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An Exact Real Space Renormalization Group and New Truncation Algorithms for Lattice Theories

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ABSTRACT

This paper discusses the theoretical basis of variational algorithms for thinning degrees of freedom in a lattice Hamiltonian theory. We show that such a thinning can--in principle--be an exact real-space renormalization group transformation to a lattice with fewer sites. This exact transformation can only be constructed given the exact ground state of the theory. However, this insight teaches us how to significantly improve previous variational algorithms. Further improvements in ability to calculate quantities of interest is achieved by introducing "look-ahead" algorithms which allow us to maintain a renormalization-group interpretation while introducing long-distance physics into the determination of variational parameters. We find that algorithms incorporating both these features are much more powerful than previous truncation algorithms. For pedagogical reasons we present our algorithms using as examples two well-understood theories namely free scalar field theory and the Ising model in a transverse field in 1 + 1 dimensions. Discussion of higher dimensions and less trivial theories is included in the final section. An appendix on generalized mean field theory is also included.

1. INTRODUCTION

Since the introduction of the Hamiltonian real space renormalization group (or lattice truncation) technique as a nonperturbative tool for analyzing cutoff field theories and quantum spin systems,[1] subsequent work has focused on applications to specific models.[2] This work has helped to establish a domain of applicability for the original ideas. However, except for the early observation that the method is a form of Rayleigh-Ritz variational calculation, little or no progress has been made in understanding the theoretical foundations of this scheme.

The lack of a theoretical framework has hampered efforts to devise systematic improvements on the simplest real space renormalization group algorithms. Brute force attempts to improve upon the accuracy of specific calculations either by keeping more states, or introducing variational parameters into the truncation procedure, demonstrated two important points. First, that high accuracy calculations of the properties of spin systems can be carried out by these methods; second, that even simple algorithms enable us to accurately calculate quantities (e.g., the spectrum of excited states of the system) which are not directly related to the ground state energy. This second fact was somewhat surprising. Experience with simpler quantum mechanical systems has taught us to expect variational calculations to yield good ground state energies, but to fail (except in exceptional circumstances) to give good estimates of either the excited state spectrum or detailed properties of the ground state wavefunction. This suggested that we were missing something important by thinking of the procedure solely in terms of a Rayleigh-Ritz calculation and led us to reinvestigate the theoretical foundations of the method.

This return to basics yielded three important results. First, we understood that an exact renormalization group scheme could be defined for Hamiltonian systems, in analogy to the Kadanoff-Wilson method for analyzing Euclidean systems.[3] Second, we understood that even the simplest real space renormalization group algorithms provide a way of approximating exact renormalization group transformations. Finally, we found that our new understanding of the theory led to the formulation of powerful new computational techniques, which subsumed all of our previous methods for doing high accuracy calculations as special cases.

The aim of this paper is to present the theoretical ideas in some detail and to indicate, by means of a simple example, the way in which they lead to the development of new calculational tools.

We begin with a discussion of the structure of free field theory. Following an argument of J. Bronzan and R. Sugar,[4] we show how knowledge of the exact ground state wave function for a lattice field theory can be used to define an exact real space renormalization transformation. Next, we discuss the original lattice truncation method and its interpretation as an approximation to the exact renormalization group transformation. We then identify features of the exact transformation which are not reproduced by naive truncation algorithms. This leads to the introduction of the concept of fast and slow modes for a block, and the observation that the slow modes must be treated as background fields for the fast modes. In this way a kind of Born-Oppenheimer approximation to the field theory emerges as an important feature of a real space renormalization group algorithm. For pedagogical reasons, this section of the paper is limited to the discussion of free Bose field theory on a lattice; however, the general discussion of approximation techniques extends straightforwardly to the case of systems with interactions.

In the third section of the paper the ideas of the preceding section are extended so as to be able to deal with quantum spin systems which differ from Bose theories in that there are only a finite number of states per site. For these systems, the identification of fast and slow modes is not as obvious as it is in the Bose case and so we introduce a new notion, that of generalized mean field theory, in order to deal with this problem. Once again, in order to present new ideas in the simplest context, we limit discussion to the simple but nontrivial case of the Ising model in a transverse magnetic field. The discussion of more interesting spin systems is put off to forthcoming papers. Comparison of exact and approximate results will make it clear that the combination of generalized mean field theory and real space renormalization group ideas produces a very powerful computational tool.

In the concluding section of this paper we briefly discuss ways to deal with problems in higher dimensions and of greater complexity. We also discuss the question of computing order parameters, transition temperatures, etc., to higher accuracy. An appendix on generalized mean field calculations is included. This technique provides a way of deciding how to best apply the truncation method to arbitrary spin systems. The generalized mean field approximation is interesting in its own right as a "quick and dirty" way of extracting physics from particular models using "back of the envelope" estimates.

2. FREE FIELD THEORY

2.1 THE VACUUM AND THE RENORMALIZATION GROUP

2.1.1 Preliminaries

The lattice theory of a free scalar field is simply a system of coupled harmonic oscillators. There are many ways in which the gradient terms[5] can be transcribed to the lattice; however, for our present purposes the differences between these methods is unimportant and we use a simple nearest neighbor definition. Thus, for the Hamiltonian of free scalar field theory we take

$$H = \sum_j \frac{p_j^2 + \mu^2 x_j^2 + (x_{j+1} - x_j)^2}{2} \tag{2.1}$$

where the operators x_j and p_m obey the canonical commutation relations

$$[x_j, p_m] = i\delta_{jm} \tag{2.2}$$

This Hamiltonian is diagonalized by Fourier transforming to the variables x_k and p_k. In terms of these variables the Hamiltonian becomes

$$H = \sum \frac{p_{-k}p_k + \{ 2(1 - \cos(k)) + \mu^2 \} x_{-k}x_k}{2} \tag{2.3}$$

At this point it is customary to rewrite this expression in terms of annihilation and creation operators, and the Hamiltonian as a sum over number operators. To relate knowledge of the groundstate wavefunction

to an exact real space renormalization group procedure, we avoid this step, and instead observe that we are dealing with a set of decoupled two dimensional Schroedinger equations; hence, the unnormalized ground state wave function for the system is a product

$$\prod_k \exp\{-\gamma_k x_k^* x_k\} \tag{2.5}$$

where the variable γ_k is defined to be

$$\gamma_k = \left[2(1 - \cos(k)) + \mu^2 \right]^{1/2} \tag{2.6}$$

This expression for the ground state wave function can be rewritten in terms of the original position space variables by performing the inverse Fourier transform to obtain the expression

$$\Psi(\ldots x_j \ldots) = \exp\{ -\frac{1}{2} \sum_{j,m} x_j \Delta(j - m) x_m \} \tag{2.7}$$

where the function $\Delta(j-k)$ is defined as

$$\Delta(j - m) = (2\pi)^{-1} \int dk \, e^{i(j-m)k} \gamma_k$$

2.2 AN EXACT RENORMALIZATION GROUP

Given the exact form of the ground state wave function one can compute the expectation values of all operators and therefore all equal time Green's functions. This information gives us, for example, the rate of fall off of correlation functions and therefore, some

information about the spectrum of excited states. Our purpose in this section is to rewrite the procedure whereby one computes expectation values in the language of a real space renormalization group calculation. By comparing the formulae derived in this way with those of earlier approximate renormalization group calculations we will be able to identify the important physics which was missed in naive approaches. We begin by introducing what we will call (for reasons which will become clear in the next section) 'slow' and 'fast' block variables, u_p and v_p,

$$u_p = (x_{2p} + x_{2p+1})/\sqrt{2} \quad ,$$
$$v_p = (x_{2p} - x_{2p+1})/\sqrt{2} \quad . \tag{2.8}$$

The exact ground state wavefunction can be rewritten, in terms of these variables, as

$$\Psi(\ldots u_p, v_p, \ldots) = \exp\{-\sum u_p \Delta_{uu}(p-r) u_r\}^* \times \exp\{-2\sum u_p \Delta_{uv}(p-r) v_r - \sum v_p \Delta_{vv}(p-r) v_r\} \tag{2.9}$$

where, Δ_{uu}, Δ_{uv}, Δ_{vu} and Δ_{vv} have the obvious definitions.[6]

The ground state expectation value of the Hamiltonian or any functions of the variables x are given by integrals of the form

$$\langle H \rangle = \int \prod_s dx_s \Psi^*(\ldots x_n \ldots) \sum_j \{-\frac{1}{2}\frac{\partial^2}{\partial x_j^2} + \frac{1}{2}\mu^2 x_j^2 + \frac{1}{2}(x_{j+1} - x_j)^2\} \times \Psi(\ldots x_n \ldots) \tag{2.10}$$

and for example,

$$\langle x^4 \rangle = \int \prod_s dx_s \; \Psi^*(\ldots x_n \ldots) \left[\sum_j x_j^4 \right] \Psi(\ldots x_n \ldots) \tag{2.11}$$

These can be rewritten in terms of the fast and slow variables as follows:

$$\langle H \rangle = \int \prod_j (du_j dv_j) \; \Psi^*(\ldots u_n, v_n \ldots) \sum_p \left\{ -\frac{1}{2} \frac{\partial^2}{\partial v_p^2} - \frac{1}{2} \frac{\partial^2}{\partial u_p^2} + \frac{1}{2} (\mu^2 + 3) v_p^2 \right.$$

$$\left. + \frac{1}{2} (\mu^2 + 1) u_p^2 \right) - \frac{1}{2} (u_p u_{p+1} - v_p u_{p+1} + u_p v_{p+1} - v_p v_{p+1}) \Big\} \; \Psi(\ldots u_n, v_n \ldots) \tag{2.12}$$

and

$$\langle x^4 \rangle = \int \prod_j (du_j dv_j) \; \Psi^*(\ldots u_n, v_n \ldots) \left[\frac{1}{2} \sum_p (u_p^4 + 6 u_p^2 v_p^2 + v_p^4) \right] \Psi(\ldots u_n, v_n \ldots) \tag{2.13}$$

