Anharmonic analysis of lattice field theories

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A new calculational procedure for polynomial lattice field theories is discussed that utilizes an anharmonic basis and a general orthogonal transformation of coordinates. The standard blocking procedure is shown to correspond to a discrete Haar transform of the field coordinates. Some generalizations of the Haar transform are given which allow one to block an arbitrary number of sites. This is applied to both the energy density and to the correlation functions. In this paper only an "unperturbed" problem will be discussed, but the unperturbed Hamiltonian will be chosen using a variational principle—it includes couplings and nonharmonic effects in a very nontrivial way. Numerical results will be given for certain critical indices for a ϕ^4 theory in one space dimension.

I. INTRODUCTION

In this series of papers, we shall develop a variation-perturbation approach to lattice field theories. The fundamental idea is to formulate such theories in an anharmonic-oscillator basis (actually a quartic oscillator with arbitrary mass term for the particular applications in this paper). In order to carry out this program in a convenient way it is necessary to consider the effects of a general orthogonal transformation on the Hamiltonian. We shall find that some quite simple transformations have a remarkable analog to the well-discussed "blocking" procedures[1-5] and that generalizations (with hopefully higher accuracy) are easy to generate.

Since we use an anharmonic-oscillator basis in our calculation, we expect (but have not been able to prove) that the resultant perturbation theory has a finite radius of convergence. That is, since we are expanding in what is effectively a λx^4 type of perturbation on an unperturbed Hamiltonian with an x^4 term, the series in λ should be convergent with a unit radius of convergence. In fact, we use a standard variational principle to choose the optimum unperturbed Hamiltonian. In this paper, only the optimum "unperturbed" results will be discussed—corrections will be dealt with in a later note.

First, a brief review of the properties of a single general quartic oscillator is given. In the subsequent applications to lattice theories, all we shall actually need are the energy and $\langle x^2\rangle$ for such an oscillator.

Second, a simple 2-site blocking procedure will be discussed for a one-dimensional ϕ^4-type lattice theory and conditions for a phase transition, or a massless excitation, will be described. Both the energy and correlation function will be evaluated. Numerical results are then given, with maps of the ordered and disordered phases, selected critical indices, and the correlation function.

The 2-site blocking procedure is then reinterpreted as a particular orthogonal transformation—the Haar transform.[6] The Haar transform is then generalized to blocking M sites at a time and applied to $M=4$. This case leads naturally to the introduction of the discrete Walsh transform[7] which will be fully discussed in the next paper in the series.

Finally, some concluding remarks and a brief discussion is given.

II. THE ANHARMONIC OSCILLATOR

In this section we present a brief summary of known results for the one-dimensional anharmonic oscillator and also establish our notation which will be used heavily in subsequent sections. We define the oscillator by its Hamiltonian

$$H(\lambda,f^2)=p^2+\lambda(x^2-f^2)^2\,, \tag{2.1}$$

and its orthonormal eigenfunctions $\phi_m(\lambda,f^2;x)$ with eigenvalues $E_n(\lambda,f^2)$ that satisfy

$$H(\lambda,f^2)\phi_n(\lambda,f^2;x)=E_n(\lambda,f^2)\phi_n(\lambda,f^2;x)\,, \tag{2.2}$$

where

$$E_{n+1}(\lambda,f^2)\geq E_n(\lambda,f^2)\,,\quad n=0,1,2,\ldots\,.$$

We also define the diagonal moments $Q_m^N(\lambda,f^2)$ by

$$Q_m^N(\lambda,f^2)=\int_{-\infty}^{\infty}dx\,|\phi_m(\lambda,f^2;x)|^2x^N\,. \tag{2.3}$$

The moments $Q_m^N(\lambda,f^2)$ are related to the energy eigenvalues through the relation[8,9]

$$\begin{aligned}4\lambda[(N+3)Q_m^{N+4}(\lambda,f^2)-2f^2(N+2)Q_m^{N+2}(\lambda,f^2)\\ +f^4(N+1)Q_m^N(\lambda,f^2)]=4(N+1)E_m(\lambda,f^2)Q_m^N(\lambda,f^2)\\ +(N+1)N(N-1)Q_m^{N-2}(\lambda,f^2)\,.\end{aligned} \tag{2.4}$$

This equation for $N=0$ is the familiar virial theorem.

It is interesting to note that given the function $E_m(\lambda,f^2)$, *all* of the moments $Q_m^N(\lambda,f^2)$ (even N) are determined. An application of the Feynman-Hellman theorem yields

$$\frac{\partial}{\partial f^2}E_m(\lambda,f^2)=2\lambda[f^2-Q_m^2(\lambda,f^2)]\,, \tag{2.5}$$

which determines $Q_m^2(\lambda,f^2)$ from $E_m(\lambda,f^2)$. Using these and the fact that $Q_m^0(\lambda,f^2)=1$, is sufficient to determine all of the moments from Eq. (2.4). Even though there are no "closed-form" expressions (at the time of this writing) for the $E_m(\lambda,f^2)$, there exist techniques[9,10] for their practical computation to *any* desired accuracy (i.e., at least to twice the precision to which the reader has the decimal digits of π committed to memory).

