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NUMERICAL CALCULATIONS IN QUANTUM FIELD THEORIES

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Numerical Calculations in Quantum Field Theories

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LECTURE NOTES

Contents

First Lecture

Quantum field theories in continuous space-time.

Dynamical variables are matter fields, such as scalar fields $\phi_i(x)$, $\bar{\phi}_i(x)$ and spinor fields $\psi_{si}(x)$, $\bar{\psi}_{si}(x)$, and gauge fields $A_\mu(x)$. i denotes indices labelling internal degrees of freedom, s is a spinor index.

The gauge field strength is

$$F^i_{\mu\nu}(x) = \partial_\mu A^i_\nu(x) - \partial_\nu A^i_\mu(x) + g f_{ijk} A^j_\mu(x) A^k_\nu(x)$$

If τ^i are infinitesimal generators of the algebra then f_{ijk} is defined by

$$[\tau^j, \tau^k] = - f_{ijk} \tau^i .$$

g is the coupling constant.

Throughout the lectures we shall use units with $\hbar = c = 1$.

The gauge potential is used to define gauge invariant couplings between matter fields at different space-time locations.

These are given by expressions of the type

$$\bar{\psi}(y)\ P\ e^{ig \int_{x,\gamma}^{y} A_\mu{}^i \tau_i\, dx^\mu} \psi(x),$$

where the integration is along some path γ joining the points x and y, the exponential is path ordered and the internal indices of the matter fields have been omitted. The matter fields belong to the representation of the gauge group for which the τ_i are infinitesimal generators.

The action of the gauge field is given by

$$S = \frac{1}{4} \int d^4x\, F^i_{\mu\nu} F^{\mu\nu}_i .$$

The total action contains also a term involving the matter fields; it turns out however that some of the most important dynamical features of the systems we shall be considering are determined by the gauge part of the action and we shall concentrate therefore on the quantum mechanical properties of a gauge system per se. Considerations involving the matter field part of the action will be presented in fourth lecture.

Vacuum expectation values (or quantum averages) of observables O are expressed through functional integrals in Euclidean space-time, after a Wick rotation $t \to it$ has been performed. (Relevant quantities are analytically continued back to Minkowski space-time, if neccessary, at the end of the computations).

$$\langle O \rangle = \frac{\int \mathcal{D}A \, O(A) \, e^{-S(A)}}{\int \mathcal{D}A \, e^{-S(A)}}$$

Numerator and denominator in the above formula must be given precise mathematical meaning. This is achieved by the process of regularization, which relies on a perturbative expansion

$$\int \mathcal{D}A \, e^{-S} = \int \mathcal{D}A \, e^{-A^2 - gA^3 - g^2A^4} =$$

$$= \int \mathcal{D}A \, e^{-A^2} (1 - gA^3 - g^2A^4 \ldots\ldots) .$$

The regularization requires the introduction of a cut-off parameter M

$$\langle O \rangle = \langle O \rangle (g, M) = O_0 + gO_1 + g^2 O_2 \cdots$$

Eventually a renormalization is performed: the cut-off parameter M is sent to infinity with $g = g(M)$ so that O tends to a well defined limit.

The whole procedure may be invalidated if one needs to study phenomena which are governed by intrinsically large values of the coupling constant or, at an even more fundamental level, if the observables under investigation are given by expressions with an essential singularity at $g = 0$, e.g.

$$\langle O \rangle = M \, e^{-\frac{\text{const}}{g^2}} (1 + O(g))$$

The lattice formulation achieves a non-perturbative regularization.[1,2] The continuum of points in space-time is replaced by the discrete set of vertices of a generally hypercubical lattice[3]

We shall denote by x the integer valued coordinates of the lattice, by symbols $\hat{\mu}$, $\hat{\nu}$ unit displacements in the μ, ν direction and by a the length of the lattice spacing.

Matter fields $\varphi_x, \bar{\varphi}_x, \psi_x, \bar{\psi}_x$ are associated with the vertices of the lattice. The gauge fields, which are now finite elements U_x^μ of the gauge group, are associated with the oriented links of the lattice.

(U_x^μ is defined on the link with origin in x and end point in $x + \hat{\mu}$).

They reduce to exponentiated potentials in the limit of very small lattice spacing

$$U_x^\mu \approx e^{i g A_\mu^i a \tau_i} .$$

Of particular importance are plaquette variables, defined as follows

$$U_x^{\mu\nu} \text{ (or } U_\square) = U_x^\nu U_{x+\nu}^\mu U_{x+\mu}^{\nu\dagger} U_x^{\mu\dagger}$$

which reduce to exponentiated field strengths in the continuum limit

$$U_x^{\mu\nu} \approx \exp i g F_{\mu\nu}^i a^2 \tau_i .$$

The action is defined through the plaquette variables. One constructs first an "internal energy"

$$E_\square = 1 - \mathrm{Tr}\, U_\square ,$$

where the trace is suitably defined and normalized. $E_\square$ is always larger or equal to 0 and equals zero if the plaquette variable reduces to the identity. In the continuum limit

$$E_\square \approx g\, a^4\, F^2 ;$$

this motivates the definition of the lattice action (of the pure gauge field)

$$S = \frac{\text{const}}{g^2} \sum_\square E_\square .$$

Because of an analogy with statistical mechanics, the quantity $\frac{\text{const}}{g^2}$ is very frequently denoted by β. We shall refer to g as the coupling constant, to β as the coupling parameter.

The expectation value of the observables are now given by multiple integrals over the gauge manifolds. If one restricts the system to a finite volume V, which is let to infinity only at the end of the calculation, the expressions for the quantum averages are mathematically well defined, independently of any perturbative expansion.

$$\langle \mathcal{O} \rangle = \frac{\int \prod_{x,\mu} dU_x^\mu \; \mathcal{O}(U)\, e^{-S(U)}}{\int \prod_{x,\mu} dU_x^\mu \; e^{-S(U)}}$$

The following examplifies the definition of the lattice gauge system in the two cases where the gauge group is the discrete group Z_2 or the group U(1).

If the group is Z_2 the link variables U_x^μ can be represented by ± 1, the group operation being ordinary multiplication. The plaquette variables are then also either +1 or −1. With a terminology taken from the theory of spin glasses, one says that the plaquettes for which $U_\square = -1$ are frustrated. As internal energy we may define

$$E_\square = 1 - U_\square \; .$$

$E_\square$ takes value 0 for a non-frustrated plaquette, 2 for a frustrated one. The total action

$$S = \frac{1}{g^2} \; \Sigma_\square E_\square \equiv \beta \; \Sigma_\square E_\square$$

equals then $\frac{2}{g^2}$ (or 2β) times the number of frustrated plaquettes.

The link variables U_x^μ in a U(1)-gauge theory can be represented by complex numbers of unit modulus: $U_x^\mu = e^{i\theta^\mu_\nu}$. We then have

$$U_\square = e^{i(\theta_x^\mu + \theta^\nu_{x+\hat{\mu}} - \theta^\mu_{x+\hat{\nu}} - \theta_x^\nu)} \equiv e^{i\theta_\square} \; .$$

A frequently used (but not unique) definition of $E_\square$ and S is

$$E_\square = 1 - \mathrm{Re}\; U_\square = 1 - \cos\theta_\square \; .$$

$$S = \frac{1}{g} \sum E_\square \equiv \beta \; \Sigma_\square E_\square \; .$$

The expressions for the quantum expectation value of the observables in the lattice theory

$$\langle O \rangle = \frac{\int \pi dU \; O(U) \; e^{-\frac{c}{g^2} \Sigma_\square E_\square}}{\int \pi dU \; e^{-\frac{c}{g^2} \Sigma_\square E_\square}}$$

are formally analogous to the expressions giving the thermal averages in the statistical formulation of thermodynamics, with the correspondence $c/g^2 \leftrightarrow 1/kT$. (Hence the notation $\beta \equiv \frac{c}{g^2}$). The dimensionality (4) of the lattice system is however a reminder that we are dealing with a quantum field theory.

Strong coupling calculations, corresponding to high temperature expansions in the above analogy, can be performed. Weak coupling expansions, corresponding to low temperature expansions, are also possible and are quite similar to the perturbative expansions of the continuum theory. The lack of rotational invariance introduces however substantial complications in the perturbative expansions and the formalism based on the continuum is more convenient for such expansions

The regularization provided by the lattice must be eventually removed to achieve a continuum limit. This is done by the process of renormalization. The lattice spacing a is sent to 0, but the coupling constant g must also be correspondingly modified.
Assume that one can calculate a definite physical quantity, e.g. a quantity r with dimension of a length. It will be given by an expression

$$r = a f(g).$$

For the existence of a continuum limit there must exist a critical value of the coupling constant g_0 such that

$$f(g) \to \infty \quad \text{for} \quad g \to g_0.$$

One can then set

$$a = a(g) = r/f(g)$$

and obtain the continuum limit by letting $a \to 0$ while $g \to g_0$ with

$$a = a(g) \quad \text{or} \quad g = g(a).$$

The relationship $r = a f(g)$ only sets a scale, i.e. allows one to assign a definite value to the lattice spacing in correspondence to definite values of g close to g_0. However if one can also calculate other quantities, e.g. a mass $m = a^{-1} f_1(g)$, then specific predictions follow for the continuum limit. One finds for instance

$$m r = \lim_{g \to g_0} f(g) f_1(g).$$

Notice that the function $f_1(g)$, as well as all the corresponding functions appearing in the expressions for other observables, must behave for $g \to g_0$ in a way such that a finite continuum limit ensues for m. We express this property by saying that g_0 is a scaling critical point.

It is apparent from all of the above discussion that in the definition of a continuum limit g cannot be taken arbitrarily, but must approach a scaling critical point g_0. For non-Abelian models, relevant to the theory of strong interactions, $g_0 = 0$. Strong coupling results must therefore be extrapolated to weak coupling, and one faces the always difficult task of obtaining information on the system for intermediate values of the coupling constants. During the last few years it has been found that such information can be obtained by the use of numerical methods, which effectively simulate with high speed computers the quantum fluctuations of a physical system.

