ANHARMONIC ANALYSIS OF LATTICE FIELD THEORIES, II *

R. Blankenbecler and John L. Richardson[†] Stanford Linear Accelerator Center Stanford University, Stanford, California 94305

ABSTRACT

In a previous paper we showed that a class of real space renormalization group calculations could be reinterpreted as an orthogonal transformation of coordinates followed by an approximate (variational) evaluation of the resulting hamiltonian. Here we shall discuss the orthogonal transform method and concentrate on analytic rather than numerical results. The transform method may ultimately be more accurate because even though similar approximations are made in coupling the lattice oscillators, at no time is the system split into noninteracting finite sized blocks.

Approximate variational solutions to a ϕ^4 lattice field theory in 2, 3 and 4 spacetime dimensions are constructed using an anharmonic oscillator basis. The solutions exhibit an ordered and a disordered phase. Analytic expressions are obtained for certain critical surfaces of these theories in regions of parameter space where a spin approximation would be invalid. The continuum limit of our solutions is discussed. The resultant perturbation expansion is also discussed and a method for its evaluation is described.

Submitted to Physical Review D.

This work was supported by the Department of Energy under Contract Number DE-AC03-76SF00515.

[†]Address after 15 September 1979: Institute of Theoretical Physics, University of California at Santa Barbara, Santa Barbara CA 93106.

I. INTRODUCTION

In this paper, which is a continuation of a previous one¹ hereafter referred to as I, we proceed to analyze polynomial quantum field theories defined on a spatial lattice, in terms of an anharmonic oscillator basis. There exists at present, two established procedures for analyzing such theories. The first is a weak coupling expansion which expands in terms which are higher than degree two in the field variables and the second consists of a strong coupling expansion which expands in the coupling or derivative matrix. The first of these suffers from the drawback that the perturbation expansion has zero radius of convergence,² even in the 0+1 dimensional theory.³ The second has the disadvantage that one is effectively expanding in the inverse lattice spacing, which grows without bound in the continuum limit.⁴ Our approach discussed here may be considered as intermediate to the two just discussed. The method involves the use of an orthogonal transformation to handle the dominant terms in the derivative (or coupling) matrix, while at the same time makes use of an anharmonic oscillator basis to handle terms which are higher than quadratic in the field variables. We exhibit some useful but simple orthogonal transformations that correspond roughly to "blocking" procedures but that are not well known in the physics literature. The hope of such an ambitious yet simple approach is that the resulting perturbation expansion may even have a finite radius of convergence. A version of perturbation theory will be described that utilizes a variational approach and which can be applied to an anharmonic basis.

In I we studied a 1+1 dimensional¹ theory and estimated numerically the critical surface of the theory. These results depended on an

-2-

<u>accurate</u> knowledge of the quantum anharmonic oscillator (actually on E and $\langle x^2 \rangle$ where needed). In this paper we approach a similar theory but in D apacetime dimensions with particularly simple choices for the orthogonal transformation (the Walsh and Haar transformation) which is susceptible to a more analytic treatment. The results we present are approximate and can be improved with a modest amount of effort.

In Section II we describe our variational method which involves a particular product form of a trial variational wave function. In Section III the equations which determine the anharmonic parameters in the trial wave function are derived for a general orthogonal transformation, the Walsh^{5,6} transform, and in Section V we discuss the Walsh solutions to the variational equations which were derived in Section III. We then construct the solutions for the Haar⁷ transformation in Section VI. Section VII is concerned with general excitation energy bounds. Finally in Section VIII we discuss a form of variational perturbation theory that can be used to improve our anharmonic solutions. Section IX contains a brief conclusion.

II. THE METHOD

The Hamiltonian we wish to study is the familiar ϕ^4 theory

$$H = \int d^{D-1}x \left[\pi^{2}(x) + (\nabla \phi)^{2}(x) + \lambda_{0} (\phi(x)^{2} - f_{0}^{2})^{2} \right] , \qquad (2.1)$$

where D is the number of space-time dimensions. Going to a cubic lattice of N $^{D-1}$ points, and lattice spacing a, yields

$$H = \sum_{\substack{\rightarrow \\ n \in V}} a^{D-1} \left[\pi_{\rightarrow}^{2} + a^{-2} \sum_{\substack{\rightarrow \\ m \in V}} \phi_{\rightarrow} D_{\rightarrow} \phi_{\rightarrow} + \lambda_{0} \left[\phi_{\rightarrow}^{2} - f_{0}^{2} \right]^{2} \right], \quad (2.2)$$

-3-

where V is the set of D-1 - tuples of integers such that each component lies between 0 and N-1, that is

$$V = \left\{ \vec{n} \in \mathbb{Z}^{D-1} \mid 0 \le n^{1} \le N \right\} , \qquad (2.3)$$

The coupling matrix $D_{n,\vec{m}}$ is chosen so that the continuum limit of the lattice Hamiltonian is a local one.

In order to write the lattice Hamiltonian in terms of dimensionless fields we perform the transformations

$$\phi_{\overrightarrow{n}} = \left(\lambda_0 a^{4-D}\right)^{-1/6} a^{\frac{2-D}{2}} q_{\overrightarrow{n}}$$

$$\pi_{\overrightarrow{n}} = \left(\lambda_0 a^{4-D}\right)^{1/6} a^{-\frac{D}{2}} p_{\overrightarrow{n}}$$
(2.4)

and the Hamiltonian becomes

ł,

$$H = a^{-1} \lambda^{1/3} \sum_{\substack{\stackrel{\rightarrow}{n} \in \mathbb{V}}} \left[p_{\stackrel{\rightarrow}{n}} \Delta \sum_{\substack{\stackrel{\rightarrow}{m} \in \mathbb{V}}} q_{\stackrel{\rightarrow}{n}} D_{\stackrel{\rightarrow}{n},\stackrel{\rightarrow}{m},\stackrel{\rightarrow}{m}} q_{\stackrel{\rightarrow}{m}} + \left(q_{\stackrel{\rightarrow}{n}}^2 - f^2 \right)^2 \right], \quad (2.5)$$

where $\lambda = \lambda_0 a^{4-D}$, $\Delta = \lambda^{1/3}$ and $f^2 = \lambda^{1/3} a^{D-2} f_0^2$. The dimensionless variables p_n and q_n satisfy

The basis of our approach is very simple. We will construct a variational ground state wave function of H, which is of the product form

$$\psi \begin{pmatrix} q \\ n \end{pmatrix} = \prod_{\substack{\rightarrow \\ n \in V}} \phi \begin{pmatrix} r \\ n \end{pmatrix} \begin{pmatrix} f^2 \\ n \end{pmatrix} \begin{pmatrix} r \\ n \end{pmatrix}$$

where the r_{\rightarrow} are related to the q_{\rightarrow} through an orthogonal transformation n

$$\mathbf{q}_{\vec{n}} = \sum_{\vec{m} \in \mathbf{V}} \mathbf{t}_{\vec{n}, \vec{m}} \mathbf{r}_{\vec{m}}$$
(2.8)

and

$$\sum_{\substack{\substack{n\\m\in V}}} t_{\substack{n\\m\in M}} t_{\substack{n\\m\in M}} = \delta_{\substack{n\\m\in M}}$$
(2.9)

The functions $\phi(\lambda, f^2; q)$ which appear in Ψ are ground state <u>anharmonic</u> oscillator wave functions, which satisfy

$$\begin{bmatrix} -\frac{d^2}{2} + \lambda (q^2 - f^2)^2 \\ dq \end{bmatrix} \phi(\lambda, f^2; q) = E(\lambda, f^2) \phi(\lambda, f^2; q) , \quad (2.10)$$

and were discussed in I.⁸ The main problems associated with constructing such a variational wave function are in determining the orthogonal transformation $t_{\vec{n},\vec{m}}$ and the parameters $\lambda_{\vec{n}}, f_{\vec{m}}^2$ which appear in Ψ . In our previous paper we showed that the standard blocking procedure could be interpreted in the above terms. For example, a two site blocking procedure was shown to correspond to a particular orthogonal transformation, the Haar transform, along with a simple sequential procedure for determining the anharmonic parameters which appear in Ψ . Thus in our approach a blocking procedure is not essential; it is simply one way of choosing the orthogonal transformation and of determing the parameters of the base problem. In this paper we shall discuss procedures which are more general than blocking.

