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LOWER BOUNDS FOR QUANTUM HAMILTONIANS IN LATTICE FIELD THEORIES[†]

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ABSTRACT

A method for approximately including quantum effects on the solution to lattice field theories is presented. The formalism is an extension of the semiquantum approximation of Sachrajda, Weldon and Blankenbecler to obtain lower bounds for quantum Hamiltonians. This approach yields classical-like equations in which the effects of quantum fluctuations is included in a variational manner. The energies obtained by this method should be lower bounds to the true eigenvalues. Vacuum and single kink solutions are treated in detail, both analytically and numerically.

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I. INTRODUCTION

The study of methods for finding nonpertubative approximate solutions to quantum field theories has been of much interest in recent years, in particular for those theories that have classical, time independent, space dependent solutions such as kinks, etc.

Approximate solutions to scalar $\lambda \phi^4$ field theory have been extensively studied by Dashen, Hasslacher and Neveu[1] (DHN) and Goldstone and Jackiw[2] in the weak coupling limit, by quantizing small vibration around the classical limit. More recently Drell, Weinstein and Yankielowicz[3] have developed a variational method for treating one dimensional $\lambda\phi^4$ theories in the lattice and Scalapino and Stoeckly[4] (SS) considered a quantum mechanical solution to a truncated theory on a lattice comparing it to a semiclassical approximation in which they linearized the equations of motion about the classical minimum and then added the energy of each resultant normal mode.

Similar problems, that appear in statistical mechanics, have been earlier treated by other method by Onsager[5] and Fisher and Ferdinand[6]. Finally, extensive work on the theory of classical and quantum solitons have been done by Christ, Lee, and coworkers.[7]

In a previous paper,[8] hereafter called SWAB, a new method for including quantum effects in a classical-like limit was developed. The method is based on approximating the effects of quantum fluctuations to the energy in a variational way which is not equivalent to an expansion in powers of $\hbar$. The values of the energy thus obtained are lower bounds to the corresponding true eigenvalues. In a way, the SWAB method is equivalent to a generalization of well known uncertainty principle arguments for estimating the ground state energy of quantum systems. A further advantage of this approach is that the resulting equations

can be solved by simple methods since the problem is one of finding a purely classical equilibrium configuration. For reasonable choices of the trial functions, the resulting values for the energy of quantum Hamiltonians are lower bounds to the quantum energy levels, and thus the method complement the Raleigh-Ritz variational calculations which provide upper bounds for those eigenvalues.

In this paper we further develop these methods by applying them to one dimensional field theories on a lattice. The extension to higher dimensions is straightforward.

In Section II we present a general description of the application of the semi-quantum approximation to lattice field theories, and apply it to free field theory in Section III. In order to make clear the physical interpretation of our results we discuss in Section IV the meaning of the equilibrium semiquantum coordinates. Section V and VI are devoted to describing analytical and numerical methods for solving the classical like equations obtained. In Sections VII and VIII we study in detail the Dashen, Hasslacher and Neveu and the Stoeckly and Scalapino problems respectively. Section IX presents our conclusions and outlook.

II. LATTICE FIELD THEORY

Let us now consider the application of our method to field theory. This will not be a full discussion but merely a brief exposition of the general approach. Of course one hopes that the inclusion of some quantum effects in an otherwise classical solution will be of interest in itself as well as providing a new starting point for an expansion of quantum effects. Since some of these important effects have been included in the zeroth order, one might hope that the expansion would be more rapidly convergent. We shall be particularly interested in the local, or classical-like, solutions and for purposes of illustration will work in one space

dimension but it is said that the extension to higher dimensions is straightforward.

Ignoring normal ordering terms, the Hamiltonians under discussion are

$$H = \int dx \left[\frac{1}{2} \pi^2(x) + \frac{1}{2} \left(\nabla \phi(x) \right)^2 + V(\phi(x)) \right] . \tag{1}$$

Since the conjugate momentum π does not commute with ϕ, our object here is to estimate π^2 (or better yet to bound it from below) by a function of the field variable ϕ only, as in the earlier discussion of Schroedinger theory. Since the new Hamiltonian then would depend only on the field variable, both H and ϕ would be diagonal in the same coherent set of states. The quantum effects of the π^2 term have not been completely neglected as they are in the usual classical limit.

In order to implement this program, it is convenient to work on a lattice with spacing a and write

$$H = a \sum_{i=1}^{N} \left[\frac{1}{2} \pi_i^2 + \frac{1}{2} (\nabla \phi)_i^2 + V(\phi_i) \right] , \tag{2}$$

where any version of the gradient operator may be employed[9] and where

$$[\pi_i, \phi_i] = -i \delta_{ij}/a . \tag{3}$$

It is convenient to introduce a vector notation at this stage, $\phi = (\phi_1, \phi_2, \ldots, \phi_N)$, where ϕ_i is the field value at site i, and write

$$\nabla^2 \equiv \sum_{1}^{N} \frac{d^2}{d\phi_i^2}$$

$$\phi \cdot D \cdot \phi \equiv a^2 \sum (\nabla \phi)_i^2$$

$$V[\phi] = \sum V(\phi_i) ,$$

where D is an N x N matrix. The Hamiltonian becomes

$$aH = -\frac{1}{2}\nabla^2 + \frac{1}{2}\phi \cdot D \cdot \phi + a^2 V[\phi] \quad . \tag{4}$$

The familiar interpretation of a set of oscillators coupled by the derivative matrix D is clear. Since the procedure worked well for single oscillators, one might expect that the same will be true here in this much more complicated case.

Using the SWAB procedure, the first term can be estimated by a localized function of ϕ:

$$\pi^2 \longrightarrow \pi^2[\phi] = \sum_i \pi^2(\phi_i) \quad ,$$

where π^2 is of the form $\pi_i^2(\phi_i) = \frac{1}{4}(g_i'(\phi_i)/g_i(\phi_i))^2$.