We can reduce the number of degrees of freedom in the problem by doing all integrals over the fast variables, leaving the slow variable integrations undone. This is easily done by completing the square in Eqs. (2.12) and (2.13). To do this we define new variables v'_p by the equation

$$v_p = v'_p + c_p(\ldots u_m \ldots) \tag{2.14}$$

where the function c is defined to be

$$c_p(\ldots u_m \ldots) = - \sum_{r,n} \Delta_{vv}^{-1}(p-r) \; \Delta_{vu}(r-n) \; u_n \tag{2.15}$$

In this way, we find the ground state expectation value of the original Hamiltonian is equivalent to the expectation value of a more complicated Hamiltonian, involving half the number of degrees of freedom, in its ground state. The new Hamiltonian is obtained from the identity

$$\langle\Psi|H|\Psi\rangle = \int \prod_j du_j \chi^*(\ldots u_m \ldots) \sum_p \{-\frac{1}{2}\frac{\partial^2}{\partial u_p^2} + \frac{1}{2}(\mu^2+1)u_p^2 c_p^2 - \frac{1}{2}u_p u_{p+1} + \frac{1}{2}c_p(u_{p+1}-u_{p-1}) + c_p c_{p+1}\}\chi(\ldots u_m \ldots) + \text{const} \tag{2.16}$$

by simply ignoring the u_p-integrations. Similarly, we find the ground state expectation value of any function of the operators p_j and x_j is equal to the expectation value of a more complicated function of half the number of variables, computed in the ground state of the new Hamiltonian. For example,

$$\langle\sum x_j^4\rangle = \frac{1}{2}\int \prod_s du_s \chi^*\{\sum_p [u_p^4 + 6u_p^2 c_p^2 + c_p^4]\}\chi + \text{const} \tag{2.17}$$

where c_p is the nonlocal function of the u_m's defined in Eq. (2.15).

There are several important points to be made about the preceding discussion. First, that this very trivial example has shown the problem of computing ground state expectation values of various operators for a system of n-degrees of freedom can be replaced by an equivalent problem for a system involving n/2 degrees of freedom, with no loss of information. We were able to do this only because we had knowledge of the exact ground state wavefunction of the system, and so in a sense this remark is trivial. There is, however, an important sense in which this remark is far from trivial: namely, we have shown that one way of

parametrizing the information contained in the exact ground state wavefunction is to specify the structure of the exact real space renormalization group equation which it definesfor all operators, including polynomials in the Hamiltonian. Hence, any algorithm for generating a real space renormalization group transformation, generates an approximation to the exact ground state wave function. Moreover, in distinction to atomic or molecular physics problems, modifying such an algorithm so that it produces the best bound on the ground state energy density, can be expected to simultaneously produce a better approximation to the true renormalization group transformation and therefore better information about correlation lengths, etc. This expectation is borne out by explicit calculations.

The second point to be abstracted from this calculation is the fact that we had to shift the v_p-variables by function of the u_p-variables in order to be able to do the v_p-integrations. One way of thinking about this shift, is to think of the configuration of the u_p-variables as defining a background field for the v_p-variables, and observing that the v_p-variables shift their mean values in response to this background field. In the next sections of the paper we relate this fact to a kind of Born-Oppenheimer approximation to the exact renormalization group transformation. We then show how this picture can be carried over to spin systems by defining the notion of a generalized mean-field calculation.

A third point, directly related to the necessity of shifting the v_p-variables, is that the exact renormalization group transformation takes a field theory with nearest neighbor couplings into a theory with long range couplings. Thus, even if we begin with a nearest neighbor

theory any good real space renormalization group algorithm quickly leads to long range gradient terms like that introduced by Drell et al.[8] This should not be a surprise since that gradient was obtained by integrating out all high momentum degrees of freedom in a free field theory. The above example provides a way of seeing that gradient terms with a long range form are in no way unnatural in a lattice field theory.

2.3 REVIEW OF THE NAIVE R.S.R.G.-ALGORITHM FOR FREE FIELDS

As already observed, the results of the preceding section required a knowledge of the exact form of the ground state wave function. Obviously, no matter how interesting such results may be, one has learned nothing more about theories with interactions, if one has to have the exact wave function in order to procede. These ideas become useful only because we can incorporate them in schemes for computing accurate approximations to these exact transformations.

In order to make our discussion of the development of approximation techniques self-contained we first review the naive way of thinning degrees of freedom for the example of a free Bose field theory. We then discuss how one incorporates the lessons of the preceding section into such calculations. The idea behind the original lattice truncation algorithms was one could get a pretty good idea of how to eliminate variables by first considering a block of finite size. For the specific case of the Hamiltonian defined in Eq. (2.1) we will discuss blocks containing two sites each, as shown in Figure 1.

These blocks are labelled by integers 'p' and the sites within a block by an integer 'r' taking the values 0 or 1. In this way the original lattice Hamiltonian can be rewritten as

$$H = \sum_p \{ H_{block}(p) + V_p^{int} \} \tag{2.18}$$

where $H_{block}(p)$ is given by

$$H_{block}(p) = \{ -\frac{1}{2}\frac{\partial^2}{\partial x_{2p}^2} - \frac{1}{2}\frac{\partial^2}{\partial x_{2p+1}^2} + \frac{1}{2}(\mu^2+2)(x_{2p}^2 + x_{2p+1}^2) - x_{2p}\, x_{2p+1} \} \tag{2.19}$$

and the block-to-block recoupling term, V_p^{int}, is given by

$$V_p^{int} = x_{2p+1}\, x_{2(p+1)} \tag{2.20}$$

$H_{block}(p)$ can be diagonalized by going to the fast and slow variables defined in Eq. (2.8). If we make this substitution H_{block} becomes

$$H_{block}(p) = \{ -\frac{1}{2}\frac{\partial^2}{\partial v_p^2} - \frac{1}{2}\frac{\partial^2}{\partial u_p^2} + \frac{1}{2}(\mu^2+3)\, v_p^2 + \frac{1}{2}(m^2+1)\, u_p^2 \} \tag{2.21}$$

and the recoupling term, V_p^{int}, becomes

$$V_p^{int} = -\frac{1}{2}\{ u_p u_{p+1} - v_p u'_{p+1} + u_p v_{p+1} - v_p v_{p+1} \} \tag{2.22}$$

Examination of Eq. (2.21) shows the eigenfunctions of H_{block} are products of harmonic oscillator wavefunctions in the variables u_p and v_p respectively. The reason for the appelations 'fast' and 'slow' now become clear, since from the point of view of H_{block} the v-oscillator is a higher frequency oscillator than the u-oscillator [i.e., $\omega_v = (\mu^2+3)^{1/2}$ and $\omega_u = (\mu^2+1)^{1/2}$].

The next step was to assume that excited states of the higher frequency oscillators would play no important role in determining the structure of the ground state wavefunction. This entirely reasonable assumption, from the point of view of a Rayleigh-Ritz calculation, led us to truncate our Hilbert space to states of the form

$$\Psi(\ldots u_p, v_p \ldots) = F(\ldots u_p \ldots) \prod_p \exp\{-\frac{1}{2} \gamma_v v_p^2\} \tag{2.23}$$

i.e., states which have arbitrary functional dependence on the variables u_p and which are simple products of independent Gaussians[9] in the variables v_p. The renormalization group transformation is defined by computing the matrix elements of the original Hamiltonian $H_{block} + V$ between arbitrary states of this form. This yields a new Hamiltonian,

$$H' = \sum_p \{-\frac{1}{2} \frac{\partial^2}{\partial u_p^2} + \frac{1}{2} (\mu^2 + 1) u_p^2 - u_p u_{p+1}\} + C_o \tag{2.24}$$

The mapping of the original Hamiltonian into a Hamiltonian, H', having exactly the same form with different coefficients, is the naive real space renormalization group algorithm for the free field discussed in Ref. 1. One derives a general form of this algorithm, for the case of an initial Hamiltonian with arbitrary coefficients, in the same way. By accumulating the coefficient of the unit operator and dividing by the volume,[10] after many iterations one obtains the ground state energy density. The limiting form of the coefficient of the single site term, x_p^2, gives the mass gap. As discussed in Ref. 1, the results of carrying out this procedure gives the ground state energy density to about 7% and gives the mass gap exactly. Given the crude nature of the truncation algorithm these results are quite impressive.

Unfortunately, the naive real space renormalization group algorithm has several defects. The most important of these defects is it fails to give the correct falloff of correlation functions, e.g., $\langle x_i x_j \rangle$, as a function of $|i-j|$. In particular, for the case of massive free field theory it gives power law as opposed to exponential falloff; and, in the case of the massless free field theory it gives power law falloff but with the wrong exponent.[11] This inablility to get the correct falloff of correlation functions has dangerous implications when one studies the structure of two-dimensional (i.e., one space + one time) field theories and asks whether the theory can exhibit spontaneous symmetry breaking. It is important to be able to obtain the correct behavior.

