Magnon wave function and impurity effects in $S=1$ antiferromagnetic chains: A large-n approach

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A large-n approximation to the $S=1$ antiferromagnetic chain, using the symmetric tensor representation and its conjugate, is developed to order $1/n$ in order to calculate the magnon wave function and to study the effect of modifying the exchange coupling from J to J' on a single link. It is shown that a magnon bound state exists below the Haldane gap for arbitrarily small negative $J'-J$ but only above a certain critical value of $J'-J$ for positive values. In the former case the binding energy vanishes as $(J-J')^2$. [S0163-1829(99)09005-0]

I. INTRODUCTION AND REVIEW

Many features of $S=1$ Heisenberg antiferromagnetic chains have been understood in considerable detail using a combination of numerical techniques, approximate field theory methods and a model with bilinear plus biquadratic exchange for which the exact ground state is a simple valence bond solid (VBS).[1] There is considerable interest in the first excited state, the triplet magnon, separated from the ground state by the Haldane gap. However, this state is not known exactly even for the VBS model.

Investigations have been made of the Heisenberg model with the exchange coupling, J, modified to a different value, J', on a single link. It can be seen that a magnon bound state exists, localized near the modified link, whose energy goes to zero in the limit $J'/J \ll 1$ or $J'/J \gg 1$. However controversy remains over whether this bound state continues to exist for $|J'-J| \ll J$. The numerical results in Ref. 2 suggest that a critical value of $J'-J$ is required, for either sign of $J'-J$, in order for the bound state to exist. On the other hand, the more detailed numerical analysis of Ref. 3 suggests that this is only true for $J'>J$ while for $J'<J$ a magnon bound state exists for arbitrarily small values of $J-J'$. There is a well known theorem of one dimensional quantum mechanics which states that an arbitrarily weak attractive potential produces a bound state. (For a general and rigorous version of this theorem see Ref. 4.) Since the magnon behaves in many ways like an ordinary stable massive particle, one might expect that this theorem should be applicable to the modified link problem, but this connection has not been established.

The valence bond solid state was in fact encountered earlier[5] as the ground state of the bilinear exchange model in a certain large-n limit. This is defined by placing the symmetric 2-tensor representation of SU(n) on the even sites and its conjugate representation on the odd sites. This is sometimes referred to as a type of ''fermionic'' large-n limit because it arises in a model with 2 ''colors'' of fermions and n ''flavors'' with a projection onto color singlets on each site with 2 particles on the even sites and 2 holes ($n-2$ particles)

on the odd sites. This must be distinguished from various other large-n limits including the fermionic case with $n/2$ fermion of each color on each site and the bosonic model with n bosons on even sites and n anti-bosons on odd sites. In Ref. 5 the model was solved only to leading order in $1/n$. In this order, there remains a threefold ground state degeneracy which is lifted in higher orders. The VBS ground state is degenerate, to leading order in $1/n$, with the two fully dimerized ground states.[5] The Haldane gap of $O(1)$ was calculated in Ref. 5 but a determination of the corresponding magnon wave function requires going to order $1/n$, due to an infinite degeneracy at lowest order.

The purpose of this paper is to develop this large-n approximation to next order in $1/n$. We show that indeed the VBS state is the actual large-n ground state, the dimerized states having energy higher by $O(1/n)$. [It was erroneously claimed in Ref. 5 that this splitting only occurs at $O(1/n^2)$.] We also solve for the magnon wave function in the large-n approximation. In this approximation it corresponds to a type of soliton-antisoliton bound state held together by a linear potential. Our results allow us to estimate the accuracy of the large-n approximation for the physical case $n=2$. The results are somewhat encouraging. In any event, this approximation is useful because it qualitatively captures the essential physics. As an application, we show that the large-n approximation allows for a simple analytic treatment of the single modified link problem. We show that a bound state exists for arbitrarily small negative $J'-J$ but for positive $J'-J$ only when $J'-J$ is greater than a critical value, in agreement with Wang and Mallwitz[3] with the binding energy vanishing as $(J-J')^2$ in the $J'<J$ case. This result follows essentially from the theorem of one-dimensional quantum mechanics that an arbitrarily weak attractive potential always produces a bound state. The simplicity and generality of the argument suggests that it may remain true for all n.

For general n, the states on even sites are labeled by a pair of symmetric SU(n) particle indices:

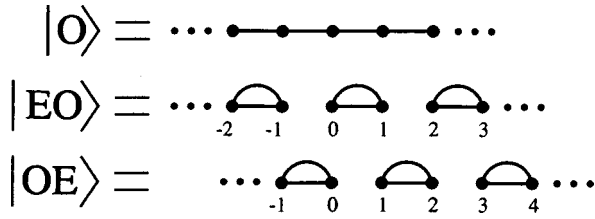$$|^{ij}\rangle = |^{ji}\rangle \qquad (1.1)$$

FIG. 1. Candidate ground states.

and on odd sites by a pair of symmetric hole indices:

$$|_{ij}\rangle = |_{ji}\rangle. \tag{1.2}$$

For all $n \geq 3$ even and odd sites are inequivalent. However, in the $n=2$ case they are equivalent with the 3 states on each link corresponding to the usual S^z eigenstates:

$$|^{11}\rangle = |_{22}\rangle = |S^z = 1\rangle,$$

$$|^{12}\rangle = |_{12}\rangle = |S^z = 0\rangle,$$

$$|^{22}\rangle = |_{11}\rangle = |S^z = -1\rangle. \tag{1.3}$$

For the 2-site model the Hamiltonian acts as

$$H|^{ij}{}_{,kl}\rangle = -(1/n)[\delta^i_k|^{mj}{}_{,ml}\rangle + \delta^i_l|^{mj}{}_{,km}\rangle + \delta^j_k|^{im}{}_{,ml}\rangle$$
$$+ \delta^j_l|^{im}{}_{,km}\rangle]. \tag{1.4}$$

For the case $n=2$,

$$H = \vec{S}_1 \cdot \vec{S}_2 - 1. \tag{1.5}$$

Throughout this paper we use the Einstein summation convention for a pair of repeated indices one upper and one lower. All SU(n) singlet states for the chain can be written with all upper indices contracted with lower indices. States with uncontracted upper and lower indices can be projected into irreducible representations of SU(n) by the usual processes of symmetrization and subtracting of traces.

For the 2-site model it is quite easy to see that the ground state is the SU(n) singlet $|^{ij}{}_{,ij}\rangle$ with energy -2 in the large-n limit. The factor of $1/n$ in Eq. (1.4) is canceled by $\delta^i_i = n$. Now consider a chain of arbitrary length. We may represent an arbitrary SU(n) singlet state by drawing a line (''valence bond'') between pairs of sites (one even and one odd) representing each contracted pair of indices. In the large-n limit the energy of such a state is simply equal to (-1) times the number of nearest neighbor valence bonds. Hence there are three degenerate ground states in the large-n limit, each of which has one nearest neighbor valence bond per link, on average. Two of these states are the dimerized states with a pair of valence bonds between each even site and the odd site to its right (or left). (See Fig. 1.) The third degenerate ground state is the valence bond solid state with a single valence bond between each neighboring pair of sites. (See Fig. 1). Only by going to higher order in $1/n$ will the degeneracy between the dimerized and VBS ground states be lifted. We show in the next section that the VBS state is the true unique ground state once $O(1/n)$ corrections are included.

In the large-n limit, the lowest excited state has one fewer nearest neighbor bond and hence an excitation energy of 1.

Assuming the VBS wave function at positive and negative spatial infinity, we see that all such states correspond to configurations with a string of dimers between the VBS states and dangling bonds separating the VBS regions from the dimer regions. (See Fig. 4.) These dangling bonds correspond to solitons between the nearly degenerate VBS and dimer approximate ground states. Such states are labeled by 2 indices, one upper and one lower corresponding to the two dangling bonds, $|^i{}_{,j}\rangle$. Subtracting the trace, $|^i{}_{,j}\rangle - (\delta^i_j/n)|^k{}_{,k}\rangle$ gives a state in the adjoint representation of SU(n). In the $n=2$ case this reduces to the spin-1 (triplet) representation. To lowest order in $1/n$, all such soliton-antisoliton ($s\bar{s}$) states have the same excitation energy, $+1$. It is necessary to go to $O(1/n)$ to split the degeneracy. Note that, if the soliton and antisoliton are separated by a distance, x, then the energy will grow as x/n because there is a region of size x which is in the ''wrong'' (dimerized) ground state, whose energy is higher by an amount of $O(1/n)$. Since the kinetic energy for the soliton and antisoliton is also $O(1/n)$, it follows that the binding energy is $O(1/n)$. We essentially must solve a lattice version of the Schrödinger equation for a particle in a linear potential. In general this will give several soliton-antisoliton bound states, each corresponding to an adjoint representation magnon. The number of stable bound states grows with increasing n.

In the next section we study the translationally invariant case, calculating the ground state and magnon states to $O(1/n)$. In Sec. III we consider the single modified link. A preliminary version of Sec. II appeared in Ref. 6.

II. GROUND STATE AND MAGNON STATES

A. Ground state

We label the candidate ground states as follows:

$$|0\rangle = |\ldots {}^{i_1 i_2}{}_{,i_2 i_3},{}^{i_3 i_4}{}_{,i_4 i_5}\ldots\rangle,$$

$$|EO\rangle = |\ldots {}^{i_1 i_2}{}_{,i_1 i_2},{}^{i_3 i_4}{}_{,i_3 i_4}\ldots\rangle,$$

$$|OE\rangle = |\ldots {}^{i_1 i_2}{}_{,i_3 i_4},{}^{i_3 i_4}{}_{,i_5 i_6}\ldots\rangle. \tag{2.1}$$

Thus the $|EO\rangle$ and $|OE\rangle$ states are related by a translation of one site. $|EO\rangle$ is the state in which the double bonds have even sites on the left and odd sites on the right and vice versa for $|OE\rangle$ (see Fig. 1). We expect the energy of the nonsymmetric states to be identical and that of the symmetric state to be different (since no symmetry connects it to the nonsymmetric states). Note that all three states have one bond per link on average. We now show that the VBS state $|0\rangle$ is the true ground state for large n.