For example, one may choose

$$\pi^2(\phi_i) = 1/4\phi_i^2 \tag{5}$$

or

$$\pi^2(\phi_i) = \frac{1}{4\phi_i^2}\left(\frac{\phi_i^2 + A}{\phi_i^2 - A}\right)^2 \quad . \tag{6}$$

A more general choice is to consider a linear combination of field variables and write

$$\pi^2[\phi] = \frac{1}{4}\sum_{n=1}^{N}(v(n)\cdot\phi)^{-2} \quad , \tag{7}$$

where the v(n) are a complete set of orthonormal vectors in N dimensions. The final approximate form of H in this "almost quantum theory" approximation is

$$a H_B = \frac{1}{2}\,\pi^2[\phi] + \frac{1}{2}\,\phi \cdot D \cdot \phi + a^2\, V[\phi] \quad . \tag{8}$$

Recall that the object here is to choose $g(\phi)$, and hence $\pi^2[\phi]$, so that H_B is as large as possible. Then its minimum will be as close as possible to the exact energy value. Criteria to be used in the choice of the function $g(\phi)$ was discussed in detail in reference 8.

III. FREE FIELD THEORY

As is customary for all approximation schemes, the method will first be applied to free field theory as an aid in interpreting the nature of the approximations involved and as a guide to the choice of $\pi^2[\phi]$. The potential is

$$V[\phi] = \frac{1}{2} M^2 \phi \cdot \phi \quad .$$

If the estimate (5) is used for $\pi^2[\phi]$, then a variation of the ϕ_i's yields the minimum condition

$$\frac{1}{4\phi_i^3} - a^2 M^2 \phi_i = \sum_j D_{ij}\phi_j \quad .$$

The solution for ϕ is a vector with constant components, $\phi_i^2 = 1/2aM$, and

$$H_B(\min) = \frac{1}{2} \sum M = \frac{1}{2}\, MN \quad . \tag{9}$$

This approximation has neglected completely the kinetic energy of each oscillator. The basic reason was that the choice for $\pi^2[\phi]$ did not prevent the solution for ϕ from being orthogonal to the eigenvectors of D with large eigenvalues (indeed ϕ was orthogonal to all eigenvectors except the one corresponding to D = 0).

This defect is easily remedied. Introduce the eigenvectors of D such that

$$Dv(n) = D_n v(n) \equiv a^2 k_n^2 v(n)$$

for $n = 1, \ldots N$ and define

$$r_n = v(n) \cdot \phi \quad .$$

Using the form (5) for $\pi^2[\phi]$, the Hamiltonian becomes

$$H_B = \frac{1}{2a} \sum_{n=1}^{N} \left[\frac{1}{4r_n^2} + a^2 k_n^2 r_n^2 + a^2 M^2 r_n^2 \right] , \qquad (10)$$

a set of uncoupled eigenmodes. The minimum with respect to the r_n is easily found:

$$H_B(\min) = \frac{1}{2} \sum_{n=1}^{N} (M^2 + k_n^2)^{\frac{1}{2}} \quad .$$

This is the exact result and the coordinates r_n are just the fourier transforms of the ϕ_i. The exact form of this transform is, of course, defined by the choice made for the derivative operator D.

Excited states of the free field are also straightforward to treat. Consider the case in which only the m^{th} mode is excited to its first level. For the π_n^2 one obviously chooses (see reference 8) the same as the above for $n \neq m$, but for the excited mode

$$\pi_m^2 = \frac{1}{4r_m^2} \left(\frac{r_m^2 + b^2}{r_m^2 - b^2} \right)^2$$

where b^2 is chosen after the minimization with respect to the r_n. It is chosen to maximize H_B. Since the modes are decoupled, this is a simple problem and

at the optimum point one finds $b^2 = 1/a\sqrt{M^2+k_m^2}$ and

$$H_B(\min) = \frac{1}{2} \sum_{n=1}^{N} (M^2 + k_n^2)^{\frac{1}{2}} + (M^2 + k_m^2)^{\frac{1}{2}} ,$$

the correct result, as expected.

For a general potential, the optimum choice for $g(\phi)$ and therefore $\pi^2[\phi]$ depends upon which terms in the Hamiltonian are large. If the potential is large and has a deep minimum, then $g(\phi)$ should be chosen so that ϕ cannot take maximum advantage of this minimum. On the other hand, if the derivative term is dominant, then one must force ϕ to mix in the large eigenvalues of D. The former condition is most easily expressed in coordinate space, the latter in k-space. Hence their simultaneous satisfaction requires some ingenuity in the choice for g.

IV. PHYSICAL INTERPRETATION

In order to aid in the physical interpretation of the equilibrium solution for the field variables ϕ_i, or the r_n, it is instructive to add a source term $\sum J_i\phi_i = \sum j_n r_n$ to the Hamiltonian and to generate expectation values of the field using the Feynman-Hellman theorem, $\langle\phi_i\rangle = \partial E/\partial J_i \,_{J=0}$. Consider a Hamiltonian of the form

$$H_B(j=0) = \frac{1}{2a} \sum_n \left[\pi_n^2 (r_n) + a^2 k_n^2 r_n^2\right] + a\, V[r]$$

which is assumed invariant under the simultaneous transformation of <u>all</u> the $r_n \longrightarrow -r_n$. Now in the presence of the source term, this symmetry is lost and the optimum choice for the π_n^2 should reflect this fact. Therefore, we introduce a shift in π^2 and define

$$H_B(j) = \frac{1}{2a} \sum_n \left[\pi_n^2 (r_n + j_n b_n) + a^2 k_n^2 r_n^2 + 2 j_n r_n\right] + a\, V[r] \qquad (11)$$

The procedure now is to minimize with respect to the r_n's, and then choose the b_n to maximize the resultant energy values. Working to first order in j, one finds that the new equilibrium coordinates are

$$r_n = r_n^0 + \sum_m R_m(n)\, j_m + 0(j^2) \quad ,$$

where the r_n^0's are the solution for $j = 0$, and

$$R_m(n) = -\frac{\partial^2 V}{\partial r_n \partial r_m} \Big/ \frac{\partial^2 H}{\partial r_n^2} \qquad (m \neq n)$$

$$R_n(n) = -\left[1 + b_n \frac{d^2 \pi_n}{dr_n^2}\right] \Big/ \frac{\partial^2 H}{\partial r_n^2} \quad ,$$

where all the variables are evaluated at $r_n = r_n^0$.