Even though the energy eigenvalues and the moments appear to depend on *two* parameters, λ and f^2, this can be simplified to *one* through the scaling relations[11]

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

and (2.6)

$$Q_m^N(\lambda,f^2)=\lambda^{-N/6}Q_m^N(1,f^2\lambda^{1/3})\,.$$

In Fig. 1 we have plotted $E_m(1,f^2)$ and $Q_m^2(1,f^2)$ for $m=0$ and 1. These were computed using the methods of Ref. 10.

Asymptotic expansions for E and Q^2 in limiting regimes are easily computed from perturbation theory using the techniques of Swenson and Danforth.[8] For $f^2\gg 1$ and $\lambda=1$, the result is

$$\begin{aligned}E_0(f^2)&\simeq 2f\left(1-\frac{1}{4f^3}-O(f^{-6})\right),\\ Q_0^2(f^2)&\simeq f^2-\frac{1}{2f}\left(1+\frac{1}{2f^3}+O(f^{-6})\right),\end{aligned} \tag{2.7}$$

whereas for $f^2\ll -1$, the relevant expansions are

$$\begin{aligned}E_0(f^2)&\simeq f^4+\sqrt{2}\,|f|\left(1+\frac{3}{8\sqrt{2}\,|f|^3}-O(f^{-6})\right),\\ Q_0^2(f^2)&\simeq\frac{1}{2\sqrt{2}\,|f|}\left(1-\frac{3\sqrt{2}}{8|f|^3}+O(f^{-6})\right).\end{aligned} \tag{2.8}$$

For notational simplicity we shall sometimes omit the subscript m when referring to the ground state $m=0$, and omission of the argument λ will imply $\lambda=1$.

III. AN EXAMPLE

In this section a simple calculation scheme will be developed that is analogous to blocking two sites at a time. In latter sections this will be reinterpreted in terms of orthogonal transformations, improved and generalized. Consider a one-dimensional periodic chain of $N=2^n$ coupled anharmonic oscillators, whose Hamiltonian is given by

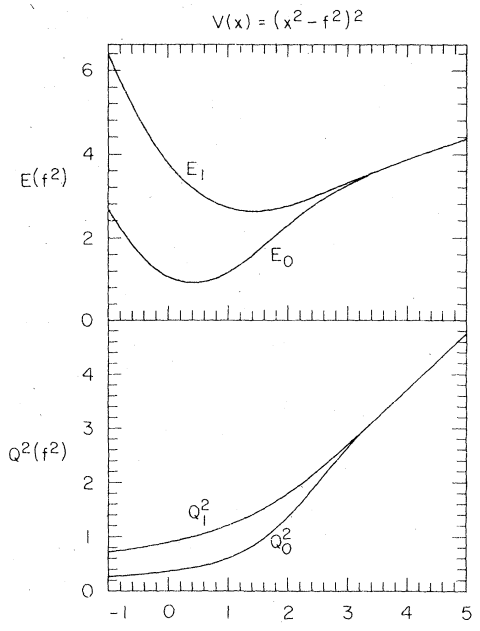

FIG. 1. A plot of $E(f^2)$ and $Q^2(f^2)$ for the double oscillator potential for the ground and first (odd) excited state.

$$H=\sum_{l=0}^{N-1}\left[p_l^{\,2}+\lambda(x_l^{\,2}-f^2)^2+\Delta(x_{l+1}-x_l)^2\right], \tag{3.1}$$

with $x_N=x_0$.

Our procedure will be to perform a transformation on pairs of coordinates and to "integrate" or "freeze out" the resulting oscillators which have the highest frequencies. This procedure is then repeated, and after each such iteration, the number of "active" oscillators is decreased by a factor of 2. After m such iterations, there are 2^{n-m} oscillators remaining, and the effective Hamiltonian takes the form

$$\begin{aligned}H_m=\sum_{l=0}^{2^{n-m}-1}\{&\epsilon_m+p_l^0(m)^2+\lambda_m[x_l^0(m)^2-f_m^{\,2}]^2\\&+\Delta_m[x_{l+1}^0(m)-x_l^0(m)]^2\},\end{aligned} \tag{3.2}$$

with

$$\epsilon_0=0\,,\quad \lambda_0=\lambda\,,\quad f_0^{\,2}=f^2\,,\quad \Delta_0=\Delta\,.$$

and

$$x_l^0(0)=x_l\,.$$

The notation used here is somewhat cumbersome but will prove convenient when generalizations are

considered in later sections of the paper.

