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THE STUDY OF THE FERMION MATRIX  
SPECTRAL DENSITY IN LATTICE  
QUANTUM CHROMODYNAMICS

Thesis by

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Master of Science

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To: my Mother, YAMINA, and Father, ABDELKADER

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"Thirty-one years ago, Dick Feynman told me about his 'sum over histories' version of quantum mechanics. 'The electron does anything it likes', he said. 'It goes in any direction at any speed, forward or backward in time, however it likes, and then you add up the amplitudes and it gives you the wave-function'. I said to him, 'You're crazy'. But he wasn't."

F.J. Dyson, 1979.



## ABSTRACT

One has developed a new method which enables us to implement dynamical lattice fermions in Monte-Carlo Simulation; and it is simply based on the analytical formulation of the spectral density of the eigenvalues of the fermion matrix in the Kogut-Susskind scheme (4).

The ratio of the determinants is predicted, then compared to the ratio calculated via the lanczos method (8).

This is done in  $SU(3)$ , in the chirally broken phase (9), in a  $4^4$  lattice at  $\beta = 5.4$ , and in a  $6^4$  lattice at  $\beta = 5.5$ .

## I. Path formulation (1)

Path formulation is an alternative quantization approach, which has the advantage of describing quantum field theory by using only functional integrals. However, before one reaches this result, let us introduce this formalism in the simplest quantum mechanical system in order that it will be simpler to generalise it.

### I.1 One dimension quantum mechanical system

One of the interests of quantum mechanics is the transition probability of the system from an initial state to a final state. It is expressed by the quantity as follows.

$$\langle x', t' | x, t \rangle = \langle x' | e^{-iH(t'-t)} | x \rangle \quad (1.1)$$

where  $H$  is the Hamiltonian of the system and  $|x\rangle$  is one of the eigenstates of the position operator  $\mathcal{X}$  in the Schrödinger picture so that

$$\mathcal{X} |x\rangle = x |x\rangle \quad (1.2)$$

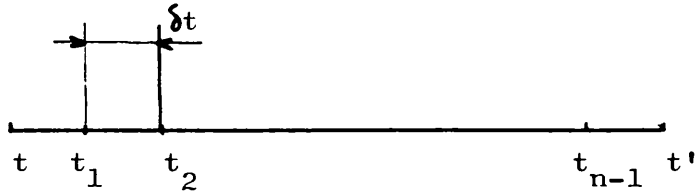
$$\text{and } |x, t\rangle = e^{iHt} |x\rangle \quad (1.3)$$

The set of  $\{|x\rangle\}$  is supposed to be an orthonormal basis in the Hilbert space  $\mathcal{H}$ . That is to say

$$\int |x\rangle \langle x| dx = I \quad (1.4)$$

$$\text{and } \langle x' | x \rangle = \delta(x' - x) \quad (1.5)$$

Let us divide the interval of time  $|t'-t|$  into  $n$  equal segments each of duration  $\delta t$ .



$$\delta t = \frac{|t'-t|}{n}$$

Use equation (1.4), then equation (1.1) can be written as

$$\begin{aligned} \langle x', t' | x, t \rangle &= \langle x' | e^{-iH(t'-t)} | x \rangle \\ &= \int dx_1 \dots dx_{n-1} \langle x' | e^{-iH\delta t} | x_{n-1} \rangle \langle x_{n-1} | e^{-iH\delta t} | x_{n-2} \rangle \dots \\ &\quad \dots \langle x_1 | e^{-iH\delta t} | x \rangle \end{aligned} \quad (1.6)$$

One has considered that the position  $x_i$  corresponds to the time  $t_i$ .

As the number of time-segments goes to infinity, which means that  $\delta t$  is sufficiently small, one has

$$\langle x' | e^{-iH\delta t} | x \rangle = \langle x' | \mathbf{1} - iH\delta t | x \rangle + o(\delta t)^2 \quad (1.7)$$

One takes as an example  $H = \frac{p^2}{2m} + V(x)$ . Then

$$\begin{aligned} \langle x' | H | x \rangle &= \langle x' | \frac{p^2}{2m} | x \rangle + V\left(\frac{x+x'}{2}\right) \delta(x-x') \\ &= \int \frac{dp}{2\pi} \langle x' | p \rangle \langle p | \frac{p^2}{2m} | x \rangle + V\left(\frac{x+x'}{2}\right) \int \frac{dp}{2\pi} e^{ip(x'-x)} \\ &= \int \frac{dp}{2\pi} e^{ip(x'-x)} \left[ \frac{p^2}{2m} + V\left(\frac{x+x'}{2}\right) \right] \end{aligned} \quad (1.8)$$

So far, one has used the well-known relations

$$\langle x' | x \rangle = \delta(x'-x) \text{ and } \langle x | p \rangle = e^{ipx}$$

Then

$$\begin{aligned} \langle x' | e^{-iH\delta t} | x \rangle &\simeq \int \frac{dp}{2\pi} e^{ip(x'-x)} \left\{ 1 - i\delta t \left[ \frac{p^2}{2m} + V\left(\frac{x+x'}{2}\right) \right] \right\} \\ &\simeq \int \frac{dp}{2\pi} e^{ip(x'-x)} e^{-i\delta t H\left(p, \frac{x+x'}{2}\right)}. \end{aligned} \quad (1.9)$$

Back to equation (1.6), and with reference to (1.9) one obtains the following.

$$\begin{aligned} \langle x' | e^{-iH(t-t')} | x \rangle &= \int \left( \frac{dp_1}{2\pi} \right) \dots \left( \frac{dp_n}{2\pi} \right) \dots (dx_{n-1}) \chi \\ &\quad \times \exp \left\{ i \sum_i \left[ p_i (x_i - x_{i-1}) - \delta t H\left(p_i, \frac{x_i + x_{i-1}}{2}\right) \right] \right\} \end{aligned} \quad (1.10a)$$

As a result of this, the transition amplitude can then be written as

$$\langle x' | e^{-iH(t-t')} | x \rangle = \lim_{n \rightarrow \infty} \int \left( \frac{dp_1}{2\pi} \right) \dots \left( \frac{dp_n}{2\pi} \right) \int dx_1 \dots dx_n \chi$$

$$\times \exp \left\{ i \sum_i \delta t \left[ p_i \left( \frac{x_i - x_{i-1}}{\delta t} \right) - H\left(p_i, \frac{x_i + x_{i-1}}{2}\right) \right] \right\} \quad (1.10b)$$

One would almost obtain the final result if one can perform the momentum-space part of the relation 1.10b. However, it can be written differently as  $n$  tends to infinity.

$$\langle x' | e^{-iH(t'-t)} | x \rangle = \int \left[ \frac{dp dx}{2\pi} \right] \exp \left\{ i \int_t^{t'} d\tau (p\dot{x} - H) \right\} \quad (1.10c)$$

One must treat  $(i \delta t)$  formally as real, because of the oscillation of the integrand (equation 1.10c) and an analytical continuation to Euclidean space becomes possible.

As a result all <sup>Momentum</sup> integrals are of the form

$$\int_{-\infty}^{+\infty} \frac{dy}{2\pi} e^{-ay^2 + by} = \frac{1}{\sqrt{4\pi a}} e^{b^2/4a}$$

And one obtains

$$\int \frac{dp_i}{2\pi} \exp \left[ -\frac{i\delta t}{2m} p_i^2 + i p_i (x_i - x_{i-1}) \right] = \sqrt{\frac{m}{2\pi i \delta t}} \exp \left[ \frac{im(x_i - x_{i-1})^2}{2\delta t} \right]$$

With this procedure (1.10c) leads to

$$\langle x, t | x', t' \rangle = \langle x' | e^{-iH(t'-t)} | x \rangle = \lim_{n \rightarrow \infty} \left( \frac{m}{2\pi i \delta t} \right)^{n/2} \int \prod_i dx_i e^{i \sum \delta t \left[ \frac{m}{2} \left( \frac{x_i - x_{i-1}}{\delta t} \right)^2 - V \right]}$$

or symbolically

$$\langle x, t | x', t' \rangle = N \int [dx] e^{i \int_t^{t'} d\tau \left[ \frac{m\dot{x}^2}{2} - V(x) \right]} \quad (1.11)$$

One could mention that  $\mathcal{L} = \frac{m}{2} \dot{x}^2 - V(x)$  is the Lagrange function.

Then

$$\langle x' | e^{-iH(t'-t)} | x \rangle = N \int [dx] e^{i \int_t^{t'} \mathcal{L}(\dot{x}, x) dz} \quad (1.12)$$

or

$$\langle x, t | x', t' \rangle = N \int \mathcal{D} x(t) e^{i \int_t^{t'} \mathcal{L} dz} \quad (1.13)$$

The quantity like  $\langle x, t | x', t' \rangle$  in equation (1.13) is a functional integral. The left-hand side of the equation is a number; so the integral associates a number with each function  $x(t)$ , and this integral is called a functional.

With the same procedure one can translate the previous result to the Green's functions. In the simplest case one will deal with the 2-points functions. It is given by

$$G(t_1, t_2) = \langle 0 | T(\chi^H(t_1) \chi^H(t_2)) | 0 \rangle \quad (1.14)$$

where  $|0\rangle$  represents the vacuum state, which is the ground state,  $T$  the time ordering product operator of  $\chi^H(t_1)$ ,  $\chi^H(t_2)$ .

One will obtain the following result in equation (1.14) if one uses the property in equation (1.4)

$$G(t_1, t_2) = \int dx dx' \langle 0 | x', t' \rangle \langle x', t' | T(\chi^H(t_1) \chi^H(t_2)) | x, t \rangle \langle x, t | 0 \rangle \quad (1.15)$$

It is clear that

$$\begin{aligned} \langle 0 | x', t' \rangle &= \langle 0 | e^{iHt} | x' \rangle = e^{-iE_0 t} \langle 0 | x' \rangle = e^{-iE_0 t} \psi_0(x') \\ &= \psi_0(x', t') \end{aligned}$$

Let us suppose that  $t' > t_1 > t_2 > t$

$$\begin{aligned} \text{Then } \langle x', t' | T(\chi^H(t_1) \chi^H(t_2)) | x, t \rangle &= \langle x' | e^{-iH(t'-t_1)} \chi^s e^{-iH(t_1-t_2)} \chi^s e^{-iH(t_2-t)} | x \rangle \\ &= \int \langle x' | e^{-iH(t'-t_1)} | x_1 \rangle \langle x_1 | \chi^s e^{-iH(t_1-t_2)} | x_2 \rangle \langle x_2 | \chi^s e^{-iH(t_2-t)} | x \rangle dx_1 dx_2 \end{aligned}$$

It is understood that  $|x_i, t_i\rangle = e^{iHt_i} |x_i\rangle$

then it becomes clear that

$$\begin{aligned} \langle x', t' | T(\chi^H(t_1) \chi^H(t_2)) | x, t \rangle &= \int \left[ \frac{dp dx}{2\pi} \right] x_1(t_1) x_2(t_2) \times \\ &\quad \times \exp \left\{ i \int_t^{t'} dt [p\dot{x} - H(p, x)] \right\} \end{aligned} \quad (1.17)$$

As a result of this, one will obtain from equation (1.15)

$$\begin{aligned} G(t_1, t_2) &= \int dx dx' \psi_0(x', t') \psi_0^*(x, t) \int \left[ \frac{dp dx}{2\pi} \right] x_1(t_1) x_2(t_2) \times \\ &\quad \times \exp \left\{ i \int_t^{t'} dt [p\dot{x} - H(p, x)] \right\} \\ &= \int \left[ \frac{dp dx}{2\pi} \right] \psi_0(x', t') \psi_0^*(x, t) x_1(t_1) x_2(t_2) e^{i \int_t^{t'} dt (p\dot{x} - H)} \end{aligned} \quad (1.18)$$

However, it is proved that

$$\begin{aligned} \lim_{\substack{t' \rightarrow -i\infty \\ t \rightarrow i\infty}} \langle x', t' | T(\chi^H(t_1) \chi^H(t_2)) | x, t \rangle &= \psi_0^*(x') \psi_0(x) e^{-\epsilon_0 t'} e^{-\epsilon_0 t} \\ &\quad \cdot \langle 0 | T(\chi^H(t_1) \chi^H(t_2)) | 0 \rangle \end{aligned}$$

Then equation (1.18) could be transformed into

$$G(t_1, t_2) = \lim_{\substack{t' \rightarrow -i\infty \\ t \rightarrow i\infty}} \frac{1}{\langle x', t' | x, t \rangle} \int \left[ \frac{dp dx}{2\pi} \right] x(t_1) x(t_2) e^{i \int_t^{t'} dt [p\dot{x} - H]} \quad (1.20)$$

The result obtained so far, can be intuitively generalised to the n-point Green's functions

$$\begin{aligned} G(t_1, \dots, t_n) &= \langle 0 | T(x^H(t_1) \dots x^H(t_n)) | 0 \rangle \\ &= \lim_{\substack{t' \rightarrow -i\infty \\ t \rightarrow i\infty}} \frac{1}{\langle x', t' | x, t \rangle} \int \left[ \frac{dp dx}{2\pi} \right] x(t_1) \dots x(t_n) \times \\ &\quad \times \exp \left\{ i \int_t^{t'} dt [p\dot{x} - H(p, x)] \right\} \end{aligned} \quad (1.21)$$

The set of Green's functions can be generated as follows

$$G(t_1, \dots, t_n) = \frac{(-i)^n \delta^n W[J]}{\delta J(t_1) \dots \delta J(t_n)} \Big|_{J=0} \quad (1.22)$$

where

$$W[J] = \lim_{\substack{t' \rightarrow -i\infty \\ t \rightarrow i\infty}} \frac{1}{\langle x', t' | x, t \rangle} \int \left[ \frac{dp dx}{2\pi} \right] e^{i \int_t^{t'} dt [p\dot{x} - H] + J(t) x(t)}$$

$W[J]$  can be considered as the transition amplitude from  $|0\rangle$  state at time "t" to  $|0\rangle$  state at time "t'" in the presence of an external source  $J_i(\mathcal{C})$ .



i.e. 
$$W[J] = \langle 0 | 0 \rangle_J \quad (1.23)$$

with the condition of normalisation

$$W[0] = 1 \quad (1.24)$$

The result (1.22) can be also generalised this time for a system of N degrees of freedom in the presence of external sources  $J_i(\zeta)$ .

Consequently one will have

$$W[J_1, \dots, J_N] = \lim_{\substack{t' \rightarrow -i\infty \\ t \rightarrow i\infty}} \int \prod_{i=1}^N [dx_i dp_i] \exp i \int_t^{t'} d\zeta [\mathcal{L} + \sum J_i(\zeta) \cdot x_i(\zeta)] \quad (1.25)$$

## I.2 Translation of P.I. formulation in Q.F.T.

One believes that Q.F.T. is the treatment of the physics of quantum systems with infinite degrees of freedom. As a result of the above one can change the classical physical quantities into their corresponding expressions in terms of field.

$$\prod_{i=1}^N [dx_i dp_i] \quad \text{will be} \quad [d\phi(x) d\pi(x)]$$

$$\text{and } L(x_i, \dot{x}_i) \quad \text{will be} \quad \int d^3x \mathcal{L}(\phi, \partial_\mu \phi)$$

$$\text{or } H(x_i, p_i) \quad \text{will be} \quad \int d^3x \mathcal{H}(\phi, \pi)$$

Then the path formulation can be naively obtained as follows.

$$W[J] \sim \int [d\phi] e^{i \int d^4x [\mathcal{L}(\phi(x)) + J(x)\phi(x)]} \quad (1.2.1)$$

Furthermore, a Wick rotation to imaginary time  $t \rightarrow -i t$  can be performed in such a way that one will obtain a very interesting result familiar to statistical physicists.

$$W_E[J] \sim \int [d\phi] e^{-\int d^4x [\mathcal{L}(\phi(x)) + J(x)\phi(x)]} \quad (1.2.2)$$

or

$$W_E[J] \sim \int [d\phi] e^{-S_E(\phi, J)} \quad (1.2.3)$$

where  $S_E$  is the Euclidean action of the system.

$W_E[J]$  reminds us that the fundamental quantity " $\mathcal{Z}$ " known as the partition function in statistical mechanics.

This means that one has made a direct connection between statistical physics and field theory. The Euclidean generating functional  $W_E[J]$  in field theory considered as a fundamental quantity corresponds to the partition function  $\mathcal{Z}$  in statistical physics. The only difference remains only on the dimension of the space on which one will work. One will deal with a four dimensional continuous Euclidean space whereas it is only a three-dimensional Euclidean space which is used in statistical physics.

### I.3 Application to the fermionic fields

The generating functional for the fermionic fields is

$$W[\eta, \bar{\eta}] = \int [d\psi(x)] [d\bar{\psi}(x)] e^{i \int \mathcal{L}(\psi, \bar{\psi}) + \bar{\eta}\psi + \bar{\psi}\eta \, d^4x} \quad (1.3.1)$$

with the usual anti-commutation relations between the fields

$$[\psi(x), \psi(x')]_+ = [\psi(x), \bar{\psi}(x')]_+ = [\bar{\psi}(x), \bar{\psi}(x')]_+ = 0 \quad (1.3.2)$$

The field of the sources is taken as having the same nature of the fermionic field, then

$$[\eta(x), \eta(x')]_+ = [\eta(x), \bar{\eta}(x')]_+ = [\bar{\eta}(x), \bar{\eta}(x')]_+ = 0 \quad (1.3.3)$$

The above fields are non-abelian, therefore they respect Grassman algebra and the integral involved in (1.3.1) is not that trivial.

However, one can briefly give some results and properties of the Grassman variables. In a  $n$ -dimensional Grassman algebra with its  $n$  generators  $\alpha_1 \dots \alpha_n$ , one has the useful properties.

$$[\alpha_i, \alpha_j]_+ = 0 \quad i, j = 1, 2, \dots, n$$

$$\frac{d}{d\alpha_i} (\alpha_1 \alpha_2 \dots \alpha_n) = \delta_{i,1} \alpha_2 \dots \alpha_n - \delta_{i,2} \alpha_1 \alpha_3 \dots \alpha_n + \dots + (-)^{n-1} \delta_{i,n} \alpha_1 \dots \alpha_{n-1}$$

$$(\alpha_1 \alpha_2 \dots \alpha_n) \frac{\overleftarrow{d}}{d\alpha_i} = \delta_{i,n} \alpha_1 \dots \alpha_{n-1} - \dots + (-)^{n-1} \delta_{1,i} \alpha_2 \dots \alpha_n$$

$$\int d\alpha_i = 0$$

$$\int d\alpha_i \alpha_j = \delta_{i,j}$$

$$\int d\beta_n \dots d\beta_1 p(\beta) = \int d\alpha_n \dots d\alpha_1 \left[ \det \left( \frac{d\beta}{d\alpha} \right) \right]^{-1} p(\beta(\alpha))$$

where

$$\beta_i = b_{ij} \alpha_j$$

In order that one can use these relations for the purpose of path calculations (in particular for fermionic fields), one will need to evaluate the following expression of the form

$$G(A) = \int d\alpha_n \dots d\alpha_1 e^{\frac{1}{2} \alpha_i A_{ij} \alpha_j}$$

One can take the simplest illustration with a 2 x 2 matrix A. A is supposed to be antisymmetric.

$$A = \begin{bmatrix} 0 & A_{12} \\ -A_{12} & 0 \end{bmatrix}$$

then

$$G(A) = \int d\alpha_2 d\alpha_1 e^{\frac{1}{2} \alpha_1 \alpha_2 A_{12}}$$

$$\begin{aligned} \text{Because } \alpha_i A_{ij} \alpha_j &= \alpha_1 A_{11} \alpha_1 + \alpha_1 A_{12} \alpha_2 + \alpha_2 A_{21} \alpha_1 + \alpha_2 A_{22} \alpha_2 \\ &= \frac{1}{2} (\alpha_1 A_{12} \alpha_2 - \alpha_2 A_{12} \alpha_1) \end{aligned}$$

$$\text{and } [\alpha_1, \alpha_2]_+ = 0$$

$$\text{One obtains } \frac{1}{2} \alpha_i A_{ij} \alpha_j = \alpha_1 \alpha_2 A_{12}$$

$$\begin{aligned} G(A) &= \int d\alpha_2 d\alpha_1 e^{\alpha_1 \alpha_2 A_{12}} \\ &= \int d\alpha_2 d\alpha_1 (1 + \alpha_1 \alpha_2 A_{12}) \\ G(A) &= A_{12} = \sqrt{\text{Det } A} \end{aligned}$$

Then

$$G(A) = \int d\alpha_2 d\alpha_1 e^{\frac{1}{2} \sum_{i,j} \alpha_i A_{ij} \alpha_j} = (\text{Det } A)^{\frac{1}{2}} \quad (1.3.5)$$

This result can be extended to the general result with a  
N x N antisymmetric matrix

$$\int d\alpha_1 \dots d\alpha_n e^{\frac{1}{2} \sum_{i,j} \alpha_i A_{ij} \alpha_j} = (\text{Det } A)^{1/2} \quad (1.3.6)$$

This result is the inverse of what one obtains with abelian  
real variables

$$\int \frac{dx_1}{\sqrt{2\pi}} \dots \frac{dx_n}{\sqrt{2\pi}} e^{-\frac{1}{2} (x_i A_{ij} x_j)} = 1 / \sqrt{\text{Det } A} \quad (1.3.7)$$

With complex Grassman variables one has

$$\int d\alpha_1 d\bar{\alpha}_1 \dots d\alpha_n d\bar{\alpha}_n e^{(\bar{\alpha}_i A_{ij} \alpha_j)} = (\text{Det } A) \quad (1.3.8)$$

as well as with abelian complex variables

$$\int \frac{dx_1}{\sqrt{\pi}} \dots \frac{dx_n}{\sqrt{\pi}} \frac{dx_1^*}{\sqrt{\pi}} \dots \frac{dx_n^*}{\sqrt{\pi}} e^{-x_i^* A_{ij} x_j} = 1 / \text{Det} A \quad (1.3.9)$$

In the case of fermion fields, one deals with Complex Grassman variables but they belong to an infinite-dimensional Grassman algebra and so, one will obtain the following

$$W_E = \int [d\psi] [d\bar{\psi}] e^{-\int \bar{\psi} M \psi} \propto \text{Det}(M) \quad (1.4.0)$$

#### I.4 Vacuum expectation value of an observable

When the Euclidean action of a physical system has the form,

$$S_E = \bar{\psi} M \psi + S_G \quad (1.4.1)$$

where the fermion action has a quadratic form, one can express the vacuum expectation value of an observable "O".