We wish to calculate the energy of the symmetric ground state including the first order correction. This is

$$E_0^{(1)} = \langle 0|H|0\rangle / \langle 0|0\rangle. \tag{2.2}$$

Now, we first consider the action of the Hamiltonian on just two sites of the symmetric ground state. That is, we calculate $H_r|0\rangle$ where H_r is defined to be the term in H acting on sites r and $r+1$. We consider only the two sites on which H_r acts.

FIG. 2. β state.

FIG. 3. α state.
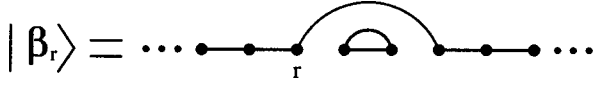
$$H_r|_{i_1i_2},^{i_2i_3}\rangle = -(1/n)[\delta_{i_1}^{i_2}|_{mi_2},^{mi_3}\rangle + \delta_{i_2}^{i_2}|_{i_1m},^{mi_3}\rangle + \delta_{i_1}^{i_3}|_{mi_2},^{i_2m}\rangle$$

$$+ \delta_{i_2}^{i_3}|_{i_1m},^{i_2m}\rangle]$$

$$= -(1/n)[|_{mi_1},^{mi_3}\rangle + n|_{i_1m},^{mi_3}\rangle + \delta_{i_1}^{i_3}|_{mi_2},^{i_2m}\rangle$$

$$+ |_{i_1m},^{i_3m}\rangle]. \qquad (2.3)$$

Renaming indices yields

$$H_r|_{i_1i_2},^{i_2i_3}\rangle = -(1+2/n)|_{i_1i_2},^{i_2i_3}\rangle - (1/n)\delta_{i_1}^{i_3}|_{mi_2},^{i_2m}\rangle. \qquad (2.4)$$

The first term is simply a multiple of the original state. The second term consists of a double bond and a delta function. This delta function serves to contract the two sites on either side of the two sites considered here thus producing a $|\beta_{r-1}\rangle$ state (see Fig. 2). Thus the action of the Hamiltonian on the entire symmetric ground state (L sites) is

$$H|0\rangle = -L(1+2/n)|0\rangle - (1/n)\sum_r|\beta_r\rangle. \qquad (2.5)$$

If we assume that the states $|0\rangle$ and $|\beta_r\rangle$ are orthogonal,

$$\langle 0|H|0\rangle = -L(1+2/n)\langle 0|0\rangle. \qquad (2.6)$$

And so

$$\langle 0|H|0\rangle/\langle 0|0\rangle = -L(1+2/n). \qquad (2.7)$$

In fact, the states $|0\rangle$ and $|\beta_r\rangle$ are not orthogonal. However, their overlap (divided by $\langle 0|0\rangle$) is order $1/n$ (see Appendix A) and thus the effect of the nonorthogonality is order $1/n^2$.

We now consider the nonsymmetric ground state. As above, we wish to calculate

$$E_{EO}^{(1)} = \langle EO|H|EO\rangle/\langle EO|EO\rangle \qquad (2.8)$$

which is the energy of the nonsymmetric ground state including the first order correction. Now, in this case we need to consider the action of the Hamiltonian on two inequivalent types of pairs of sites, those possessing a double bond between each other and those not. For a chain of L sites, there are $L/2$ of each type (assuming L is even).

First consider H_r with r even. Then H_r acts on a pair of sites possessing a double bond between each other. We need only consider the two sites on which the Hamiltonian acts.

$$H_r|_{i_1i_2},^{i_1i_2}\rangle = -(1/n)[\delta_{i_1}^{i_1}|_{mi_2},^{mi_2}\rangle + \delta_{i_2}^{i_1}|_{i_1m},^{mi_2}\rangle + \delta_{i_1}^{i_2}|_{mi_2},^{i_1m}\rangle$$

$$+ \delta_{i_2}^{i_2}|_{i_1m},^{i_1m}\rangle]$$

$$= -(1/n)[n|_{mi_2},^{mi_2}\rangle + |_{i_1m},^{mi_1}\rangle + |_{mi_1},^{i_1m}\rangle$$

$$+ n|_{i_1m},^{i_1m}\rangle]. \qquad (2.9)$$
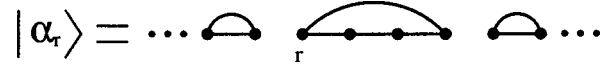
We see that all of the states in the above expression are simply the original state with a change of dummy variables. Therefore,

$$H_r|_{i_1i_2},^{i_1i_2}\rangle = -2(1+1/n)|_{i_1i_2},^{i_1i_2}\rangle. \qquad (2.10)$$

Now consider H_r with r odd. Then H_r acts on a pair of sites not possessing a double bond between each other. Again, we only consider the two sites on which the Hamiltonian acts. Remembering that the indices of the leftmost site are contracted to the left and those of the rightmost site are contracted to the right,

$$H_r|_{i_1i_2},^{i_3i_4}\rangle = -(1/n)[\delta_{i_1}^{i_3}|_{mi_2},^{mi_4}\rangle + \delta_{i_2}^{i_3}|_{i_1m},^{mi_4}\rangle + \delta_{i_1}^{i_4}|_{mi_2},^{i_3m}\rangle$$

$$+ \delta_{i_2}^{i_4}|_{i_1m},^{i_3m}\rangle]. \qquad (2.11)$$

In each of the states in the above expression, there exists a single bond between the two sites considered (that is, sites r and $r+1$), a single bond between sites $r-1$ and r resulting from one of the original dummy indices on site r remaining and a single bond between sites $r+1$ and $r+2$ resulting from one of the original dummy indices on site $r+1$ remaining. Also, in each case, the delta function serves to contract the indices on sites $r-1$ and $r+2$. Thus, the action of the Hamiltonian on the state $|EO\rangle$ is

$$H|EO\rangle = -L(1+1/n)|EO\rangle - (4/n)\sum_r|\alpha_{2r}\rangle, \qquad (2.12)$$

where $|\alpha_r\rangle$ is defined in Fig. 3.

If we assume the states $|EO\rangle$ and $|\alpha_{2r}\rangle$ are orthogonal,

$$\langle EO|H|EO\rangle = -L(1+1/n)\langle EO|EO\rangle. \qquad (2.13)$$

And so

$$\langle EO|H|EO\rangle/\langle EO|EO\rangle = -L(1+1/n). \qquad (2.14)$$

In fact, the states $|EO\rangle$ and $|\alpha_r\rangle$ are not orthogonal. However, their overlap (divided by $\langle EO|EO\rangle$ is order $1/n$ (see Appendix A) and thus the effect of the nonorthogonality is order $1/n^2$. Therefore, the above result holds to order $1/n$.

Comparing the values found in Eqs. (2.7) and (2.14) we see that the symmetric ground state is the true ground state (having the lower energy) which agrees with known results. The energy difference per site is $1/n + O(1/n^2)$.

Considering states of the form

$$|\psi_1\rangle = |0\rangle + (a/L)\sum_r|\beta_r\rangle,$$

$$|\psi_2\rangle = |EO\rangle + [b/(2L)]\sum_r|\alpha_{2r}\rangle \qquad (2.15)$$

and calculating the ground state energies variationally produces the same results as those found above to $O(1/n)$ (see Appendix B). Extrapolating the large-n approximation to $n = 2$, and taking into account the shift of the Hamiltonian by

FIG. 4. Soliton-antisoliton state. Note that an uncontracted upper index is represented by an upwards facing free link while an uncontracted lower index is represented by a downwards facing free link.

a constant noted in Eq. (1.5), the estimates of the ground state per site to 0th and 1st order in $1/n$ are 0 and -1, respectively. The numerical result for $n=2$ is -1.401485.[8] Thus we see that the inclusion of the terms of first order in $1/n$ brings us closer to the numerical result.

B. The first excited states

Since our Hamiltonian counts the number of nearest neighbor bonds to leading order in $1/n$, the excited states consist of an uncontracted lower index at some site and an uncontracted upper index at some other site (that is, they have one fewer nearest neighbor bond). These uncontracted indices can be thought of as solitons/antisolitons interpolating between two "ground states." We label such sites as in Fig. 4.

Note that r labels the uncontracted upper index and s labels the uncontracted lower index. We will assume that the indices on sites r and s are different to eliminate mixing with the singlet states (in which the indices on sites r and s are contracted). Thus these states transform under the adjoint representation of SU(n), reducing to spin 1 in the SU(2) case. We define

$$x \equiv r-s. \quad (2.16)$$

Note that r must be even and s must be odd implying that x is odd. Since the energy of the nonsymmetric state is higher than that of the symmetric state by $1/n(+O(1/n^2))$, we expect the soliton-antisoliton pair to experience a linear (in x) confining potential like that encountered in quark confinement.

Let us first consider $H|\widetilde{r,s}\rangle$ for $|s-r|>1$. We need only consider the effects of $H_{r-1}, H_r, H_{s-1}, H_s$. The effects of the terms in the Hamiltonian acting on the other links have already been calculated.