The question of computing correlation functions was discussed in detail by Drell and Weinstein[12] and a scheme which involved keeping more oscillators per block was introduced to solve the problem. While this method proved quite satisfactory, it is definitely more cumbersome to deal with than the naive algorithm. In the next section we show that comparison of the exact renormalization group algorithm and the one obtained by this naive procedure leads to a scheme of sufficient power obtain correct results for correlation functions without sacrificing the computational advantage of having to keep only one degree of freedom per site in a renormalization group calculation. A detailed study of such algorithms for the case of a free Bose field has been carried out by Shahar Ben-Menachem and will be published separately.[13]

2.4 A BORN-OPPENHEIMER APPROACH TO THE RENORMALIZATION GROUP

Comparison of the exact renormalization group transformation and that just discussed makes it easy to see what is wrong with the naive

algorithm. In the naive algorithm we only kept trial wavefunctions which were products of independent Gaussians in the v_p-variable; and furthermore, the v_p-dependence of these wavefunctions was independent of the u_p-variables. This is, quite different from the situation in the exact transformation; where, due to the shift, we saw that the form of the v_p-part of the wavefunction depended explicitly upon the particular values of the u_p-variables at all points. We lost this information by focusing solely upon the structure of H_{block}, and not allowing block-to-block recoupling to influence our choice of trial wavefunction.

Implicit in our choice of a wave function of the form specified in Eq. (2.23), was the assumption that the interactions of the slow modes took place on a longer time scale than interactions among the fast modes; moreover, it was assumed that fast-fast and fast-slow recoupling was unimportant. This second assumption is incorrect, for reasons we will now discuss. If we only accept the intuitive notion that changes in the slow modes take place adiabatically on the scale of the fast modes, then we are led to an ansatz for the trial wavefunction which like the naive form, Eq. (2.25), is separable in the variables v_p; but, where the form of the trial wave function for each v_p-variable is allowed to depend on the values of the u_p-variables in other blocks. We thus make the ansatz that the groundstate wavefunction has the form

$$|\Psi\rangle = F(u_p) \prod_p \Phi_p(v_p + c_p\{u_n\}) \ . \qquad (2.25)$$

where F and ϕ are arbitrary functions. This form allows shifts of the type encountered in the exact truncation [Eq. (2.14)]. However, since we are pretending that we have no knowledge of the exact groundstate

wavefunction the parameters $c_p(\{u_n\})$ will be determined by a variational prescription.

By far the simplest procedure to follow is to assume that the function $c_j(u_p)$ is a linear function of the u_p's, i.e.

$$c_j(u_p) = \sum_p C_{jp} u_p \tag{2.26}$$

where the variables C_{jp} are left undetermined. If we compute the expectation value of H in this state and vary over the matrix determining the function $c_j(u_j)$ it will be clear that the values of the matrix, C_{jp}, will depend upon the specific function $F(\ldots u_p \ldots)$. If one chooses, for simplicity, a trivial product form

$$F(\ldots u_p \ldots) = \prod_p \exp\left\{ - \frac{\gamma u_p^2}{2} \right\} \tag{2.27}$$

it is straightforward to derive an equation for the coefficients C_{jp}, and verify that $C_{jp} = 0$ does not miminize the expectation value of H. Hence, we see from this argument that even if we had not known about the structure of the exact renormalization group equations, careful analysis of the original naive algorithm would have revealed the necessity for shifting the fast variables so that they could follow the field set up by the slow variables. This treatment of slow variables as adiabatically changing with respect to the fast variables is reminiscent of the way in which one treats molecular problems; hence, we have chosen to refer to renormalization group algorithms which incoporate this observation as Born-Oppenheimer algorithms.

In general it is difficult to carry out the renormalization group procedure for arbitrary linear functions, C_{jp}, and even more difficult to allow these variables to remain undetermined until the end of the calculation. Furthermore, this problem becomes even greater when one carries this technique over to spin systems. For this reason, we will limit our present discussion to a simple variant of the general approach which we call a nearest neighbor look-ahead algorithm. The virtues of this algorithm are, first that it is an interpolation between the naive algorithm and the one we have just discussed; and second, it is easy to implement for spin systems. A comparison of the full range of algorithms for the free scalar field will appear in the forthcoming paper by This paper will show that this variant of the general algorithm provides considerable improvement over the naive algorithm and comes quite close to the best estimates. It will further show that by "looking more steps ahead" the accuracy one obtains improves dramatically. The accuracy of all of these methods is much better than anything achieved by naive blocking algorithms.

The simplest version of the nearest neighbor look-ahead algorithm is the following:

(i) first, make the approximation that only $C_{j,j+1}$, $C_{j,j}$ and $C_{j,j-1}$ are different from zero;

(ii) next, for a one-step look-ahead procedure, define the state

$$|\Psi\rangle = \prod_p \exp\{-\frac{1}{2}\gamma_u u_p^2\}\{-\frac{1}{2}\gamma_v(v_p + \sum_m C_{pm} u_m)^2\}\ ; \qquad (2.28)$$

(iii) compute $\langle\Psi|H|\Psi\rangle$ as a function of γ_u, γ_v, $C_{j,j+1}$, $C_{j,j}$ and $C_{j,j-1}$ and minimize over these variables;

(iv) using these values for γ_v, $C_{j,j+1}$, $C_{j,j}$ and $C_{j,j-1}$ compute H truncated between arbitrary states of the form

$$|\Phi\rangle = |F(\ldots u_p \ldots) \prod_p \exp\{-\gamma_p(v_p + \sum_m c_{pm} u_m)\}\rangle \ . \qquad (2.29)$$

(v) Having computed a new Hamiltonian, H', go to step (i) and repeat.

To summarize, the single step look-ahead algorithm determines the values of the parameters used in the truncation process, by assuming a product of Gaussians provides a good approximation to the groundstate of the Hamiltonian, H', obtained by carrying out one truncation. While this assumption is not bad for some regions of parameters in the original Hamiltonian, it clearly is not the best one can do for the general case. This leads one to invent two-step,three-step, etc., nearest neighbor look-ahead algorithms as straightforward generalizations of steps (i) through (v). The basic idea in an n-step look-ahead algorithm is that one performs the fast-slow thinning n-times, introducing four unspecified parameters $(\gamma_v, C_{j,j+1} \ C_{j,j}, \ C_{j,j-1})$ for each step and then chooses a simple product of Gaussians in the remaining variables as an input to for a trial wavefunction. Using this ansatz, the expectation value of H is a function of 4n+1 unknown parameters, which are to be determined by minimizing the expectation value of H in this trial state. The first four of these parameters determine the first truncation step, the second four determine a subsequent step, etc. In general the first four parameters will have different values for an n-step look-ahead than those obtained from a single-step algorithm. Having obtained these parameters, there is no need to ever use the final

product form of the wavefunction. Instead, one uses these first four parameters to define a single step renormalization group transformation to obtain a new H'. Having obtained the new H', the original n-step calculation is forgotten about and a new n-step look-ahead procedure is initiated in order to define the next single-step renormalization group transformation which will yield an H'',etc.

It is not difficult to imagine that one could systematically go about improving upon this sort of procedure; both by increasing the number of steps one looks ahead, and by allowing more of the variables C_{pm} to be non-vanishing. We refer the interested reader to the paper of Shahar Ben-Menachem for a detailed comparison of various schemes of this sort.

The point that we wish to emphasize is that, once one has taken into account what we have called the Born-Oppenheimer aspects of the truncation problem, thinning degrees of freedom using simple product wavefunctions becomes a highly accurate procedure.

3. SPIN SYSTEMS AND THE BORN-OPPENHEIMER RENORMALIZATION GROUP

3.1 ISING MODEL IN A TRANVERSE FIELD

We now turn to the discussion of a 1+1-dimensional quantum spin system. Our purpose is to show how one incorporates insights gained from the real space renormalization group treatment of Bose field theory, into the treatment of lattice systems having only a finite number of degrees of freedom per site. If we let 'n' denote the number of states per site of a spin system, then there are n^m states associated with a block of m-sites. A renormalization group transformation for

such a system is defined by an algorithm for choosing a subset of these n states per block, and truncating the original Hamiltonian to the subspace spanned by tensor products over this limited set of states. A good algorithm is one for which the subspace spanned by this set of tensor products contains a state with a large overlap with the true groundstate wavefunction. The spin-system analogue of the naive truncation calculation discussed in Section 2.3 is to divide the Hamiltonian into $H_{block} + V$, where H_{block} contains only terms referring to sites within a block, and then to choose the restricted number of states per block to be the 'r' lowest eigenstates of H_{block}, where $r < n^m$ for a block of length 'm'. The discussion of the previous section suggests that this algorithm should not be expected to work too well since it does not retain the effects of block-to-block recouplings while choosing the small set of states per block to be kept in the truncation process. As before, we would expect that a better procedure is to identify slow and fast-variables for each block, and then truncate in a way which takes the Born-Oppenheimer aspects of the problem into account.

The identification of slow and fast-variables is not as obvious for a spin system as for a Bose field theory and so we need to generalize our technique to allow for this fact. We do this by introducing the notion of a generalized mean field state and identifying the parameters which define this state with the slow-variables of the Bose field theory. Fast variables will be taken into account by keeping extra states per block; these states will be generated by considering position dependent mean-field configurations, and so they can be thought of as including the effects of configurations exhibiting spatial variation over a single block.

3.2 MEAN FIELD THEORY AND THE RENORMALIZATION GROUP

The discussion to follow describes truncation calculations for the 1+1-dimensional Ising model in a transverse magnetic field. We present this example because comparison of our calculations with known exact results allows us to demonstrate the power of the method, and not because these approximate calculations tell us anything new about this model. Our purpose is to show that having a theoretical understanding of the physics of truncation algorithms does, in actual calculations, lead to more effective computational techniques.

