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G. Parisi : CORRELATION FUNCTIONS AND COMPUTER SIMULATIONS.

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ABSTRACT.

If the equilibrium properties of a statistical system are obtained by solving numerically the associated Langevin equation describing the approach to equilibrium, the connected correlations functions can be computed directly with small effort and high precision.

1. - INTRODUCTION.

Computer simulation of statistical systems start to be popular also among high energy physicists[1]; they are mostly interested to compute the correlation length $\xi = m^{-1}$: if A(x) is a local operator one can prove that

$$\langle A(x)\,A(y)\rangle_c \equiv \langle A(x)\,A(y)\rangle - \langle A(x)\rangle\langle A(y)\rangle \longrightarrow$$
$$\longrightarrow \exp(-m_A |x-y|)/|x-y|^{\frac{D-1}{2}} \qquad (1)$$

where m_A is the minimum mass of the state created from the vacuum by the operator A; the power law in the prefactor is correct only if the minimum mass state is a one-particle state[2].

In order to extract the value of the mass from the connected correlations functions and to compute the mass spectrum, it is necessary to control the correlation function at large $|x-y|$, i.e. in the region

where it is small. This fact is particularily sad; a typical Montecarlo simulation[1,2] has a random statistical error proportional to $N_T^{-1/2}$, N_T being the total number of extractions, in many physically interesting cases, in particular gauge theories, it is impossible to give reasonable extimates of the mass, also using very high statistics.

In this paper I present a new algorithm which allows the direct computation of connected correlation functions for continuous systems, the algorithm being based on the Langevin equation. I have not done a systematic study of the advantages presented by this new algorithm: after the description of the method (Section 2) I present the results which I have obtained in some simple casess (Section 3). The difficulties in extending this method to more interesting cases are briefly discussed in Section 4.

2. - THE LANGEVIN EQUATION FOR CORRELATION FUNCTIONS.

Let us consider a statistical system, with Hamiltonina $H[\phi]$; ϕ_i $(i = 1, N)$ being N continuous variables. The equilibrium expectation value of a function $f[\phi]$ is given by:

$$\langle f[\phi] \rangle = \int d[\phi] \exp(-H[\phi]) f[\phi] \Big/ \int d[\phi] \exp(-H[\phi]) . \qquad (2)$$

For semplicity we have set $\beta = (KT)^{-1} = 1$.

A practical way of computing $\langle f[\phi] \rangle$ is based on the Langevin equation[3]:

$$\dot{\phi}_i = - \frac{\partial H}{\partial \phi_i} + \eta_i(t) \qquad \langle \eta_i(t)\, \eta_j(t) \rangle = 2\, \delta_{ij}\, \delta(t - t') \qquad (3)$$

$\phi_i(t)$ being a function of the "time" t and $\eta_i(t)$ being a random gaussian variable. Indeed we have:

$$\langle f[\phi] \rangle = \lim_{\tau \to \infty} \frac{1}{\tau} \int_0^{\tau} dt\, f[\phi(t)] , \qquad (4)$$

where $\phi(t)$ is the solution of eq. (3) for a given random choice of η.

Eqs. (3, 4) are a practical tool to compute the statistical expectation value, alternative to the standard Montecarlo technique.

Before actually solving eq. (3) we must discretize the time:

$$\phi_i^{k+1} = - \varepsilon \frac{\partial H}{\partial \phi_i} \left[\phi^k\right] + \sqrt{2\varepsilon}\, R_i^k \quad , \tag{5}$$

where we have set $t = \varepsilon k$ and the R_i^k are gaussian random variables:

$$\langle R_i^k R_{i'}^{k'} \rangle = \delta^{kk'} \delta_{ii'} \ . \tag{6}$$

The computer time is proportional to ε^{-1} and the errors on the final result are proportional to ε. If accurate results are needed, this procedure is slower that the standard Montecarlo: the time discretized Langevin equation is very similar to the Montecarlo method with small steps proportional to $\varepsilon^{1/2}$.