The lower bound to the energy becomes

$$H_B = H_B(j=0) + \frac{1}{a} \sum_n j_n \left[r_n^0 - \left(2D_n r_n^0 + \frac{\partial V}{\partial r_n^0}\right) b_n\right] + O(j^2) \qquad (12)$$

Now since the original Hamiltonian possessed a symmetry in r, if the set r_n^0 is a solution to the minimization problem, so is $-r_n^0$. Now the optimum value for b_n must be such that the value of dH_B does not depend upon which of these minima one expands around (otherwise one would be smaller) and hence

$$b_n = \left[2D_n + \frac{1}{r_n^0} \frac{\partial V}{\partial r_n^0}\right]^{-1} \quad .$$

The odd term in j in the energy vanishes identically. Thus

$$\langle r_n \rangle = \langle \phi_i \rangle = 0$$

and clearly one should not identify r_n^0 with the quantum expectation value $\langle r_n \rangle$.

On the other hand, if a term $\sum_n j_n r_n^2$ is added to the Hamiltonian, one finds approximately that $\langle r_n^2 \rangle \cong (r_n^0)^2$. This root mean square relation for r_n^0 is a reasonable and intuitive interpretation of the equilibrium values of the fields and this momentum space connection should be kept in mind while interpreting our results.

V. KINK SOLUTIONS - COORDINATE SPACE

In this section, a few general remarks will be made for kink-type solutions although no specific examples will be discussed in detail. We shall be interested in the difference in behavior between the solutions using our approach and the purely classical ($\pi^2 = 0$) limit. For $\pi^2[\phi]$ of the form given by Equation (5), that treats all lattice points the same, the minimization of (24) yields the equation

$$\sum_j \frac{1}{a^2} D_{ij} \phi_j + \frac{d}{d\phi_i} W(\phi_i) = 0 \quad , \tag{13}$$

where

$$W(\phi_i) = V(\phi_i) + \frac{1}{2a^2} \pi^2(\phi_i) \quad .$$

This difference equation is most easily treated by passing back to the continuum limit in which $\phi_i = \phi(x)$, but the explicit factor of a^2 is retained in the effective quantum potential $W(\phi)$. The result is

$$\nabla^2 \phi(x) = \frac{d}{d\phi} W(\phi) \quad .$$

The requirement that ϕ approach a constant value at infinity is that this constant F satisfy

$$\frac{d}{dF} W(F) = 0 \quad . \tag{14}$$

The equation for $\phi(x)$ can be integrated once to yield

$$\frac{1}{2}\left(\phi'(x)\right)^2 = W(\phi) - W(F), \tag{15}$$

and the field ϕ is a solution of the familiar implicit equation

$$\int_{\phi(y)}^{\phi(x)} d\phi \left[W(\phi) - W(F)\right]^{-\frac{1}{2}} = \sqrt{2}(x-y) \quad .$$

The Hamiltonian density can be written as

$$\mathcal{H}_B(x) = \left[V(F) + \frac{1}{2a^2}\,\pi^2(F)\right] + \left(\phi'(x)\right)^2 \quad , \tag{16}$$

where the last term is given by Equation (15). It is easy to show that this term vanishes like $(\phi - F)^2$ for large x.

For the "vacuum" state, defined by $\phi' \equiv 0$, the energy density is constant and given by the first terms. This is not the same as the classical result since F is to be computed by finding the minimum of the effective quantum potential W that includes effects of the π^2 term. The asymptotic field is therefore renormalized. The energy, back on the lattice, is

$$H_B = a\sum_1^N \mathcal{H}(x_i) = aNW(F) + a\sum_i \left[\phi'(x_i)\right]^2 \quad . \tag{17}$$

This will now be examined for kink-type solutions.

For such a solution, i.e., in which $\phi(\pm\infty) = \pm F$, the function ϕ must vanish at some point. Since $\phi = 0$ is a symmetry point, most choices for $\pi^2[\phi]$ blow up there. This has an important effect on the energy which is quite different from standard classical theories. To explore this point further, consider π^2 of the form (5) or (6). Near the vanishing point of ϕ, the equation for ϕ' is

$$\phi' \simeq \frac{1}{2a} (\phi^2)^{-\frac{1}{2}} + 0(\phi^2)^{\frac{1}{2}} \quad ,$$

and hence

$$\phi(x) \sim \left| \frac{x - x_0}{a} \right|^{\frac{1}{2}} + \ldots$$

Note that in the limit ϕ depends only on a, i.e., the quantum effects from π^2 completely dominate the effect of the potential. The energy density for $x \sim x_0$ has the behavior

$$\mathcal{H}(x) \sim (4a|x-x_0|)^{-1} \quad .$$

Therefore there is a logarithmic infinity in the energy arising from the forced vanishing of $\phi(x)$. One expects that quantum fluctuations will have their largest relative effects when the field ϕ itself is small, and indeed this is the case. This divergence may be due to the fact that our starting Hamiltonian was not normal ordered and there is still a mass renormalization to be performed.