Second Lecture

We shall illustrate methods of numerical simulation considering for definiteness lattice gauge theories where the gauge group is Z_N, i.e. the subgroup of U(1) consisting of rotations by multiples of $2\pi/N$.

The link variables U_x^μ can be represented by complex numbers (of unit modulus)

$$U_x^\mu = e^{\frac{2\pi i\, n_x^\mu}{N}} \qquad n_x^\mu = 0, \ldots N-1,$$

or, simply, by the integers n_x^μ. The group operation is addition modulus N

$$e^{\frac{2\pi i\, n_1}{N}}\; e^{\frac{2\pi i\, n_2}{N}} = e^{\frac{2\pi i\, n_3}{N}} \qquad \text{with } n_3 = n_1 + n_2 \pmod N.$$

Our considerations extend indeed very easily to any system with discrete gauge group. The group elements U can be labelled by integers n and the composition law can be codified in a multiplication table

$$(n_1, n_2) \Rightarrow n_3 = MT(n_1, n_2).$$

Plaquette variables and vacuum expectation values are defined as follows

$$n_\Box = n_x^\mu + n_{x+\hat\mu}^\nu - n_{x+\hat\nu}^\mu - n_x^\nu \pmod n$$

$$E_\Box = 1 - \cos 2\pi \frac{n_\Box}{N}$$

$$\langle \mathcal{O} \rangle = \frac{\sum_{\{n_x^\mu\}} \mathcal{O}(n)\, e^{-\beta \sum_\Box E_\Box}}{\sum_{\{n_x^\mu\}} e^{-\beta \sum_\Box E_\Box}}$$

The sums appearing in the above equation are finite but, if the lattice extends for M sites in each dimension the number of terms in the sums is N^{4M^4} and a direct summation, even with the highest speed computers, is impossible but for extremely small values of M.

One resorts to methods of numerical sampling, or Monte Carlo simulations (which apply also to spin systems). The collection of gauge variables is defined as a configuration C

$$C \equiv \{ n_x^r \}.$$

We have

$$\langle O \rangle = \sum_C O(C)\, e^{-S(C)} \Big/ \sum_C e^{-S(C)} ;$$

the denominator in the above equation will be frequently denoted by Z. If we can define a stochastic sequence

$$C_1 \to C_2 \to \dots C_i \to C_{i+1} \to \dots ,$$

with the property that the probability $P^{(i)}(C)$ of encountering a definite configuration C at the i^{th} step approaches

$$P^{(i)}(C) \to \frac{e^{-S(C)}}{Z}$$

for $i \to \infty$, then it will be possible to approximate the quantum averages with averages taken of a larger number N of configurations occurring in the sequence

$$\langle O \rangle \simeq \frac{1}{N} \sum_{i=i_1}^{i_1+N} O(C_i).$$

Requirements are that all of relevant parts of phase space are explored and that N is large enough to garantee a sufficiently accurate determination of $\langle O \rangle$.

The passage from one configuration to the next is effected according to a transition probability $p(C \to C')$, satisfying

$$p(C \to C') \geq 0 \quad , \quad \Sigma_{C'}\, p(C \to C') = 1 .$$

If p obeys a property of detailed balance

$$p(C \to C') / p(C' \to C) = e^{-S(C')} / e^{-S(C)}$$

then $e^{-S(C)}/Z$ is an eigenvector of the stochastic process. Indeed

$$P(C') = \sum_C \frac{e^{-S(C)}}{Z}\, p(C \to C') = \sum_C \frac{e^{-S(C')}}{Z}\, p(C' \to C) =$$

$$= \frac{e^{-S(C')}}{Z}$$

Although detailed balance is not an absolute requirement for convergence to the appropriate distribution, it is satisfied by all the algorithms used in practical simulations.

The most widely used algorithm is an application of the algorithm originally introduced by Metropolis et al.[4] It proceeds as follows.

Upgrade U_x^μ with all other $U_{x'}^{\mu'}$ fixed:

select a new candidate $\hat{U}_x^\mu$ according to $p_0(U \to \hat{U})$

p_0 obeys $p_0(U \to \hat{U}) = p_0(\hat{U} \to U)$

evaluate $\Delta S = S(\hat{U}; U' \ldots) - S(U; U' \ldots)$ (this requires only a local computation)

if $\Delta S \leq 0$ accept and $U \to \hat{U}$

if $\Delta S > 0$ accept (and $U \to \hat{U}$) with probability $e^{-\Delta S}$, otherwise reject.

Proceed to another link variable $U_{x'}^{\mu'}$.

The algorithm satisfies detailed balance:

$$\frac{p(U \to \hat{U})}{p(\hat{U} \to U)} \overset{\text{(assuming } S(\hat{U}\ldots) > S(U\ldots)\text{)}}{=} \frac{p_0(U \to \hat{U}) e^{-\Delta S}}{p_0(\hat{U} \to U)} = e^{-[S(\hat{U},\ldots) - S(U,\ldots)]} = \frac{e^{-S(\hat{U},\ldots)}}{e^{-S(U,\ldots)}}$$

For the computer inplementation one keeps all of the n_x^μ in memory. Then the steps are as follows

→ select link variable n_x^μ, calculate contribution to S from all plaquettes involving n_x^μ (appropriate boundary conditions must be implemented)

extract new candidate $\hat{n}_x^\mu$

calculate same contribution to S with $\tilde{n}_x^\mu$ replacing n_x^μ

calculate $\exp(-\Delta S)$

extract r $\quad 0 \leq r \leq 1$

if $r \leq \exp(-\Delta S)$ $\quad n_x^\mu \to \hat{n}_x^\mu$

↑

Alternative algorithms which are frequently used are the modified Metropolis algorithm:

the step $U_x^\mu \to \hat{U}_x^\mu$ is performed m times at fixed x,μ before proceeding to new $x'\mu'$;

the heat bath algorithm:

if we let $m \to \infty$, then

$$p(U \to \tilde{U}) = p(\tilde{U}) \propto e^{-S(\tilde{U};\ U' \text{ fixed})};$$

the heat bath method may be convenient if a fast algorithm is available to extract $\tilde{U}$ according to $p(\tilde{U})$.

Results for four-dimensional Z_N lattice gauge models.

Monte Carlo simulations can be used to evaluate $E \equiv \langle E_\square \rangle$ as function of β (as a reminder: $e^{-S} = e^{-\beta \Sigma_\square E_\square}$ $0 \le E_\square \le 2$,

($\langle E_\square \rangle = 0$ for $\beta = \infty$, $\langle E_\square \rangle = 1$ for $\beta = 0$).

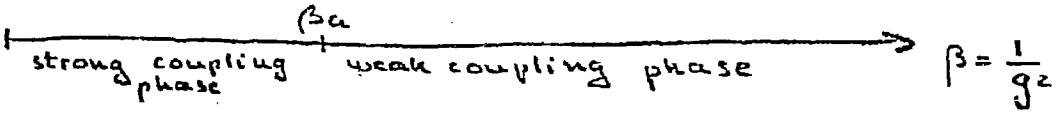
Results obtained by varying β very slowly in the course of the simulation exhibit hysteresis loops which signal phase transitions. Figures 1, 2 and 3 illustrate MC results for the Z_2 Z_3 Z_4 Z_5 Z_6 and Z_8 models.[5]

The Z_2 Z_3 and Z_4 systems exhibit a structure of two phases separated by a first order transition; the Z_N systems, for $N>4$, exibit a 3 phase structure, with 2 continuous phase transitions at

$$\left.\begin{aligned} \beta_{c2}' &\to \text{const} \\ \beta_{c2}'' &\sim N^2 \end{aligned}\right\} \text{ for } N \to \infty.$$

MC simulations where the initial configuration has a mixed phase structu can be used to investigate the nature of the phase transitions (see figure 4). Simulations done at several values of β in the neighbourhoo of a phase transition show a rather linear drift of E as function of the number of iterations if the transition is of first order. This corresponds to the stable phase expanding and overtaking the whole system. A markedly different behaviour is observed with continuous phase transitions.

The U(1) gauge system, which can also be considered to be the limit of a Z_N system for $N \to \infty$, has a 2 phase structure.[5,6]



For $\beta < \beta_{cr}$ the system is in a strong coupling phase: the force between static charges tends to a constant value as the separation increases to infinity and electric charges are confined. For $\beta > \beta_{cr}$ the system is in a weak coupling phase: the force between static charges exhibits a Coulombic behaviour. The continuum limit (i.e. the free quantized photon field) is recovered for $\beta > \beta_{cr}$.

Simulations of systems with continuous gauge group can be done along the lines illustrated above, but require more memory to represent the gauge dynamical variables and much more arithmetic to implement the group multiplications needed for the evaluation of ΔS. By separating the dynamical variables into suitable subsets, the upgrading of all the variables belonging to the same subsets can be done simultaneously (red-black algorithms). This allows optimal utilization of vectorized, parallel or special purpose processors.[7]

Third Lecture

Quantum Chromo Dynamics or QCD, the gauge theory of strong interactions, is based on quark matter fields, $\psi_{x,c}$ $\bar{\psi}_{x,c}$, which transform according to the fundamental representation of SU(3), and gauge fields $U_{x,cc}$, which transform according to the adjoing representation of SU(3). (Spin and other internal indices of ψ and $\bar{\psi}$ are left implicit.)

A typical gauge invariant coupling would be given by

$$\varepsilon_{cc'}\ \bar{\psi}_{x+\hat{\mu},c}\ U^{\mu}_{x,cc'}\ \psi_{x,c}\ .$$

Many important dynamical effects are already present at the level of the pure gauge system. We shall therefore consider a theory with gauge dynamical variables only, in this lecture, and postpone the treatment of systems with quark fields to the next one.