The theory under discussion is the theory with two states per lattice site. These states are usually described by two component spinors and the Hamiltonian of the system is

$$H = \sum_j \left[\frac{1}{2} \varepsilon \sigma_z(j) - \sigma_x(j)\, \sigma_x(j+1) \right] \qquad (3.1)$$

where, by the notation $\sigma_x(j)$ we mean the Pauli matrix σ_x operating on the spin associated with site 'j'. We remark that this Hamiltonian commutes with the symmetry operator

$$PZ = \prod_j \sigma_z(j) \qquad (3.2)$$

and with the parity transformation (i.e. left-right reflection)

To introduce the concept of slow-modes for the spin system we begin by defining a block mean-field approximation for the groundstate wave-function. To define a block mean-field state we imagine the lattice divided into blocks of n-sites, so that there is a 2^n dimensional vector

space associated with each block.[14] If we number the blocks by the integer 'j', a block mean-field state is defined to be a state of the form

$$|\Phi\rangle = \prod_j |\phi_j\rangle \tag{3.3}$$

where the state $|\phi_j\rangle$ is assumed to be the same state in each block. The block mean-field approximation to the groundstate wavefunction is defined to be that state $|\Phi\rangle$ which minimizes the expectation value

$$\frac{\langle\Phi|H|\Phi\rangle}{\text{volume}} = \frac{1}{n}\langle\phi_j|H_{\text{block}}|\phi_j\rangle - \langle\phi_j|\sigma_x(1)|\phi_j\rangle\langle\phi_j|\sigma_x(n)|\phi_j\rangle \tag{3.4}$$

where the label j=1,..,n runs over the sites of the block from left to right, and we have used the assumption that $|\phi_j\rangle$ is independent of 'j' to replace $\langle\phi_{j=1}|\sigma_x(1)|\phi_{j+1}\rangle$ by $\langle\phi_j|\sigma_x(1)|\phi_j\rangle$. Moreover, we have defined H to be

$$h_{\text{block}} = \sum_j \left[\frac{1}{2}\varepsilon\sigma_z(j) - \sigma_x(j)\,\sigma_x(j+1)\right] \tag{3.5}$$

From Eq. (3.5) we see that H_{block} contains those terms in H which involve interactions among sites within a single block, and that the second term on the right-hand side of Eq. (3.4) gives the effects of block-to-block recoupling.

The variational problem of finding the state $|\phi\rangle$ which minimizes Eq. (3.4) can be carried out very simply. Straightforward variation of Eq. (3.4) with respect to the normalized state $|\phi\rangle$ tells us that $|\phi\rangle$ satisfies the nonlinear equation

$$\left[H_{block} - \langle\phi|\sigma_x(1)|\phi\rangle\ \sigma_x(n) - \langle\phi|\sigma_x(n)|\phi\rangle\ \sigma_x(1)\right]\ |\phi\rangle \;=\; \mu|\phi\rangle \quad . \tag{3.6}$$

This problem can be linearized by introducing, what we will refer to as a shadow Hamiltonian, $H_s(\alpha,\beta)$:

$$H_s(\alpha,\beta) \;=\; H_{block} + \frac{\alpha\left(\sigma_x(1) + \sigma_x(n)\right)}{2} + \frac{\beta\left(\sigma_x(1) - \sigma_x(n)\right)}{2} \quad , \tag{3.7}$$

and defining the two parameter family of trial states $|\phi(\alpha,\beta)\rangle$ as the lowest eigenstate of H_s, i.e.

$$H_s(\alpha,\beta)|\phi(\alpha,\beta)\rangle \;=\; \kappa(\alpha,\beta)|\phi(\alpha,\beta)\rangle \quad . \tag{3.8}$$

We then determine the values of the parameters α and β by minimizing the expectation value of the true Hamiltonian, H, in the block mean-field state $|\Psi(\alpha,\beta)\rangle$

$$|\Psi(\alpha,\beta)\rangle \;=\; \prod_j |\phi(\alpha,\beta)\rangle \tag{3.9}$$

[This procedure is closely related to that in Section 2.4 used to obtain the trial wavefunction defined in Eq. (2.29).] Using the fact that

$$\frac{\partial\kappa(\alpha,\beta)}{\partial\alpha} \;=\; \langle\phi(\alpha,\beta)|\ \frac{1}{2}\left(\sigma_x(1) + \sigma_x(n)\right)|\phi(\alpha,\beta)\rangle \tag{3.10}$$

and

$$\frac{\partial\kappa(\alpha,\beta)}{\partial\beta} = \langle\phi(\alpha,\beta)| \frac{1}{2}\left(\sigma_x(1) - \sigma_x(n)\right)|\phi(\alpha,\beta)\rangle \qquad (3.11)$$

and substituting Eqs. (3.10) and (3.11) into Eq. (3.4), we obtain an equivalent expression for the energy density

$$\frac{\langle\psi|H|\psi\rangle}{\text{Volume}} =$$

$$\frac{1}{n}\left\{ \kappa(\alpha,\beta) - \frac{\alpha\partial\kappa(\alpha,\beta)}{\partial\alpha} - \frac{\beta\partial\kappa(\alpha,\beta)}{\partial\beta} - \left(\frac{\partial\kappa(\alpha,\beta)}{\partial\alpha}\right)^2 + \left(\frac{\partial\kappa(\alpha,\beta)}{\partial\beta}\right)^2 \right\} . \qquad (3.12)$$

It is easy to see that the state $|\phi(\alpha,\beta)\rangle$ which minimizes Eq. (3.12) is a solution to the original nonlinear Eq. (3.6), and that this state is the lowest eigenstate of $H_s(\alpha_o,\beta_o)$ where α_o and β_o satisfy the equations

$$\alpha_o = -2\frac{\partial\kappa(\alpha_o,\beta_o)}{\partial\alpha_o} \qquad (3.13)$$

and

$$\beta_o = 2\frac{\partial\kappa(\alpha_o,\beta_o)}{\partial\beta_o} \qquad (3.14)$$

Moreover, it is clear that for ε large enough the only possible solution to the minimization problem occurs for $\alpha_o = \beta_o = 0$. One can prove that for general ε the minimum of the energy density is obtained for $\beta_o = 0$, and so one really only has to deal with a one parameter variational problem. For sufficiently small ε the minimum of the energy density as a function of α will not occur for $\alpha_o = 0$. Since the original Hamiltonian commutes with the symmetry operation PZ, whenever there is a minimum for the energy for an α_o different from zero there is another degenerate

minimum for $-\alpha_o$. Heuristically, for two site blocks, we see that the variable α is conjugate to the expectation value of what we would be tempted to think of as the 'slow' field variable $(\sigma_x(1) + \sigma_x(2))$; and furthermore, the values $\pm\alpha_o$ correspond to extremal "classical field configurations".

Now that we have defined the notion of a block mean-field theory we turn to the problem of combining this idea with that of the real-space renormalization group. In particular, we want to develop algorithms which incorporate the insights obtained from our discussion of the free Bose field. We can introduce a 2-state renormalization group algorithm which is the analogue of the naive truncation procedure for the free Bose field in that it ignores the Born-Oppenheimer aspects of the problem. To do this we form the two orthonormal states

$$|s_z = +1\rangle = \frac{(1 + PZ)|\phi(\alpha,0)\rangle}{\sqrt{2(1+\eta)}}$$

and

$$|s_z = -1\rangle = \frac{(1 - PZ)|\phi(\alpha,0)\rangle}{\sqrt{2(1-\eta)}} \tag{3.15}$$

where $\eta = \langle\phi(\alpha_o,0)|PZ|\phi(\alpha_o,0)\rangle$; and then, truncate the Hamiltonian to the subspace spanned by taking arbitrary tensor products of these two states per block. Since H_{block} commutes with PZ, i.e., PZ H_{block} PZ = H_{block}, and PZ $\sigma_x(j)$ PZ = $-\sigma_x(j)$ it follows that the truncated Hamiltonian also takes the form of an Ising model,[15]

$$H' = \sum_p \left[c_1 1(p) + \frac{1}{2}\varepsilon\sigma_z(p) - \Delta_1\sigma_x(p)\,\sigma_x(p+1)\right] \tag{3.16}$$

The coefficients in H' are functions of the coefficients in H and the variational parameters α.

To obtain the spin system analogue of the one-step look-ahead procedure defined for the Bose theory we can choose $\alpha = \alpha_o$; however, as we found in the free field case a much more accurate result can be achieved by looking ahead several steps before fixing on a choice of the parameter "α". In the multi-step look-ahead procedure on retains α as a variational parameter, forms the truncated Hamiltonian, H', and then repeats the calculation which led from H to H'as many times as one wishes. Of course, at each step of the procedure we introduce an independent varational parameters, e.g., α', α'', etc. In this way we obtain, at the m-th step of the process, a truncated Ising Hamiltonian whose coefficients depend upon the original values of ϵ and Δ and all of the variational parameters α, α', α'', etc. To determine the best values to choose for these parameters, we do a block mean-field calculation for this truncated Hamiltonian, varying over the α-parameters to minimize the expectation value of the original Hamiltonian. Having determined the best values for the α-parameters in this way the first full iteration can be regarded as completed. The value of the first parameter, α, determined by the m-step look-ahead can then be use to define the simple two state renormalization group transformation. Given the new Hamiltonian, H', we can proceed to do another m-step look-ahead calculation and define a new Hamiltonian H'', and so on ad-infinitum. Note, that even though we look m-steps ahead to define the first truncation parameter, we <u>do not</u> use anything but the first α-parameter to define our renormalization group transformation. In this way the procedure remains a single step procedure for mapping a Hamiltonian

$H^n \to H^{n+1}$ and the coefficients of the new Hamiltonian are determined as functions of the coefficients of the Hamiltonian of the previous step alone. Because of this we can carry over all of the techniques of Kadanoff and Wilson for discussing renormalization group flows and use them to enable us to accurately locate the critical point of the theory and evaluate critical exponents. The results of such a calculation using a 3-step look-ahead algorithm are presented in Table 1, for some representative choices for the starting value of ε.

