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# QUANTUM FIELD THEORIES ON A LATTICE: VARIATIONAL METHODS FOR ARBITRARY COUPLING STRENGTHS AND THE ISING MODEL IN A TRANSVERSE MAGNETIC FIELD*

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## ABSTRACT

This paper continues our studies of quantum field theories on a lattice. We develop techniques for computing the low lying spectrum of a lattice Hamiltonian using a variational approach, without recourse either to weak or strong coupling expansions. Our variational methods, which are relatively simple and straightforward, are applied to the Ising model in a transverse magnetic field as well as to a free spinless field theory. We demonstrate their accuracy in the vicinity of a phase transition for the Ising model by comparing with known exact solutions.

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## I. INTRODUCTION

Interest in the study of non-abelian color gauge theories has been spurred by hopes that a fundamental theory of strong interactions will emerge from that class of theories. A primary goal in the study of such theories is to determine whether they confine the quarks and gluons that are their basic degrees of freedom. To study this question one needs an approach that does not rely on perturbative methods for calculating the spectrum of low lying physical states. This paper is the third in a series[1] concerned with the development of more general techniques applicable to problems of this type and to the study of specific examples in order to gain an understanding as to how well these techniques work. In particular in papers I and II we focused upon the problem of constructing lattice theories unitarily equivalent to cutoff continuum theories and we analyzed several models in the strong coupling limit. In this paper we develop straightforward and relatively simple variational methods for finding the spectrum of a lattice Hamiltonian without recourse either to strong or weak coupling expansions. We show that these methods—which were described and sketched out in Section IV. D of paper I—can be applied to calculations of basic properties with reasonable accuracy even in the vicinity of a phase transition.

The key to the success of any attempt to apply variational methods to the study of systems with a large number of degrees of freedom is the ability to make an appropriate choice of the class of trial states. The procedure we will describe is essentially an algorithm for constructing an appropriate class of trial functions. To demonstrate this constructive procedure we will study two soluble theories—free field theory and the one space-one time dimensional Ising model with a transverse applied magnetic field. We compare our variational calculations with known properties of the exact solutions, and discuss

methods for systematically improving upon our results. The application of these methods to the more interesting lattice gauge theories remains to be done.

The idea behind our constructive approach is very simple.[2] We begin by dissecting the lattice into small blocks containing a few sites which are coupled together via the gradient terms in the Hamiltonian. The Hamiltonian for the resulting few degree of freedom problem is diagonalized and the degrees of freedom "thinned" by a truncation procedure which amounts to keeping only an appropriate set of low lying states. An effective Hamiltonian is then constructed by computing the matrix elements of the original Hamiltonian in the space of states spanned by the lowest lying states in each block. The process is then repeated for this effective Hamiltonian. At each step the coupling parameters of the effective Hamiltonian change and the basic procedure is repeated until we enter either a very weak or strong coupling regime. As we shall see the calculation quickly brings the Hamiltonian to a fixed form. Formally the "thinning" of degrees of freedom at each step is equivalent to choosing an incomplete orthonormal set of states spanning a subspace of the Hilbert space. Thus, the variational problem of finding that linear combination of states which minimizes the expectation value of H is equivalent to the problem of diagonalizing the truncated Hamiltonian obtained by restricting H to this subspace.

## II. GENERAL METHOD APPLIED TO FREE FIELD THEORY

In this section we describe our general approach to the problem of finding the ground state and lowest lying excited states of a lattice field theory. To demonstrate the general procedure we begin by applying it to the trivial example of the field theory of free spinless particles on a lattice in 1x-it dimensions.

We first rewrite the free field Hamiltonian in terms of dimensionless canonical variables (see Eq. (3.17) of I), i.e.,

$$H = \Lambda \sum_{j=-N}^{N} \left\{ \frac{1}{2} p_j^2 + \frac{1}{2} \mu^2 x_j^2 + \frac{1}{2} (x_j - x_{j+1})^2 \right\} \tag{2.1}$$

where $\Lambda^{-1} = a$ is the lattice spacing, $L = (2N+1)/\Lambda$ is the length of the lattice in a 1x-it dimensional model, and $\mu$ is the mass parameter in units of $\Lambda$. The gradient operator has, for simplicity, been defined in terms of nearest neighbor differences. The exact solution of (2.1) describes a system of noninteracting oscillators of frequency

$$\omega_k = \sqrt{\mu^2 + 4 \sin^2 \frac{k}{2}} \qquad k = \frac{2\pi n}{2N+1} \tag{2.2}$$

$$n = 0, \pm 1, \pm 2, \ldots \pm N$$

with ground state energy density[3]

$$\epsilon_0 = \frac{1}{2\pi} \int_0^{\pi} dk \sqrt{\mu^2 + 4 \sin^2 \frac{k}{2}} \tag{2.3}$$

Our approximate constructive technique for solving (2.1) can be described as follows:

1. Introduce creation and annihilation operators at each lattice site j by the standard definition

$$x_j = \frac{1}{\sqrt{2\omega_j}} \left( a_j + a_j^\dagger \right)$$

$$p_j = -i \sqrt{\frac{\omega_j}{2}} \left( a_j - a_j^\dagger \right) \tag{2.4}$$

where $\omega_j$ is an arbitrary frequency. Define the state

$$|\Omega\rangle = \prod_{j=-N}^{N} |\Omega_j\rangle$$

$$a_j |\Omega_j\rangle = 0 \quad . \tag{2.5}$$

2. Divide the lattice into blocks containing several adjacent sites and solve for the eigenstates of H restricted to just these (two or three) lattice sites.

3. Make a canonical transformation on the $x_j$, $p_j$ for each such block and choose a trial state as a linear combination of all the states formed from $|\Omega>$ by application of the lowest, and only the lowest, mass oscillator for each block. Compute the Hamiltonian in this restricted set of states.

4. Repeat this process on the truncated problem by once again coupling adjacent blocks.

5. Iterate until the successive rescaling of eigenfrequencies leads either to a very weak or strong coupling regime in which the remaining coupling terms between neighboring blocks that arise from the gradient term of (2.1) can be treated perturbatively—either by weak or strong coupling approximation methods.

The general formulation of this procedure was presented in Section IV. D of Paper I. Its application to (2.1) will show it to be a very accurate technique. Specifically, we begin by dividing the lattice into blocks of 2 sites apiece as shown in Fig. 1 and label each block by the variable "$\ell$". Hence, each point of j can be written as

$$j = 2\ell + r \qquad \text{where } r = 0, 1 \tag{2.6}$$

We then define

$$x_0(\ell) = x_{2\ell}\,; \qquad p_0(\ell) = p_{2\ell}$$

$$x_1(\ell) = x_{2\ell+1}\,; \qquad p_1(\ell) = p_{2\ell+1}$$

and rewrite H as

$$\frac{1}{\Lambda} H = \sum_{\ell} \left[ \frac{1}{2} p_0^2(\ell) + \frac{1}{2} p_1^2(\ell) + \frac{1}{2}(\mu^2+2) \left[ x_0^2(\ell) + x_1^2(\ell) \right] - x_0(\ell)\, x_1(\ell) \right] - \sum_{\ell} x_0(\ell+1) x_1(\ell) \tag{2.7}$$

Our next step is to define variables $x_+(\ell)$ and $x_-(\ell)$ so that the part of H made up of operators referring to a single block $\ell$ is diagonal, i.e.,

$$x_+(\ell) \equiv \frac{x_0(\ell) - x_1(\ell)}{\sqrt{2}} \qquad p_+(\ell) \equiv \frac{p_0(\ell) - p_1(\ell)}{\sqrt{2}}$$
$$x_-(\ell) \equiv \frac{x_0(\ell) + x_1(\ell)}{\sqrt{2}} \qquad p_-(\ell) \equiv \frac{p_0(\ell) + p_1(\ell)}{\sqrt{2}} \tag{2.8}$$

In terms of these variables H becomes

$$\frac{1}{\Lambda}H = \sum_{\ell}\left[\frac{1}{2}p_+^2(\ell) + \frac{1}{2}(\mu^2+3)\,x_+^2(\ell) + \frac{1}{2}p_-^2(\ell) + \frac{1}{2}(\mu^2+1)\,x_-^2(\ell)\right]$$
$$- \frac{1}{2}\sum_{\ell}(x_+(\ell+1) + x_-(\ell+1))(x_-(\ell) - x_+(\ell)) \tag{2.9}$$

Our basic approximation is to freeze out the higher frequency oscillators $x_+(\ell)$ in each block $\ell$ by choosing as our smaller space of trial states only those states $|\psi\rangle$ generated by applying arbitrary powers of $p_-(\ell)$ and $x_-(\ell)$ to $|\Omega\rangle$. This amounts to replacing all powers of $p_+(\ell)$ and $x_+(\ell)$ by their ground state expectation values. Doing this we obtain a truncated Hamiltonian

$$\frac{1}{\Lambda}H^{(tr)}(1) = \sum_{\ell}\left\{\frac{1}{2}\sqrt{\mu^2+3} + \frac{1}{2}p_-^2(\ell) + \frac{1}{2}(\mu^2+1)\,x_-^2(\ell)\right\} - \frac{1}{2}\sum_{\ell}x_-(\ell)\,x_-(\ell+1) \tag{2.10}$$

Iterating this procedure (n+1) times one obtains a truncated Hamiltonian of the form

$$\frac{1}{\Lambda}H^{(tr)}(n+1) = \sum_{\ell'}\left[d_{n+1} + \frac{1}{2}p_-^2(\ell') + \frac{1}{2}\omega^2(n+1)\,x_-^2(\ell')\right] - \sum_{\ell'}\frac{1}{a_{n+1}}x_-(\ell'+1)\,x_-(\ell') \tag{2.11}$$

where

$$d_{n+1} = 2d_n + \frac{1}{2}\sqrt{\mu^2 + \frac{3}{2^n}}\,; \qquad d_0 \equiv 0$$
$$\omega(n) = \sqrt{\mu^2 + \left(\frac{1}{2}\right)^{n-1}} \qquad \text{for } n \geq 1 \tag{2.12}$$

$$a_n = (2)^n$$

and $\ell'$ denotes the variable for the $(n+1)^{th}$ iterated block. Clearly, for large n, $H^{(tr)}(n+1)$ becomes a Hamiltonian for which the last, or gradient term, is multiplied by a factor of $1/2^n$. Hence, it can be treated as a small perturbation on the single-site terms which describe oscillators of mass $\sim\mu$. In this way we see that the $n \to \infty$ limit evidently describes a theory of particles of "mass" $\mu$ with ground state energy density (henceforth expressed in units of $\Lambda$)

$$\epsilon_g(\mu^2) \equiv \lim_{n\to\infty} \frac{1}{2^n} d_n \tag{2.13}$$

The prediction of the mass $\mu$ of the single particle states for this system is exactly correct. It is easy to see from (2.11) that for $\mu^2 >> 1$, the ground state energy approaches the exact value of $\epsilon_g(\mu^2 >> 1) = (1/2)\mu$ in accord with (2.3); whereas for $\mu^2 = 0$, $\epsilon_g(0) = .67$ which is a reasonably good approximation to the exact result $\epsilon_0(0) = \frac{2}{\pi} \cong .64$ in the $\mu^2 = 0$ limit. This general idea of grouping lattice sites into blocks, then thinning out the number of states per block is the foundation of our method.[2]