III. GENERAL ORTHOGONAL TRANSFORMATION

In this section we will determine the conditions on the parameters $\lambda_{\overrightarrow{n}}$, $f_{\overrightarrow{n}}^2$ which appear in Ψ and decompose H into an unperturbed part H_0 and a perturbation H_1 which will be useful for discussing the induced perturbation expansion later. H_0 will be determined using a variational principle so that $(\Psi, H_2, \Psi) = 0$ by design.

Since our trial state Ψ is simple in terms of the r,'s it is convenient to express H in terms of the r's. One finds that

$$H = (a^{-1}\lambda^{1/3}) \left[\sum_{\substack{n \in V \\ n \in V}} \left(p_{\frac{1}{n}}^2 - 2f^2 r_{\frac{1}{n}}^2 + f^4 \right) + \Delta \sum_{\substack{n,n' \in V \\ n,n' \in V}} r_{\frac{1}{n}} d_{\frac{1}{n},n'} r_{\frac{1}{n},n'} r_{\frac{$$

where

$$d_{\vec{n},\vec{m}} = \sum_{\vec{k},\vec{k}' \in V} t_{\vec{k},\vec{n}} D_{\vec{k},\vec{k}'} t_{\vec{k}',\vec{m}}$$
(3.2)

To determine the optimal set of anharmonic parameters one must minimize $E = (\Psi, H \Psi)$. One might also consider the parameters that characterize the orthogonal transformation $t_{\vec{n},\vec{m}}$ as parameters to be varied. However, it is then very difficult to solve the resulting equations. It is far simpler to assume a form for the orthogonal transformation that does not do violence to the anharmonic nature of the problem nor to the coupling between oscillators, and it is this latter procedure that we shall pursue. Using the simple product form of Ψ in terms of the $r_{\rm m}{\,}'s$ and the above expression for H, we find that

$$\frac{E}{a^{-1}\lambda^{1/3}} = \sum_{\overrightarrow{n}\in V} E\left[\lambda_{\overrightarrow{n}}, f_{\overrightarrow{n}}^{2}\right] + \left[T_{\overrightarrow{n}} - \lambda_{\overrightarrow{n}}\right] Q^{4}\left[\lambda_{\overrightarrow{n}}, f_{\overrightarrow{n}}^{2}\right] + \left[f^{4} - \lambda_{\overrightarrow{n}}, f_{\overrightarrow{n}}^{4}\right] + \left[2\lambda_{\overrightarrow{n}}, f_{\overrightarrow{n}}^{2} - 2f^{2} + \Delta d_{\overrightarrow{n},\overrightarrow{n}}\right] Q^{2}\left[\lambda_{\overrightarrow{n}}, f_{\overrightarrow{n}}^{2}\right] + \left[f^{4} - \lambda_{\overrightarrow{n}}, f_{\overrightarrow{n}}^{4}\right] + 3\sum_{\overrightarrow{n}, \overrightarrow{n}\in V} Q^{2}\left[\lambda_{\overrightarrow{n}}, f_{\overrightarrow{n}}^{2}\right] Q^{2}\left[\lambda_{\overrightarrow{n}}, f_{\overrightarrow{n}}^{2}\right] T_{\overrightarrow{n},\overrightarrow{m}}, \qquad (3.3)$$

where

ł

$$T_{\overrightarrow{n}} = \sum_{\overrightarrow{k} \in V} \left[t_{\overrightarrow{n}, \overrightarrow{k}} \right]^{4}$$
(3.4)

and

$$T_{\vec{n},\vec{m}} = \sum_{\vec{\ell} \in V} t^2_{\vec{n},\vec{\ell}} t^2_{\vec{m},\vec{\ell}} \left(1 - \delta_{\vec{n},\vec{m}}\right) \qquad (3.5)$$

Finally

$$Q^{N}(\lambda, f^{2}) = \int_{-\infty}^{\infty} |\phi(\lambda, f^{2}; q)|^{2} q^{N} dq . \qquad (3.6)$$

Varying this expression with respect to λ_{1} , f_{1}^{2} , that is by setting

$$\frac{\partial E}{\partial \lambda} = 0 \quad \text{and} \quad \frac{\partial E}{\partial f_{\star}^2} = 0 ,$$

one finds after a few manipulations and an application of the Feynman-Hellman theorem that

$$\begin{array}{ccc} \lambda &= T \\ \stackrel{\rightarrow}{n} & n \end{array}$$

and

$$\lambda_{\overrightarrow{n}} \stackrel{f^2}{\xrightarrow{n}} = f^2 - \frac{1}{2} \land d_{\overrightarrow{n},\overrightarrow{n}} - 3 \sum_{\overrightarrow{m} \in V} T_{\overrightarrow{n},\overrightarrow{m}} Q^2 \begin{pmatrix} \lambda_{\overrightarrow{m}}, f_{\overrightarrow{m}}^2 \end{pmatrix}$$

Using this optimal set of anharmonic parameters one obtains an upper bound on the ground state energy of the vacuum

$$E_{true} \leq \left(\lambda^{1/3} a^{-1}\right) E , \qquad (3.8)$$

(3.7)

where

$$E = \sum_{\substack{n \in V \\ n \in V}} \left[E \left(\lambda_{\overrightarrow{n}}, f_{\overrightarrow{n}}^2 \right) + \left(f^4 - \lambda_{\overrightarrow{n}} f_{\overrightarrow{n}}^4 \right) \right] - 3 \sum_{\substack{n \to \infty \\ n, m \in V}} Q^2 \left(\lambda_{\overrightarrow{n}}, f_{\overrightarrow{n}}^2 \right) Q^2 \left(\lambda_{\overrightarrow{n}}, f_{\overrightarrow{m}}^2 \right) T_{\overrightarrow{n}, \overrightarrow{m}}.$$

It will prove interesting to decompose H into an unperturbed part H_0 to which Y and E are the exact energy eigenstate and eigenvalue, and H_1 the perturbation; that is

$$H = \left(\lambda^{1/3} a^{-1}\right) \left(H_0 + H_1\right)$$

where

$$H_{0} = \sum_{\substack{\rightarrow \\ n \in V}} \left[p_{\rightarrow}^{2} + \lambda_{\rightarrow} \left[r_{\rightarrow}^{2} - f^{2} \right]^{2} + J_{\rightarrow} \right]$$
(3.9)
$$J_{\rightarrow} = f^{4} - T_{\rightarrow} f_{\rightarrow}^{4} - 3 \sum_{\substack{\rightarrow \\ m \in V}} T_{\rightarrow} q^{2} \left[\lambda_{\rightarrow}, f_{\rightarrow}^{2} \right] q^{2} \left[\lambda_{\rightarrow}, f_{\rightarrow}^{2} \right]$$

and

where

$$\Gamma_{\vec{k},\vec{\ell},\vec{m},\vec{n}} = \sum_{\vec{j} \in V} t_{\vec{k},\vec{j}} t_{\vec{\ell},\vec{j}} t_{\vec{n},\vec{j}} t_{\vec{n},\vec{j}}$$

since (Ψ, H_1, Ψ) vanishes by construction it will first contribute to the energy in second order. In a later section we shall show how to calculate this correction to any desired accuracy.