By arguments based on perturbative expansions[8] one can show that $g_{cr} = 0$ defines a possible continuum limit and that, if the continuum theory is indeed recovered for vanishing coupling constant, the lattice spacing must behave for small g as follows:

$$a(g) \propto \left(\frac{8\pi^2}{33}\ \frac{6}{g^2}\right)^{\frac{51}{121}}\ e^{-\frac{4\pi^2}{33}\ \frac{6}{g^2}}$$

$$\text{or} \quad \propto \left(\frac{8\pi^2}{33}\beta\right)^{\frac{51}{121}}\ e^{-\frac{4\pi^2}{33}\beta} \qquad \left(\beta = \frac{6}{g^2}\right).$$

It is convenient to define a lattice scale parameter Λ by

$$a(\beta) = \frac{1}{\Lambda}\left(\frac{8\pi^2}{33}\beta\right)^{\frac{51}{121}} e^{-\frac{4\pi^2}{33}\beta}\left(1 + O(1/\beta)\right)$$

If a physical quantity q has dimensions of $[\text{mass}]^d = [\text{length}]^{-d}$ it will be given by an expression

$$q(\beta) = f(\beta) a^{-d}.$$

One then expects a scaling behaviour $f(\beta) \sim c[\Lambda a(\beta)]^d$

which implies that the continuum value of q is $c\Lambda^d$.

Very early MC simulations gave evidence for the absence of a phase transition in the SU(3) model (and also in the SU(2) system, which for many aspects behaves similarly to the SU(3) system itself[9]). This implies that the properties of the strong coupling phase extend all the way to the scaling domain and persist in the continuum limit. Then numerical simulations were used to produce evidence for the scaling behaviour of many observables as $\beta \to \infty$ and to calculate their continuum values.

We illustrate now the calculation of the force between static quarks and of the string tension, i.e. the limiting value of the force for very large separation, using results from a very recent MC study done with a Cyber 205 vectorized processor by D.Barkai, K.Moriarty and the author.[10]

Let us define by U_{ij} the product of $U_\mu^{\pm}$ dynamical variables along a rectangular closed path, extending for i and j links, and by W_{ij} the quantity

$$W_{ij} = \frac{1}{3} \operatorname{Re} \operatorname{Tr} U_{ij} .$$

By expressing the vacuum expectation value of W_{ij} as the result of the propagation in time of a quark-antiquark pair created at a separation of j lattice links and by using an expansion into a complete set of physical states, one can prove

$$\langle W_{ij} \rangle \approx |\langle q\bar{q}|0\rangle| \, e^{-E_{q\bar{q}} t} \quad \text{for large } t.$$

It follows

$$E_{q\bar{q}}(r = ja) = \lim_{i\to\infty} -\frac{1}{a} \ln \frac{\langle W_{ij}\rangle}{\langle W_{i-1,j}\rangle}$$

and

$$F(\sqrt{j(j-1)}\, a) = \frac{E(ja) - E((j-1)a)}{a} =$$

$$= \lim_{i\to\infty} -\frac{1}{a^2} \ln \frac{\langle W_{ij}\rangle \langle W_{i-1,j-1}\rangle}{\langle W_{i-1,j}\rangle \langle W_{i,j-1}\rangle} \equiv \lim_{i\to\infty} -\frac{1}{a^2} \chi_{ij}$$

In particular if $F(r) \underset{r\to\infty}{\to} \sigma$ (string tension), then

$E(r) \underset{r\to\infty}{\sim} \sigma r$ and, for $i,j \to \infty$

$$\langle W_{ij} \rangle \sim e^{-\sigma r t} = e^{-\sigma A}$$

with A = area of the rectangle enclosed by the path.

This generalizes to any closed path γ. One expects a behaviour

$$\langle W_\gamma \rangle \sim e^{-\sigma A}$$

as the area A enclosed by γ becomes larger and larger.

A nonvanishing σ (area law) signals confinement.

The expectation values $\langle W_{ij} \rangle$ have been calculated on a $16^3 \times 32$ lattice for sizes up to $i = j = 8$ at the values $\beta = 5.6,\ 5.8,\ 6,\ 6.2, 6.4,\ 6.6$. These values of the coupling parameter are known to span the domain where the transition toward the scaling regime takes place. Over 1100 MC iterations, i.e. upgradings per dynamical variable, have been performed at each of the values of β, and the expectation values $\langle W_{ij} \rangle$ have been calculated averaging over 100 configurations separated by 10 iterations each.
To evaluate the force one needs to extrapolate

$$\chi_{ij} \underset{i \to \infty}{\Rightarrow} \frac{F\left(a\sqrt{j(j-1)}\right)}{a^2}$$

to large values of i. A simple functional form

$$\chi_{ij} \approx b_j + \frac{c_j}{i(i-1)}$$

(motivated by the expected behaviour for small i) has been assumed and fit through the data points. Figure 5 illustrates this fitting procedure for $\beta = 6.2$.
The values thus found for b_j are in turn consistent, for all β, with an expression for the force

$$b_j \approx \frac{\alpha}{j(j-1)} + \sigma a^2$$

or equivalently

$$F(r) \approx \frac{\alpha}{r^2} + \sigma,$$

consisting of the superposition of a constant and a Coulombic term. This behaviour is illustrated, always for $\beta = 6.2$, in the bottom graph of figure 5 and in figure 6.
The values found for σa^2 appear to scale as

$$(\Lambda a)^2(\beta) = \left(\frac{8\pi^2}{33}\beta\right)^{\frac{51}{121}} e^{-\frac{4\pi^2\beta}{33}},$$

substantial
with no $\Lambda O(\frac{1}{\beta})$ corrections for $\beta \geq 6$. One can thus determine

$$\Lambda \approx 9.6 \times 10^{-3} \sqrt{\sigma}.$$

The scaling behaviour of σa^2 is illustrated in figure 7.

(The fact that the last point, for $\beta = 6.6$, is above the scaling curve is attributed to an overestimate of the asymptotic value of the force, due to the smallness of the lattice spacing for such value of β)

The above results allow one to express the lattice spacing a in function of β and σ. Then all the values found for the force (at all values of β) can be re-expressed in physical units of σ, for the force, and $\sigma^{-\frac{1}{2}}$, for the separation. The data so rescaled are shown in figure 8. All of the points lie, within statistical errors, on a universal curve, which conforms the scaling behaviour.

Perturbative arguments[11] can be used to determine the expected short distance behaviour of the force, with no free parameters once Λ is fixed. The line in figure 8 represents the theoretical prediction for the short distance behaviour and one sees that theory and numerical results are in agreement.

In a confining pure gauge system the spectrum of states (also referred to as glueballs) begins with a lowest stable state of mass $m_g > 0$. m_g is the mass-gap of the theory. It can be evaluated from the numerical calculation of

$$G_{\vec{x},t} = \langle E^{\mu\nu}_{\vec{x}t} \; E^{\mu\nu}_{0} \rangle - \langle E_0 \rangle^2$$

where $E^{\mu\nu}_{\vec{x},t}$ represents the energy of a plaquette at $\vec{x},t$.
By insertion of a complete set of physical states, $G_{\vec{x},t}$ can be re-expressed as follows

$$G_{\vec{x},t} = \sum_{n \neq \emptyset} |\langle n | E_0 | \emptyset \rangle|^2 \, e^{-E_n t + i \vec{p}_n \cdot \vec{x}}$$

It is even better to consider

$$\tilde{G}_t = \sum_{\vec{x}} G_{\vec{x},t} = \sum_{\substack{n \neq \emptyset \\ \vec{p}_n = 0}} |\langle n | E_0 | 0 \rangle|^2 \, e^{-m_n t}$$

Clearly information on the lower masses in the spectrum of pure gauge exitations can be obtained from a study of the rate of decay of $\tilde{G}_t$ for large t.
MC evaluations of $\tilde{G}_t$, or of similar quantities, related in any case to the response of the system to a perturbation and therefore to the correlation $G_{\vec{x},t}$, have allowed several investigators to estimate m_g.[12]

Thermodynamical effects in a quantum field theory can be calculated by expressing the partition function

$$Z(T) = \sum_n \langle n | e^{-\frac{H}{T}} | n \rangle$$

as a functional integral

$$Z(T) = \int\!\!\int_{\text{configurations}} e^{-S},$$

where the propagation occurs for a finite extent $t = \frac{1}{T}$ in time and periodic boundary conditions in time are imposed.
Thus one can study thermodynamical properties of lattice quantum field theories by considering a system extending for n_t spacings in time, n_s spacings along the spatial directions, and $n_t \ll n_s$.
This describes a medium at a physical temperature

$$T = \frac{1}{n_t a}.$$

(These considerations also imply a warning on the use of very small lattices)
The free energy of an individual quark can be evaluated recalling that a static source at $\vec{x}$ implies a modification of the action

$$S \to S + ig \int A^0(\vec{x},t)\, dt$$

in the continuum case.

The free energy of an isolated quark relative to the vacuum is therefore formally given in the continuum theory by

$$e^{-\frac{\Delta F}{T}} = \frac{\sum_n \langle n | e^{-\frac{H}{T}} e^{i\int A_0 dt} | n \rangle}{\sum_n \langle n | e^{-\frac{H}{T}} | n \rangle} = \langle e^{i\int A_0 dt} \rangle .$$

But the lattice analogy of $e^{i\int A_0 dt}$ is the product of the $U^{\mu=4}_{\vec{x},t}$ gauge variables along a line extending in the time direction (a path closed by virtue of the periodic boundary conditions). Let such product be denoted by $U_{\vec{x}}$ and let

$$W_{\vec{x}} = \frac{1}{3} \mathrm{Tr}_2 U_{\vec{x}} .$$

We then have

$$e^{-\frac{\Delta F}{T}} = \langle W_{\vec{x}} \rangle$$

If quarks are confined $\Delta F = \infty$ and $\langle W_{\vec{x}} \rangle = 0$.
If thermal fluctuations deconfine quarks ΔF = finite and $\langle W_{\vec{x}} \rangle > 0$.

MC simulations have shown that $\langle W_{\vec{x}} \rangle = 0$ for large enough n_t and small enough $a(\beta)$ (remember $T = 1/n_t a(\beta)$), but a transition to $\langle W_{\vec{x}} \rangle > 0$ is observed when, modifying n_t or β, T is brought above a critical value T_c.
Thus the thermodynamical properties of the gauge medium and in particular the presence of a confining phase transition can be and have been studied by MC numerical techniques.[13]

Fourth Lecture

Numerical calculations involving fermionic matter fields.