3.3 MULTISTATE ALGORITHMS AND FAST MODES OF THE THEORY

Two questions arise at this point. First, what determines the right number of steps to look-ahead? Second, how can we generalize this calculation to a multistate, rather than two state per block algorithm? The answer to the first question leads naturally to the second, and furthermore it simultaneously solves the problem of incorporating our insights about the Born-Oppenheimer aspects of the physics into our renormalization group scheme.

If one adopts a look-ahead algorithm wherein one looks too many steps ahead the calculation just described begins to behave strangely, at least for values of ε not far from the critical point. What happens is that the formula for the energy density develops secondary minima which at a critical value of ε become lower than the minima one has been following from small . This effect of looking too many steps ahead signals the fact that at a sufficiently large distance scale, states other than simple block mean-field states become physically important. The physics behind the formation of such states is easily understood if one slightly generalizes our block mean-field formalism.

Below a critical value of ε we have two degenerate mean-field states

$$|\psi(\pm \alpha_o)\rangle = \prod_j |\phi_j(\pm \alpha_o)\rangle \tag{3.17}$$

For small ε the two states $|\phi(\pm \alpha_o)\rangle$ are essentially left polarized and right polarized spin states (i.e., states such that the expectation values of $\sigma_x(j)$ are very nearly all ± 1). Now, when there are two degenerate "groundstates" per block, an obviously important low lying state is the "kink" state, which interpolates between two regions which are in different block "groundstates". We can define such a kink state of zero momentum as

$$|\psi_{kink}\rangle = N_o \sum_p \prod_{j<p} |\phi_j(-\alpha_o)\rangle |\phi_p^*\rangle \prod_{j>p} |\phi_j(\alpha_o)\rangle \tag{3.18}$$

where N_o is a normalization factor. The state $|\phi_p^*\rangle$ is inserted at site 'p' to interpolate between the two polarized states. A natural question which arises at this point is, does the expectation value of the Hamiltonian in a state of the form specified in Eq. (3.18) lie higher than the expectation value of H in the mean field state? If we choose, for the sake of convenience, to make the state $|\phi^*\rangle$ orthogonal to the state $|\phi_{-\alpha}\rangle$ this calculation is easily carried out for the simple single site mean-field approximation and one finds that

$$\langle\psi_{kink}|H|\psi_{kink}\rangle - \langle\psi(\alpha_o)|H|\psi(\alpha_o)\rangle \propto 2 - \varepsilon \tag{3.19}$$

Thus we see that for ε greater than 2 the kink states in motion actually cross the mean-field ground state and the mean-field calculation is

expected to break down. The remarkable fact is that $\varepsilon = 2$ is the exact critical point of the theory, and so even though at first glance mean field theory would seem to give a bad value for the location of the phase transition in this model, a slight generalization of the method allows us to see why this happens. This calculation is discussed in detail in the Appendix.

From this discussion we see that it is very important to allow states which can play the role of the interpolating state $|\phi^*\rangle$ into our block-spin algorithm. We will now discuss how this kind of physics can be incorporated in a natural way.

The prescription obtained by minimizing the energy of $|\Psi_{kink}\rangle$ for a given $|\phi_\alpha\rangle$ is quite clumsy. However, within the context of the shadow Hamiltonian and a look-ahead algorithm, we can readily accomodate the need for such states. We remark that an n-site block state which sits between $|\phi_\alpha\rangle$ on one side and $|\phi_{-\alpha}\rangle$ on the other, will not be a parity even state due to the effects of neighboring blocks. This suggests that such states can only be accomodated if we extend our block-spin truncation algorithm so as to keep more than two states per block. Heuristically, we see that keeping such states is analogous to choosing the 'fast modes' differently in the presence of different position dependent 'slow modes'. Since the states to be kept in the presence of left-right and right-left kinks are not parity eigenstates, both the α and β parameters in the shadow Hamiltonian can be expected to have nonzero values for the best choice of states. Thus, in order to avoid breaking any of the discrete symmetries, PZ or parity, we must keep a minimum[16] of six states, i.e., $|\phi(\alpha,0)\rangle$, $|\phi(-\alpha,0)\rangle$, $|\phi(\alpha',\beta)\rangle$, $|\phi(-\alpha',\beta)\rangle$, $|\phi(\alpha',-\beta)\rangle$, $|\phi(-\alpha',-\beta)\rangle$, where now, α,α' and β are all kept

as variational parameters. Note that in general these six states are not an orthonormal set of states and they must be orthonormalized prior to carrying out the truncation process. It turns out that from the six states constructed in this fashion one only obtains four orthonormal states which span the six.

Combining the multistate algorithm with the m-step look-ahead procedure removes the problem of degenerate minima, because the condensation of kink-states in motion has now been taken into account. At this point the question of how big to make 'm' becomes merely a computational problem. If one looks too many steps ahead the numerical problem of minimizing a function of many variables, which is a relatively insensitive function of most of the variables, becomes extremely difficult. One therefore stops the look-ahead procedure when the values of the first-step parameters become insensitive to an additional look-ahead step. The results of carrying out a three step look-ahead presented in Table 2.

This concludes our presentation of general material in the context of this simple model. The increase in accuracy obtained by incorporating the insights obtained from the study of Bose field theory examples into renormalization group calculations for spin systems speaks for itself. There are, however, a few points which are worth making. First, since the zeroth-order input into the new class of renormalization group calculations amounts to incorporating mean-field (or semiclassical) information into the procedure, we should expect that as the mean field approximation becomes a better one, our new algorithms should also increase in accuracy. Thus, we expect these new methods to improve in accuracy as one studies problems in higher dimensions, and as one passes from spin systems having very few states per site to ones having large

number of states per site. This expectation is born out by specific calculations. In order to give the reader some feeling for how this works the results,for the 2+1-dimensional Ising model, of a single site mean-field, four site mean-field and two state renormalization group calculation with no look-ahead are given in Table 3 along with results obtained from high order perturbation theory calculations.[17]

4. CONCLUSION

This paper introduces a new way of looking at Hamiltonian real-space renormalization group calculations; namely, as an approximation to an, in principle, exact procedure which can be defined if on has knowledge of the groundstate wavefunction of the system in question. In addition, it establishes the relationship between the exact renormalization group transformation and various schemes for approximating it. By doing so we identify the concept of 'fast' and 'slow' block modes and what we referred to as the Born-Oppenheimer aspects of the renormalization group problem. From a conceptual point of view these are the two most important ideas we wish to present.

In order to incoporate this new understanding into algorithms for spin systems we introduced another new idea, that of the shadow Hamiltonian and the look ahead algorithm. It is important to point out that while we believe these techniques provide powerful new tools for carrying out explicit computations in specific models, we believe the way we used them to analyze the example of the Ising model in a transverse field only scratches the surface of what can be done. Certainly, there is much more to be learned both theoretically and practically about incorporating the results of generalized mean-field theory calculations

into the generation of real-space renormalization group algorithms. The methods we used, i.e., keeping more states and therefore more parameters in a look-ahead algorithm, are only a first crude step towards more effective procedures. Furthermore, there is the whole question of development of techniques of using these methods to calculate quantities such order parameters, correlation functions, etc., to the same accuracy as the ground state energy density. Finally, there is the question of how to best carry out higher dimensional calculations.

While it is true that we are nowhere near having the final word to say about any of these questions, we have done enough work on each of them to have learned some interesting facts. We will conclude this paper with a series of brief comments about each of these points, indicating what we already know and suggesting what we believe to be interesting directions in which to procede.

4.1 GOING TO HIGHER DIMENSIONS

There is no problem in generalizing all of our discussions in the preceding sections to the case of 2+1 and 3+1-dimensional field theories and spin systems. However, one does run into the computational problem of dealing with large numbers of states, since the smallest two dimensional unit having the symmetries of the original lattice is the square containing four points; and the smallest three dimensional unit with these properties is the cube with eight points (or a star with seven). If one must use shadow Hamiltonians based upon these fundamental units, then the size of the matrices one must diagonalize in order to carry out the real-space renormalization group procedure grows very rapidly indeed. Certainly, with the development of methods for dealing with

large matrices[18] this may still be practicable, but it is amusing to note that the shadow Hamiltonian techniques seem to make it possible to avoid much of this work. One can entertain the possibility of executing asymetrical blocking procedures. For example, one could carry out a blocking for the 2+1-dimensional Ising model wherein one first blocks in the x-direction and then in the y-direction, as indicated in Fig. 2. Hence, after two truncation steps one would have effectively carried out a truncation over the degrees of freedom of a single square. If one did this for 3-site blocks, using the naive truncation procedure, one would find that after a few iterations the truncated Hamiltonian became assymetrical under 90° rotations, and so one would obtain spurious results for the behavior of Green's functions, etc. However, if one uses the shadow Hamiltonian method and at least a two step look ahead procedure, one finds that the variational parameters adjust themselves to dramatically reduce this effect. This happens because the true ground state wavefunction of the system is invariant with respect to 90° rotations.