The procedure for obtaining H_{m+1} from H_m is as follows. Write H_m in terms of the "slow" and "fast" coordinates

$$x_l^0(m+1)=\frac{x_{2l}^0(m)+x_{2l+1}^0(m)}{\sqrt{2}}, \qquad l=0,1,\ldots,2^{n-m-1}-1, \quad (3.3)$$

$$x_l^1(m+1)=\frac{x_{2l}^0(m)-x_{2l+1}^0(m)}{\sqrt{2}},$$

with $x_l^0(0)=x_l$, and the corresponding momenta $p_l^0(m+1), p_l^1(m+1)$. The next step is to find the variationally best wave function of the form

$$\psi=\prod_{l=0}^{2^{n-m-1}-1}\phi(\lambda_0(m+1),F_0^2(m+1);x_l^0(m+1))\times\phi(\lambda_1(m+1),F_1^2(m+1);x_l^1(m+1)). \quad (3.4)$$

The four parameters $\lambda_{0,1}(m+1), F_{0,1}^2(m+1)$ are determined by minimizing $(\psi, H_m\psi)$. One finds easily that

$$\lambda_0(m+1)=\lambda_1(m+1)=\lambda_m/2\equiv\lambda_{m+1},$$

and

$$F_0^2(m+1)=2f_m^2-3Q^2(\lambda_{m+1},F_1^2(m+1))-\frac{\Delta_m}{\lambda_m}, \quad (3.5)$$

$$F_1^2(m+1)=2f_m^2-3Q^2(\lambda_{m+1},F_0^2(m+1))-3\frac{\Delta_m}{\lambda_m},$$

where $\Delta_m/\lambda_m=\Delta_0/\lambda_0=\Delta/\lambda$.

Finally, one determines H_{m+1} by freezing out the fast coordinates $x_l^1(m+1)$,

$$H_{m+1}=\int\left[\prod_{l=0}^{2^{n-m-1}-1}dx_l^1(m+1)\phi(\lambda_{m+1},F_1^2(m+1);x_l^1(m+1))\right]H_m\left[\prod_{l=0}^{2^{n-m-1}-1}\phi(\lambda_{m+1},F_1^2(m+1);x_l^1(m+1))\right]. \quad (3.6)$$

This Hamiltonian achieves the same form as Eq. (3.2) with

$$f_{m+1}^2=F_0^2(m+1)+\frac{\Delta_m}{\lambda_m}, \quad \Delta_{m+1}=\frac{\Delta_m}{2}, \quad \lambda_{m+1}=\frac{\lambda_m}{2}, \quad (3.7)$$

and

$$\epsilon_{m+1}=2\epsilon_m+E(\lambda_{m+1},F_1^2(m+1))+\lambda_{m+1}[4f_m^4-f_{m+1}^4-F_1^4(m+1)-6Q^2(\lambda_{m+1},F_1^2(m+1))Q^2(\lambda_{m+1},F_0^2(m+1))].$$

One continues this procedure until n iterations have been achieved. The "mass" of the lightest excitation at the mth stage is determined by

$$\mu=E_1(\lambda_m,F_0^2(m))-E_0(\lambda_m,F_0^2(m)). \quad (3.8)$$

We notice that this entire "pruning" procedure is equivalent to choosing a trial wave function at the mth iteration that is given by

$$\psi_m(x_0,\ldots,x_{N-1})=\left[\prod_{k=1}^{m}\prod_{l=0}^{2^{n-k}-1}\phi(\lambda_k,F_1^2(k);x_l^1(k))\right]\left[\prod_{l=0}^{2^{n-m}-1}\phi(\lambda_m,F_0^2(m);x_l^0(m))\right], \quad (3.9)$$

where the λ_k's and the $F_{0,1}(k)$'s are given by the above equations.

Matrix elements depending on the original coordinates x_l are easy to compute by expressing the x_l's in terms of the "fast" and "slow" coordinates. This will be done in general in Sec. VI. Using the formula (to be derived in detail later) one finds that after m iterations

$$x_l=\sum_{j=1}^{m}\frac{(-1)^{l_j-1}}{2^{j/2}}x_{[l/2^j]}^1(j)+\frac{x_{[l/2^m]}^0(m)}{2^{m/2}}, \quad (3.10)$$

where $[a]$ is the largest integer not exceeding a, and l_j is the jth binary digit (0 or 1) of the integer l,

$$l=\sum_{j=0}^{m}l_j2^j \text{ or } l_j=[l/2^j]-2[l/2^{j+1}].$$

As a simple example, let us compute the two-point correlation function $(\psi_m, x_kx_l\psi_m)$ at the mth level. Using Eqs. (3.9) and (3.10) we find that

$$(\psi_m,x_kx_l\psi_m)=\sum_{j=1}^{m}(-1)^{k_j-1+l_j-1}\delta_{[k/2^j],[l/2^j]}\times\frac{Q^2(\lambda_j,F_1^2(j))}{2^j}+\frac{Q^2(\lambda_m,F_0^2(m))}{2^m}, \quad (3.11)$$

If f^2 and Δ in Eq. (3.1) are sufficiently positive, then the solutions to Eq. (3.5) have a simple behavior—$F_0^2(m)$ becomes large and positive while $F_1^2(m)$ becomes large and negative. In fact, the behavior of F_0^2 for large l is

$$F_0^2(n+l) \sim 2^l F_0^2(n) + (2^l - 1)\Delta/\lambda .$$

Thus for very large distances, the correlation function, Eq. (3.11) is dominated by the last term. Using the scaling relation and (2.7) one finds the leading behavior

$$(\psi_m | x_0 x_l | \psi_m) \simeq \frac{F_0^2(m)}{2^m} . \tag{3.12}$$

Numerical results will be given in the next section.