The complete action for QCD is the sum of the pure gauge action S_G and the action of the quark matter fields S_M. S_M will be of the form

$$S_M = \sum_{xy} \bar{\psi}_x (D+m)_{xy} \psi_y$$

where color and possible spin indices of the quark fields ψ_x, $\bar{\psi}_x$ have been left implicit and the matrix D+m represents the generalization to the lattice of Dirac's operator of the continuum theory:

$$\gamma^\mu (\partial_\mu + igA_\mu^i T_i) + m$$

Such a generalization is not obvious. A straightforward lattice-transcription of Dirac's operator, obtained by replacing first order derivatives by central differences, leads to a theory which exhibits in the continuum limit a 16-fold degeneracy of states (2^d for a d-dimensional system). A modification of the action due to Wilson[14] removes the degeneracy at the cost of breaking chiral symmetry when m=0; in another formulation, originated by Kogut and Susskind,[15] which preserves a continuum chiral symmetry for m=0, the spin components of ψ_x are distributed among the vertices in a 2^d cell. Then the fermions are represented by single component, anticommuting dynamical variables ψ_x, $\bar{\psi}_x$ ("single component" refers only to spin - ψ and $\bar{\psi}$ are still 3 component complex vectors in SU(3) color space). The Kogut-Susskind formulation reduces the unwanted degeneracy to 4. Other generalizations are possible; we need not go into details. In any event S_M will contain nearest neighbor couplings, of the type

$$\bar{\psi}_{x+\hat{\mu}} U_x^\mu \psi_x .$$

The U_x^μ variables needed to make the couplings gauge invariant render D+m explicitly dependent on the gauge fields, thus inducing the coupling between matter and gauge degrees of freedom.

For Monte Carlo simulations one needs to approximate quantum averages taken over gauge and fermionic degrees of freedom, e.g.

$$G_{x,y} = \langle \bar\psi_x \Gamma \psi_x \; \bar\psi_y \Gamma \psi_y \rangle =$$

$$= \mathcal{Z}^{-1} \int \Pi dU_x^\mu \, \Pi (d\bar\psi_x d\psi_x) \bar\psi_x \Gamma \psi_x \bar\psi_y \Gamma \psi_y \, e^{-S_G - S_M} ,$$

where Γ represents some suitable generalization of the continuum γ-matrices and

$$\mathcal{Z} = \int \Pi dU_x^\mu \, \Pi (d\bar\psi_x d\psi_x) \, e^{-S_G - S_M} .$$

From the discussion of the mass gap (Lecture 3), it should be clear that information about the quark model spectrum can be derived from the analysis of the rate of decay in time of

$$\tilde G_t = \sum_{\vec x} G_{\vec x, t, 0} =$$

$$= \sum_{\substack{n \\ \vec p_n = 0}} |\langle n | \bar\psi \Gamma \psi | 0 \rangle|^2 \, e^{-m_n t} .$$

It is however not obvious how one should sample integrals over elements of a Grassman algebra, i.e. over the anticommuting variables $\bar\psi$ and ψ. A possibility is to exploit the fact that such integrals have really been introduced to represent sums over occupation members of quark and antiquark states. Such states

are finite in number, in a lattice of finite volume, and thus the quantum averages are, for the fermionic part, sums over a finite number of binary variables, 0 and 1. This reformulation has been successfully used for the numerical simulation of 2-dimensional (1 space - 1 time) systems.[16] In more than 1 spatial dimension, however, the terms appearing in the sums are no longer positive definite, and a probabilistic interpretation as well as a practical sampling procedure become impossible.

For 4-dimensional systems all numerical computations have exploited the fact that the action S_M is, bilinear in the fermionic fields. The Gaussian integration over $\bar{\psi}_x$ and ψ_x can be done explicitely and one finds (always referring to $G_{x,y}$ for exemplification)

$$G_{x,y} = \tilde{Z}^{-1} \int \Pi dU_x^\mu \langle \bar{\psi}_x \Gamma \psi_x \, \bar{\psi}_y \Gamma \psi_y \rangle_U \times e^{-S_G} \, \mathrm{Det}\,(D(U)+m),$$

where

$$\tilde{Z} = \int \Pi dU_x^\mu \, e^{-S_G} \, \mathrm{Det}\,(D(U)+m)$$

and

$\langle \bar{\psi}_x \Gamma \psi_x \bar{\psi}_y \Gamma \psi_y \rangle_U$ stands for the expectation value of the fermionic observable in the presence of a fixed gauge field configuration U_x^μ.

This expectation value can be expressed in terms of quark propagators. For instance, assuming for simplicity that Γ is such that only connected diagrams are present,

$$\langle \bar{\psi}_x \Gamma \psi_x \bar{\psi}_y \Gamma \psi_y \rangle_U = \mathrm{Tr}\left\{ \Gamma (D(U)+m)^{-1}_{xy} \Gamma (D(U)+m)^{-1}_{yx} \right\}.$$

Thus the quantum averages have been reduced to averages over ordinary bosonic variables only (integrals over the group manifolds, as in the pure gauge system). A numerical calculation of G_{xy} still faces two serious levels of computational complexity.

I) The measure is now of the type

$$e^{-S_{eff}}$$

with

$$S_{eff} = S_G - \ln \mathrm{Det}(D(U)+m) = S_G - \mathrm{Tr} \ln (D(U)+m).$$

For a Monte Carlo simulation one needs to evaluate the change Δ induced by a change $U_x^\mu \to \hat{U}_x^\mu$. Whereas S_G is local, the second term makes S_{eff} non-local. The values of all the dynamical variables $U_{x'}^{\mu'}$ enter in the calculation of the variation ΔS_{eff} induced by any one of them. An exact calculation of ΔS_{eff}, while feasible, becomes so time consuming to make the implementation of the MC algorithm for any lattice of realistic size impossible. The only way out appears to be, at present, in replacing the exact calculation of ΔS_{eff} with some fast, but only approximate computation. While we shall be mentioning more sophisticated scheme of approximation later, the simplest approximate calculation consists, in neglecting the second term in S_{eff} altogether, and to sample the gauge field configurations according to the pure gauge measure $\exp(-S_G)$.

Such an approximation, which has been called the "quenched"[17] or "valence"[18] approximation, is not necessarily as drastic as it may seem. It corresponds to neglecting (in terms of a perturbative expansion) the effects of internal quark loops, and several arguments of phenomenological and theoretical nature have been brought to justify schemes making the same or even more restrictive (to planar diagrams) approximations.

B) Whether the gauge field configurations are sampled according to $\exp(-S_o)$ or some method taking into account the effects of internal quark loops (i.e., the effects of dynamical fermions), one still needs to evaluate

$$(D(U) + m)^{-1}_{xy}$$

This is another time consuming operation, which requires the solution of a large system of linear equations (not a full matrix inversion, since generally only a few elements of $(D+m)^{-1}$ are required, for instance all those where y is set at the origin). Relaxation methods, or methods based on the algorithm of conjugate gradients, are normally used to find the propagators. The fact remains that only few inversions (of the order of a few tens, or at most a few hundreds) can be done in a definite calculation, and then estimates of masses and similar fermionic observables are based on relatively limited samples.

Many calculations of the masses of lowest states in the quark model spectrum and of other fermionic observables, such as the chiral symmetry breaking condensate $\langle\bar{\psi}\psi\rangle$, have nevertheless been performed, in the quenched approximation[19]. The results of different calculations exhibit discrepancies larger than what can be justified by statistical fluctuations, which can however be easily understood considering the various kinds of computational limitations. Among the most important:

- the generally small extents in space and time of the lattices used for the calculations
  Only recently lattices extending for as much as $10^3 \times 20$ (space and time sizes) have been considered, and, assuming that $\beta \geq 6$ is required to have enough resolution in the lattice approximation to the continuum, and that the values quoted for the string tension in the previous lecture are correct, this makes $a \leq \sim .125$ fm, $10\ a \leq \sim 1.25$ fm, a size certainly not too large.
- the limited sampling.

- the possible distortions introduced by the lattice transcription of the Dirac equation. While all formulations ought to become equivalent in the continuum limit, the differences in the spectra determined within different formalisms may still be sizeable at the values considered for a.

Bearing the above limitations in mind, the results have been generally successful. All give evidence for a dynamical realization of chiral symmetry, with $m_\pi^2 \to 0$ as $m_q \to 0$. The other masses (m_ρ, m_p, etc.) appear to remain at finite values when $m_q \to 0$, values generally compatible with the scale set by the calculations of pure gauge observables and with the experimental mass splittings among various states. I shall not quote here specific numbers, because the situation is still too much in a state of flux to quote definite values, and a systematics of all investigations performed and all results obtained is beyond the scope of these lectures.

Finally, let me briefly mention just one[20] (among several interesting methods which have been proposed[21]) possibility to go beyond the quenched approximation.

If $\delta U_x^\mu = \hat{U}_x^\mu - U_x^\mu$ is sufficiently small (and one would think that the nature of the continuum limit is such that it should be possible to explore all of the relevant phase space with small fluctuations δU_x^μ from configuration to configuration, although this may show the simulation), one can linearize the variation of S_{eff}:

$$\Delta S_{eff} = \Delta S_G - Tr \ln (D(U) - m) \approx$$

$$\approx \Delta S_G - Tr\, (D(U) + m)^{-1} \delta D(U) =$$

$$= \Delta S_G - Tr\, (D(U) + m)^{-1} \frac{\partial D}{\partial U} \delta U \,.$$

The structure of the lattice Dirac operator is such that $\frac{\partial D}{\partial U}$ is local. Thus the linearized variation will be easily calculable if a few relevant matrix elements (involving neighbouring sites) of $(D(U) + m)^{-1}$ are known. These will be given by expectation values

$$\langle \psi_x \bar{\psi}_y \rangle_U$$

where the sites x and y are neighbouring. Indeed, to the whole expression $(D(U) + m)^{-1} \frac{\delta D}{\delta U}$, which multiplies δU_x^μ in the linearized variation of S_{eff}, one can give the form of expectation value, in the given gauge field configuration, of a fermionic current j_x^μ, involving fermions at neighbouring sites.