It can be computed in terms of a path integral

$$\langle O \rangle = \frac{1}{Z_E} \int [d\psi] [d\bar{\psi}] [d\psi] O(\bar{\psi}, \psi, \psi) e^{-(\bar{\psi} M \psi + S_G)} \quad (1.4.2)$$

where

$$\mathcal{Z}_e \equiv \int [d\psi] [d\bar{\psi}] e^{-(\bar{\psi} M \psi + S_G)} \quad (1.4.3)$$

From (1.4.0) one has

$$\langle O \rangle = \frac{\int [d\nu] \tilde{O}(\nu) \text{Det} M e^{-S_G}}{\int [d\nu] \text{Det} M e^{-S_G}} \quad (1.4.1)$$

which is a quite familiar result, if not the same, in statistical mechanics.

## II. Lattice formulation

### II.1 Lattice formulation for the gauge fields

All the experience and intuitions a statistical physicist can have, is a good background to study field theory once formulated in the lattice. This means that one simply approximates the universe by a four dimensional hypercube containing a finite number of sites separated by a constant distance "a", called the lattice spacing, (Fig. 1), and this in all the four directions of the space-time.

In statistical physics the fundamental quantity, as one has said previously, is the partition function  $\mathcal{Z}$  which is

$$\mathcal{Z} = \sum_i e^{-H_i/kT} \quad (2.1.1)$$

where  $H_i$  is the Hamiltonian at the state  $|i\rangle$ ,  $k$  is the Boltzman constant and  $T$  the temperature of the system.

In contrast with Euclidean quantum field theory, one has the generating functional and it can be written in case of pure Q.C.D. (quark effect neglected) as

$$\mathcal{Z}_{\text{pure}} = \int \mathcal{D}(u) e^{-S(u)} \quad (2.1.2)$$

where the theory is defined by  $(3 \times 3)$ ,  $SU(3)$  gauge matrices.

Once one considers the space-time as discretized the four dimensional integration will be replaced by a sum

$$\int d^4x \longrightarrow a^4 \sum_n \quad (2.1.3)$$



where "a" is the lattice spacing and a four dimensional derivative by finite differences.

$$\partial_\mu \phi(x) = \frac{1}{a} [\phi(x_n + a\hat{\mu}) - \phi(x_n)] \quad (2.1.4)$$

The expression of  $\mathcal{L}_{\text{pure}}$  can be changed now into a simple sum when the space is discretised.

$$\mathcal{L} \propto a^4 \sum_{\text{configurations}} e^{-S(\text{lattice})} \quad (2.1.5)$$

Using local gauge invariance and demanding locality of the interactions, one can postulate lattice actions which reproduce the Yang-Mills theory (Yang and Mills, 1954) once in the continuum limit ( $a \rightarrow 0$ ), <sup>and</sup> or the confinement of quarks once in the strong coupling limit.

## II.2 The action

In the lattice version, the matrix which reflects interactions between neighbouring sites  $n \rightarrow n + \mu$  is called the gauge link variable (Fig. 2).

Now, let us consider a four-dimensional hypercubic Euclidean lattice with spacing a. On each link of the lattice an SU(3) matrix is placed

$$U(n+\hat{\mu}, n) = \exp\left\{iag \frac{\lambda^i}{2} A_{n,\mu}^i\right\} \quad (2.2.1)$$

where  $\lambda^i$ ,  $i = 1, 2, \dots, 8$  are the usual Gell-mann matrices.

One has in the lattice version of gauge transformation

$$\begin{aligned}\Psi_n &\longrightarrow \phi_n \Psi_n \\ \bar{\Psi}_n &\longrightarrow \bar{\Psi}_n \phi_n^+\end{aligned}\tag{2.2.2}$$

and 
$$U(n+\hat{\mu}, n) \longrightarrow \phi_{n+\hat{\mu}} U(n+\hat{\mu}, n) \phi_n^+$$

where the SU(3) gauge symmetry is

$$\phi_n = \exp \left\{ i \frac{\lambda^i}{2} \theta_n^i \right\}\tag{2.2.3}$$

Therefore,  $\bar{\Psi}_n U(n, n+\hat{\mu}) \Psi_{n+\hat{\mu}}$  stays as a gauge-invariant quantity.

The action of pure Q.C.D. with gluons is suggested to be having the form (2), (18), (19).

$$S_G \propto -\frac{1}{2g^2} \sum_{n, \mu, \nu} \text{Tr} \left\{ U(n, n+\hat{\mu}) U(n+\hat{\mu}, n+\hat{\mu}+\hat{\nu}) U(n+\hat{\mu}+\hat{\nu}, n+\hat{\nu}) U(n+\hat{\nu}, n) \right\}\tag{2.2.4}$$

and one notices immediately that the action is simply a sum of the trace of a product of four link variables around an elementary square called a "plaquette" (Fig. 3). What is the physics of this proposed model?

- (1) Is the classical continuum limit ( $a \rightarrow 0$ ) an ordinary Yang-Mills theory?
- (2) Does the strong coupling limit confine quarks?

### II.3 The continuum limit

To take the classical limit, one must "taylor" expand the slowly varying fields  $B_\mu(n)$  which are defined as follows

$$B_\mu(n) = \frac{1}{2} a g \lambda_i A_{\mu,n}^i \quad (2.3.1)$$

Then the SU(3) gauge link matrices can be rewritten as

$$U(n+\hat{\mu}, n) = U_\mu(n) = \exp(i B_\mu(n)) \quad (2.3.2)$$

with respect to the following considerations

$$\left\{ \begin{array}{l} B_\nu(n+\hat{\mu}) \cong B_\nu(n) + a \partial_\mu B_\nu(n) + O(a^2) \\ B_{-\nu}(n+\hat{\mu}+\hat{\nu}) = -B_\mu(n+\hat{\nu}) \cong -[B_\mu(n) + a \partial_\nu B_\mu(n)] + O(a^2) \\ B_{-\nu}(n+\hat{\nu}) = -B_\nu(n) \end{array} \right. \quad (2.3.3)$$

One can transform equation (2.2.4) to the approximation

$$UUUU \cong e^{iB_\mu(n)} e^{i(B_\nu(n) + a\partial_\mu B_\nu(n))} e^{-i(B_\mu(n) + a\partial_\nu B_\mu(n))} e^{-iB_\nu(n)} \quad (2.3.4)$$

Now, by using the identity

$$e^A e^B = e^{A+B + \frac{1}{2}[A, B] + \dots} \quad (2.3.5)$$

one believes that

$$\begin{aligned} UUUU &\cong e^{(i(B_\mu(n) + B_\nu(n) + a\partial_\mu B_\nu(n)) - \frac{1}{2}[B_\mu(n), B_\nu(n)])} \\ &\cdot e^{(-i(B_\mu(n) + B_\nu(n) + a\partial_\nu B_\mu(n)) - \frac{1}{2}[B_\mu(n), B_\nu(n)])} \\ &\cong \exp\left(ia(\partial_\mu B_\nu(n) - \partial_\nu B_\mu(n)) - [B_\mu(n), B_\nu(n)]\right) \end{aligned} \quad (2.3.5)$$

Equation (2.3.5) can be redefined since one believes that

$$B_\mu(n) = \frac{1}{2} ag\lambda_i A_\mu^i(n) = ag A_\mu(n)$$

where  $A_\mu(n) \equiv \frac{1}{2} \lambda \cdot A(n)$

$$UUUU \cong e^{ia^2g\left\{\partial_\mu A_\nu(n) - \partial_\nu A_\mu(n) + ig[A_\mu^{(n)}, A_\nu^{(n)}]\right\}} \quad (2.3.6)$$

One recognises the conventional Yang-Mills field strength

$F_{\mu\nu}(n)$ .

$$UUUU \cong e^{ia^2g F_{\mu\nu}(n)}$$

This, puts the gluon action to be written as

$$S_G \cong -\frac{1}{2g^2} \sum_{\substack{\mu, \nu, \\ \gamma}} \text{Tr} \left( e^{ia^2g F_{\mu\nu}(n)} \right) \quad (2.3.7)$$

which it can be simplified to

$$\begin{aligned}
 \text{Tr} \left( e^{ia^2 g F_{\mu\nu}(n)} \right) &= \text{Tr} \left( 1 + ia^2 g F_{\mu\nu} - \frac{1}{2} a^4 g^2 F_{\mu\nu}^2 + \dots \right) \\
 &= \text{Tr} 1 + ia^2 g \text{Tr} F_{\mu\nu} - \frac{1}{2} a^4 g^2 \text{Tr} F_{\mu\nu}^2 + \dots \\
 &= \text{Tr} 1 - \frac{1}{2} a^4 g^2 \text{Tr} F_{\mu\nu}^2 + \dots
 \end{aligned}
 \tag{2.3.8}$$

∵  $F_{\mu\nu}$  is a generator then  $\text{Tr} F_{\mu\nu} = 0$ .

$$\text{Tr} F_{\mu\nu}^2 = \frac{1}{2} \left( \partial_\mu A_\nu^k - \partial_\nu A_\mu^k - g \epsilon_{ijk} A_\mu^i A_\nu^j \right)^2
 \tag{2.3.9}$$

where the fact that  $\text{Tr} \lambda_i \lambda_j = 2 \delta_{ij}$  has been used to find equation (2.3.9).

∵  $\epsilon_{ijk}$  is the usual antisymmetric Levi-Cevita tensor.

The action, now, settles on the given expression (to within a constant).

$$S_G \approx \frac{1}{2g^2} \int \frac{d^4x}{a^4} g^2 \frac{1}{2} \left( \partial_\mu A_\nu^k - g \epsilon_{ijk} A_\mu^i A_\nu^j - \partial_\nu A_\mu^k \right)^2
 \tag{2.3.10}$$

where  $\sum_{\mu, \nu}$  in (2.3.7) has been replaced by  $\int \frac{d^4x}{a^4} \sum_{\mu, \nu}$

Finally, one tends to the usual Euclidean action of classical Yang-Mills theory. (21)

$$S \equiv \frac{1}{4} \int d^4x (F_{\mu\nu}^i)^2
 \tag{2.3.11}$$

## II.4 Confinement criteria, the Wilson loop

What about the strong coupling limit? Is it characterised by quark confinement? This is what one will hope for, unless the action proposed in lattice Q.C.D. is not the adequate candidate which gives the real figure of Q.C.D. once formulated in the lattice. One believes that Wilson has made one of the most elegant formulation in lattice Q.C.D., and in fact confinement occurs in the strong coupling limit (Wilson, 1974; Polyakov, 1975; Wegner, 1971). The loop correlation function which is also the "Wilson correlation function" is the order parameter for the strong coupling limit exploration. Simply because it is related to the behaviour of the heavy potential interaction between a pair of quark and antiquark particles.

It can be formulated by the expectation value of the evolution operator  $\exp(-Ht)$  between one initial state and a final state.

$$\begin{aligned} \langle i | e^{-Ht} | f \rangle &\underset{t \rightarrow \infty}{=} e^{-V(r)t} \langle i | f \rangle \\ &\equiv \langle W(r,t) \rangle \end{aligned} \quad (2.4.1)$$

$V(r)$  is the potential and  $r$  is the distance between the pair of quarks. From the fact that one knows how to express the vacuum expectation value of an observable,  $W(r,t)$  will be computed by

$$\langle W(r,t) \rangle \equiv \frac{1}{\mathcal{Z}} \int [dU] W(r,t) e^{-S_G(U)} \quad (2.4.2)$$

In fact the action  $S_G$  from (2.2.4) is written as

$$S_G(U) = 1 - \frac{1}{N} \text{Real} (\text{Tr } U_{\square})$$

where  $\text{Tr } U_{\square} = \sum UUUU$

Then,  $S_G(U) = 1 - \frac{1}{2N} (\text{Tr } U_{\square} + \text{Tr } U_{\square}^{\dagger})$  .

And

$$e^{-S_G(U)} \simeq 1 - \frac{1}{2N} (\text{Tr } U_{\square} + \text{Tr } U_{\square}^{\dagger}) + \frac{1}{2!} \left(\frac{1}{2N}\right)^2 (\text{Tr } U_{\square} + \text{Tr } U_{\square}^{\dagger})^2$$

$$+ \dots + \frac{1}{\left(\frac{rt}{a^2}\right)!} \left(\frac{1}{2N}\right)^{\frac{rt}{a^2}} (\text{Tr } U_{\square} \text{Tr } U_{\square} \dots \text{Tr } U_{\square}) \quad (2.4.3)$$

$\therefore \left(\frac{rt}{a^2}\right)$  is the number of plaquettes (Fig. 4). Once one

uses the properties of the gauge link variables such as

$$\begin{cases} \int [dU] U_{ji} = 0 \\ \int [dU] U_{ji} U_{kl}^{-1} = \frac{1}{N} \delta_{jl} \delta_{ik} \end{cases} \quad (2.4.5)$$

Only the terms with  $\left(\frac{rt}{a^2}\right)$  contribute to the evaluation of  $\langle W(r,t) \rangle$

$$\langle W(r,t) \rangle = \left(\frac{1}{3g^2}\right)^{\frac{rt}{a^2}} = e^{-\left(\ln \frac{3g^2}{2}\right) r.t/a^2} \quad (2.4.6)$$

Once one identifies this result with (2.4.1), one will lead to the confining potential one hopefully has expected.

$$V(r) \simeq Kr \quad (2.4.7)$$

with

$$K = \frac{\ln 3g^2}{a^2} \quad (2.4.8)$$

where  $K$  is called as the string tension. The quark-antiquark potential seems to be growing without bounds.

$$V(r) \longrightarrow \infty \quad \text{for } R \longrightarrow \infty \quad (2.4.9)$$

and this obviously implies the confinement of the theory which one has to respect in view of starting lattice calculations.



### III. Monte-Carlo Simulation

#### III.1 Introduction

In lattice formulation the Feynmann path formula for the gauge theory is simply an ordinary sum for the partition function. This suggests that one attempts numerical calculations to evaluate this fundamental quantity mentioned so far.

However, the problem is not as simple as one would imagine, because a straight forward numerical computation seems to be practically impossible, and this can be given by the following example.

Consider a  $10^4$  lattice, which is a fairly reasonable lattice size, with a simple  $Z_2$  gauge theory. Such a system has, first of all, forty thousand link variables and consequently the partition function, once one tries to evaluate, becomes a sum with an enormous number of terms. Unfortunately this number is equal to

$$2^{40000} = 1.58 \times 10^{12041} \quad (3.1.1)$$

A simple way to avoid this ambiguity one must lead to statistical treatment in such a way that the computation can be feasible and this, by what one calls the Monte-Carlo simulation method.

The Monte-Carlo technique is quite an old method (24) in statistical physics and the idea, is to replace the expectation value of a physical quantity "O" which is

$$\langle O \rangle = \frac{1}{\mathcal{Z}} \sum_{[U_{ij}]} O(U_{ij}) e^{-S(U_{ij})}$$

by

$$\langle O \rangle_{h.c} = \frac{1}{N} \sum_i O(\{U\}_i) \quad (3.1.2)$$

Where the set  $\{U\}_i$  of configurations has a Boltzmann distribution law and "N" is the number of sets of configurations which significantly contribute to the average  $\langle O \rangle$ .

Note that each set of configurations  $\{U\}_i$  means a set of U matrices on all the links of the lattice. Then, it is clear that a configuration with very large value of the action does not effectively contribute to the path sum since  $e^{-\beta S}$  remains very small.

The aspect of the problem will be now shifted to the algorithm programmes which generate the set of configurations one would need.

There are two very well known computer algorithms capable of solving the problem; the first is the Metropolis algorithm and the second is the Heat bath algorithm. One will look only at the first one which is used in our calculations. (3), (20).

### III.2. The Metropolis et al. algorithm (3)

Basically, the Metropolis algorithm begins with a given configuration  $\{U\}$  of the lattice system. Then one gauge link variable is changed in order to obtain a new configuration  $\{U\}'$ . This new configuration is accepted unless it does not satisfy the rules of the algorithm and one must seek the thermal equilibrium after many "sweeps" which generate a gauge configuration  $\{U\}$  with a Boltzmann probability distribution.

Then the value of the physical quantity "O" can be calculated for the configuration  $\{U\}_1$  and recorded in the storage memory of the computer. The next step is to apply the previous procedure to the  $\{U\}_1$  configuration until one obtains another independent  $\{U\}_2$  configuration which has also a Boltzmann distribution.

Finally, the "job" is repeated several times and an average value of "O" can be estimated by

$$\begin{aligned}\langle O \rangle &= \frac{\sum_i O(\{U\}_i)}{\sum_i 1} \\ &= \frac{1}{N} \sum_i O(\{U\}_i)\end{aligned}$$

which is the equation (3.1.2).

Now, let us consider each procedure mentioned so far in more detail.

All occur at a given site, once one has a configuration  $\{U\}$  changed, (by changing a link) will obtain a new configuration  $\{U\}'$  which will be tested by the following rules. Compute the change  $\Delta S$  in the action  $S$ ; if  $\Delta S$  is negative or equal to zero, then the new configuration is accepted. If  $\Delta S$  is positive, then the  $\{U\}'$  is accepted but with a probability  $e^{-\Delta S}$  this time. (It is understood that  $S = (S\{U\}' - S\{U\})$ ).

In other words, one picks a random number "r" where  $r \in ]0, 1[$  and if  $e^{-\Delta S} > r$  the change is accepted. If  $e^{-\Delta S} < r$  the change is not accepted.

