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The t-EXPANSION: A NON-PERTURBATIVE ANALYTIC TOOL FOR HAMILTONIAN SYSTEMS*

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ABSTRACT

A systematic non-perturbative scheme is developed to calculate the ground-state expectation values of arbitrary operators for any Hamiltonian system. Quantities computed in this way converge rapidly to their true expectation values. The method is based upon the use of the operator e^{-tH} to contract any trial-state onto the true groundstate of the Hamiltonian H. We express all expectation values in the *contracted* state as a power series in t, and reconstruct the $t \to \infty$ behavior by means of Padé approximants. The problem associated with factors of spatial volume is taken care of by developing a *connected graph* expansion for matrix elements of arbitrary operators taken between arbitrary states. We investigate Padé methods for the t-series and discuss the merits of various procedures. As examples of the power of this technique we present results obtained for the Heisenberg and Ising models in 1+1 dimensions starting from simple mean-field wavefunctions. The improvement upon mean-field results is remarkable for the amount of effort required. The connection between our method and conventional perturbation theory is established; and a generalization of the technique which allows us to exploit off-diagonal matrix elements is introduced. This bi-state procedure is used to develop a t-expansion for the ground-state energy of the Ising model which is, term by term, self-dual.

1. INTRODUCTION

It has become clear that analyzing confinement and computing the properties of hadrons requires the development of non-perturbative methods for dealing with quantum field theories. Conventional renormalization techniques require a perturbative framework and so, in order to remove all divergences from the theory, Wilson[1] introduced a lattice formulation of Euclidean gauge-theories which was transcribed into Hamiltonian langauge by Kogut and Susskind If one adopts this formalism the problem becomes one of being able to analyze this sort of theory for all values of the coupling constant. It quickly became clear that strong coupling perturbation theory could not be relied upon to study the physics of the weak coupling limit, i.e. the limit of interest for the continuum theory, and other techniques would be necessary. Up to now much effort has been invested in Monte Carlo calculations in an attempt to systematically compute the quantities of physical interest. The drawback of the Monte Carlo technique is the amount of computer time required to study even small lattices; this, of course, makes it hard to trust these results as guides to the physics of the continuum. Another drawback of the Monte Carlo technique is that it is entirely numerical and one has no way of getting a feeling for what is essential and what is superfluous. In order to obtain information of this nature there would seem to be no substitute for non-perturbative analytic techniques which can be used to systematically study Hamiltonian systems in general. In this paper we present a new non-perturbative scheme which can be applied to a wide class of Hamiltonian lattice theories. While this should be of general interest to people working on many-body and condensed matter problems, we are particularly attracted to the method because it holds great promise of working well for lattice gauge-theories. For pedagogical reasons this paper will focus on some simple Hamiltonian lattice systems in order to present the basic ideas and show how well the approximation scheme converges. The application of these techniques to lattice gauge theories will be presented elsewhere.

In looking for a candidate for a non-perturbative computational scheme applicable to a wide variety of problems, one is tempted to turn to variational methods. There are many variational techniques which allow for non-perturbative calculation of the ground-state, and low-lying excited states, of a Hamiltonian system. The principal virtue of these methods is they allow the computation of effects, such as the existence of phase transitions, which cannot be treated within the framework of ordinary perturbation theory. Their principal drawback is that there is no simple scheme for systematically improving upon the initial result. In the section which follows we will show how to rectify this situation and develop a non-perturbative expansion, henceforth referred to as the t-expansion, which allows one to systematically improve upon the results of any variational, or perturbative, calculation. The application of this method to specific examples shows that successive approximations to quantities of physical interest converge rapidly to their true ground-state expectation values.

We begin by presenting the simple idea behind this scheme and establish the rules for calculating in a general theory. Next, we present the results of applying this technique to some sample problems. After the reader has gotten a feeling for the way in which the technique works, we establish the connection of this method to the usual perturbation expansion, and present a generalization of the basic scheme which may play an important role in the analysis of lattice gauge theories.

2. FUNDAMENTALS

2.1 THE BASIC IDEA

Non-perturbative techniques such as Hartree, Hartree-Fock, mean-field and real-space renormalization group approximations, are variational calculations for the ground-state of a Hamiltonian system. In each case one picks a trial state, $|\psi_0\rangle$, which depends upon a set of variational parameters, $\{\alpha\} = \alpha_1, \ldots, \alpha_n$, and determines the best values for these parameters by minimizing

$$E_0(\alpha_1, \ldots, \alpha_n) = \frac{\langle\psi_0|\ H\ |\psi_0\rangle}{\langle\psi_0|\psi_0\rangle}. \tag{2.1}$$

Assuming that we have chosen such a variational wavefunction we note that the normalized state

$$|\psi_t\rangle = \frac{1}{\langle\psi_0|\, e^{-tH}\, |\psi_0\rangle^{1/2}}\, e^{-tH/2}\, |\psi_0\rangle, \tag{2.2}$$

is, for any finite value of t, a better approximation to the true vacuum. To prove this expand $|\psi_t\rangle$ in eigenstates of H, and observe that

$$e^{-tH/2}\ |\psi_t\rangle = \sum_n c_n\, e^{-\epsilon_n t/2} |n\rangle. \tag{2.3}$$

It follows from (2.3) that the coefficient of the true vacuum state which appears in the expansion of $|\psi_t\rangle$ is larger than in $|\psi_0\rangle$. As long as the initial state $|\psi_0\rangle$ has an overlap with the true ground-state quantities like

$$O(t)\ =\ \langle\psi_t|\, O\, |\psi_t\rangle, \tag{2.4}$$

and in particular

$$E(t)\ =\ \langle\psi_t|\, H\, |\psi_t\rangle, \tag{2.5}$$

are guaranteed to converge to their true ground-state expectation values in the limit $t \rightarrow \infty$. This *contraction* of the wavefunction onto the lowest eigenstate

of the Hamiltonian rapidly eliminates states which have energies far larger than the lowest state and if accurately computed, provides an upper bound upon the ground-state energy for any finite value of t.

2.2 CLUSTER EXPANSION

Focusing on the problem of computing the ground-state energy for a system defined by a Hamiltonian, H, we see that evaluation of (2.2) and (2.5) requires the computation of ratios like

$$E(t) = \frac{\langle\psi_0| He^{-tH} |\psi_0\rangle}{\langle\psi_0| e^{-tH} |\psi_0\rangle}. \tag{2.6}$$

In general, we cannot exponentiate the Hamiltonian of a quantum system, so some way of approximating the ratio must be developed. Our approach is to expand (2.6) to a fixed order in the variable t and then use Padé approximants to reconstruct the function. This method is appealing since computing $\langle\psi_0| OH^n |\psi_0\rangle$, for $|\psi_0\rangle$ belonging to the class of variational wavefunctions under consideration, is straightforward. There is, however, an important conceptual point which must be addressed before plunging into such a calculation. This problem is that for a system of volume V, the expectation value $\langle\psi_0| H^n |\psi_0\rangle$, is proportional to V^n. Since we are interested in the limit $V \to \infty$, there seems to be a problem in defining our approximation procedure.

This problem is familiar from statistical mechanics and is due to the fact that the normalization factor

$$Z(t) = \langle\psi_0| e^{-tH} |\psi_0\rangle, \tag{2.7}$$

is, for a system of volume V, of the form

$$Z(t) = e^{-tV\mathcal{F}(t)}. \tag{2.8}$$

The powers of volume appearing in

$$Z(t) = \sum_{n=0}^{\infty} \frac{(-t)^n}{n!} \langle \psi_0 | H^n | \psi_0 \rangle \tag{2.9}$$

can be taken into account by systematically rearranging terms into a calculation of the function $\mathcal{F}$. Actually, what we want to compute are ratios of the form

$$O(t) = \frac{\langle \psi_0 | e^{-tH/2} O e^{-tH/2} | \psi_0 \rangle}{Z(t)}, \tag{2.10}$$

which must be free of such difficulties. This suggests that expanding (2.10) as a power series in t must yield expansion for $O(t)$, of the form

$$O(t) = \sum_{n} \frac{(-t)^n}{n!} \langle OH^n \rangle^c \tag{2.11}$$

wherein all of the coefficients $\langle OH^n \rangle^c$ have the same volume dependence as O. Pursuing the analogy with statistical mechanics, and for that matter with field theory in general, we refer to the coefficients, O_n^c, as *connected* coefficients. A precise formulation of this result for the case $O = H$ is:

Theorem I: *The ratio* $\langle \psi_0 | He^{-tH} | \psi_0 \rangle / \langle \psi_0 | e^{-tH} | \psi_0 \rangle$ *can be written as*

$$\frac{\langle \psi_0 | He^{-tH} | \psi_0 \rangle}{\langle \psi_0 | e^{-tH} | \psi_0 \rangle} = \sum_{n=0}^{\infty} \frac{(-t)^n}{n!} \langle H^{n+1} \rangle^c$$

where, $\langle H^{n+1} \rangle^c$ *is defined recursively,*

$$\langle H^{n+1} \rangle^c = \langle \psi_0 | H^{n+1} | \psi_0 \rangle - \sum_{p=0}^{n-1} \binom{n}{p} \langle H^{p+1} \rangle^c \langle \psi_0 | H^{n-p} | \psi_0 \rangle$$

Proof: Rewrite the ratio as

$$\frac{\langle \psi_0 | He^{-tH} | \psi_0 \rangle}{\langle \psi_0 | e^{-tH} | \psi_0 \rangle} = \frac{\sum (-t)^n \langle \psi_0 | H^{n+1} | \psi_0 \rangle / n!}{\sum (-t)^m \langle \psi_0 | H^m | \psi_0 \rangle / m!}.$$

Replace the expectation value $\langle\psi_0|\, H^{n+1}\,|\psi_0\rangle$ by

$$\langle\psi_0|\, H^{n+1}\,|\psi_0\rangle = \sum_{p=0}^{n} \binom{n}{p} \langle H^{p+1}\rangle^c \langle\psi_0|\, H^{n-p}\,|\psi_0\rangle.$$

Observe that if we let $n = m + p$, then the p and m sums can be done independently. Grouping terms and cancelling the sums over m appearing in both the numerator and denominator leads to the desired result.

Q.E.D.

This result is easily generalized to the case of an arbitrary operator O. The explicit form for the connected matrix elements appearing in (2.11) are

$$\langle OH^m\rangle^c = \langle OH^m\rangle - \sum_{p=1}^{m} \binom{m}{p} \langle OH^{m-p}\rangle^c \langle\psi_0|\, H^p\,|\psi_0\rangle\,, \tag{2.12}$$

where $\langle OH^m\rangle$ is defined to be

$$\langle OH^m\rangle = \frac{1}{2^m} \sum_{p=0}^{m} \binom{m}{p} \langle\psi_0|\, H^p O H^{m-p}\,|\psi_0\rangle. \tag{2.13}$$

2.3 Pade Approximants

Having obtained $O(t) = \langle\psi_0|\, Oe^{-tH}\,|\psi_0\rangle / \langle\psi_0|\, e^{-tH}\,|\psi_0\rangle$ as a power series in t, we must decide what to do with this information. Our approach is to Padé the series, in order to obtain a good approximation to $O(t)$ over a larger range in t. Since there is more than one way in which to Padé a function, we have to specify the particular strategy which we will adopt.

The obvious approach is to take the series

$$O(t) = \sum_{n=0}^{N} \frac{1}{n!}\, \alpha_n (-t)^n \tag{2.14}$$

and improve it by forming diagonal Padé approximants: diagonal approximants are preferred because we expect the function $O(t)$ to tend smoothly to its exact value as $t \rightarrow \infty$. There are however, several problems associated with this prescription. First, there is the problem of establishing a criterion for determining the maximum value of t for which we can trust the calculation. The natural criterion which comes to mind is that we only trust our calculation over the range in which several Padé approximants agree. Since computation of the (N, N)-Padé approximant requires the series for $O(t)$ to order t^{2N}, we see that restricting ourselves to diagonal Padé approximants requires going to rather high orders in t in order to check the convergence of the calculation. At this point we observe that the use of diagonal Padé approximants is forced only if we hope to extract the $t = \infty$ value of $O(t)$ from our calculation. If, however, we are satisfied with a reliable computation of the same quantity for a finite value of t, then the motivation for restricting attention to diagonal approximants disappears.

There is another method for using Padé approximants which liberates us from the restriction to diagonal approximants, converges better for small values of t and does not preclude extrapolation of the results to $t = \infty$. To motivate this approach let us consider the problem of computing the vacuum energy $E(t)$, defined by

$$E(t) = \frac{\langle \psi_0 | H e^{-tH} | \psi_0 \rangle}{\langle \psi_0 | e^{-tH} | \psi_0 \rangle}. \tag{2.15}$$

Begin by noting that $E(t)$ is a monotonically decreasing function of t. To prove this differentiate (2.15) with respect to t, to obtain

$$\frac{dE(t)}{dt} = -\{ \langle \psi_t | H^2 | \psi_t \rangle - \langle \psi_t | H | \psi_t \rangle^2 \}, \tag{2.16}$$

which is the negative of the expectation value of the positive operator $(H - \langle H \rangle)^2$. This piece of information is very useful since it says that if we Padé the series for (2.16), then we know for sure that the approximation is breaking down if the Padé of the derivative becomes positive. When this happens we have determined

the largest value of t for which we can expect the Padé of the ground-state energy to be reliable. We also know that the derivative (2.16) must be integrable, and so must vanish faster than t^{-1} as $t \to \infty$. This implies that we should restrict attention to $(L, L+M)$–Padé approximants for $M \geq 2$. By integrating the $(L, L+M)$–Padé approximant from 0 to t we obtain a larger set of approximations to $E(t)$ without giving up the ability to extrapolate to $t = \infty$.

There is another advantage to using Padé approximants for the derivative of the function instead of for the function itself. Namely, this method can be expected to accurately reconstruct functions like $E(t)$ over a larger range in t. This happens because the Padé approximant constructs a function with specified asymptotic behavior and a particular Taylor series around $t = 0$. In general, forcing the asymptotic behvior of the function affects its reconstruction even for moderate values of t. However, if we Padé the derivative of the function and then integrate, errors made in reconstructing the derivative for moderate values of t take longer to have an effect upon the reconstruction of the function. Another virtue of this method is that it allows accurate reconstruction of functions whose straightforward Padé approximants fail to converge well[3] ; e.g., $f(t) = \tanh(t)$. We will discuss the significance of this fact in chapter 7. Before continuing with the development of the theory behind this technique, let us turn to a specific example.