One thus finds

$$\Delta S_{eff} \approx \Delta S_G - Tr\{\langle j_x^\mu \rangle_U \delta U_x^\mu\},$$

an expression quite reminiscent of the formula for the continuum action. The physical significance of the above equation is that the dynamical reaction of the fermions manifests itself (to first order in δU_x^μ) via the current that the gauge field U_x^μ excites in the vacuum.

The crucial observation is now that the vacuum expectation value of the current is the same (given identical couplings to the gauge field) for a fermionic or for a bosonic system. It is only the sign with which

$$Tr\{\langle j_x^\mu \rangle_U \delta U_x^\mu\}$$

enters in ΔS_{eff} which differentiates between the two cases (it would be + for bosonic fields). Thus one may introduce a parallel set of bosonic variables $\bar{\phi}_x \phi_x$, the pseudofermions, and calculate $\langle j_x^\mu \rangle_U$ by a Monte Carlo simulation over these variables. The method proceeds then as follows. For a given gauge field configuration a few MC iterations over the pseudofermions are used to evaluate, approximately, $\langle j_x^\mu \rangle_U$. The values thus found are input in the upgrading of all the gauge field variables, approximating ΔS_{eff} with

$$\Delta S_G - Tr\{\langle j_x^\mu \rangle_U \delta U_x^\mu\}.$$

The method has been tested in some cases[17,22,23] and appears to produce reasonably accurate results in situations where the dynamical effects of the fermions can be computed by other reliable means; it also appears computationally implementable, in the sense that the CP-time requirements, although larger than for a pure gauge simulation, are contained enough to allow for practical calculations. The method is currently being applied to problems, where the dynamical effects of the fermions are expected to be particularly relevant.