With this procedure, one can prove that a thermal equilibrium can be reached after one repeats the process several times and the probability to find a configuration will be proportional to the Boltzmann factor. To establish this, let us consider the relationship between the Nth and the (N+1)th process (can be called sweeps). The probability to find a configuration  $\{U\}$  after (N+1) sweeps is

$$P_{N+1}(U) = \sum_{\{U'\}} W(U' \rightarrow U) P_N(U') + \{1 - W(U \rightarrow U')\} P_N(U) \quad (3.2.1)$$

where  $W(U \rightarrow U')$  is the probability for the transition  $U \rightarrow U'$

It is clear that this process must converge to some stationary values, which implies the following condition for the thermal equilibrium.

$$P_{N+1}(U) = P_N(U) \quad (3.2.2)$$

From (3.1.3) one obtains

$$\sum_{\{U'\}} [P_N(U') W(U' \rightarrow U) - P_N(U) W(U \rightarrow U')] = 0 \quad (3.2.3)$$

which leads to the result

$$P_N^{\text{eq}}(U) W(U \rightarrow U') = P_N^{\text{eq}}(U') W(U' \rightarrow U) \quad (3.2.4)$$

Successive sweeps must bring us closer to satisfying the balance (eq. (3.1.6)). In the Metropolis algorithm one defines  $W(U \rightarrow U')$  to be equal to

$$W(U \rightarrow U') = \begin{cases} 1 & \text{if } S(U) \geq S(U') \\ e^{-[S(U') - S(U)]} & \text{if } S(U) < S(U') \end{cases} \quad (3.2.5)$$

From equation (3.1.6) one leads to the final result

$$P_N^{\text{eq}}(U) \propto C \cdot e^{-S(U)} \quad (3.2.6)$$

which is the requirement of the theory. (23)

### III.3. The modified Metropolis algorithm (23)

The previous method may not be practical since quantities calculated by M.C. methods will converge as  $1/\sqrt{n}$  which is a slowly falling function of  $n$ . One can repeat the Metropolis algorithm at each site several times before moving on to the next site to proceed with the same manner. Consequently, when one searches for an acceptable configuration, which is done by the computation of  $\Delta S$ , it will involve only the neighbouring plaquettes and then the probability of finding a new candidate for  $U_{ji}$  is increased. This idea is approved in the modified Metropolis algorithm and less time will be required to obtain an acceptable configuration.

## IV. Lattice formulation for the fermion field

### IV.1. The naive action

In order to have a complete lattice model of Q.C.D one must have some schemes for including fermions on the lattice, to reproduce more or less quarks contribution in the system.

However, several difficulties occur once one starts lattice calculations. One of the difficulties is that one finds  $2^4$  degeneracy of fermions in the continuum limit instead of one fermion which one has naively expected. (22) First of all, let us introduce the original action called the naive action which leads to the difficulty (the doubling problem) mentioned so far. Obviously, one requires to discretise the Dirac action.

$$S_F^{\text{continuum}} = \int d^4x \bar{\Psi} (\not{\partial} + im) \Psi \quad (4.1.1)$$

where  $\not{\partial}$  denotes the Dirac's operator

$$\not{\partial} = \gamma^\mu (\partial_\mu + ig A_\mu) \quad (4.1.2)$$

A natural way to represent S on the lattice is to associate fermion fields with lattice sites and to substitute derivatives by finite differences. Specifically, in order to have something which is symmetric and has the same hermiticity properties as the operators in the continuum theory, one would replace the first derivative with central differences and this action leads to what one has called the naive action.

$$S_F^N = \frac{1}{2a} \sum_{x,\mu} a^4 \left( \bar{\Psi}_x \gamma^\mu U_{x,x+\hat{\mu}} \Psi_{x+\hat{\mu}} - \bar{\Psi}_{x+\hat{\mu}} \gamma^\mu U_{x+\hat{\mu},x} \Psi_x \right) + i m a^4 \sum_x \bar{\Psi}_x \Psi_x \quad (4.1.3)$$

where the gauge link variables have been introduced to make the coupling among nearest neighbours covariant.

$$\bar{\Psi}_{x+\hat{\mu}} \Psi_x \longrightarrow \bar{\Psi}_{x+\hat{\mu}} \gamma^\mu U_{x+\hat{\mu},x} \Psi_x \quad (4.1.4)$$

The doubling problem can be seen easily once one analyses the continuum limit simply with the free case; with  $U = 1$ , and it is convenient to rescale the field variable  $\Psi$  as follows:

$$\Psi \longrightarrow a^{-3/2} \Psi \quad (4.1.5)$$

Then, the action becomes

$$S_F^N = \frac{1}{2} \sum_{x,\mu} \left( \bar{\Psi}_x \gamma^\mu \Psi_{x+\hat{\mu}} - \bar{\Psi}_{x+\hat{\mu}} \gamma^\mu \Psi_x \right) + i m a \sum_x \bar{\Psi}_x \Psi_x \quad (4.1.6)$$

and now, one can mention that "a" has been incorporated with the mass term.

The continuum propagator equation for the free fermions is



$$(\gamma^\mu \partial_\mu + ma) G(x' - x) = \delta^4(x' - x) \quad (4.1.7)$$

where

$$[\gamma^\mu, \gamma^\nu]_+ = 2\delta^{\mu\nu} \quad (4.1.8)$$

As a result of this, the lattice propagator equation can be written as: (In case of free fermions)

$$\frac{1}{2} \sum_\mu \gamma^\mu [G(n+\mu) - G(n-\mu)] + ma G(n) = \delta_{n,0} \quad (4.1.9)$$

The next step is to write equation (4.1.9) in the momentum space and this can be done via the Fourier transform

$$G(n) = \sum_P e^{ip \cdot n} G(p) \quad (4.1.10)$$

Consequently, equation (4.1.9) becomes

$$\begin{aligned} \frac{1}{2} \sum_\mu \gamma^\mu \left[ \sum_P [e^{ip(n+\mu)} - e^{ip(n-\mu)}] G(p) \right] + ma \sum_P e^{ipn} G(p) \\ = \delta_{n,0} \end{aligned} \quad (4.1.11)$$

One can transform equation (4.1.11) more, as follows

$$\sum_P e^{ipn} G(p) \left[ \sum_\mu \gamma^\mu \left( \frac{e^{ip_\mu a} - e^{-ip_\mu a}}{2} \right) + ma \right] = \delta_{n,0} \quad (4.1.12)$$

where,  $p_\mu a = p \cdot \mu$  (4.1.13)

and  $-\frac{\pi}{a} \leq p_\mu \leq \frac{\pi}{a}$  for each  $\mu$  direction.

Equation (4.1.12) gives the fermion propagator in the momentum space

$$G(p) = \frac{1}{ma + \sum_\mu \gamma^\mu \sin p_\mu a} \quad (4.1.14)$$

Putting  $m = 0$  and using equation (4.1.8) one obtains

$$G(p) = \frac{\sum_\mu \gamma^\mu \sin p_\mu a}{\sum_\mu \sin^2 p_\mu a} \quad (4.1.15)$$

It is clear that  $G(p)$  has a periodic structure in the Brillouin zone ( $p_\mu \in [-\frac{\pi}{a}, \frac{\pi}{a}]$ )

There are  $16 = 2^4$  unexpected poles at

$$P = (0,0,0,0), P = (\frac{\pi}{a}, 0,0,0), \dots p = (\frac{\pi}{a}, \frac{\pi}{a}, \frac{\pi}{a}, \frac{\pi}{a})$$

Thus, in a  $D$  dimensional lattice one finds  $2^D$  species which survive in the continuum limit. The naive theory finds  $2^D - 1$  unwanted flavors as the cut-off is removed ( $a \rightarrow 0$ ). (16)

#### IV.2. Wilson's action (2)

The idea of Wilson consists in adding some terms in the naive action in order to modify the dispersion formula;

which means that the 15 poles will be decoupled from the central pole. This is done by adding the following term:

$$\frac{1}{2} \sum_{x,\mu} \bar{\Psi}_x \gamma^\mu (\Psi_{x+\hat{\mu}} - 2\Psi_x + \Psi_{x-\hat{\mu}}) \quad (4.1.17)$$

As a result, the fermion propagator equation becomes

$$\delta_{n,0} = \sum_{\mu} \left\{ (1-\gamma_{\mu}) G(n-\mu) + (1+\gamma_{\mu}) G(n+\mu) \right\} + (ma-8)G(n). \quad (4.1.18)$$

And after the Fourier transform, this equation can be rewritten in the momentum space.

$$\begin{aligned} \sum_{\mu} (1-\gamma_{\mu}) \sum_p G(p) e^{ip(n-\mu)} + \sum_{\mu} (1+\gamma_{\mu}) \sum_p G(p) e^{ip(n+\mu)} + \\ + (ma-8) \sum_p G(p) e^{ipn} = \delta_{n,0} \end{aligned} \quad (4.1.19)$$

or

$$\sum_p e^{ipn} G(p) \left[ \sum_{\mu} (1-\gamma_{\mu}) e^{ip_{\mu}a} + (1+\gamma_{\mu}) e^{ip_{\mu}a} + (ma-8) \right] = \delta_{n,0} \quad (4.1.20)$$

which leads to

$$G(p) = \frac{1}{\sum_{\mu} (1-\gamma_{\mu}) e^{-ip_{\mu}a} + (1+\gamma_{\mu}) e^{ip_{\mu}a} + (ma-8)} \quad (4.1.21)$$

Putting  $m = 0$

$$G(p) = \frac{1}{2 \sum_{\mu} \gamma_{\mu} \sin p_{\mu} a + 2 \sum_{\mu} (\cos p_{\mu} a - 1)} \quad (4.1.22)$$

Now  $G(p)$  has still a pole at  $p = (0,0,0,0)$  while the other 15 poles have been removed. However, the action has neither continuous nor discrete  $\gamma_5$  symmetry.

#### IV.3. Kogut-Susskind action with spin diagonalisation (4)

If one does a unitary transformation on the fermion field variable  $\Psi$  called spin diagonalisation, one should be able to decouple the 16 flavors of naive fermions into four groups of four fermions.

At any site  $x^{\mu} = (x,y,z,t)$  the fermion field variable  $\Psi$  should be transformed to the following variable  $\chi$

$$\Psi = \gamma_1^x \gamma_2^y \gamma_3^z \gamma_4^t \chi \quad (4.3.1)$$

And also

$$\bar{\Psi} = \bar{\chi} \gamma_4^t \gamma_3^z \gamma_2^y \gamma_1^x \quad (4.3.2)$$

It is clear that the transformation is unitary since

$$\bar{\Psi} \Psi = \bar{\chi} \chi \quad (4.3.3)$$

The four components of  $\chi$  are decoupled and can be considered as four independent fermion fields with just four species doubling each.

Then one can introduce the Kogut-Susskind action as similar to

$$S_F^{K-S} = \bar{\Psi} (M_{K-S} + 2ma) \Psi \quad (4.3.4)$$

$$= \sum_{x,\mu} f_\mu(x) \left\{ \bar{\Psi}_x U_{x,x+\mu} \Psi_{x+\mu} - h.c \right\} + 2ma \sum_x \bar{\Psi}_x \Psi_x \quad (4.3.5)$$

where  $M_{K-S}$  has been defined as

$$\bar{\Psi} M_N \Psi = \sum_{d=1}^4 \bar{\chi}_d M_{K-S} \chi_d \quad (4.3.6)$$

which is the Kogut-Susskind fermion matrix.  $\alpha$  reads for the flavor number and  $f_\mu(x)$  for the fermion sign.

$$f_\mu(x) = \begin{cases} 1 & \mu = x_1 \\ (-)^{x_1} & \mu = x_2 \\ (-)^{x_1+x_2} & \mu = x_3 \\ (-)^{x_1+x_2+x_3} & \mu = t \end{cases} \quad (4.3.7)$$

The doubling problem still remains as one has noticed so far, but chiral symmetry has been recovered for  $m = 0$ .



One can write  $\mathcal{X}$  as a set of column vector

$$\mathcal{X} = (x_1, x_2, \dots, x_N) \quad (5.1.3)$$

These vectors are called the lanczos vectors and they are orthonormal

$$x_i^+ x_j = \delta_{ij} \quad (5.1.4)$$

These properties considered all together lead to what one calls the lanczos equations from which the  $\alpha_i$ ,  $\rho_i$  and even  $x_i$  can be deduced recursively.

One has

$$\mathcal{X}^+ H \mathcal{X} = T \quad \Leftrightarrow \quad \mathcal{X} \mathcal{X}^+ H \mathcal{X} = \mathcal{X} T$$

$$\text{Consequently, } H \mathcal{X} = \mathcal{X} T \quad (5.1.5)$$

The lanczos equations can be obtained from (5.1.5) by considering the form of the matrix T in (5.1.2)

- a)  $Hx_1 = \alpha_1 x_1 + \rho_1 x_2$
- b)  $Hx_i = \rho_{i-1} x_{i-1} + \alpha_i x_i + \rho_i x_{i+1}, \quad 2 \leq i \leq N-1$
- c)  $Hx_N = \rho_{N-1} x_{N-1} + \alpha_N x_N$

The first procedure is to choose  $x_1$  to be any unit vector.

For instance

$$x_1 = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \quad (5.1.6)$$

Then, one takes the scalar product of  $X_1$  with the first lanczos equation and uses the equation (5.1.4), which is the orthonormality equation of the lanczos vectors. This will lead to the following value of  $\alpha_1$

$$\alpha_1 = X_1^+ H X_1 \quad (5.1.7)$$

It is clear that  $\alpha_1$  is real, because of the hermiticity of  $H$ .

$$\alpha_1^* = X_1^+ H^+ X_1 = X_1^+ H X_1 = \alpha_1 \quad (5.1.8)$$

The second step is to obtain  $\beta_1$  and the second lanczos vector  $X_2$ .

From the 1st lanczos equation one can compute the following.

$$\beta_1 X_2 = H X_1 - \alpha_1 X_1$$

Then, uses the fact that

$$X_2^+ X_2 = 1$$

As a result

$$\beta_1 = \left| H X_1 - \alpha_1 X_1 \right| \quad (5.1.9)$$

and 
$$X_2 = \frac{1}{\beta_1} (H X_1 - \alpha_1 X_1)$$

One can compute similarly to find the  $\alpha_i$ 's, the  $\beta_i$ 's and  $X_i$ 's after using the second lanczos equation.

$$\alpha_i = X_i^+ H X_i \quad (5.1.10)$$

$$\beta_i = \left| H X_i - \beta_{i-1} X_{i-1} - \alpha_i X_i \right| \quad (5.1.11)$$

$$X_i = \frac{1}{\beta_{i-1}} (H X_{i-1} - \beta_{i-2} X_{i-2} - \alpha_{i-1} X_{i-1}) \quad (5.1.12)$$



Finally, this defines the lanczos algorithm but it would be rather safe to check that the hermitian nature of  $H$  ensures the orthogonality of the lanczos vectors at any stage of the calculation. One has to show, for a simple illustration, that  $X_1$  is orthogonal to  $X_2$ .

$$\begin{aligned} X_1^+ X_2 &= X_1^+ \left[ \frac{1}{\beta_1} (HX_1 - \alpha_1 X_1) \right] \\ &= \frac{1}{\beta_1} (X_1^+ H X_1 - \alpha_1 X_1^+ X_1) \end{aligned}$$

So far, it has been proved that  $\alpha_1 = X_1^+ H X_1$  (equation 5.1.8), and that is due to the hermiticity of  $H$ , which includes that

$$X_1^+ X_2 = \frac{1}{\beta_1} (\alpha_1 - \alpha_1) = 0 \quad (5.1.13)$$

which is the case for all the rest of the lanczos vectors.

From the last equation, one can find that

$$\alpha_N = X_N^+ H X_N \quad (5.1.14)$$

which is the last parameter to find by the algorithm.

Nevertheless, one can fail into problems, particularly when  $\beta$  in some steps is equal to zero, then one will have a division by zero. That simply means that the first lanczos vector is orthogonal to some eigenvector of the matrix  $H$ .

The solution to this problem is to continue the calculation by choosing the next  $X_i$  to be any unit vector orthogonal to all the predecessor vectors. It seems to be slightly difficult to compute this idea practically, but since one has never failed in this situation, one has ignored it.

One has to add another procedure to the algorithm so that it increases its efficiency because it seems that after few iterations one might notice the loss of the orthogonality between the lanczos vectors  $X_i$  and it is impossible to overcome this problem by increasing the precision while the errors tend to build up exponentially. Then it is essential to reorthogonalise.

The new lanczos vector  $X_i$  can be made orthogonal to the previous lanczos vector  $X_j$  simply by the following transformation.

$$X_i \longrightarrow X_i = X_i - X_j(X_j^+ X_i) \quad (5.1.15)$$

That reduces the loss of orthogonality between lanczos vectors and it is quite reasonable not to reorthogonalise at each iteration when the eigenvalues of  $H$  are relatively well separated.

## V.2. The non-hermitian lanczos method (7)

The previous modified lanczos method can be generalised for tridiagonalising arbitrary complex matrices. One requires a bi-unitary transformation

$$\begin{aligned} T &= Y^+ H X \\ T^+ &= X^+ H^+ Y \\ Y^+ X &= I \end{aligned} \quad (5.2.1)$$

$T$  is the tridiagonal, symmetric matrix which one wants to obtain. Similarly  $X$  and  $Y$  can be written as a set of column vectors

$$\begin{aligned} Y &= (Y_1, Y_2, \dots, Y_N) \\ X &= (X_1, X_2, \dots, X_N) \end{aligned} \quad (5.2.2)$$

They are also called the lanczos vector and satisfy a bi-orthogonality property

$$Y_i^+ X_j = \delta_{ij} \quad (5.2.3)$$

As a result of this, one obtains the first lanczos equations, practically with the same way as in the previous method.

$$\begin{aligned} HX_1 &= \alpha_1 X_1 + \beta_1 X_2 \\ H^+ Y_1 &= \alpha_1^* Y_1 + \beta_1^* Y_2 \end{aligned} \quad (5.2.4)$$

The next step is also as in the first method, one simply chooses  $X_1$  and  $Y_1$  as unit vectors and by using (5.2.3) one will obtain

$$\alpha_1 = Y_1^+ H X_1 \quad (5.2.5)$$

Then, it is possible to compute

$$\begin{aligned} \beta_1 X_2 &= H X_1 - \alpha_1 X_1 \\ \text{and } \beta_1^* Y_2 &= H^+ Y_1 - \alpha_1^* Y_1 \end{aligned}$$

where it is easy to find  $\beta_1$

$$(\beta_1^* Y_2)^+ (\beta_1 X_2) = \beta_1^2 = (H^+ Y_1 - \alpha_1^* Y_1)^+ (H X_1 - \alpha_1 X_1)$$

In other words

$$\beta_1 = \left| (H^+ Y_1 - \alpha_1^* Y_1)^+ (H X_1 - \alpha_1 X_1) \right| \quad (5.2.6)$$

Finally, one can get the second lanczos vectors

$$X_2 = \frac{1}{\beta_1} (H X_1 - \alpha_1 X_1) \quad (5.2.7)$$

and

$$Y_2 = \frac{1}{\beta_1^*} (H^+ Y_1 - \alpha_1^* Y_1)$$

which will satisfy the bi-orthogonality property

$$Y_2^+ X_2 = 1$$

One can continue in a similar way to find the rest of the  $\alpha_i$ 's  $\beta_i$ 's and the lanczos vectors

$$\alpha_i = Y_i^+ H X_i \quad (5.2.8)$$

$$\beta_i = \left| \begin{array}{l} (H^+ Y_i - \alpha_i^* Y_i - \beta_{i-1}^* Y_{i-1})^+ \\ \cdot (H X_i - \alpha_i X_i - \beta_{i-1} X_{i-1}) \end{array} \right|$$

$$X_{i+1} = \frac{1}{\beta_i} (H X_i - \alpha_i X_i - \beta_{i-1} X_{i-1})$$

and 
$$Y_{i+1} = \frac{1}{\beta_i^*} (H^+ Y_i - \alpha_i^* Y_i - \beta_{i-1}^* Y_{i-1}) \quad (5.2.9)$$

Furthermore, one completes the algorithm when one obtains the value of  $\alpha_N$

$$\alpha_N = Y_N^+ H X_N \quad (5.2.10)$$

and theoretically one must check the condition (5.2.3)

between the lanczos vectors. As an example one takes

$$Y_1^+ X_2 = \frac{1}{\beta_1^*} \left[ Y_1^+ (H X_1 - \alpha_1 X_1) \right] = \frac{1}{\beta_1^*} (\alpha_1 - \alpha_1) = 0 \quad (5.2.11)$$

This is the case where there are not any rounding errors.