From the fluctuation-dissipation theorem we know that:

$$\langle \phi_i \phi_j \rangle_c = \frac{d}{d\lambda} \langle \phi_i \rangle_\lambda \Big|_{\lambda = 0} \ , \tag{7}$$

where $\langle \phi \rangle_\lambda$ is computed with the Hamiltonian $H_\lambda = H - \lambda \phi_j$. We can introduce the λ-dependent Langevin equation[6]:

$$\dot{\phi}_i(t, \lambda) = - \frac{\partial H}{\partial \phi_i} + \lambda \delta_{ij} + \eta_i(t) \ . \tag{8}$$

Expanding $\phi_i(t, \lambda)$ in powers of λ ($\phi_i(t, \lambda) = \phi_i^{(0)} + \lambda \phi_i^{(1)} + \frac{\lambda^2}{2} \phi_i^{(2)} + \cdots$) and identifying the terms we get:

$$\begin{aligned} &\dot{\phi}_i^{(0)} = - \frac{\partial H}{\partial \phi_i} + \eta_i(t) \ , \qquad \dot{\phi}_i^{(1)} = - \frac{\partial^2 H}{\partial \phi_i \, \partial \phi_l} \phi_l^{(1)} + \delta_{ij} \ , \\ &\dot{\phi}_i^{(2)} = - \frac{\partial^2 H}{\partial \phi_i \, \partial \phi_l} \phi_l^{(2)} - \frac{\partial^3 H}{\partial \phi_i \, \partial \phi_l \, \partial \phi_n} \phi_l^{(1)} \phi_n^{(1)} \ , \end{aligned} \tag{9}$$

where H and its derivatives are computed as functions of $\phi^{(0)}$ only.

We finally get :

$$\langle \phi_i \phi_j \rangle_c = \lim_{\tau \to \infty} \frac{1}{\tau} \int_0^\tau \phi_i^{(1)}(t)\, dt \ ,$$
$$\langle \phi_i \phi_j \phi_j \rangle_c = \lim_{\tau \to \infty} \frac{1}{\tau} \int_0^\tau \phi_j^{(2)}(t)\, dt \ . \qquad (10)$$

Similar expressions can be obtained for higher orders correlations functions.

We have found a direct method to compute the correlation functions ; this method cannot be implemented in the standard Montecarlo approach : we have used in an essential way the fact that the trajectory is a continuous (analytic) function of the force ; that property does not hold in Montecarlo simulations, where the force controls a probability factor which gives a yes-no answer. In the next Section we shall see the application of this method to simple examples.

3. - SOME EXAMPLES.

The simplest example we can think about is free field theory : the Hamiltonian is :

$$H = \frac{1}{2} \int d^D x \left[m^2 \phi^2(x) + (\partial_\mu \phi)^2 \right] \ , \qquad (11)$$

the field being defined on a D dimensional space.

The equations for $\phi^{(0)}$, $\phi^{(1)}$ and $\phi^{(2)}$ are respectively :

$$\dot{\phi}^{(0)}(x,t) = -(-\Delta + m^2)\, \phi^{(0)}(x,t) + \eta(x,t) \langle \eta(x,t)\ \eta(x't') \rangle =$$
$$= 2\, \delta^D(x - x')\, \delta(t - t') \ ,$$
$$\dot{\phi}^{(1)}(x,t) = -(-\Delta + m^2)\, \phi^{(1)}(x,t) + \delta^D(x) \ , \qquad (12)$$
$$\dot{\phi}^{(2)}(x,t) = -(-\Delta + m^2)\, \phi^{(2)}(x,t) \ .$$

The solution of the last two equations is trivial in momentum space:

$$\phi^{(1)}(k,t) = n\left[1 - \exp(-t(k^2+m^2))\right]/(k^2+m^2)\,,$$
$$\phi^{(2)}(k,t) = 0\,. \tag{13}$$

The boundary conditions $\phi^1(x,0) = \phi^2(t,0) = 0$ have been imposed. The same asymptotic result for $\tau \to \infty$ is obtained also if we discretize the time.

Generally speaking in the method here proposed the equation for the connected correlations functions are deterministic if the Hamiltonian is Gaussian: the convergence is therefore very fast: no random errors are present.

Let us consider an interacting case:

$$H = \int dx^D \left[\frac{m^2}{2}\phi^2(x) + \frac{1}{2}(\partial_\mu \phi)^2 + \frac{g}{4}\phi^4\right],$$
$$\phi^{(0)}(x,t) = -(-\Delta + m^2)\phi^{(0)}(x,t) + g(\phi^0(x,t))^3 + \eta(x,t)\,, \tag{14}$$
$$\phi^{(1)}(x,t) = -(-\Delta + m^2)\phi^{(1)}(x,t) + 3g(\phi^0(x,t))^2\phi^{(1)}(x,t) + \delta^D(x)\,.$$

The equations are very simple if we substitute $\langle\phi^{(0)2}\rangle$ to $(\phi^{(0)}(x,t))^2$ in the last equation we get the Hartree-Fock approximation.