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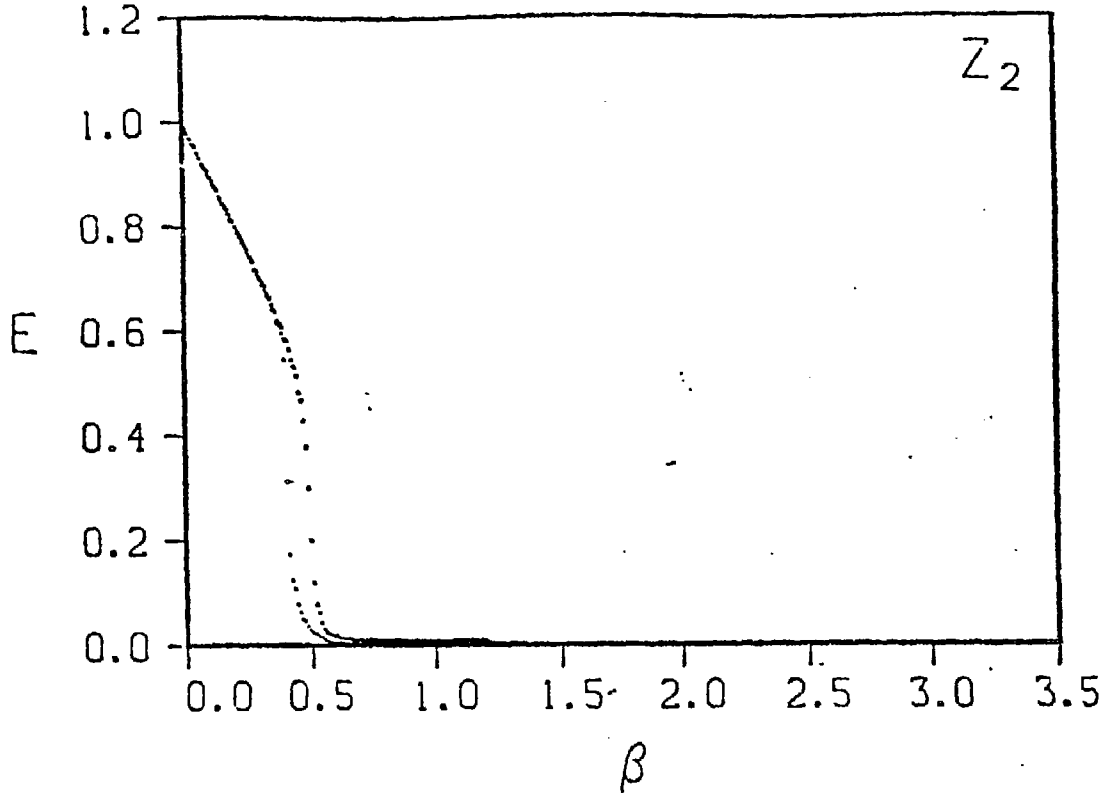
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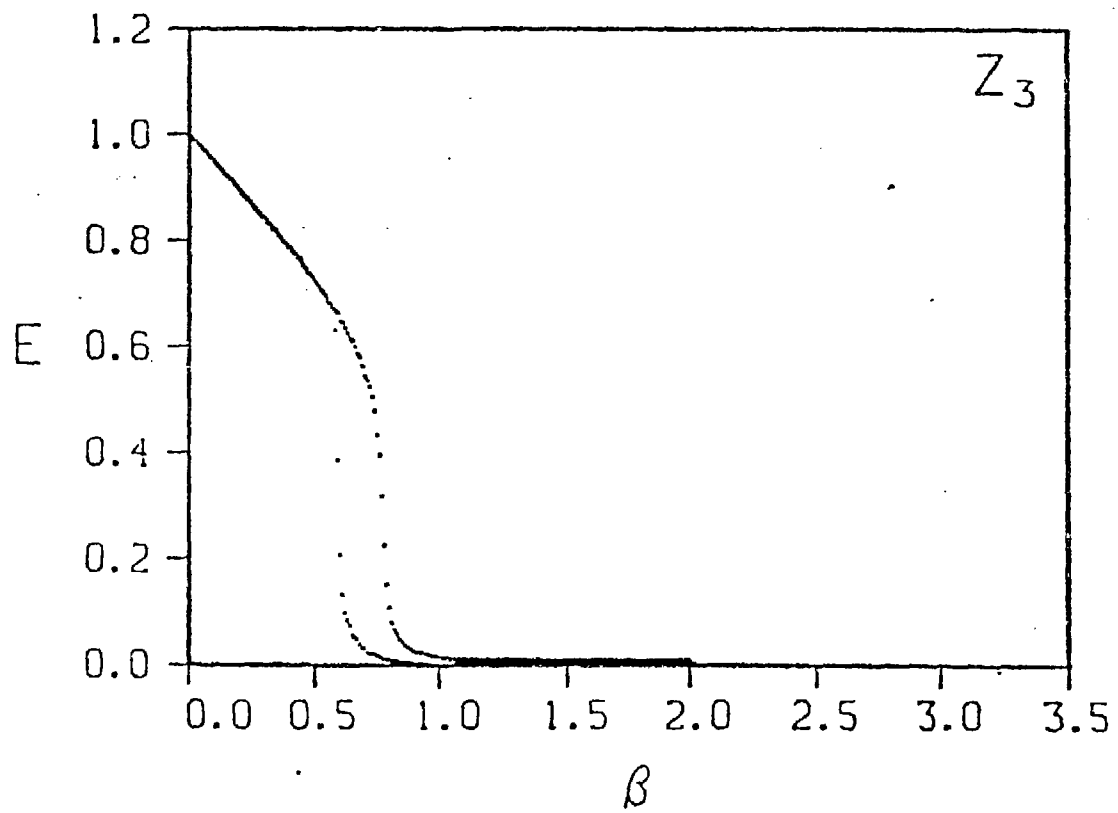
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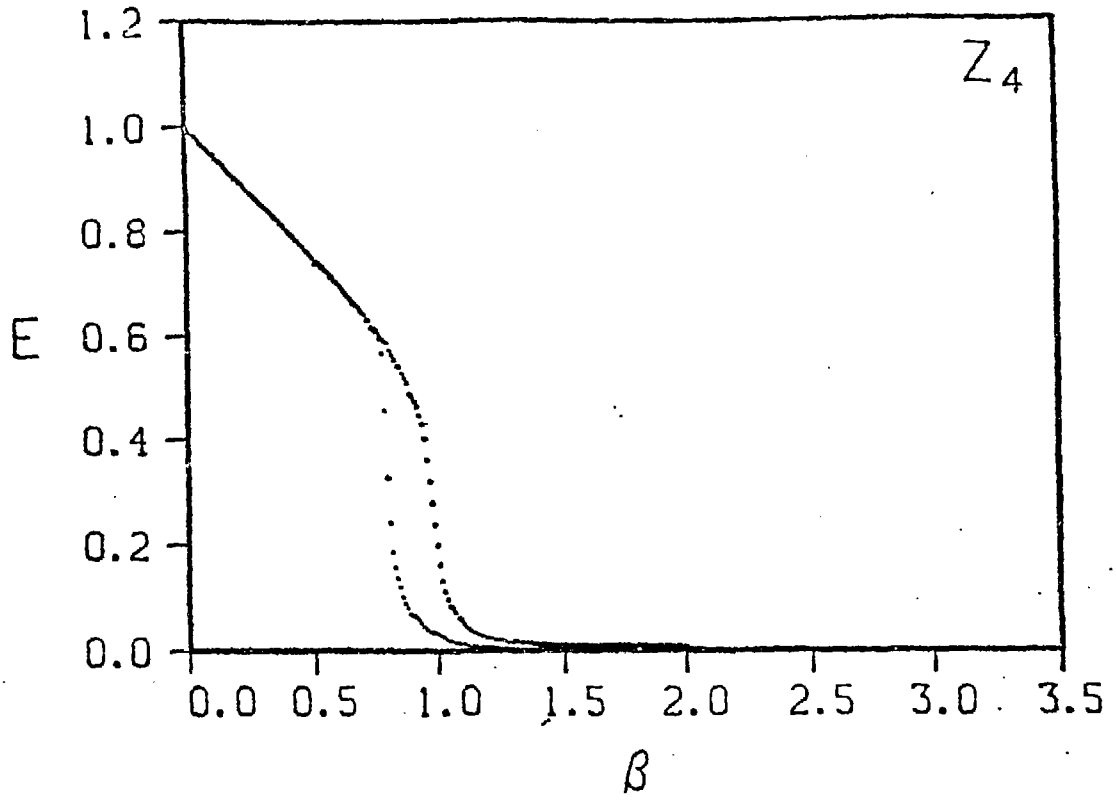
Fig 1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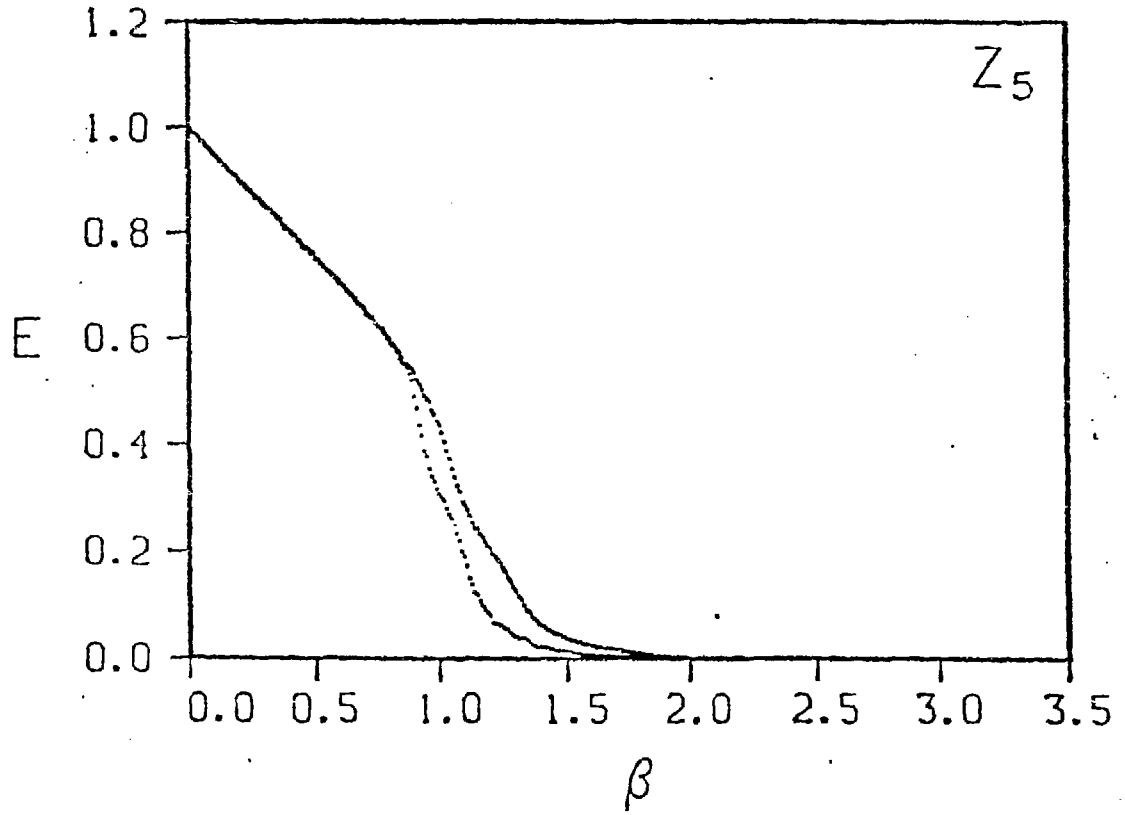