VI. LINEAR LATTICE

Let us now turn to more specific example, that of $\kappa\phi^4$ on the lattice, and perform numerical calucations in k–space in which the eigenfunction of D are used for the v(n). The solution for the vectors v(n) if D is chosen to be the nearest neighbor gradient, $(\nabla\phi_i)^2 = (\phi_i - \phi_{i+1})^2$, are given in the Appendix, case (a). We define

$$r_n = v_i^n \phi_i \tag{19}$$

and its inverse as

$$\phi_i = w_i^n r_n .$$

These vectors satisfy

$$D_{ij} v_j^n = D_n v_i^n$$

with

$$D_n = 4 \sin^2 \pi(n-1)/N \quad . \tag{20}$$

The Hamiltonian of interest is then chosen to be

$$H_L = \frac{1}{2a} \sum_{n=1}^{M} \left[\pi^2(r_n) + a^2 D_n r_n^2 \right] + a\kappa \sum_i (\phi_i^2 - f^2)^2 \quad . \tag{21}$$

One can now proceed to minimize this function of the r_n (or, equivalently the ϕ_j). This can be done by brute force but it is helpful to have approximate solutions to localize the search. Two such approximate solutions will now be discussed.

For the vacuum state, and except near the symmetry point even for the kink state, one expects that the ϕ^2 will be roughly equal (except for end effects). This suggests the approximation

$$\sum \phi_i^4 \sim \frac{1}{N} \left(\sum \phi_i^2 \right)^2 = \frac{1}{N} \left(\sum r_n^2 \right)^2 \quad .$$

The Hamiltonian is now an explicit function of the r_n. The minimization is now quite simple:

$$\frac{1}{2} \frac{d}{dr_n} \pi^2(r_n) + a^2 D_n r_n + 4a^2 \kappa \left[\frac{1}{N} \sum r_n^2 - f^2 \right] r_n = 0 \tag{22}$$

The classical solution to this problem is $\phi_i = f$ or $r_1 = \sqrt{N} f$, $r_n = 0$ $(n > 1)$.

Thus to force the quantum solution away from these values we chose

$$\pi_1^2(r_1) = \frac{1}{4} \left(r_1 - \sqrt{N} f \right)^{-2}$$

$$\pi_n^2 (r_n) = \frac{1}{4} (r_n)^{-2} \qquad n > 1$$

This choice for π, does not retain the original symmetry of the Hamiltonian under $r_n \rightarrow - r_n$ (all n simultaneously) but is closely related to the standard expansion procedure[1,7]. A better choice would be Eq. (6) with $A = nf^2$ which would retain the symmetry of the original Hamiltonian in r_1.

The solution for $n > 1$ is

$$r_n^2 = \frac{1}{2a} \left[D_n + 4\kappa \left(\frac{1}{N} R^2 - f^2 \right) \right]^{-\frac{1}{2}} , \tag{23}$$

and r_1 is the solution to

$$r_1 (r_1 - \sqrt{N} f)^3 = \left[4 a^2 \kappa \left(\frac{1}{N} R^2 - f^2 \right) \right]^{-1} , \tag{24}$$

where $R^2 \equiv \sum r_n^2$ and must be determined self-consistantly, from (23) and (24).

A second approach, which is very similar to the expansion used by DHN, is to write $\phi_i = \phi_i^c + \delta \phi_i$ or equivalently their transforms $r_n = r_n^c + \delta r_n$, where ϕ_i^c (and r_n^c) is the classical solution to the problem. The conjugate momentum operator π^2 is then chosen so as to keep the δr_n's from being too small. In this case, the Hamiltonian becomes

$$H_L = H_c + H_1 + H_2$$

$$H_c = \sum_n \frac{1}{2} a D_n (r_n^c)^2 + a\kappa \sum_i (\phi_i^{c2} - f^2)^2 , \tag{25}$$

where

$$H_1 = \frac{1}{2a}\sum_n \left[\frac{1}{4(\delta r_n)^2} + a^2 D_n (\delta r_n)^2\right] + 2a\kappa \sum_i \left[3(\phi_i^c)^2 - f^2\right](\delta\phi_i)^2 \qquad (26)$$

$$H_2 = 6a\kappa \sum_i \phi_i^c (\delta\phi_i)^3 + a\kappa \sum_i (\delta\phi_i)^4 \quad . \qquad (27)$$

If the $\delta\phi$'s are small, then H_2 can be neglected to lowest order. Also if $\phi_c^2 \approx$ constant, which is exactly true for the (classical) vacuum, then the solution for the δr_n's is

$$(\delta r_n)^2 = \frac{1}{2a}\left[D_n + 8\kappa f^2\right]^{-\frac{1}{2}} \quad . \qquad (28)$$

This should be compared with our earlier estimates, Equations (23) and (24). These two approximations are similar in character, but not identical, due to the somewhat different estimates that were used.

VII. THE DHN PROBLEM

In their classic papers[1] on the subject, DHN gave an analytic solution to the (continum) problem posed by the Hamiltonian $H_c + H_1$. In order to compare with their results in detail let us first consider this reduced problem. Our procedure is as follows:

First, we solve for the classical solution to the lattice problem by finding the minimum of H_c as a function of the ϕ_i^c (or the r_n^c) (because of the lattice, the kink solution is somewhat different from the expected f tanh ($\sqrt{2\kappa}$ fax$_i$)). Then the minimum of H_1 as a function of the δr_n was found numerically using for initial (trial) values those given by Equation (28) and then letting the program find the true minimum.

The results for the vacuum and kink state energies per site are given in Figure 1 for the values Na = 8, $\kappa = 1$ and for a range of values of f^2.

The analytic values given by DHN are, of course, infinite due to renormalization effects. If their formulas are arbitrarily cut off at a k value of $k_{max} = 2\pi/a$, in order to correspond to the effect of the lattice, one finds (N = 8) for the energies of the non-normal ordered Hamiltonian,[10]

$$\frac{E(\text{kink})-E(\text{vac})}{\sqrt{\kappa}} \cong \frac{4\sqrt{2}}{3} f^3 - f\left(\frac{3\sqrt{2}}{\pi} - \sqrt{\frac{3}{2}}\right) - \frac{3\sqrt{2}f}{n} \int_0^{q_0} dq \, \frac{(q^2+2)}{(q^2+1)\sqrt{q^2+4}} , \qquad (29)$$

where $q_0 = k_{max}/\sqrt{2\kappa}\, f \sim 2\pi/\sqrt{2\kappa}\, fa$. A rough estimate (for $\kappa = 1$) of the integral shows that (29) vanishes for $f^2 \sim 1.4$. Our calculation also has such a crossover, at a value of $f^2 \sim 1.6$, as is evident from Figure 1.