We will first consider the effect of H_{r-1}. We let i_1 be the index contracted between the sites $r-2$ and $r-1$, i_2 the index contracted between sites $r-1$ and r, and i_3 the free index on site r. Now,

$$H_{r-1}|_{i_1 i_2}{}^{,i_2 i_3}\rangle = -(1/n)[\delta_{i_1}^{i_2}|_{mi_2}{}^{,mi_3}\rangle + \delta_{i_2}^{i_2}|_{i_1 m}{}^{,mi_3}\rangle$$

$$+ \delta_{i_1}^{i_3}|_{mi_2}{}^{,i_2 m}\rangle + \delta_{i_2}^{i_3}|_{i_1 m}{}^{,i_2 m}\rangle]$$

$$= -(1/n)[|_{mi_1}{}^{,mi_3}\rangle + n|_{i_1 m}{}^{,mi_3}\rangle$$

$$+ \delta_{i_1}^{i_3}|_{mi_2}{}^{,i_2 m}\rangle + |_{i_1 m}{}^{,i_3 m}\rangle]$$

$$= -(1/n)[(n+2)|_{mi_1}{}^{,mi_3}\rangle + \delta_{i_1}^{i_3}|_{mi_2}{}^{,i_2 m}\rangle]. \quad (2.17)$$

We recognize the first term as a constant times the original state (with i_2 renamed m). The second term represents a double bond between states $r-1$ and r while the delta function serves to create a free index (equal to the free index in

the original state) on site $r-2$. Thus, from this second term, we obtain the state $|\widetilde{r-2,s}\rangle$. And so,

$$H_{r-1}|\widetilde{r,s}\rangle = -(1+2/n)|\widetilde{r,s}\rangle - (1/n)|\widetilde{r-2,s}\rangle. \quad (2.18)$$

We now consider the effect of H_r. Using the same indices as above and letting i_4 and i_5 be the indices representing the double bond between sites $r+1$ and $r+2$, we calculate

$$H_r|^{i_2 i_3}{}_{,i_4 i_5}\rangle = -(1/n)[\delta_{i_2}^{i_4}|^{mi_3}{}_{,mi_5}\rangle + \delta_{i_3}^{i_4}|^{i_2 m}{}_{,mi_5}\rangle + \delta_{i_2}^{i_5}|^{mi_3}{}_{,i_4 m}\rangle$$

$$+ \delta_{i_3}^{i_5}|^{i_2 m}{}_{,i_4 m}\rangle]. \quad (2.19)$$

Now, in the second and fourth terms above, the index i_2 will contract to the left creating a bond, the index m represents a bond between sites r and $r+1$, the indices i_5 and i_4 (respectively) produce a bond between sites $r+1$ and $r+2$, and the delta function serves to move the soliton (same free index) to site $r+2$. Thus from these terms, we obtain the state $|\widetilde{r+2,s}\rangle$. In the first and third terms above, the soliton (represented by the free index i_3) remains on site r, the index m represents a bond between sites r and $r+1$, and the indices i_5 and i_4 (respectively) produce a bond between sites $r-1$ and $r+2$. Thus, in effect, we have replaced the bond between sites $r-1$ and r and one of the bonds between sites $r+1$ and $r+2$ with one bond between sites r and $r+1$ and one between sites $r-1$ and $r+2$. Thus, we have reduced the number of nearest neighbor bonds by one. This increases the energy by order 1. Therefore, we ignore these terms in our analysis. So,

$$H_r|\widetilde{r,s}\rangle = -(2/n)|\widetilde{r+2,s}\rangle. \quad (2.20)$$

By symmetry,

$$H_s|\widetilde{r,s}\rangle = -(1+2/n)|\widetilde{r,s}\rangle - (1/n)|\widetilde{r,s+2}\rangle,$$

$$H_{s-1}|\widetilde{r,s}\rangle = -(2/n)|\widetilde{r,s-2}\rangle. \quad (2.21)$$

Therefore, neglecting terms with energy higher by an amount of order 1,

$$H|\widetilde{s,r}\rangle = -[(L-1)(1+2/n) - (|x|-1)/n]|\widetilde{r,s}\rangle$$

$$- (2/n)(|\widetilde{r+2,s}\rangle + |\widetilde{r,s-2}\rangle) - (1/n)(|\widetilde{r-2,s}\rangle$$

$$+ |\widetilde{r,s+2}\rangle) \quad (\text{for } |r-s|>1). \quad (2.22)$$

We now consider the action of the Hamiltonian on the state $|\widetilde{r,r+1}\rangle$ (that is, for $x=1$). The action on $|\widetilde{r,r-1}\rangle$ ($x=-1$) will follow by symmetry. We only need to calculate the effect of H_r; the rest are known. Assume the index i_1 is contracted to the left, i_4 is contracted to the right, and i_2, i_3 are free and consider

$$H_r|_{i_1 i_2},^{i_3 i_4}\rangle = -(1/n)[\delta_{i_1}^{i_3}|_{m i_2},^{m i_4}\rangle + \delta_{i_2}^{i_3}|_{i_1 m},^{m i_4}\rangle + \delta_{i_1}^{i_4}|_{m i_2},^{i_3 m}\rangle$$

$$+ \delta_{i_2}^{i_4}|_{i_1 m},^{i_3 m}\rangle]. \qquad (2.23)$$

Now, the first term results in the state $|r,r-1\rangle$. The second term results in a delta function times the symmetric ground state. The third term results in a state with a soliton on site r, an antisoliton on site $r+1$ and bonds between sites r and $r+1$ as well as $r-1$ and $r+2$ (this state has one fewer nearest neighbor bonds). The fourth term results in the state $|r+2,r+1\rangle$. Thus, ignoring states with higher energy of order 1 and assuming that $i_2 \neq i_3$,

$$H_r|\widetilde{r,r+1}\rangle = -(1/n)(|\widetilde{r,r-1}\rangle + |\widetilde{r+2,r+1}\rangle) \quad (2.24)$$

and similarly

$$H_r|\widetilde{r,r-1}\rangle = -(1/n)(|\widetilde{r-2,r-1}\rangle + |\widetilde{r,r+1}\rangle). \qquad (2.25)$$

At first glance, it seems as though our Hamiltonian is non-Hermitian. However, we can see that this is simply due to the normalization of the $|\widetilde{r,s}\rangle$ states. The normalization for sites $r+1$ through $s-1$ is the same as that for an $|EO\rangle$ state of length $|x|-1$. We see from Appendix A that this normalization is $[2n(n+1)]^{(|x|-1)/2}$. The normalization for the rest of the sites is the same as that for an $|0\rangle$ state of length $L-|x|+1$ (where L is the total number of sites in the state $|r,s\rangle$). It is shown in Appendix A that this normalization is $((n+1)^{L-|x|+1}-1)/n$. Thus the total normalization is

$$\langle \widetilde{r,s}|\widetilde{r,s}\rangle = [2n(n+1)]^{(|x|-1)/2}[((n+1)^{L-|x|+1}-1)/n]. \qquad (2.26)$$

In the large L and large n limits (taking L large first as usual), this reduces to $2^{(|x|-1)/2}n^{L-1}$. Thus we define the "properly" normalized states

$$|r,s\rangle = 2^{-(|x|-1)/4}n^{(1-L)/2}|\widetilde{r,s}\rangle. \qquad (2.27)$$

With this normalization, the Hamiltonian becomes

$$(H+(L-1)(1+2/n))|r,s\rangle$$

$$= [(|x|-1)/n]|r,s\rangle - (\sqrt{2}/n)(|r+2,s\rangle + |r,s-2\rangle$$

$$+ |r-2,s\rangle + |r,s+2\rangle) \quad \text{for} \quad |x|>1,$$

$$(H+(L-1)(1+2/n))|r,r+1\rangle$$

$$= -(1/n)(|r,r-1\rangle + |r+2,r+1\rangle),$$

$$(H+(L-1)(1+2/n))|r,r-1\rangle$$

$$= -(1/n)(|r-2,r-1\rangle + |r,r+1\rangle). \qquad (2.28)$$

Now, we expect the first excited states to be translationally invariant. Therefore we define the translationally invariant states

$$|x\rangle = (1/\sqrt{2L})\sum_r |2r,2r+x\rangle, \qquad (2.29)$$

where the multiplicative constant ensures that $\langle x|x\rangle = 1$. (This follows from the normalization of $|r,s\rangle$ since it is

shown in Appendix C that $\langle \widetilde{r',s'}|\widetilde{r,s}\rangle$ is of order n^{L-2} or smaller if $r' \neq r$ and/or $s' \neq s$.)

Therefore, for $|x|>1$,

$$(H+(L-1)(1+2/n))|x\rangle$$

$$= (H+(L-1)(1+2/n))\left[(1/\sqrt{2L})\sum_r \left|2r,2r+x\right\rangle\right]$$

$$= (1/\sqrt{2L})\sum_r [((|x|-1)/n)|2r,2r+x\rangle$$

$$- (\sqrt{2}/n)(|2r+2,2r+x\rangle + |2r,2r+x-2\rangle$$

$$+ |2r-2,2r+x\rangle + |2r,2r+x+2\rangle)]$$

$$= [(|x|-1)/n]|x\rangle - (2\sqrt{2}/n)(|x-2\rangle + |x+2\rangle). \qquad (2.30)$$

And for $x = \pm 1$

$$(H+(L-1)(1+2/n))|1\rangle = -(2/n)|-1\rangle - (2\sqrt{2}/n)|3\rangle,$$

$$(H+(L-1)(1+2/n))|-1\rangle = -(2/n)|1\rangle - (2\sqrt{2}/n)|-3\rangle. \qquad (2.31)$$

Although the assumption will prove to be a poor one in future calculations, if we assume that our wave function varies slowly, we can change our Hamiltonian into continuous form by Taylor expanding the states involved to obtain

$$|x \pm 2\rangle \approx |x\rangle \pm 2(d/dx)|x\rangle + 2(d^2/dx^2)|x\rangle. \qquad (2.32)$$

Therefore,

$$|x+2\rangle + |x-2\rangle \approx 2|x\rangle + 4(d^2/dx^2)|x\rangle + \cdots. \qquad (2.33)$$

Making this substitution into the expression for our Hamiltonian and ignoring the fact that the action of the Hamiltonian is slightly different for $x = \pm 1$ than it is for $|x|>1$,

$$H = -[(L-1)(1+2/n) - 4\sqrt{2}/n] + (|x|-1)/n$$

$$- (8\sqrt{2}/n)d^2/dx^2. \qquad (2.34)$$

This is the Hamiltonian for a particle in a linear potential with x corresponding to the difference coordinate of the soliton-antisoliton pair. Thus, in this approximation, the soliton-antisoliton pair experiences a linear confinement potential similar to that encountered in quark confinement. If the pair becomes too separated, it splits into two pairs much like the quark-antiquark pair comprising a meson (this will be discussed in more detail later). The exact Hamiltonian (in the large-n limit) is of this form but the kinetic energy term is not equal to p^2 as the above approximation would suggest.