However, it seems to be the case after some iterations and the process needs the re-orthogonalisation again, as previously mentioned. It is done simply by the projection of the lanczos vectors  $X_i, Y_j$  on the earlier ones  $X_j$  and  $Y_j$

$$\begin{aligned} X_i &\longrightarrow X_i \equiv X_i - X_j (Y_j^+ X_i) \\ Y_i &\longrightarrow Y_i \equiv Y_i - Y_j (X_j^+ Y_i) \end{aligned} \quad (5.2.12)$$

### V.3. Application of the method in lattice Q.C.D.

After one has introduced the lattice formulation in the previous chapters, one can see the use of lanczos algorithm in our calculation.

If  $N_s$  and  $N_t$  are the number of sites along the spatial and temporal directions respectively, and if  $a_s$  and  $a_t$  are the lattice spacing along the spatial and temporal directions respectively, one would write the complete action discretized as follows:

$$S = S_F + S_G$$

where

$$S_G = \frac{2N_c}{g^2} \frac{a_t}{a_s} \sum_{\text{spatial plaquettes}} \left[ 1 - \frac{1}{N_c} \text{Real} (\text{Tr} UUUU) \right] \\ + \frac{2N_c}{g^2} \frac{a_s}{a_t} \sum_{\text{temporal plaquettes}} \left[ 1 - \frac{1}{N_c} \text{Real} (\text{Tr} UUUU) \right]$$

which is the well-known gluon action

and

$$S_F \propto \sum_{n,\mu} \bar{\Psi}_n U_{n,n+\mu} \int_{n,n+\mu} \Psi_{n+\mu} \quad - \quad \text{hermitian conjugate}$$

which is the fermion action in the Kogut-Susskind scheme.

This means

∴  $\Psi_n$  is the single colour triplet sited at

$$n = (x_1, x_2, x_3, t)$$

∴  $\mu$  is the 4 directions index in the space - time.

- ∴  $\mu$  is the displacement vector of length  $a$ , in direction  $\mu$ .
- ∴  $\mu_{n, n + \hat{\mu}}$  is a  $3 \times 3$  gauge matrix joining sites  $n$  and  $n + \mu$
- ∴  $f_{n, n + \hat{\mu}}$  is the fermion sign factor.

The fermion action can be simply written as

$$S_F = - \bar{\Psi} (M + 2ma) \Psi \quad (5.3.1)$$

Since  $S_F$  has a quadratic form the integral involved in the calculation of the fundamental quantity which is the partition function appears as a Gaussian, then it is natural to integrate out Grassmann fermion fields variable in that case. Then,  $\mathcal{Z}$  is written as

$$\mathcal{Z} \equiv \int \mathcal{D}[U] e^{-S_G} \text{Det } H \quad (5.3.2)$$

where  $H = M + 2ma$ .

This reminds us that  $\text{Det} H$  contains the dynamics of Q.C.D in lattice and to simulate this dynamical effect in M.C. simulation means the computation of the determinant of  $H$  at each change of link because it is needed at any trial of new configuration accepted by the Metropolis algorithm.

This is called the updating of dynamical fermions in M.C. simulation. As far as the application of Lanczos algorithm is concerned, the inversion of the matrix  $H$  is needed, then performed this time in the updating. (8)

In fact, the ratio of the determinant of H corresponding respectively to two configurations is computed

$$\begin{aligned}
 R &= \frac{\det(H + \Delta)}{\det(H)} \\
 &= \det(1 + H^{-1} \Delta) \qquad \qquad \qquad 5.3.3)
 \end{aligned}$$

where  $\Delta$  is the change in the fermion matrix once the link is changed. It is important to notice that  $\Delta$  is different from zero only in the 6 x 6 block corresponding to the two end points of the link involved in the change. Then, once one has the value of  $H^{-1}$  in this region, will be able to update the same link as many times as wanted.

Indeed, it is possible to modify the lanczos method and try to make it much faster in its execution for the updating purpose.

One has not discussed the inversion of a sparse matrix by the lanczos method because it is not used to compare the results with the new method in our calculations.

Nevertheless, the candidate for the inversion of H is called the block lanczos method and has already been developed for both cases, the hermitian and the non-hermitian case. Basically, it consists of considering the alphas and betas as elementary matrices and the lanczos equations will be modified with respect to the new hypothesis.

The block lanczos method stays as a standard method with good convergence properties for the updating in M.C. procedure, but one is not going to introduce it because it is not used in our trial on setting the new method. However, one must point out that, in our "trial of setting the new method" for the updating purpose, one will need the lanczos method for tridiagonalising the fermion matrix  $H$  and evaluate  $\text{Det } H$  (equation 5.3.3). On the basis of the results obtained by the lanczos method like the distribution function of the eigenvalues, the maximum eigenvalue, the determinant of  $H$ , and the ratio of two determinants corresponding respectively to two configurations differing only on one link changed; one will try to introduce the new method which really does not need a long time to compute these results. Therefore, it will be practical to update dynamical fermion in M.C. simulation with less time required than in the block lanczos method. (25)



## VI. The new method

The method consists simply of studying the form of the spectral density function which is the distribution function of the eigenvalues of the fermion matrix. One is in the case of the Kogut-Susskind scheme, where only the neighbouring sites can interact between each other, in the lattice, via the gauge link matrices which correspond to the colour interaction transported by the gluons. Then, the fermion matrix has the following form

$$H = (M + 2mai) = \begin{pmatrix} 2mai & M \\ M^+ & 2mai \end{pmatrix} \quad (6.1.1)$$

For the calculations below, one will consider first  $m = 0$  in order to work out the trace of matrices like  $H^2$ ,  $H^4$ ,  $H^6$ .

### VI.1 The fermion matrix

One is interested in the computation of the trace of the fermion matrix at any power, in terms of elementary loops of different orders, and this will depend on the accuracy required by the new method. One can prove easily that traces of  $H^4$ ,  $H^6$ , ...,  $H^{2n}$  are formulated by calculating simply the average value of loops of order, 4, 6, ...,  $2n$  in the lattice.

An example can be shown clearly in a 2-dimensional lattice of 16 sites which is in fact a  $4^2$  lattice, and an extension of the idea becomes clearer for a four dimensional lattice.

In the case of a  $4^2$  lattice, and with respect to the Kogut-Susskind scheme, one has the form of the fermion matrix shown in Figure 5, with the 32 links representing the gauge interaction.\* In fact this implies  $32 \times 32$  non-zero elements in the matrix, which one is going to deal with.

Consequently, the trace of  $H^4$  can be found easily, once one knows the form of  $H$  (or  $M$ , in fact) and furthermore, only the top diagonal element of  $M^4$  has to be known, because of the symmetry of the lattice.

Now, the problem becomes simple, and the element  $M_{1,1}^4$  of the matrix  $M$  is equal to

$$\begin{aligned}
 M_{1,1}^4 = & 16 + (U_1 U_5 U_5^\dagger U_1^\dagger + U_1 U_5 U_8 U_2^\dagger + U_2 U_8^\dagger U_5^\dagger U_1^\dagger + U_2 U_8^\dagger U_8 U_2^\dagger) \\
 & + (U_1 U_6 U_6^\dagger U_1^\dagger + U_1 U_6 U_{13}^\dagger U_3^\dagger + U_3 U_{13}^\dagger U_6^\dagger U_1^\dagger + U_3 U_{13}^\dagger U_{13}^\dagger U_3^\dagger) \\
 & + (U_2 U_{11} U_{11}^\dagger U_2^\dagger + U_2 U_{11} U_{14}^\dagger U_3^\dagger + U_3 U_{14}^\dagger U_{11}^\dagger U_2^\dagger + U_3 U_{14}^\dagger U_{14}^\dagger U_3^\dagger) \\
 & + (U_3 U_{15} U_{15}^\dagger U_3^\dagger + U_3 U_{15} U_{23}^\dagger U_4^\dagger + U_4 U_{23}^\dagger U_{15}^\dagger U_3^\dagger + U_4 U_{23}^\dagger U_{23}^\dagger U_4^\dagger) \\
 & + (U_1 U_7 U_7^\dagger U_1^\dagger + U_1 U_7 U_{29}^\dagger U_4^\dagger + U_4 U_{29}^\dagger U_7^\dagger U_1^\dagger + U_4 U_{29}^\dagger U_{29}^\dagger U_4^\dagger) \\
 & + (U_2 U_{12} U_{12}^\dagger U_2^\dagger + U_2 U_{12} U_{30}^\dagger U_4^\dagger + U_4 U_{30}^\dagger U_{12}^\dagger U_2^\dagger + U_4 U_{30}^\dagger U_{30}^\dagger U_4^\dagger).
 \end{aligned}
 \tag{6.1.2}$$

One recognises different species of loops in equation (6.1.2), and it is important to classify them to formulate the trace of  $M^4$ .

One recognizes the loop like  $(U_1 U_5 U_5^\dagger U_1^\dagger)$  as a constant because of the property of the gauge links

$$U_i^\dagger U_j = \delta_{ij} \tag{6.1.3}$$

\*See Figure 5'.

then  $(U_1 U_5 U_5^+ U_1^+) = 1$  for example.

One also recognizes the loop like  $(U_1 U_5 U_8 U_2^+)$  as a polyakov loop which is non-zero, and there are four of them in the expression of  $M_{1,1}^4$ .

The final loops are the well-known "plaquettes" which are the loops like  $U_1 U_6 U_{13}^+ U_3^+$  or  $U_2 U_{12} U_{30}^+ U_4^+$  etc..., and there are eight of them in total.

This idea concerns only a site in the lattice or one element of the diagonal of  $M^4$  but it is the same case for all the sites. The trace of  $M^4$  is then  $3 N_S$  times the average values of the loops which occur in a similar manner in the calculations.  $N_S$  is the number of sites in the lattice, and 3 corresponds to the dimension of the SU(3) group. As a result, one has

$$\text{Tr } M^4 = 48(16 - 8 \langle \square \rangle) + \sum \text{Polyakovs}$$

where  $\langle \square \rangle$  is the average plaquettes value and the associated (-) sign arises from the Dirac gamma matrices. One has to notice that the trace of  $M^4$  or  $M^6$ , or even higher degrees of power, can be worked out only by computing the number of possible loops with their values. Especially, when one works on a 4-dimensional lattice, the access to the computer becomes crucial to count the possible loops, and this is not trivial, in particular for higher order loops in the lattice.

However, in a 4-dimensional lattice it is easy to find that there are 48 possible plaquettes per site, 24 in one direction and 24 in the other direction and Trace  $M^4$  can be

expressed by

$$\text{Tr } M^4 = 3N_S(8^2 + 8 \times 7 - 48 \langle \square \rangle) + \sum \text{Polyakovs} \quad (6.1.5)$$

for example, in a  $4^4$  lattice  $N_S = 4^4 = 256$  sites.

For higher degrees of the trace  $M^n$ , computer calculations are required to find the number of loops of different species in the lattice. But one has to be careful on finding all the possible kinds of loops which are in the expression of  $\text{Tr } M^n$ . A good example of this is that one has worked out the formula for  $\text{Tr } M^6$ , where the loops like the one shown in Figure (6) have to be computed.

Finally  $\text{Tr } M^6$  is given by the following expression.

$$\text{Tr } M^6 = 3N_S(2192 - 2016 \langle \square \rangle + 912 \text{ loop6}) + \sum \text{Polyakovs} \quad (6.1.6)$$

for example in a  $6^4$  lattice,  $N_S = 6^4 = 1296$  sites.

It is also clear that Trace  $M^4$  in a  $6^4$  lattice is given by

$$\text{Tr } M^4 = 3N_S(8^2 + 8 \times 7 - 48 \langle \square \rangle) \quad (6.1.7)$$

One has noticed immediately the difference from equation (6.1.6); this is simply due to the reason that in a  $6^4$  lattice the polyakov loops of order 4 cannot exist and then,  $\text{Tr } M^4$  is simpler.

After all, one can prove the exactness of these formulae by computing  $\text{Tr } M^4$  and  $\text{Tr } M^6$  via the Lanczos method which will give the eigenvalue of  $M$  and one has

$$\begin{aligned} \text{Tr } M^4 &= \sum_i \lambda_i^4 \\ \text{and } \text{Tr } M^6 &= \sum_i \lambda_i^6 \end{aligned} \quad (6.1.8)$$

Finally the results confirm each other, so that one could say that equations (6.1.6), (6.1.7) and (6.1.5) are correct.

For instance, one obtains that the total sum of the eigenvalues to the power six and four are

$$\sum \lambda_i^6 = 515861350$$

$$\sum \lambda_i^4 = 370601.20$$

and that the trace of  $M^6$  or  $M^4$  obtained from equation (6.1.8) and (6.1.9) respectively are the following

$$\text{Tr } M^6 = 5156830.0$$

$$\text{and } \text{Tr } M^4 = 370638.25$$

$$\text{where } \langle \square \rangle = -0.51398402$$

$$\text{Pol} = 68.955$$

$$\text{Loop6} = 0.6630476 \cdot 10^6$$

This was in a  $6^4$  lattice at  $\beta = 5.5$ .

## VI.2 The spectral density

The aim of our research is to find out the actual real form of the spectral density function of the eigenvalue of the fermion matrix and predict analytically the value of the determinant at any configuration of the lattice, then the ratio to implement dynamical fermion in M.C. simulation. (8)

After several observations on the form of the function  $\rho(\lambda)$  which is the spectral density, one proposes the following analytical form of it

$$\rho(\lambda) = (A + B\lambda^2 + C\lambda^4 + \dots) \sqrt{\lambda_M^2 - \lambda^2} \quad (6.2.1)$$

The odd powers of  $|\lambda|$  could be included in the polynomial part of  $\rho$ , but since  $\rho(\lambda)$  in (6.2.1) has fitted the set

of eigenvalues of the diagonalised form of  $M$ , one has to say that they do not contribute in the calculations. The anti-hermiticity of  $M$  implies that the eigenvalues come in pairs of equal and opposite sign; then one is going to treat to positive eigenvalues distribution which is the same for the negative eigenvalues. Obviously, one assumes in the above and below that one is in the chirally broken phase, which means that the spectro-function  $\rho(\lambda)$  is non-zero between 0 and  $\lambda_M$ , but the formulation of the spectro function could be easily extended to the unbroken phase by considering that  $\rho(\lambda)$  is equal to zero at a particular minimum eigenvalue  $\lambda_{\min}$ . (9)

In equation (6.2.1),  $\rho(\lambda)$  is parametrised by the unknown variables  $A, B, C, \dots$  and  $\lambda_{\max}$  which is the maximum positive eigenvalue of  $M$ , and they can be evaluated by setting up a system of equations. These equations come from the fact that one knows some properties of the normalised spectro-function. First of all one has

$$\int_{-\lambda_{\max}}^{\lambda_{\max}} \rho(\lambda) d\lambda = 1 \quad (6.2.2)$$

and

$$\int_{-\lambda_{\max}}^{\lambda_{\max}} \lambda^2 \rho(\lambda) d\lambda = \frac{\text{Tr } M^2}{3 N_S} = 8 \quad (6.2.3)$$

$$\int_{-\lambda_{\max}}^{\lambda_{\max}} \lambda^4 \rho(\lambda) d\lambda = \frac{\text{Tr } M^4}{3 N_S} \quad (6.2.4)$$

$$\int_{-\lambda_{\max}}^{\lambda_{\max}} \lambda^6 \rho(\lambda) d\lambda = \frac{\text{Tr } M^6}{3N_S} \quad (6.2.5)$$

$$\int_{-\lambda_{\max}}^{\lambda_{\max}} \lambda^{2n} \rho(\lambda) d\lambda = \frac{\text{Tr } M^{2n}}{3N_S} \quad (6.2.6)$$

The limit has been made when one considers that

$\sum \lambda_i^n \longrightarrow \int \lambda^n \rho(\lambda) d\lambda$ . which is for an infinite lattice.

The application of this idea could be made if, for example, one has  $\rho(\lambda)$  given by

$$\rho(\lambda) = (A + B\lambda^2) \sqrt{\lambda_M^2 - \lambda^2}$$

and

$$\int_0^{\lambda_{\max}} \rho(\lambda) d\lambda = 1/2$$

$$\int_0^{\lambda_{\max}} \lambda^2 \rho(\lambda) d\lambda = 8/2$$

$$\int_0^{\lambda_{\max}} \lambda^4 \rho(\lambda) d\lambda = \frac{1}{2} \left( \frac{\text{Tr } M^4}{3N_S} \right) = p/2 \quad (6.2.7)$$

This gives,

$$\left\{ \begin{array}{l} \frac{\pi \lambda_M^2}{32} (8A + 2B\lambda_M^2) = 1/2 \\ \frac{\pi \lambda_M^4}{256} (16A + 8B\lambda_M^2) = 4 \\ \frac{\pi \lambda_M^6}{512} (16A + 10B\lambda_M^2) = p/2 \end{array} \right. \quad (6.2.8)$$

and finally the parameters A, B and  $\lambda_{\max}$  are

$$\left\{ \begin{array}{l} \lambda_{\max} \text{ obtained from the equation } \lambda_M^4 - 96\lambda_M^2 + 16p = 0 \\ \text{and} \\ A = \frac{2}{\pi \lambda_M^2} \left( 3 - \frac{2^7}{\lambda_M^2} + \frac{2^4 p}{\lambda_M^4} \right) \\ B = -\frac{32}{\pi \lambda_M^4} \left( 1 - 5 \cdot \frac{2^4}{\lambda_M^2} + 3 \frac{2^2 p}{\lambda_M^4} \right) \end{array} \right. \quad (6.2.9)$$

In the equation which computes  $\lambda_{\max}$ , one has to choose one real root closer to the value of the maximum eigenvalue given by the lanczos method which has been always around 4.5. Note that equation (6.2.9) implies that the maximum eigenvalue  $\lambda_{\max}$  is given by

$$\lambda_{\max} = \sqrt{48 - 8 \sqrt{6(1 + 2 \langle \square \rangle)}}$$

and therefore, the expression of the parameter A will be

$$A = \frac{4}{\pi \lambda_M^4} (\lambda_M^2 - 16)$$

which means that for  $\langle \square \rangle = 5/6$ , one has  $\lambda_{\max} = 4$ , then  $A = 0$ . This assumption leads to the fact that chiral transition occurs at the value 0.83 for the average plaquette and this result depends neither on the size of the lattice nor the temperature of the lattice.

It is then necessary to go to a higher order parametrisation of  $\mathcal{F}(\lambda)$  and include higher order loops in order to avoid this ambiguity.

The inclusion of higher order loops is possible as long as the trace of  $M^n$  (with  $n > 4$ ) can be worked out.