We notice that for m^2 positive, the second derivative $\frac{\delta^2 H}{\delta\phi(x)\,\delta\phi(y)}$ is a positive operator and an absolute bound on $\phi^{(1)}(x,t)$ can easily obtained. The method may fail (although I do not believe that it fails) when m^2 is negative; $\phi^{(1)}(x,t)$ may oscillate and become larger and larger increasing the time and the limit $\tau \to \infty$ in eq. (10) may not exist; this problem deserves a more accurate study.

In order to verify the efficiency of the method I have done a very simple test. I have considered an one-dimensional system, the Hamiltonian is:

$$H = \sum_{1}^{N}{}_{i} \left(\frac{\phi_i^4}{4} + 4(\phi_i - \phi_{i+1})^2 \right) , \qquad (15)$$

periodic boundary conditions have been imposed, N has been taken equal to 98.

Computer simulations of eqs. (5, 6) have been done in two cases:

$$\begin{aligned} &\text{a)} \quad \varepsilon = 0.01 , \qquad \tau = 500 ; \\ &\text{b)} \quad \varepsilon = 0.0025 , \qquad \tau = 125 . \end{aligned} \qquad (16)$$

The results for the correlation function as function of the distance are shown in Fig. 1 for case b. The typical statistical error is of a few percent, the systematic error is proportional to ε. Going from case a to case b the correlations functions change of about 10%, so also the systematic error can be estimated in the few percent range.

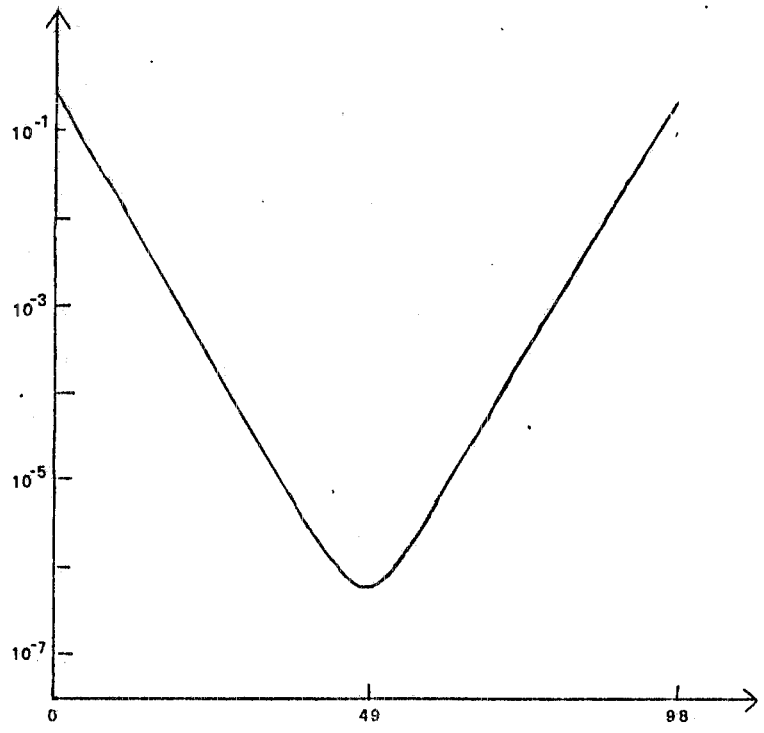

FIG. 1 - The correlation function $\langle \phi(c)\, \phi(k) \rangle$ as function of the distance i-k. The periodic boundary condition implies the invariance under the transformation i-k $\longrightarrow$ N - (i-k) ; (N = 98).

As a check of the consistency of the approach, I have computed $\langle \phi^0(x)^2 \rangle$ and $\langle \phi^1(0) \rangle$, these two quantities must coincide in the limit $\varepsilon = 0$. I have found:

$$\text{a)} \quad \langle \phi^{(0)}(x)^2 \rangle = 0.245 \pm 0.002 \,, \quad \langle \phi^{(1)}(0) \rangle = 0.218 \pm 0.002 \,,$$
$$\text{b)} \quad \langle \phi^{(0)}(x)^2 \rangle = 0.234 \pm 0.004 \,, \quad \langle \phi^{(1)}(0) \rangle = 0.232 \pm 0.006 \,. \tag{17}$$

The error being purely statistical. We clearly see that in case a the two results do not agree, while in case b good agreement is found.

In cases a and b the mass is estimated to be 0.285 and 0.289 respectively.

4. - OPEN PROBLEMS.

If the method I propose gives good results also for higher dimensional systems, it would be rather interesting to extend it to both to discrete system, as the Ising model, and to constrained systems like the non linear σ-model or gauge theories.