The same technique can also be applied just as readily if the nearest neighbor approximation to the gradient operator on the lattice is replaced by the form constructed in I (see (3.10)), which makes the lattice and cutoff versions of the free field theory isomorphic. This introduces long range interactions (see Eqs. (3.10)-(3.12) in I), viz. the gradient term becomes

$$\int \frac{1}{2}(\nabla\phi)^2 dx \to \frac{1}{2}\Lambda \sum_{j_1, j_2=-N}^{N} D(j_1 - j_2)\, x_{j_1} x_{j_2} \tag{2.14}$$

with

$$D(j) = \pi^2/3 \qquad \text{for } j=0$$
$$= \frac{2(-)^j}{j^2} \qquad \text{for } j\neq 0 \tag{2.15}$$

in the $N\to\infty$ limit. In place of (2.2) and (2.3) we obtain the exact cutoff frequencies

$$\omega_k = \sqrt{\mu^2+k^2}$$

and ground state energy density

$$\tilde{\epsilon}_0 = \frac{1}{2\pi}\int_0^\pi dk\,\sqrt{\mu^2+k^2}$$

In this case we can also apply the truncation procedure just described even though the gradient operator couples distant lattice sites. The results as derived in the appendix are similar to what we found above for (2.1). The correct single particle mass is found, as is also the ground state energy for $\mu^2 >> 1$. In the massless limit we calculate $\tilde{\epsilon}_g(0) = 0.84$ which is larger than the exact result $\tilde{\epsilon}_0 = \pi/4 = .785$ by ~7%.

Evidently this simple-minded procedure of diagonalizing the 2-site Hamiltonian and keeping only the states generated by the lowest "mass" oscillators can be furthered improved on. In the next section we apply this technique to a spin lattice problem which differs from (2.1) in that there are only a finite number of eigenstates at each lattice site. We study the accuracy of this method in this example by comparing with known exact solutions of the model, and we improve its accuracy by a simple generalization of the variational procedure in Section IV.

## III. TRANSVERSE ISING MODEL: A SIMPLE TRUNCATION PROCEDURE

We begin this section by considering the 1-space, 1-time Ising model in a transverse magnetic field and adopting an intuitive and simple truncation procedure. This is an interesting example for testing our method for three reasons:

1. The known exact solution of this model exhibits a phase transition so we can measure the predictions of our method against the exactly computed critical indices and transition temperature.

2. There are only a finite number of states for the spin degree of freedom at each lattice site in common with theories of spin 1/2 particles such as quarks.

3. The simple truncation procedure for thinning the degrees of freedom to be discussed in this section is very different from the free field case since there are just two eigenstates at each lattice site instead of an infinite sequence of oscillator states.

The explicit form of the Hamiltonian for this model is written in terms of the usual Pauli matrices[4]

$$\frac{1}{\Lambda} H = \sum_{j=-N}^{N} \left\{ \frac{1}{2} \epsilon_0 \, \mathbb{1}_j + \frac{1}{2} \epsilon_0 \sigma_z(j) - \Delta_0 \sigma_x(j) \, \sigma_x(j+1) \right\} \tag{3.1}$$

Before studying (3.1) for arbitrary constants $\epsilon_0$ and $\Delta_0$ let us make some observations about limiting cases. In the strong coupling limit, $\Delta_0/\epsilon_0 \to 0$, (3.1) describes an assembly of noninteracting spins that all line up with spin down in the nondegenerate ground state

$$|0\rangle = \prod_j \begin{pmatrix} 0 \\ 1 \end{pmatrix}_j \tag{3.2}$$

of energy density (in units of $\Lambda$) $\mathcal{E}_0(\Delta_0/\epsilon_0 \to 0) = 0$. The particle-like excitations lie $+\epsilon_0$ above the ground state for each site excited to the spinup configuration, $\begin{pmatrix} 1 \\ 0 \end{pmatrix}_j$.

In the opposite, or weak coupling extreme, $\epsilon_0/\Delta_0 \to 0$, the eigenstates

$$|\rightarrow\rangle_j \equiv \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}_j \tag{3.3}$$

and

$$|\leftarrow\rangle_j \equiv \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}_j \tag{3.4}$$

diagonalize the Hamiltonian. The ground state is doubly degenerate, being formed as a product of states (3.3) at each site, or all states (3.4) at each site. For each "wall" between two adjacent sites, one formed as (3.3) and the other reversed as (3.4), there is an excitation of $+2\Delta_0$ units of energy. In this extreme the excitations are kink-like as illustrated by Fig. 2. These low lying excitations in the strong coupling limit correspond to collective "kink" states rather than single particle excitations.

From a study of the exact H in (3.1) it is known[5] that a second order phase transition occurs between the nondegenerate ground state (3.2) and the degenerate configurations (3.3) and (3.4). The transition occurs when $\epsilon_0 = 2\Delta_0$. The behavior of the order parameter, or "magnetization," in this model is given by

$$\begin{aligned} \langle\sigma_x\rangle &= \left(1 - \left[\epsilon_0/2\Delta_0\right]^2\right)^{1/8} \qquad \text{for } \frac{\epsilon_0}{2\Delta_0} \lesssim 1 \\ \langle\sigma_x\rangle &= 0 \qquad\qquad\qquad\qquad\quad \text{for } \frac{\epsilon_0}{2\Delta_0} > 1 \ . \end{aligned} \tag{3.5}$$

Keeping these exact results in mind, let us now apply our iterative variational procedure to (3.1) for arbitrary coupling $(\epsilon_0/\Delta_0)$. Again we construct a suitable trial state by the iterative procedure of coupling small spin blocks, or boxes, containing neighboring lattice sites; diagonalizing the "box" Hamiltonian; and dropping all but a subset of the low lying eigenstates with which to form a

block basis for the truncated Hamiltonian. We then iterate the procedure. The simplest application of this procedure to (3.1) is to form blocks containing just two lattice sites and $2^2=4$ eigenstates which we determine exactly. We then discard two of these eigenstates retaining just the lowest two states which will be mixed together when we add back in the terms in (3.1) linking different boxes. In terms of these two states we construct a new effective truncated Hamiltonian of the same form and continue the iterative process. We can think of this procedure as successively eliminating higher momentum states from the problem. Hence the series of truncated Hamiltonians describe the physics of low momentum states alone.

To begin we note that within one block of two adjacent sites in (3.1) there are four independent states which we denote by $|\uparrow\uparrow>$, $|\uparrow\downarrow>$, $|\downarrow\uparrow>$, and $|\downarrow\downarrow>$, where $|\uparrow\uparrow> \equiv |\uparrow>_1 |\uparrow>_2$, etc. The problem of diagonalizing the 2-site Hamiltonian reduces simply to one of diagonalizing two $2\times 2$ matrices, since $|\downarrow\downarrow>$ mixes only with $|\uparrow\uparrow>$, and $|\downarrow\uparrow>$ with $|\uparrow\downarrow>$. The eigenstates and eigenvalues are simply found and are given in Table I. Step (i) of our general procedure will be to choose this set of four eigenstates as the new orthonormal system which we will use to construct a basis for H. Step (ii), the thinning out procedure, is simply accomplished by retaining only the two lowest energy states in Table I for each box when we add back the terms linking different boxes in (3.1). It is reasonable to expect that the most important part of the true ground state will be in the subspace spanned by these two states in each box. In order to implement this approximation we need only construct the truncated or effective Hamiltonian for this choice of trial states and see if we can solve it.

To compute $H^{(tr)}$ we label each 2-site box by an integer 'p' and divide the Hamiltonian into two parts, $H_1$ and $H_2$. $H_1$ contains only those terms in (3.1)

which refer to single boxes and $H_2$ contains the remaining interaction terms in (3.1) which couple sites in adjacent boxes; i.e.,

$$H_2 = -\Delta_0 \sum_p \sigma_x(p,1)\,\sigma_x(p+1,0) \tag{3.6}$$

where $\sigma_x(p,\alpha)$ operates on the spin in box p and at site $\alpha$=0, 1 within each box. In keeping with our approximation of retaining only the two lowest states in each box, the truncated $H_1^{(tr)}$ can be written as a sum of 2×2 matrices operating on the two states we keep for each box. In particular referring to Table I we see that $H_1^{(tr)}$ can be written as

$$H_1^{(tr)} = \sum_p \begin{pmatrix} \epsilon_0-\Delta_0 & \\ & \epsilon_0-\sqrt{\epsilon_0^2+\Delta_0^2} \end{pmatrix}_{(p)}$$

$$= \sum_p \left\{ \left(\epsilon_0 - \frac{1}{2}\left[\Delta_0+\sqrt{\epsilon_0^2+\Delta_0^2}\right]\right) \mathbb{1}(p) + \frac{1}{2}\left(\sqrt{\epsilon_0^2+\Delta_0^2}-\Delta_0\right)\sigma_z(p) \right\} . \tag{3.7}$$

The eigenstates of (3.7) can be written as products over boxes of the two lowest eigenstates in Table I; i.e.,

$$|\Psi_1\rangle = \prod_{\text{boxes } p} |\psi_p\rangle . \tag{3.8}$$

Hence the interaction (3.6) can now be re-expressed in terms of the truncated basis (3.8) by evaluating its matrix elements for flipping one "spin" in each of two adjacent boxes. To compute this we take the matrix element of $\sigma_x(p,1)$ between the states

$$|\psi_0(p)\rangle = \frac{(|\downarrow\downarrow\rangle + a_0|\uparrow\uparrow\rangle)}{\sqrt{1+a_0^2}} \tag{3.9}$$

and

$$|\psi_1(p)\rangle = \frac{(|\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle)}{\sqrt{2}} \tag{3.10}$$

The actual computation is quite trivial:

$$\sigma_x(p,1)|\psi_0(p)> = \frac{1}{\sqrt{1+a_0^2}}\,[|\downarrow\uparrow>+a_0|\uparrow\downarrow>]_p \tag{3.11}$$

and so

$$<\psi_1(p)|\sigma_x(p,1)|\psi_0(p)> = \frac{(1+a_0)}{\sqrt{2}\,\sqrt{1+a_0^2}} \tag{3.12}$$