The great virtue of this observation is that it frees one to consider carrying out multi-state renormalization group calculations in any number of dimensions without having to face very great numerical problems. The price one pays for this is the introduction of additional variational parameters. Many other ways of combining asymetrical blocking procedures with the method of shadow Hamiltonians suggest themselves, especially for treating high dimensional problems involving continuous internal symmetry groups; the general question of how well the variational parameters of the scheme compensate for asymetries introduced by the computational procedure is under study.

4.2 FERMIONS AND MEAN FIELD THEORY METHODS

Much of the discussion of Bose free field theory can be carried out for the case of fermion free field theory; however, the phase factors coming from the anticommuting nature of the fermion variables make the problem more complicated. At present there seems to be no simple way to avoid the fact that after one renormalization group transformation one is dealing with a spin system with very complicated, but tractable, long range interactions. What is clear is that the physics of models such as the 1+1-dimensional Schwinger model cannot be correctly obtained from truncation calculations without including this physics. The question of what is the best way of including this sort of effect in approximate renormalization group transformations is under study.

4.3 MORE ABOUT MEAN FIELD THEORY

The way to incorporate more of the physics of the generalized mean-field theory into the generation of renormalization group algorithms remains a very important open question. Many earlier calculations, such as the Anderson[19] calculation of the properties of the Heisenberg antiferromagnet can be nicely rewritten in terms of a generalized mean-field theory calculation; and furthermore, this format suggests how one can systematically go beyond this approximation and treat generalizations of the asymetrical model accurately. In addition, the generalized mean-field theory approximation provides a good zeroth order approximation to such diverse phenomena as the Kosterlitz-Thouliss transition in the 1+1-dimensional U(1)-model,[20] and the fascinating physics, for which the ANNNI-models provide a paradigm.[21] The mechanism of the

ANNNI-models would be particularly interesting to understand well, since they provide examples of theories which generate a discrete infinity of physical scales as a function of a dimensionless parameter. If an analagous mechanism can be incorporated into lattice field theories it would greatly enlarge the possibilities for constructing theories wherein quarks and leptons are composite. For this reason application of our shadow Hamiltonian real-space renormalization group ideas to this class of theories is one of the problems we will be studying in the near future. Preliminary investigation of this theory has shown that the generalized mean field theory formalism already incorporates much of what is known about this model, and so the problem of finding a better formalism for melding this set of ideas into the renormalization group procedure is very interesting.

4.4 COMPUTING ORDER PARAMETERS, ETC., TO HIGHER ACCURACY

As is evident from the results presented in Tables 1 and 2, the error in the computation of quantities like the magnetization of the ordered phase of the Ising model, is in general significantly greater than that in the computation of the energy. The reason for this is easy to understand. We have done a variational calculation of the ground-state energy, so the error in this quantity is second order in the error in the groundstate wavefunction; however, quantities such as the magnetization are not stationary under variation of the parameters used to compute the renormalization group transformation and so the error in these quantities is of first order in the error in the groundstate wavefunction. There are many ways one can go about improving this situation;[22] one simple one which suggests itself is to simply carry

along enough extra states so that the first order perturbation correction to the magnetization can be computed at any stage of the truncation process. To be precise, suppose we have carried out a p-state procedure to determine the variational parameters of the look-ahead calculation. In order to calculate the expectation value of an operator,X, to the same order of accuracy as the groundstate energy we then carry out a 2p-state truncation procedure for the computation of X as follows:

(i) using the parameters determined in the p-state procedure introduce a shadow Hamiltonian, $H_{shad}(\alpha)$ and use this Hamiltonian and its symmetry transforms to find the p-states used in the original truncation algorithm;

(ii) having found these p-states, $\{v_p\}$, apply the operator X to them to obtain an additional p-states $\{Xv_p\}$;

(iii) orthonormalize the set of 2p-states $\{v_p, Xv_p\}$ and use the resulting set of states to truncate the Hamiltonian H^n to obtain H^{n+1} and to take X^n to X^{n+1};

(iv) at each succeding stage carry out a p-state look ahead to fix the parameters to be used in the shadow Hamiltonians, and then choose 2p-states to carry out the truncation process

The results of augmenting the calculation summarized in Table 3 by this method are shown in Table 4. As expected we see that the improvement in accuracy for the computation of the magnetization, and therefore the location of the critical point and critical exponents, is much greater than the change in the computation of the groundstate energy density.

This procedure for carrying out computations of quantites other than the groundstate energy to high accuracy is easily generalizeable, and much work remains to be done along these lines.

4.5 FINAL REMARKS

Besides the topics discussed in the preceding paragraphs, many other important questions about the possibility of extending these ideas in other directions remain unanswered. Of particular interest to field-theorists is the general question of whether these methods can be further developed and applied to the computation of the properties of gauge theories with fermions. Unfortunately, at present, we are in no position to give a yes or no answer to this question. The results of preliminary work along these lines suggests that one must be at least capable of incorporating the mean-field ideas into the renormalization group algorithms used for these theories, or one will not be able to answer such questions as whether or not the gauge theory spontaneously breaks itself. We are hopeful that gauge theories will prove to be amenable to analysis by future generalizations of these techniques.[23] We believe that considerable improvements both in the understanding of the theory of the real-space renormalization group transformation and in the development of new computational techniques are possible.

4.6 ACKNOWLEDGEMNTS

We would like to thank Prof. L. Kadanoff for insisting that we should be able to develop variational renormalization group algorithms introduced in another context,[24] in order to make it possible to adapt conventional techniques for computing critical exponents, etc. The attempt to understand if this could be done led to the work reported in this paper. In addition, we gratefully acknowledge discussions with Prof D. Horn, which led us to think about using mean-field methods as input to renormalization group transformations; and, many helpful conversations with Prof. R. Blankenbecler about the general subject of computing matrix elements of general operators to the same accuracy as the ground state energy.

Appendix A

GENERALIZED MEAN-FIELD CALCULATIONS

One by-product of the development of these algorithms for block-spin calculations is that we have learned a great deal about the properties of what we have called generalized mean-field calculations. The results of some of these calculations are interesting enought that we include them here to show the power of this approach alone. We hope that the discussion of the simple examples presented in this appendix will make it clear why the combination of these ideas with that of the block-spin truncation algorithm provides such a powerful computational technique.

A.1 THE 1+1-DIMENSIONAL ISING MODEL

The purpose of this section is to carry out a single site mean-field calculation for the Ising model in a transverse field, relate this to familiar calculations, generalize this to block mean-field calculations and finally show how to improve these results by including effects of "position dependent" mean-field state.

A single site mean-field state is defined to be a state of the form

$$|\psi(\theta)\rangle = \prod_j \left[\cos\theta|\sigma_z=-1\rangle + \sin\theta|\sigma_z=1\rangle\right]_j \qquad \text{(A1)}$$

The value of theta which defines the mean-field approximation to the groundstate wavefunction is obtained by minimizing the energy density

$$\varepsilon(\theta) = \frac{\langle\psi(\theta)|H|\psi(\theta)\rangle}{\text{volume}} \quad . \tag{A2}$$

Because of the symmetry of H under $PZ = \Pi\, \sigma_z(j)$ minima corresponding to nonzero values of theta are twofold degenerate. A trivial calculation yields

$$\theta_o = \pm \frac{1}{2} \arccos \frac{\varepsilon}{4} \quad \text{for } \varepsilon < 4$$

and

$$\theta_o = 0 \quad \text{for } \varepsilon \geq 4 \quad . \tag{A3}$$

Thus, the single site mean-field calculation finds degenerate vacua for all $\varepsilon < 4$ and a unique vacuum for all ε larger than 4. Since the exact critical value of ε is $\varepsilon_c = 2$, the single site mean-field calculation of the critical point is in error by a factor of two.

One way to improve on this trivial calculation is to form block mean-field states as described in Section 3. The critical values of ε for two, four and six site block mean-field calculations are given in Table 5. Table 5 also includes a comparison of the exact groundstate energy density for $\varepsilon = 1.8$ and the estimate obtained from each of these block mean-field calculations. Clearly, by using block mean-field states as a starting point for truncation calculations we take advantage of the considerable improvement they provide over single site mean-field calculations.

In Section 3 we remarked that the parameter β in the multistate truncation algorithm allowed us to include the effects of kink-states in motion, because it provided us with states which interpolated between regions of one mean-field vacuum and another. We will now show that the

role of such states is clear, even within the framework of a single-site mean-field calculation if one generalizes the calculation to include the possibility of "position dependent" mean-field states. By a position dependent mean-field state we mean, a state $|\psi(\theta_j)\rangle$

$$|\psi(\theta_j)\rangle = \prod_j [\cos\theta_j |\sigma_z(j)=-1\rangle + \sin\theta_j |\sigma_z(j)=+1\rangle] \qquad \text{(A4)}$$

If we compute the expectation value, $\langle\psi(\theta_j)|H|\psi(\theta_j)\rangle$ and extremize over arbitrary functions θ_j, we find that in addition to the solutions $\theta_j = \pm\,\theta_o$ there are "kink-like" solutions for which

$$\text{gap} = \langle\psi(\theta_j)|H|\psi(\theta_j)\rangle - \langle\psi(\theta_o)|H|\psi(\theta_o)\rangle \qquad \text{(A5)}$$

is a finite quantity. Those states which give finite gaps are of the form $\theta_j = -\,\theta_o$ for $j < j_1$ and $\theta_j = \theta_o$ for $j > j_2$, with a transition or kink region interpolating between j_1 and j_2 (Clearly antikink configurations which go from θ_o to $-\,\theta_o$ also give finite gaps.) Simple variational estimates of the width of the transition region for these states indicates that for all $\varepsilon < 3$ the transition takes place over one intervening site. This suggests that one can estimate the effects of allowing the kink-configurations to move by forming zero-momentum states of the form

$$|\psi_{\text{kink}}\rangle = (\text{norm})\{\sum_p \prod_{j<p} [|\phi_j(-\theta_o)\rangle]|\phi_p^*\rangle \prod_{j<p} |\phi_j(\theta_o)\rangle\} \qquad \text{(A6)}$$

where

$$|\phi(\pm\theta_o\rangle = \pm\cos\theta_o|\sigma_z=-1\rangle + \sin\theta_o|\sigma_z=1\rangle \qquad \text{(A7)}$$

and $|\phi_p^*\rangle$ is a state at site 'p' satisfying the condition

$$\langle\phi_p^*|\phi_p(\theta_o)\rangle = 0 \qquad \text{(A8)}$$

and θ_o is the value determined for theta by the position independent mean-field calculation.