For instance, one can include Trace  $M^6$  in the parametrisation of  $\rho(\lambda)$  and obtains from

$$\rho(\lambda) = (A + B\lambda^2 + C\lambda^4) \sqrt{\lambda_m^2 - \lambda^2} \quad (6.2.10)$$

$$\int_0^{\lambda_{\max}} \rho(\lambda) d\lambda = 1/2$$

and

$$\int_0^{\lambda_{\max}} \lambda^2 \rho(\lambda) d\lambda = 8/2$$

$$\int_0^{\lambda_{\max}} \lambda^4 \rho(\lambda) d\lambda = 1/2 \frac{\text{Tr } M^4}{3N_S} = p/2$$

$$\int_0^{\lambda_{\max}} \lambda^6 \rho(\lambda) d\lambda = 1/2 \frac{\text{Tr } M^6}{3N_S} = f/2$$

the following:

$$97\lambda_M^6 - 9408 \lambda_M^4 + 1616 p \cdot \lambda_M^2 - 64 \cdot f = 0$$

which gives  $\lambda_{\max}$

and

$$\begin{bmatrix} A \\ B\lambda_M^2 \\ C\lambda_M^4 \end{bmatrix} = \mathcal{M}^{-1} \begin{bmatrix} 128/\pi\lambda_M^2 \\ 2048/\pi\lambda_M^4 \\ 1024p/\pi\lambda_M^6 \end{bmatrix} \quad (6.2.11)$$

where

$$\mathcal{M}^{-1} = \begin{bmatrix} 64 & 16 & 8 \\ 32 & 16 & 10 \\ 64 & 40 & 28 \end{bmatrix}^{-1}$$

### VI.3 Application to a $4^4$ lattice

Once one has evaluated the analytical expression of the spectral density (Fig. 1-a), the determinant of the fermion matrix can be calculated analytically without any problems. One is in the case of a  $4^4$  lattice at  $\beta = 5.4$  in  $SU(3)$ .

$$\begin{aligned} \text{Det}(M + 2ma) &= e^{\text{Tr}(\ln(M + 2ma))} \\ &\simeq e^{\int_0^{\lambda_{\max}} \ln(\lambda^2 + m^2) \rho(\lambda) d\lambda} \quad (6.3.1) \end{aligned}$$

where  $2ma \equiv m$

In our case  $\rho(\lambda) = (A + B\lambda^2) \sqrt{\lambda_M^2 - \lambda^2}$

Then

$$\int_0^{\lambda_{\max}} \ln(\lambda^2 + m^2) \rho(\lambda) d\lambda = \int_0^1 (A + Bd^2x^2) d^2 \sqrt{1-x^2} \ln \left[ (m^2) \cdot (1+b^2x^2) \right] dx$$

where  $d = \lambda_{\max}$ ;  $b = \frac{\lambda_{\max}^2}{m^2}$  and  $x = \frac{\lambda}{\lambda_{\max}}$

Consequently

$$\begin{aligned} \int_0^{\lambda_{\max}} \ln(\lambda^2 + m^2) \rho(\lambda) d\lambda &= 2d^2 \ln(m) \int_0^1 (A + Bd^2x^2) \sqrt{1-x^2} dx \\ &\quad + d^2 \int_0^1 (A + Bd^2x^2) \sqrt{1-x^2} \ln(1+b^2x^2) dx \\ &= 2d^2 \ln(m) \left[ A \frac{\pi}{4} + Bd^2 \frac{\pi}{16} \right] + d^2 \left[ AI_1 + Bd^2 I_2 \right] \end{aligned}$$

$$\text{where } I_1 = \frac{\pi}{2} \left\{ \frac{1}{2} \frac{1 - \sqrt{1+b^2}}{1 + \sqrt{1+b^2}} + \ln \frac{1 + \sqrt{1+b^2}}{2} \right\}$$

$$\text{and } I_2 = \frac{\pi}{8b^2} \left\{ \frac{3-b^2}{2+\sqrt{1+b^2}} - \frac{2}{1+\sqrt{1+b^2}} \right\} + \frac{\pi}{8} \ln\left(\frac{1+\sqrt{1+b^2}}{2}\right) + \frac{\pi}{32}$$

(6.3.2)

So the determinant can be predicted at any configuration of the lattice (Fig. 1-b), once  $\rho(\lambda)$  is formulated by the given values of the corresponding loops which occur in the computation of  $\text{Tr } M^n$ . The computation time is not very long and the method seems to be useful. However, the determinant at zero-mass is calculated separately but still in an analytical way and it is given by

$$\begin{aligned}
 D_0 &= \exp \int_0^d (A + B\lambda^2) \sqrt{d^2 - \lambda^2} \ln \lambda \, d\lambda \\
 &= \exp \frac{\pi d^2}{2} \left\{ \ln\left(\frac{d}{2}\right) \left(A + \frac{Bd^2}{4}\right) - \frac{1}{2} \left(A - \frac{Bd^2}{8}\right) \right\} \quad (6.3.3)
 \end{aligned}$$

The next step of the calculation is to evaluate the determinant of  $M$  as many times as the link is changed to give another configuration. This means, that when a new spectro-function is given with its new parameters, (Fig. 1-c), the determinant corresponding to a new configuration is evaluated (Fig. 1-d). Finally, the ratio of the determinants is calculated. This process does not need a lot of time to be computed and the implementation of dynamical fermions becomes operational.

$$\text{Ratio} = \frac{e \int_0^{\lambda_{\max}} \hat{\rho}(\lambda) \ln(\lambda^2 + m^2) d\lambda}{e \int_0^{\lambda_{\max}} \rho(\lambda) \ln(\lambda^2 + m^2) d\lambda} \quad (6.3.4)$$

(See Fig. 1-e).

The results are confirmed when one compares them with the results obtained from Lanczos. Nevertheless, there is a difference between them for small masses between 0 and 0.2 in lattice unit.

#### VI.4 Application to a $6^4$ lattice

The procedure is similar to the previous one but one is going to use the method in a  $6^4$  lattice at  $\beta = 5.5$ . The aim of this is that one proves that  $\rho(\lambda)$  form, is still correct in the calculation of the determinant or the ratio.

One takes  $\rho(\lambda) = (A + B\lambda^2 + C\lambda^4) \sqrt{(\lambda_M^2 - \lambda^2)}$  (Figs. 2-a, 2-c and 2-f), where the computation of loop6 is required. The determinant is then given by

$$\text{Det} = \exp(I), \text{ where}$$

$$I = 2d^2 \ln(m) \left\{ A \frac{\pi}{4} + Bd^2 \frac{\pi}{16} + Cd^4 \frac{\pi}{32} \right. \\ \left. + d^2 \left\{ A I_1 + Bd^2 I_2 + Cd^4 I_3 \right\} \right\} \quad (6.4.1)$$

where

$$I_1 = \frac{\pi}{2} \left\{ \frac{1}{2} \frac{1 - \sqrt{1+b^2}}{1 + \sqrt{1+b^2}} + \ln \left( \frac{1 + \sqrt{1+b^2}}{2} \right) \right\}$$

$$I_2 = \frac{\pi}{8b^2} \left\{ \frac{3-b^2}{2 + \sqrt{1+b^2}} - \frac{2}{1 + \sqrt{1+b^2}} \right\} + \frac{\pi}{8} \ln \left( \frac{1 + \sqrt{1+b^2}}{2} \right) + \frac{\pi}{32}$$

$$\text{and } I_3 = \frac{\pi}{48b^6} \left\{ (3b^4 - 8)(1 - \sqrt{1+b^2}) - 2b^2(3 - \sqrt{1+b^2}) + \frac{\pi}{16} \ln \right. \\ \left. \left( \frac{1 + \sqrt{1+b^2}}{2} \right) + \frac{5\pi}{192} \right\}$$

And the determinant at zero mass is given by the following

$$D_0 = e^{I_0}$$

$$\text{where } I_0 = \frac{\pi d^2}{2} \left\{ A \left( \ln \frac{d}{2} - \frac{1}{2} \right) + \frac{Bd^2}{4} \left( \ln \frac{d}{2} + \frac{1}{4} \right) + \frac{Cd^4}{8} \left( \ln \frac{d}{2} + \frac{5}{12} \right) \right\} \quad (6.4.2)$$

Finally the ratio is given by

$$\text{Ratio} = \frac{\hat{D}}{D} \quad (6.4.3)$$

where  $\hat{D}$  is the determinant corresponding to a configuration differing by one link from the previous configuration.

The results are confirmed by lanczos results but the difference at small masses remains again. This concludes that the computation of higher order loops like loop8, loop10 etc. is needed to explore the interval of quark masses between 0 and 0.25 in lattice units.

\*See figures (2-b; 2-d; 2-f; 2-g; 2-h; and 2-i).

## VI.5 Conclusion

From this method, with its trivial and simple formulation, one has nearly discovered the results obtained by Lanczos method to update dynamical fermions at quark masses bigger than 0.2 in lattice unit. Although, one has included only small loops of order four and six, one has obtained similar results. Consequently, the updating of dynamical fermion of masses larger than 0.2, loops of order higher than six, do not seem to contribute substantially.

However, higher order loops are crucially needed in the method for the implementation of light dynamical fermions because the predicted ratios at small masses as shown in Figures (1-e; 2-g; 2-h; 2-i) differ from the ratios obtained by Lanczos method quite clearly. Nevertheless, finite size effect can be also a factor in the predicted ratios, and as one knows, that on any finite lattice this effect will dominate

the low eigenvalues which will manifest themselves at small quark mass (Fig. 3-a). (13)

As far as the time of the computation of these loops is concerned, it becomes longer for higher order paths, especially for bigger lattices. The time can be reduced to a big factor, however, because one is searching on the change of the loops once a link is changed in a configuration. This change occurs only in the neighbouring loops to the link involved in the change. Then

$$\sum \text{loopn}_2 = \sum \text{loopn}_1 + \sum \Delta \text{loopn} \quad (6.5.1)$$

where  $\sum \Delta \text{loopn}$  has to be computed in view of evaluating the trace of  $M^n$ . The computation of  $\sum \Delta \text{loopn}$  is fast, then the time required for finding a configuration accepted by the Metropolis algorithm, with dynamical fermions implemented, is minimised.

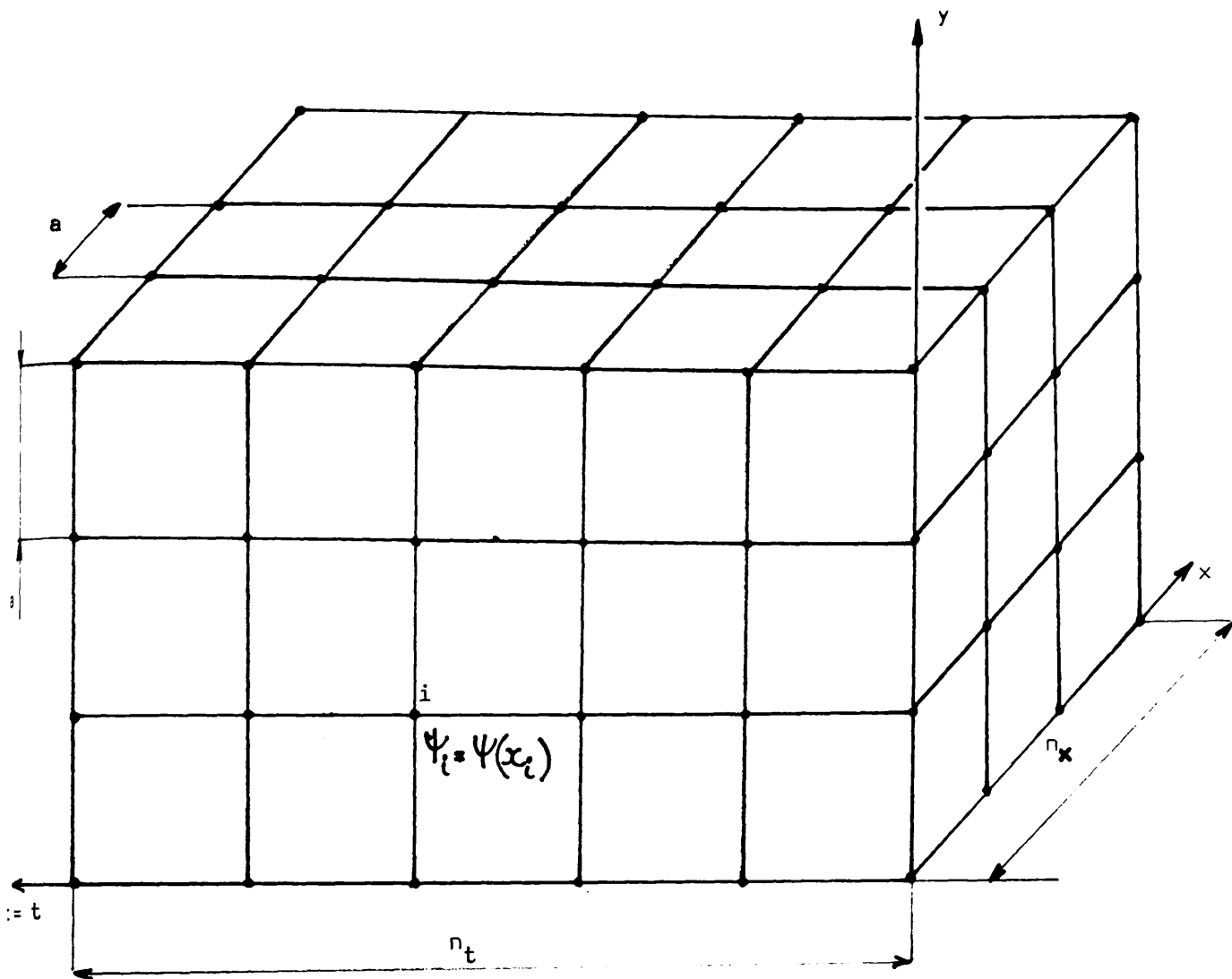


Fig. 1  $A_{4^2 6}$  Lattice

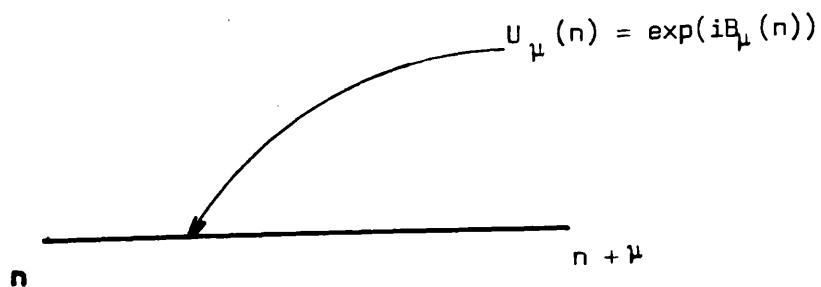
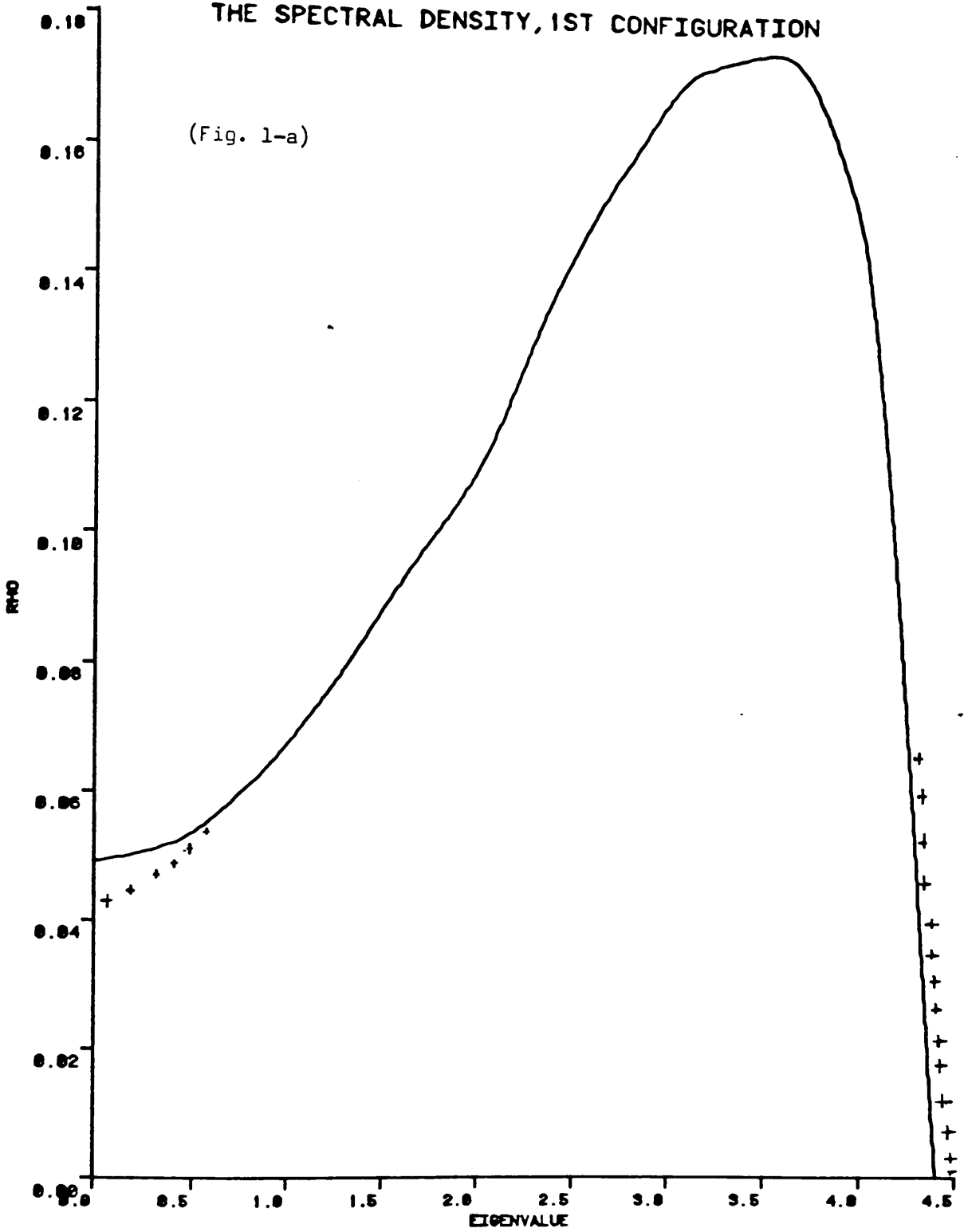


Fig. (2)

# THE SPECTRAL DENSITY, 1ST CONFIGURATION



\* The spectral density without any change in links

\*  $\beta = 5.4$ ;  $4^4$  lattice

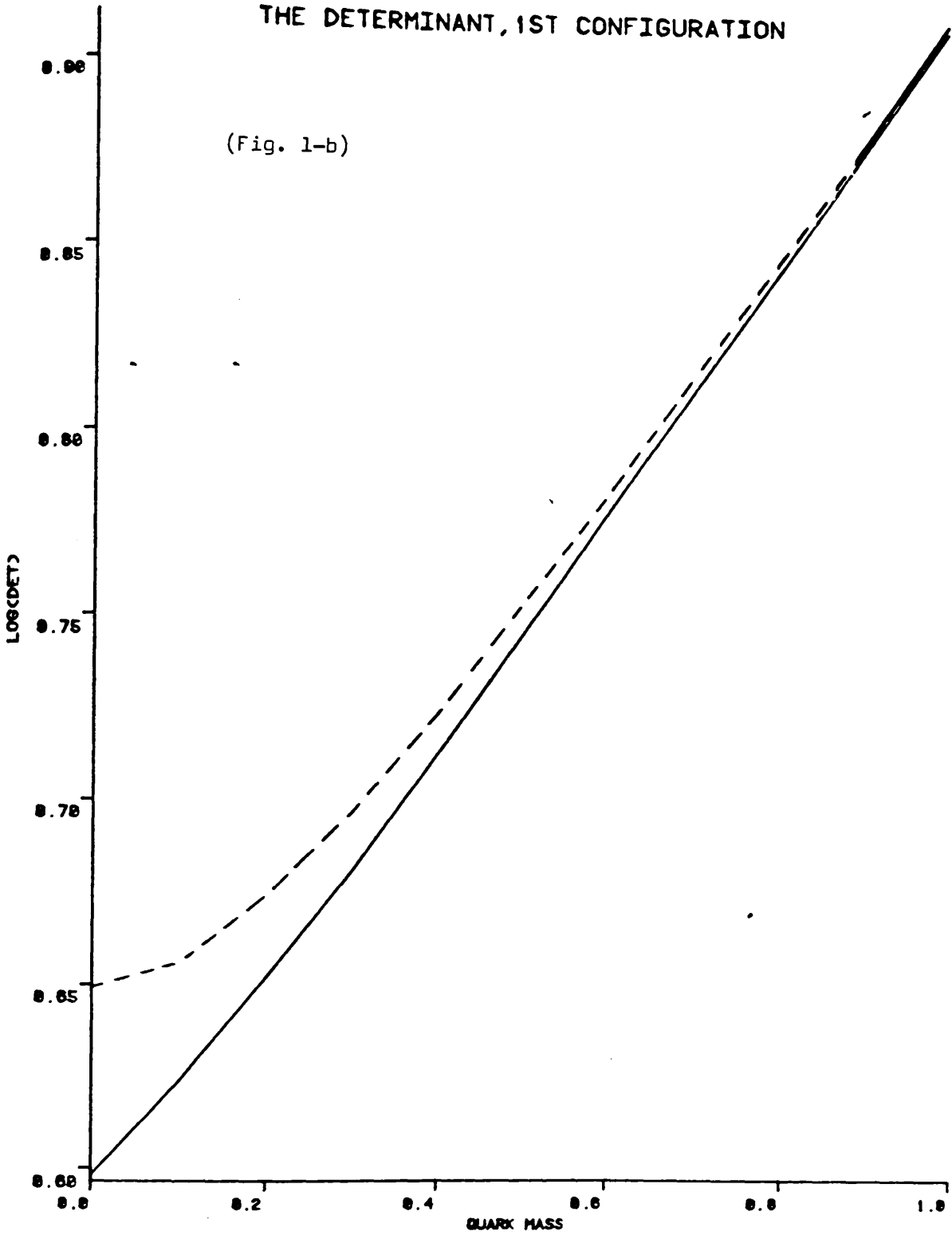
— The new method

+ Lanczos method



# THE DETERMINANT, 1ST CONFIGURATION

(Fig. 1-b)