3. THE HEISENBERG ANTIFERROMAGNET

3.1 THE MODEL:

As a first test of the application of this formalism let us consider the Heisenberg anti-ferromagnet in 1+1-dimensions. This model is defined by the Hamiltonian

$$H = \frac{1}{4}\sum_i \vec{\sigma}(i)\cdot\vec{\sigma}(i+1)\,. \tag{3.1}$$

Using the Bethe ansatz[4] one can solve this model exactly and show that the ground-state energy density is

$$\mathcal{E}_{exact} = -\ln(2) + 0.25 = -0.4431\,. \tag{3.2}$$

We will now study the application of the method just outlined to the problem of computing $\mathcal{E}(t)$ starting from a wavefunction $|\Psi_0\rangle$ which is a tensor product of single site wavefunctions; i.e., a Hamiltonian mean field state. The particular state we choose is an eigenstate of $\sigma_z(i)$ for every point i, with eigenvalues

$$\sigma_z(i)\,|\psi_0\rangle = (-1)^i\,|\psi_0\rangle\,. \tag{3.3}$$

Since the expectation values of σ_x and σ_y vanish for this choice of wavefunction, the energy density is

$$\mathcal{E}_0 = \frac{1}{V}\langle\psi_0|\,H\,|\psi_0\rangle = -\frac{1}{4} \tag{3.4}$$

which differs by almost a factor of two from (3.2) .

3.2 THE CALCULATION:

In order to compute the term of order t^p in the expansion of $\mathcal{E}(t)$ we must evaluate the expectation values $\langle H^{p+1}\rangle^c$. Thus, the coefficient of the term of order t^0 is just $\langle\psi_0|\,H\,|\psi_0\rangle$, or $-.25$. To compute the term of order t we evaluate

$$\begin{aligned}\langle H^2\rangle^c &= \langle\psi_0|\,H^2\,|\psi_0\rangle - \langle\psi_0|\,H\,|\psi_0\rangle^2 \\ &= \sum_{\substack{i,j\\ \alpha,\beta}} \frac{1}{16}\Big[\langle\psi_0|\,\sigma_\alpha(i)\sigma_\alpha(i+1)\sigma_\beta(j)\sigma_\beta(j+1)\,|\psi_0\rangle \\ &\qquad - \langle\psi_0|\,\sigma_\alpha(i)\sigma_\alpha(i+1)\,|\psi_0\rangle\,\langle\psi_0|\,\sigma_\beta(j)\sigma_\beta(j+1)\,|\psi_0\rangle\Big].\end{aligned} \tag{3.5}$$

At this point the virtue of working with a simple product wave-function becomes obvious; for the particular state which we have chosen,

$$\langle\psi_0|\prod_{p=1,\ldots,n}\sigma_{\alpha_p}(i_p)\,|\psi_0\rangle = \prod_{p=1,\ldots,n}\langle\psi_0|\,\sigma_{\alpha_p}(i_p)\,|\psi_0\rangle \tag{3.6}$$

so long as $i_1 \neq i_2 \neq \cdots \neq i_n$. Hence, the terms in (3.5) for which $i \neq j$ or $j \pm 1$ cancel exactly, leaving

$$\begin{aligned}\langle H^2\rangle^c = \frac{1}{16}\sum_{i,\alpha,\beta}\Big[&\langle\sigma_\alpha\rangle\,\langle\sigma_\alpha\sigma_\beta\rangle\,\langle\sigma_\beta\rangle + \langle\sigma_\alpha\sigma_\beta\rangle\,\langle\sigma_\alpha\sigma_\beta\rangle + \langle\sigma_\beta\rangle\,\langle\sigma_\alpha\sigma_\beta\rangle\,\langle\sigma_\alpha\rangle \\ &- 3\,\langle\sigma_\alpha\rangle\,\langle\sigma_\alpha\rangle\,\langle\sigma_\beta\rangle\,\langle\sigma_\beta\rangle\Big]\end{aligned} \tag{3.7}$$

where the dependence of each of the terms on the points $i, i+1, \ldots$ has been suppressed because of the translation invariance of the trial wave function.

This example exhibits a general feature of a calculation done using a mean-field wavefunction; namely, in this case *connected* means keeping only terms in H^n in which the operators touch one another. One can adopt a graphical notation wherein a link stands for a term $\sigma_\alpha(i)\sigma_\alpha(i+1)$, and then the set of graphs which contribute up to order t^2 are shown in Fig. 1 Clearly the graphs

corresponding to higher order terms in the Taylor expansion in t are obtained by *decorating* the lower order graphs, being careful to take combinatoric factors into account. In this way it is a straightforward problem to generate the various terms of the t-expansion for $\mathcal{E}(t)$.

Before discussing the results obtained from these calculations there is one fact which we should point out, since it greatly simplifies the task of carrying out these calculations. We have just observed that for a mean-field wave function connected matrix elements correspond to terms which are connected in the obvious sense that the all operators touch at least one other operator. This implies that for the example being considered, computing $\langle H^p \rangle^c$ for an infinite lattice and a periodic lattice having only $p+1$ sites, is the same. This is true because only terms which correspond to chains of operators which completely wrap around the lattice distinguish one situation from the other. It follows that one can evaluate the terms of order t^p in our expansion, i.e. expectation values of H^{p+1}, by computing on a finite lattice having $p+2$ sites. This allows us to use a computer to carry out our computation without loss of generality. We emphasize that this trick is very different from calculating exact results for a finite lattice. The finite lattice we use is nothing more than a computational device to allow us to numerically, as opposed to symbolically, exactly compute the terms $\langle H^p \rangle^c$ for the theory defined on an infinite lattice.

By making use of this trick we compute the connected coefficients for the ground-state energy density to order t^7. In Fig. 2 we contrast the results obtained by directly forming diagonal Padé approximants to the energy density, to the results obtained by forming off diagonal Padé approximants to the derivative of the energy density and then integrating. We also plot both the behavior of the Taylor series in the same range and the exact answer. In figure 2 we display all of the diagonal Padés which can be formed with our data, and it is clear their convergence to the exact answer is fairly slow. This should be contrasted with the single curve which shows that many of the off-diagonal Padés agree with one an-

other and converge rapidly to the correct result. Of the integrable approximants which correspond to calculations carried out to order t^7, the 1-5 and 2-4 Padés best approximate the exact answer; i.e., $\mathcal{E}_{15} = -.43982$ and $\mathcal{E}_{24} = -.441892$, versus $\mathcal{E}_{exact} = -.44315$. The fractional errors for these two case are .75% and .27% respectively; this should be compared with Anderson's[6] calculation of this quantity in the spin-wave approximation which is on the order of 4% .

Note that in this example the wavefunction $|\psi_0\rangle$ had no variational parameter associated with it. We will now turn to a second example in order to see how the method works when there is a variational parameter to play with.

4. THE 1+1–DIMENSIONAL ISING MODEL

4.1 THE MODEL

The Ising Model in $1+1$ dimensions has long been used to compare different computational techniques. It is defined by the Hamiltonian

$$H = -\sum_i \sigma_z(i) - \lambda \sum_i \sigma_x(i)\sigma_x(i+1) \,. \tag{4.1}$$

Our mean-field (MF) variational state is a product state

$$|\psi_0\rangle = \prod_j |\theta_j, \phi_j\rangle \tag{4.2}$$

where the single site states $|\theta_j, \phi_j\rangle$ are defined in terms of eigenstates of the operator $\sigma_z(j)$ to be

$$|\theta_j, \phi_j\rangle = \cos(\tfrac{1}{2}\,\theta_j)\,|\,\sigma_z(j) = 1\,\rangle + e^{i\phi_j}\sin(\tfrac{1}{2}\,\theta_j)\,|\,\sigma_z(j) = -1\,\rangle \,. \tag{4.3}$$

If we choose θ and ϕ to be constants, independent of the point j, it follows that

$$\begin{aligned} z &= \langle\sigma_z\rangle = \cos\theta \\ x &= \langle\sigma_x\rangle = \sin\theta\cos\phi \\ y &= \langle\sigma_y\rangle = \sin\theta\sin\phi \end{aligned} \tag{4.4}$$

The MF approximation amounts to

$$\langle\psi_0|\, H\,|\psi_0\rangle = -V\,(z+\lambda x^2)\,. \tag{4.5}$$

Note, that y does not appear here and so must be chosen to vanish (which also means $\phi = 0$) in order to minimize (4.5) . Minimization of (4.5) with respect to θ gives a disordered phase ($x = 0, z = 1$) for $0 \leq \lambda \leq 1/2$ and an ordered phase with a broken symmetry ($x \neq 0$) for $\lambda \geq 1/2$. It is known from the exact solution to this model that the model has a second order phase transition between these phases located at $\lambda = 1$. This differs by factor of 2 from the location of the phase transition predicted by the mean field approximation. In addition to missing the location of the phase transition the mean field approximation also fails to give correct critical indices, and only gives a good approximation to the energy density for $\lambda > 1$, i.e. deep within the ordered phase.

4.2 The Contraction Operator Calculation

Applying our method we find the following first few terms of the perturbative energy density by calculating the connected matrix elements of H

$$\begin{aligned}\mathcal{E}^{(2)}_{\text{Taylor}} = &-(z+\lambda x^2) - t[1 - z^2 - 4\lambda x^2 z + \lambda^2(1 + 2x^2 - 3x^4)] \\ &+\tfrac{1}{2}\,t^2\,[-2(z^3 - z) - \lambda(18z^2x^2 - 4x^2 - 2y^2) \\ &\qquad - \lambda^2(36zx^4 - 16zx^2 - 4z) - \lambda^3(20x^6 - 24x^4 + 4x^2)]\ .\end{aligned} \tag{4.6}$$

It is interesting to note that y dependence shows up for the first time in the λt^2 term and is quite insignificant. For all practical purposes one may choose $y = 0$. This continues to be true even to the next few orders in t.

Using (4.6) one can evaluate the 1-1 Padé approximant. This alone causes a considerable shift of the critical point. However, in order to do better, we would like to compute higher Padé approximants. To avoid the complexity of

a hand calculation we again turn to the computer in order to evaluate the desired connected matrix elements. As before this is done by computing connected coefficients for a theory defined on a finite lattice. In what follows we work to order t^6 and therefore must compute $\langle H^7 \rangle^c$. This means that for our numerical calculation we work on a lattice with eight sites. The computation was carried out for various values of the parameter θ; the resulting Padé approximants are studied for fixed t as functions of θ. However, before discussing the results of these computations there is an important technical point which should be made which relates to the question of determining the range in t for which our Padés can be expected to converge.

For the Hamiltonian defined in (4.1), the parameter λ is taken to range over the region $0 \leq \lambda \leq \infty$. A problem which arises at this juncture is that we compute an approximation to $\mathcal{E}(t)$ by terminating a Taylor series at a finite order in t, hence we do not expect the Padé approximants formed from this series to converge for the same range in t for all values of λ. The problem is to find a way of rescaling t so as to minimize this effect. We observe that for $\lambda \gg 1$ the Taylor series to order t^n, which consists of terms up to order λ^{n+1}, diverges strongly as $\lambda \to \infty$. This can be avoided if we rewrite the Hamiltonian, H, so as to compactify the range of the coefficients; e.g., use a Hamiltonian of the form

$$H(\alpha) = -\sum_j \Big[\cos\alpha\, \sigma_z(j) + \sin\alpha\, \sigma_x(j)\sigma_x(j+1) \Big]. \tag{4.7}$$

In fact, it is only necessary to use $H(\alpha)$ in the contraction operator, and continue to evaluate all expectation values as before. The precise way in which we implement this procedure is to let $\cos\alpha = 1/\sqrt{1+\lambda^2}$, $\sin\alpha = \lambda/\sqrt{1+\lambda^2}$ and define $\mathcal{E}(t,\theta)$ to be

$$\mathcal{E}(t,\theta) = \frac{\langle \Psi_\theta | H e^{-tH/\sqrt{1+\lambda^2}} | \Psi_\theta \rangle}{\langle \Psi_\theta | e^{-tH/\sqrt{1+\lambda^2}} | \Psi_\theta \rangle}. \tag{4.8}$$

For fixed t the functions $\mathcal{E}(t,\theta)$ provide a θ - dependent upper bound upon the true vacuum energy. For a fixed value of t we obtain a *best* bound by

minimizing $\mathcal{E}(t,\theta)$ with respect to θ. In this sense, the functions $\mathcal{E}(t,\theta)$ computed for a fixed value of t play the role of *effective potentials*, and we will refer to them as such. Note that since we do not compute the functions $\mathcal{E}(t,\theta)$ exactly, but attempt to reconstruct them using Padé approximants, the functions we plot are not necessarily true bounds. In particular, these potentials are reliable guides to the location of the true minimum in θ only to the degree in which the Padé approximants have converged. For this reason the way in which we extract information from our calculation is to compare the curves obtained by constructing various Padé approximants. We define the range of θ for which we can trust these effective potentials by requiring several Padé approximants to agree. Examples of effective potentials are presented in figures 3-6.

4.3 Discussion of Results

Figure 3 displays results obtained for a value of λ deep in the *ordered* phase. The uppermost dashed curve is $\mathcal{E}(0,\theta)$, which corresponds to the familiar Hamiltonian mean-field calculation. The three curves which appear below it correspond to effective potentials $\mathcal{E}(1,\theta)$, $\mathcal{E}(3,\theta)$ and $\mathcal{E}(5,\theta)$ respectively. Solid lines represent curves obtained by integrating the 0-5 Padé approximant to $d\mathcal{E}(t,\theta)/dt$, and points signify values obtained by integrating the 1-4 Padé approximants. Different symbols have been chosen to indicate the results of the 1-4 Padé approximant for the three different t values. This was done in order to make it easy to see what is happening when the 0-5 and 1-4 Padé approximants no longer agree with one another. Obviously, for figure 3 this is completely unnecessary.