Straightforward computation of the quantity "gap" defined in (A5) yields the result

$$\text{gap} \propto \varepsilon - 2 \qquad \text{(A9)}$$

Hence, we see that this "generalized mean-field calculation" tells us that a plane wave state of one kink in motion has a lower energy than that of the position independent mean field state for $\varepsilon > 2$. It follows trivially, that a state with a separated kink antikink pair, each having $k = 0$, lies still lower, etc. Thus, we see that at $\varepsilon = 2$ the position independent mean-field groundstate has become unstable to the condensation of multiple kink antikink pairs, and the ordinary mean field approximation can no longer be trusted.

In this way we see that a simple generalization of the position independent mean field calculation produces a correct prediction of the critical point and predicts a "mass gap" which vanishes like $|\varepsilon-2|$, which is of course the correct answer.

The simplest way to carry out the generalized mean-field calculation is to observe that

$$[-\cos\theta_o|\sigma_z=-1\rangle + \sin\theta_o|\sigma_z=1\rangle] = \sigma_z[\cos\theta_o|\sigma_z=-1\rangle = \sin\theta_o|\sigma_z=1\rangle] \tag{A10}$$

and that the state $|\psi^*\rangle$, which is orthogonal to $|\psi(\theta_o)\rangle$, must be

$$|\psi^*\rangle = [\sin\theta_o|\sigma_z=-1\rangle + \cos\theta_o|\sigma_z=1\rangle] = \sigma_x|\psi(\theta_o)\rangle \tag{A11}$$

hence, the state $|\psi_{kink}\rangle$ can be written in operator form, as

$$|\psi_{kink}\rangle \propto \sum_p O_x(p)|\psi(\theta_o)\rangle$$

where

$$O_x(p) = \left[\prod_{j<p} \sigma_z(j)\right] \sigma_x(p) \tag{A12}$$

Readers familiar with the exact solution of the Ising model will recognize that the operators $O_x(p)$ are linear combinations of the fermion operators obtained by performing a Jordan-Wigner transformation[25] on the spin operators, and will recall that the exact solution of the theory can be given in terms of the operators $O_x(p)$ and the analagous operators defined by replacing with σ_x with σ_y.

A.2 MEAN-FIELD APPROXIMATION TO U(1)-THEORY

The theory we wish to consider is a 1+1-dimensional lattice theory of coupled planar rigid rotors. This theory can be obtained by taking the $\lambda \to \infty$ limit for the theory of a self-coupled complex scalar field, having an interaction term of the form $V(\phi) = \lambda(\phi^*\phi - f^2)^2$. The Hamiltonian for this problem can be written as

$$H = \frac{1}{2f^2} \sum_i \left[J_z(i)^2 - \frac{f^2}{2} \left(J^+(i)J^-(i+1) + J^-(i)J^+(i+1) \right) \right] \qquad (A13)$$

where a complete basis for the system is generated by taking tensor products over the single-site states, $|m_i\rangle$, defined by the conditions

$$J_z(i)|m_i\rangle = m|m_i\rangle \qquad (A14)$$

where the m's are integers and $-\infty < m_i < \infty$, and

$$J^+(i)|m_i\rangle = |(m+1)_i\rangle \quad \text{and} \quad J^-(i)|m_i\rangle = |(m-1)_i\rangle \ . \qquad (A15)$$

Following the general procedure outlined for the Ising model, we see that a single-site mean-field approximation to this model corresponds to evaluating the expectation value of H in a product state of the form

$$|\Phi\rangle = \prod_j |\phi\rangle_j \qquad (A16)$$

Taking this expectation value yields an expression of the energy of the form

$$\varepsilon = \text{volume}\left[\langle\phi| \frac{1}{2f^2} J_z^2 |\phi\rangle - f^2 \langle\phi|J^+|\phi\rangle\langle\phi|J^-|\phi\rangle \right] \qquad (A17)$$

Varying ε with respect to $\langle\phi|$ we see that at the extremum $|\phi\rangle$ satisfies the Schroedinger equation

$$\left[\frac{1}{2f^2} J_z^2 - \eta\{\exp(i\alpha)J^+ + \exp(-i\alpha)J^-\} \right] |\phi\rangle = \mu|\phi\rangle \qquad (A18)$$

where we have defined $\langle\phi|J^{+}|\phi\rangle = \eta[\exp(-i\alpha)/f^{2}]$. Observing that Eq. (A18) is just another way of writing the Mathieu differential

$$\left[\frac{1}{2f^{2}} - \frac{\partial^{2}}{\partial\theta^{2}} - 2f^{2}\cos(\theta-\alpha)\right]\phi(\theta) = \mu\phi(\theta) \qquad \text{(A19)}$$

In the limit $f\to 0$ the solution to this problem is the unique state specified by the condition $m_{i} = 0$ everywhere; however, in general there can be a 1-parameter family of states $|\Phi(\alpha)\rangle$ which extremize ε. Since the overlaps of states corresponding to distinct values of α are smaller than unity, it follows that in the infinite volume limit there can be in general an infinite number of degenerate ground states of the system characterized by the order parameters $\langle\phi|J^{+}|\phi\rangle$. This result is in conflict with Coleman's theorem and one must turn to the generalized mean-field calculation to fully understand the situation.

In order to make it simple to understand what is happening in terms of explicit calculations, we will not deal with the solutions to the Mathieu equation, but rather, estimate these solutions by periodic Gaussians, i.e., wavefunctions of the form

$$|\phi(\alpha)\rangle = \sum_{m} \exp\{im(\theta-\alpha)\}\exp\{-\frac{m^{2}}{2\gamma}\} \qquad \text{(A20)}$$

where the normalization of this state is given by

$$\int \phi^{*}\theta\ \phi\theta = \sum_{m} \exp\{(-\frac{m^{2}}{\gamma})2\pi^{2}\} \qquad \text{(A21)}$$

Evaluating $\langle\phi|H|\phi\rangle/\langle\phi|\phi\rangle$ in the state defined by Eq. (A20) we obtain

$$\varepsilon(\gamma,f) = \langle\phi|\phi\rangle^{-1} \sum_m \left[\frac{1}{2f^2} m^2 \exp\left\{-\frac{m^2}{\gamma} - 2f^2\right\} \exp\left\{-\frac{1}{4\gamma}\right\} \exp\left\{-\left(m + \frac{1}{2}\right)^2\right\}\right] \tag{A22}$$

The problem which faces us is to minimize $\varepsilon(\gamma,f)$ over the parameter γ for each value of the parameter 'f' appearing in the definition of the Hamiltonian.

This formula is easily evaluated numerically for various values of f^2 and γ; the results of such a calculation are shown Fig. 3. We see that for $f < .69$ the solution $\gamma = 0$ provides the lowest energy for the variational wavefunction, whereas for $f > .695$ we see that the absolute minimum occurs for different from zero. This would indicate that the location of the phase transition for this model would be estimated to be around f = .695 which is not far from the answer obtained by Kogut et al.[26] which in our units corresponds to f = .96. As we indicated, since the solutions corresponding to different values of the parameter α have overlap less than unity, the existence of a minimum for γ different than zero would seem to indicate the existence of an infinite number of degenerate groundstates in the infinite volume limit. What is worse, the expectation value of exp ($i\theta$) in these states would appear to be non-vanishing in contradiction to what is required by the Mermin-Wagner theorem. However, this is where generalized mean-field theory enters the game.

It is easy to show that, for the Hamiltonian defined in (A18), whenever the minimum of $\varepsilon(\gamma,f)$ is for different from zero then the energy of a "kink-in-motion" state lies lower still. To be specific, if we define the state

$$\psi_{kink} = \text{Norm} \sum_p \prod_{j<p} |\phi_\delta(\alpha)\rangle_\delta \prod_{j>p} |\phi(\alpha+\delta)\rangle_\delta \quad . \qquad \text{(A23)}$$

then it follows that $\langle\psi_{kink}|H|\psi_{kink}\rangle/\langle\psi_{kink}|\psi_{kink}\rangle$ is less than $\langle\phi|H|\varepsilon\rangle/\langle\phi/\phi\rangle$ for small enough δ. In fact, one can quickly see that two kinks in motion lie still lower in energy, etc. Hence, as in the case of the Ising model, generalized free field theory tells us that the mean-field approximation is breaking down due to the condensation of kink states before the mean-field calculation alone signals a phase transition (i.e., in this case the transition to the condensate of kinks occurs for an f greater than that given by the mean-field calculation). It is straightforward to show that the situation encountered for $f > .694$ is just what one would encounter if one tried to do a simple mean-field calculation for a massless free field theory, and in fact the various one-kink, two-kink state energies occur in the same way. Of course it is well known that for massless free field theory the expectation value of $\exp(i\theta)$ does vanish, and that is presumably the way in which generalized mean-field theory contrives to satisfy the Mermin-Wagner theorem.