\* The determinants without any change in links

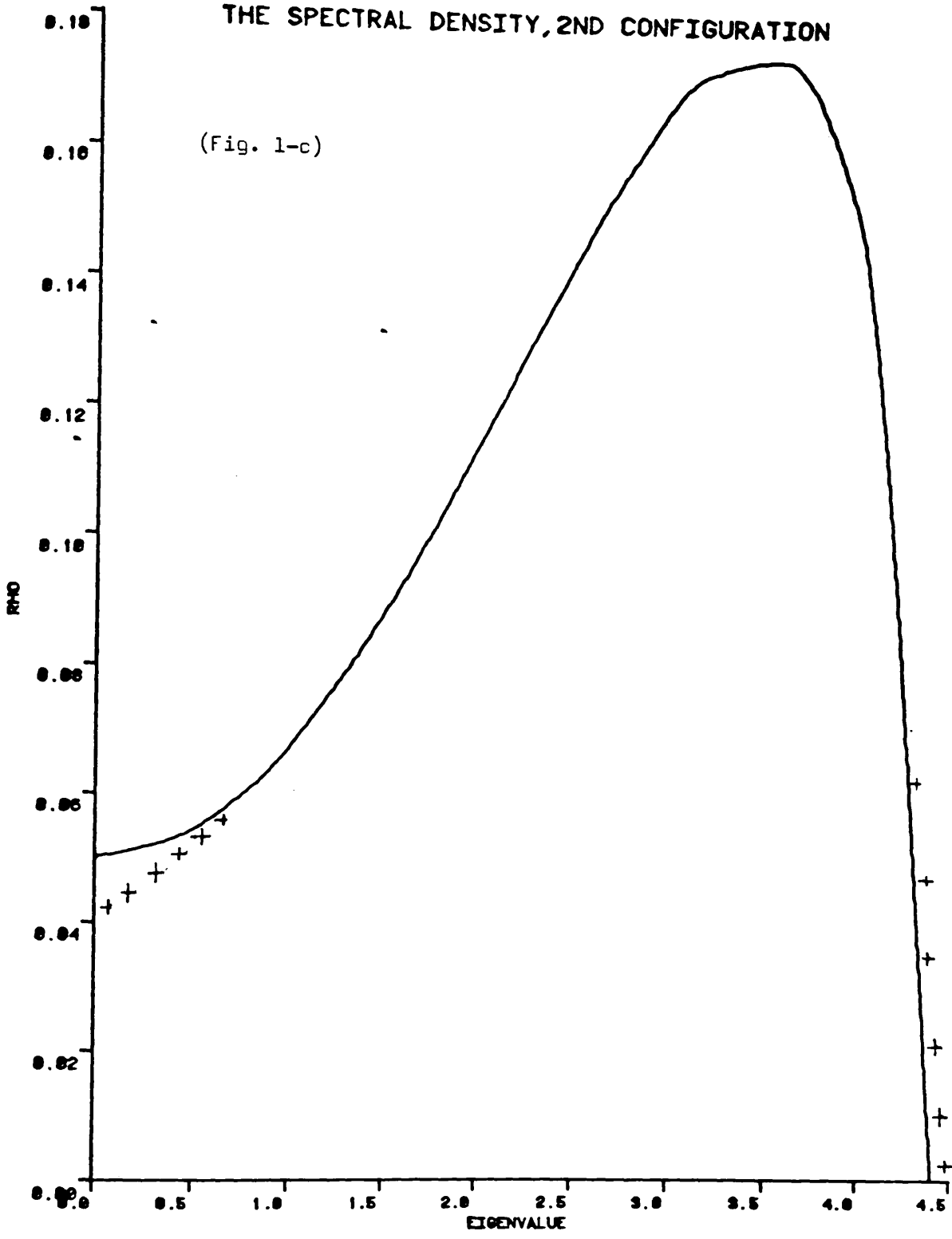
\*  $\beta = 5.4$ ;  $4^4$  lattice

— The new method

— Lanczos method

# THE SPECTRAL DENSITY, 2ND CONFIGURATION

(Fig. 1-c)



\* The spectral density at one link changed

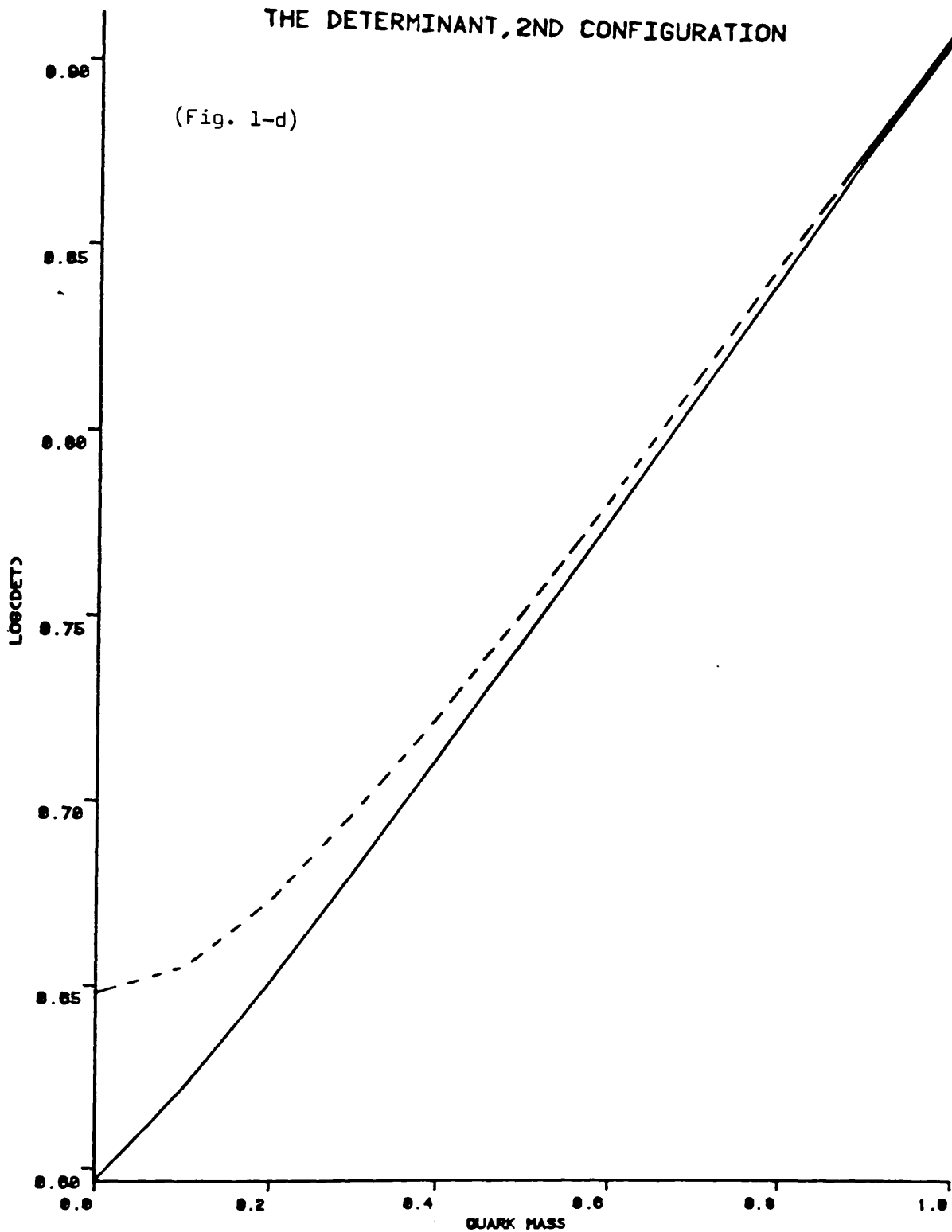
\*  $\beta = 5.4$ ;  $4^4$  lattice

— The new method

+ Lanczos method

# THE DETERMINANT, 2ND CONFIGURATION

(Fig. 1-d)



\* The determinants at one link changed, the first link

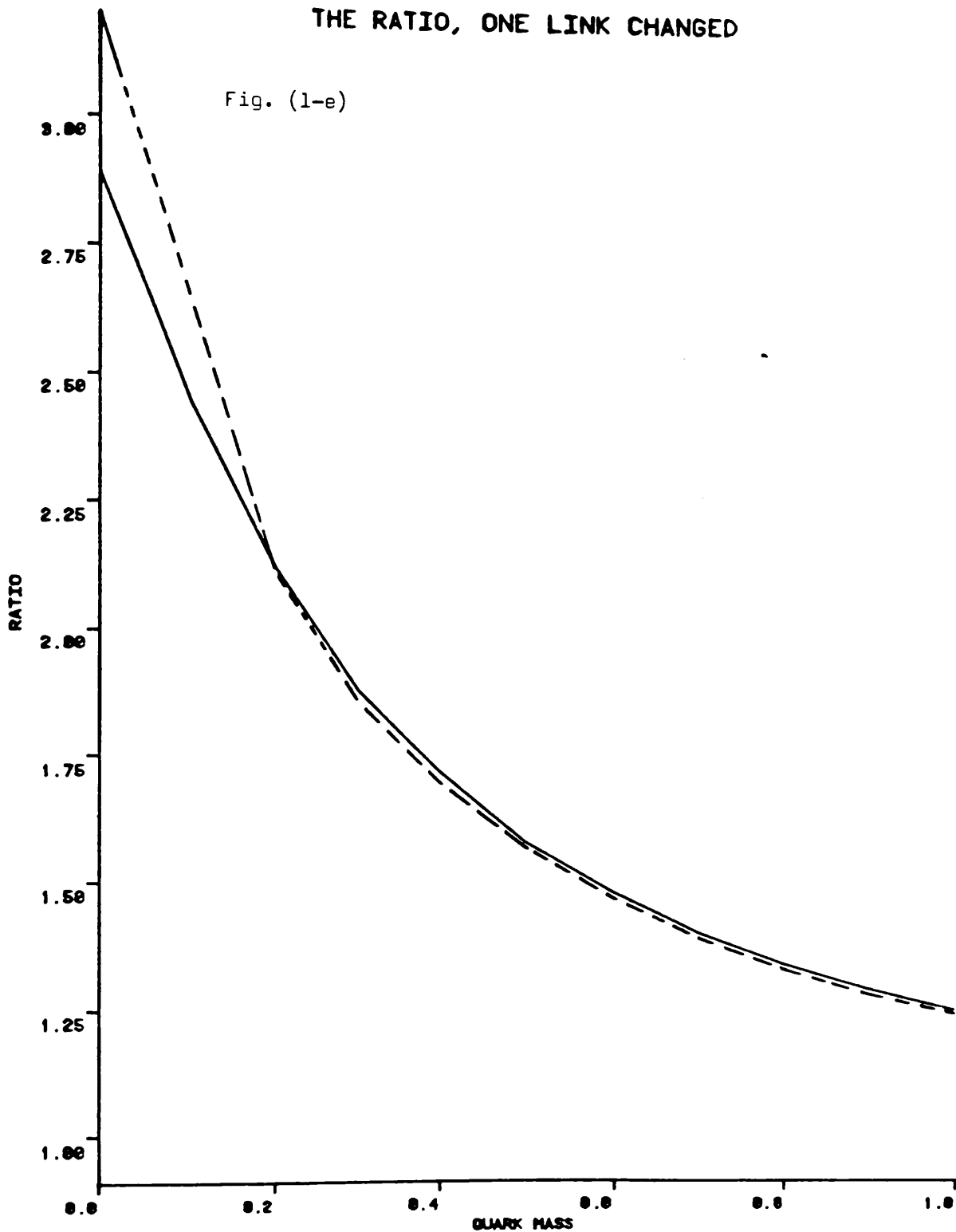
\*  $\beta = 5.4$ ;  $4^4$  lattice

— The new method

— Lanczos method

# THE RATIO, ONE LINK CHANGED

Fig. (1-e)



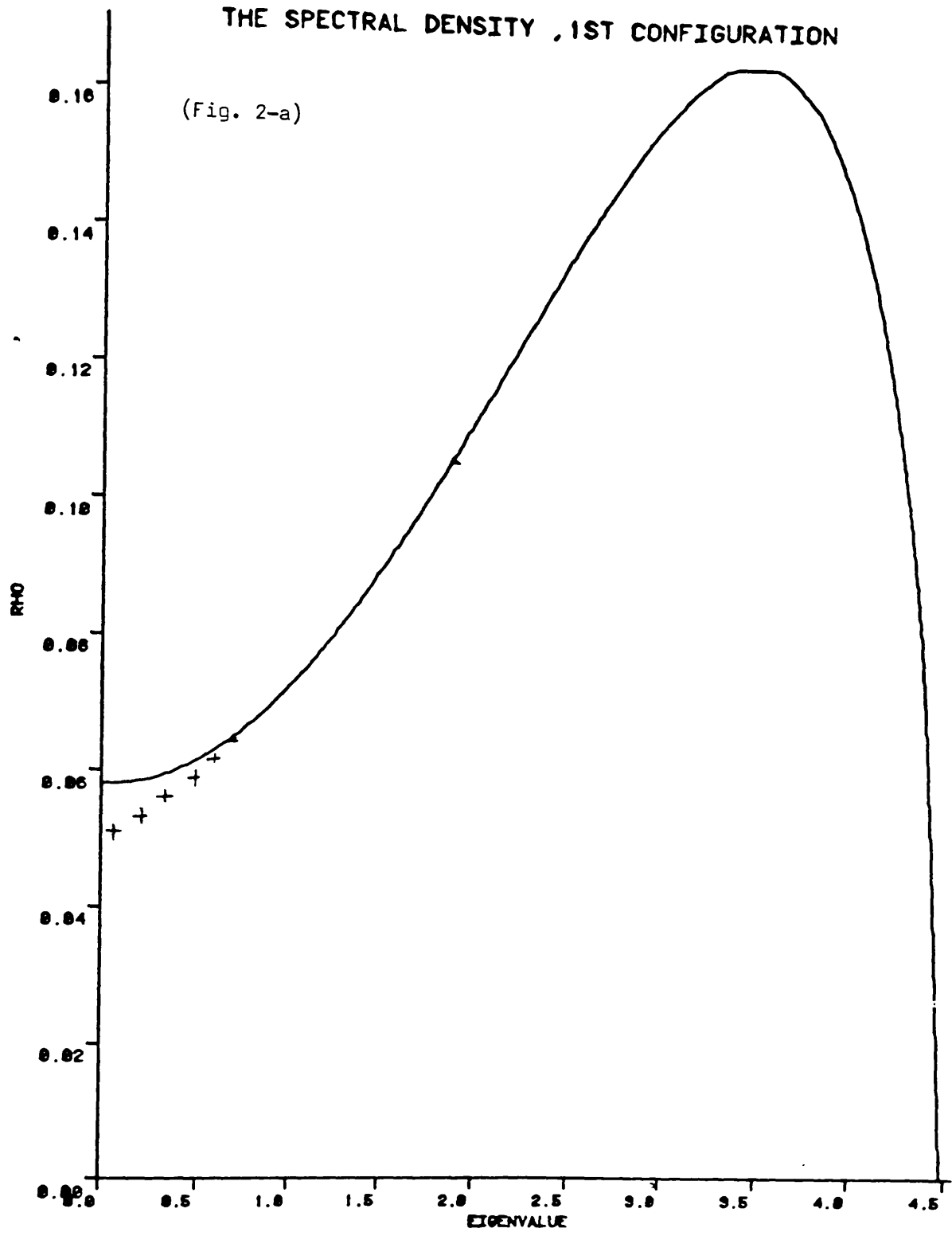
\*  $\beta = 5.4$ ;  $4^4$  lattice

— New method

- - - Lanczos method

# THE SPECTRAL DENSITY ,1ST CONFIGURATION

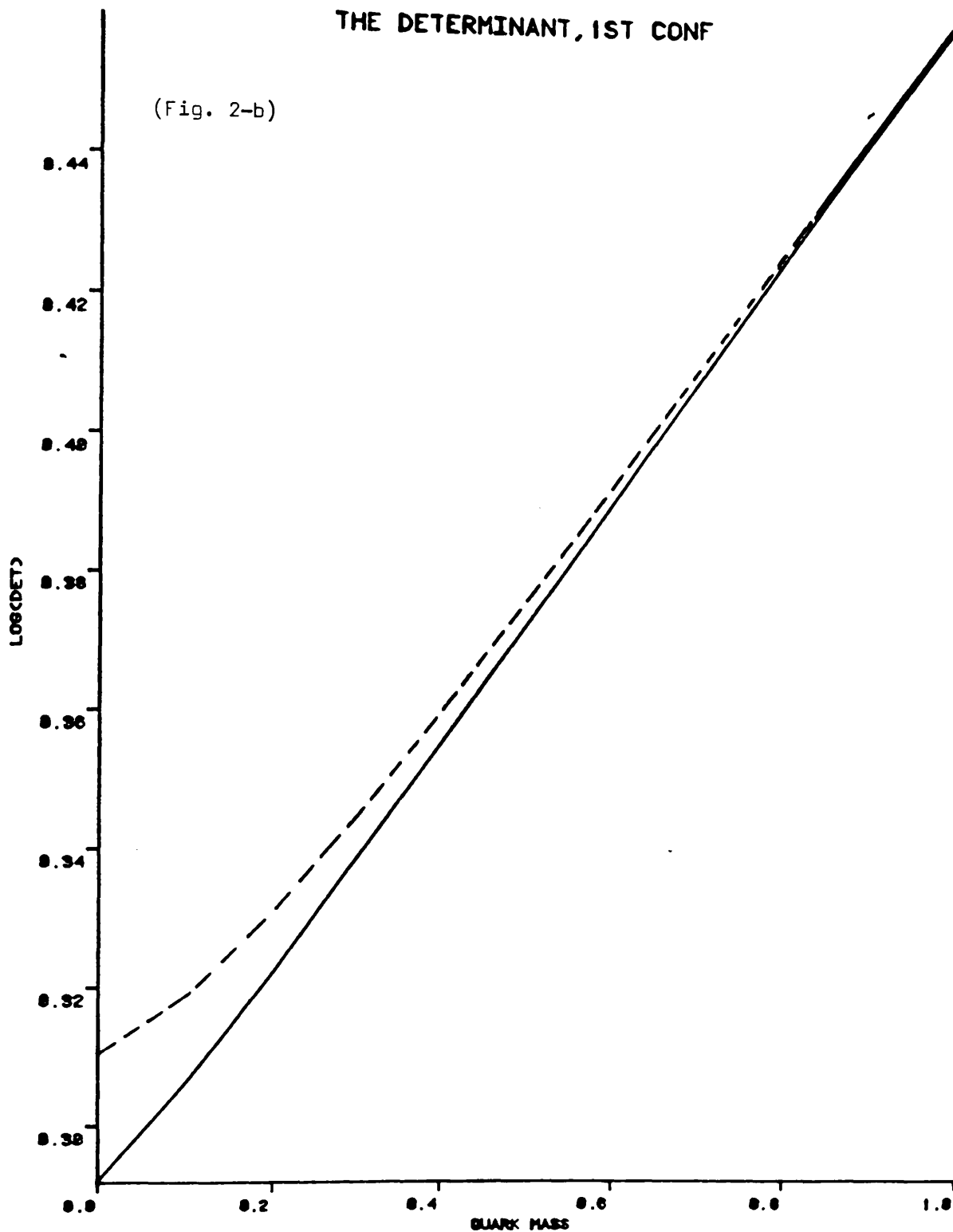
(Fig. 2-a)



- \* The spectral density, without any change of links
- \*  $\rho = 5.5$ ;  $6^4$  lattice
- The new method
- + Lanczos method

# THE DETERMINANT, 1ST CONF

(Fig. 2-b)