Figure 3(a) exhibits the behavior of the various effective potentials over the entire range in θ, and figure 3(b) shows what these potentials look like when they are magnified to more clearly exhibit the structure of the results in the region of the minimum. These pictures are typical of the behavior seen in the region of $\lambda > 1.5$. In this region the Padés agree with one another to high precision and the location of the minimum of all of the effective potentials is quite close

to the value obtained from the simple mean-field calculation. The actual best values of the energy density,however, become increasingly accurate for larger values of t. The interesting feature of this particular class of curves is the way in which the effective potentials change as we go to larger values of t. Figure 3 clearly exhibits the fact that the greatest improvements in the estimate of the vacuum energy occur for trial states which lie far away from the true eigenstate, and that the total variation of the estimate of the energy density over the entire range in θ gets progressively smaller. This is just what one would expect if our approximation is working correctly, since the result one would obtain for $t = \infty$ should be the completely flat lower dot-dash line, which is simply a plot of the exact ground-state energy density for this value of λ.

Turning to figures 4(a) and 4(b) we see a much more complicated situation. Once again, the dashed curve is the $t = 0$, or mean-field, effective potential; and the three curves lying below it give the effective potentials corresponding to $t = 1, 3$ and 5 respectively. In this figure we see that the 0-5 and 1-4 $t = 5$ Padé approximants strongly disagree with one another for $\theta < 1$. This same sort of disagreement would have been seen in the picture for $\lambda = 10$ had we plotted potentials for t's greater than 5. Presumably, the extrapolation to large t values would be more stable if one calculated to t^8 or t^{10}. This conjecture is supported by 10-site calculations carried out for a much smaller set of θ values.

The most striking feature of the curves shown in figure 4 is the enormous disagreement between the $t = 5$, 0-5 and 1-4 Padé approximants for $\theta < .5$. In fact the 0-5 approximant undershoots the exact energy. As mentioned previously this signifies the breakdown of our approximation since we know that the exact effective potential must be an upper bound on the ground-state energy density for all values of t. From this we see a typical feature of all the calculations, one Padé approximant can be very inaccurate for a range of t and θ, however comparison of several Padés usually allows us to resolve any ambiguity. Figure 4(b) exhibits the complicated structures that can occur in any one Padé approximant.

Note that a reliable estimate of the energy density comes from the point where the various approximations agree. Had we plotted effective potentials for more values in the region $0 \leq t < 3$ we would have seen that the minimum for each of these functions would be contained in the interval $1.19 < \theta < 1.4$. When the curves split apart the different approximants develop secondary minima. When this starts to happen one has no reliable way to choose among them. The most cautious approach in this event would be to limit the value of t which one uses to be less than or equal to the first t value at which the splitting occurs. Inspection of figure 4(b), however, shows that one can be somewhat bolder. Namely, one can follow the minimum through increasing t values, then choose the best approximation for larger t-values to be the value of $\mathcal{E}(t)$ at the point at which the various Padés continue to agree. In this way, one is able to reliably extend the calculation to higher values of t than the straightforward approach would allow. Note, that in figure 4(b) the best point according to this criterion is a local extremum for some of the Padés .

Figure 5 exhibits the same set of curves for the critical value $\lambda = 1$. Now, if we follow the minimum in through increasing values of t we find that the reliable region corresponds to $\theta \leq 1$. There is nothing particularly striking about these curves. The only point worth making is that for $t < 5$ the minimum occurs for a non-zero value of θ; hence, this calculation incorrectly predicts the critical point of the theory to be below 1.

The last set of effective potentials diplayed in Fig. 6are typical of the region $.5 \leq \lambda \leq .9$. We see that for $t \geq 3$ the minima of the various effective potentials all move to $\theta = 0$. In fact, more careful study shows that if we limit ourselves to $t = 3$, then the phase transition occurs for $\lambda \sim .9$. Since we know that the mean-field transition occurs at $\lambda = .5$, the minimum of all Padés must be at $\theta = 0$ in the region $0 \leq \lambda \leq .5$. As before, the values of $\mathcal{E}(t)$ at the minimum improve with increasing t. Considering that we have only computed our expansion to order t^6, we feel that these results represent a significant improvement over mean-field

results for a modest effort. This improvement is made much more striking if we compare these results to what is obtained by using more complicated block-mean field or real-space Hamiltonian renormalization group techniques; these methods require one to work very hard to get results which are not this good.

Having discussed the various effective potentials, we will now explain how we obtained our values for the ground-state energy density, magnetization, etc.. In figure 7 we exhibit the energy density obtained from the 1-4 Padé evaluated for $t = 3$. The choice of the 1-4 Padé versus the 0-5 Padé is completely arbitrary, since for this value of t the difference between the two functions at the minimum is on the order of a few times 10^{-4}. Obviously, errors of this magnitude are not visible on the plot shown in figure 7. It is obvious that the agreement between this calculation and the exact answer is quite good. In fact, over most of the range $0 \leq \lambda \leq \infty$ the relative difference between our calculation and the exact answer is on the order of 10^{-4}, and it grows to $4 \cdot 10^{-3}$ in a very narrow region surrounding the point $\lambda = .9$. This small discrepancy shifts the singularity of the second derivative of the energy density (i.e., the specific heat) from $\lambda = 1$ to $\lambda \simeq .9$.

The last two curves are plots of our computation of the magnetization; i.e., the expectation value of the operator $\sum\langle\sigma_x(j)\rangle/V$ computed according to equations (2.11), (2.12) and (2.13). The crosses in figure 8 corresponds to the values of the magnetization computed for asymptotic t, i.e. values of t for which the magnetization has become a constant. Since the 0-5 and 1-4 Padés agree with one another to an accuracy which would not be visible on the plot we do not bother to indicate which is plotted. The solid curve shown in figure 8 is a plot of the function

$$M(\lambda) = \left(1 - \left(\frac{.87}{\lambda}\right)^2\right)^{.18} \tag{4.9}$$

which is to be compared to the dot-dash curve which is the exact magnetization

as a function of λ i.e.

$$\frac{1}{V}\sum_j \langle \sigma_x(j) \rangle = \left(1-(1/\lambda)^2\right)^{.125}. \tag{4.10}$$

The crosses in figure 9 present the same data, except that we are plotting $\log M(\lambda)$ versus the variable $\log\left(1-(\frac{.87}{\lambda})^2\right)$. The solid curve is a straight line of slope .18 chosen to pass exactly through the point in the lower left hand corner of the graph. It is clear from this graph that it fits a power law of the type (4.9).

While the results presented in this section are by no means in perfect agreement with the exact answer for the 1+1-dimensional Ising model the reader should recall that they are to be compared to the results of the mean-field expansion which predicts a phase transition at $\lambda_c = 0.5$ and a magnetization, $M(\lambda)_{MF}$ which is given by

$$M(\lambda)_{MF} = \left(1-\left(\frac{0.5}{\lambda}\right)^2\right)^{.5}. \tag{4.11}$$

By computing out to sixth order in t we are able to significantly improve these predictions in a systematic way.

5. TWO PARAMETER EXPANSIONS

5.1 THE CONNECTION TO PERTURBATION THEORY

The contraction technique we have introduced is based upon expanding in a parameter t which does not appear in the Hamiltonian. Therefore, it is applicable even when there is no identifiable small parameter which can be exploited to develop the more familiar perturbation expansion. Nevertheless there are situations, such as in the case of the 1+1–dimensional Hamiltonian Ising model, where such an identifiable parameter does exist and so one is tempted to ask how our method relates to more familiar techniques. This section has two purposes: first, we will establish the precise connection between our expansion and the usual perturbative expansion; second, we will indicate the way in which one can exploit this connection to simplify the problem of computing connected coefficients for a class of interesting problems.

Begin with a Hamiltonian

$$H = H_0 + xV \tag{5.1}$$

where x is to be identified with the small parameter appearing in the usual perturbation expansion. The operator H_0 is referred to as the *unperturbed Hamiltonian*, and its complete set of eigenstates will be denoted as $|\phi_n\rangle$, with eigenvalues E_n^0. In particular, the lowest eigenstate of H_0 will be denoted by $|\phi_0\rangle$. For the case of the Ising model discussed in the preceding section x is to identified with λ or $1/\lambda$ depending upon whether we are considering the weak or strong-coupling expansion. Since the connected coefficient of the term of order t^n in our expansion for the ground-state energy density is obtained by computing expectation values of $(H_0 + xV)^{n+1}$, it is obvious that each term of order t^n is a polynomial of order $n+1$ in the parameter x. Hence, it follows that our series can be rewritten as

$$E(t) \equiv E(x,t) = \langle H_0 \rangle + \sum_{n,p=0}^{\infty} \frac{(-t)^{n+p}}{(n+p)!} x^{n+1} \langle H_0^p V^{n+1} \rangle^c, \tag{5.2}$$

where the symbol $(H_0^p V^{n+1})^c$ stands for the appropriate sum of connected matrix elements. The next question is, how must this series be resummed in order to obtain the usual perturbation expansion. To do this in the most straightforward manner we will present the discussion in a way which directly parallels the usual development of a perturbation expansion.

To establish the connection between our contraction formula and perturbation theory in x we consider the operator $e^{-tH/2}$ applied to the lowest eigenstate of H_0, $|\phi_0\rangle$; i.e., consider ratios of the form

$$O(t) = \frac{\langle\phi_0| e^{-tH/2} O e^{-tH/2} |\phi_0\rangle}{\langle\phi_0| e^{-tH} |\phi_0\rangle}. \tag{5.3}$$

For now focus on the energy $E(t)$ which can be written as

$$E(t) = \frac{\langle\phi_0| H e^{-tH} |\phi_0\rangle}{\langle\phi_0| e^{-tH} |\phi_0\rangle}. \tag{5.4}$$

In analogy with the construction of the interaction representation we define the operator

$$U(t, t_0) = e^{tH_0} e^{(t_0 - t)H} e^{-t_0 H_0}. \tag{5.5}$$

This is not a unitary operator, as in the Schrödinger problem, however it does obey the same group property

$$U(t_1, t_2) U(t_2, t_3) = U(t_1, t_3). \tag{5.6}$$

The operator $U(t) \equiv U(t, 0)$ satisfies the differential equation

$$-\frac{dU(t)}{dt} = xV(t)U(t) \tag{5.7}$$

where

$$V(t) = e^{tH_0} V e^{-tH_0}. \tag{5.8}$$

The solution to (5.7) is the time-ordered exponential

$$U(t) = Te^{-x\int_0^t V(\tau)d\tau}. \tag{5.9}$$

Expanding $U(t)$ in x one obtains a power series in x whose coefficients are complicated functions of t. It follows from (5.7) that the function $E(t)$ is simply

$$E(t) = \frac{\langle\phi_0|\, He^{-tH}\,|\phi_0\rangle}{\langle\phi_0|\, e^{-tH}\,|\phi_0\rangle} = E_0^0 + x\frac{\langle\phi_0|\, V(t)U(t)\,|\phi_0\rangle}{\langle\phi_0|\, U(t)\,|\phi_0\rangle} \tag{5.10}$$

Substituting the Taylor expansion for $U(t)$ in both the numerator and denominator of (5.10) we obtain an expression for $E(t)$ which suffers from the the same problem addressed by Theorem I, namely the coefficients of x^n diverge as V^{n+1}. The solution of this problem proceeds as before; we observe that the ratio (5.10) must, term by term as a power series in x, be free of all volume divergences. Hence, we know that

$$\frac{\langle\phi_0|\, V(t)U(t)\,|\phi_0\rangle}{\langle\phi_0|\, U(t)\,|\phi_0\rangle} = \sum_{n=0}^{\infty}\frac{(-x)^n}{n!}\langle V^{n+1}(t)\rangle^c \tag{5.11}$$

where each *connected* matrix element appearing on the right hand side of (5.11) is proportional to one power of the volume. Once again, connected matrix-elements are defined recursively by

$$\begin{aligned}\langle V^{n+1}(t)\rangle^c =& \langle\phi_0|\, V(t)T(\int_0^t V(\tau)d\tau)^n\,|\phi_0\rangle \\ &- \sum_{p=1}^{n}\binom{n}{p}\langle V^{n+1-p}(t)\rangle^c\langle\phi_0|\, T(\int_0^t V(\tau)d\tau)^p\,|\phi_0\rangle.\end{aligned} \tag{5.12}$$

We have now established two equivalent expansions for $E(x,t)$; namely,

$$E(x,t) = E_0^0 + x\sum_{n=0}^{\infty}\frac{(-x)^n}{n!}\langle V^{n+1}(t)\rangle^c = \sum_{n=0}^{\infty}\frac{(-t)^n}{n!}\langle H^{n+1}(x)\rangle^c. \tag{5.13}$$

Expanding $\langle V^{n+1}(t)\rangle$ as a power series in t, and $\langle H^{n+1}(x)\rangle$ as a power series in x we obtain the double power series expansion of equation (5.2). Now, however, we are able to identify the connected matrix element $\langle H_0^p V^{n+1}\rangle^c$ either as the coefficient of t^{n+p} appearing in the expansion of $\langle V^{n+1}(t)\rangle^c$, or as the term of order x^{n+1} appearing in the coefficient of t^{n+p} in our original t-expansion.

We now argue that by inserting a complete set of intermediate states into (5.11) using the recursive definition (5.12) and taking the limit $t \to \infty$ we obtain the familiar perturbation expansion. To see how this works consider the first few terms of the expansion; i.e.,

$$E(x,t) = E_0^0 + x\langle\phi_0|\,V\,|\phi_0\rangle - x^2 \sum_{n\neq 0} |\langle\phi_0|\,V\,|\phi_n\rangle|^2 \frac{1-e^{t(E_0^0-E_n^0)}}{E_n^0-E_0^0} + \ldots \quad , \quad (5.14)$$

where we have inserted a complete set of intermediate states and explicitly carried out the necessary integrations over the τ-variables. It is this integration which converts an expression free of energy denominators into one with such denominators. Taking the limit $t \to \infty$ we see that the decreasing exponential in the term of order x^2 vanishes leaving us with the familiar result of second-order perturbation-theory. Note that expanding this term around $t = 0$ one finds that it starts like t , as it should, and that the energy denominators disappear, as they must, when we expand this result as a Taylor-series in t.