IV. NUMERICAL RESULTS

Let us first make a simple numerical check of the transformation procedure by discussing N *uncoupled* anharmonic oscillators. That is, if one sets $\Delta = 0$, Eq. (3.6) has degenerate solutions, $F_0^2(m+1) = F_1^2(m+1)$. The perturbation that is neglected at each stage in the procedure is of the form

$$W = 3\lambda_{m+1} \sum_i [x_i^0(m)^2 - Q^2(\lambda_m, F_0^2(m))] \times [x_i^1(m)^2 - Q^2(\lambda_m, F_1^2(m))] .$$

This perturbation vanishes in the ground state (by design) but does contribute to second order via the excitation of both anharmonic oscillators to their second excited state (it is only the first excited state that can become degenerate with the ground state as $F^2 \to \infty$). This energy shift will be computed shortly for one illustrative case.

Let us denote the energy per site in the mth level of blocking by $e(m)$. At the zeroth level, since no transformation has been made, $e(0)$ is the exact energy of one oscillator. The question is how do the errors in $e(m)$ build up as $m \to \infty$? We find that $e(m)$ grows and saturates as m increases. The numerical results for $f^2 = 0$ and $\lambda = 1$ are $e(0) = 1.0604$, $e(1) = 1.0758$, $e(2) = 1.0779$, $e(4) = 1.0782$, and $e(20) = 1.0782$. Thus the error after 20 stages is only ~1.7%. For $f^2 = 1$, the error is somewhat larger: $e(0) = 1.1378$, $e(1) = 1.2204$, $e(2) = 1.2306$, $e(4) = 1.2322$, and $e(20) = 1.2323$, a final error of ~8.3%, whereas for $f^2 = -1$, the error is smaller: $e(0) = 2.6778$, $e(1) = 2.6823$, $e(2) = 2.6830$, $e(4) = 2.6831$, and $e(20) = 2.6831$, a final error on only 0.2%. We therefore conclude that there is no tendency for the error in the energy to continue to grow as $m \to \infty$. In fact, as one adds in a coupling between the sites, most of the $F^2(m)$'s become more negative, and the error probably even decreases.

One can easily estimate the second-order energy shift due to the W_i given above by using standard closure arguments. The result for $\lambda = 1$, $f^2 = 0$, and $m = 1$ is a negative correction to $e(1)$ given by

$$E(m=1) = 1.075\,76 - 0.018\,26 = 1.0575 ,$$

which reduces the zeroth-order error of 1.5% to an error of only 0.3%. Details of this simple calculation will be given later. The analogous calculation for $f^2 = 1$ is

$$E(m=1) = 1.220\,44 - 0.096\,52 = 1.123\,92 ,$$

an error reduction from 7.3% to 1.2% and for $f^2 = -1$ the result is

$$E(m=1) = 2.6823 - 0.005\,12 = 2.6772 ,$$

an error reduction from 0.2% to 0.02%.

In this section we examine the general numerical behavior of the recursion relations which were derived in the previous section. Given a pair of coupling constants f^2, Δ we investigate the large-m behavior of λ_m and f_m^2. It is sufficient to consider the case $\lambda = 1$ since other values of λ may be handled by the scaling relations used in Sec. II. We find two distinct behaviors of the f_m^2 as $m \to \infty$ which depends on the Δ and f^2 values: in case *one* we find that

$$\lim_{m\to\infty} f_m^2 \to \infty ,$$

whereas in case *two* we find that

$$\lim_{m\to\infty} f_m^2 \to -\infty .$$

In case *one*, since $f_m^2 \to +\infty$, we see that the mass gap $E_1 - E_0$ is going to zero. We call this the *ordered* phase. It is analogous to the magnetized phase of a ferromagnet for $T < T_c$. In case *two*, f_m^2 becomes large and negative (at the same time that λ_m decreases), so that the physical mass μ is finite and is given by

$$\mu^2 = \lim_{m\to\infty} (-4\lambda_m f_m^2) . \tag{4.1}$$

Numerically we find that this converges to a constant independent of m for large m. This phase is analogous to the disordered phase of a ferromagnet with $T > T_c$, in which the correlation length is finite.

The two phases are separated by a one-dimensional critical surface (*a* line). We have computed the approximate location of this line (the dashed line in Fig. 2) using the method described in the previous section. Note that this line behaves incorrectly in the region $\Delta \to 0$, $f^2 > 0$. This is be-

cause it is variationally disadvantageous to transform to the "fast" and "slow" coordinates in this region. Indeed, here it is better to use a local wave function.

This leads to another possible criterion for determining the phase of the system. One determines the best wave function ψ_m for which $(\psi_m, H\psi_m)$ is a minimum. If this minima is reached only when $m \to \infty$ (that is, the best variational wave function correlates oscillators which are infinitely separated) then we call the system ordered. On the other hand, if the best wave function is attained for a finite m, then oscillators which are infinitely far apart are not correlated; the correlation length is finite, and we call the system disordered. This is shown in the solid curve in Fig. 2.