In terms of the variational wave function Ψ , the two point correlation function is quite simple to evaluate, to lowest order in H_1 :

$$\left\langle \Psi, q, q, \Psi \right\rangle = \sum_{\vec{k} \in V} t_{\vec{n}, \vec{k}} t_{\vec{m}, \vec{k}} Q^2 \left(\lambda, f_{\vec{k}}^2 \right)$$
(3.12)

The lowest mode of the system is the d.c. component $t_{\vec{0},\vec{n}} = N^{-(D-1)/2}$. The behavior of the correlation function at large distances is strongly affected by the $\vec{k} = 0$ mode. For example if f_0^2 is large and positive, $Q^2 \left(\lambda_{\vec{0}}, f_0^2\right) \approx f_0^2$; this contribution to $\langle q_{\vec{1}} q_{\vec{1}} \rangle$ becomes

$$\left\langle \mathbf{q}_{\overrightarrow{\mathbf{n}} \overrightarrow{\mathbf{m}}} \right\rangle = \frac{\mathbf{f}_{0}^{2}}{\mathbf{N}^{D-1}} + \sum_{\substack{\overrightarrow{\mathbf{k}} \in \mathbf{V} \\ \overrightarrow{\mathbf{k}} \neq \mathbf{0}}} \mathbf{t}_{\overrightarrow{\mathbf{n}}, \overrightarrow{\mathbf{k}}} \mathbf{t}_{\overrightarrow{\mathbf{m}}, \overrightarrow{\mathbf{k}}} \mathbf{Q}^{2} \left\{ \lambda_{\overrightarrow{\mathbf{k}}}, \mathbf{f}_{\overrightarrow{\mathbf{k}}}^{2} \right\}$$
(3.13)

Therefore the signal for a constant correlation function at large distances $|\vec{n} - \vec{m}| \rightarrow \infty$ is that $f_{\vec{0}}^2$ grow like N^{D-1} as $N \rightarrow \infty$.

In I we showed that blocking two sites at a time corresponds to choosing $t_{\lambda,m}$ to be the classical Haar transform and gave generalization of this transform that corresponds to blocking M sites at a time. One can and should treat M as a variational parameter, since the optimum size "block" clearly depends on the values of the parameters f^2 , λ and Δ . In Section IV the Walsh transform eill be discussed and in Section V we present a solution to the variational equations which utilizes this transform. In Section VI, a short discussion of the Haar transform and its solution will be given.

IV. WALSH TRANSFORM

The Walsh transform is an orthogonal transformation with elements equal to (± 1) only.⁶ Since it was defined in I, only a brief review will be given here. Define the base 2 representation of the integer as $(0 \le l \le N-1 = 2^n - 1)$,

$$k = \sum_{r=0}^{n-1} k_r 2^r , \qquad (4.1)$$

where by definition $l_n = 0$. The Walsh function on 2^n points can then be written as (sequency ordered)

Wal(l,j) =
$$\prod_{r=0}^{n-1} (-1)^{l_r (j_{n-r} + j_{n-r-1})}$$
 (4.2)

where

$$Wal(l,j) = Wal(j,l)$$

$$(Wal(l,j))^{2} = 1$$

$$(4.3)$$

and

$$\sum_{j=0}^{N-1} Wal(k,j) Wal(j,l) = N \delta_{kl} .$$
 (4.4)

The Walsh functions obey the multiplication relation

$$Wal(k,j) Wal(\ell,j) = Wal(k \oplus \ell,j) , \qquad (4.5)$$

where $(k \oplus l)$ is bit by bit addition Modulo 2 under the rules 0 + 1 = 1 + 0 = 1, and 1 + 1 = 0 = 0 + 0. It is also the logical exclusive OR operation. Clearly the Walsh functions are closely associated with the discrete dyadic group.

Even though the Walsh functions take on the values of (± 1) only, it is possible to define a derivative operation. This has been termed the "logical derivative" by Gibbs.⁶ It is a difference operation defined by

$$v'(x) = \sum_{r=0}^{n-1} 2^{r-1} \left[v(x) - v(x \oplus (2^{n-r} - 1)) \right] . \quad (4.6)$$

The Walsh functions are easily shown to satisfy

$$(Wal(l,x))' = l Wal(l,x)$$
 (4.7)

A Walsh lattice theory is defined by choosing

$$t_{lj} = \frac{1}{\sqrt{N}} Wal(l,j) , \qquad (4.8)$$

and one easily finds

$$T_{g} = 1/N$$
, (4.9)

$$T_{\ell,n} = \left(1 - \delta_{\ell n}\right) / N \tag{4.10}$$

and for k, l, m and n distinct and unequal

$$T_{klmn} = \delta_{k \oplus l, m \oplus n} , \qquad (4.11)$$

where δ is the Knoenecker delta function.

There are several convenient choices for the derivative matrix D in the Hamiltonian. In general an interesting type of D to consider is one that is strongly correlated with the choice of the orthogonal transformation t and its associated basis functions. In the present case, if D is the square of the logical derivative operator then (in one space dimension)

$$D_{k\ell} = D_0 \delta_{k\ell} (\ell/N)^2 \qquad (4.12)$$

If the more familiar nearest neighbor derivative is chosen then

$$D_{k\ell} = \frac{1}{N} \sum_{ab} Wal(k,a) \Delta_{ab} Wal(\ell,b) , \qquad (4.13)$$

where

$$\Delta_{ab} = \left(2 \, \delta_{a,b} - \delta_{a,b+1} - \delta_{a,b-1} - \delta_{a,0} \delta_{b,N-1} - \delta_{a,N-1} \delta_{b,0} \right) \, .$$

One finds that the D matrix is not fully diagonal, but its diagonal part is given by

$$D_{ll} = \frac{2}{N} \left(2 l + 1 - (-)^{l} \right)$$
$$= \frac{8}{N} \left[\frac{l + 1}{2} \right] , \qquad (4.14)$$

where [z] is the nearest integer below or equal to Z. It is straight forward to explicitly see that the D matrix is diagonal for N = 2 and 4, and that the zeroth and $(N-1)^{st}$ modes are uncoupled for any N:

$$D_{\ell 0} = 0$$

$$D_{\ell,N-1} = 4 \delta_{\ell,N-1}$$

As an example of our technique, and to motivate the choice of the coupling between lattice sites (the D matrix) consider a free scalar field theory. The transformed Hamiltonian is

$$H = \sum_{\ell} \left[p_{\ell}^{2} + m^{2} r_{\ell}^{2} \right] + \sum_{k,\ell} r_{k} D_{k\ell} r_{\ell}$$

and if the D matrix is chosen to be the square of the "logical" derivative⁶

$$D_{k\ell} = \delta_{k\ell} \left(\frac{2 \pi \ell}{a N} \right)^2 ,$$

Then H can be directly diagionalized. The result for the ground state is

$$E = \sum_{\ell=0}^{N-1} \left[m^2 + \left(\frac{2 \pi \ell}{a N} \right)^2 \right]^{1/2}$$

The continuum limit is easily performed by defining $K = 2\pi / Na$, and the sum becomes $\frac{2\pi}{a} \left(1 - \frac{1}{N} \right)$ $E = Na \int \frac{dk}{2\pi} \left[m^2 + k^2 \right]^{1/2}$

which is the exact result in the limit $a \rightarrow 0$, Na = L.