While it is very difficult to include the H_2 terms in an exact treatment, it is a straightforward matter to include them in the semi-quantum approach. The results for the energies are shown in Figure 2 for N = 8. The full energy values have risen slightly and the crossover has moved to $f^2 \sim 1.2$.

To find these minima of H_L we have used a computer program based on a quasi-Newton method that minimizes a scalar function of N variables. The method is iterative and therefore requires an initial estimate of the position of the minimum. Since the function to be minimized must be continuous with continuous first derivatives, we have regularized the kinetic energy term by adding a small positive parameter ($\approx 10^{-10}$) to the denominators. Changes of the value of that parameter do not change the solutions. The initial estimate of the minimum is multiplied by a parameter that is increased by steps from 10^{-5} to 1. The kinetic energy term is also multiplied by the same parameter and the search is started at one of the

classical solutions, either constant or kink. The search stops when all components of the gradient are smaller than 10^{-7}.

Since the ϕ_i's are linear combinations of the r_i's, there are several local minima depending on the signs of the r_i's. To find the true minimum we have started the search with each of the 2^N possible combinations of signs. Because of end point effects, we have selected only those solutions that maintain the constant or kink character as the absolute value of f^2 is decreased to well below the critical point.

VIII. THE SS PROBLEM

A quantum mechanical solution to an interesting one dimensional lattice model, a truncated $\lambda \phi^4$ theory on a ring, has been discussed by B. Stoeckly and D. J. Scalapino.[4] In order to facilitate comparison with their work, the Hamiltonian will be rewritten in their notation

$$H = H_c + H_q \quad , \tag{30}$$

where the classical and quantum Hamiltonian are (a = 1)

$$H_c = \sum_i \left[\frac{1}{2} c (\nabla \phi_i^c)^2 + \frac{1}{2} \tau (\phi_i^c)^2 + \frac{1}{4} (\phi_i^c)^4 \right]$$

and

$$H_q = \sum_n \left[\frac{1}{2} \pi_n^2 + \frac{1}{2} (\tau + c D_n) (\delta r_n)^2 \right]$$

$$+ \sum_j{}' \left[\frac{3}{2} (\phi_i^c)^2 (\delta \phi_i)^2 + \phi_i^c (\delta \phi_i)^3 + \frac{1}{4} (\delta \phi_i)^4 \right] \quad . \tag{31}$$

The relation to the DHN problem is obvious. The estimate of the energy due to the conjugate momentum is chosen to be the familiar

$$\pi_n^2 = \frac{1}{4}(\delta r_n)^{-2} \quad .$$

It is now a somewhat simple matter to solve for the minimum energy configuration by varying the δr_n. However, the transformation between the coordinate and momentum space field variables, $r_n = v_i^n \phi_i$, depends now on the boundary conditions. The vacuum state requires symmetric boundary conditions on the ring, whereas the kink state demands antisymmetric boundary conditions. The solutions for the v's for these two situations are given in the Appendix case (b) and (c). Note that since the problem is posed on a ring, there are many translation and inversion degeneracies in the solution.

The energies and configurations for the minimum energy vacuum and kink boundary conditions we obtained numerically for $N = 8$, $c = 0.1$ and a range of τ and are compared with the results of SS in Figure 3. The kink energy is above the vacuum energy for sufficiently negative τ but they become equal for $\tau \cong -2.6$. This is to be compared with the calculation of SS which found this degeneracy occurring at $\tau \simeq -2.2$.

It is reassuring to see that, if as in the Stoeckley- Scalapino calculation, the energy of the vacuum is taken as the origin of the energy variable, then our calculation should give a lower bound to the energy of the kink, as is the case. Of course the two problems are slightly different since SS obtains a quantum mechanical solution to a truncated problem. However, for small values of ϵ (see Reference 4) the approximation of considering only the ground state and the first excited state of each anharmonic oscillator should be quite good and therefore the truncated problem should be a reasonable approximation to the full Hamiltonian.

In addition, Pfeuty[11] has shown that for the ground state $\langle\phi\rangle \sim (\tau_c - \tau)^{1/8}$ for $\tau < \tau_c$, corresponding to $\beta = 1/8$ in the Onsager[5] calculation of the two dimensional Ising model. Since the kink energy goes as $(\tau_c - \tau)$ for $\tau \approx \tau_c$, we obtain from our solution a value of $\beta = 1/8$ which is the Onsager result.

IX. CONCLUSIONS

A simple semiquantum approach to lattice theories has been developed and applied to several examples. This approach provides lower bounds to the true quantum energy (except for possible end point problems discussed in Reference 1). Comparison with the results of conventional treatments and solutions of the examples shows reasonable agreement. It is hoped that the semiquantum approach can be used to develop insight and physical intuition into the effects of quantum fluctuations on purely classical solutions as well as to provide convenient lower bounds to test the accuracy of conventional calculations of the energies of quantum systems. Further applications of the method to the Sine-Gordon problem, fermions, etc., may prove very instructive.

It may be possible to use these classical-like configurations as a new expansion point for quantum effects that are then treated perturbatively. Such an expansion would be expected to converge more rapidly since some quantum are already included in lowest order. As yet, we have not been able to carry out this program satisfactorily due to some formal problems. In any case, the method stands on its own as a useful technique to estimate and even to bound from below the energies of simple field theories.