We now define a general state

$$|\psi\rangle = \sum_{x \text{ odd}} \psi(x)|x\rangle. \qquad (2.35)$$

We then seek the lowest energy eigenstate of this form. This will be the first excited state. Thus, we wish to find the function $\psi(x)$, defined on the odd integers such that

$$(H-(E_0+1+2/n))|\psi\rangle = \delta E|\psi\rangle$$

$$\Rightarrow \sum_{x \text{ odd}} \psi(x)(H-(E_0+1+2/n))|x\rangle = \delta E \sum_{x \text{ odd}} \psi(x)|x\rangle,$$

$$(2.36)$$

where $E_0 = -L(1+2/n)$ is the ground state energy. Thus

$$-(2/n)[\psi(-1)|1\rangle + \psi(1)|-1\rangle] - (2\sqrt{2}/n)[\psi(1)|3\rangle$$

$$+\psi(-1)|-3\rangle] + \sum_{x \text{ odd},|x|>1} \psi(x)[((|x|-1)/n)|x\rangle$$

$$-(2\sqrt{2}/n)(|x+2\rangle + |x-2\rangle)]$$

$$= \delta E \sum_{x \text{ odd}} \psi(x)|x\rangle. \qquad (2.37)$$

We now take the overlap of both sides with the state $\langle x'|$. We have from the calculations of Appendix C that the overlap $\langle x'|x\rangle$ is order n^{L-1} if $x'=x$ and is of smaller order in n if $x' \neq x$. Thus, from the overlap with $|1\rangle$ we obtain, to order $1/n$,

$$-(2/n)\psi(-1)-(2\sqrt{2}/n)\psi(3) = \delta E\psi(1) \Rightarrow \psi(3)$$

$$= -(2\psi(-1)+n\delta E\psi(1))/(2\sqrt{2}). \qquad (2.38)$$

And for $|x|>1$ we obtain, to order $1/n$,

$$-(2\sqrt{2}/n)[\psi(x-2)+\psi(x+2)] + ((|x|-1)/n)\psi(x)$$

$$= \delta E\psi(x) \Rightarrow \psi(x+2)$$

$$= [(|x|-n\delta E-1)/(2\sqrt{2})]\psi(x)-\psi(x-2). \qquad (2.39)$$

Now, since the Hamiltonian is an even function of x, we expect $\psi(x)$ to be either an even or an odd function of x. We can easily prove that the first excited state is even by a contradiction argument inspired by Feynman. Assume that the first excited state is odd [that is, $\psi(x)$ is an odd function of x]. Now define

$$g(x) = -\psi(x), \quad x<0$$

$$= \psi(x), \quad x>0 \qquad (2.40)$$

which is obviously an even function of x. Now, the two states defined by these functions obviously have the same normalization. Thus, we can ignore this normalization when comparing the energies of the two states. The energy of the state $|\psi\rangle$ relative to E_0+1+2/n is

$$E_\psi = -(4/n)\psi(-1)\psi(1) + \sum_{x \text{ odd},|x|>1} [((|x|-1)/n)\psi(x)^2$$

$$-(2\sqrt{2}/n)(\psi(x)\psi(x-2)+\psi(x)\psi(x+2))]$$

$$= (4/n)\psi(1)^2 + 2\sum_{x \text{ odd},x>1} [((|x|-1)/n)\psi(x)^2$$

$$-(2\sqrt{2}/n)(\psi(x)\psi(x-2)+\psi(x)\psi(x+2))] \qquad (2.41)$$

while the energy of the state defined by $g(x)$ is

$$E_g = -(4/n)g(-1)g(1) + \sum_{x \text{ odd},|x|>1} [((|x|-1)/n)g(x)^2$$

$$-(2\sqrt{2}/n)(g(x)g(x-2)+g(x)g(x+2))]$$

$$= -(4/n)\psi(1)^2 + 2\sum_{x \text{ odd},x>1} [((|x|-1)/n)\psi(x)^2$$

$$-(2\sqrt{2}/n)(\psi(x)\psi(x-2)+\psi(x)\psi(x+2))]$$

$$= E_\psi - (8/n)\psi(1)^2. \qquad (2.42)$$

Thus the function defined by $g(x)$ has a lower [or equal if $\psi(1)=0$] energy than the state $|\psi\rangle$. This contradicts the claim that $|\psi\rangle$ is the first excited state. Thus the first excited state is an even function of x.

Therefore, to find the first excited state, we can set $\psi(1) = 1$ and need only determine $\psi(x)$ for positive x. Since ψ is even, $\psi(-1) = \psi(1) = 1$ and so Eq. (2.38) becomes

$$\psi(3) = -(n\delta E+2)/2\sqrt{2}. \qquad (2.43)$$

Equation (2.43) gives $\psi(3)$ in terms of $\psi(1)=1$ and $n\delta E$. Equation (2.39) is a recursion relation defining the $\psi(x)$ for x odd. Now, in order for the state $|\psi\rangle$ to be normalizable, we need the sum $\Sigma_{z=0}^{\infty}\psi(2z+1)^2$ to converge. We expect that this will only occur for discrete values of $n\delta E$. Thus, using the above recursion relation, we plot the value of a partial sum of the above series for various values of $n\delta E$. This plot is shown is Fig. 5.

We find that the first excited state has $n\delta E \approx -3.747$ (see Fig. 6). The wave function for this energy is shown in Fig. 7.

Thus the energy gap of the first excited state to order $1/n$ is

$$\Delta = E_1 - E_0 = 1 + 2/n + \delta E \approx 1 + 2/n - 3.747/n = 1 - 1.747/n. \qquad (2.44)$$

Thus, for $n=2$, $\Delta \approx 0.1265$. Numerically and experimentally, this value is found to be 0.41050.[7] Since we obtain $\Delta = 1$ to leading order, and $\Delta \approx 0.1265$ to order $1/n$ it seems plausible that were one to include higher orders, the calculated value of Δ might approach 0.41050 in an oscillatory manner.

Using our numerical results to order $1/n$ we can also calculate how many bound states exist. We assume that a necessary and sufficient condition for the stability of a given state is that it has less than twice the energy of the first excited state (otherwise, it would decay into two or more states of lower energy). Thus, the mth excited state will be stable if and only if

$$1 + 2/n + (n\delta E)_m/n < 2(1-1.747/n) \Rightarrow (n\delta E)_m < n - 5.494. \qquad (2.45)$$

Now, we find that the second excited state is a parity odd state with $(n\delta E)_2 \approx 0.467$. Thus, the second excited state is stable if and only if

$$0.467 < n-5.494 \Rightarrow n > 5.96. \qquad (2.46)$$

Thus, for $n=2$ there exists only one stable magnon in agreement with σ model, numerical and experimental results.
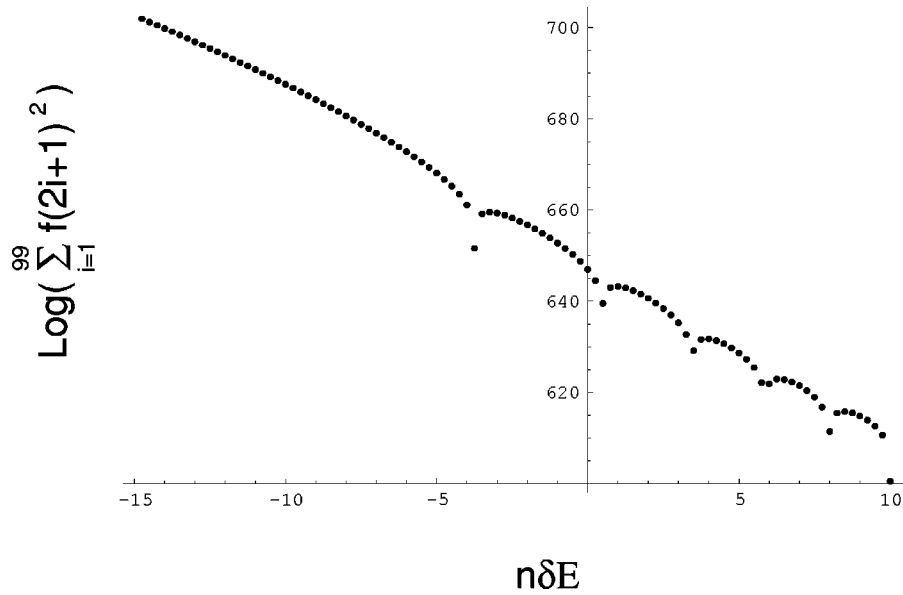
FIG. 5. Log of partial normalization sum versus $n\,\delta E$. The log of the sum is plotted to allow the wide range to be displayed more clearly.

III. SINGLE MODIFIED LINK

We now consider the case in which one of the links in our chain has a coupling which may differ from that of the other links. In the following discussion, we will find it useful to use the coordinates

$$x \equiv s - r,$$

$$y \equiv s + r - 1 \qquad (3.1)$$

rather than r and s to label our magnon states. The fact that r must be even and s must be odd implies that either $x = 4p + 1, y = 4q$ or $x = 4p + 3, y = 4q + 2$ where p and q are both integers. Thus although x must be odd and y must be even, not all combinations of odd x and even y are allowed.

We define the coupling between sites 0 and 1 to be J' and between all the other sites to be J. As in the previous calcu-lations, we will choose our units of energy so that $J = 1$. We assume that $J' - 1$ is $O(1/n)$. This implies that the ground state will remain unchanged to leading order in $1/n$ and that its energy will be (to order $1/n$)

$$E_0 = -(L + J' - 1)(1 + 2/n). \qquad (3.2)$$

Note that this redefinition of E_0 corresponds with our earlier definition in the case $J' = 1$. We now define H_0 to be the Hamiltonian without the modified link with the new gener-alized E_0 substituted for the old [that is, we define $H_0 - E_0$ $-(1 + 2/n)$ to be the right sides of Eq. (2.28)].