5.2 Exploiting The Double Expansion

Note, that it is often true that V connects $|\phi_0\rangle$ to one, or at most a small number of other eigenstates of H_0. When this happens then it is quite simple to compute the analogue of (5.14) directly and use it to generate the t-expansion. From a computational point of view this observation can greatly simplify the task of computing connected matrix elements for the general t-expansion.

A more important point relating to the general structure of the two parameter expansion has to do with the general question of convergence, both of Taylor

series and sets of Padé approximants. On the one hand, the general t-expansion amounts to first summing over all orders in x corresponding to the same power in t and then constructing Padés to the resulting Taylor series in t. On the other hand, perturbation theory corresponds to summing over all terms multiplied by the same power of x in order to obtain a sum of decreasing exponentials in t; then, taking the limit $t \to \infty$. Which of these procedures can be expected to work best obviously depends upon the region of x and t under consideration. In the region $x \ll 1$, where we might expect perturbation theory to be rapidly convergent, it is in general preferable to use the Taylor-expansion in x, leaving the t-dependence in the form of decreasing exponentials. In this case one is not exploiting the contraction approach at all. However, when x is large and simple perturbation theory in x can no longer be trusted, the contraction approach comes into its own. In addition, perturbation theory is usually only an asymptotic series; the fact that the contraction approach is expected to converge gives us a prescription for resumming the finite t perturbation expansion in order to render it more convergent. We will discuss questions of convergence in chapter 7.

Another point is that there is no reason why the parameter t appearing in our general formulae cannot be replaced by a complex parameter z, so long as we take the limit $\Re(z) \to \infty$. This would correspond to the usual Gell-Mann Low[7] expansion, if we take matrix elements between two different states defined by taking $z = t(\epsilon + i)$ and $z^* = t(\epsilon - i)$. The next section is devoted to the theory of such expansions and we will delay discussion of this point to that section.

Finally we would like to point out that the perturbative technique combines with the variational approach in a straightforward fashion. The trick is to replace the variation of the parameters in $|\psi_0\rangle$ by an equivalent variation of parameters in a "shadow-Hamiltonian";[8-9] i.e., an unperturbed Hamiltonian H_0 whose lowest eigenstate is $|\psi_0\rangle$. This is useful since in a general case it is easier to change parameters in the Hamiltonian than in the wave-function. Another virtue of this approach is that it is often easier to guess, on physical grounds, what operators

(or order parameters) should be varied in H_0; whereas it may be quite difficult to find the correct direction to choose in Hilbert-space. Subtracting the shadow-Hamiltonian from the true Hamiltonian we obtain a separation of the type of (5.1), however in general this no longer leads to a simple perturbation theory and can prove cumbersome in practice. The decision of whether to use the perturbative technique or directly calculate the t-expansion should be made on the basis of the problem to be studied.

6. BI-STATE CONTRACTION SCHEME

To this point we have focused on a contraction scheme based upon taking diagonal matrix elements of operators. This method is powerful and easy to implement for a wide variety of Hamiltonians; nevertheless, there are problems for which it is desireable to be able to compute with off-diagonal matrix elements. For example consider the problem of computing the ground-state energy density or string-tension for a non-abelian lattice gauge theory. For a non-abelian theory there is only one gauge-invariant mean-field state which can be written down, i.e., the infinite coupling vacuum. If we restrict our analysis to diagonal matrix elements and product wavefunctions, then we lose the ability to introduce a variational parameter. As we have already seen, however, without a variational parameter we give up a considerable amount of accuracy. A variational parameter can be introduced by using a mean-field wavefunction which is non-trivial but such a wavefunction is no longer gauge-invariant; hence, we are unable to trust computations of the string-tension, etc., obtained in this way. It is therefore highly desireable to develop a scheme which allows us to introduce a variational parameter without abandoning the explicit gauge-invariance of the computation. The technique which we will now discuss, which exploits two states and computes off-diagonal matrix elements, has this virtue. The application of this approach to the study of lattice gauge-theories is currently under investigation, and will be presented elsewhere. We will show here that this bi-state computational scheme

is useful whenever we can construct a good approximation to the vacuum wave-function of a Hamiltonian system for two widely different values of the coupling constant, because in that case it allows us to construct an expansion about both points simultaneously. As an example of this aspect of the scheme we will show how it can be used to construct an explicitly self-dual series for the energy density of the Ising model in 1+1 dimensions.

6.1 General Formalism

Begin by considering two different states $|\psi_0\rangle$ and $|\chi_0\rangle$. Using either of these states by themselves we can construct the improved states $|\psi_t\rangle$ and $|\chi_t\rangle$, and use them to construct two independent approximations to the vacuum energy; i.e.,

$$E_\psi(t) = \langle\psi_t| H |\psi_t\rangle = -\frac{d(\ln\langle\psi_0| e^{-tH} |\psi_0\rangle)}{dt}, \tag{6.1}$$

and

$$E_\chi(t) = \langle\chi_t| H |\chi_t\rangle = -\frac{d(\ln\langle\chi_0| e^{-tH} |\chi_0\rangle}{dt}, \tag{6.2}$$

both of which have the true vacuum energy as an asymptotic limit. Next consider the expression

$$E_{\psi\chi}(t) = -\frac{d(\ln\langle\psi_0| e^{-tH} |\chi_0\rangle)}{dt}. \tag{6.3}$$

We will refer to this as the bi-state contracted energy. As a matter of convenience we will assume that $|\psi_0\rangle$ and $|\chi_0\rangle$ have been chosen so that $E_{\psi\chi}(t)$ is real. In contradistinction to E_ψ and E_χ, (6.3) is not, by itself, an upper-bound on the vacuum-energy. It is, however, guaranteed to converge to the true energy in the limit $t \to \infty$. To convert this information into a form which does provide a bound we make use of the Schwartz inequality

$$|\langle\psi_0| e^{-tH} |\chi_0\rangle|^2 \leq \langle\psi_0| e^{-tH} |\psi_0\rangle \langle\chi_0| e^{-tH} |\chi_0\rangle. \tag{6.4}$$

Integrating (6.1), (6.2) and (6.3) with respect to t we can solve for the various quantities which appear in (6.4). For example, we find

$$\langle\psi_0|\, e^{-tH}\,|\psi_0\rangle = \langle\psi_0|\,\psi_0\rangle e^{-\int_0^t E_\psi(\tau)d\tau}, \tag{6.5}$$

and analogous expressions for the other matrix elements of e^{-tH}. Inserting them into the Schwartz inequality leads to the result

$$2\Re\int_0^t E_{\psi\chi}(\tau)d\tau + \ln\frac{\langle\psi_0|\,\psi_0\rangle\langle\chi_0|\,\chi_0\rangle}{|\langle\psi_0|\,\chi_0\rangle|^2} \geq \int_0^t (E_\psi(\tau)+E_\chi(\tau))d\tau \geq 2tE_{vac}, \tag{6.6}$$

which tells us that the lefthand side of (6.6) is an upper bound upon the true vacuum energy. In addition, it tells us that this quantity is always greater than or equal to the minimum diagonal approximation to the energy. Having recast the bi-state computation into the form of an upper bound we may exploit this bound by varying the left-hand side of (6.6) to fix the choice of the parameters in $|\psi_0\rangle$ and $|\chi_0\rangle$. Note that it is necessary to integrate to large t-values if one wishes to render the role of the logarithmic term in (6.6) negligible. To do this reliably, however, will generally require computation of many connected matrix elements. If one can extrapolate to large t one may apply the criterion of a stationary point in parameter-space to $2\Re\int E_{\psi\chi}(\tau)d\tau$ directly, although it is not truly an upper bound. In practice there should not be much difference between these two methods for reasonable t values.

The Schwartz inequality (6.4) can also be used to obtain

$$|E_{\psi\chi}(t)| \geq |\langle\psi_t|\, H\,|\chi_t\rangle|. \tag{6.7}$$

The right-hand side is yet another expression that tends to the desired asymptotic limit; which, however, cannot be exploited since our treatment of the cancellation

of volume factors in the t-expansion does not apply to this quantity, whereas it does apply to $E_{\psi\chi}(t)$. We should point out that since our proof of Theorem I did not make use of the state appearing on the left and right hand sides of the expectation value, and in fact did not even require that they be the same state, the result of Theorem I generalizes to the bi-state situation. Hence, all of the tools which we have developed carry over directly. The only change which must be made is that there is an arbitrariness in the definition of connected matrix elements having to do with the normalization one chooses for the states $|\psi_0\rangle$ and $|\chi_0\rangle$. Since these normalizations are arbitrary one may choose, without any loss of generality,

$$\begin{aligned} \langle\psi_0|\psi_o\rangle &= 1 \\ \langle\psi_0|\,\chi_0\rangle &= 1. \end{aligned} \tag{6.8}$$

In this case, all definitions of connected matrix elements are as before except that all operators are to be taken between $\langle\psi_0|$ and $|\chi_0\rangle$.

6.2 Application To The Ising Model

As an example of the application of the bi-state method to a specific problem let us consider our previous example, the Ising model in 1+1 dimensions. In this model we know the form of the vacuum wave-function at opposite extrema of the coupling λ (i.e. strong and weak couplings), the problem is to construct a way of simultaneously interpolating from both ends of parameter space to the region $\lambda = 1$. This kind of extrapolation is just what the bi-state scheme does for us. If we let $|\psi_0\rangle$ and $|\chi_0\rangle$ be the exact strong- and weak-coupling groundstates, respectively, we have a systematic procedure that allows us to approach the true vacuum throughout the entire range of couplings. More specifically we choose these states to satisfy

$$\sigma_3(i)\,|\psi_0\rangle = |\psi_0\rangle \qquad \sigma_1(i)\,|\chi_0\rangle = |\chi_0\rangle \tag{6.9}$$

It is obvious that $|\psi_0\rangle$ is the vacuum of the Ising Hamiltonian

$$H = -\sum_i \sigma_3(i) - \lambda \sum_i \sigma_1(i)\sigma_1(i+1) \tag{6.10}$$

in the limit $\lambda = 0$; and $|\chi_0\rangle$ is one of the two degenerate vacuua in the limit $\lambda = \infty$.

Perhaps the most amusing feature of this application of the bi-state technique is that the t-expansion which is generated has the very interesting property of being term by term self-dual. To our knowledge this is the only systematic expansion which exhibits this discrete symmetry of the exact theory. For non-experts we point out that the duality transformation for the Ising model in 1+1 dimensions amounts to replacing the point- variables σ by another set of Pauli spin-matrices τ associated with the links of the lattice. If one denotes every link by the point to its left, the relations between these two sets of operators should be

$$\begin{aligned} \sigma_3(i) &= \tau_1(i-1)\tau_1(i) \\ \tau_3(i) &= \sigma_1(i)\sigma_1(i+1) \end{aligned} \tag{6.11}$$

It follows that $H(\lambda)$ turns into $\lambda H(\lambda^{-1})$ for the one-dimensional system in which the links (which are dual to the lattice points) form an equivalent system to the one we started with. The duality relation should hold for every energy level of the Hamiltonian

$$E_n(\lambda) = \lambda E_n(\lambda^{-1}). \tag{6.12}$$

Performing the duality transformation on $|\psi_0\rangle$ and $|\chi_0\rangle$ one finds that they interchange their roles. Since in this basis all the matrix elements that we need will be real it follows that they will automatically be self-dual; thus guaranteeing that the resulting energy-function will obey (6.12) .

In our treatment of the Ising model as a bi-state calculation we fixed the two states $|\psi_0\rangle$ and $|\chi_0\rangle$, and therefore have no variational parameters with which

to play. As a result the energy, calculated to the same order in t as in chapter 3, is less accurate over the entire range in λ. There, the biggest error was on the order of 10^{-3} at the phase transition, and on the order of 10^{-4} elsewhere; here, on the other hand, the relative error is on the order of 10^{-3} throughout. Another feature of this result is that to this order in t the calculation does not show a phase-transition. The second derivative of the energy-density, however, does peak at $\lambda = 1$, the self-dual point. This means that consecutive higher orders in t are required to slowly build up the singularity associated with the second-order phase-transition at the correct point.

6.3 Gauge Theories

We expect the bi-state calculational scheme to be particularly useful for local gauge theories. Characteristically such models can be easily solved in the strong-coupling regime, but they are very difficult to tackle in the weak-coupling regime, which happens to be the one of interest. The difficulty arises because local gauge-invariance has to be maintained by the vacuum wave-function. This rules out a mean-link ansatz, that could otherwise be appropriate for the weak-coupling region unless it is properly projected onto its gauge-invariant part. While one can formulate a gauge-projected mean field calculation[10] it is in general prohibitively complicated to implement. The bi-state approach manages to allow us to use non-trivial product wave-functions without going through such a complicated procedure. If one uses the strong-coupling wave-function for $|\psi_0\rangle$, one is free to use any state for $|\chi_0\rangle$ without worrying about its gauge properties. The fact that $|\psi_0\rangle$ and H are gauge-invariant, guarantees that only the gauge-invariant part of $|\chi_0\rangle$ will be involved in the calculation. This provides an enormous simplification of the problem.

A particularly straightforward series is developed if one uses a mean-link state for $|\chi_0\rangle$. In this case, since both $|\psi_0\rangle$ and $|\chi_0\rangle$ have no link-link correlations, we find that connected diagrams are still ones which touch in configuration-

space. With this ansatz the bi-state approach allows for calculations in the weak-coupling regime that were up to now unique to strong-coupling perturbation theory.

6.4 COMPLEX t

Finally let us return to the remark that we are free to choose the parameter t to be a complex variable z. In particular we could choose z to be $z = (i + \epsilon)t$, where epsilon is a small positive real number. In this case the state

$$|\psi(z)\rangle = e^{-t(\epsilon+i)H} |\psi_0\rangle \tag{6.13}$$

becomes the usual time dependent state of the Schroedinger representation in the limit $\epsilon \to 0$. Now let us recall that the usual formulation of perturbation theory for Green's functions, etc. involves the computation of time-ordered products of fields between states $|\psi(t)\rangle$ and $|\psi(-t)\rangle$ in the limit $t \to \infty$. Clearly, this can be thought of as an example of a bi-state calculation take between states $|\psi(z)\rangle$ and $|\psi(z^*)\rangle$, where z is taken as indicated and the limit $\epsilon \to 0$ is to be understood. Aside from the fact that it is always interesting to be able to establish the connections between different approaches, this observation is interesting because it raises the question of whether or not this formalism can be used to calculate scattering amplitudes as well as energy levels. It also raises the question of if the series in the complex variable z and perturbative parameter x can be rendered even more convergent by resumming it in a manner which is different from the one we have used in this paper.