These relations are easy to generalize for higher spacetime dimensions. In D spacetime dimensions one defines

$$\mathbf{t}_{\overrightarrow{l},\overrightarrow{n}} = \prod_{i=1}^{D-1} \mathbf{t}_{\underset{i=1}{l} \overrightarrow{n}_{i}}$$
(4.15)

Most of the previous formula are generalized by replacing the scalar indices by vector ones(i.e., $\delta_{l,n} \stackrel{\rightarrow}{\rightarrow} \stackrel{\delta_{\rightarrow}}{\underset{l,n}{\rightarrow}}$, etc.). The generalization of

and

2

the Walsh transformed nearest neighbor derivative, Eq. (4.14), becomes

$$d_{\vec{k},\vec{k}} = \frac{8}{N} \sum_{i=1}^{D-1} \left[\frac{\ell_i + 1}{2} \right]$$
(4.16)

which we shall utilize in the next section. Note that N is the number of lattice points in any one direction. The total number of lattice points in V is therefore N^{D-1} .

V. WALSH SOLUTIONS

In this section we provide the solutions to the variational equations which were derived in Section III, for a particular choice of the orthogonal transformation, the Walsh transformation. The solutions are particularly simple, due to the fact that the Walsh matrices contain only the elements ±1. The solutions are analytical in nature and we are able to compare the critical regions of these solutions with the numerical ones obtained in paper I. As will be evident from the solutions, choosing the full Walsh transform is equivalent to a block size of N; hence the solutions will share certain good and bad features with the mean field approximation.

As was shown in Section IV, one has the relations for the Walsh transform that

$$T_{n} = N^{1-D}$$
(5.1)

$$\Gamma_{\vec{k},\vec{n}} = N^{1-D} \left(1 - \delta_{\vec{k},\vec{n}} \right)$$

One finds that with this choice of the orthogonal transformation that the variational equations of Section III take the simple form

$$N^{1-D}f_{\vec{n}}^{2} = f^{2} - \frac{1}{2} \Delta \vec{d}_{\vec{n},\vec{n}} - 3N^{1-D} \sum_{\vec{m} \in V} Q^{2} \left(N^{1-D}, f_{\vec{m}}^{2} \right)$$
(5.2)

where the prime on the sum means that the term with $\dot{m} = \dot{n}$ is omitted. It is convenient to rewrite this in the form

$$N^{1-D} f_0^2 = f^2 - 3N^{1-D} \sum_{\substack{m \in V - \{0\}}} Q^2 \begin{pmatrix} N^{1-D}, f_{\frac{m}{m}}^2 \end{pmatrix}$$
(5.3)

and

$$N^{1-D} f_{\vec{k}}^{2} = N^{1-D} f_{0}^{2} - \frac{1}{2} \Delta d_{\vec{k},\vec{k}} - 3N^{1-D} \left[Q^{2} \left[N^{1-D}, f_{\vec{k}}^{2} \right] - Q^{2} \left[N^{1-D}, f_{0}^{2} \right] \right].$$
(5.4)

For the case that $f^2 \le 0$, one sees that $f_0^2 \le 0$ and thus $f_{\frac{1}{2}}^2 \le 0$ for all $\frac{1}{4}$. Hence if f^2 is not too positive, one can define a mass by $\mu^2 = -2N^{1-D}f_0^2$. Using the fact that

$$Q^{2}(\lambda, f^{2}) = \lambda^{-1/3} Q^{2}(1, \lambda^{1/3}, f^{2})$$

where

$$\lim_{g^2 << -1} Q^2(1,g^2) = \frac{1}{2\sqrt{-2g^2}} \left[1 - \frac{3\sqrt{2}}{8|g|^3} + \mathscr{O}\left(|g|^{-6}\right) \right]$$

one sees that

$$-N^{1-D}f_{\overrightarrow{\ell}}^{2} = \frac{1}{2}\mu^{2} + \frac{1}{2}\Delta d_{\overrightarrow{\ell},\overrightarrow{\ell}} + \mathscr{O}\left(N^{1-D}\right)$$

Neglecting the small corrections which go to zero in the infinite volume limit where $N \rightarrow \infty$, one has the self consistency condition that

$$\mu^{2} = -2f^{2} + \frac{3}{N^{D-1}} \sum_{\vec{k} \in V} \frac{1}{\sqrt{\mu^{2} + \Delta d_{\vec{k},\vec{k}}}} .$$
 (5.6)

The energy becomes

$$E = \sum_{\ell} \sqrt{\mu^{2} + \Delta d_{\ell\ell}} + N^{D-1} \left[f^{2} - \frac{1}{3} \left(f^{2} - \frac{1}{2} \mu^{2} \right)^{2} \right] + \frac{3}{4} N^{1-D} \sum_{\ell} \left(\mu^{2} + \Delta d_{\ell\ell} \right)^{-1} .$$
 (5.7)

and the last term is negligible as N $\rightarrow \infty$.

By extrapolating these results to larger f^2 , we may estimate the point at which the mass μ^2 vanishes (the critical point). This occurs when f^2 reaches f_c^2 where

$$f_{c}^{2} = \frac{3}{2} \frac{1}{N^{D-1}} \sum_{\vec{k} \in V} \left(\frac{1}{\sqrt{\Delta d_{\vec{k},\vec{k}}}} \right)$$
(5.8)

In order to compare with the numerical results which were obtained in paper I, we make use of the nearest neighbor derivative where $d_{\overrightarrow{k},\overrightarrow{k}} = (8/N) \sum_{i=1}^{D-1} [(l_i+1)/2]$. In this case the infinite volume limit of the previous equation may be taken explicitly and one finds that l_i

$$\mu^{2} = -2f^{2} + 3 \int_{0}^{\pi} dx_{1} \dots dx_{D-1} \frac{1}{\sqrt{\mu^{2} + 4\Delta \sum_{i=1}^{D-1} x_{i}}}$$
(5.9)

The critical point is obtained by requiring that $\mu^2 = 0$ or

$$f_{c}^{2} = \frac{3}{2} \frac{1}{\sqrt{\Delta}} I_{D}$$
 (5.10)

with

$$I_{D} = \frac{1}{2} \int_{0}^{1} dx_{1} \dots dx_{D-1} \frac{1}{\sqrt{\sum_{i=1}^{D-1} x_{i}}}$$
(5.11)

and one finds $I_2 = 1$, $I_3 = (4/3)(\sqrt{2} - 1)$, $I_4 = (4/5)(1 + 3\sqrt{3} - 4\sqrt{2})$, etc. With D = 2, we see that

$$\sqrt{\Delta} f_c^2 = 3/2$$
 (5.12)

which we can compare with the numerical results of I. For $\Delta = 10$ we found that $\sqrt{\Delta} f_c^2 = 1.483$ to be compared with the above, an error of only 1%. We expect that the accuracy of these results should be improved at larger Δ ; for smaller Δ the reverse is true and indeed one finds a larger discrepancy at $\Delta = 2$, about 5% (see Fig. 2 in I).