In the region $\Delta \to 0$, $f^2 \to \infty$ one may alternatively invoke a spin-$\frac{1}{2}$ approximation which involves a diagonalization of H within the restricted basis spanned by states of the form

$$\prod_{l=0}^{N-1} \phi_{m_l}(\lambda, f^2 - \Delta; x_l),$$

where $m_l = 0, 1$. Following Stoeckly and Scalapino[5] one writes

$$H = \sum_{l=0}^{N-1} \{p_l^2 + [x_l^2 - (f^2 - \Delta)]^2 - 2\Delta x_l x_{l+1} + f^2 - (f^2 - \Delta)^2\}.$$

and with respect to this restricted basis, the Hamiltonian becomes

$$H_T = N\left(\frac{E_1 + E_0}{2} + f^4 - (f^2 - \Delta)^2\right) - \sum_{l=0}^{N-1} \left(\frac{E_1 - E_0}{2}\sigma_3(l) + 2\Delta T \sigma_1(l)\sigma_1(l+1)\right),$$

where T is the square of the transition matrix element between $m_l = 0$ and 1,

$$T = |\langle 0|x|1\rangle|^2.$$

The exact solution to this truncated problem is well known. There is a second-order phase transition at the point where

$$\Delta_c = \frac{1}{4T}[E_1(f_c^2) - E_0(f_c^2)]. \tag{4.2}$$

If $f^2 \gg 1$ then[12]

$$E_1 - E_0 \simeq \frac{32}{3}\left(\frac{2\ln 6}{\pi}\right)^{1/2} f^{5/2} e^{-4f^3/3},$$

and $T \simeq f^2$. Thus the critical value of Δ for $f = f_c \gg 1$ behaves as

$$\Delta_c \simeq \frac{8}{3}\left(\frac{\pi}{2\ln 6}\right)^{1/2} f_c^{1/2} e^{-4f_c^3/3}.$$

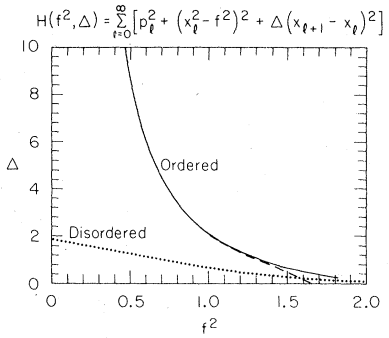

FIG. 2. A plot of the boundary between the ordered and disordered phases as a function of f^2 and Δ for $\lambda = 1$. The solid curve is using the criteria of comparing the rotated to the local energy. The dashed line is a straight iteration of the equations. The dotted line is the result of the spin-$\frac{1}{2}$ approximation.

We have used this form for large f_c^2 and the "exact" numerical results (cf., Ref. 10) in Eq. (4.2) to yield the dotted line in Fig. 2.

Using Eqs. (3.11) and (3.12), we have also computed the magnetization, M, which is defined in terms of the correlation function as the limit

$$M^2 = \lim_{l \to \infty} \langle \psi | x_0 x_l | \psi \rangle, \tag{4.3}$$

The number of iterations (or "prunings") was chosen sufficiently large so that the numerical result had converged to several significant decimal digits.

For f near its critical value f_c, the magnetization behaves as

$$M \sim (f^2 - f_c^2)^\beta, \tag{4.4}$$

where one might expect $\beta \sim \frac{1}{8}$. In Fig. 3, the magnetization to the eighth power is plotted vs f^2 for $\Delta = 10$. One sees that the series of points is essentially linear, implying that β is very close to $\frac{1}{8}$. We have not bothered to estimate an error. A calculation for $\Delta = 1$ yields a similar result.

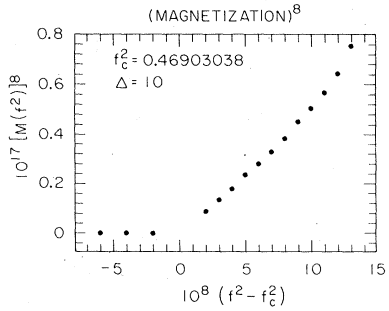

FIG. 3. A plot of the eighth power of the magnetization vs f^2. The critical exponent for the magnetization seems to be quite close to $\frac{1}{8}$.

V. A REINTERPRETATION–THE HAAR TRANSFORM

The preceding blocking procedure first involved an orthogonal transformation (a 45° rotation and inversion). This then allowed one to find in a simple way the variationally optimum λ, F^2 values for the unperturbed Hamiltonian for each variable of the form $H_0 = p^2 + \lambda(x^2 - F^2)^2$. The essential point to be emphasized in this method is the orthogonal transformation of coordinates given by Eq. (3.3). Is there a useful characterization of such transformations, and can they be generalized to blocking larger number of sites together? The answer to both these questions is in the affirmative as we shall now show.