7. ANALYTICITY OF THE t-EXPANSION

Up to now we have discussed the t-expansions as if $E(t)$ and $Z(t)$ are guaranteed to be analytic functions of t, independently of the initial states $|\psi_0\rangle$ and $|\chi_0\rangle$. This is not necessarily the case. If one starts with a wavefunction which is a sufficiently bad approximation to the true ground-state of the system, then $Z(t)$, etc. may be non-analytic. If this occurs it will affect the convergence of the Padé approximants, and so it is important to be aware of this possiblity.

The simplest way to see that this can happen is to expand the state $|\psi_0\rangle$ in a complete set of eigenstates of H; i.e.,

$$|\psi_0\rangle = \sum_n c_n |n\rangle \tag{7.1}$$

and rewrite the norm $Z(t)$ as

$$\begin{aligned} Z(t) &= \langle\psi_0| e^{-tH} |\psi_0\rangle \\ &= \sum_n c_n^* c_n e^{-tE_n} \\ &= \sum_{E_n} e^{-tE_n + S(E_n)} \quad ; \end{aligned} \tag{7.2}$$

$S(E_n) = \log(\sum c_n^* c_n)$ is the sum over all eigenstates of H having energy E_n. This procedure maps the problem of computing $Z(t)$ into the problem of computing the partition function for a classical system at temperature $1/t$, with entropy $S(E_n)$. Thus, if this equivalent classical system exhibits a finite temperature phase transition, then quantities like $\mathcal{E}(t)$ will be non-analytic in t; higher derivatives of this function will exhibit singularities. Obviously, if the c_n's vanish sufficiently rapidly as a function of E_n there will be no problem, the extreme case being that all but a finite number of the c_n's vanish. Our discussion of theories in one spatial dimension was protected from this problem because in one spatial dimension there are no phase transitions at finite temperature.

We hasten to emphasize the fact that while this is a possible problem, this lack of analyticity only manifests itself for some choices of a trial wavefunction; in general, it can be avoided if one chooses a wavefunction with some care. Presumably, this sort of effect will be signaled by the fact that several Padé approximants will exhibit singular behavior at the *same* value of t .

We will now discuss several examples and present a criterion for telling when, within a class of trial wavefunctions, one may encounter non-analyticity in t. This criterion is a conjecture and certainly doesn't have the status of a theorem, but we believe that it generally provides a guide to when we can get into trouble. Our basic aim is to use this criterion to compare lattice spin systems and lattice gauge-theories. We will argue that the spin system can present some difficulties as soon as the dimension of the spatial lattice is greater than or equal to 2. On the other hand, the non-abelian lattice gauge theory can be expected to present no particular difficulties if the spatial dimension of the lattice is less than or equal to 5. We reemphasize that this argument does not mean that one cannot use the t-expansion to analyze spin systems in two and more dimensions; rather, it says that if one does, one has to be more careful in choosing the starting wavefunction for a spin system than for a gauge theory. We conclude with the example of similar problems which can be encountered for a quantum mechanical system with a single degree of freedom. This example is included in order to show how changing the wavefunction can avoid difficulties.

7.1 Spin Models

Consider a higher dimensional spin system of the Ising type; i.e., theories defined by Hamiltonians of the form

$$H = \sum_{\vec{j},\hat{n}} \Big[-\sigma_z(\vec{j}) - \lambda \sigma_x(\vec{j})\sigma_x(\vec{j}+\hat{n}) \Big]. \tag{7.3}$$

As in the 1+1 dimensional Ising model, these theories exhibit ordered and disordered phases. The completely disordered phase corresponds to the case $\lambda = 0$,

and the completely ordered phase to the case $\lambda = \infty$. We denote the vacua of the $\lambda = 0$ and $\lambda = \infty$ Hamiltonians by $|\phi_0\rangle$ and $|\phi_\infty\rangle$ respectively. As in the 1+1 dimensional theory, we can use the general class of mean-field wavefunctions which depend on the single parameter θ to interpolate between $|\phi_0\rangle$ and $|\phi_\infty\rangle$.

We now ask what happens if we attempt to use the contraction technique to construct $|\phi_\infty\rangle$ starting from $|\phi_0\rangle$. More precisely, we wish to compute the t-dependence of the function

$$Z(t) = \langle\phi_0|e^{-tH}|\phi_0\rangle, \tag{7.4}$$

where the state $|\phi_0\rangle$ is defined to be the state for which

$$\sigma_z(i)|\phi_0\rangle = |\phi_0\rangle. \tag{7.5}$$

In effect we want to know if we get the correct ground-state energy, etc., using that wavefunction which lies furthest from the true vacuum. Our conjecture is that if this works, then we can expect our general calculation to be free of trouble. Conversely, if this calculation exhibits a phase transition in t, then we can expect to have problems.

Note that the state, which is an eigenstate of all $\sigma_z(\vec{i})$ with eigenvalue 1, can be rewritten in terms of eigenstates of $\sigma_x(\vec{i})$ as

$$|\phi_0\rangle = \prod_{\vec{i}} \left(\frac{1}{\sqrt{2}}\right)^V \Big[|\rightarrow\rangle + |\leftarrow\rangle\Big], \tag{7.6}$$

where V stands for the number of lattice sites. This product state is, up to the normalization factor of $(1/\sqrt{2})^V$, just a sum over all of the eigenstates of the $\lambda = \infty$ Hamiltonian

$$\tilde{H} = -\sum_{(\vec{i},\vec{j})} \sigma_x(\vec{i})\sigma_x(\vec{j}). \tag{7.7}$$

Hence, we see that with this choice of $|\phi_0\rangle$

$$\begin{aligned} Z(t) &= \langle\phi_0|e^{-t\tilde{H}}|\phi_0\rangle \\ &= \sum_{\substack{m(\vec{i})=-1,1 \\ \langle\vec{i},\vec{j}\rangle}} e^{tm(\vec{i})m(\vec{j})} \end{aligned} \tag{7.8}$$

which is immediately recognizable as the classical Ising model in d-dimensions (where d is the spatial dimension of our lattice).

It is easy to show that in the case of one spatial dimension

$$Z(t) = (\cosh(t))^V \tag{7.9}$$

and

$$\mathcal{E}(t) = \tanh(t); \tag{7.10}$$

which explains our interest in being able to Padé functions of this type. The fact that this function is analytic for all finite values of t is just a specific example of the fact that there are no phase transitions at finite temperature in one dimension. If the spatial dimension of our lattice is 2 or greater, however, then we know that the classical statistical mechanics problem does exhibit a phase transition. Hence, for these theories if one uses the $\lambda = 0$ wave-function to calculate physical quantities one can run into problems with analyticity in t. Presumably, a variational ansatz, is capable of avoiding such problems.

Note that if one chooses for $|\psi_0\rangle$ the wavefunction

$$|\phi_\infty\rangle = \prod_{\vec{(i)}} |\rightarrow\rangle$$

and chooses for $\tilde{H}$ the $\lambda = 0$ Hamiltonian

$$\tilde{H} = \sum_{\vec{j}} \sigma_z(\vec{j}), \tag{7.11}$$

the same sort of argument indicates that there is nothing to worry about. In this case we obtain $\mathcal{E}(t) = \tanh(t)$, as in the case of the one dimensional theory, and everything is completely analytic. Apparently, the difference between these cases is that when starting from the disordered vacuum the contraction operation has no way of choosing between the two possible ordered vacua of $\tilde{H}$. Obviously, if we start from one of the two ordered states and try to contract onto the single totally disordered state the situation will be better. In any event, the lesson we wish to leave the reader with is that one can, if one is not careful, run into problems with analyticity in t; however, simple modifications of the starting wavefunction can in general avoid these problems.

7.2 GAUGE-THEORIES

Let us now apply the same argument to the case of a lattice gauge theory. In this case the basic variables, the fields of the model, are continuous functions taking values on a compact Lie group. We will show that for these gauge theories a t-expansion built upon the simplest strong coupling wave-function can be expected to generate a non-analytic function of t when the spatial dimension of the theory is greater than a critical dimension, d_c. Fortunately, we will find that for an abelian theory $d_c = 4$ and for a non-abelian theory $d_c = 5$. Thus, for the theories of physical interest we do not expect to have any difficulty with the application of our methods in their simplest possible form.

Consider a lattice gauge-theory defined by a Hamiltonian of the form

$$H = \frac{g^2}{2} \sum_{l,\alpha} E_\alpha^2 - \frac{1}{g^2} \sum_p (\mathrm{Tr} U_p + h.c.), \tag{7.12}$$

where l stands for lattice links, and p for plaquettes. Choose for $|\psi_0\rangle$ the wave function which is annihilated by all of the electric field variables. Following the logic used for the spin models let us analyze the zero coupling Hamiltonian $\tilde{H}$ obtained by dropping the E_α^2 term from (7.12). As before this represents

the worst possible mismatch between wavefunction and Hamiltonian, and so our conjecture is that if the $Z(t)$ is analytic in this case it will be analytic for finite g. Evaluating the norm of the contracted state we obtain

$$\langle\psi_0|\, e^{-t\tilde{H}}\, |\psi_0\rangle = \int \prod_l dU_l\, e^{t/g^2 \sum_p (\mathrm{Tr}U_p + h.c.)}, \tag{7.13}$$

which can be immediately recognized as the Wilson action for a Euclidean lattice gauge theory in d–dimensions; recall our problem is assumed to be formulated in $d+1$ space-time dimensions. If the gauge theory under consideration is abelian, then we know that for $d = 4$ the theory exhibits a phase transition; hence, we could expect problems for t-expansion for an abelain theory in five space-time dimensions. For a non-abelian theory the belief is that the Wilson theory does not have a phase-transition below $d = 5$, and so the t-expansion is expected to converge for all theories in the interesting case of four space-time dimensions. Hence, we believe that this method will run into no difficulties for the case of a pure gauge theory in 3+1–dimensions.

7.3 The Anharmonic Oscillator

We will now show that one can run into difficulties even when dealing with quantum mechanical problems of one degree of freedom when the quantum variables of the problem are continuous and non-compact. To see how this occurs, and to see what must be done to avoid it, we consider the anharmonic oscillator. The anharmonic oscillator is defined by a Hamiltonian of the form

$$H = p^2 + x^4\,. \tag{7.14}$$

Clearly, in this example we will run into no difficulties with volume factors, so much of the formalism of connected graphs is not essential. Nevertheless, one still has to divide the expectation value of H by the norm of the improved state, and so the formula is still useful.

Let us choose $|\psi_0\rangle$ to be a Gaussian wave-function, i.e., the ground state of some harmonic oscillator shadow-Hamiltonian

$$\begin{aligned} H_0 &= p^2 + \frac{1}{4}\omega^2 x^2 \\ H_0\psi_0 &= \frac{1}{2}\omega\,\psi_0 \end{aligned} \quad . \tag{7.15}$$

Since ω is directly related to the width of the wave-function we see that we may vary ω so as to obtain the best expectation value for

$$E_0 = \int \psi_0^* H \psi_0 \, dx \; . \tag{7.16}$$

It is a straightforward matter to compute the t-expansion for this problem; unfortunately, the results are quite disappointing since the straight Padé approximants fail to converge well near $t = 0$, and so it is difficult to understand how to continue to larger t's. The difficulty encountered in this calculation can be easily understood if we apply our conjecture and study the properties of the $Z(t)$ which corresponds to contracting an arbitrary gaussian wavefunction using the simplified Hamiltonian $\tilde{H} = x^4$. In this case the problem of computing $\langle\psi_0| e^{-t\tilde{H}} |\psi_0\rangle$ reduces to the computation of an integral of the form

$$\int e^{-tx^4} e^{-\alpha x^2} dx \tag{7.17}$$

which diverges for $t < 0$. This is the problem which the Padé approximants were trying to reproduce, and since it is an effect due to choosing a bad wavefunction no clever modification of the Padé prescription will really be able to rescue the situation.

Clearly, the problem encountered here is simple to solve; one only has to choose for $|\psi_0\rangle$ a wavefunction which vanishes sufficiently rapidly as $x \to \infty$. This is the route that should be chosen for multi-dimensional models with non-compact variables where one has to rely on the t-expansion to deal with problems

associated with factors of volume. However, it is interesting to note that for the simple quantum mechanics problem there exists an alternative to choosing a better behaved starting wavefunction. We will conclude our discussion by presenting this alternative since it is a useful technique for a class of interesting problems.

The fact that the Taylor series for the exponential of the Hamiltonian has no radius of convergence around $t = 0$ does not reflect on the logic of the contraction technique; it merely implies that approximation of e^{-tH} by a power series in t is not possible. There is another approximation of the exponential which can be used in this situation, and that is to approximate it by polynomials, $P_n(t)$ defined by

$$P_n(t) = \left(1 - \frac{Ht}{2n}\right)^n, \tag{7.18}$$

since

$$e^{-tH/2} = \lim_{n\to\infty} P_n(t). \tag{7.19}$$

To use (7.18) and (7.19) we approximate the norm of $|\psi_t\rangle$ by

$$\langle\psi_t| e^{-tH} |\psi_t\rangle \simeq \langle\psi_0|\left(1 - \frac{Ht}{2n}\right)^n |\psi_0\rangle \tag{7.20}$$

and hold $\epsilon = t/2n$ fixed while increasing n. With this prescription the limit $n \to \infty$ coincides with the limit $t \to \infty$.

This approximation has two advantages:

1. Using it in (7.20) yields a positive norm for every value of n.

2. It is free of any singularity in t yet it converges uniformly as $n \to \infty$.

If one computes with this procedure for $\epsilon \lesssim 0.01$ and $n = 20$ one obtains the ground-state energy to fifteen significant figures. The convergence is extremely rapid.