Specializing to the case D = 2 we have

$$\mu^{2} = -2f^{2} + \frac{3}{2\sqrt{\Delta}} \int_{0}^{1} dx \frac{1}{\sqrt{(\mu^{2}/4\Delta) + x}}$$
$$= -2f^{2} + \frac{3}{\sqrt{\Delta}} \left(\sqrt{1 + (\mu^{2}/4\Delta)} - \sqrt{(\mu^{2}/4\Delta)} \right) . \quad (5.13)$$

For $\mu^2 << 1$ we may invert this relation to obtain

$$\mu = \frac{2\sqrt{\Delta}}{f_c^2} \left[f_c^2 - f^2 \right] \left(1 + \mathcal{O} \left[f_c^2 - f^2 \right] \right)$$
(5.14)

which implies that the critical exponent ν is one. This is what one might expect since this theory should belong to the same universality class as the two-dimensional Ising model where $\nu = 1$ exactly. A similar analysis for D = 3 and 4 implies that $\nu = 1/2$ in both cases. Numerical studies have hinted toward $\nu_3 = 0.638$, and $\nu_4 = 0.5$. If f^2 is sufficiently positive we may define a positive magnetization by $M^2 = N^{1-D} f_0^2$. In this regime we may use the previous scaling relations and the fact that

$$\lim_{f^2 \to 1} Q^2(1, f^2) = f^2 - \frac{1}{2f} \left[1 + \mathcal{O}(f^{-3}) \right]$$
(5.15)

to find a solution in which the $f_{\vec{l}}$'s are negative for $\vec{l} \neq 0$ and

$$-N^{1-D} f_{\frac{1}{2}}^{2} = 2M^{2} + \frac{1}{2} \Delta d_{\frac{1}{2},\frac{1}{2}} \quad (\vec{k} \neq 0) \quad (5.16)$$

along with a self consistency condition

$$M^{2} = f^{2} - \frac{1}{N^{D-1}} \frac{3}{2} \sum_{\vec{k} \neq 0} \frac{1}{\sqrt{\frac{4M^{2} + \Delta d}{\vec{k}, \vec{k}}}}$$
(5.17)

In this case we call the system <u>ordered</u> and the two-point function goes to the constant M^2 at large distances. The energy can be easily evaluated to leading order in N:

$$E = \sum_{l} \sqrt{\frac{4M^2 + \Delta d_{ll}}{4M^2 + \Delta d_{ll}}} + \frac{2}{3} N^{D-1} \left(f^2 - M^2 \right)^2 \quad .$$
 (5.18)

To compare to the previous results for the disordered phase we again take the infinite volume limit $N \rightarrow \infty$ and make use of the nearest neighbor derivative to obtain

$$M^{2} = f^{2} - \frac{3}{2} \int_{0}^{1} dx_{1} \dots dx_{D-1} \left[M^{2} + 4\Delta \sum_{i=1}^{D-1} x_{i} \right]^{-1/2} (5.19)$$

Note that the magnetization M vanishes at precisely the same point where the mass μ vanished in the disordered region, i.e., in this approximation the two critical points coincide. This is perhaps fortuitous because the magnetization itself behaves incorrectly near the critical point. There are two possible values of M^2 for a given f^2 (for f^2 near f_c^2). This region of double valuedness decreases as Δ increases. Indeed the solution M^2 (f^2) should be single valued. A more detailed analysis shows that the wave function with the larger of the two M^2 's is the one with the lowest energy. This flaw is perhaps reminiscent of the first order behavior found by Drell et al.,⁹ where a variational principle was also applied. This result is surprising to us since the numerical result of paper I predicted essentially the "correct expected" behavior for the magnetization using the Haar transform with the simple parameter determination given by the 2-site blocking scheme. Perhaps the problem here is in our approximate analytic solution.

VI. HAAR TRANSFORM SOLUTION

The Haar transform was discussed in some detail in I. In this section a brief review of its properties will be given and the resulting form of the Hamiltonian and its lowest order solution. For reasons of simplicity, only one case of D=2, or one space dimension, will be discussed in detail. The Haar transform is constructed by first "blocking" two sites at a time; that is, one forms the sum and difference coordinates and then proceeds by re-"blocking" the sum coordinates two at a time until the top of the coordinate pyramid is reached. Thus the discrete Haar transform is an orthogonal matrix made up on the elements 0 and $\pm(\sqrt{2})^p$ only. Examples and a complete definition were given in I.

If the above construction procedure is applied to $N = 2^n$ coordinates, at the first stage, or level, there are N/2 difference coordinates that

-19-

are not affected by later steps in the construction. At the second level, there are N/4 difference coordinates that are fixed and at the L^{th} level, there are 2^{n-L} difference coordinates. The magnitude of the nonzero elements of the Haar matrix depend only on the level; one finds (2)^{-L/2} for the size of all elements in level L.

In the equation the F's, one needs T_{ℓ} , $T_{\ell,n}$, and the sum over the Q^2 's. First note that $T_{\ell,\ell}$ can depend only on the respective levels that ℓ and ℓ ' are in. If $\ell(\ell')$ is in level L(L'), then one finds that

$$T_{\ell,\ell'} = T_{L,L'} = 2^{-L_{>}} \left(1 - \delta_{\ell\ell'} \right),$$
 (6.1)

where $L_{>}$ is the larger of L or L', and

$$T_{l} = T_{L} = 2^{-L}$$
 (6.2)

In the equation of the F's, Eq. (3.7), one needs a sum S_{g} of the form W-1 n

$$S_{\ell} = \sum_{\ell'=1}^{W-1} T_{\ell,\ell'}, q_{\ell'}^2, = \sum_{L'=1}^{H} T_{L,L'}, q_{\ell'}^2,$$
 (6.3)

since λ_{ℓ}^{2} , F_{ℓ}^{2} , and hence Q_{ℓ}^{2} , depend only on the level L of the coordinate r_{ℓ} . This sum is easy to evaluate by dividing it into two terms in which L' > L and L' < L. For the latter case, one needs to know the number of terms in level L' that contribute to a given L, this is seen to be $2^{L-L'}$. Thus the sum becomes

$$S_{\ell} = \sum_{L' \neq L} 2^{-L'} Q^2 \left(\lambda_{L'}, F_{L'}^2 \right)$$
(6.3)

where $\lambda_{L} = \lambda 2^{-L'}$ and L' runs from 1 to n.

The nearest neighbor derivative term is straightforward to evaluate after some thought. Its diagonal elements are found to be

$$D_{ll} = 2^{-n} (0, 8, 3 \cdot 2^2, \dots, 3 \cdot 2^{n+1-L}, \dots, 3 \cdot 2^n) , \qquad (6.4)$$

where the 0 value is for the variable $r_0 = \sum_{i=0}^{N-1} x_i$, etc.