Consider the case of four sites, $N = 2^n = 4$. The 2×2 blocking procedure applied twice in this case results in a transformation of the individual site coordinates x_j to the final coordinates, r_l, of the following form

$$r = H_4 x\,,$$

where

$$H_4 = \frac{1}{2}\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 \\ \sqrt{2} & -\sqrt{2} & 0 & 0 \\ 0 & 0 & \sqrt{2} & -\sqrt{2} \end{pmatrix}. \tag{5.1}$$

This is the well-known discrete Haar transformation.[13] This transformation follows naturally from the expansion of an arbitrary function in terms of the Haar functions,[6] which are a complete set of orthogonal functions in the interval $[0, 1]$ and which take on only the values, $0, \pm 1, \pm\sqrt{2}, \pm 2$, etc. They are defined as (for $0 < t < 1$, and extended periodically outside this interval)

$$\text{Haar}(2^n + j, t) = \chi_n^{(j)}(t)\,,$$

with $n = 1, 2, \ldots$ and $j = 0, 1, \ldots, 2^n - 1$, where

$$\chi_0^{(0)}(t) = 1\,,$$

$$\chi_0^{(1)}(t) = \begin{cases} 1\,, & 0 < t < \frac{1}{2} \\ -1\,, & \frac{1}{2} < t < 1\,, \end{cases}$$

$$\chi_1^{(0)}(t) = \begin{cases} \sqrt{2}\,, & 0 < t < \frac{1}{4} \\ -\sqrt{2}\,, & \frac{1}{4} < t < \frac{1}{2} \\ 0\,, & \frac{1}{2} < t < 1\,, \end{cases} \tag{5.2}$$

$$\ldots$$

$$\chi_n^{(j)}(t) = \begin{cases} 2^{n/2}\,, & j2^{-n} < t < (j+\frac{1}{2})2^{-n} \\ -2^{n/2}\,, & (j+\frac{1}{2})2^{-n} < t < (j+1)2^{-n} \\ 0\,, & \text{elsewhere}\,. \end{cases}$$

As a further example, the discrete Haar transform for eight sites can be written in the convenient product form

$$H_8 = \frac{1}{\sqrt{8}}\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \sqrt{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \sqrt{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 \end{pmatrix}\begin{pmatrix} + & + & + & + & + & + & + & + \\ + & + & + & + & - & - & - & - \\ + & + & - & - & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & + & + & - & - \\ + & - & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & + & - & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & + & - & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & + & - \end{pmatrix}, \tag{5.3}$$

where $+ = +1$. One notices that the top rows of the matrix H look not unlike squared-off sinusoidal waves but the bottom rows, the high-frequency part, do *not* resemble such waves. This is as one expects from any blocking procedure; the longest wavelengths are treated more accurately than the short wavelengths.

This transformation can be performed directly on the Hamiltonian and then the expectation value taken in a selected set of states. The most natural one is a set diagonal in the r's with adjustable parameters (λ, F^2). Note that for N sites, there are N independent coordinates and N independent F's to choose. The 2 by 2 blocking scheme is highly degenerate in choosing the F values—there are $N/2$ degenerate F's at the first step, $N/4$ at the second, $N/8$ at the third, etc. The last two F's are not degenerate. This degeneracy pattern

changes with the number of sites in the blocking scheme.

In the 2-site blocking scheme of Sec. III, the choice is made for the F's at each stage or level by neglecting the (further) couplings between the slow modes. This is not necessarily the optimum choice, as we shall see later, but is a simple one and is in any event variational. This means that while the energy values may be satisfactory, other quantities, such as the correlation function, may have considerably larger errors. In a later paper we shall show how to compute all such quantities with an accuracy that approaches that of the energy.

Let us now turn to a generalization of the Haar transform which corresponds to blocking M sites together and retaining the "slowest" oscillator coordinate.

VI. M-SITE BLOCKS

In this section we will consider a more ambitious blocking calculation in which M sites are considered together and then the $M-1$ fastest oscillators are frozen out. The remaining slowest oscillators are in turn coupled to each other in blocks of M and the process repeated. In this section we shall work out the general coordinate transformation implied by this blocking scheme and its inverse. The explicit correlation function will then be discussed.

The block size will be denoted by M and the total number of lattice sites will be N, where $N=M^n$. As the blocking process is carried out, one needs a coordinate notation that provides three pieces of information: m, which is the position within a block of M sites ($0 \leq m \leq M-1$); l, which denotes which particular block the site is in; and k which denotes the level or stage of the procedure. Thus we introduce

$$x_l^m(k) \tag{6.1}$$

as the general coordinate notation, where $0 \leq l \leq M^{n-m}-1$. The original site variable x_l is given by

$$x_l \equiv x_l^0(0)\,. \tag{6.2}$$

At the first stage one performs a general orthogonal transformation T among M sites:

$$x_l^m(1) = \sum_{j=0}^{M-1} \frac{T^{mj}}{\sqrt{M}}\, x^0_{M\cdot l+j}(0)\,, \tag{6.3}$$

where we have normalized T to have all $+1$'s in its top row, i.e., $T^{0j}=1$. The $M-1$ fastest oscillators are frozen out and only the slowest, labeled $m=0$, is retained for the next level. At a general level, we define

$$x_l^m(k+1) = \sum_{j=0}^{M-1} \frac{T^{mj}}{\sqrt{M}}\, x^0_{M\cdot l+j}(k)\,. \tag{6.4}$$