This concludes what we have to say about questions of convergence of the t-expansion, except to emphasize that this is a subject which merits considerably more study.

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FIGURE CAPTIONS

1. Connected diagrams for the Heisenberg anti-ferromagnet up to order t^2.

2. Comparison of various ways for using the t-expansion to obtain the groundstate energy density. The curve marked E^6_{Taylor} is a plot of the Taylor series. The curves (1,1), (2,2) and (3,3) are diagonal Padé approximants. Four curves obtained by integrating the (0,4), (1,4), (1,5) and (2,4) Padé approximants to the derivative of the energy density coincide with one another on this scale, and all have asymptotic values which are very close to the exact answer.

3. (a) Effective potentials for$\lambda = 10$. The curves showing the t=0 (mean field theory), $t = 1$,$t = 3$ and $t = 5$ effective potentials monotonically converge to the exact answer represented by the straight line. Solid curves correspond to the result obtained from the (0,5)-Padé approximant, and symbols indicate the result of using the (1,4)-Padés . The circles mark the curve obtained from the 1-4 Padé approximation to the $t = 1$ data, the crosses mark the 1-4 Padé approximation to the $t = 3$ data, and the sharp-signs denote the results of the 1-4 Padé approximation to the derivative integrated to $t = 5$. (b) Same plots where the region of the minimum is magnified

4. (a) Effective potentials for $\lambda = 1.428$. The notation is as in Fig. 3. (b) This is a magnification of the region around the minimum. Note that the 0-5 and 1-4 Padés for $t = 3, 5$ disagree substantially except at the location of the minimum of the $t = 1$ curves.

5. Plot of effective potentials for $\lambda = 1$.

6. (a) Effective potentials for $\lambda = .833$. Notation as before.Effective potentials for higher t-values have a minimum at $\theta = 0$, indicating a transition to the disordered phase has occured.

7. Energy density from (1,4)-Padé evaluated at $t = 3$

8. Linear plot of magnetization versus λ . The broken curve is the exact result, and the solid curve represents a fit to our calculated values by a function having the same form but with a different exponent and λ_c.

9. A log-log plot of our results for the magnetization

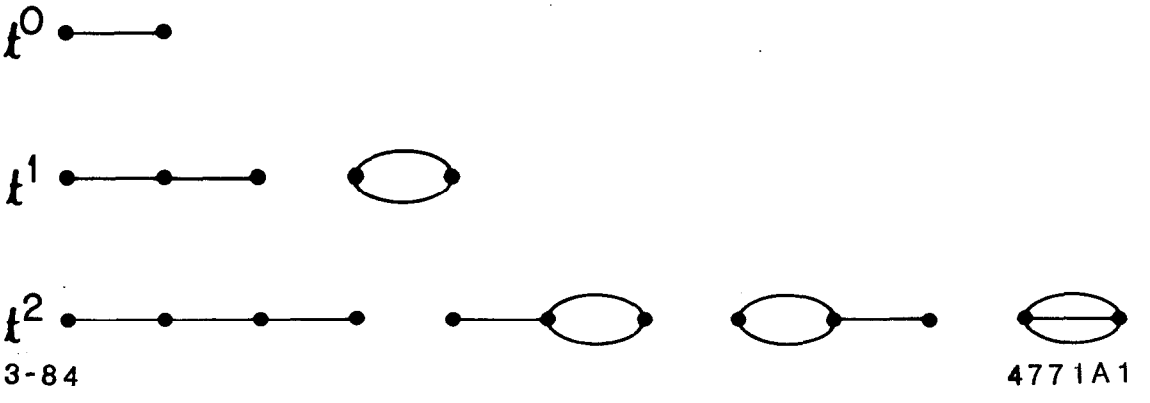

Fig. 1

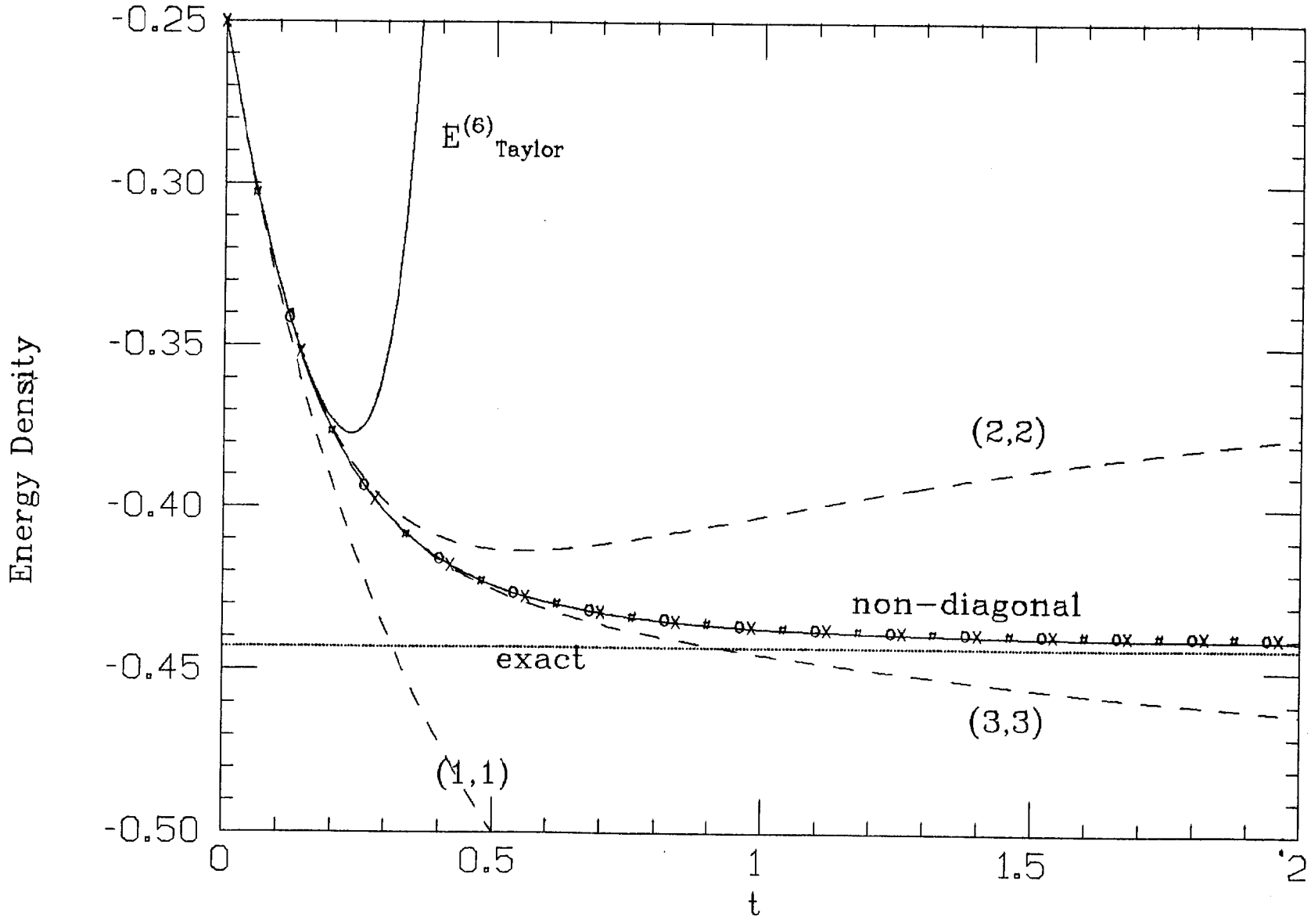
-0.25
-0.30
-0.35
-0.40
-0.45
-0.50
Energy Density
0
0.5
1
1.5
2
t
$E^{(6)}_{Taylor}$
(2,2)
non−diagonal
exact
(3,3)
(1,1)