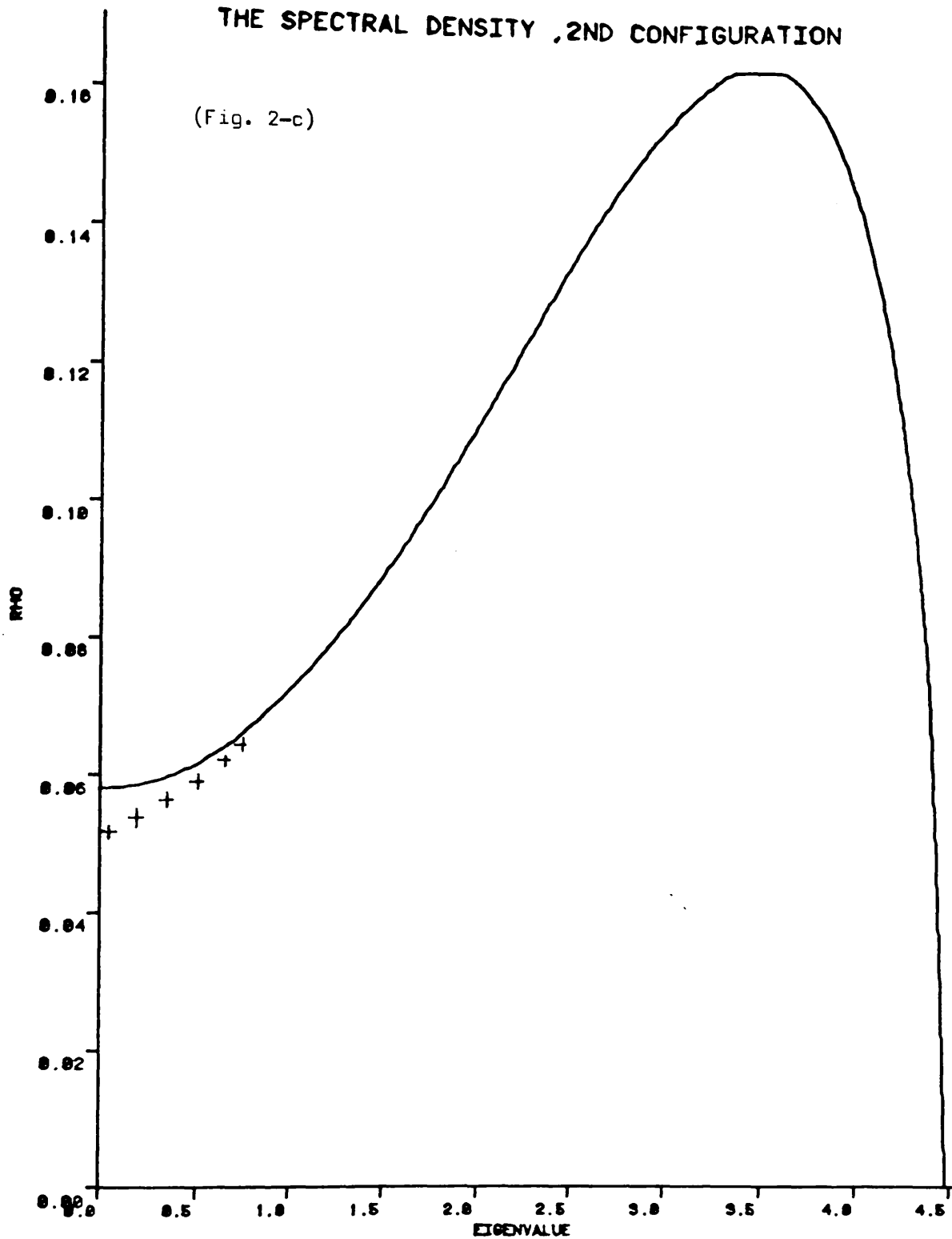
\* The Determinants without any change in links

\*  $\beta = 5.5$ ;  $6^4$  lattice

— The new method

- - - Lanczos method

# THE SPECTRAL DENSITY ,2ND CONFIGURATION



\* The spectral density at one link changed, the first link

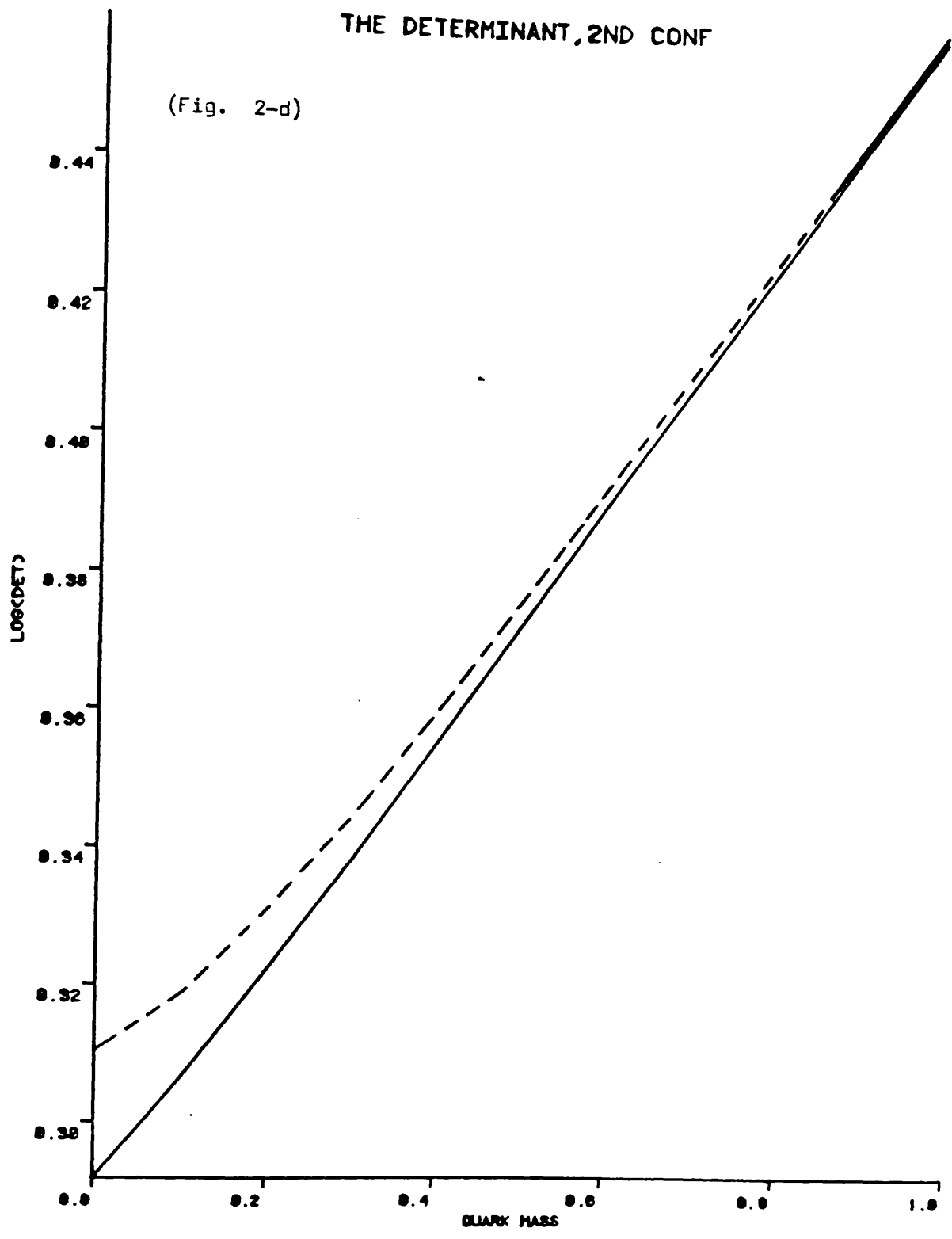
$\rho = 5.5; 6^4$  lattice

— The new method

--- Lanczos method

# THE DETERMINANT, 2ND CONF

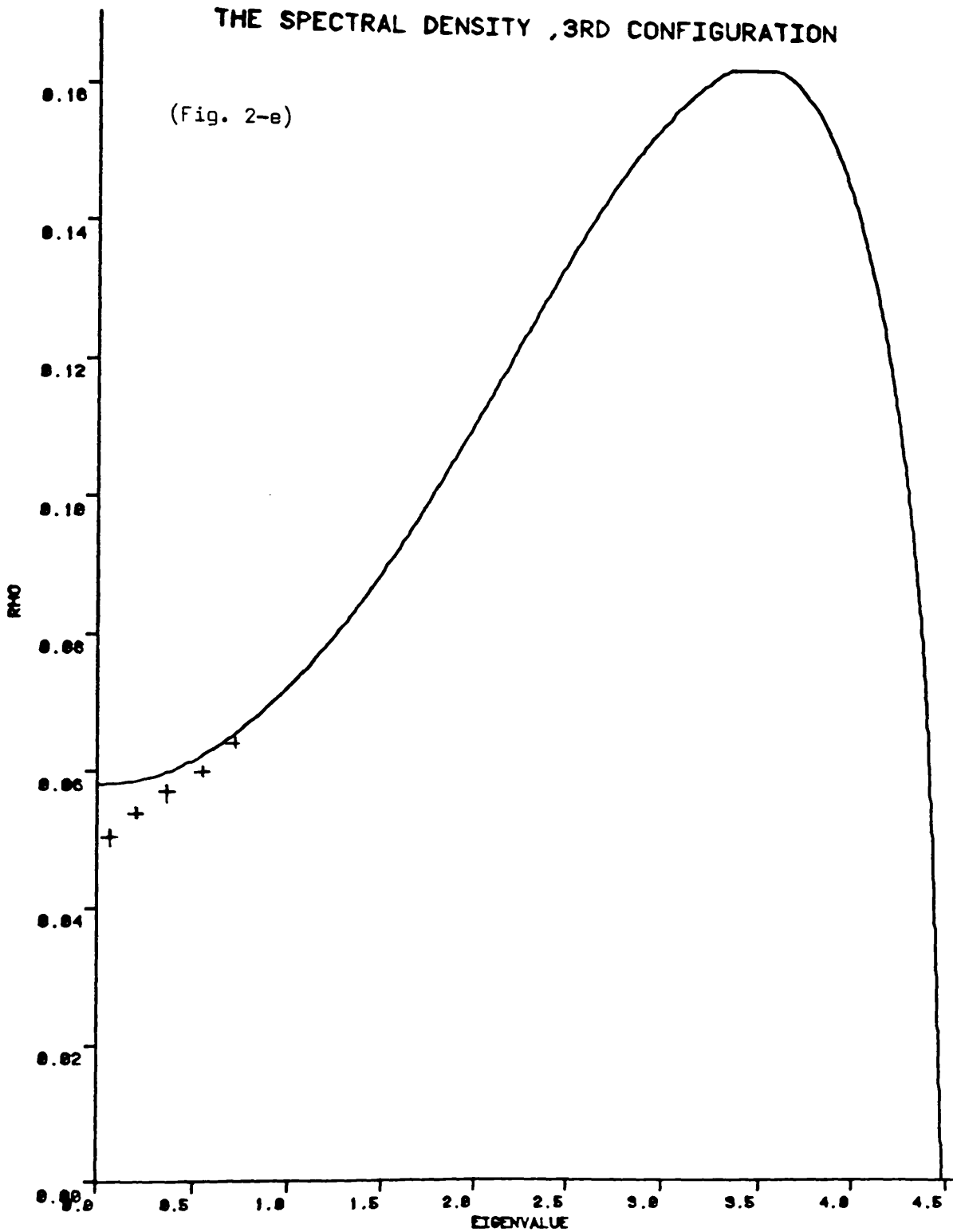
(Fig. 2-d)



- \* The determinants at one link changed, the first link
- \*  $\beta = 5.5$ ;  $6^4$  lattice
- The new method
- - - Lanczos method



# THE SPECTRAL DENSITY ,3RD CONFIGURATION



\* The spectral density at one link changed, the second link

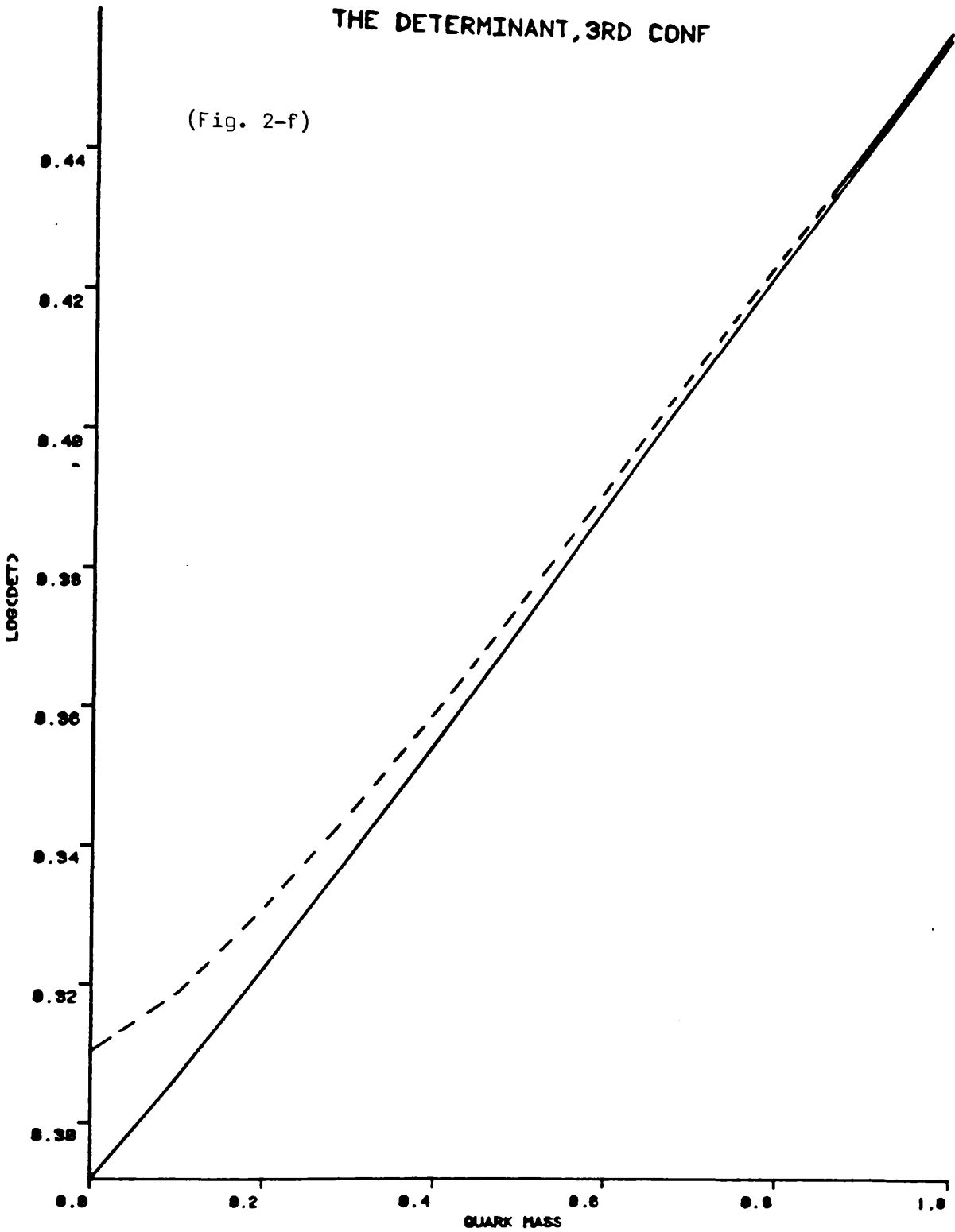
$\rho = 5.5$ ;  $6^4$  lattice

— The new method

+ Lanczos method

# THE DETERMINANT, 3RD CONF

(Fig. 2-f)



\* The spectral density at one link changed, the second link

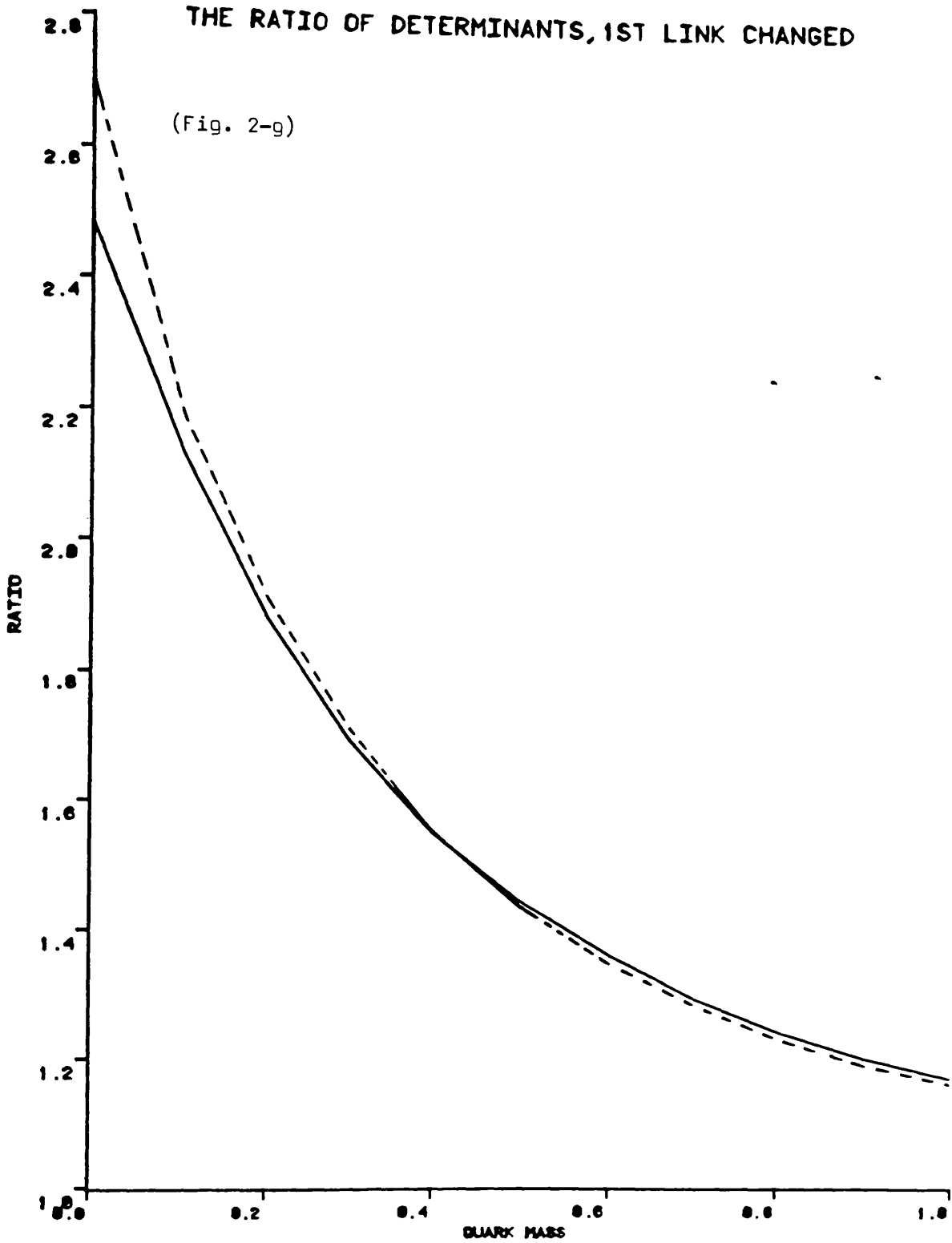
$\beta = 5.5; 6^4$  lattice

— The new method

- - - Lanczos method

# THE RATIO OF DETERMINANTS, 1ST LINK CHANGED

(Fig. 2-g)