We can write the true Hamiltonian (with the modified link) as H_0 plus terms correcting for the modified link. That is, we can write the true Hamiltonian H as

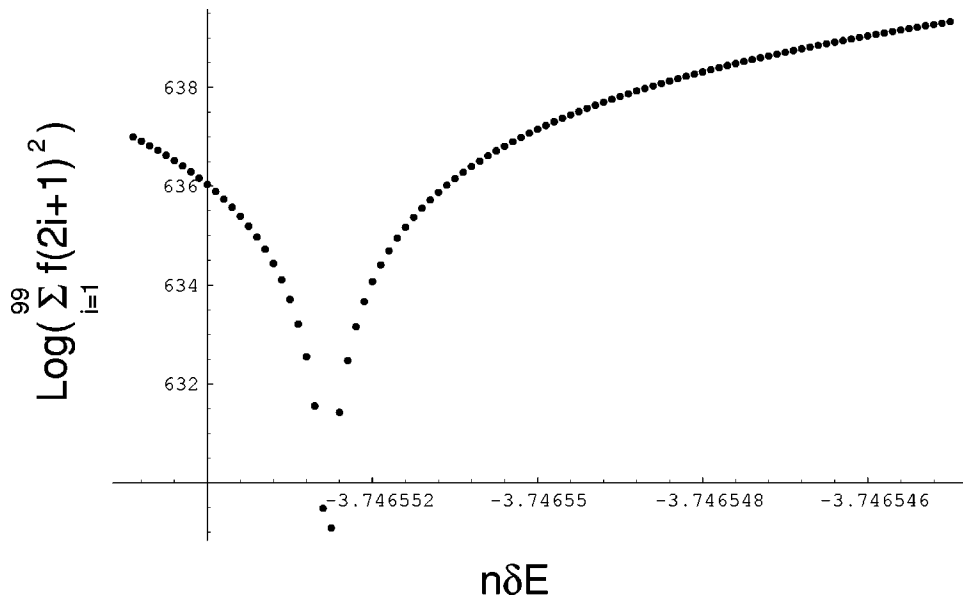$$H = H_0 + \lambda H_k + \lambda V, \qquad (3.3)$$

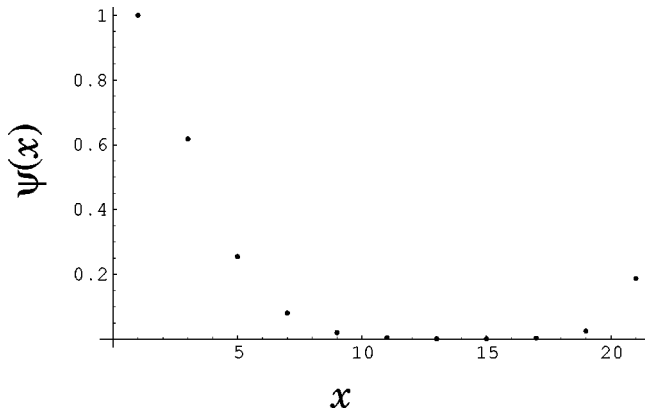FIG. 6. A blow up of Fig. 5 near the first minimum.

FIG. 7. Ground state wave function. Since the wave function is even, it is only plotted for positive x. Note that the wave function starts to diverge at about $x = 19$. This is due to the fact that the eigenvalue found is merely a numerical approximation to the true eigenvalue.

where $\lambda = 1 - J' = O(1/n)$ and

$$H_k|r,s\rangle = (\sqrt{2}/n)|r+2,s\rangle \quad \text{for} \quad r=0, \quad s\neq 1$$
$$= (\sqrt{2}/n)|r,s-2\rangle \quad \text{for} \quad s=1, \quad r\neq 0$$
$$= (1/n)[|r+2,s\rangle + |r,s-2\rangle] \quad \text{for} \quad r=0, \quad s=1$$
$$= 0 \quad \text{otherwise},$$

$$V|r,s\rangle = -(1+2/n)|r,s\rangle, \quad \text{for} \quad r\leq 0, \quad s\geq 1$$
$$= +(1+2/n)|r,s\rangle, \quad \text{for} \quad r\geq 2, \quad s\leq -1$$
$$= 0 \quad \text{otherwise.} \tag{3.4}$$

Thus λH_k is a modified kinetic energy operator and λV is a modified potential. Now, since we are considering the large n limit, we can neglect H_k and drop the $2/n$ term in V since these are lower order in n. [Recall that λ is $O(1/n)$.] Thus, if we now change coordinates to x and y, Eq. (3.4) becomes to leading order in $1/n$

$$H_k|x,y\rangle = 0,$$

$$V|x,y\rangle = -|x,y\rangle, \quad \text{for} \quad x\geq 1, \quad |y|\leq x-1$$
$$= +|x,y\rangle, \quad \text{for} \quad x\leq -3, \quad |y|\leq -(x+3)$$
$$= 0 \quad \text{otherwise.} \tag{3.5}$$

Thus, the modified link not only breaks translational symmetry, it also breaks parity symmetry (reflection about a site) since V is not symmetric with respect to parity. Our potential arises from the fact we have defined our energy such that zero energy corresponds to the modified link being outside the soliton-antisoliton pair where there is a single bond between neighboring sites. If the modified link is instead between the soliton and the antisoliton, it is either between two sites not bonded together (in this case, $V = -1$) or between two sites with a double bond (in this case $V = +1$). We see from Eq. (3.5) and Fig. 8 that if the modified link is between the soliton and antisoliton (that is, V is nonzero) then, it must lie between two sites not bonded together if $x\geq 1$ and on a double bond if $x\leq -3$.
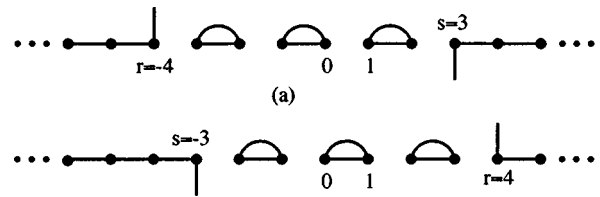

(a)

FIG. 8. (a) Typical configuration with $r\leq 0, s\geq 1 (\Rightarrow x\geq 1)$. There is no bond on the modified link 01. (b) Typical configuration with $r\geq 2, s\leq -1 (\Rightarrow x\leq -1)$. There is a double bond on the modified link 01.

Our goal is to determine the nature of possible bound states of the Hamiltonian given above. Let us define

$$|\psi_0\rangle = \sum_{\text{allowed } x,y} \psi_0(x)|x,y\rangle \tag{3.6}$$

to be the translationally invariant state we found in the case of the unmodified Hamiltonian, normalized so that

$$\sum_{x \text{ odd}} \psi_0(x)^2 = 1. \tag{3.7}$$

We see that in the limit of large L (recall L is the length of our chain), $|\psi_0\rangle$ has energy $E_0 + \Delta$ (note the change in the definition of E_0 here) since the state is spread along the entire length of the chain (that is, it is independent of y) while the modified link occurs only between two sites and thus its effect becomes negligible. Therefore, we expect that an eigenstate of the modified Hamiltonian will be bound (that is, be normalizable) if and only if it has energy less than $E_0 + \Delta$. Let $|\phi\rangle$ be such a bound eigenstate where

$$|\phi\rangle = \sum_{\text{allowed } x,y} \phi(x,y)|x,y\rangle. \tag{3.8}$$

Since $|\phi\rangle$ is a bound state, we know that $\langle\phi|\phi\rangle < \infty$. Thus, the energy of the state $|\phi\rangle$ is

$$E_\phi = \langle\phi|H_0|\phi\rangle/\langle\phi|\phi\rangle + \lambda\langle\phi|V|\phi\rangle/\langle\phi|\phi\rangle$$
$$\geq E_0 + \Delta + \lambda\langle\phi|V|\phi\rangle/\langle\phi|\phi\rangle, \tag{3.9}$$

where the inequality is due to the fact that, by definition, Δ is the lowest energy eigenstate of $H_0 - E_0$ (and therefore $E_0 + \Delta$ is the lowest energy eigenstate of H_0). Now, we know that $\phi(x,y)$ must decay rapidly at large $|x|$ due to the linear potential present in the Hamiltonian. We see from Eq. (3.5) and Fig. 9 that for small x, the potential V is only non-zero for small y. Since our perturbation is small (order λ), we expect that for small x and y, $\phi \approx \psi$ (that is, the corrections are order λ and thus can be ignored to leading order). Therefore Eq. (3.9) becomes, to leading order in λ,

$$E_\phi \geq E_0 + \Delta + \lambda\langle\psi_0|V|\psi_0\rangle/\langle\phi|\phi\rangle. \tag{3.10}$$

The fact that $\psi_0(x)$ is independent of y makes $\langle\psi_0|V|\psi_0\rangle$ particularly easy to calculate. Since $\psi_0(x)$ is an even function of x, both signs of x are weighted evenly in the sum $\langle\psi_0|V|\psi_0\rangle$. Also, the fact that $\psi_0(x)$ is independent of y means that the weighting is the same (for a given value of $|x|$) no matter where the modified link is. Now, for a given $|x|$, there is always one more link with no bond than with a double bond. This can be seen easily in Fig. 8. Thus, for each
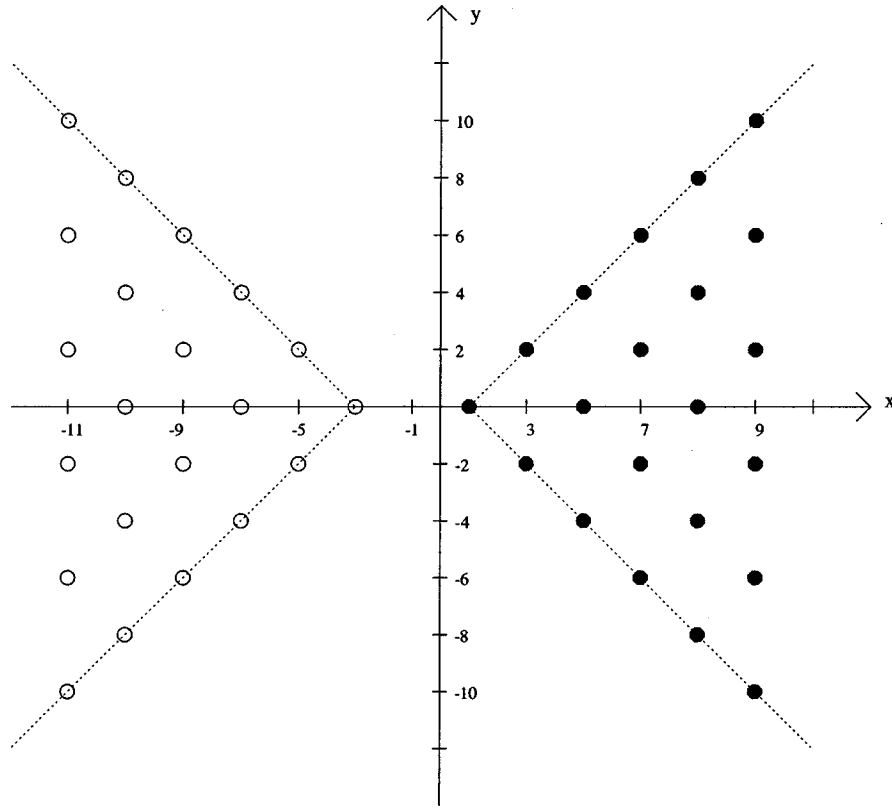
FIG. 9. Modified potential V. An open circle denotes a coordinate at which V has the value $+1$ and a closed circle denotes a coordinate at which V has the value -1.