Fig. 2

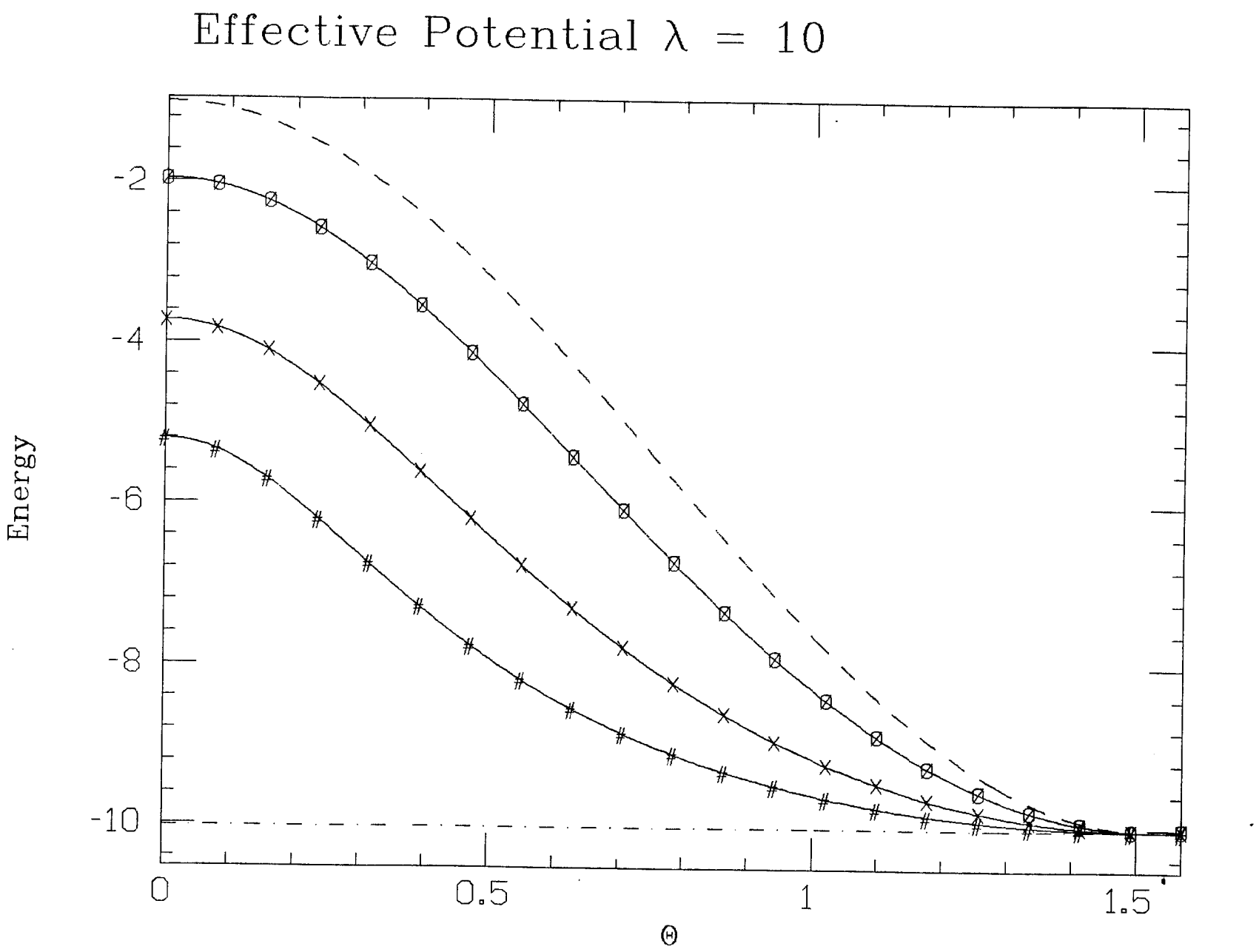

Fig. 3a

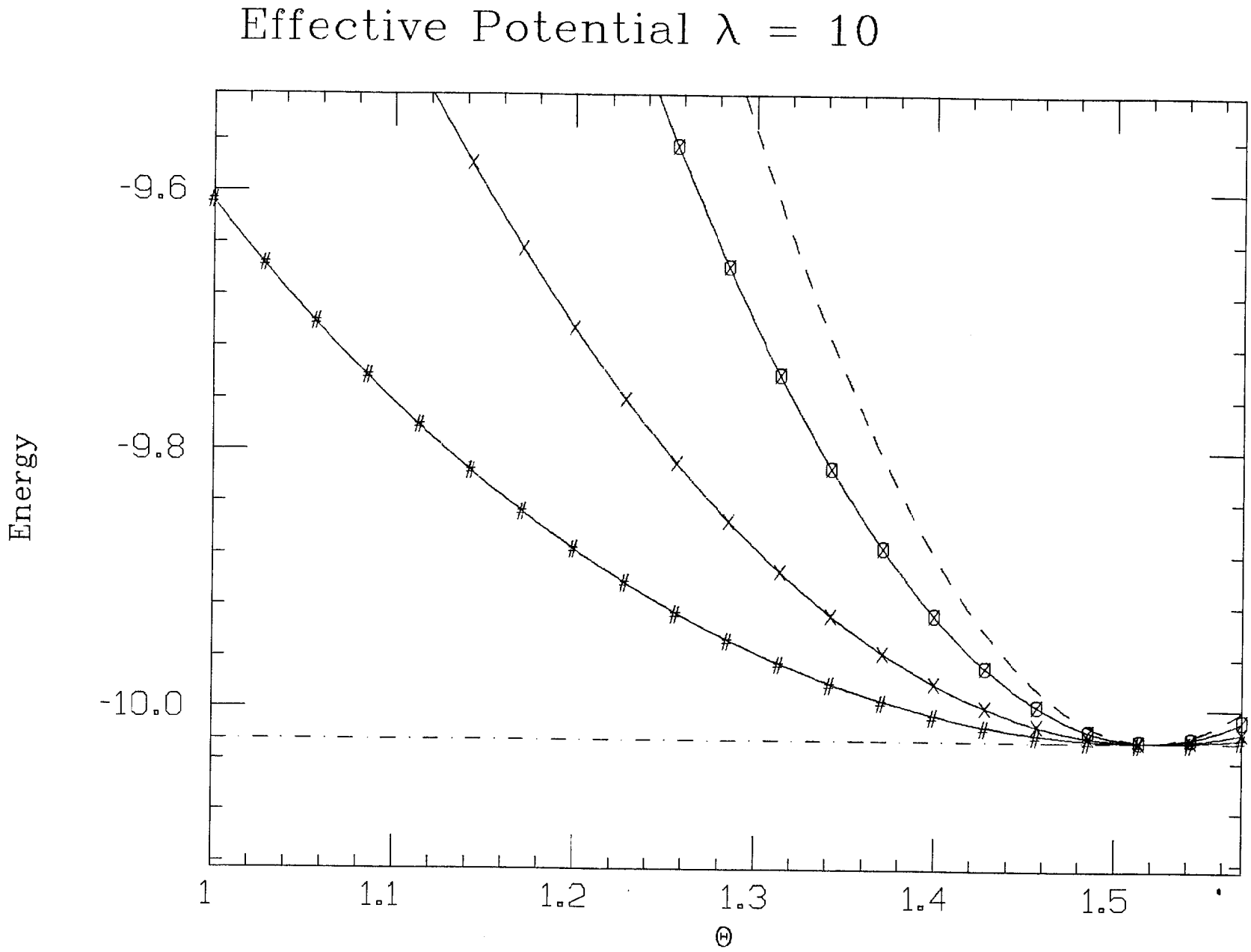

Fig. 3b

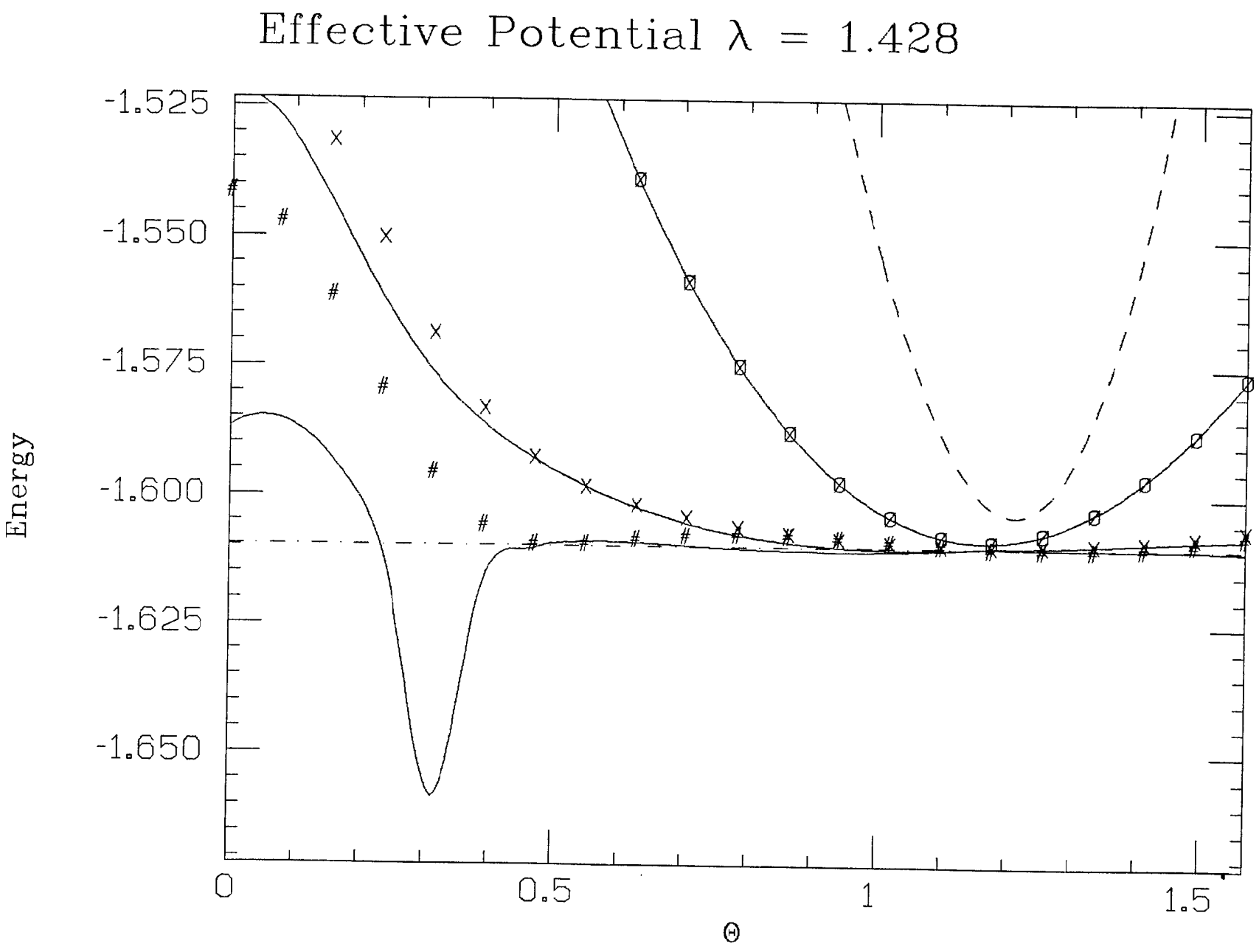
Effective Potential λ = 1.428
-1.525
-1.550
-1.575
-1.600
-1.625
-1.650
Energy
0
0.5
1
1.5
Θ

Fig. 4a

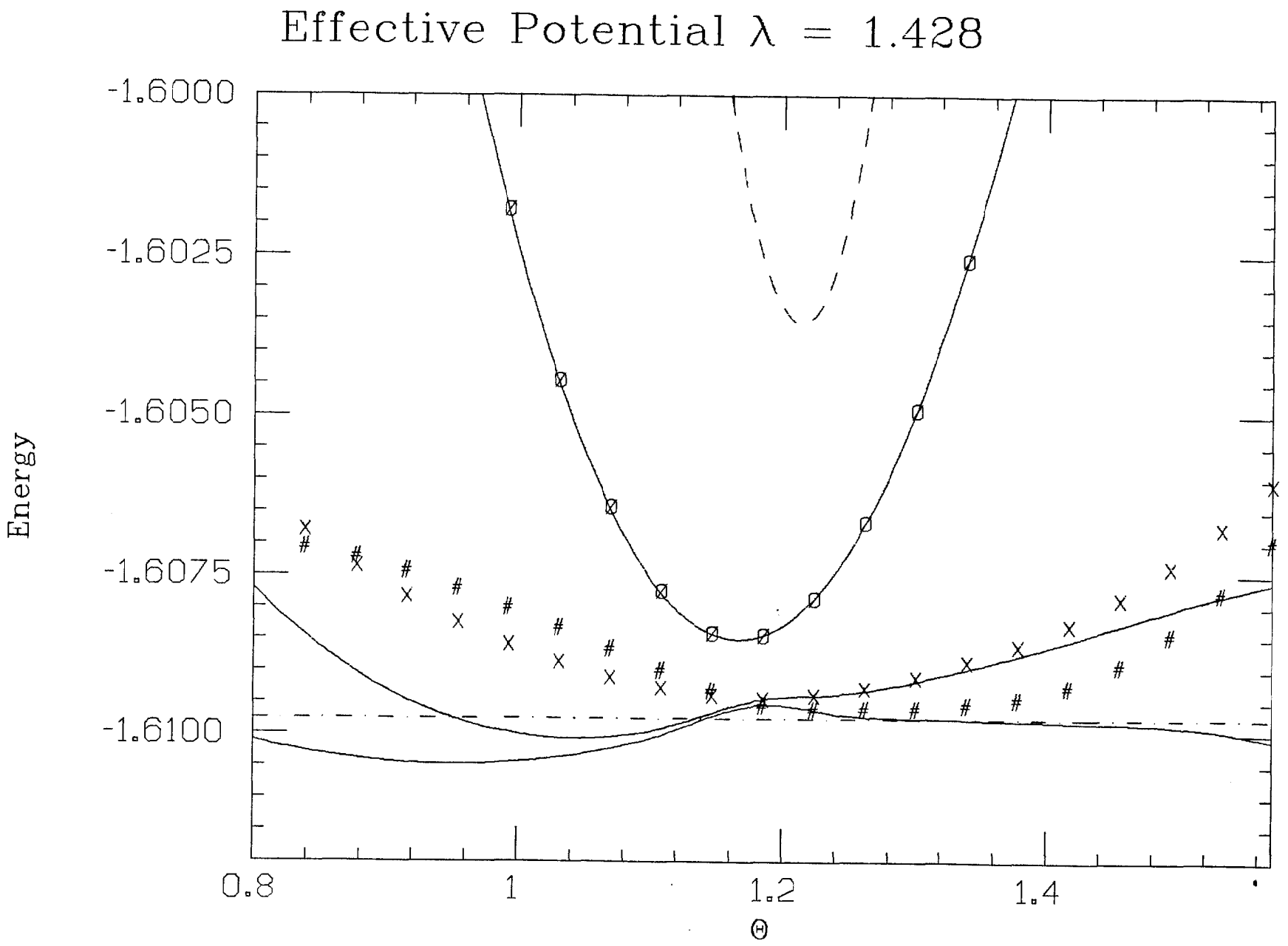
Effective Potential λ = 1.428
-1.6000
-1.6025
-1.6050
-1.6075
-1.6100
Energy
0.8
1
1.2
1.4
Θ