Similarly

$$\sigma_x(p+1,0)|\psi_0(p+1)> = \frac{1}{\sqrt{1+a_0^2}}\,[|\uparrow\downarrow>+a_0|\downarrow\uparrow>] \tag{3.13}$$

and so

$$<\psi_1(p+1)|\sigma_x(p+1,0)|\psi_0(p+1)> = \frac{(1+a_0)}{\sqrt{2}\,\sqrt{1+a_0^2}} \tag{3.14}$$

which is identical with (3.12). It follows from this that for 'j' in the $p^{th}$ box, and for both cases $\alpha$=0 and 1,

$$\begin{aligned}\sigma_x^{(tr)}(j) &= \frac{1+a_0}{\sqrt{2(1+a_0^2)}}\,\sigma_x(p)\\ \sigma_x^{(tr)}(j+1) &= \frac{1+a_0}{\sqrt{2(1+a_0^2)}}\,\sigma_x(p+1)\end{aligned} \tag{3.15}$$

Thus we have reduced the problem of finding the best upper bound which one can obtain by choosing trial states from the set of states spanned by forming all possible tensor products of the lowest two states in Table I, to the problem of diagonalizing a new Hamiltonian, $H^{(tr)}$. Since our truncation procedure retained just two states per box we again have a spin form for the truncated Hamiltonian. $H^{(tr)}$ has exactly the same form as the original Hamiltonian but different coefficients:

$$H^{(tr)} = \sum_p \left[c_1 \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}(p) + \frac{1}{2}\epsilon_1 \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}(p) - \Delta_1 \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}(p)\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}(p+1)\right] \tag{3.16}$$

where

$$c_1 = \epsilon_0 - \frac{1}{2}\left(\Delta_0 + \sqrt{\epsilon_0^2+\Delta_0^2}\right) \tag{3.17}$$

$$\epsilon_1 = \sqrt{\epsilon_0^2+\Delta_0^2} - \Delta_0$$

and

$$\Delta_1 = \frac{\Delta_0(1+a_0)^2}{2(1+a_0^2)}$$

At this point we face one of two possibilities. Either the values of $\epsilon_1$ and $\Delta_1$ are such that we can treat the resulting effective Hamiltonian, $H^{(tr)}(1)$ by perturbation theory for $\epsilon_1/\Delta_1 > 1$ or $\epsilon_1/\Delta_1 < 1$; or, we may repeat the same procedure that we just went through, but this time combining neighboring pairs of blocks p in the Hamiltonian $H^{(tr)}$ and thereby including additional interaction terms in a new basis to which we again apply the same state-thinning steps as in (3.6) to (3.16). One readily sees in the comparison of (3.16) with the original (3.1) that each successive restriction of our class of trial wave functions by this procedure leads us to a new effective Hamiltonian of the same <u>form</u> as the original Hamiltonian, and with the coefficients of the effective Hamiltonian given by (3.17) in terms of the coefficients found in the preceding step of the calculation.

The general result is that after 'n' successive truncations our variational problem reduces to the problem of diagonalizing the effective lattice Hamiltonian

$$H_n^{(tr)} = \sum_{p_n}\left[d_n\begin{pmatrix}1&0\\0&1\end{pmatrix}_{p_n} + \frac{1}{2}\epsilon_n\begin{pmatrix}1&0\\0&-1\end{pmatrix}_{p_n} - \Delta_n\begin{pmatrix}0&1\\1&0\end{pmatrix}_{p_n}\begin{pmatrix}0&1\\1&0\end{pmatrix}_{(p_n+1)}\right] \tag{3.18}$$

where

$$\epsilon_{n+1} = \left(\epsilon_n\left(1-a_n^2\right) - \Delta_n(1-a_n)^2\right)/\left(1+a_n^2\right)$$

$$\Delta_{n+1} = \frac{\Delta_n}{2}\frac{(1+a_n)^2}{(1+a_n^2)} \quad ,$$

$$a_n = \sqrt{\left(\frac{\epsilon_n}{\Delta_n}\right)^2 + 1} - \left(\frac{\epsilon_n}{\Delta_n}\right) \quad ,$$

$$c_{n+1} = -\left[\frac{\epsilon_n\left(1-a_n^2\right) + \Delta_n(1+a_n)^2}{2\left(1+a_n^2\right)}\right]$$

and

$$d_{n+1} = c_{n+1} + 2d_n; \quad d_0 = \frac{1}{2}\epsilon_0 \tag{3.19}$$

Clearly, each step of our iteration procedure includes additional interaction terms between adjacent lattice sites in $H_1^{(tr)}(n)$, leaving fewer in the remaining $H_2(n)$. This is illustrated in Fig. 3. Hopefully, as in the free field theory example of the previous section, at some state of this process one of the $H_n^{(tr)}$'s will prove to have a ratio of $\epsilon_n/\Delta_n$ which is solvable or can be handled in perturbation theory. We borrow from Wilson and Kadanoff[2] and call the process of generating a new effective Hamiltonian from the one which was obtained in a previous step a "renormalization group transformation." The recursion relations given (3.18) - (3.19), which define the parameters in $H_n^{(tr)}$ obtained from successive iterations, will be referred to—for want of a better name—as renormalization group equations.

Analyzing the Renormalization Group Equations

In the preceding discussion we reduced the problem of constructing a set of $|\psi_n>$'s by means of a successive thinning out process to the equivalent problem of computing a series of renormalization group transformations on the coefficients of an effective Hamiltonian. In order to extract all of the information contained in (3.18) - (3.19) the recursion relations must be studied numerically.

However, there are several points which can be understood directly. First, we note that both ($\epsilon_0$=0, $\Delta_0$ arbitrary) and ($\epsilon_0$ arbitrary, $\Delta_0$=0) are fixed points of the renormalization group transformation since in either case $\epsilon_n=\epsilon_0$ and $\Delta_n=\Delta_0$ for all 'n'. In fact, we have already seen that both of these cases can be solved exactly; and it is easy to convince oneself that our algorithm for constructing the ground state wave function constructs the exact eigenstate for these two limiting cases. Second, we observe that a great deal of information can be extracted without completely solving the renormalization group equations if we know whether the ratio $\epsilon_n/\Delta_n$ increases or decreases with successive iterations.

To study this we define

$$y_n \equiv \left(\frac{\epsilon_n}{\Delta_n}\right) \tag{3.20}$$

The Hamiltonian (3.1) depends only on the ratio ($\epsilon/\Delta$) up to a scale factor; hence (3.19) gives $y_{n+1}$ as a function of $y_n$ alone:

$$y_{n+1} = \frac{2\left(\sqrt{1+y_n^2} - 1\right)\left(1 - 2y_n\left(\sqrt{1+y_n^2} - y_n\right)\right)}{\left(1 + \sqrt{1+y_n^2} - y_n\right)^2} \equiv F(y_n) \tag{3.21}$$

We need only study the function defined by

$$R(y) \equiv F(y) - y \tag{3.22}$$

in order to see if $y_n = \epsilon_n/\Delta_n$ increases or decreases with each iteration and see what it looks like for all y. R(y) is plotted schematically in Fig. 4, and its general shape yields the following useful information. A "fixed point" of the transformation occurs at values of $\epsilon$ and $\Delta$ which reproduce themselves under the renormalization group transformation; i.e., for $R(y)=R(\epsilon/\Delta)=0$. There is also a fixed point if $\epsilon/\Delta=\infty$ and $R(\infty)$ 0 so that this value cannot be reduced. Hence Fig. 4 shows that there are three fixed points for our transformation; namely, $\epsilon/\Delta$=0, $\epsilon/\Delta=\infty$ and $\epsilon/\Delta=2.55348456\ldots$ . Actually the condition R(y)=0 only requires that the

ratio $(\epsilon/\Delta)$ is unchanged by the iteration, and so the Hamiltonian may change by an overall scale factor at such a point if $\epsilon_{n+1} = \lambda\epsilon_n$ and $\Delta_{n+1} = \lambda\Delta_n$. As we have already seen y=0 and y=∞ are true fixed points of (3.18) - (3.19). A more careful analysis shows that $y_c = 2.55\ldots$ is a point at which the Hamiltonian is reproduced up to a scale factor $\lambda(y_c)$, which is another critical constant of the theory.

There is additional qualitative information which can be extracted from R(y). In particular, R(y)<0 implies that the ratio $(\epsilon/\Delta)$=y decreases for that iteration and so the new $(\epsilon'/\Delta')$ lies to the left of the y we started with. Since, as shown in Fig. 4, R(y) is negative for all $y < y_c$ we see that if we start at any point in this range, successive iterations of our truncation procedure will drive us to a form for the effective Hamiltonian which we have studied in weak coupling perturbation theory. On the other hand, for $y > y_c$ successive iterations drive us to y=∞ since, in this case, $R(y) > 0$. This implies $\epsilon/\Delta \gg 1$ which is the strong coupling limit of the Hamiltonian which we have also studied.[1] Hence those theories described by (3.1) for which the initial $y < y_c$ are theories with a degenerate ground state and spontaneously broken symmetry. On the other hand, for $y > y_c$ we have a unique ground state. Clearly $y_c$ is the point at which the nature of the ground state changes, and so $y_c$ is the <u>critical point</u> of this theory.

The result $y_c = 2.55348\ldots$ which is obtained from our simple procedure is not far from the exact transition point $y_c^{exact} = 2$. The fixed points y=0 and y=∞ are the stable fixed points of this renormalization group transformation, and the fixed point at $y=y_c$ is an <u>unstable fixed point</u>. The fact that at $y=y_c$ the Hamiltonian continues to reproduce itself up to a scale factor says that at this critical point the physics going on at different length scales is essentially the same.

There is still more information to be gleaned from the recursion relations in (3.18) - (3.21). In particular, these relations allow us to compute $\epsilon_n$ and $\Delta_n$ separately. If one examines the result of iterating (3.18) - (3.21) one finds that for initial values, $\epsilon_0/\Delta_0 < y_c$, the successive renormalization group transformations lead to $\lim_{n=\infty} \epsilon_n = 0$ and $\lim_{n=\infty} \Delta_n = \Delta_\infty(\epsilon_0/\Delta_0) \neq 0$, whereas for $(\epsilon_0/\Delta_0) > y_c$, $\lim_{n=\infty} \epsilon_n = \epsilon_\infty(\epsilon_0/\Delta_0) \neq 0$ and $\lim_{n=\infty} \Delta_n = 0$.