$|x|$, the sum over $+x$ and $-x$ and the respective allowed values of y in $\langle \psi_0 | V | \psi_0 \rangle$ equals -1 since V takes on the value -1 one more time than it takes on the value $+1$. Thus,

$$\langle \psi_0 | V | \psi_0 \rangle = -\sum_{x \geq 1 \text{ odd}} \psi_0(x)^2 = -1/2 \qquad (3.11)$$

since this sum is equal to half the normalization sum in Eq. (3.7). Therefore,

$$E_\phi \geq E_0 + \Delta - \lambda/(2\langle \phi | \phi \rangle). \qquad (3.12)$$

Since $\langle \phi | \phi \rangle > 0$, if $\lambda < 0$ then $E_\phi \geq E_0 + \Delta$ which is a contradiction since this implies $|\phi\rangle$ is not a bound state. Thus, in the small λ limit, it is only possible for a bound state to occur if $\lambda > 0$ (that is, if $J' < J$). However, we do not yet know that a bound state *does* exist in this case. To see this, we will use a variational argument.

We choose as our variational state the normalized wave function,

$$|\psi\rangle = \sum_{\text{allowed } x,y} \psi(x,y)|x,y\rangle$$

$$\text{where} \quad \psi(x,y) = A\psi_0(x)e^{-\epsilon|y|}$$

$$\text{and} \quad A \to \sqrt{4\epsilon} \quad \text{as} \quad \epsilon \to 0. \qquad (3.13)$$

To see how the normalization constant A (chosen so that $\langle \psi | \psi \rangle = 1$) was obtained, recall that either $x=4p+1, y=4q$ or $x=4p+3, y=4q+2$ where p and q are integers. Thus,

$$\sum_{\text{allowed } y} (e^{-\epsilon|y|})^2$$

$$= \sum_{q \in Z} e^{-8\epsilon|q|} = 2\sum_{q=0}^{\infty} e^{-8\epsilon q} - 1$$

$$= 2/(1 - e^{-8\epsilon}) - 1 = (1 + e^{-8\epsilon})/(1 - e^{-8\epsilon}) \approx 1/(4\epsilon)$$

$$\text{or} \ = 2e^{-4\epsilon} \sum_{q=0}^{\infty} e^{-8\epsilon|q|} = 2e^{-4\epsilon}/(1 - e^{-8\epsilon}) \approx 1/(4\epsilon)$$

$$\qquad (3.14)$$

which gives us our normalization constant A in the small ϵ limit. We choose the trial wave function given above since it reduces to the translationally invariant wave function in the limit $\epsilon \to 0$ (we expect $\epsilon \to 0$ as $\lambda \to 0$). We will minimize the energy of this trial wave function with respect to ϵ.

In terms of the coordinates x and y and using the same normalization for the $|x,y\rangle$ states as was used for the $|r,s\rangle$ states, H_0 is given by

$$(H_0 - (E_0 + 1 + 2/n))|x,y\rangle$$

$$= ((|x| - 1)/n)|x,y\rangle$$

$$- (\sqrt{2}/n)(|x+2,y+2\rangle + |x+2,y-2\rangle$$

$$+ |x-2,y+2\rangle + |x-2,y-2\rangle) \quad \text{for} \ |x| > 1,$$

$$(H_0 - (E_0 + 1 + 2/n))|1,y\rangle$$

$$= -(\sqrt{2}/n)(|3,y+2\rangle + |3,y-2\rangle)$$

$$- (1/n)(|-1,y+2\rangle + |-1,y-2\rangle),$$

$$(H_0 - (E_0 + 1 + 2/n))|-1,y\rangle$$

$$= -(\sqrt{2}/n)(|-3,y+2\rangle + |-3,y-2\rangle) - (1/n)(|1,y+2\rangle$$

$$+ |1,y-2\rangle). \qquad (3.15)$$

We would like to separate H_0 into its x and y components. One possible method for doing this would be to introduce lattice derivatives. However, a problem arises when we attempt this. We would like to add and subtract the states $|x+2,y\rangle$ and $|x-2,y\rangle$ from the right hand side of Eq. (3.15). However, given that the state $|x,y\rangle$ exists, neither of the states $|x+2,y\rangle$ or $|x-2,y\rangle$ can exist (this follows from the permissible values of x and y). However, the states $|-(x+2),y\rangle$ and $|-(x-2),y\rangle$ do exist. Although adding and subtracting these states from the right hand side of Eq. (3.15) may seem counterintuitive, the fact that $\psi(x,y)$ is an even function of x allows us to effectively separate H_0 into its x and y components in this way. Thus, we rewrite the $|x|>1$ portion of Eq. (3.15) as

$$(H_0 - (E_0 + 1 + 2/n))|x,y\rangle$$

$$= ((|x|-1)/n)|x,y\rangle - (\sqrt{2}/n)(|x+2,y+2\rangle$$

$$+ |x+2,y-2\rangle - 2|-(x+2),y\rangle + |x-2,y+2\rangle$$

$$+ |x-2,y-2\rangle) - 2|-(x-2),y\rangle)$$

$$- (2\sqrt{2}/n)(|-(x+2),y\rangle + |-(x-2),y\rangle$$

$$- 2|x,y\rangle) - (4\sqrt{2}/n)|x,y\rangle$$

$$= ((|x|-1)/n - 4\sqrt{2}/n)|x,y\rangle - (\sqrt{2}/n)(\Delta_y|x+2,y\rangle$$

$$+ \Delta_y|x-2,y\rangle) - (2\sqrt{2}/n)\Delta_x|x,y\rangle, \qquad (3.16)$$

where

$$\Delta_x|x,y\rangle = |-(x+2),y\rangle + |-(x-2),y\rangle - 2|x,y\rangle,$$

$$\Delta_y|x,y\rangle = |x,y+2\rangle + |x,y-2\rangle - 2|-x,y\rangle \qquad (3.17)$$

are our lattice second derivative operators. Similarly,

$$(H_0 - (E_0 + 1 + 2/n))|1,y\rangle$$

$$= -(\sqrt{2}/n)\Delta_y|3,y\rangle - (1/n)\Delta_y|-1,y\rangle - (2\sqrt{2}/n)|-3,y\rangle$$

$$- (2/n)|1,y\rangle,$$

$$(H_0 - (E_0 + 1 + 2/n))|-1,y\rangle$$

$$= -(\sqrt{2}/n)\Delta_y|-3,y\rangle - (1/n)\Delta_y|1,y\rangle - (2\sqrt{2}/n)|3,y\rangle$$

$$- (2/n)|-1,y\rangle. \qquad (3.18)$$

We can now roughly separate H_0 into its x and y components. Define H_0^y as the sum of the terms in Eqs. (3.16) and (3.18) involving Δ_y and H_0^x as the sum of the remaining terms. Since $\psi_0(x)$ is an even function of x and is independent of y, $\Delta_y|\psi_0\rangle = 0$. Thus $H_0^y|\psi_0\rangle = 0$ and so H_0^x is precisely the Hamiltonian we encountered in the case $J' = J$ up to a constant relating to the redefinition of E_0.

We now calculate the expectation energy of our trial wave function:

$$E_\epsilon = \langle\psi|H|\psi\rangle$$

$$= E_0 + \Delta + \langle\psi|H_0^y|\psi\rangle + \lambda\langle\psi|V|\psi\rangle. \qquad (3.19)$$

Now, although Δ_y is defined as an operator on the state $|x,y\rangle$, through a change of variables, we can treat it as an operator on the coefficients $\psi(x,y)$. For $y>0$ (note that y is always even),

$$\Delta_y\psi(x,y) = \sqrt{4\epsilon}\,\psi_0(x)[e^{-\epsilon(y+2)} + e^{-\epsilon(y-2)} - 2e^{-\epsilon y}]$$

$$= \psi(x,y)[e^{-2\epsilon} + e^{2\epsilon} - 2]$$

$$= \psi(x,y)[4\epsilon^2 + O(\epsilon^4)], \qquad (3.20)$$

where we have used the fact that $\psi_0(x)$ is an even function. Similarly, for $y<0$,

$$\Delta_y\psi(x,y) = \psi(x,y)[4\epsilon^2 + O(\epsilon^4)]. \qquad (3.21)$$

Now, for $y=0$,

$$\Delta_y\psi(x,0) = \sqrt{4\epsilon}\,\psi_0(x)[2e^{-2\epsilon} - 2]$$

$$= \psi(x,0)[-4\epsilon + 4\epsilon^2 + O(\epsilon^3)]. \qquad (3.22)$$

Notice that the case $y=0$ agrees with the case $y\neq0$ in the ϵ^2 term. Therefore, dropping terms of order ϵ^3 and higher and using the fact that $\psi(x,y)$ is an even function of x we see that

$$\langle\psi|H_0^y|\psi\rangle = -(\sqrt{2}/n)4\epsilon^2 \sum_{\text{allowed } |x|>1,y} [\psi(x,y)\psi(-(x-2),y) + \psi(x,y)\psi(-(x+2),y)]$$

$$- (\sqrt{2}/n)(-4\epsilon) \sum_{\text{allowed } |x|>1} [\psi(x,0)\psi(-(x-2),0) + \psi(x,0)\psi(-(x+2),0)]$$

$$- 4\epsilon^2 \sum_{\text{allowed } y} [(\sqrt{2}/n)\psi(1,y)\psi(-3,y) + (1/n)\psi(1,y)\psi(1,y)] + 4\epsilon[(\sqrt{2}/n)\psi(1,0)\psi(-3,0)$$

$$+ (1/n)\psi(1,0)\psi(1,0)]$$

$$- 4\epsilon^2 \sum_{\text{allowed } y} [(\sqrt{2}/n)\psi(-1,y)\psi(3,y) + (1/n)\psi(-1,y)\psi(-1,y)]. \qquad (3.23)$$