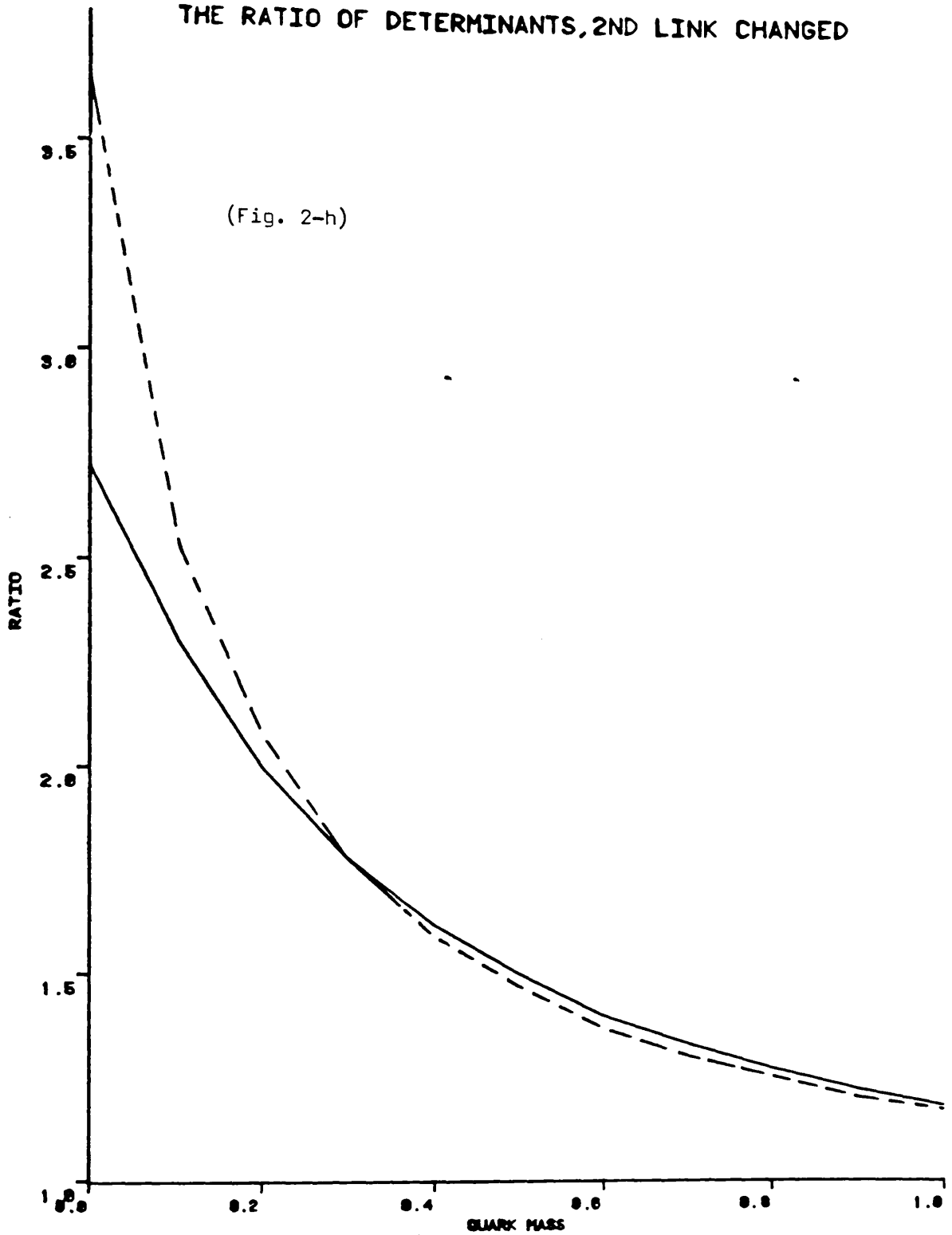


\*  $\beta = 5.5$ ;  $6^4$  lattice

— The new method

- - - Lanczos method

# THE RATIO OF DETERMINANTS, 2ND LINK CHANGED



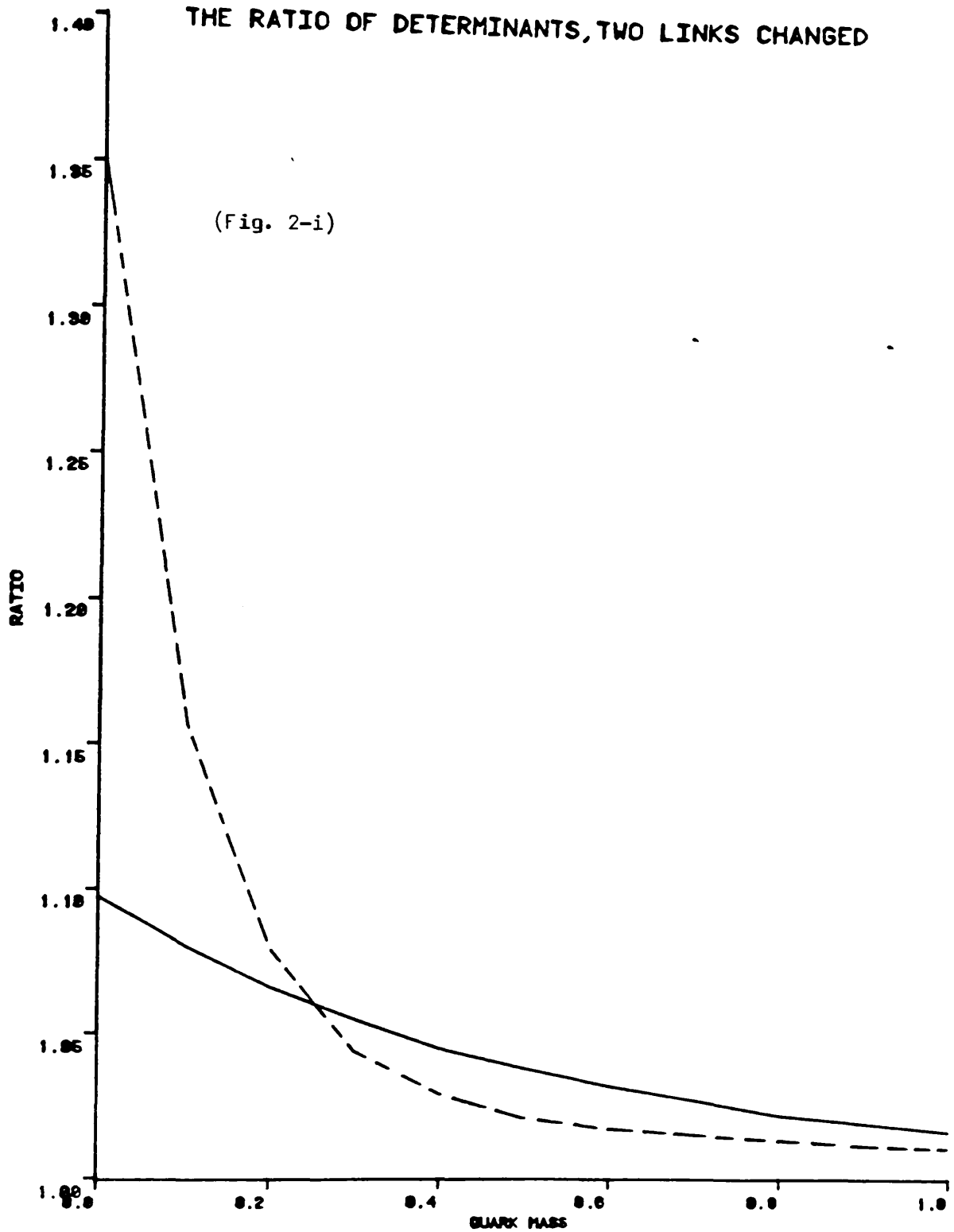
\*  $\beta = 5.5$ ;  $6^4$  lattice

— The new method

- - - Lanczos method

# THE RATIO OF DETERMINANTS, TWO LINKS CHANGED

(Fig. 2-i)

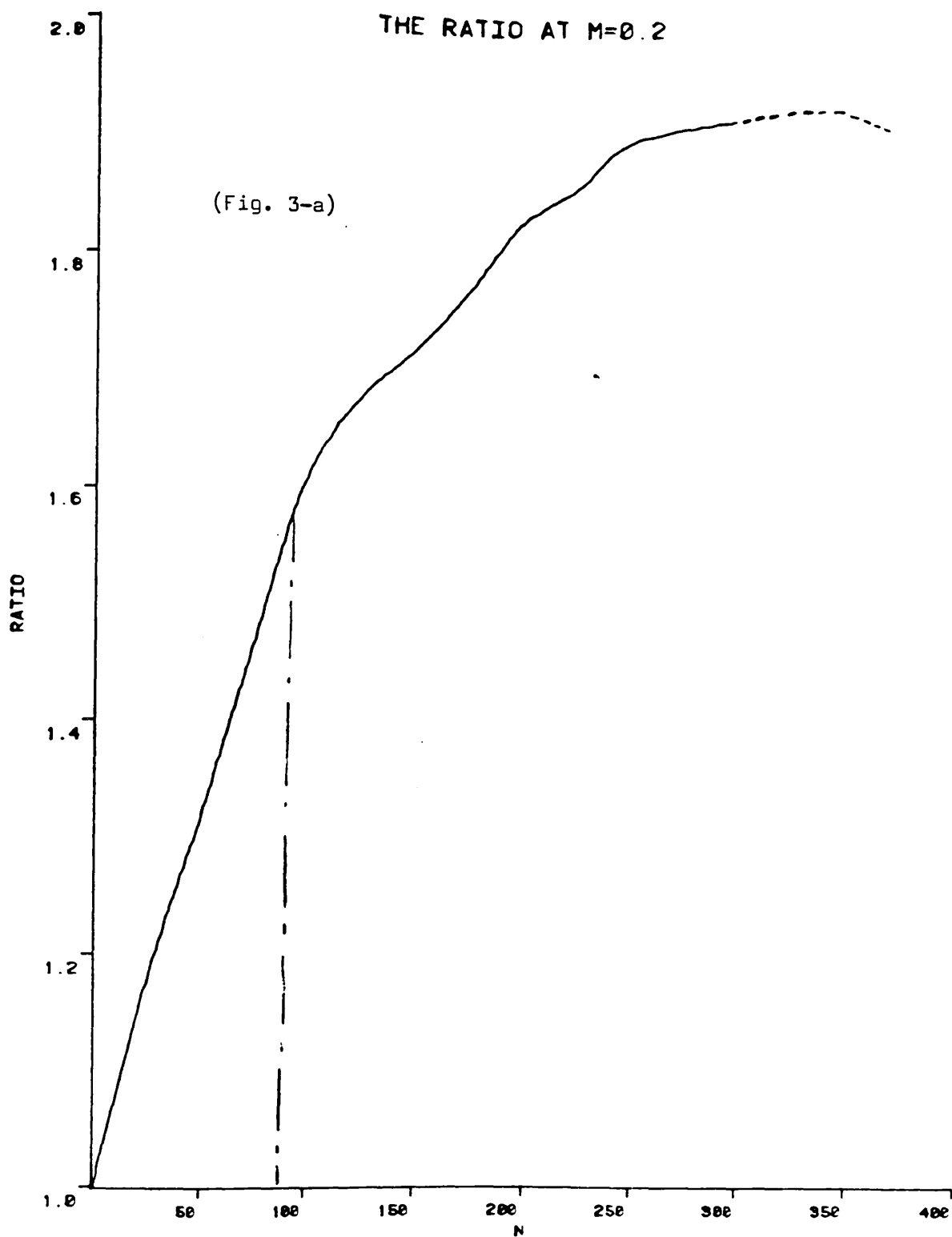


\*  $\beta = 5.5$ ;  $6^4$  lattice

— The new method

- - - Lanczos method

# THE RATIO AT $M=0.2$



The ratio at  $\beta = 5.4$ ,  $4^4$  lattice. One can see that the variation of ratio is rapid from 1st eigenvalue to 85th eigenvalue, and becomes slower after that.

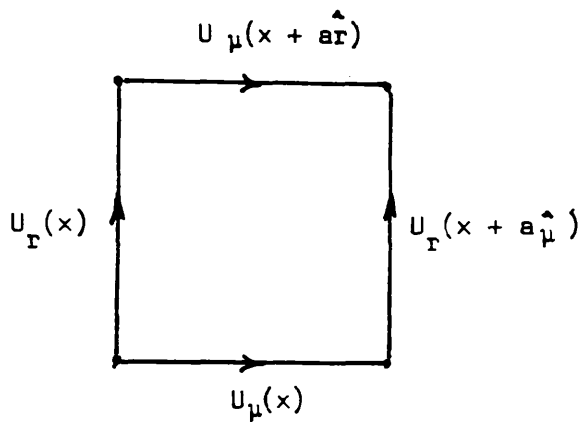


Fig. 3. "The Plaquette".

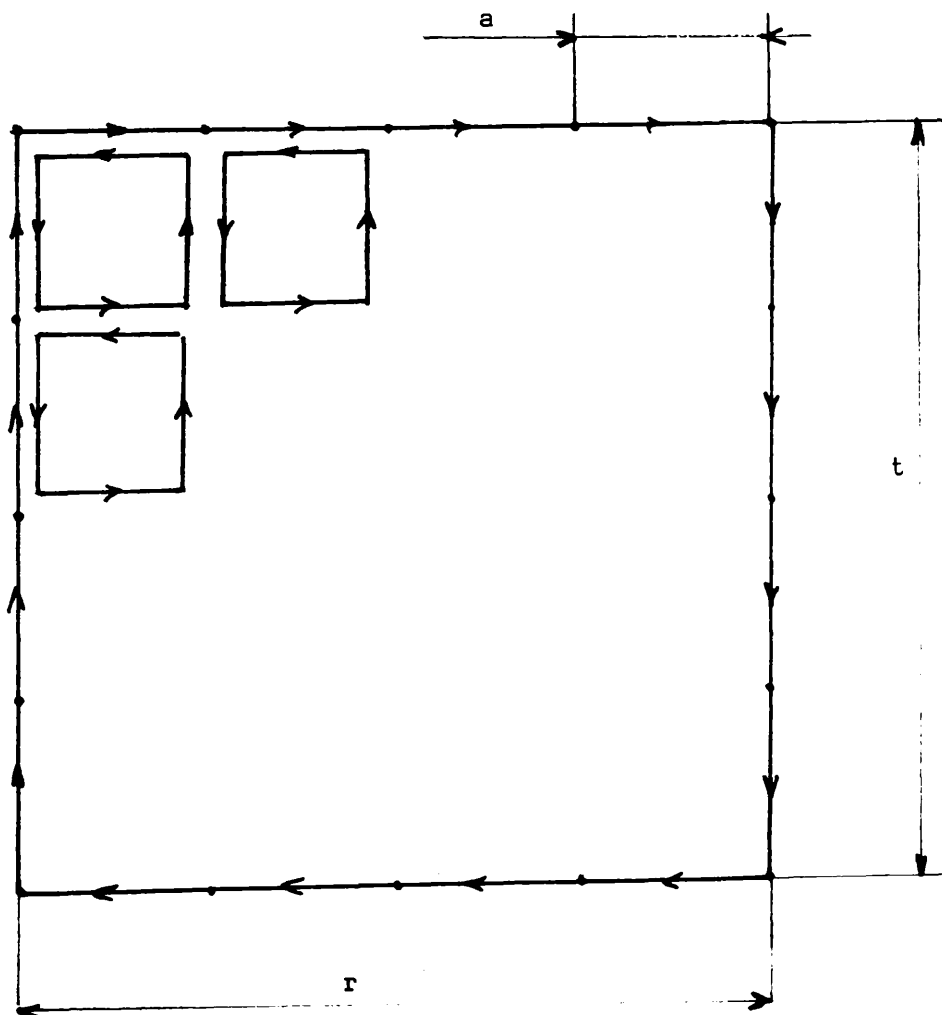


Fig. 4. Number of plaquettes is  $rt/a^2$ .

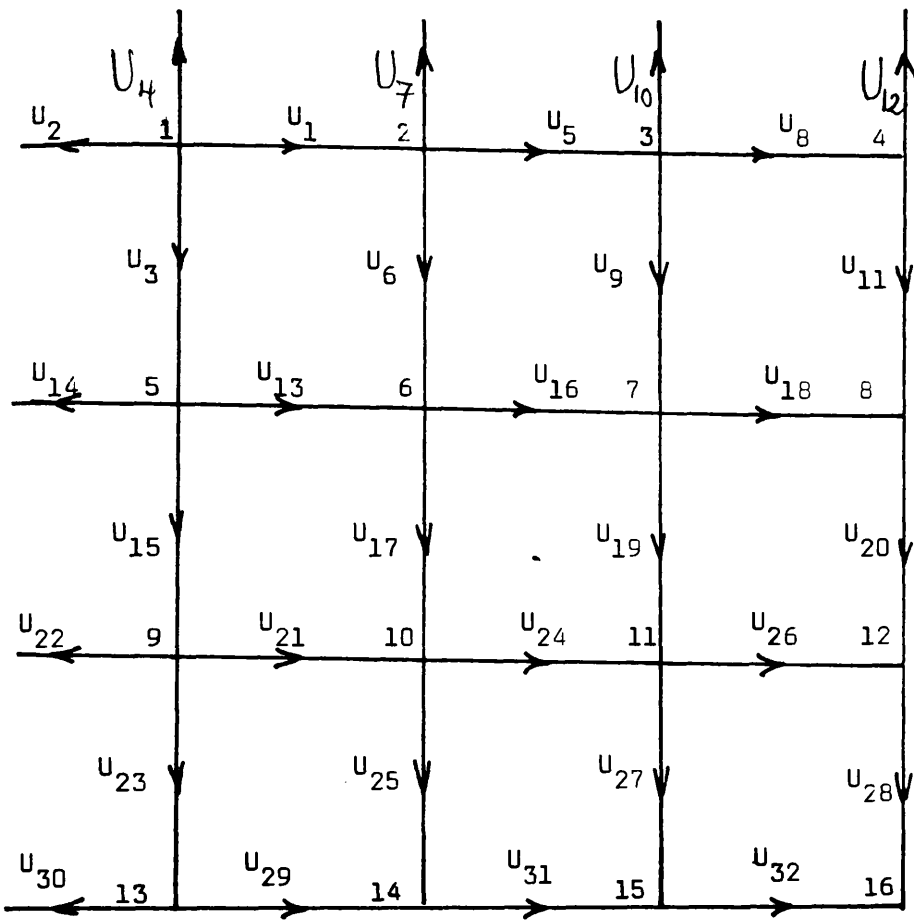


Fig. 5. A  $4^2$  lattice with its 16 sites and 32 links.

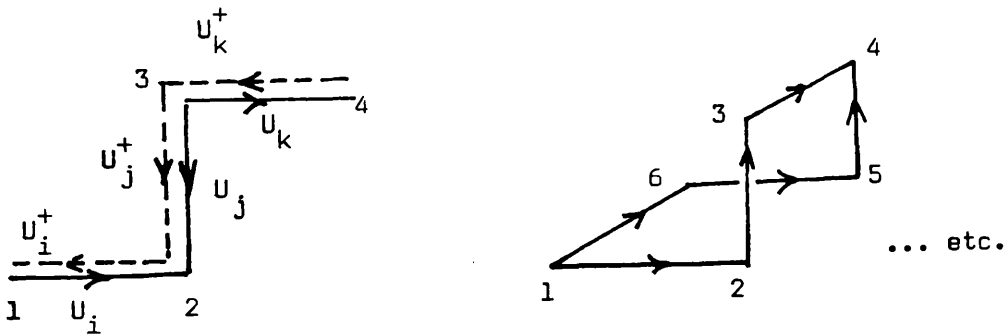


Fig. 6. Loops of order six. (Left) is a constant. (Right) is loop6.





## Appendix

### Abbreviations

- 1) M.C simulation is Monte Carlo simulation.
- 2) Q.F.T is QUATUM<sup>n</sup> field theory.
- 3) P.I is Path integral.
- 4) Q.C.D Quantum chromodynamics.

### Numerical results

In the graphs of the determinants, one should read the value of the determinants as in  $10^3$  units in a  $4^4$  lattice, and in  $10^4$  units in a  $6^4$  lattice.

From "Table of Integrals", I.S. Gradshteyn/I.M. Ryzhik, Fourth edition, Academic Press, New York and London, 1965.

One has:

$$\int_0^1 x^{2n} \sqrt{1-x^2} \ln x \, dx = \frac{(2n-1)!!}{(2n+2)!!} \frac{\pi}{2} \left( \sum_{k=1}^{2n} \frac{(-)^{k-1}}{k} - \frac{1}{2n+2} - \ln 2 \right)$$

$$\int_0^{\pi/2} \sin^{2m} x \, dx = \frac{(2m-1)!!}{(2m)!!} \frac{\pi}{2}$$

$$\int_0^{\pi/2} \frac{\cos^2 x}{1+a^2 \sin^2 x} \, dx = \frac{\pi}{2(1+\sqrt{1+a^2})}$$

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