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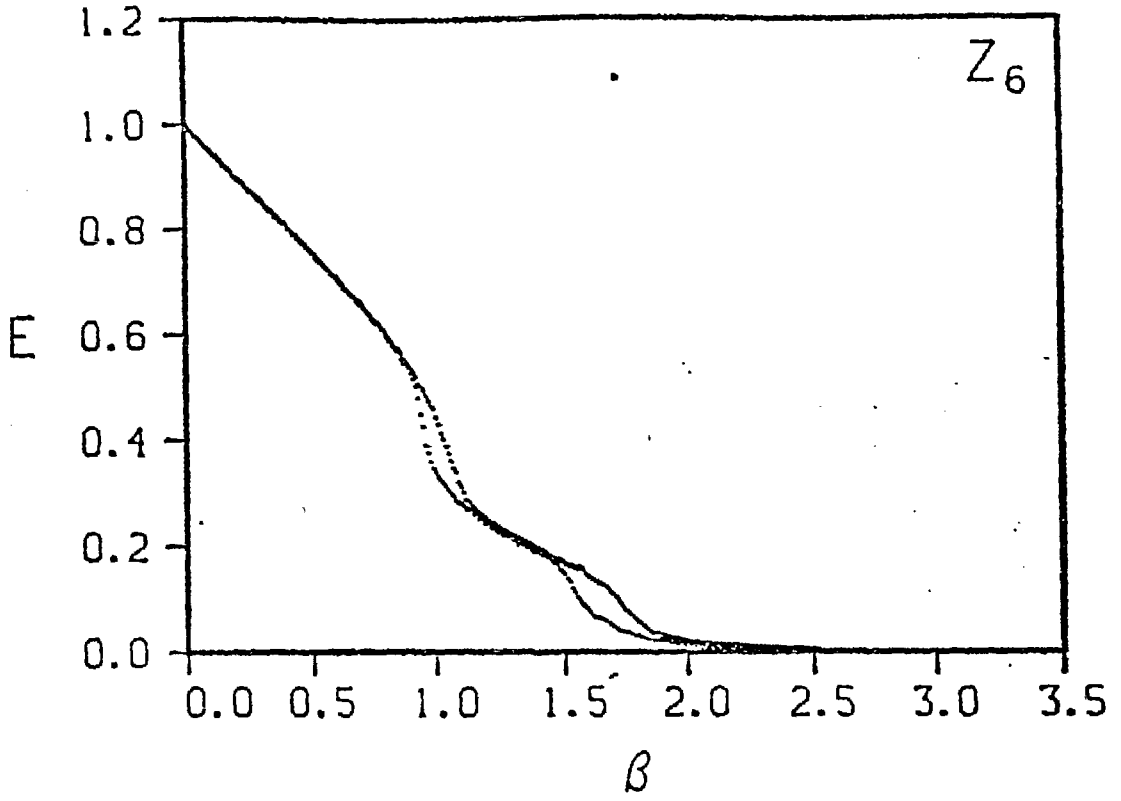
Fig 2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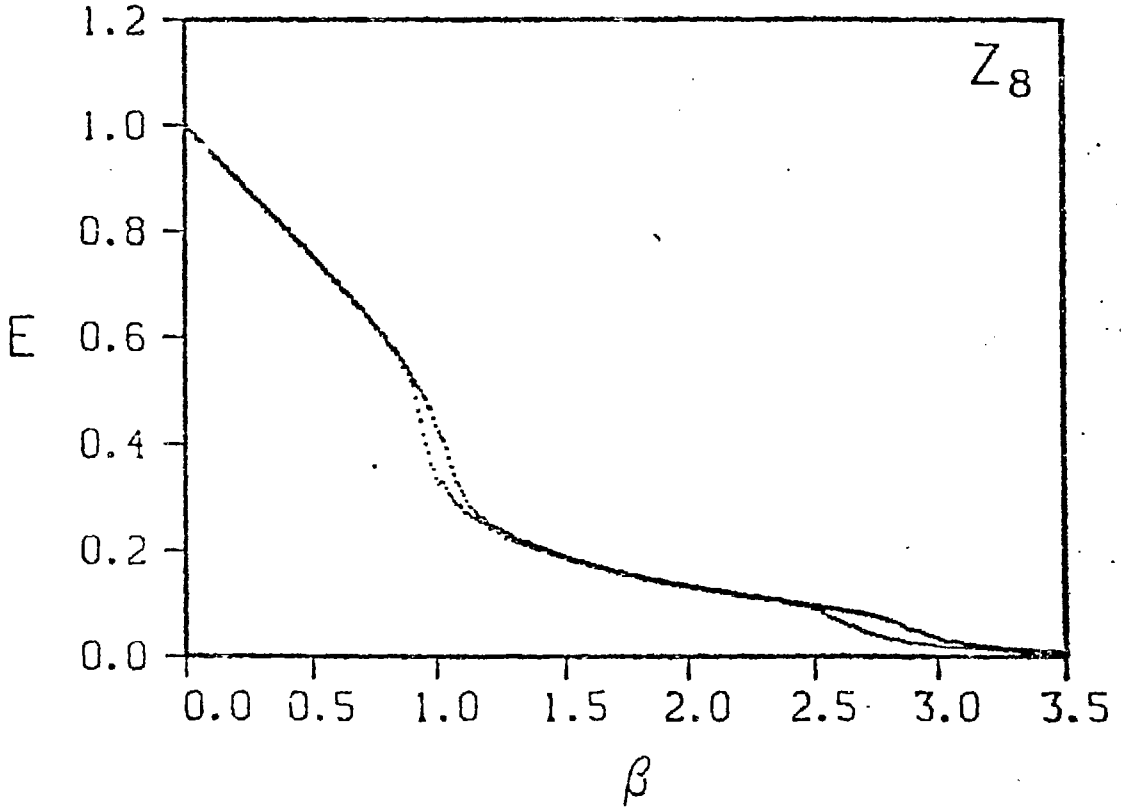
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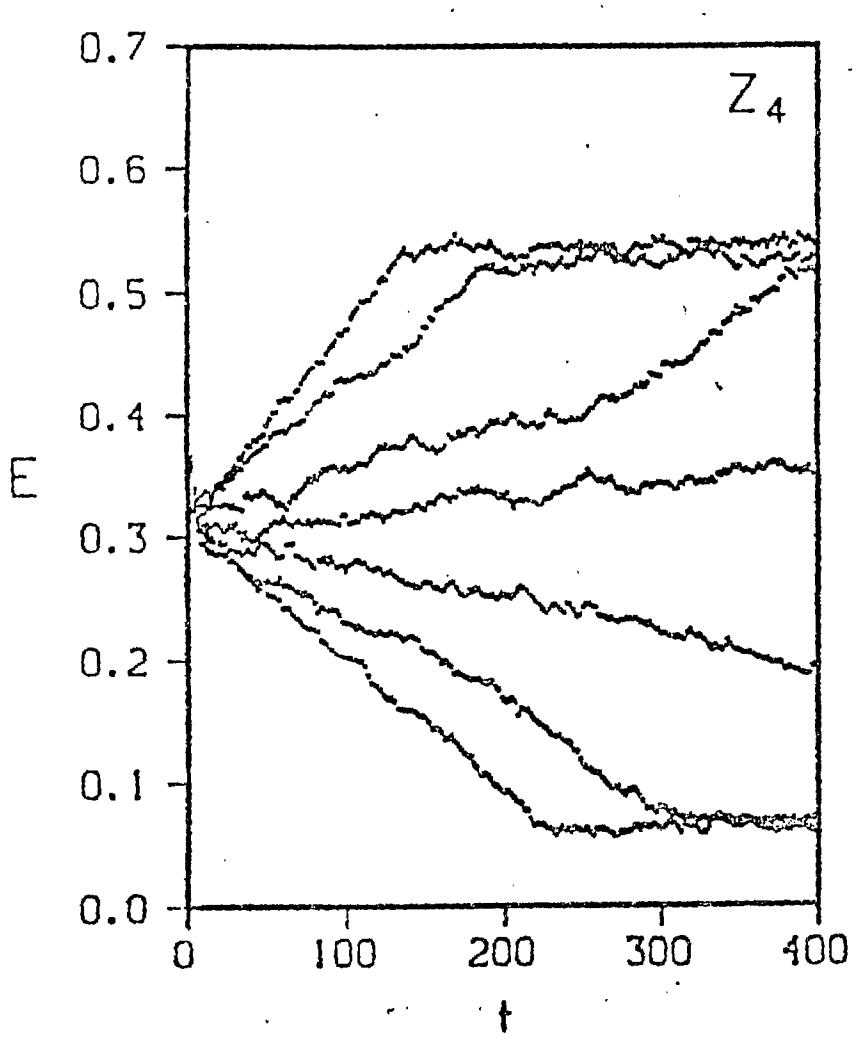
Fig 3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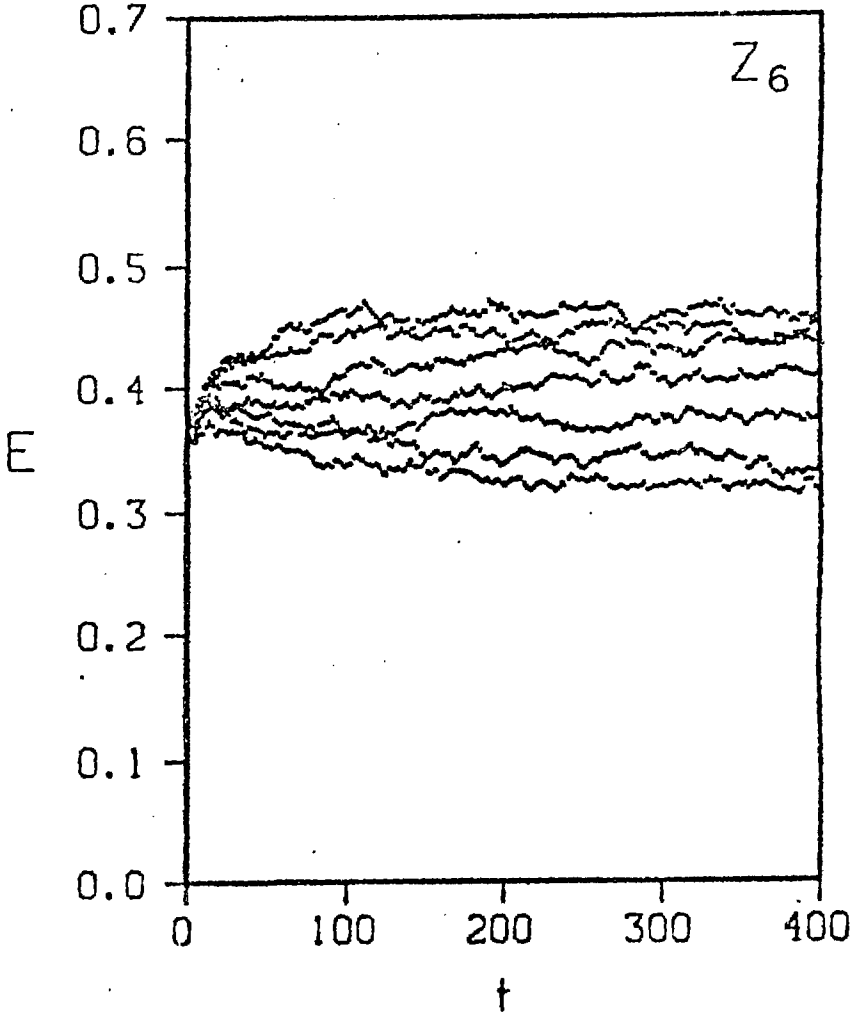
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Fig 4

