)\,dt \,. \qquad (2)$$

If one simulates the Langevin equation on a computer the statistical fluctuations in the time average are proportional to $1/\tau^{1/2}$ and this method is rather inconvenient for computing correlations functions at large distance, where the correlation is small. It was realized in ref. (1) that a more accurate method consistes in considering an action A_h dependent on an extra parameter h:

$$A_h(\Phi) = A(\Phi) + h f(\Phi) \,. \qquad (3)$$

An h dependent Langevin equation can be written:

$$\dot{\Phi}_h(x,t) = - \frac{\partial A}{\partial \Phi} + \eta(x,t) \,. \qquad (4)$$

From the dissipation fluctuation theorem we get:

$$\langle g(\Phi)\, f(\Phi)\rangle_c = \lim_{h \to 0} \overline{(g(\Phi_h) - g(\Phi_0))}/h \,. \qquad (5)$$

This method works better that the conventional one only if the statistical fluctuations in time of the r.h.s. of eq. (4) are much smaller than those of $g(\Phi)\, f(\Phi)$.

In ref. (1) it was shown that the method works very well for the field-field correlations functions in the free case or not too far from the free case; explicite computer simulations were reported for the one dimensional anharmonic oscillator. The results for two dimensional σ-model are presented in the Section 2 of this paper. In Section 3 we discuss the difficulties in extending this method to the energy-energy correlations. Finally in Section 4 we briefly discuss an alternative method for computing the correlation functions also of composite operators in theories like the Φ^4 interaction.

2. - THE NON LINEAR σ-MODEL.

The non linear σ-model is characterized by the following action

$$A(\sigma) = -\frac{1}{2}\,\beta\,\Sigma_{i,k}\,J_{ik}\,\sigma_i^a\,\sigma_k^a \qquad (6)$$

where the σ_i^a are unit vectors belonging to the n dimensional unit sphere $(\sum_1^n{}_a(\sigma_i^a)^2 = 1)$; in the simplest version of the model the index i runs over the points of a square lattice and the elements of the matrix J_{ik} are different from zero and equal to 1 only when i and k are nearest neighbour.

The associated Langevin equation is:

$$\dot{\sigma}_i^a = \beta\Sigma_k J_{ik}\sigma_k^a + \lambda_i\,\sigma_i^a + \eta_i^a \quad , \qquad \langle \eta_i^a(t)\,\eta_j^b(t')\rangle = 2\,\delta^{a,b}\delta_{i,j}\delta(t-t') \qquad (7)$$

where λ_i is a Lagrange multiplier which enforce the validity of the constraint and η_i^a is a white noise such that at $\beta = 0$ the spins describe a Brownian motion on the sphere.

In order to implement the Langevin equation on a computer, it is convenient to transform it in a finite difference eqaution by discretizing the time. If we call ε the time step we get:

$$\sigma_i^a(m+1) = \tilde{\sigma}_i^a(m+1)/\left[\sum_1^n{}_a(\tilde{\sigma}_i^a(m))^2\right]^{1/2} ,$$

$$\tilde{\sigma}_i^a(n+1) = \varepsilon\left[\delta^{ab} - \sigma_i^a(n)\,\sigma_i^b(n)\right]\left[\beta\,\Sigma_k J_{ik}\sigma_k^b + R_i^b\right] . \qquad (8)$$

$$\overline{R_i^b\,R_j^a} = (2 + c\,\varepsilon)/\varepsilon\,\delta_{ij}\delta_{ab} .$$

The parameter c is irrelevant in the limit $\varepsilon \to 0$, empirically we have found convenient to set $c = 2$ in order to decrease the dependence on ε for finite ε. We have verified that for this choice of a one finds the same results of standard Montecarlo simulations for $n = 3$. The algorithm is slower of a factor 2-3 compared to the one used in the Montecarlo simulations of ref. (3).

We have tried to compute the spin spin correlation functions for different temperatures, for $n = 3, 4, 5, 8$ on lattices of various dimensions ranging from 6×6 to 30×30. At this end we have defined the quantities

$$S(1) = \sqrt{\frac{n}{N}} \Sigma_r \sigma^1(1, r) \tag{9}$$

where r labels the rows of the lattice and 1 labels the columns (in an $N \times N$ lattice both 1 and r range from 1 to N). The correlation function $\langle S(1) S(1') \rangle$ can be easyly written in terms of the correlation function of simple spins:

$$\begin{aligned} &\langle S(1) S(1') \rangle = \Sigma_r G(1 - 1', j) \\ &\langle \sigma^a(1, j) \sigma^b(1', j') \rangle = \delta^{ab} G(1 - 1', j - j') \, . \end{aligned} \tag{10}$$

We have computed the expectation value of each of the S(1) in presence of extracontribution to the action equal to S(1). Typical values of h are 0 and 10^{-4}. Using eq. (5) we easyly obtain the correlation functions, the effects of the rounding error are expected to be of the order of 10^{-10} (we are working on a CDC 7600, a 60 bit machine). We have done runs with $\tau = 100$.