We can also calculate the order parameter $\langle\sigma_x(j)\rangle$ which can have a non-vanishing ground state expectation value when $y < y_c$ and the ground state is doubly degenerate. At each step of the iteration $\sigma_x(j)$ will connect the two lowest states in Table I with one another since $\sigma_x$ flips the spin at one site. Therefore we need only calculate

$$\lim_{N\to\infty} \langle\psi^N_{even}|\sigma_x(j)|\psi^N_{odd}\rangle \equiv \langle\sigma_x(j)\rangle \tag{3.23}$$

Going back to the discussion leading to (3.19) we see that because $\sigma_x^{(tr)}(j)$ is a purely off-diagonal $2\times 2$-matrix, calculating $\langle\psi^{(1)}_{even}|\sigma_x(j)|\psi^{(1)}_{odd}\rangle$ is the same as computing

$$[\sigma_x(j)]^{1st\text{-}trunc.} = \frac{(1+a_1)}{\sqrt{2\left(1+a_1^2\right)}}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} = \sqrt{\frac{\Delta_1}{\Delta_0}}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} \tag{3.24}$$

Hence in successive transformations we find that

$$[\sigma_x(j)]^{Nth\text{-}trunc.} = \prod_{p=1}^{N}\sqrt{\frac{\Delta_p}{\Delta_{p-1}}}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} = \sqrt{\frac{\Delta_N}{\Delta_0}}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} \tag{3.25}$$

We conclude therefore that if $\Delta_\infty \equiv \lim_{N\to\infty} \Delta_N$, the order parameter for a theory such that $y_0 = \epsilon_0/\Delta_0 < y_c$, is given by

$$\left\langle\sigma_x\left(\frac{\epsilon_0}{\Delta_0}\right)\right\rangle = \sqrt{\frac{\Delta_\infty}{\Delta_0}} \tag{3.26}$$

Explicit numerical iteration of (3.18) - (3.19) gives the following form as a very good fit to the order parameter

$$\left\langle \sigma_x\left(\frac{\epsilon_0}{\Delta_0}\right)\right\rangle \cong \left(1-\left(\frac{y}{y_c}\right)^2\right)^{.39} \tag{3.27}$$

with $y_c = 2.55348456\ldots$ . The agreement of (3.27) with the exact result (see (3.5))

$$\langle \sigma_x \rangle_{\text{exact}}(y) = \left[1 - \left(\frac{y}{2}\right)^2\right]^{.125}$$

is not too bad considering the simplicity of this calculation and the crudity of our approximation.

We now can ask what it takes to do better, particularly for the critical index by modifying our truncation algorithm. In the next section we show how a simple modification of our general approach does in fact produce a significant improvement in these results.

## IV. A MORE SOPHISTICATED ALGORITHM

The key point to be made in this section is that our variational technique can be systematically improved upon and the procedure for implementing this methodically is not much more difficult than the original naive procedure.

We will find that we can significantly improve the critical exponent (by a factor of 2) while moving the critical point only very slightly further away from the exact value. We also make a dramatic improvement in the general behavior of the ground state energy. In particular we find that $\epsilon_0(y)$ possesses a singularity in its second derivative at the critical point—a result which cannot be obtained from the preceding more naive calculation.

To begin, let us note that there are in fact two distinctly different pieces to our algorithm, both susceptible to change and improvement. First we

committed ourselves to grouping lattice sites into boxes containing two sites each. We then constructed "box states" and thinned out our complete set by throwing away two out of the four possible states per box. One simple way to generalize this approach would be by grouping sites into bigger boxes and by keeping more states. However, for now let us assume that this part of our procedure will be left unmodified, so that successive truncations of our space of trial wave functions shall always lead to an effective Hamiltonian of the same form as the original one.[6] Instead we turn to the question of improving upon our algorithm for throwing away states.

There are four states for a two-site box and these may be divided into two classes: $|\uparrow\uparrow>$, $|\downarrow\downarrow>$; and $|\downarrow\uparrow>$, $|\uparrow\downarrow>$, which are even and odd eigenstates, respectively, of the unitary transformation

$$U = e^{i\frac{\pi}{2}\sum_i \sigma_z(j)} \tag{4.1}$$

under which the Hamiltonian (3.1) is invariant. Whatever truncation procedure we employ in selecting just two of these four states in thinning the degrees of freedom we will want to choose one state from each of these two classes. This is because the box-box interaction terms being sequentially added to $H^{(tr)}$ by our iterative procedure link only the even and odd states under U to one another; i.e., $\sigma_x(j)$ flips one spin only and is odd under U. The question is which state to choose from each class.

In order not to destroy the reflection-symmetry of the theory we choose for the odd eigenstate under U the symmetric combination identical with Table I

$$|\psi_1> \equiv \frac{1}{\sqrt{2}}(|\downarrow\uparrow> + |\uparrow\downarrow>) \tag{4.2}$$

For the even eigenstate we generalize the construction in the preceding section by writing

$$|\psi_0> = \frac{1}{\sqrt{1+a^2(\epsilon,\Delta)}} \{|\downarrow\downarrow> + a(\epsilon,\Delta)\,|\uparrow\uparrow>\} \tag{4.3}$$

Equation (4.3) has the same form as before but we shall now choose the coefficient $a(\epsilon,\Delta)$ variationally by minimizing the ground state energy after a fixed (large) number of iterations rather than by simply diagonalizing the $2\times 2$ box Hamiltonian in each successive step. This procedure is computationally feasible as a result of an important observation by R. Pearson of Fermilab who noted that on the basis of (3.19) we can choose $a(\epsilon,\Delta)$ as a function of the ratio $(\epsilon/\Delta)$ alone. This is equivalent to the statement that the overall scale of the Hamiltonian does not matter for our analysis.

Using (4.2) and (4.3) we can carry out the renormalization group transformation and repeat precisely the same steps leading to the earlier result (3.18) and (3.19) with one single difference. The coefficient $a(\epsilon/\Delta)$ is now no longer given after the nth iteration as expressed in (3.19) but $a_n(\epsilon_n/\Delta_n)$ remains free to be determined variationally by minimizing the ground state eigenvalue of the effective truncated lattice Hamiltonian after a suitable number of iterations.

In order to give a more explicit formulation of this idea we note from the first of Eqs. (3.19) that the term in the Hamiltonian proportional to $d_{n+1}$ increases by a power of 2 for each iteration in contrast to the behavior of $\epsilon_n$ and $\Delta_n$. Hence, for N sufficiently large this term swamps the remainder of the Hamiltonian. This divergence in the coefficient of the unit matrix is just the renormalization group transformation's way of telling us that translation invariance of the ground state implies that its energy is proportional to the volume of the lattice times a finite number, $\mathscr{E}_0$, which is the ground state energy

density. Since each point of the effective Nth-lattice is $2^N$-points in the original lattice, the energy density is the limit

$$\mathscr{E}_0 = \lim_{N\to\infty} \left(\frac{1}{2^N} d_N\right)$$

or, from (3.19)

$$\mathscr{E}_0 = \lim_{N\to\infty} \sum_{n=0}^{N} \left(\frac{c_n}{2^n}\right. \tag{4.4}$$

In order to actually implement this procedure we perform a straightforward numerical calculation using a simple variational guess for $a(\epsilon/\Delta)$ that meets its known limiting values for $\epsilon/\Delta \to 0$ and $\to \infty$. A convenient parametrization in terms of two parameters $\rho$ and u is

$$\tan^{-1} a\left(\frac{\epsilon}{\Delta}\right) = \frac{\pi}{4}\left\{\frac{1 - \tanh\left(\frac{\epsilon}{\Delta}\rho - u\right)}{1 - \tanh(-u)}\right\} \tag{4.5}$$

This choice automatically satisfies the limits explored in Section III:

$$a \to 1 \quad \text{for } \epsilon/\Delta \to 0$$

$$a \to 0 \quad \text{for } \epsilon/\Delta \to \infty$$

We then minimize the ground state energy density (4.4) by varying the two free parameters $\rho$ and u in (4.5) and iterating to $N \approx 100$ which gives us $\mathscr{E}_0$ to an accuracy of roughly one part in $2^{100}$.

In Fig. 5 we show a comparison of our calculation of the ground state energy density to the exact answer. Values of $\epsilon/\Delta$ smaller than 1 and greater than 3 are suppressed because for these regions agreement is much better than one-part in $10^3$. Examination of these curves shows that our worst disagreement with the exact answer is on the order of 3%. This is a significant improvement over the naive calculation. In Fig. 6 we compare our computation

of the order parameter $\langle\sigma_x\rangle$ with the exact answer. As shown the critical value of $\epsilon/\Delta \cong 2.75$ which is somewhat further from the exact value of 2 than we found via our naive calculation that gave 2.55. The critical index however is improved by a factor of $\approx 2$ as seen from the accurate power law fit to $\langle\sigma_x\rangle$:

$$\langle\sigma_x(\epsilon/\Delta)\rangle = \left(1 - \left(\frac{y}{y_c}\right)^2\right)^{.21}$$

Finally we also see in Fig. 7 that our relatively simple variational approach reproduces the singularity in $\partial^2$ (ground state energy density/$\partial\epsilon^2$) which occurs at the critical point. This is quite a subtle property of the theory which was missed by our original naive renormalization group procedure described in Section III.

One can carry these methods further; in particular by working with larger blocks comprising three or more sites, and/or by retaining more states in the process of thinning the degrees of freedom, and by introducing more detailed trial functions than (4.5) with more than two parameters. A program of such calculations using more complex algorithms in our renormalization group variational approach is in progress.[6] Those calculations already completed further improve the agreement between our results and the known exact solution and will be reported later. Having already demonstrated the power of this approach for deducing the basic features of a theory that cannot be studied perturbatively our primary interest at this time is to extend their application to fermions (e.g., quark theories) and gauge models as well as to higher dimensional lattices.[7]

## V. SUMMARY AND FUTURE DIRECTIONS

In this paper we have demonstrated how one can study—by variational methods and without recourse to perturbation expansions—a lattice field theory formulated by imposing momentum and volume cutoffs on a local continuum field theory. Our principle goal was to show that the problem of finding a good basis for constructing such trial-wave functions can be converted to a renormalization group calculation in which the renormalization group itself is to be determined by means of the variational procedure. In effect, the only choices needed for such a calculation are the way in which to group single sites into blocks of sites and the assumption of how many states to keep at each truncation. Having constructed this equivalent renormalization group transformation we then study what happens to the form of the truncated or effective Hamiltonian as we successively thin out our family of linear trial wave functions. As we saw in the two specific examples of the Ising model and free field theory the key first point to understand in these transformations is what happens to the strength of the gradient (site-site recoupling) terms relative to the potential (single-site) terms in the Hamiltonian.