The final reduced form for the equations that determine the parameters in H_0 are easily written down in terms of F^2 (associated with the variable r_0) and G_L^2 , $n \le L \le 1$, associated with the (degenerate) difference coordinates at level L. The result is

$$F^{2} = 2^{n} \left[f^{2} - 3 \sum_{L'=1}^{n} 2^{-L'} Q^{2} \left[\lambda_{L'}, G_{L'}^{2} \right] \right]$$
(6.5)

and

$$G_{L}^{2} = 2^{L} \left[f^{2} - 3 \cdot 2^{-n} Q^{2} \left(\lambda_{n}, F^{2} \right) - \sum_{L' \neq L} 2^{-L'} Q^{2} \left(\lambda_{L'}, G_{L'}^{2} \right) \right] - \frac{\Delta}{\lambda} \left(3 + \delta_{Ln} \right).$$

Approximate solution for these equations can be found if the parameters are in suitable domains. For example, if \triangle is large and F^2 is not too near zero, one may write

$$F^2 = 2^n M^2,$$

where M is the magnetization and then by taking the difference of (6.5),

$$G_{L}^{2} \cong -\left[2^{L+1} M^{2} + \frac{\Delta}{\lambda} \left(3 + \delta_{Ln}\right)\right] , \qquad (6.6)$$

If $|G_L^2|$ is large enough so that the term $3Q_L^2$ can be neglected compared to $2^L M^2$.

Some useful relations for the quartic oscillator which can be used to derive and discuss these solutions for F^2 and G_L^2 are: for $g^2 \rightarrow +\infty$, $Q^2 \left(\Lambda, g^2\right) \cong q^2 - \frac{1}{2\sqrt{\Lambda g^2}} + \dots$ and for $g^2 \rightarrow -\infty$,

$$Q^2\left(\Lambda,g^2\right) \simeq \frac{1}{\sqrt{8\Lambda|g^2|}} \left[1 - \frac{3\Lambda}{2\left(2\Lambda|g^2|\right)^{3/2}}\right]$$

or to this order

$$3Q^{2}\left(\Lambda,g^{2}\right) - g^{2} \cong \left[8\Lambda\left(Q^{2}\left(\Lambda,g^{2}\right)\right)^{2}\right]^{-1}$$

The consistency relation that determines $M^2(f^2)$ to this approximation is then

$$M^{2} = f^{2} - \frac{3}{\sqrt{8\Delta}} \sum_{L=1}^{n} 2^{-L/2} \left[3 + \delta_{Ln} + 2^{L+1} \lambda M^{2} / \Delta \right]^{-1/2} .$$
 (6.7)

For $M^2 = 0$, the critical value of f^2 is

$$f^{2} = f_{c}^{2} = \frac{3}{\sqrt{8\Delta}} \sum_{l}^{n} 2^{-L/L} \left[3 + \delta_{Ln} \right]^{-1/2}$$

or

$$\sqrt{\Delta} f_c^2 = \frac{\sqrt{6}}{4(\sqrt{2} - 1)} + \mathscr{O}\left(2^{-n/2}\right)$$
 (6.8)

The numerical value of the first term is 1.478. Recall that the Walsh transform gave the result 1.50, and the iterative numerical Haar transform used in I gave the value 1.483 (at $\Delta = 10$, $\lambda = 1$). Again, just as in the Walsh transform case, while the value of f_c^2 is given quite accurately by these analytical results, the critical exponent is not very satisfactory.

The energy estimate takes the form $(\lambda = 1)$

$$E = 2M + \sum_{L=1}^{n} 2^{n-L} \sqrt{4M^2 + \Delta e_{LL}} + \frac{2}{3} \cdot 2^n \cdot \left(f^2 - M^2\right)^2, \qquad (6.9)$$

where

$$e_{LL} = 2^{1-L} \left(3 + \delta_{Ln}\right)$$

These should be compared with the result for the Walsh transform given in equation (5.18) for D=2. As one expects, the main difference is in the form of the Δ term. This kinetic term has a geometric spectrum $(\sim 2^{-L} \Delta)$ for the Haar transform and a linear spectrum ($\sim \ell \Delta$) for the Walsh transform.

VII. EXCITATION ENERGY BOUNDS

In this section we shall show how to bound and to estimate the excitation energies of quantum systems. An exact bound between the excitation energy and the correlation function will be derived. The techniques to be used are probably familiar in the literature but we will reformulate them for convenient application to the present lattice theory. The feature we will use is the fact that for $f^2 \leq 0$, the quartic oscillator has matrix elements and moments that are quite different in magnitude from a harmonic oscillator but the selection rules are very accurately satisfied.

First consider a single general oscillator in which the exact ground state $|0\rangle$ is known:

$$H|0\rangle = E_0|0\rangle$$

Define an "excited" state by

$$|h\rangle = h(x)|0\rangle$$
,

then one finds by simple manipulation that

$$E_{h} \leq \langle h | H | h \rangle / \langle h | h \rangle$$

satisfies

$$E_{h} - E_{0} \le \langle 0 | (h')^{2} | 0 \rangle \langle 0 | h^{2} | 0 \rangle$$
 (7.1)

For example, choosing h = x, $(x^2 - \langle 0 | x^2 | 0 \rangle)$ respectively, yields bounds on the excitation energies

$$E_{1} - E_{0} \leq 1/\langle 0 | x^{2} | 0 \rangle$$

$$E_{2} - E_{0} \leq 4\langle 0 | x^{2} | 0 \rangle / (\langle 0 | x^{4} | 0 \rangle - \langle 0 | x^{2} | 0 \rangle^{2}).$$
(7.2)

If $V = (x^2 - f^2)^2$ the first inequality is only off by 0.8% and the second by 1.8% for $f^2 = 0$. They are more accurate for f^2 negative and less accurate for f^2 positive. For large positive f, a more sensible choice for h is h = tanh ax, where a ~ 2f. The resultant energy gap is exponentially small in f $(E_1 - E_0 \sim \exp(-f^3))$.

Now consider a general lattice theory. Using the above line of argument one finds $(h = h(q_0 \dots q_{N-1}))$

$$E_{1} - E_{0} \leq \sum_{i=0}^{N-1} \langle 0 | \left(\frac{\partial h}{\partial q_{i}} \right)^{2} | 0 \rangle / \langle 0 | h^{2} | 0 \rangle$$

Now consider the choice

$$h = \sum_{i=1}^{n} q_{i}$$

and then

$$\sum_{\mathbf{i}} \langle \mathbf{0} | \left(\frac{\partial \mathbf{h}}{\partial \mathbf{q}_{\mathbf{i}}} \right)^2 | \mathbf{0} \rangle = \mathbf{N}$$

$$\langle 0 | h^{2} | 0 \rangle = \sum_{i,j} \langle 0 | q_{i} q_{j} | 0 \rangle$$

= N $\sum_{j} \langle 0 | q_{0} q_{j} | 0 \rangle$

by translational invariance. The bound on the excitation energy is

$$E_1 - E_0 \le 1 / \sum_j \langle 0 | q_0 q_j | 0 \rangle$$
 (7.3)

The denominator is the volume integral of the correlation function (which is also its Fourier transform at k = 0). Thus if the correlation function is infinite at k = 0., then E_1 and E_0 <u>must</u> be degenerate.

VIII. VARIATIONAL PERTURBATION THEORY

Let us now turn to perturbation theory and show how to improve the zeroth order (but variational) results of the previous sections. The methods we shall use are straightforward extensions of familiar and well tested ideas in lower dimensional contexts.¹⁰ Since the first order energy shift due to the perturbation H_1 is zero, it first contributes to second order. If one is not going to compute third order, it hardly makes sense to evaluate the second order shift exactly. Therefore we will review the derivation of a variational principle for the second order energy shift due to H_1 . The main feature we can utilize here is that the anharmonic oscillator satisfies the harmonic oscillator selection rules to high accuracy.