For $n = 3$ the results are deceiving, the results for the correlations functions are not better than the direct average. For $n \geq 4$ much better results are obtained: a typical example is shown in Figs. 1 and 2, where we plot the correlation function and their ratio for $\beta = 0.4$ and $n = 4$ on a 30×30 lattice.

How this results compare with Montecarlo? We have done 1000 upgradings of the spins, which corresponds to 1000 Montecarlo steps for spin. At the best we would have 10^6 different values for the correlations functions to average so that the statistical error would be 10^{-3}. The estimated error on the last correlation function we can see, is 10^{-9}; we have gained at least a factor 10^6 in precision which corresponds to a factor 10^{12} in time. Similar results are obtained at higher values of N and different value of β.

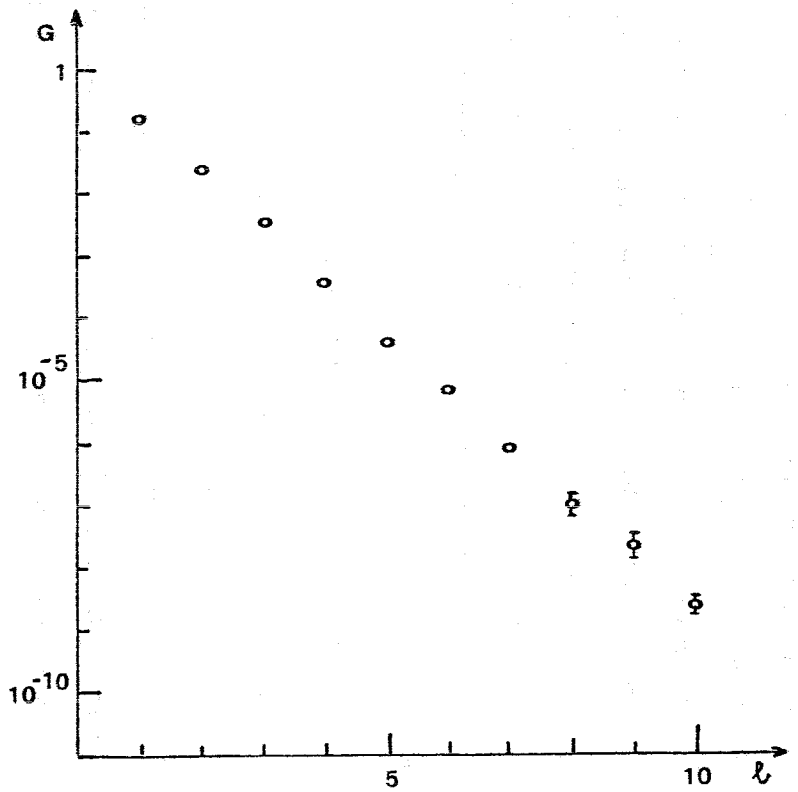

FIG. 1 - The $\langle S(1)\,S(1+l)\rangle$ correlation function in a logarithmics scale on a 30×30 lattice for $n = 4$, $\beta = 0.4$. The errors are only statistical.