REFERENCES

1. R. F. Dashen, B. Hasslacher and A. Neveu, Phys. Rev. D10, 4114 (1974), D10, 4130 (1974), D10, 4138 (1974). See also the excellent review by R. Rajaraman, Phys. Reports 21, 227 (1975).
2. J. Goldstone and R. Jackiw, Phys. Rev. D11, 1486 (1975).
3. S. P. Drell, M. Weinstein and S. Yankielowicz, Phys. Rev. D14, 487 (1976).
4. D. J. Scalapino and B. Stoeckly, Phys. Rev. D14, 3367 (1976).
5. L. Onsager, Phys. Rev. 65, 117 (1944).
6. M. E. Fisher and A. E. Ferdinand, Phys. Ref. Letters 19, 169 (1967).
7. N. Christ and T. D. Lee, Phys. Rev. D12, 1606 (1975). R. Friedberg and T. D. Lee, Phys. Rev. D15, 1694 (1977).
8. C. Sachrajda, A. Weldon and R. Blankenbecler, SLAC-PUB-2015 , submitted to Phys. Rev.
9. For example, the nearest neighbor difference approximation or the "SLAC" gradient of Reference 3 (which follows directly from the cardinal interpolation formula of Whittaker) can be used, or any other.
10. See the concise derivation of formulas of this type by K. Cahill, A. Comtet, and R. J. Glauber, Phys. Letters, 64B, 283 (1976).
11. P. Pfeuty, Ann. Phys. (N.Y.) 57, 79 (1970).

APPENDIX

In term of the field variables, the gradient term in the Hamiltonian was written as:

$$(\nabla\phi_j)^2 = (\phi_j - \phi_{j+1})^2 = \phi_j \left(\sum_{k=1}^{N} D_{jk}\phi_k\right) \qquad \text{(A-1)}$$

Where the matrix D depends on the boundary conditions imposed.

We have considered three cases.

a) Linear system with free end point conditions:

$$D_{ij} = \begin{cases} 2\,\delta_{ij} & i, j = 2, \ldots, N-1 \\ \delta_{ij} & i, j = 1 \text{ or } N \\ -1 & i = j \pm 1 \\ 0 & \text{otherwise .} \end{cases}$$

b) Closed ring with symmetric boundary conditions:

$$D_{ij} = \begin{cases} 2\,\delta_{ij} & i, j = 1, \ldots, N \\ -1 & i = j \pm 1;\ \begin{cases} i = 1,\ j = N \\ i = N,\ j = 1 \end{cases} \\ 0 & \text{otherwise .} \end{cases}$$

c) Closed ring with antisymmetric boundary conditions (kink solutions):

$$D_{ij} = \begin{cases} 2\,\delta_{ij} & i, j = 1, \ldots, N \\ 1 & \begin{cases} i = 1,\ j = N \\ i = N,\ j = 1 \end{cases} \\ -1 & i = j \pm 1 \\ 0 & \text{otherwise .} \end{cases}$$

The eigenvalue equations are:

$$(2 - D_n)\, v_i^n = v_{i+1}^n + v_{i-1}^n$$

with the following boundary conditions:

Case a: $v_0 = v_1$; $v_{n+1} = v_n$

Case b: $v_{n+1} = v_1$; $v_0 = v_n$

Case c: $v_{n+1} = v_1$; $v_0 = -v_n$.

Writing

$$v_j^n = M_n \sin(j a_n + \phi_n) ,$$

one obtains

$$D_n = 4 \sin^2 (\frac{a_n}{2})$$

and the following solutions for each case:

Case a:

$$a_n = \frac{n-1}{N} \pi \qquad n = 1, \ldots , N$$

$$M_n = \sqrt{\frac{2}{N}} \qquad n = 1, \ldots , N$$

$$\phi_n = \frac{N - n + 1}{N} \pi \qquad n \neq 1$$

$$\phi_1 = \frac{\pi}{2}$$

Case b:

$$\begin{cases} a_1 = \frac{\pi}{4} \\ \phi_1 = 0 \\ M_1 = \frac{1}{\sqrt{N}} \end{cases}$$

$$\begin{cases} a_n = \frac{2(n-1)}{N}\pi \\ \phi_n = 0 \end{cases} \qquad n = \begin{cases} 2, \ldots, \frac{N}{2} \; ; \; N \text{ even} \\ 2, \ldots, \frac{N+1}{2} \; ; \; N \text{ odd} \end{cases}$$

$$\begin{cases} a_{\frac{N}{2}+1} = \pi \\ \phi_{\frac{N}{2}+1} = \frac{\pi}{4} \end{cases}$$

$$\begin{cases} a_n = \frac{2(N-n+1)}{N} \\ \phi_n = \frac{\pi}{4} \end{cases} \qquad n = \begin{cases} \frac{N}{2}+2, \ldots, N; \; N \text{ even} \\ \frac{N+3}{2}, \ldots, N; \; N \text{ odd} \end{cases}$$

$$M_n = \sqrt{\frac{2}{N}} \qquad n = 2, \ldots, N$$

Case c:

$$\begin{cases} a_n = \dfrac{2n-1}{N}\,\pi \\ \phi_n = -\,(2n-1)\dfrac{N+1}{N}\,\pi \\ M_n = \sqrt{\dfrac{2}{N}} \end{cases} \qquad n = \begin{cases} 1, \ldots, \dfrac{N}{2}\ ; \ N \text{ even} \\ 1, \ldots, \dfrac{N-1}{2}\ ; \ N \text{ odd} \end{cases}$$

$$\begin{cases} a_{\frac{N+1}{2}} = \pi \\ \phi_{\frac{N+1}{2}} = \dfrac{N\pi}{2} \\ M_{\frac{N+1}{2}} = \dfrac{1}{\sqrt{N}} \end{cases}$$

$$\begin{cases} a_n = \dfrac{2(N-n+\frac{1}{2})}{N}\,\pi \\ \phi_n = 2(N-n+\tfrac{1}{2})\dfrac{N+1}{N}\,\pi \\ M_n = \sqrt{\dfrac{2}{N}} \end{cases} \qquad n = \begin{cases} \dfrac{N}{2}+1, \ldots, N; \ N \text{ even} \\ \dfrac{N+3}{2}, \ldots, N; \ N \text{ odd} \end{cases}$$

FIGURE CAPTIONS

1. The difference between the energy per site of
for the truncated problem of DHN with $\kappa = 1$, :
2. The energy per site of the vacuum and kink sta
Hamiltonian of the DHN problem for $\kappa = 1$, N =
3. The results of the semiquantum method for the t
are compared to the calculation of Scalapino and
τ values.