Write the first order change in the wave function as a function F(q) times the unperturbed $|\psi\rangle$. The second order energy shift can be written in the equivalent forms $(H_1 \equiv W)$

$$\mathbf{E}_{2} = \langle \psi | \mathbf{WF} | \psi \rangle = \langle \psi | \mathbf{FW} | \psi \rangle = - \langle \psi | | \vec{\nabla}\mathbf{F} |^{2} | \psi \rangle$$

by simple manipulation. A stationary principle for E₂ can be constructed out of these forms:

$$\begin{bmatrix} E_2 \end{bmatrix} = \langle \psi | WF + FW + | \vec{\nabla}F |^2 | \psi \rangle , \qquad (8.1)$$

which is stationary with respect to variations in F. This can be derived directly from equation (7.1) of the previous section by writing h = 1+F, $H = H_0 + W$, and choosing $|\psi\rangle$ to be an eigenstate of H_0 . An expansion in powers of F then yields (8.1)

A. The first type to be considered is the nondiagonal part of the derivative matrix

$$W_{A} = \sum_{k,l} r_{k} D_{kl} r_{l}$$

where $D_{ll} = D_{l0} = 0$ and D is symmetric. Assume F is of the form

$$\mathbf{F}_{\mathbf{A}} = \sum_{\mathbf{k}, \mathbf{\ell}} \left[\mathbf{r}_{\mathbf{k}} \mathbf{A}_{\mathbf{k} \mathbf{\ell}} \mathbf{r}_{\mathbf{\ell}} \right]$$

where $A_{ll} = A_{l0} = 0$. The stationary form for E_2 takes the form

$$\begin{bmatrix} E_2 \end{bmatrix} = \sum_{k,\ell} \left[4 A_{k\ell} D_{k\ell} Q_k^2 Q_\ell^2 + 2 A_{k\ell} A_{\ell k} \left[Q_k^2 + Q_\ell^2 \right] \right]$$

The stationary solution for ${\bf F}_{\!\!A}$ is

$$A_{k\ell} = -D_{k\ell} \left[\frac{1}{Q_k^2} + \frac{1}{Q_\ell^2} \right]^{-1}$$

and

$$\begin{bmatrix} E_2 \end{bmatrix} = -2 \sum_{k,l} D_{kl} D_{lk} Q_k^2 Q_l^2 \left[\frac{1}{Q_k^2} + \frac{1}{Q_l^2} \right]^{-1} . \quad (8.2)$$

Using the previous bounds for $E_1 - E_0$, this form can alternatively be interpreted as a closure approximation to the familiar second order sum over states. However, more general forms for F allow one to calculate E_2 to any desired accuracy using only properties of the ground state $|\psi\rangle$. The first order correction to the correlation function is

$$\langle q_{0}q_{j} \rangle = \frac{1}{N} \sum_{k,\ell} t_{0k} t_{j\ell} \langle \psi | (1+F) r_{k} r_{\ell} (1+F) | \psi \rangle$$

$$= \frac{1}{N} \sum_{k,\ell} t_{j\ell} \langle \psi | r_{k} r_{\ell} (1+2F+\ldots) | \psi \rangle$$

$$= \frac{1}{N} \sum_{\ell} t_{j\ell} Q_{\ell}^{2} + \frac{4}{N} \sum_{k,\ell} t_{j\ell} A_{\ell k} Q_{\ell}^{2} Q_{\ell}^{2} + \ldots \qquad (8.3)$$

Recall that $D_{\ell 0} = 0$, hence $A_{\ell 0} = 0$ and therefore there is <u>no first order</u> <u>correction</u> to the magnetization from this perturbation (as in fact required by the structure of $D_{k\ell}$).

B. The second term in W is of the form (recall $T_{ll} \equiv 0$)

$$W_{\rm B} = 3\lambda \sum T_{\ell n} \left(r_{\ell}^2 - Q_{\ell}^2 \right) \left(r_n^2 Q_n^2 \right)$$

đ

Since the operators of the form $(r^2 - Q^2)$ excite the modes to even states, it is natural to try an F of the form

$$F_{B} = \sum_{\ell n} B_{\ell n} \left[r_{\ell}^{2} - Q_{\ell}^{2} \right] \left[r_{n}^{2} - Q_{n}^{2} \right]$$

where $B_{q,q} = 0$. The stationary solution for B is

$$B_{\ell n} = -\frac{3\lambda}{4} T_{\ell n} \left[\frac{Q_{\ell}^2}{R_{\ell}} + \frac{Q_n^2}{R_n} \right]^{-1} ,$$

where $R_{\ell} = Q_{\ell}^4 - Q_{\ell}^2 Q_{\ell}^2$, and the resultant energy shift is

$$E_{2}^{B} = -\frac{9\lambda^{2}}{2} \sum_{\substack{\left(T_{\ell n}\right)^{2}}} R_{\ell} R_{n} \left[\frac{Q_{\ell}^{2}}{R_{\ell}} \frac{Q_{n}^{2}}{R_{n}} \right]^{-1} . \quad (8.4)$$

This is also easy to interpret in terms of a sum over states by recalling that $E_2 - E_0 \simeq 4Q^2/R$. This formula has been applied to two coupled quartic oscillators in I and found to substantially increase the accuracy of the energy calculation.

Finally, we note that F_B does not effect the correlation function to first order since $\langle \psi | F_B | \psi \rangle = 0$.

C. The final type of term in W is of the form

$$W_{\rm C} = \lambda \sum_{\neq} T_{\rm klmn} r_{\rm k} r_{\rm l} r_{\rm m} r_{\rm n}$$

And for simplicity we will assume that $T_{k\ell mn}$ is of the Walsh form-that is, T vanished if any two indices are equal. A more general T only requires a more general notation. Now since the 0th mode could have a large positive F_0^2 , it is necessary to separate the terms in the sum that involve r_0 and those that do not; thus we write

$$W_{C} = W_{C}^{0} + W_{C}^{1} ,$$

where

$$W_{C}^{0} = 4\lambda \sum T_{0 \ell m n} r_{0} r_{\ell} r_{m} r_{n}$$

and

$$W_{C}^{1} = \lambda \sum_{\neq 0} T_{k \ell m n} r_{k} r_{\ell} r_{m} r_{n}$$

Consider the second term in ${\tt W}_C$ first. It is natural to assume an ${\tt F}_C^1$ of the form

$$\mathbf{F}_{\mathbf{C}}^{1} = \sum_{\neq 0} \mathbf{C}_{k \ell m n}^{1} \mathbf{r}_{k} \mathbf{r}_{\ell} \mathbf{r}_{m} \mathbf{r}_{n}$$

and one easily finds that the stationary solution for C^1 is

$$C_{klmn}^{1} = -\lambda T_{klmn} \left[\frac{1}{Q_{k}^{2}} + \frac{1}{Q_{k}^{2}} + \frac{1}{Q_{m}^{2}} + \frac{1}{Q_{n}^{2}} \right]^{-1} . \qquad (8.5)$$

The stationary form for this contribution to E_2 is simple to write down.