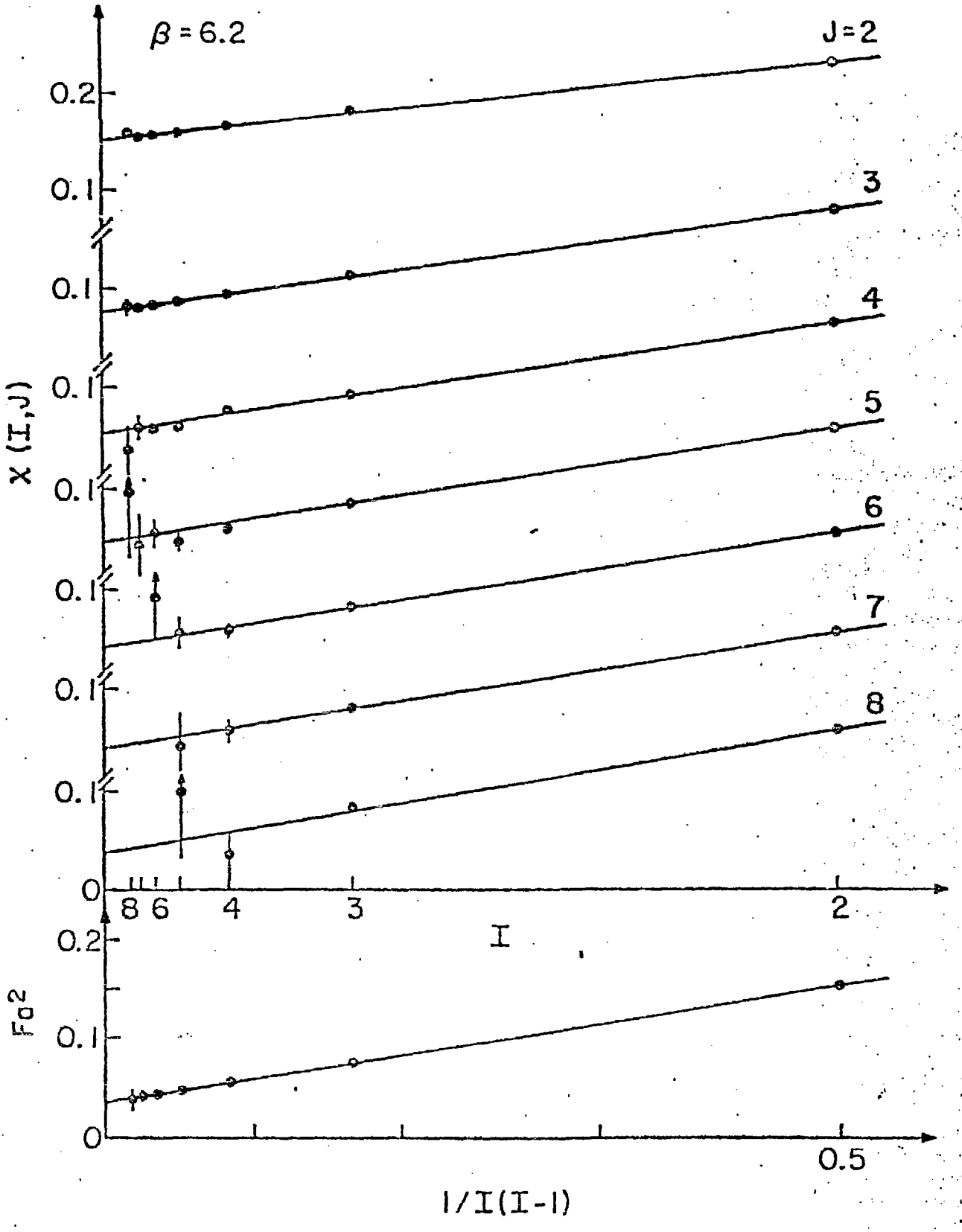


Fig 5

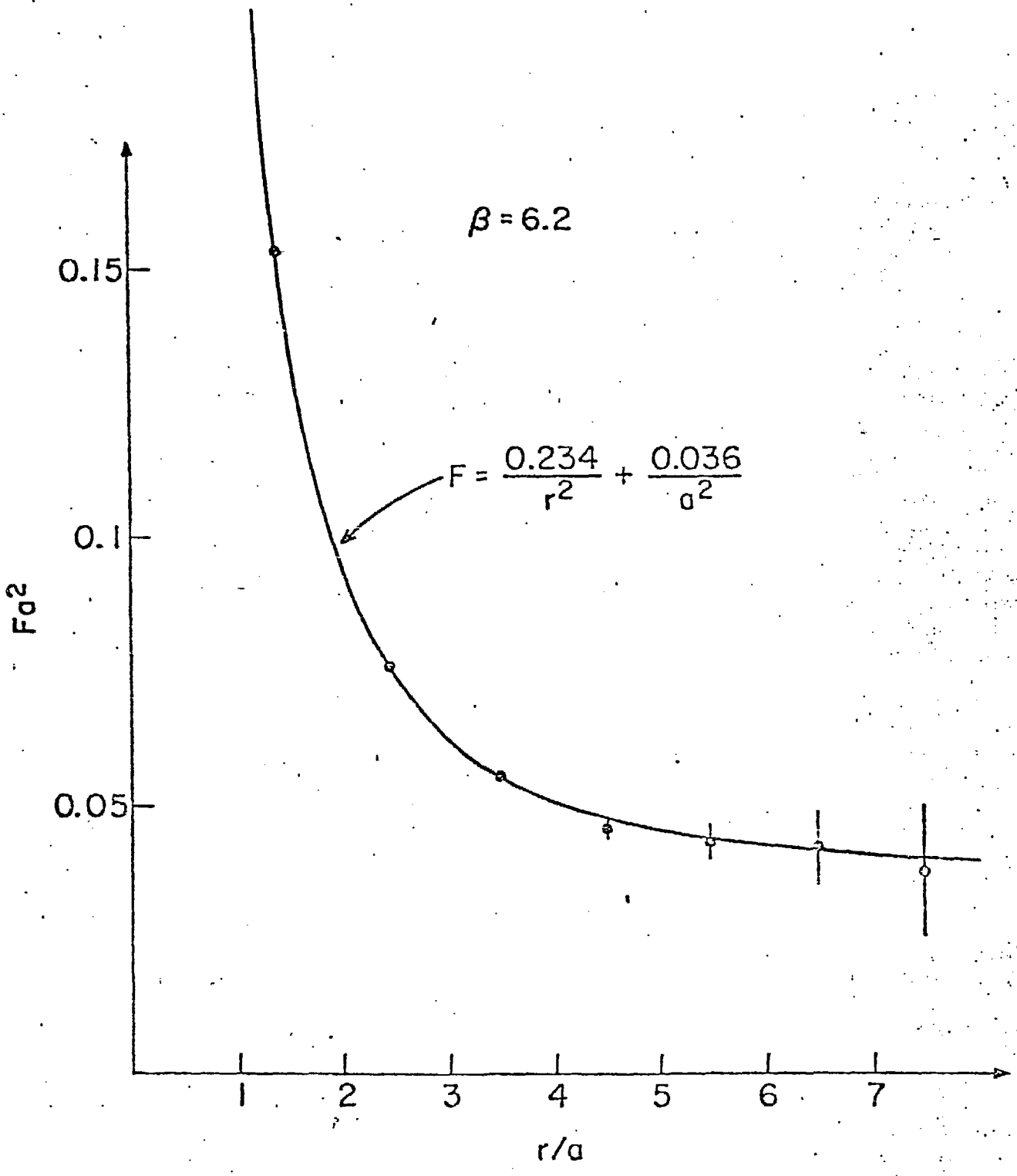
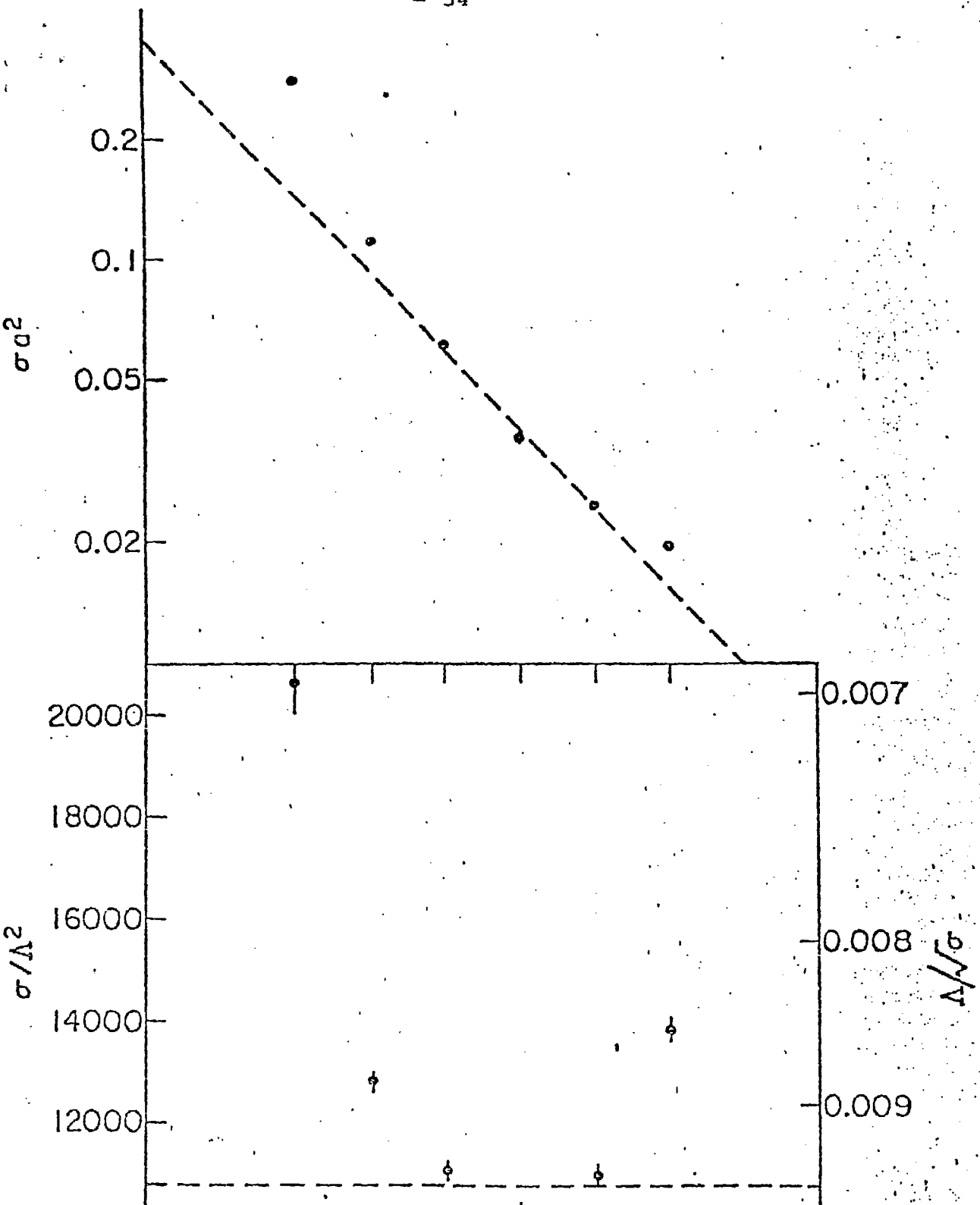


Fig 6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β

Fig 7

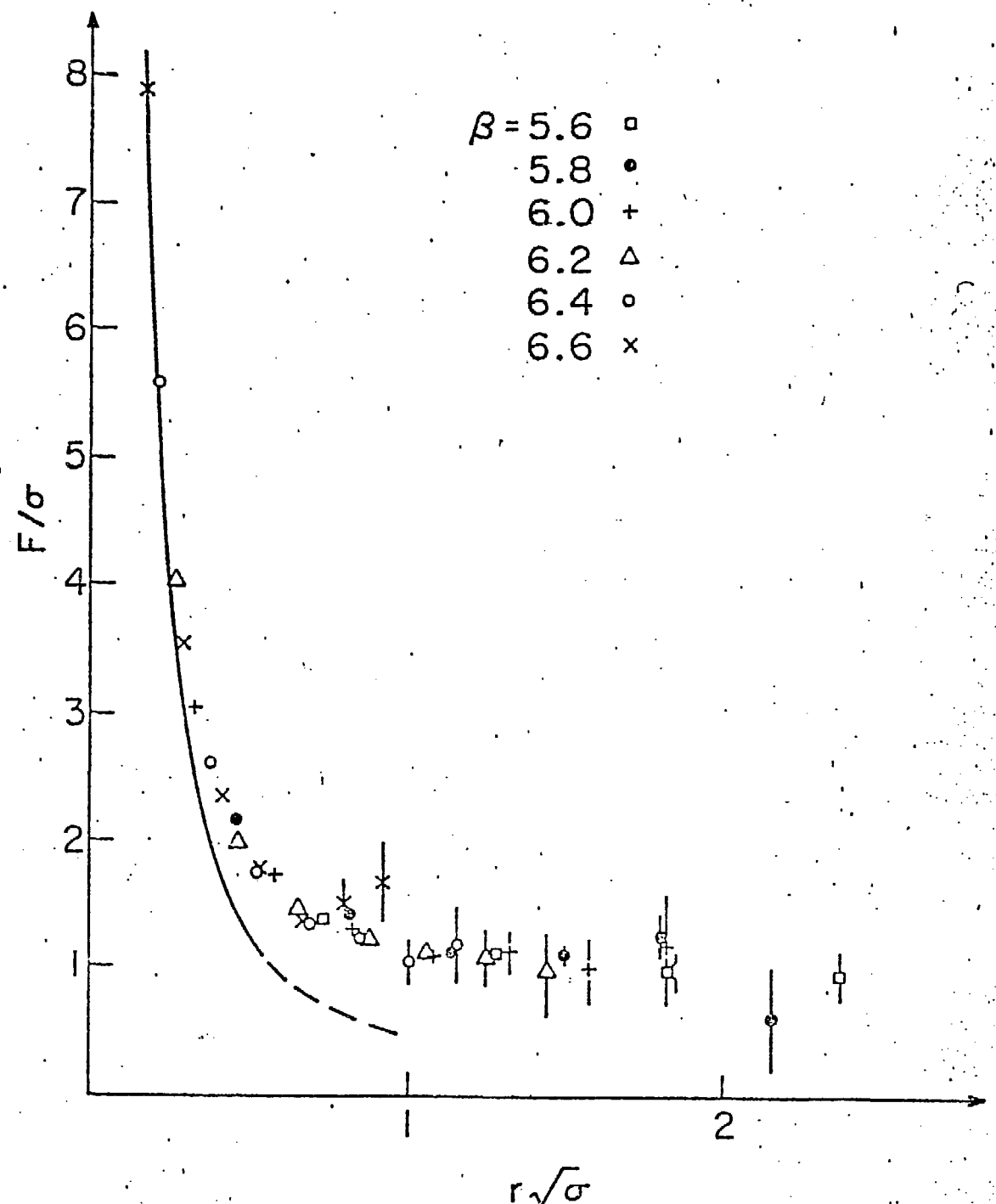

Fig 8