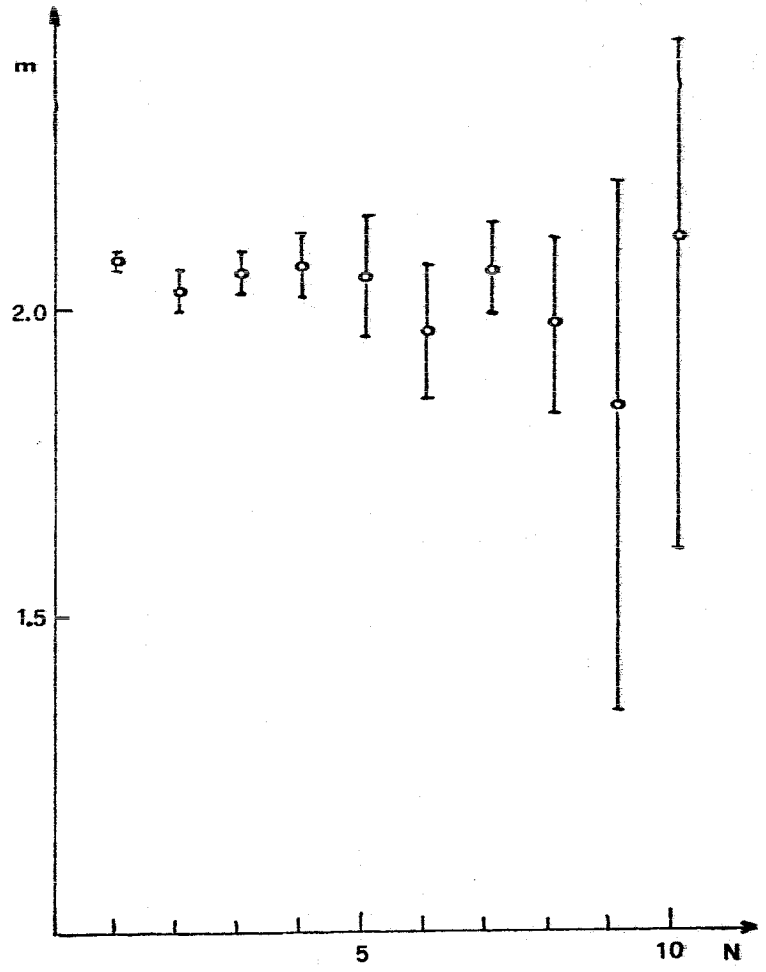

FIG. 2 - The function $m(l) = \ln \frac{\langle S(0)\,S(l-1)\rangle}{\langle S(0)\,S(l)\rangle}$. For large l we expect $m(l) \to m + 0(\exp(-2\,ml))$.

It is not easy to understand why the method does not work for $n = 3$. It is possible however to understand why it work for higher values of n. Indeed in the limit $n \to \infty$ the theory becomes the free one and the method work perfectly in the free case[1]. It is however surprising than going from $n = 3$ to $n = 4$ one gains a factor 10^6; an analytic study of this effect would be welcome.

The method can be applied without difficulties to non abelian gauge theories, at least for the SU(2) group. In the SU(3) case one should careful implement the unitarity constraint on the 3×3 matrices ; also the construction of the Brownian motion on the group is not so trivial[4] (the SU(2) group is isomorphic to the sphere, which is constant curvature manifold).

It is not clear if the results for SU(2) would be more similar to the O(3) or to the O(4) non linear σ-model.

3. - HIGH ORDER CORRELATION FUNCTIONS.

Very satisfacted with the results obtained in the previous section we have tried to use the method to compute the energy energy correlations functions (e.g. $\langle \sigma_1^a J_{1k} \sigma_k^a \; \sigma_1^b J_{1k'} \sigma_{k'}^b \rangle$). Unfortunately by doing explicite computations we have obtained results which at the best are only slightly better that these corresponding to the direct average; in this case the reason of the failure is very clear, but it is very difficult to remove. Asymptotically the correlation two spins decrease like $\exp - m|x|$, while the energy enérgy correlations functions should behave like

$$\exp(-2m|x|) + \langle \sigma \rangle^2 \exp(-m|x|). \qquad (11)$$

Now in a computer simulation the mean value of the magnetization ($\langle \sigma \rangle$) is a small non zero number also in absence of a magnetic field. This means that the signal is covered by a random noise which is leading at large distance. A similar (hopefully attenuated) disaster may happen if one tries to use this method to compute the

plaquette-plaquette correlation function; one would obtain a much larger contribution at large distance from the link-link correlation function. Indeed the link-link correlation function would be zero in a gauge invariant theory, however in doing a simulation the computer would take some time to realize that the theory is exactly gauge invariant. One can hope that as far as gauge invariance is a local symmetry, (compared to the global O(n) symmetry of the previous example) one would get a faster convergence to zero for non gauge invariant objects.

Coming back to the non linear σ model, it is clear that the same pathology is present if we try to compute a 4 spins correlation functions in spite of the fact that by successive differentiations we can extract the connected correlations functions. We should instead compute the one particle irreducible correlations functions.

In principle this can be done doing a Legendre transformation. In reality Legendre transformation is not easy to do unless we stay at zero external momentum.

4. - A DIFFERENT APPROACH.

It would be interesting to find an alternative method which does not suffer of the drawbacks described in the previous Section. This can be done in certain case for operators which are non singlect under the action of some group. We are not going to present computer simulations for this method, but we discuss it for compleateness.