The term in W_C involving r_0 must be treated differently because this mode may have a large positive F^2 and a different choice for F_C is necessary. Based on our previous discussion, we will write

$$\mathbf{F}_{C}^{0} = \sum \mathbf{C}_{0 \, \ell \, \mathrm{mn}}^{0} \, \mathbf{h}(\mathbf{r}_{0}) \, \mathbf{r}_{\ell} \, \mathbf{r}_{\mathrm{m}} \, \mathbf{r}_{\mathrm{n}}$$

where $h(r_0)$ will be chosen below and neither l, m, nor n can be equal to zero. The solution for C⁰ is

$$C_{0\,\ell mn}^{0} = -\lambda T_{0\,\ell mn} \frac{\langle r_{0}h(r_{0}) \rangle}{\langle h^{2}(r_{0}) \rangle} \left[\frac{1}{Q_{\ell}^{2}} + \frac{1}{Q_{m}^{2}} + \frac{1}{Q_{n}^{2}} + \frac{\langle (h')^{2} \rangle}{\langle h^{2} \rangle} \right]^{-1}$$

If F^2 is very large and positive this form can be simplified. Since a reasonable choice for h is h = tanh (ar₀), one sees that $\langle h'^2 \rangle / \langle h^2 \rangle$ is exponentially small in F^2 , and that $\langle r_0 h \rangle / \langle h^2 \rangle \sim F$, to a very high accuracy (exponential in F^2). Thus

$$c_{0\ell mn}^{0} \cong -\lambda T_{0\ell mn} F \left[\frac{1}{Q_{\ell}^{2}} + \frac{1}{Q_{m}^{2}} + \frac{1}{Q_{n}^{2}} \right]^{-1}$$

and its contribution to E_2 is

$$\left[E_{2}(C^{0})\right] \simeq -\lambda^{2}(3!)Q_{0}^{2}F \sum_{n} \left[T_{0\ell mn}\right]^{2} Q_{\ell}^{2}Q_{m}^{2}Q_{n}^{2}\left[\frac{1}{Q_{\ell}^{2}} + \frac{1}{Q_{m}^{2}} + \frac{1}{Q_{n}^{2}}\right]^{-1} . \quad (8.6)$$

One again sees that W_C does not affect the two point correlation function to first order. The above choice for $h(r_0)$ includes the important contribution of the (almost degenerate) odd excited state to the sum over intermediate states. A more general choice will do a better job of including the less important higher excited odd states. D. In this paragraph a counting of the terms in the second order energy shifts in the case of the Walsh transform will be given in order to estimate the importance of the various terms in the perturbation W. We shall perform the counting by setting the Q's and R's equal to their average values and take them outside the sum over modes. (By setting the Q's and R's equal to their extreme values one can get bounds on E_2 but this will not be pursued here.) Again, the l=0 mode will be treated differently from the l>0 modes. The Haar transform can be discussed in a similar way.

Proceeding in the above manner one finds

$$\begin{bmatrix} E_2^A \end{bmatrix} \sim -(\bar{Q}^2)^3 \sum_{k \neq l} D_{kl} D_{lk}$$

where the average of $Q^2 = \overline{Q}^2$ for l > 0. For the nearest neighbor form for the gradient, the sum can be performed with the result

$$\begin{bmatrix} E_{2}^{A} \end{bmatrix} \simeq -(\bar{Q}^{2})^{3} \quad \frac{8}{3} \quad \Delta^{2} \quad N$$
(8.7)

Thus W_A can contribute to the energy density as $N \rightarrow \infty$.

The perturbation $W_{\rm B}$ contributes terms of the form

$$\begin{bmatrix} E_{2}^{B} \end{bmatrix} \sim -\frac{9\lambda^{2}}{2} \frac{N-1}{N^{2}} \begin{bmatrix} \frac{2R_{0}\bar{R}}{\left[\frac{Q_{0}^{2}}{R_{0}} + \frac{\bar{Q}^{2}}{\bar{R}}\right]} + \frac{\bar{R}^{3}}{\bar{Q}^{2}} \frac{N-2}{2} \end{bmatrix}$$
(8.8)

Finally, the term W_{C} is computed by using the explicit form of the WALSH matrices and one finds

$$\begin{bmatrix} E_2^{\vec{C}} \end{bmatrix} = -\lambda^2 4(4!) \frac{(N-1)(N-2)}{N^2} \left[\frac{(\bar{Q}^2)^4 Q_0^2}{3} \right] - \lambda^2 (4!) \frac{(N-1)(N-2)}{N} \left(1 - \frac{4}{N} \right) \left[\frac{(\bar{Q}^2)^5}{4} \right] (8.9)$$

IX. CONCLUSION

In this paper we have constructed some non-trivial variational wave functions for a ϕ^4 field theory in terms of an anharmonic oscillator basis. Our results seem qualitatively correct and we hope that these results may be improved upon with a modest amount of effort.

In I, we gave a general procedure for constructing orthogonal transforms that corresponded to an arbitrary block size M. It was applied to the case M=2 and numerical results were given for the ϕ^4 theory in D = 2. In this paper, the full Walsh transform was applied and shown to correspond to a block size which was the same as that of the sample, M = N. Approximate analytic solutions were given for the Walsh and Haar transform cases which are valid in restricted regimes of the parameters. A more exact numerical treatment is necessary. However, one significant feature of these solutions is that they are analytic in nature and there is no need for accurate computation involving anharmonic oscillators. The disadvantages of our analytic solutions is that they behave incorrectly near the critical point. In particular, the Walsh case with M=N is essentially the same as mean field theory. It is clearly possible to improve these results by discussing an arbitrary block size M and then choosing M variationally (i.e., the optimum M value will depend on f^2 , Δ and D). Further improvements will result from performing a more accurate analytic treatment and by applying the perturbation expansion as outlined in Section VIII.

-31-

ACKNOWLEDGMENT

This work was supported by the Department of Energy under Contract Number DE-AC03-76SF00515.

REFERENCES

- J. L. Richardson and R. Blankenbecler, SLAC-PUB-2317, to be published in Phys. Rev. D. (see references therein).
- 2. A. M. Jaffe, Comm. Math. Phys. 1, 127 (1965).
- 3. C. M. Bender and T. T. Wu, Phys. Rev. 184, 1231 (1964).
- C. M. Bender, F. Cooper, G. S. Guralnik and D. H. Sharp,
 Phys. Rev. <u>D19</u>, 1865 (1979); N. Parga, D. Toussiant and
 J. R. Fulco, Phys. Rev. <u>D20</u>, 887 (1979) and references therein.
- 5. J. L. Walsh, Am. J. Math. <u>45</u>, 5 (1923).
- 6. For a general review, see H. F. Harmuth, "Transmission of Information by Orthogonal Functions-" Second edition, Springer-Verlag (1972). In particular the "logical", or Gibbs derivative is discussed.
- 7. A. Haar, Math. Annalen <u>69</u>, 331 (1910).
- 8. For a general analysis, see B. Simon, Ann. Phys. <u>58</u>, 76 (1970).
- S. D. Drell, M. Weinstein and S. Yankielowicz, Phys. Rev. <u>D14</u>, 1627 (1976); M. Weinstein, Lectures presented at the Banff Summer Institute on Particles and Fields, Banff, Alberta, Canada, 25 August - 5 September, 1977. See also references therein.
- For a general review of practical perturbation theory see
 J. Killingbeck, Rept. Progr. Phys. <u>40</u>, 963 (1977), and also
 C. Schwartz, Ann. of Phys. 2, 156 and 170 (1959).