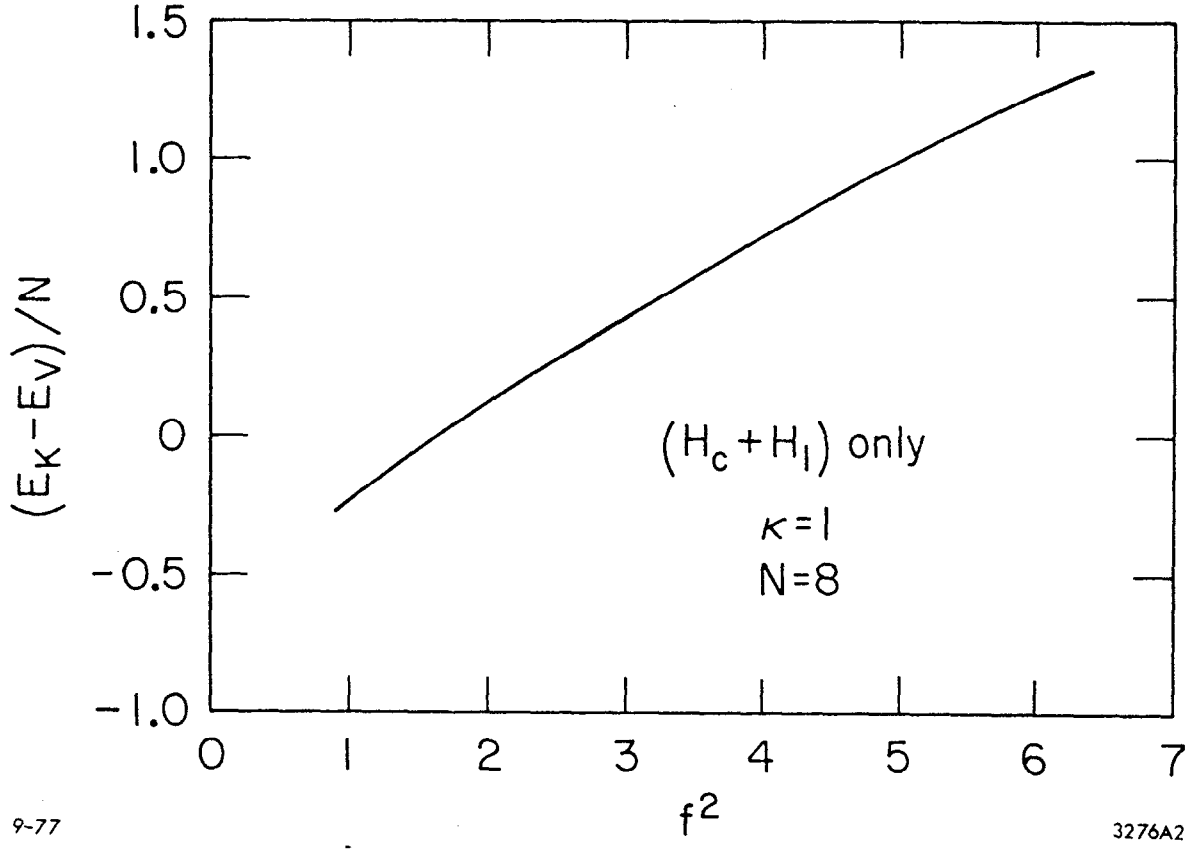
1.5
1.0
0.5
0
-0.5
-1.0
0
1
2
3
4
5
6
7
$(E_K - E_V)/N$
f^2
$(H_c + H_1)$ only
$\kappa = 1$
N=8
9-77
3276A2

Fig. 1

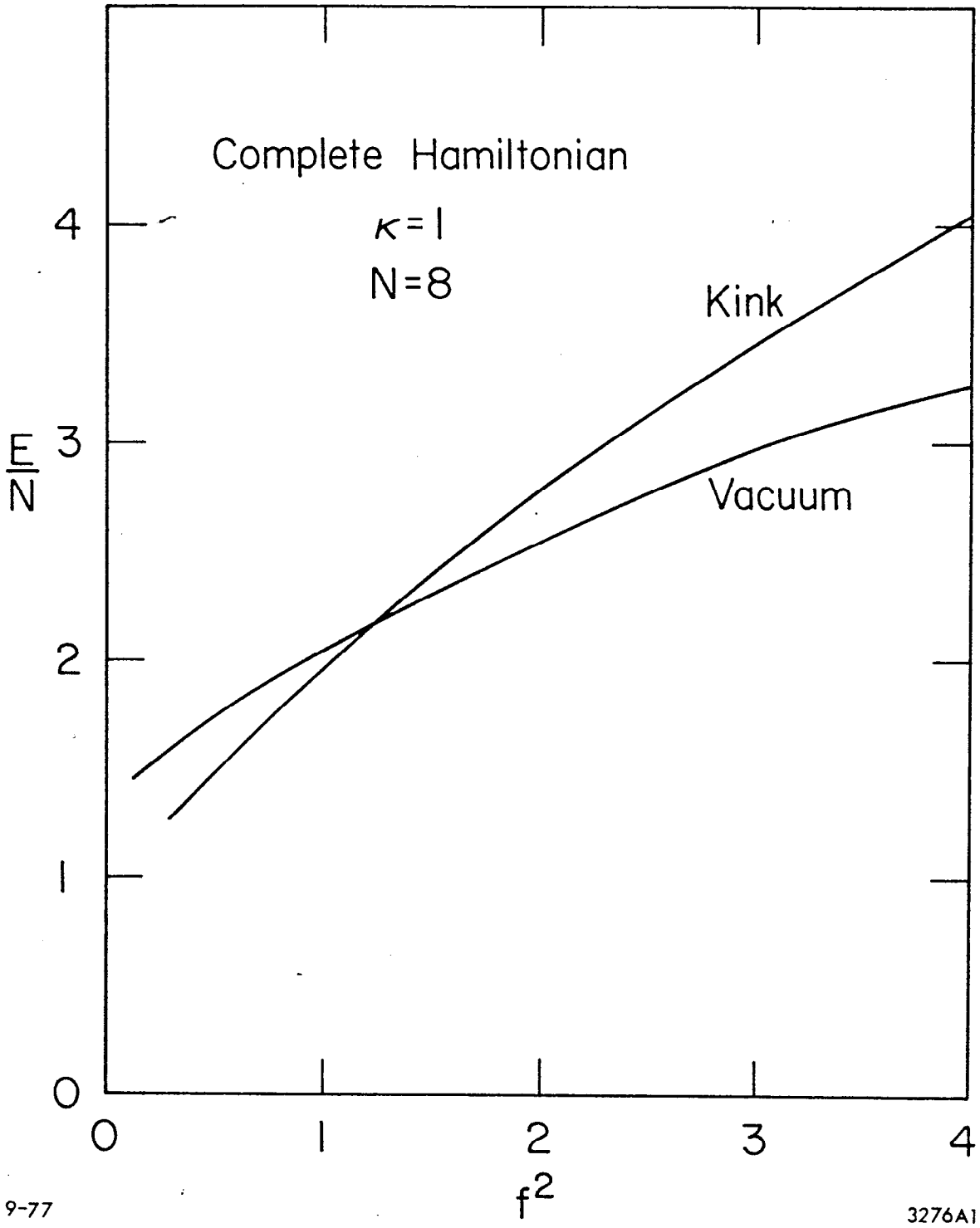
Complete Hamiltonian
κ=1
N=8
Kink
Vacuum
E/N
f²
0
1
2
3
4
9-77
3276A1