More generally, it proves useful to study the function R(y) which gives the change in the ratio of the potential to the gradient terms after a finite number of iterations, since, as we saw in our specific examples, one can learn a great deal about qualitative features of a theory from this information alone. Suppose for illustrative purposes, we assume that there is only one single-site, or potential, coupling constant in a theory. Then, defining y to be the ratio of the strength of the single-site coupling to the gradient term, we can plot the general form of the function R(y) = (change of y in finite number of iterations) as defined in (3.22); viz., $R(y_N) = y_{N+1} - y_N$. A few examples of simple forms for R(y)

are given in Figs. 8a-8c and lead to different conclusions about the theories they are assumed to characterize.

In Fig. 8a we see that $R(y) \geq 0$ for all values of $0 \leq y \leq \infty$. If a theory has this form for R(y) we can conclude two things. First, the points y=0 and y=∞ are the only fixed points of the theory. The Hamiltonian at y=0, i.e., zero coupling constant, is a "free field theory," and can presumably be solved exactly. The y=∞ Hamiltonian becomes the single-site Schrœdinger problem with neglect of the gradient terms. Second, we observe that if we start at some finite value of y successive iterations drive us to larger value of y; i.e., $R(y) > 0$. Eventually after a finite number of iterations our problem can be studied by treating the gradient terms as a perturbation on the single-site terms. Hence, in any theory for which $R(y) > 0$ we can conclude that the low energy (or long-wavelength) physics is described by an effectively strong-coupling constant Hamiltonian. It follows from this discussion that the mass gap in such a theory will be given by calculating the gap between the first two eigenstates of the effective single-site Schrœdinger problem. The gap is thus a function of the effective single-site coupling $g_\infty$, where the subscript denotes the many iterations $N \gg 1$ to reach the strong coupling behavior. In general, since the scale of H is set by the cutoff $\Lambda$, this means that the lowest mass gap in the theory will be $\approx \Lambda g_\infty$. However, the scale of physical masses should be negligible with respect to the maximum momentum $\Lambda$ if we are to retain practical Lorentz invariance for the low lying eigenstates in spite of our cutoff procedure. Therefore we are only interested in theories for which $g_\infty \ll 1$, or in other words, $g_\infty \Lambda$ finite (and perhaps ≈1 GeV).

Generally the Hamiltonian at a fixed point reproduces itself up to a scale factor $\rho$, and after N iterations the overall scale of $H_N$ is $\Lambda \rho^N$. Since this

should be finite ($\approx 1$ GeV) this suggests that the question of the practical relativistic invariance of a theory for which R(y) behaves as in Fig. 8a can be settled by computing the scale parameter $\rho$ in the y=0 limit. If we find $\rho < 1$ then we can take the cutoff $\Lambda \to \infty$ and still keep the masses of the lowest states finite if we choose the original bare coupling constant $g_0$ to tend appropriately to zero as a function of increasing $\Lambda$. This is an example of a theory whose short distance behavior is "free" but whose long wavelength behavior is not.

If we next look at R(y) for Fig. 8b we come up with the opposite conclusion. If $R(y) < 0$ each successive set of N-iterations will make it smaller. Hence the large wavelength or low energy physics of this theory is given by weak coupling perturbation theory, whereas the single-site or short distance behavior is governed by a strong coupling constant.

Figure 8c tells us that the two different cases can occur depending upon the starting value for y, i.e., whether $y_0 < y_c$ or $y_0 > y_c$. This is just the form of R(y) calculated for our Ising model in Fig. 4 and one can refer back to the exact solution of this theory[5] to see how an effectively relativistic theory emerges.

The use of the function R(y) to catalogue types of theories has its analogue in the study of the renormalization group equations in momentum space, where one encounters the well known $\beta(g)$ function in terms of which the asymptotic behaviors of field theories are described. Both functions, $\beta(g)$ and R(y), describe the change in coupling constant (g or y) as we change the scale of distance in the theory. The two functions are complementary to one another in that we have introduced R(y) here in coordinate space, whereas $\beta(g)$ normally appears in the momentum space analysis of the renormalization group equations. In our renormalization group procedure on a lattice we build larger and larger blocks at each state of the calculation so that we are studying the behavior of the theory

at lower and lower momenta. When working in momentum space one normally studies the renormalization group equations by scaling up the momenta to higher and higher values at each stage, and correspondingly to smaller and smaller values of the underlying lattice spacing. In our approach Fig. 8a describes a theory which is asymptotically free (high momenta) and Fig. 8b describes one that is infrared stable. The $\beta$ function has just the complementary behavior as illustrated by Figs. 9 for asymptotically free and infrared stable theories.

In our preceding papers[1] we have systematically studied strong coupling limiting behavior for lattice theories. Their relevance is clear in the light of the above discussion. Our next task is to apply our variational renormalization group approach to fermion and gauge models and to verify in particular if asymptotically free color gauge theories satisfy the folklore based on continuum perturbation theory; i.e., asymptotic freedom at short distances and color confinement at large distances.

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3. Equation (2.3) is the exact continuum cutoff theory result for $\mu >> \pi$ and is reduced by a factor of $8/\pi^2 \approx 0.8$ from the exact result as $\mu \to 0$ because of the approximation of the gradient operator by nearest neighbor differences. In I the lattice gradient leading to an exact free particle dispersion relation, $\omega_k = \sqrt{\mu^2 + k^2}$, was introduced and can be used here also as we shall describe shortly.

4. As is generally known the Ising model Hamiltonian represents an approximation to the $\phi^4$ field theory in the 1x-1t dimension if we are far into the spontaneously broken symmetry region with strong coupling. To show this we write this theory on the lattice in terms of dimensionless canonical variables and using the nearest neighbor gradient:

$$\frac{1}{\Lambda} H = \sum_{j=-N}^{N} \left[ \frac{1}{2} p_j^2 + \lambda_0 \left( x_j^2 - f_0^2 \right)^2 + \frac{1}{2} (x_j - x_{j+1})^2 \right]$$

The lowest two eigenlevels of the single-site Schrœdinger problem (neglecting the gradient term) lie deep in the potential well if the zero point energy is very small compared with the height of the center bump; i.e.,

$$\lambda_0^{1/2} f_0 \ll \lambda_0 f_0^4 \qquad \text{(a)}$$

These two low lying levels are, respectively, symmetric and antisymmetric under reflection. The energy gap between them is proportional to the tunneling between the two minima in the double-bottomed potential $\lambda_0 \cdot \left( x_j^2 - f_0^2 \right)^2$ at $\pm f_0$. Since condition (a) means that there is very little tunneling this gap is very small—i.e.,

$$\Delta \mathscr{E}_{gap} \sim \lambda_0^{1/2} f_0 e^{-\lambda_0^{1/2} f_0^3} \ll \lambda_0^{1/2} f_0 \qquad \text{(b)}$$

if $\lambda_0^{1/2} f_0^3 >> 1$. When conditions (a) and (b) are satisfied we can neglect higher excitations at each lattice site. The two states retained correspond to the spin down and up configurations in the Ising model (3.1). The gradient term induces mixing between the symmetric and antisymmetric solutions which is approximately given by

$$<\text{sym}|x_j|\text{antisym}>^2 \approx f_0^2 \qquad \text{(c)}$$

When this mixing is comparable to the gap separating the levels—i.e., for

$$\lambda_0^{1/2} f_0 e^{-\lambda_0^{1/2} f_0^3} \approx f_0^2 \qquad \text{(d)}$$

the gradient term is comparable to the single site terms and we can make neither a weak nor strong coupling limiting approximation. Condition (d) requires $f_0^2 \ll 1$, $\lambda_0 >> 1$, consistent with $\lambda_0^{1/2} f_0^3 >> 1$.

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## APPENDIX

We sketch here the procedure of Section II applied to the free field Hamiltonian transcribed to a lattice using (2.14) - (2.15) for the gradient. In place of (2.1) we have

$$H = \Lambda \sum_{j=-N}^{N} \left\{ \frac{1}{2} p_j^2 + \frac{1}{2}(\mu^2 + D(0)) x_j^2 \right\} + \Lambda \sum_{j_1 > j_2} D(j_1 - j_2) x_{j_1} x_{j_2} \qquad \text{(a)}$$

Dividing the lattice into 2-site blocks and repeating the steps leading from (2.7) to (2.10) we transform (a) into

$$\frac{1}{\Lambda} H^{(tr)}(1) = \sum_{\ell} \left\{ \frac{1}{2} \sqrt{\mu^2 + D(0) - D(1)} + \frac{1}{2} p_-^2(\ell) + \frac{1}{2}(\mu^2 + D(0) + D(1)) x_-^2(\ell) \right\}$$

$$+ \frac{1}{2} \sum_{\ell} \sum_{p \geq 1} \sum_{r=0,1} D\left(2^p + r_{\ell+p} - r_\ell\right) x_1(\ell)\, x_-(\ell+p) \qquad \text{(b)}$$

We can now iterate this procedure as we did following (2.10). The ground state energy is built up following the pattern indicated in Fig. A—i.e.,

$$\mathcal{E}_0(\mu) = \left\{ \frac{1}{2} \sqrt{\mu^2 + D(0) - D(1)} \right\} \frac{1}{2}$$

$$+ \left\{ \frac{1}{2} \sqrt{\mu^2 + D(0) + D(1) - \frac{1}{2}\left[D(1) + 2D(2) + D(3)\right]} \right\} \frac{1}{2^2}$$

$$+ \left\{ \frac{1}{2} \sqrt{\mu^2 + D(0) + D(1) + \frac{1}{2}\left[D(1) + 2D(2) + D(3)\right] - \frac{1}{2^2}\left[D(1) + 2D(2) + 3D(3) + 4D(4) + 3D(5) + 2D(6) + D(7)\right]} \right\} \frac{1}{2^3}$$

$$+ \ldots \qquad \text{(c)}$$

The numerically summed series (c) leads to the values quoted in the text.

Table I

| State | Energy | Energy Relative to Lowest State |
|---|---|---|
| $\frac{1}{\sqrt{1+a_0^2}}(\lvert\downarrow\downarrow\rangle + a_0\lvert\uparrow\uparrow\rangle)^* \equiv \lvert\downarrow'\rangle$ | $\epsilon_0 - \sqrt{\epsilon_0^2+\Delta_0^2}$ | 0 |
| $\frac{1}{\sqrt{2}}(\lvert\uparrow\downarrow\rangle + \lvert\downarrow\uparrow\rangle) \equiv \lvert\uparrow'\rangle$ | $\epsilon_0 - \Delta_0$ | $\sqrt{\epsilon_0^2+\Delta_0^2} - \Delta_0$ |
| $\frac{1}{\sqrt{2}}(\lvert\downarrow\uparrow\rangle - \lvert\uparrow\downarrow\rangle)$ | $\epsilon_0 + \Delta_0$ | $\sqrt{\epsilon_0^2+\Delta_0^2} + \Delta_0$ |
| $\frac{1}{\sqrt{1+a_0^2}}(-a_0\lvert\downarrow\downarrow\rangle + \lvert\uparrow\uparrow\rangle)$ | $\epsilon_0 + \sqrt{\epsilon_0^2+\Delta_0^2}$ | $2\sqrt{\epsilon_0^2+\Delta_0^2}$ |

*$a_0 = \left(\sqrt{\epsilon_0^2+\Delta_0^2} - \epsilon_0\right)/\Delta_0$.