Let us consider the case of an n components Φ^4 theory in continuum, the action being

$$A(\Phi) = \int \frac{1}{2} \sum_{1}^{n}{}_{i} (\partial_u \Phi_i)^2 + \frac{m^2}{2} \Sigma_i \Phi_i^2 + \frac{g}{2} (\Sigma_i \Phi_i^2)^2 \qquad (12)$$

Following Symanzik one easyly obtain [5]:

$$\langle \Phi_i(x)\, \Phi_j(y) \rangle = \int d\mu \left[\Phi, \sigma\right] \langle x \left| D^{-1} \right| y \rangle \delta_{ij} \qquad (13)$$

$$\langle \Phi_i(x)\,\Phi_j(x)\Phi_l(y)\,\Phi_m(y)\rangle = \int d\mu\,[\Phi,\sigma]\,\Big\{\,\big|\langle x|D^{-1}|y\rangle\big|^2\,\cdot$$

$$\cdot\,(\delta_{il}\delta_{jm}+\delta_{im}\delta_{jl}) + \langle x|D^{-1}|x\rangle\langle y|D^{-1}|y\rangle\,\delta_{ij}\delta_{ml}\Big\},$$

where $d\mu[\Phi,\sigma]$ is a measure normalized to 1 :

$$d\mu[\Phi,\sigma] \propto d[\Phi]\,d[\sigma]\,\exp\Big[-A(\Phi) - \int d^D x\,\frac{1}{2}\,\sigma^2(x)\Big] \qquad (14)$$

and D is the differential operator :

$$D = -\Delta + m^2 + g\sum_1^n{}_i\Phi_i^2 + (-g)^{1/2}\sigma\ . \qquad (15)$$

One should compute typical equilibrium configuration of Φ using the standard Montecarlo method and after computing the matrix elements of D^{-1} using a fast approximate method (e. g. a relaxation method)[6,7,8]. If $m^2 > 0$ the exponential decay of the two point correlation functions is authomatic. If one consider the correlation function of $(\Phi_i\,\Phi_j - \frac{1}{n}\,\delta_{ij}\,\Sigma_k\,\Phi_k^2) \equiv \Phi^2_{I=2}$ with itself (the isospin two combination) only the first term contributes (discontinued contributions are equal to zero for symmetry reasons). In this case one should obtain naturally that $\langle \Phi^2_{I=2}(x)\,\Phi^2_{I=0}(0)\rangle$ is near to $\langle \Phi(x)\,\Phi(0)\rangle^2$.

Of course we could also use this method to compute the correlation function $\langle \Phi(x)\,\Phi(0)\rangle$. Let us discuss the case $n = 0$ on the lattice, i. e. the so called self avoiding problem.

We get :

$$\langle \Phi_i(x)\,\Phi_j(0)\rangle = \delta_{ij}\,G(x)\ , \qquad (16)$$

$$G(x) = \int d[\sigma]\,\Big\langle x\Big|\frac{1}{-\Delta+m^2+ig^{1/2}\sigma}\Big|0\Big\rangle \exp -\int \frac{1}{2}\,\sigma^2(y)\,d^D y\ .$$

On the lattice the equivalent problem would consists (after rescaling) in finding the inverse D^{-1}_{lj} of the operator :

$$D_{lj} = -\beta J_{lk} + \delta_{lk}(1 + i g^{1/2} \sigma_l) \ , \qquad (17)$$

where J_{lk} connects only nearest neighbour points. Among the possible relaxation methods we can chose the one giving:

$$D^{-1}_{lk} = M_l \delta_{lk} + \beta M_l J_{lk} M_k + \beta^2 M_l J_{ln} M_n J_{nk} M_k + \cdots \qquad (18)$$

It is easy to see that if we stop the computation at the order β^k we have reproduced after the mean on σ, the first k orders of the high temperature expansion.

The method proposed may be usefull when the Lagrangian is quadratic in the fields or it can be reduced to a quadratic one by a simple transformation, so it is not apted for pure gauge theories.

No "very" efficient method has been found in this paper for computing the plaquette-plaquette correlation function. I hope that such a method exists and that it will be found by someone else.

I am very hapy to thank G. Martinelli and R. Petronzio; we have written together the computer program for Montecarlo simulations, which with the substitutions of only few cards, was used to simulate the Langevin equation.

REFERENCES.

1) G. Parisi, Correlations functions and computer simulations, Frascati preprint, to be published.
2) See for example G. Parisi and Wu Yong-Shi, Perturbation theory without gauge fixing, Scientia Sinica (1981).
3) G. Martinelli, G. Parisi and R. Petronzio, Phys. Letters B, to be published.
4) D. Dohrn and F. Guerra, Lett. Nuovo Cimento 22, 121 (1978).
5) K. Symanzik, Proc. of the Enrico Fermi School, Course XLV, ed by R. Jost (Academic Press, 1969).
6) D. J. Scalapino and R. L. Sugar, Phys. Rev. Letters 46, 519 (1981).
7) D. H. Weingarten and D. N. Petcher, Indiana preprint IUHET-61 (1980).
8) E. Marinari, G. Parisi and C. Rebbi, CERN preprint 3080 (1981).