Now, we can use the fact that $\psi(-x,y)=\psi(x,y)$ to convert sums over all x to (two times) sums over positive x. Also, the $x=\pm 1$ cases missing in the first two sums above, are present in the third and fourth sums. Finally, in the second sum of Eq. (3.23), we must remember that only certain values of x are allowed if $y=0$. The allowed values are $\ldots, -7, -3, 1, 5, 9, \ldots$. Thus, using the fact that $\psi_0(x)$ is an even function of x, we can convert a sum over these allowed values into a sum over all odd positive x. Thus, we may simplify the above expression to

$$\langle\psi|H_0^y|\psi\rangle = -(\sqrt{2}/n)4\epsilon^2\left[4\sum_{\text{allowed } x\geq 1,y}\psi(x,y)\psi(x+2,y)\right]$$

$$+(\sqrt{2}/n)(4\epsilon)\left[2\sum_{\text{odd } x\geq 1}\psi(x,0)\psi(x+2,0)\right]$$

$$-(1/n)4\epsilon^2\left[2\sum_{\text{allowed } y}\psi(1,y)\psi(1,y)\right]$$

$$+(4\epsilon/n)\psi(1,0)\psi(1,0). \qquad (3.24)$$

Now, a factor of ϵ occurs from the normalization of ψ which is canceled when a sum over y is performed. Thus, all the terms in the above end up being $O(\epsilon^2)$. Thus, the above becomes

$$\langle\psi|H_0^y|\psi\rangle = -(\sqrt{2}/n)16\epsilon^2\sum_{\text{odd } x\geq 1}\psi_0(x)\psi_0(x+2)$$

$$+(\sqrt{2}/n)8\epsilon\sum_{\text{odd } x\geq 1}4\epsilon\psi_0(x)\psi_0(x+2)$$

$$-(8\epsilon^2/n)\psi_0(1)^2+(16\epsilon^2/n)\psi_0(1)^2$$

$$=(\epsilon^2/n)[16\sqrt{2}\theta+8\psi_0(1)^2], \qquad (3.25)$$

where

$$\theta=\sum_{\text{odd } x\geq 1}\psi_0(x)\psi_0(x+2)>0. \qquad (3.26)$$

It is shown in Appendix D that ψ_0 is everywhere positive and so we know θ is positive.

We now consider the term V, using the same reasoning as when we were calculating $\langle\phi|V|\phi\rangle$ [that is, for small x, y and $\epsilon, \psi(x,y)\approx A\psi_0(x)$], we see that

$$\langle\psi|V|\psi\rangle\approx A^2\langle\psi_0|V|\psi_0\rangle=(4\epsilon)(-1/2)=-2\epsilon. \qquad (3.27)$$

Therefore, the expectation energy of our trial wave function is

$$E_\epsilon=E_0+\Delta+8\kappa\epsilon^2/n-2\lambda\epsilon,$$

$$\text{where} \quad \kappa=2\sqrt{2}\theta+\psi_0(1)^2>0. \qquad (3.28)$$

In order to minimize this quantity with respect to ϵ, we set $dE/d\epsilon=0$ to obtain

$$0=16\kappa\epsilon/n-2\lambda$$

$$\Rightarrow\epsilon=n\lambda/(8\kappa) \qquad (3.29)$$

which gives an energy of (to leading order in n)

$$E_{\min}=E_0+\Delta-n\lambda^2/(8\kappa)<E_0+\Delta. \qquad (3.30)$$

Thus, we know that the true magnon state of the modified link Hamiltonian has an energy which is less than $E_0+\Delta$ and thus is bound. Note that our minimizing value of ϵ is positive which is necessary for our trial wave function to be normalizable. Numerically, θ is calculated to be approximately 0.279 and thus κ is approximately 1.134. Therefore, for $n=2$ and $\lambda>0$,

$$E_{\min}\approx E_0+\Delta-0.221\lambda^2. \qquad (3.31)$$

So far we have presented the wave function of Eq. (3.13) as merely a variational one so that the energy $E_{\min}$ is just an upper bound. However, we expect the variational wave function to become sufficiently accurate that the actual bound state energy is given by Eq. (3.30) in the limit $\lambda\to 0^+$. This follows from the following observations. First of all, $\psi(x,y)$ is an exact eigenfunction in the translationally invariant case, $\lambda=0$, for any ϵ. Secondly, even for $\lambda\neq 0$, $\psi(x,y)$ satifies exactly the Schrödinger equation outside the dotted lines in Fig. 9. For any fixed value of x and sufficiently small λ [and hence ϵ as determined by Eq. (3.29)] $\psi(x,y)$ is nearly constant as a function of y between the dotted lines of Fig. 9. The true bound state wave function must also have this property in order for $\langle\psi|H_0^y|\psi\rangle$ to be small. Thus the actual value of the wave function in this region is not important as long as it is nearly constant and joins smoothly with the wave function outside the dotted lines, properties enjoyed by $\psi(x,y)$. At $|x|\geq 1$, $\psi(x,y)$ goes to 0 rapidly. [From the continuum form of the Hamiltonian in Eq. (2.34) we may estimate $\psi_0(x)\propto e^{-|x|^{3/2}/(3\times 2^{3/4})}$.] Again we expect the actual bound state wave function to have this property so $\psi(x,y)$ should be a sufficient approximation in the large $|x|$ region. Therefore we expect $\psi(x,y)$ [with ϵ given by Eq. (3.29)] to be a good first approximation to the actual bound state wave function at small λ and the energy of Eq. (3.30) to be asymptotically correct. The situation is similar to the case of one-dimensional quantum mechanics with a weak potential, the single dimension corresponding to y. Despite the fact that ψ depends on 2 coordinates x and y, the present problem is rather different than the two-dimensional case with a short-range potential due to the confining x-dependent potential. Essentially, x acts as an internal degree of freedom of the magnon whereas y represents its location. In particular, the quadratic dependence of the binding energy on the strength of the potential also occurs in the one-dimensional case.

Thus, if we assume that $E_{\min}$ is not merely an upper bound on the energy but actually a good approximation to it, we can plot the energy as a function of $\lambda=(J'-J)/J$. This is done in Fig. 10. Note that the critical value of $\lambda>0$ at which the energy becomes negative (implying the existence of a bound state) has not been calculated and so no significance should be attributed to the value indicated on the plot. Also, the exact form of the energy dependence for $\lambda>0$ is unknown. In Fig. 10 it is plotted with the same quadratic dependence as in the case $\lambda<0$. Based on our experience in the previous section with extrapolating large-n results to $n=2$, we might expect the prefactor of 0.221 in Eq. (3.31) to
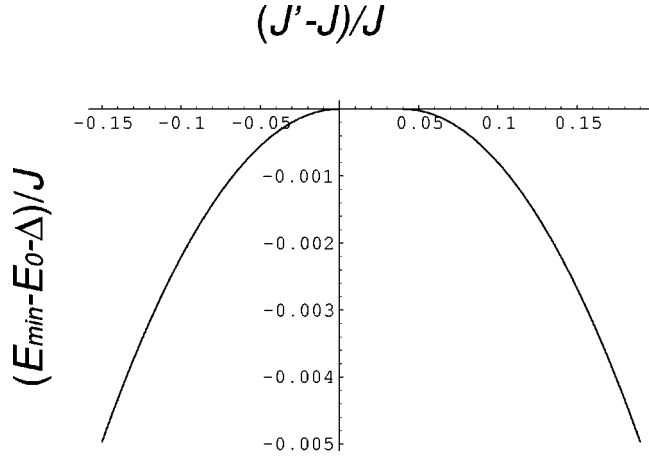
$(J'\text{-}J)/J$

FIG. 10. $E_{\min}$ versus $(J'-J)/J$. The critical value of $J'>J$ for which the energy becomes negative has been assigned an arbitrary value. The form of the energy dependence for J' larger than this critical value has been assumed to be the same as the dependence for $J'<J$.

only be accurate to within a factor of 2 or so. However, the fact that the functional dependence is quadratic in $(J'-J)$ is likely to be exact, since it is a general result for one-dimensional quantum systems, as emphasized above. The numerical results in Ref. 3 are probably consistent with quadratic behavior at small negative $(J'-J)$ but with a smaller prefactor.

Therefore, we have shown that in the case of a modified link, in the limit $J'\to J$, a bound state exists if and only if $J'<J$. This results from the fact that between the antisoliton and soliton there is one more pair of neighboring sites with no bond between them than with a double bond.