Generally speaking it is impossible to extend the method to a general discreate system, the continuity and the differentiability of the time evolution being a prerequisite for applying this method. However in simple cases, like the Ising model, something can be done: indeed the partition function of the Ising model can be written as[8]:

$$\sum_{\{\sigma = \pm 1\}} \exp\left[\beta \frac{1}{2} \sum_{i,k} \sigma_i \sigma_k V_{ik}\right]$$
$$= \int d\phi_i \exp\left[-\frac{\beta}{2} \sum_{i,k} \phi_i \phi_k V_{ik} + \sum_i \ln \operatorname{ch}\left(\sum_k \beta V_{ik} \phi_k\right)\right],$$

$$\langle \sigma_i \rangle = \langle \operatorname{ch}\left(\sum_k \beta V_{ik} \phi_k\right) \rangle \,, \tag{18}$$

$$\langle \sigma_i \sigma_j \rangle = \langle \operatorname{ch}\left(\sum_k \beta V_{ik} \phi_k\right) \operatorname{ch}\left(\sum_l \beta V_{jl} \phi_l\right) + \delta_{ij} \operatorname{ch}^{-2}\left(\sum_k \beta V_{ik} \phi_k\right) \rangle \,.$$

The correlation functions of the σ spins can be easyly reconstructed from the correlations functions of ϕ fields, which may be computed using the method here proposed.

The evolution equation for ϕ is

$$\dot{\phi}_i = - \Sigma_k V_{ik} \left[\phi_k - \mathrm{ch}\left(\Sigma_l \beta V_{kl} \phi_l \right) \right] + \eta_i \langle \eta_i(t) \eta_k(t') \rangle = \tag{19}$$

$$= 2 \delta_{ik} \delta(t - t')/\beta \ .$$

If we neglect the noise term (η_i) we recover the mean field equations.

Unfortunately this operation of substituting a discrete variable with a continuous one can easily done only if the interaction is quadratic. Serious difficulties would be present in an Ising model with a 4-spins interaction.

For constrained systems, if the above described trick does not work, we have many possibilities, whose respective advantages and disavantages unclear to me, the simplest one consisting in replacing the delta function of the constraint with a strongly peaked functions. This question deserves more investigations.

An other problem comes from the Langevin equation itself: in order to simulate it on a computer we must discretize the time, introducing a non zero ε; in the algorithm described in the previous Section the error is proportional to ε; there are algorithms for which the error is of order ε^2 but they are rather complicated. In reality we need only that the error on the asymptotic behaviour is small: we are not interested to know with high precision the time dependence of the solution of the Langevin equation. In order to reach thermodynamic equilibrium we need to enforce the detailed balance principle for the transition probabilities $P(x, x')$:

$$\exp - H(x)\, P(x, x') = P(x, x') \exp - H(x) \ , \tag{20}$$

as can be seen from the corresponding master equation[9].

For example in the one dimensional case we can write the equation:

$$\phi^{(k+1)} - \phi^{(k)} = - \varepsilon \frac{\partial H}{\partial \phi} C(\phi) + S(\phi) \sqrt{2\varepsilon} R^{(k)} , \tag{21}$$

where the corrections factors ($C(\phi)$ and $S(\phi)$) are chosen in such a way to enforce the detailed balance at the order ε^2.

Possible choices are:

$$C(\phi) = 1 + \frac{\varepsilon}{2} \frac{\partial^2 H}{\partial \phi^2} , \qquad S(\phi) = 1 ; \qquad \text{or}$$
$$C(\phi) = 1 , \qquad S(\phi) = 1 - \frac{\varepsilon}{4} \frac{\partial^2 H}{\partial \phi^2} . \tag{22}$$

In the quadratic case ($H = \frac{1}{2} m^2 \phi^2$) the recurrence equation would be:

$$\phi^{(k+1)} - \phi^{(k)} = - A \phi^{(k)} + \sqrt{2\varepsilon} B R^{(k)} , \tag{23}$$

where A and B are given by the condition:

$$A - \frac{A^2}{2} = m^2 \varepsilon B^2 \tag{24}$$

No solutions are found for $B = 1$ if $m^2\varepsilon > 1$. It would be interesting to extend this procedure to the general case in an efficient way, bypassing the condition $m^2\varepsilon < 1$. This step may be crucial if we want to replace the constraints by a stiff potential.

It is also possible to avoid the introduction of the constraint and to write directly the Langevin equation on the constrained system.

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(6) - This approach is very similar to the technique of ref. (7) for computing time dependent correlation function in the molecular dynamics approach; their method fails to compute static correlation functions, the time evolution of the system being ergodic.

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(9) - See for example the discussion in K. Binder, Montecarlo Methods, ed. by K. Binder (Springer, 1979).