The inverse transformation is also easily derived by a recursive procedure. Since T is orthogonal,

$$\sum_{m=0}^{M-1} T^{mi}T^{mj} = M\delta_{ij}\,. \tag{6.5}$$

Thus, for example, the inverse of (6.3) is

$$\begin{aligned} x_l &= x_l^0(0) \\ &= \sum_{m=1}^{M-1} \frac{T^{ml_0}}{\sqrt{M}} x^m_{[l/M]}(1) + \frac{1}{\sqrt{M}}\, x^0_{[l/M]}(1)\,, \end{aligned} \tag{6.6}$$

where l_0 is the zeroth-base M digit of the integer l, or, in other words,

$$l_0 = l - M[l/M]\,,$$

where $[z]$ is again the greatest integer not exceeding z. After the repeated application of Eqs. (6.6) and (6.4), one achieves

$$\begin{aligned} x_l = \sum_{j=1}^{k}\sum_{m=1}^{M-1} M^{-j/2} T^{m,l_{j-1}} x^m_{[l/M^j]}(j) \\ + M^{-k/2} x^0_{[l/M^k]}(k)\,, \end{aligned} \tag{6.7}$$

where l_j is the jth digit in base M of the integer l,

$$l_j \equiv [l/M^j] - M[l/M^{j+1}]\,. \tag{6.8}$$

Note that for $M=2$, and

$$T = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

we recover Eq. (3.9).

The generalization of Eq. (3.7) for the wave function to blocks of size M is given by

$$\psi_k(x_0,\ldots,x_{N-1}) = \left(\prod_{j=1}^{k}\prod_{l=0}^{M^{n-j}}\prod_{m=1}^{M-1} \phi(\lambda_m(j), F_m^2(j); x_l^m(j))\right) \prod_{l=0}^{M^{n-k}-1} \phi(\lambda_0(k), F_0^2(k); x_l^0(k))\,. \tag{6.9}$$

The couplings at the stage j are determined recursively in terms of those of the previous stage $(j-1)$ by the variational principle [e.g., the generalization of (2.9)].

In terms of these parameters, the correlation function is given by

$$\langle\psi_k|x_l x_{l'}|\psi_k\rangle = \sum_{j=1}^{k}\sum_{m=1}^{M-1} M^{-j} T^{ml_{j-1}} T^{ml'_{j-1}} \delta_{[l/M^j],[l'/M^j]} Q^2(\lambda_m(j), F_m^2(j)) + M^{-k}\delta_{[l/M^k],[l'/M^k]} Q^2(\lambda_0(k), F_0^2(k))\,. \tag{6.10}$$

These relations are easier to apply than to write.

One can easily apply these formulas to more general blocking procedures. For example, after coupling M sites together in a block, one could freeze out $M-2$ variables and leave 2 oscillators free to couple at the next stage. Further generalizations are straightforward.

VII. FOUR-SITE BLOCKS

It is quite interesting to apply the previous discussion to the case $M=4$. In this case, there is an orthogonal transformation that is very convenient to use since it diagonalizes the periodic derivative term exactly and puts the quartic interaction into a convenient form for our method. This transform is called the discrete *Walsh* transform.[14] For example, for 4 sites, the coordinates transform as

$$r = W_4 x \tag{7.1}$$

where

$$W_4 = \frac{1}{2}\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \\ 1 & -1 & 1 & -1 \end{pmatrix}. \tag{7.2}$$

This transformation is defined with respect to the discrete Walsh functions. It is straightforward to define them in the continuum but the discrete situation is all that we will need here. For the case of $N=2^n$ points, we define the base 2 representation of the integers k and j as

$$k = \sum_0^{n-1} k_r 2^r, \qquad j = \sum_0^{n-1} j_r 2^r, \tag{7.3}$$

where k_r and j_r only take on the values 0 or 1. The Walsh function on the interval $[0, N]$ can then be written as

$$\mathrm{Wal}(k,j) = \prod_{r=0}^{n-1} (-1)^{j_r(k_{n-r}+k_{n-r-1})}. \tag{7.4}$$

The label j is the position label and k is the analog of the momentum or frequency label. Obviously $\mathrm{Wal}(k,j) = \mathrm{Wal}(j,k)$, and

$$[\mathrm{Wal}(k,j)]^2 = 1.$$

With the orthogonal transformation given by (7.2), the periodic derivative coupling term becomes ($x_4 \equiv x_0$)

$$\sum_{i=0}^{3} (x_{i+1}-x_i)^2 = 2(r_1^2+r_2^2)+4r_3^2,$$

and the quartic term is

$$4\sum_{i=0}^{3} x_i^4 = \sum_{l=0}^{3} r_l^4 + 3\sum_{l'\neq l} r_l^2 r_{l'}^2 + 24 r_0 r_1 r_2 r_3$$

and of course, since W_4 is orthogonal,

$$\sum_0^3 x_i^2 = \sum_0^3 r_l^2.$$

As a simple example, the transformed Hamiltonian of Eq. (3.1) for $N=4$ becomes (with $\lambda = 1$)

$$H = \vec{p}^2 + \tfrac{1}{4}\sum_{l=0}^{3} r_l^4 + 3\sum_{l'\neq l} r_l^2 r_{l'}^2 - 8f^2 r_l^2 + 4f^4 + 2\Delta(r_1^2+r_2^2+2r_3^2) + 6 r_0 r_1 r_2 r_3. \tag{7.5}$$