Actually, once one has seen the physics of the generalized mean field calculation one is led to ansatz a trial wave-function of the general Hartree-Fock form

$$|\psi\rangle = \sum_i \left[\exp\{i \sum m_i\theta_i\} \exp\{-\sum_j m_i\Delta(i-j)\, m_j\}\right] \qquad \text{(A24)}$$

where for the function $\Delta(i-j)$ we can use the inverse propagator for a massless free field theory. It is easy to show that this ansatz gives a lower estimate of the groundstate energy than that given by mean-field

theory for f less than unity. By allowing the form of $\Delta(i-j)$ to vary between the extreme case of mean-field theory, i.e., $\Delta(i-j) = \text{const} \times \delta_{ij}$, and the free field form, one could do a much better job in determining both the location and the nature of the true phase transition. That, however, takes us beyond the discussion of generalized mean-field theory and we will terminate our treatment of the problem at this point.

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7. The well known fact that a field theory is defined by its Green's functions which are just groundstate expectation values of various operators, is the essential point here; all time independent Green's functions are, in principle, amenable to calculation by the methods we will describe.

8. See Ref. 5.

9. This assumed wave function renders the block-to-block recoupling terms involving v-operators inoperative.

10. i.e., 2^n where n equals the number of iterations performed.

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TABLE I

Results from a two-state calculation with three-step look-ahead for the 1+1 Dimensional Ising Model. [Numbers in brackets are last digits of exact results, where these differ from calculated numbers.]

ε	Energy Density	Magnetization
.4	-1.010000 [25]	.99493 [1]
.8	-1.040306 [417]	.97883 [44]
1.8	-1.2108 [60]	.8604 [125]
2.0	-1.2629 [732]	nonzero [0]

Critical parameters from this calculation

$\varepsilon_c = 2.5957$ [2.0]

$\gamma = .215$ [.125] $\qquad$ Mag $= \left[1 - \left(\frac{\varepsilon}{\varepsilon_c}\right)^2\right]^\gamma$

$\nu = .85$ from correlation length [1.0]

$= .783$ from gap

TABLE II

Results from a four-state calculation with three-step look-ahead for the 1+1 Dimensional Ising Model.

ε	Energy Density	Magnitization	Gap
.4	-1.010019 [25]	.994926 [1]	1.599981 [1.6]
.8	-1.04032 [42]	.97872 [44]	1.19959 [1.2]
1.0	-1.06331 [51]	.9654 [47]	.99884 [1.0]
1.8	-1.2134 [60]	.81443 [254]	.16237 [.2]
2	-1.2702 [32]	0	0

$\varepsilon_c \approx 1.91$ [2.0]

TABLE III

2+1 Dimensional Ising - Comparison of critical value for ε obtained in various calculations.

Calculation	ε_c
Single site mean field	8
Four-site mean field	7.45
Four-site two-state block spin	7.11
High Temperature Series expansion	6.22 ± .06

TABLE IV

Results from an eight-state calculation with improved magentization operator for 1+1 Dimensional Ising Model.

ε	Energy Density	Magnetization	Gap
1.8	-1.2149 [60]	.8135 [25]	.2099 [00]
2.0	-1.2716 [32]	.4427 [0]	.0255 [0.0]

$\varepsilon_c = 2.01$

$\gamma = .127$

$\nu = .965,$ from gap.

TABLE V

Results of block mean field calculations for 1+1 Dimensional Ising Model in a Transverse field with varying block size.

Number of Sites per Block	ε [Naive m.f.]
1	4.0
2	$3.4 < \varepsilon_c < 3.5$
4	$3.0 < \varepsilon_c < 3.1$
6	$2.9 < \varepsilon_c < 3.0$

At $\varepsilon = 1.8$

Number of Sites	Energy Density
2	-1.2072
4	-1.2108
6	-1.2124
[Exact]	[-1.2160]

Figure Captions

Fig. 1. Division of a one-dimensional lattice into two-site blocks.

Fig. 2. Division of a two-dimensional lattice into four-site blocks by blocking one dimension at a time.

Fig. 3. The groud state energy density as a function of the variational parameter γ for (a) f = .694, (b) f = .695, and (c) f = .7.

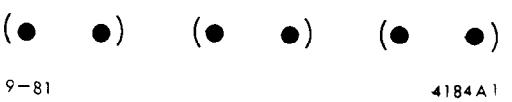
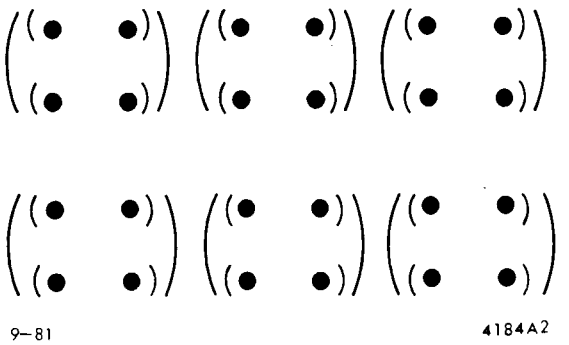


Fig. 1



9–81

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Fig. 2

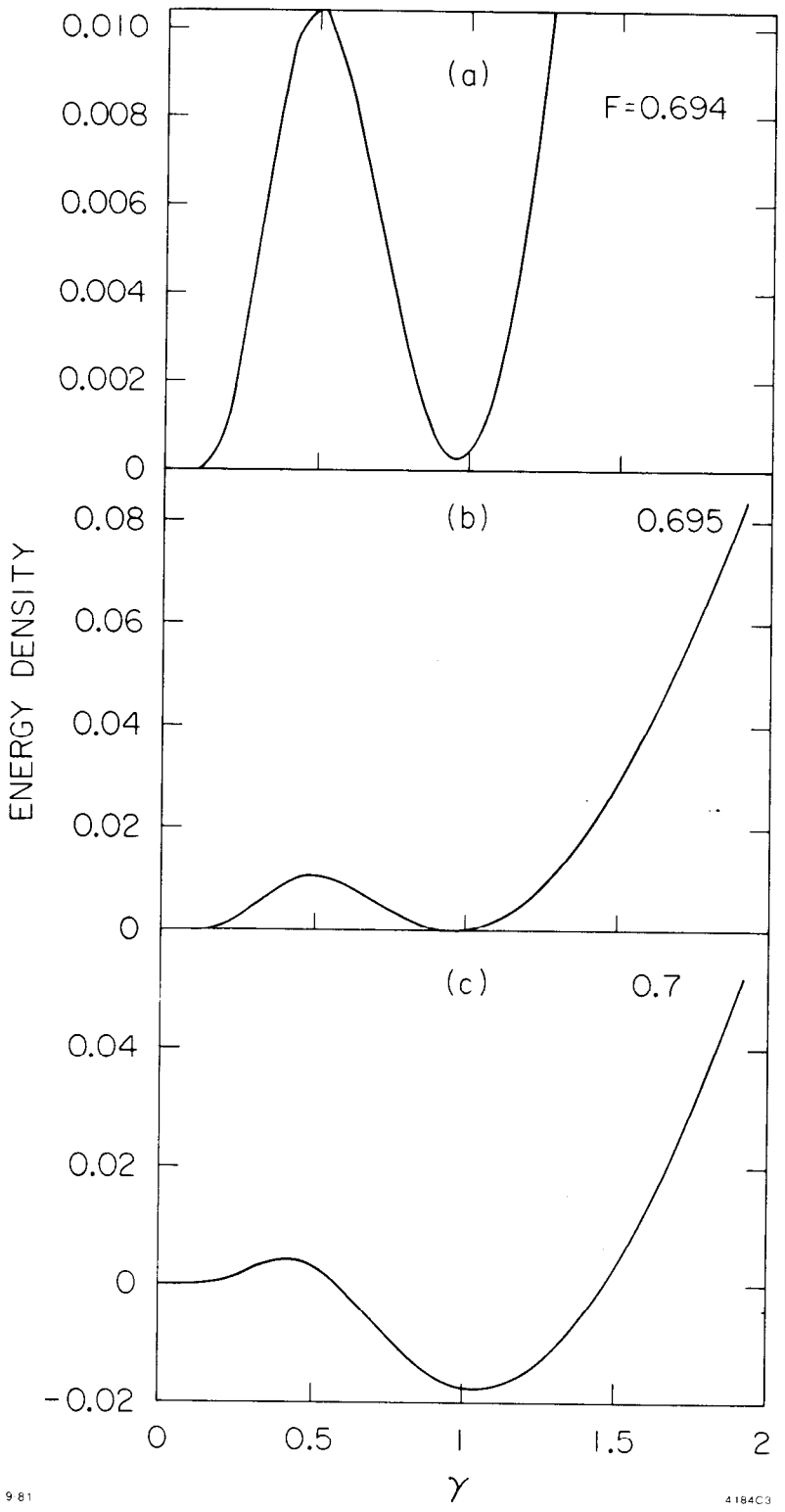
0.010
0.008
0.006
0.004
0.002
0
(a)
F=0.694
0.08
0.06
0.04
0.02
0
(b)
0.695
ENERGY DENSITY
0.04
0.02
0
-0.02
(c)
0.7
0
0.5
1
1.5
2
γ
9 81
4184C3

Fig. 3