FIGURE CAPTIONS

1. Notation for a one-dimensional lattice divided into 2 site blocks. The block is labeled by $\ell$ and the site in each block by r=0, 1. Each point j along the lattice is labeled by $j=2\ell+r$.
2. One and two kink-like excitations on the lattice. These, rather than single particle-like excitations, are the low lying configurations in the "weak coupling" limit, $\epsilon_0/\Delta_0=0$, of Eq. (3.1).
3. Interaction terms between adjacent lattice sites are indicated together with the iteration order, n, in which they are included in $H_2(n)$ in Eq. (3.6).
4. R(y) in Eq. (3.22) is plotted schematically vs. $y=\epsilon/\Delta$ showing the three fixed points at y=0, 2.553, and $\infty$.
5. Comparison of the ground state energy density as a function of y for the exact calculation and for our approximate variational calculation using (4.5).
6. Comparison of the order parameter $\langle\sigma_x(y)\rangle$ vs. y for the exact and approximate variational calculations.
7. Comparison of singularities in the second derivative of the ground state energy density vs. y for the exact and approximate variational calculations.
8. These figures show different behaviors for R(y), the ratio of the single site (binding) to the gradient (kinetic energy) terms in the Hamiltonian with successive steps of iteration; i.e., $R(y_N)\equiv y_{N+1}-y_N$ vs. $y_N=(\epsilon/\Delta)_N$. In (a) R(y) monotonically increases corresponding to a theory whose long wave length (low energy) behavior is given by the strong coupling limit $y\to\infty$ but whose short distance behavior starting at $y\ll 1$ is asymptotically free. In (b) R(y) is monotonically decreasing corresponding to a theory that is asymptotically free at low energy and large distances, i.e., infrared

stable. (c) describes a theory with a finite critical point such that one is driven to strong or weak coupling limits depending on whether the bare coupling is $y_0 > y_c$ or $y_0 < y_c$ respectively.

9. Standard renormalization group results for the $\beta(g)$ function corresponding to asymptotically free (a) and infrared stable (b) theories.

A. Pattern of coupling of different lattice sites using the long range gradient as defined in Eqs. (2.14)-(2.15).

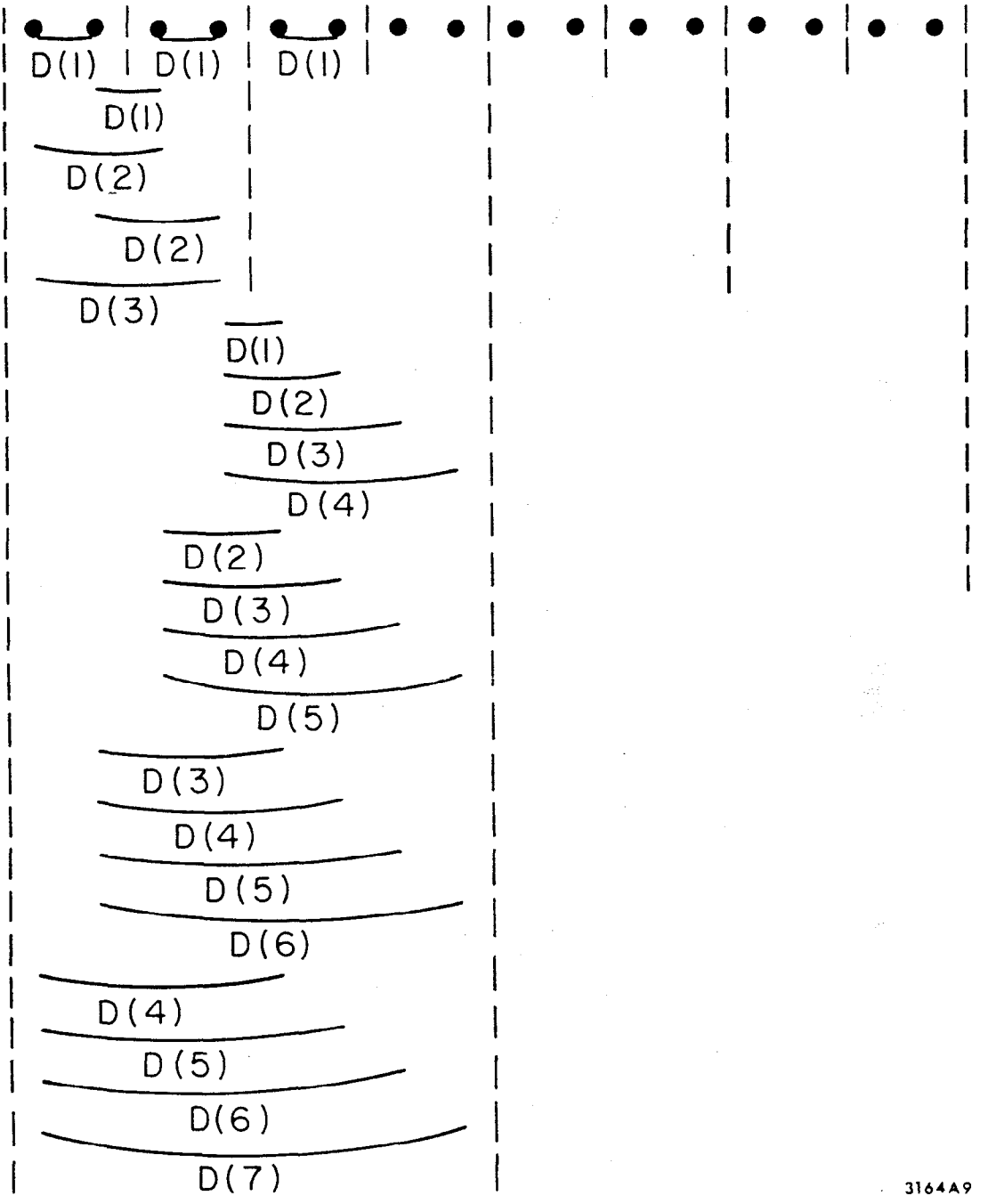
D(1)
D(1)
D(1)
D(1)
D(2)
D(2)
D(3)
D(1)
D(2)
D(3)
D(4)
D(2)
D(3)
D(4)
D(5)
D(3)
D(4)
D(5)
D(6)
D(4)
D(5)
D(6)
D(7)
5-77
3164A9