Fig. 4b

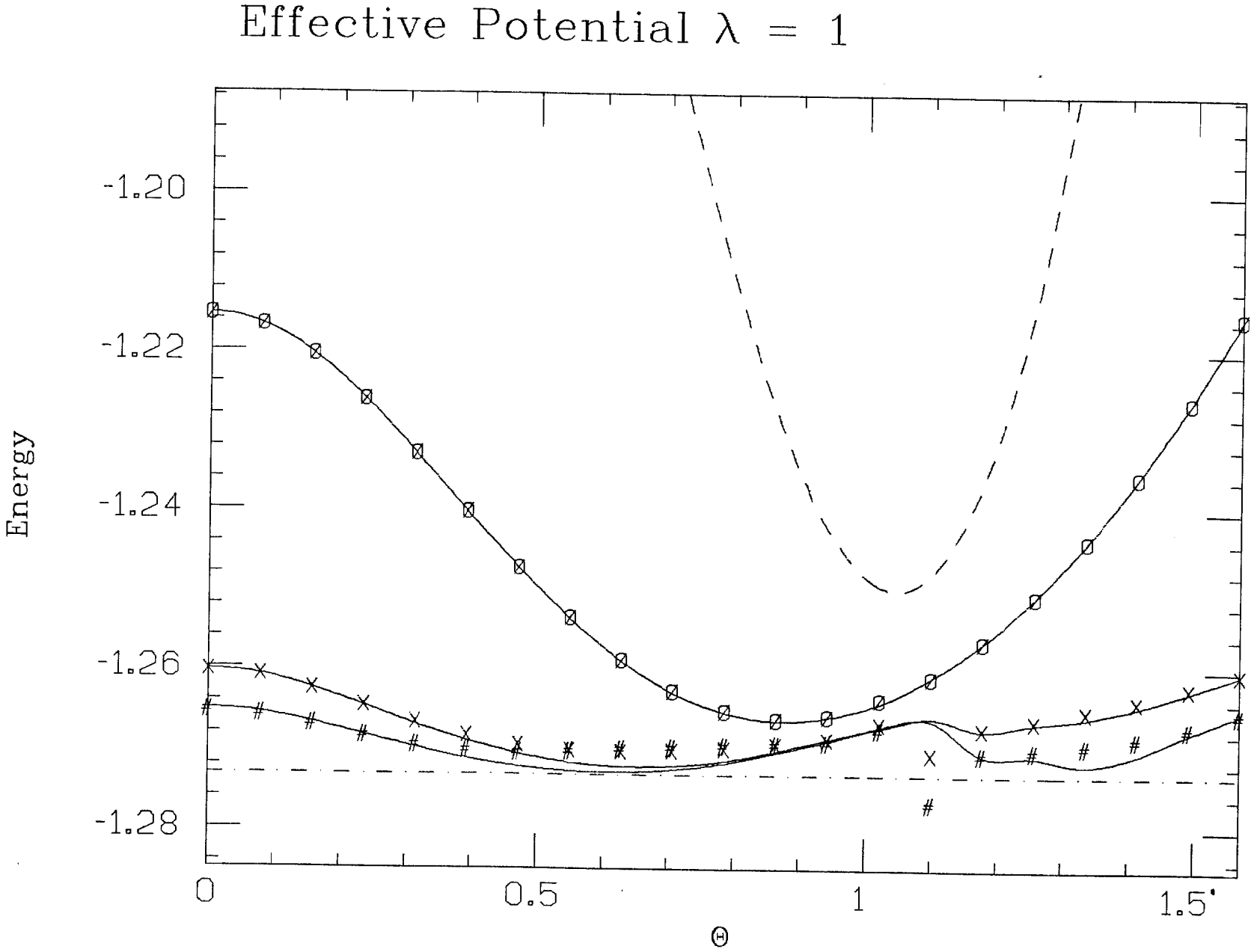

Fig. 5

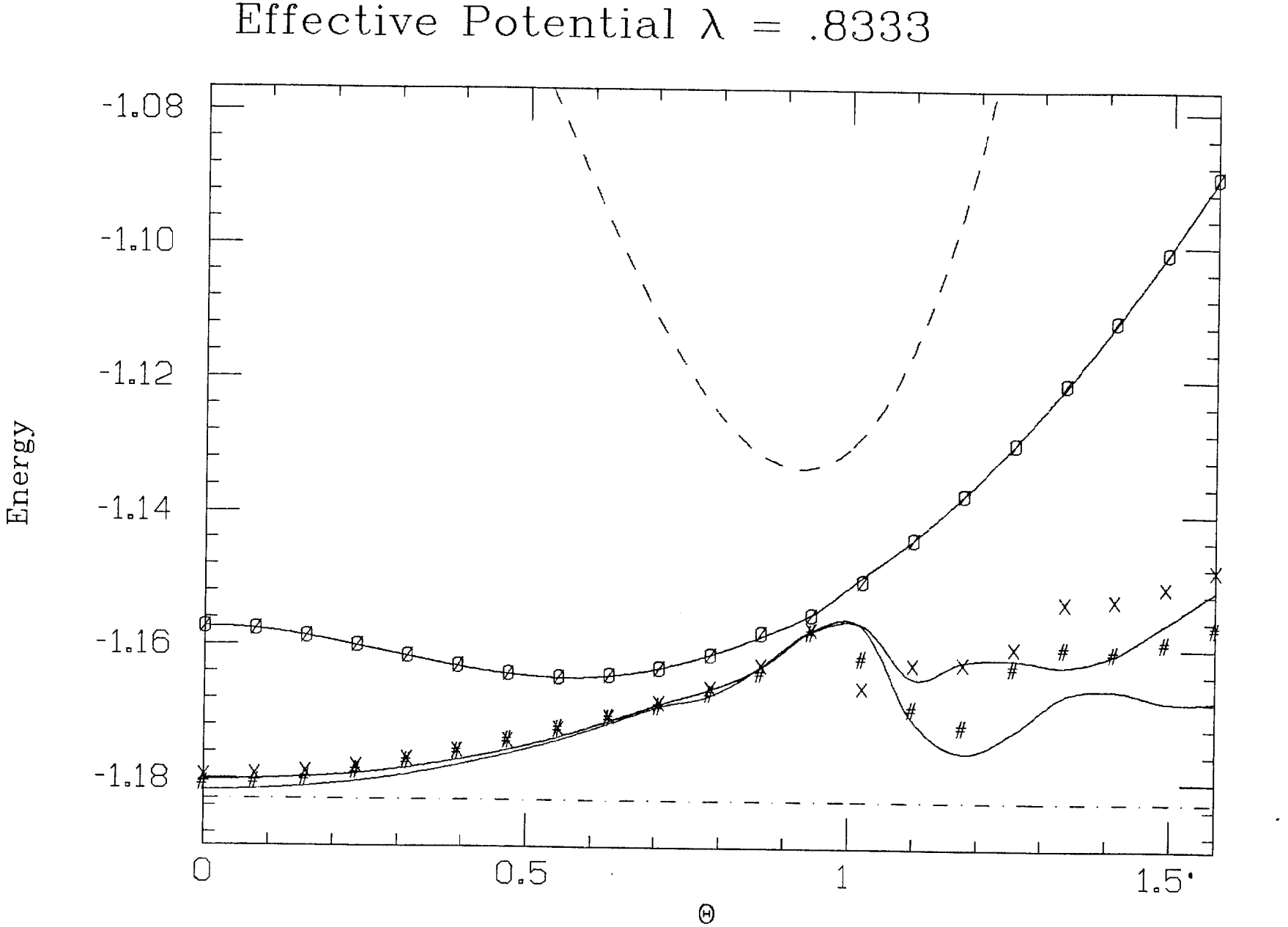
Effective Potential λ = .8333
-1.08
-1.10
-1.12
-1.14
-1.16
-1.18
Energy
0
0.5
1
1.5
Θ

Fig. 6

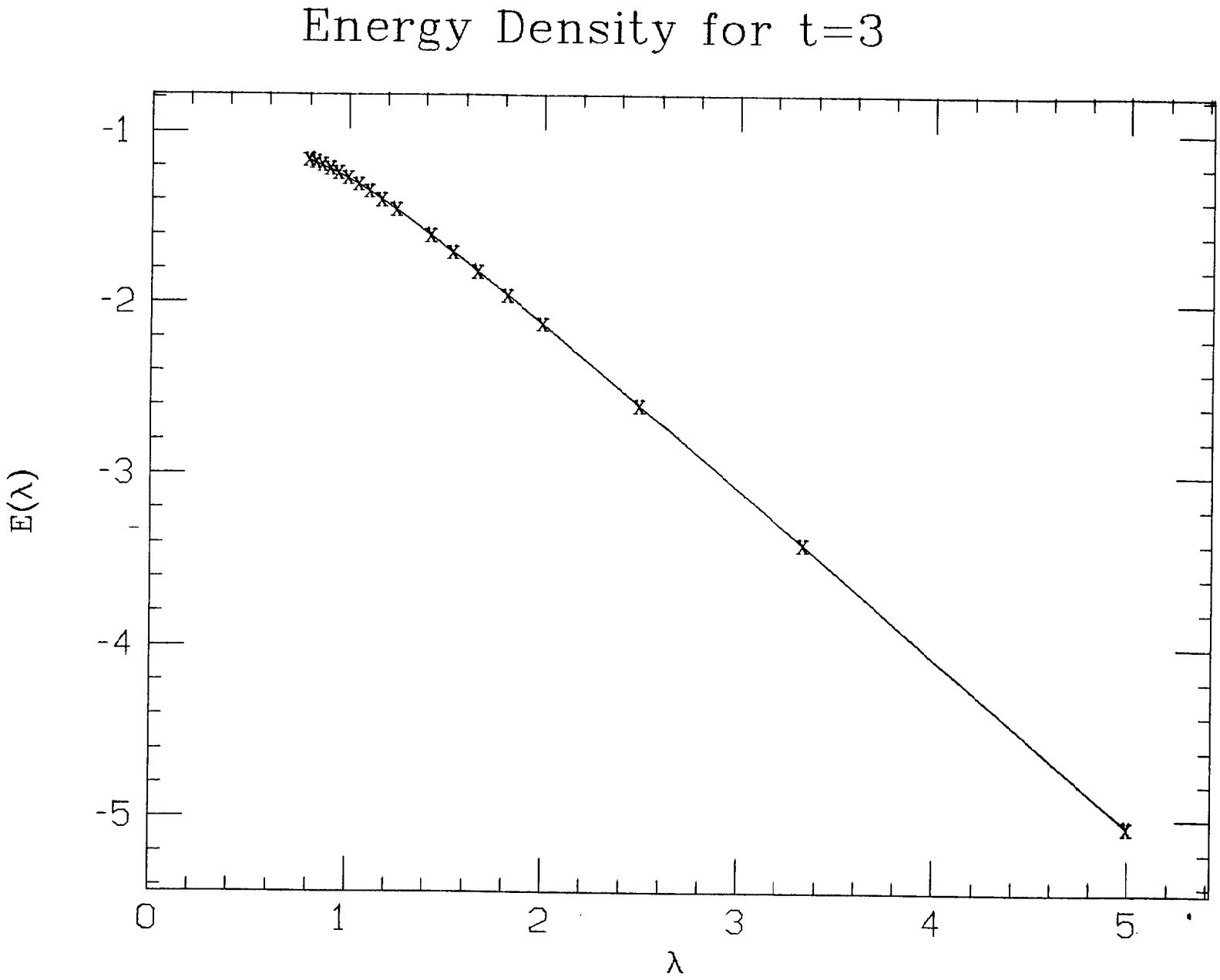

Fig. 7

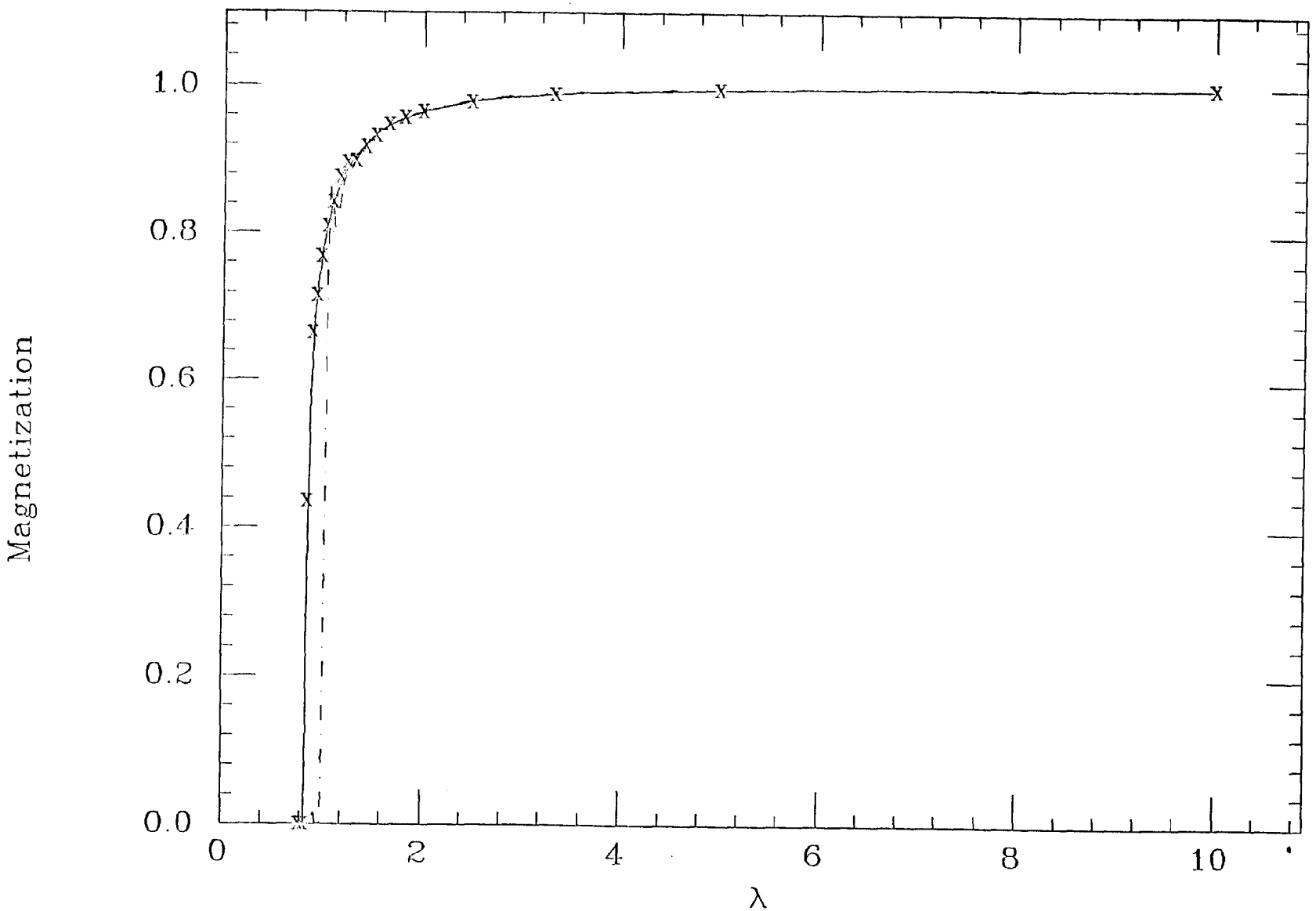

Fig. 8

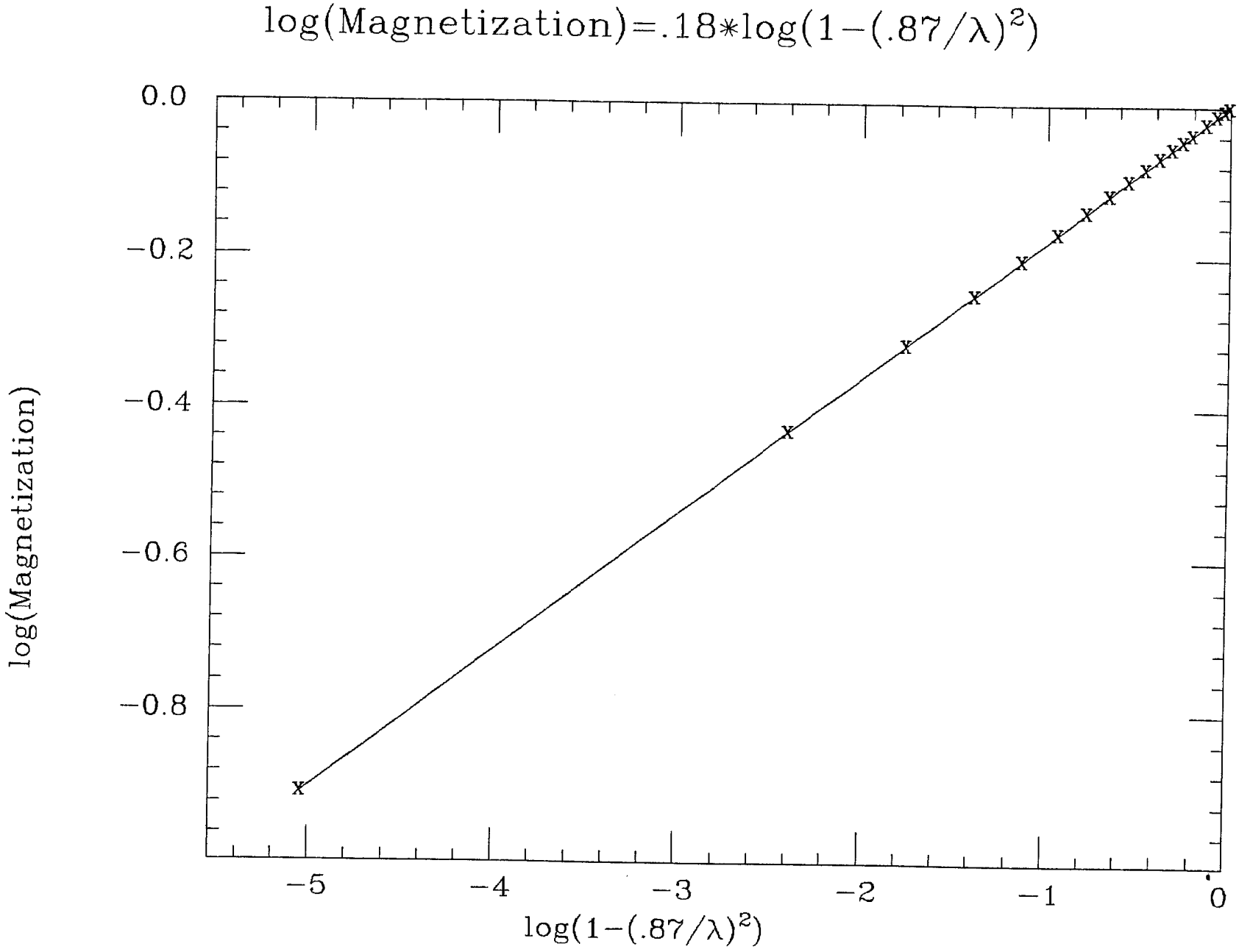
log(Magnetization)=.18*log(1−(.87/λ)²)
0.0
−0.2
−0.4
−0.6
−0.8
log(Magnetization)
−5
−4
−3
−2
−1
0
log(1−(.87/λ)²)

Fig. 9