Using the anharmonic trial functions, one finds $\lambda = \frac{1}{4}$ and

$$\begin{aligned} F_0^2 &= 4f^2 - 3\sum_{l\neq 0} Q^2(\tfrac{1}{4}, F_l^2) - \Delta/\lambda, \\ F_1^2 &= 4f^2 - 3\sum_{l\neq 1} Q^2(\tfrac{1}{4}, F_l^2) - 4\Delta/\lambda, \\ F_2^2 &= 4f^2 - 3\sum_{l\neq 2} Q^2(\tfrac{1}{4}, F_l^2) - 4\Delta/\lambda, \\ F_3^2 &= 4f^2 - 3\sum_{l\neq 3} Q^2(\tfrac{1}{4}, F_l^2) - 8\Delta/\lambda. \end{aligned} \tag{7.6}$$

These are easily solved.

To proceed to the $N>4$ case, one must include the further coupling term in Eq. (2.3), freeze out F_1^2, F_2^2, and F_3^2, and then proceed to the next stage by blocking the slowest oscillators with coordinates r_0. The coupling terms between the blocks of 4 change the Δ terms and the equations satisfied by the F's at the $(j+1)$st level take the simple form ($l = 0, \ldots, 3$)

$$F_l^2(j+1) = 4f_j^2 - 3\sum_{l'\neq l} Q^2(\lambda_{j+1}, F_{l'}^2(j+1)) - (2l+1)\Delta/\lambda, \tag{7.7}$$

where $\lambda_{j+1} = \lambda_j/4$, $\Delta_{j+1} = \Delta_j/4$, and the f^2 parameter for the r_0 coordinate in the pruned Hamiltonian is

$$f_{j+1}^2 = F_0^2(j+1) + \Delta/\lambda. \tag{7.8}$$

Numerical results for this model will be presented in another paper.

To clarify the connection and differences between the $M=4$ and the $M=2$, or Haar transform, cases, it is interesting to compare the $N=8$ case given by Eq. (5.3) to the 4-site blocking just discussed with $N=16$. The orthogonal transformation

for this latter case is

$$r = M_{16} x ,$$

where

$$M_{16} = \frac{1}{4} \begin{bmatrix} u & u & u & u \\ u & u & -u & -u \\ u & -u & -u & u \\ u & -u & u & -u \\ 2w & 0 & 0 & 0 \\ 0 & 2w & 0 & 0 \\ 0 & 0 & 2w & 0 \\ 0 & 0 & 0 & 2w \end{bmatrix},$$

with

$$u = (1 \;\; 1 \;\; 1 \;\; 1)$$

and

$$w = \begin{bmatrix} -1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \\ 1 & -1 & 1 & -1 \end{bmatrix}.$$

VIII. DISCUSSION

Since this is only the first paper in a series, the conclusion will be kept brief. In this paper, we have discussed a one-dimensional ϕ^4 lattice theory using a general anharmonic basis with a selected orthogonal transformation of variables. Both the energy density and the correlation function were discussed and evaluated numerically. The calculation of other critical exponents and order parameters can easily be carried out. The choice of the parameters in H_0 were made by imposing a variational principle at each stage of the "pruning" procedure which neglected higher-level couplings of the "slow" coordinates. This procedure could clearly be improved.

Some good points of our procedure described in this paper is that it is expected to be good for large Δ and since an infinite number of states (i.e., a complete oscillator) are retained after each "pruning" step, it should certainly be better than truncating to a finite number of levels. It is also possible to compute higher-order corrections to the energy and correlation functions as will be shown later. Among its deficiencies are those of any finite blocking procedure, the high-frequency part of the spectrum is poorly treated—the ultraviolet and renormalization properties are certainly wrong. This defect will be remedied in paper II in this series. Another shortcoming is the fact that the F's are not chosen so as to minimize the final energy, but for reasons of simplicity are computed at each stage by neglecting further couplings. One undesirable feature of our rather extreme orthogonal transformations is that as $\Delta \to 0$, the calculational procedure chooses either a full transform or a local wave function (which ever yields the best energy value). This poses no problem but is not as smooth as one might wish.

In further papers we shall demonstrate how to improve the lowest-order (but variational) results given here by unusual versions of perturbation theory to improve other observables, such as the correlation functions, so that they are as accurate as the energy. We shall also apply this approach to treat other models, higher dimensions, and the high-frequency part of the spectrum.

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