Fig. A

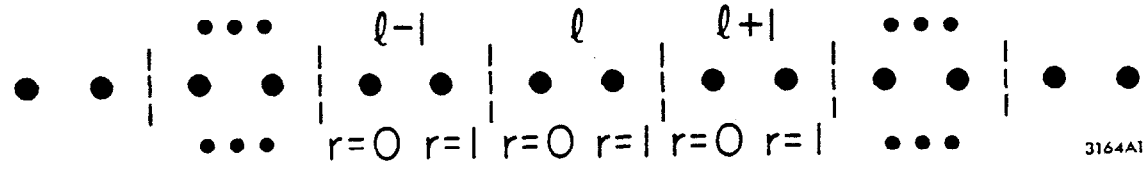


Fig. 1

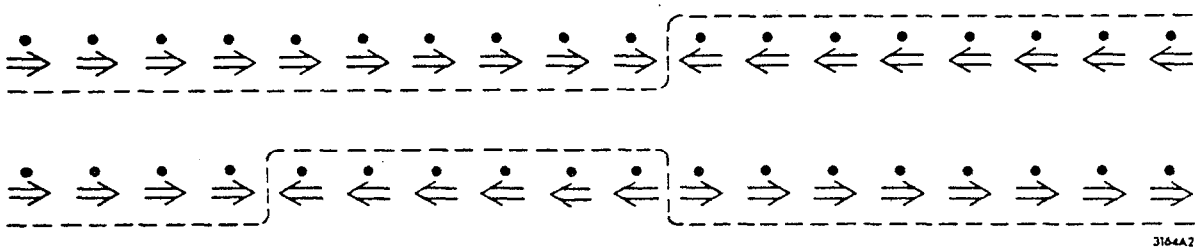


Fig.2

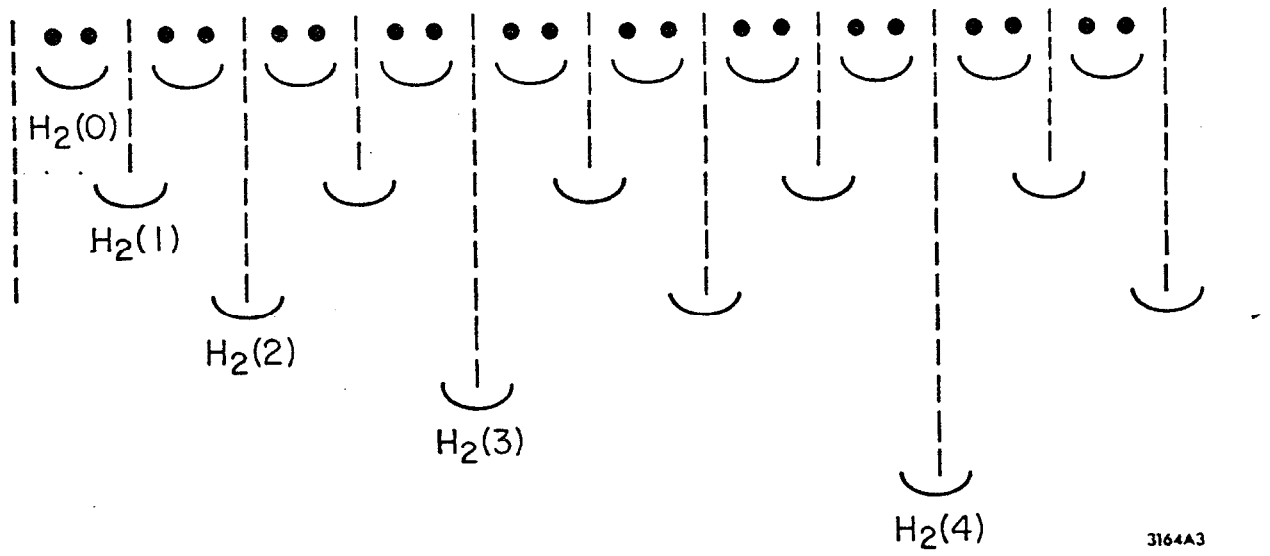


Fig. 3

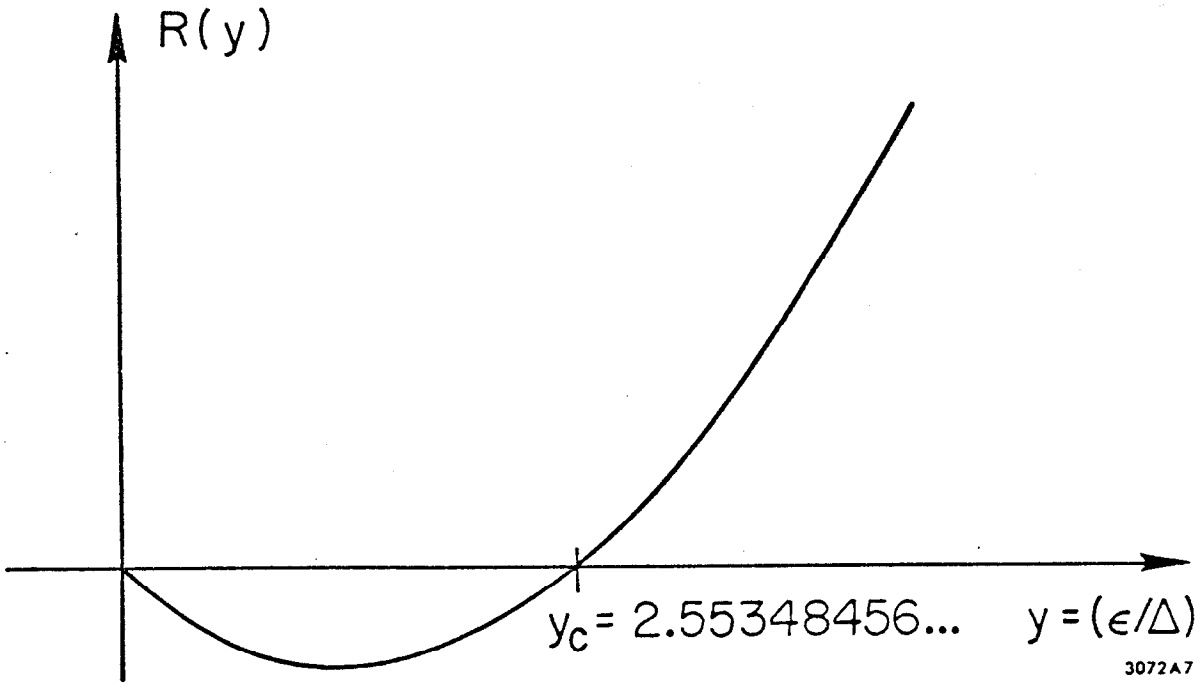


Fig. 4

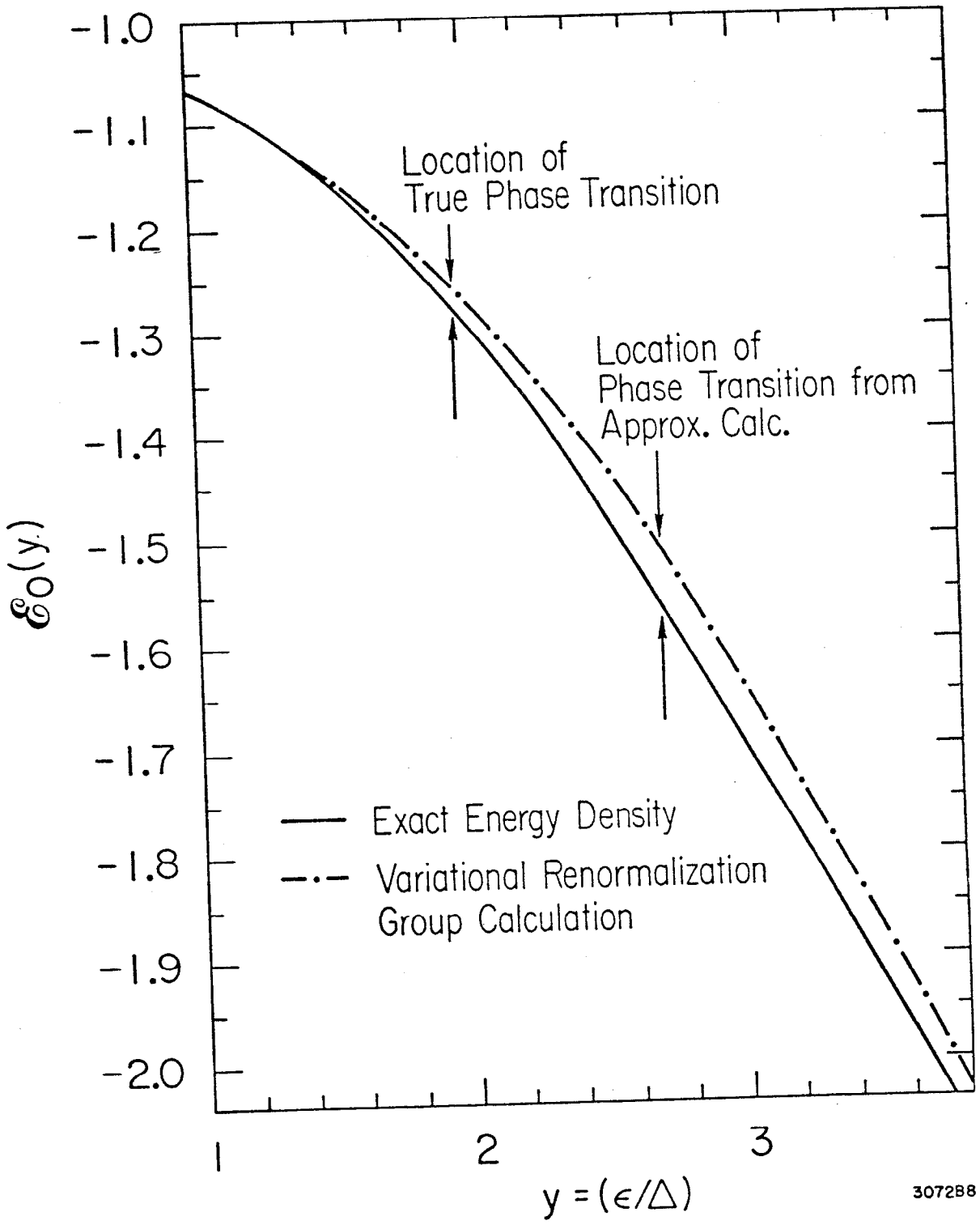
-1.0
-1.1
-1.2
-1.3
-1.4
-1.5
-1.6
-1.7
-1.8
-1.9
-2.0
$\mathcal{E}_0(y)$
Location of
True Phase Transition
Location of
Phase Transition from
Approx. Calc.
Exact Energy Density
Variational Renormalization
Group Calculation
1
2
3
$y = (\epsilon/\Delta)$
307288

Fig. 5

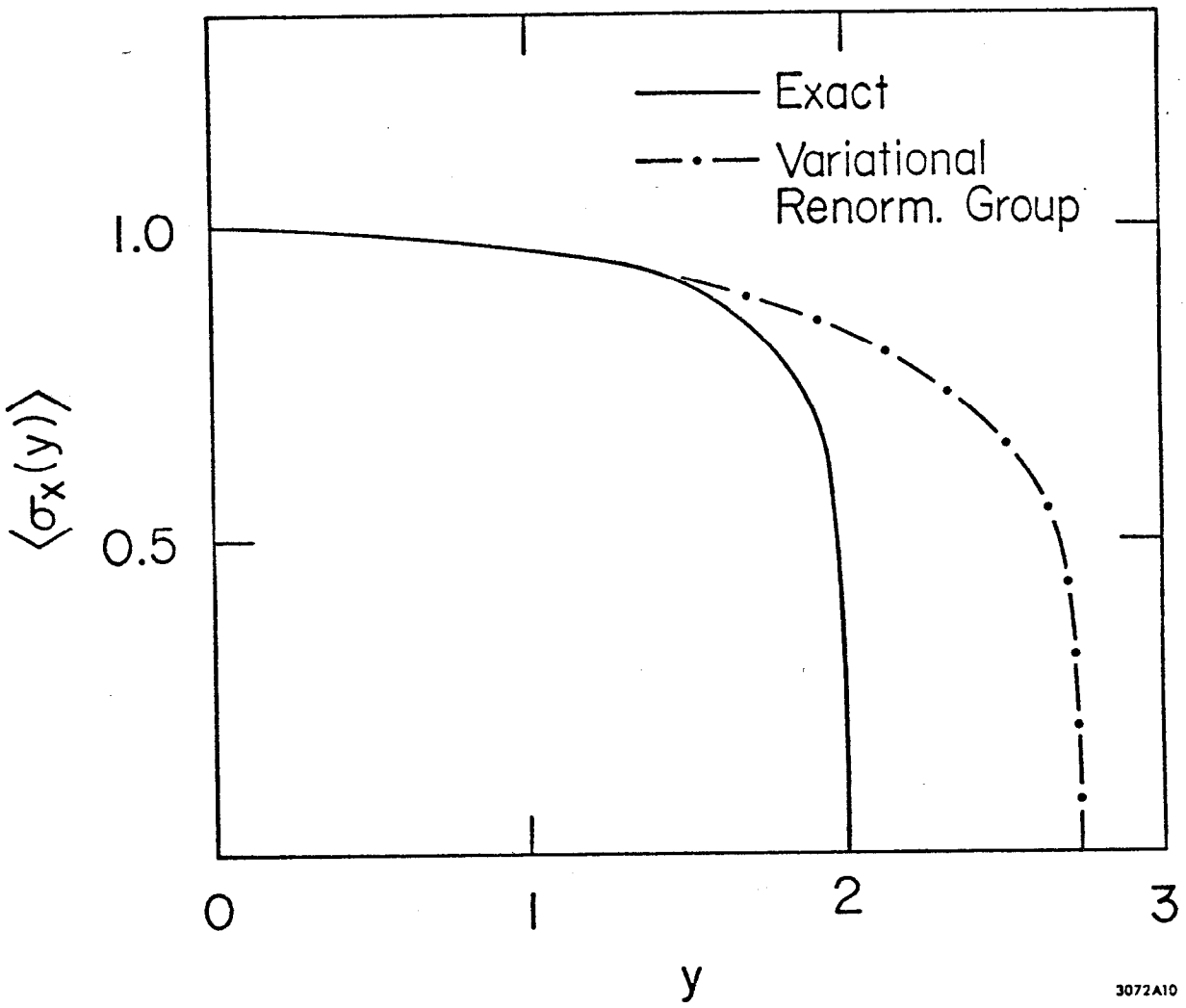
Exact
Variational
Renorm. Group
1.0
0.5
$\langle\sigma_x(y)\rangle$
0
1
2
3
y
3072A10