Fig. 2

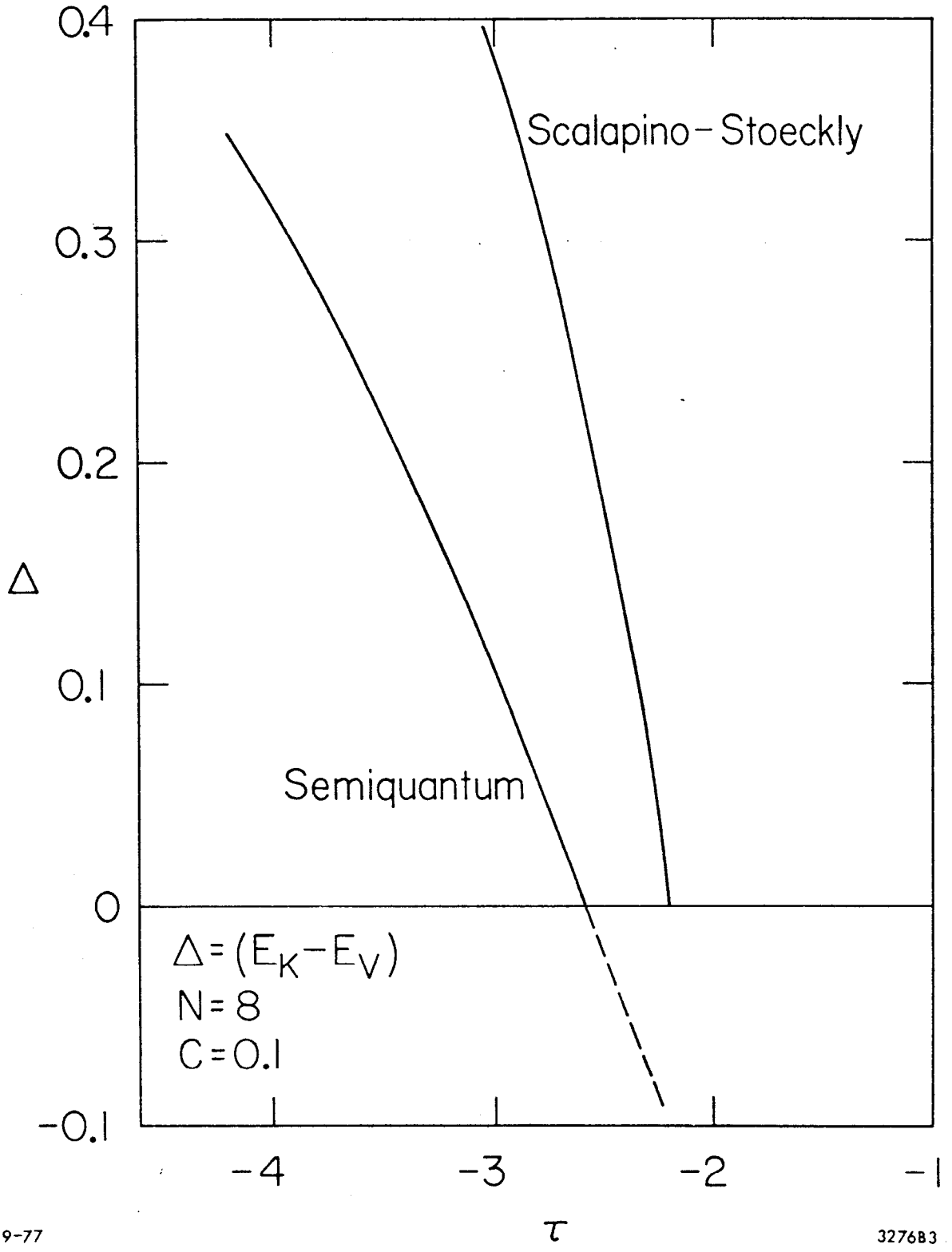
0.4
0.3
0.2
0.1
0
-0.1
Δ
Scalapino-Stoeckly
Semiquantum
Δ=(E_K-E_V)
N=8
C=0.1
-4
-3
-2
-1
τ
9-77
3276B3

Fig. 3