Fig. 6

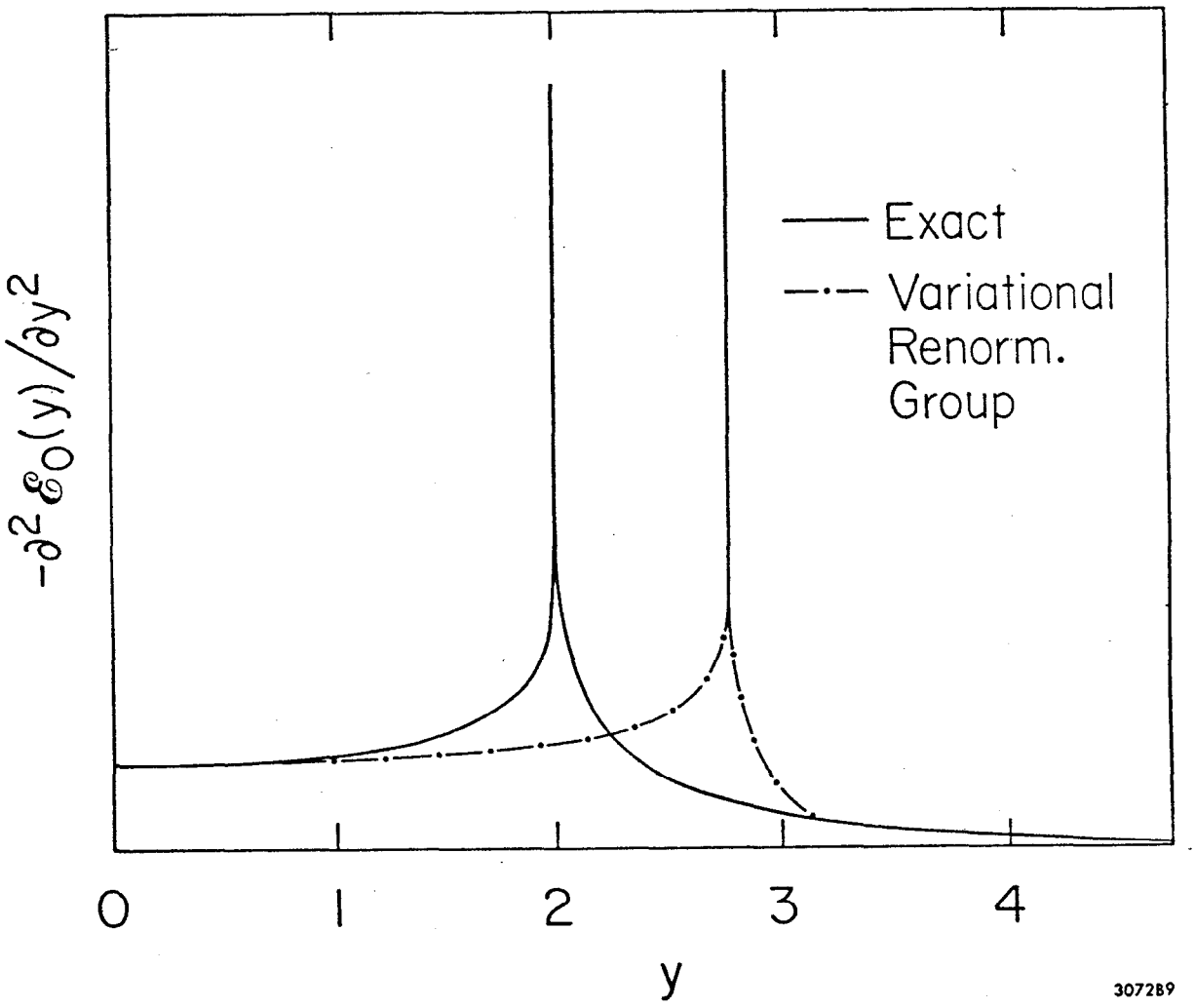
Exact
Variational
Renorm.
Group
$-\partial^2 \mathcal{E}_0(y)/\partial y^2$
0
1
2
3
4
y
307289

Fig. 7

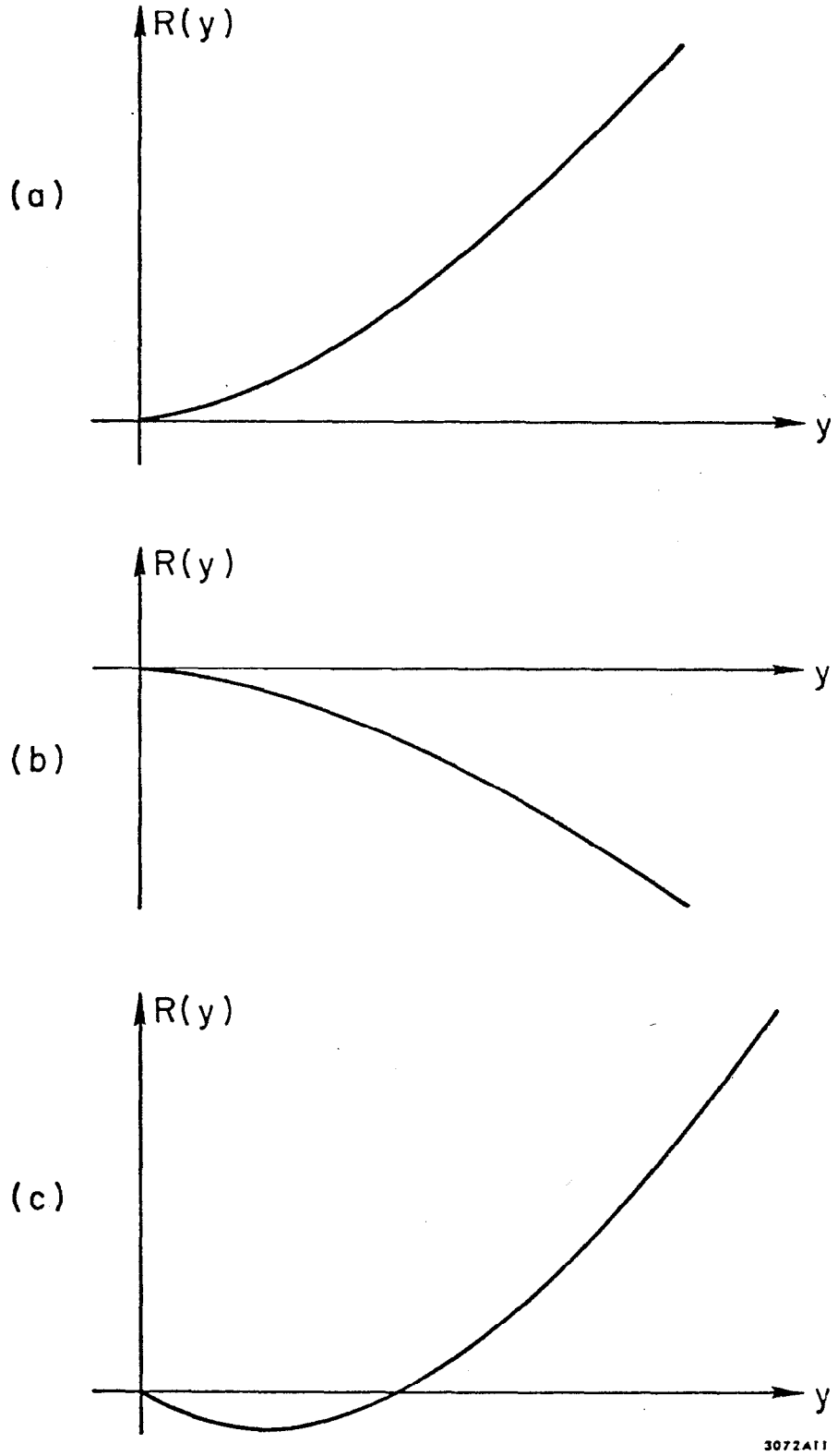


Fig. 8

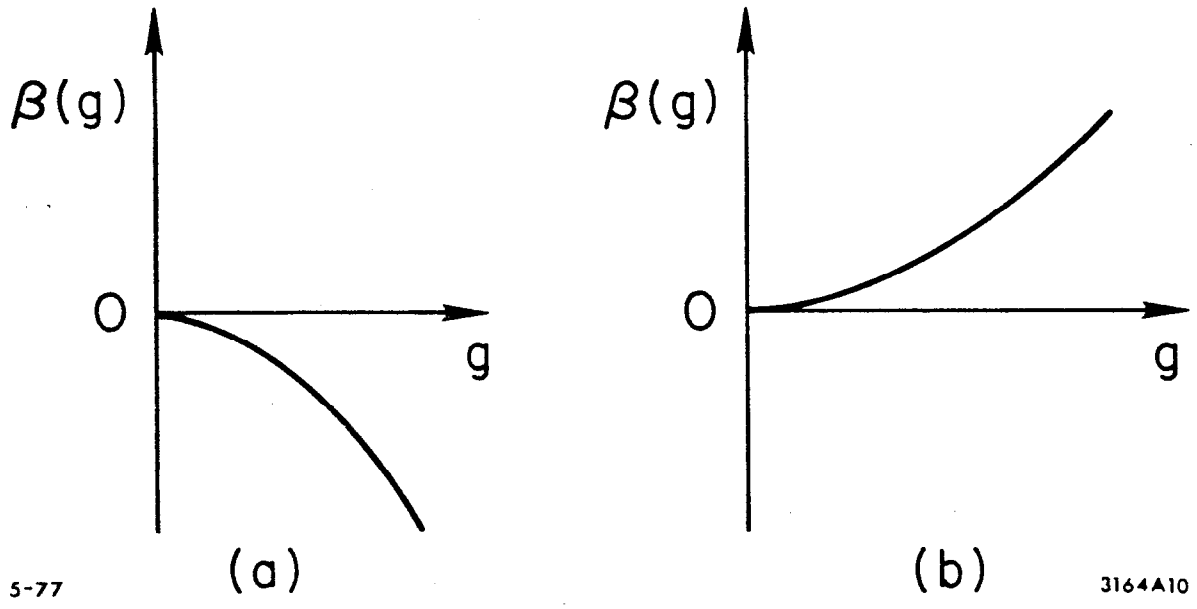


Fig. 9