APPENDIX A: CALCULATION OF OVERLAPS ARISING IN DETERMINATION OF TRUE GROUND STATE

1. Calculation of $\langle 0|0\rangle$

For the symmetric ground state, we first consider just two of the sites:

$$\langle {}^{i_1 i_2}, {}_{i_2 i_3}|{}_{j_1 j_2}, {}^{j_2 j_3}\rangle = (\delta^{i_1}_{j_1}\delta^{i_2}_{j_2}+\delta^{i_1}_{j_2}\delta^{i_2}_{j_1})(\delta^{j_2}_{i_2}\delta^{j_3}_{i_3}+\delta^{j_2}_{i_3}\delta^{j_3}_{i_2})$$
$$= (n+2)\delta^{i_1}_{j_1}\delta^{j_3}_{i_3}+\delta^{i_1}_{i_3}\delta^{j_3}_{j_1}. \quad (A1)$$

We then consider three sites:

$$\langle {}^{i_1 i_2}, {}_{i_2 i_3}, {}^{i_3 i_4}|{}_{j_1 j_2}, {}^{j_2 j_3}, {}_{j_3 j_4}\rangle$$
$$= (\delta^{i_1}_{j_1}\delta^{i_2}_{j_2}+\delta^{i_1}_{j_2}\delta^{i_2}_{j_1})(\delta^{j_2}_{i_2}\delta^{j_3}_{i_3}+\delta^{j_2}_{i_3}\delta^{j_3}_{i_2})(\delta^{i_3}_{j_3}\delta^{i_4}_{j_4}+\delta^{i_3}_{j_4}\delta^{i_4}_{j_3})$$
$$= [(n+2)\delta^{i_1}_{j_1}\delta^{j_3}_{i_3}+\delta^{i_1}_{i_3}\delta^{j_3}_{j_1}](\delta^{i_3}_{j_3}\delta^{i_4}_{j_4}+\delta^{i_3}_{j_4}\delta^{i_4}_{j_3})$$
$$= [(n+1)(n+2)+1]\delta^{i_1}_{j_1}\delta^{i_4}_{j_4}+\delta^{i_1}_{j_4}\delta^{i_4}_{j_1}. \quad (A2)$$

We see that this pattern will continue. That is, for L sites, with L even, we obtain

$$\langle 0|0\rangle = a_L\delta^{i_1}_{j_1}\delta^{j_{L+1}}_{i_{L+1}}+\delta^{i_1}_{i_{L+1}}\delta^{j_{L+1}}_{j_1}, \quad (A3)$$

where a_L is given by the recursion relation

$$a_{L+1}=(n+1)a_L+1. \quad (A4)$$

However, this is simply a geometric series:

$$a_1=1,$$

$$a_2=(n+1)+1,$$

$$a_3=(n+1)^2+(n+1)+1,$$

$$a_L=\sum_{i=0}^{L-1}(n+1)^i=[(n+1)^L-1]/n. \quad (A5)$$

Thus for a finite chain of L sites,

$$\langle 0|0\rangle = [((n+1)^L-1)/n]\delta^{i_1}_{j_1}\delta^{j_{L+1}}_{i_{L+1}}+\delta^{i_1}_{i_{L+1}}\delta^{j_{L+1}}_{j_1}. \quad (A6)$$

If we now wish to impose periodic boundary conditions, this is equivalent to replacing i_{L+1} by i_1 and j_{L+1} by j_1 in the above expression. Doing this, and contracting the indices yields

$$\langle 0|0\rangle = [((n+1)^L-1)/n]n+n^2=(n+1)^L+n^2-1. \quad (A7)$$

Taking $L\to\infty$ first, then large n, this may be approximated as

$$\langle 0|0\rangle = (n+1)^L. \quad (A8)$$

2. Calculation of $\langle EO|EO\rangle$

To calculate this matrix element, we can use the previous result. Each double bond can be thought of as a two site $|0\rangle$ state with periodic boundary conditions. Thus, for L even

$$\langle EO|EO\rangle = [(n+1)^2+n^2-1]^{L/2}=[2n(n+1)]^{L/2}. \quad (A9)$$

3. Calculation of $\langle\alpha_r|\alpha_r\rangle$

We again use our previous results to calculate this matrix element. The four sites which comprise the soliton-antisoliton pair can be thought of as a four site $|0\rangle$ state with periodic boundary conditions while the remainder of the $|\alpha_r\rangle$ state is identical to the $|EO\rangle$ state. Thus, for L even

$$\langle\alpha_r|\alpha_r\rangle = [(n+1)^4+n^2-1][2n(n+1)]^{(L-4)/2}. \quad (A10)$$

4. Calculation of $\langle\beta_r|\beta_r\rangle$

The overlap of $|\beta_r\rangle$ with itself consists of the overlap of a two site $|EO\rangle$ state (or equivalently a two site $|0\rangle$ state) with itself and an $(L-2)$ site $|0\rangle$ state with itself. Thus, for L even

$$\langle\beta_r|\beta_r\rangle = 2n(n+1)[(n+1)^{L-2}+n^2-1]. \quad (A11)$$
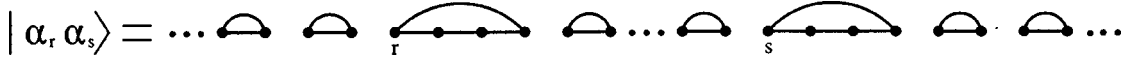
FIG. 11. Double alpha state.

5. Calculation of $\langle 0|\beta_r\rangle$

We need only consider the four sites which comprise the soliton-antisoliton pair. The remainder of the matrix element is identical to $\langle 0|0\rangle$:

$$\langle {}^{i_1 i_2},_{i_2 i_3},{}^{i_3 i_4},_{i_4 i_5}|_{j_1 j_2},{}^{j_3 j_4},_{j_3 j_4},{}^{j_2 j_5}\rangle$$

$$= (\delta_{j_1}^{i_1}\delta_{j_2}^{i_2} + \delta_{j_2}^{i_1}\delta_{j_1}^{i_2})(\delta_{i_2}^{j_3}\delta_{i_3}^{j_4} + \delta_{i_3}^{j_3}\delta_{i_2}^{j_4})(\delta_{j_3}^{i_3}\delta_{j_4}^{i_4} + \delta_{j_4}^{i_3}\delta_{j_3}^{i_4})$$

$$\times(\delta_{i_4}^{j_2}\delta_{i_5}^{j_5} + \delta_{i_5}^{j_2}\delta_{i_4}^{j_5})$$

$$= (\delta_{j_1}^{i_1}\delta_{j_2}^{j_3}\delta_{i_3}^{j_4} + \delta_{j_1}^{i_1}\delta_{i_3}^{j_3}\delta_{j_2}^{j_4} + \delta_{j_2}^{i_1}\delta_{j_1}^{j_3}\delta_{i_3}^{j_4} + \delta_{j_2}^{i_1}\delta_{i_3}^{j_3}\delta_{j_1}^{j_4})$$

$$\times(\delta_{j_3}^{i_3}\delta_{j_4}^{j_2}\delta_{i_5}^{j_5} + \delta_{j_3}^{i_3}\delta_{i_5}^{j_2}\delta_{j_4}^{j_5} + \delta_{j_4}^{i_3}\delta_{j_3}^{j_2}\delta_{i_5}^{j_5} + \delta_{j_4}^{i_3}\delta_{i_5}^{j_2}\delta_{j_3}^{j_5})$$

$$= (2n^2 + 6n + 4)\delta_{j_1}^{i_1}\delta_{i_5}^{j_5} + 2(n+1)\delta_{i_5}^{i_1}\delta_{j_1}^{j_5}$$

$$= 2(n+1)[(n+2)\delta_{j_1}^{i_1}\delta_{i_5}^{j_5} + \delta_{i_5}^{i_1}\delta_{j_1}^{j_5}]. \tag{A12}$$

We now note that this is precisely $2(n+1)$ times the expression we obtain from a two site $\langle 0|0\rangle$ aside from a renaming of indices. Thus, since the remaining $L-4$ sites of the $|\beta_r\rangle$ state are identical to those for the $|0\rangle$ state

$$\langle 0|\beta_r\rangle = 2(n+1)[(n+1)^{L-2} + n^2 - 1] \approx [2/(n+1)]\langle 0|0\rangle. \tag{A13}$$

6. Calculation of $\langle EO|\alpha_r\rangle$

As in the previous calculation, we need only consider the four sites which comprise the soliton-antisoliton pair. The remainder of the matrix element is identical to $\langle EO|EO\rangle$:

$$\langle {}^{i_1 i_2},_{i_1 i_2},{}^{i_3 i_4},_{i_3 i_4}|_{j_1 j_2},{}^{j_2 j_3},_{j_3 j_4},{}^{j_4 j_1}\rangle$$

$$= (\delta_{j_1}^{i_1}\delta_{j_2}^{i_2} + \delta_{j_2}^{i_1}\delta_{j_1}^{i_2})$$

$$\times(\delta_{i_1}^{j_2}\delta_{i_2}^{j_3} + \delta_{i_2}^{j_2}\delta_{i_1}^{j_3})(\delta_{i_3}^{j_3}\delta_{j_4}^{i_4} + \delta_{j_4}^{i_3}\delta_{j_3}^{i_4})(\delta_{i_3}^{j_4}\delta_{i_4}^{j_1} + \delta_{i_4}^{j_4}\delta_{i_3}^{j_1})$$

$$= [(2n+2)\delta_{j_1}^{j_3}][(2n+2)\delta_{j_3}^{j_1}]$$

$$= 4n(n+1)^2. \tag{A14}$$

Recall that for a four site $|EO\rangle$ chain,

$$\langle EO|EO\rangle = 4n^2(n+1)^2. \tag{A15}$$

Thus, adding in the other $L-4$ sites, we obtain

$$\langle EO|\alpha_r\rangle = (1/n)\langle EO|EO\rangle = (1/n)[2n(n+1)]^{L/2}$$

$$\approx (1/n)\langle EO|EO\rangle. \tag{A16}$$

7. Calculation of $\langle \alpha_r|\alpha_s\rangle$ and $\langle EO|\alpha_r\alpha_s\rangle$ for $|r-s|>3$

In this case, the two soliton-antisoliton pairs do not overlap. Thus, comparison with the calculation of $\langle EO|\alpha_r\rangle$ yields

$$\langle \alpha_r|\alpha_s\rangle = (1/n^2)[2n(n+1)]^{L/2} \approx (1/n)^2\langle EO|EO\rangle. \tag{A17}$$

8. Calculation of $\langle \alpha_t|\alpha_r\alpha_s\rangle$ for $|r-s|>3, |r-t|>3, |s-t|>3$

Here $|\alpha_r\alpha_s\rangle$ is defined in the obvious way in Fig. 11. In this case, none of the soliton-antisoliton pairs overlap. Thus, comparison with the calculation of $\langle EO|\alpha_r\rangle$ yields

$$\langle \alpha_t|\alpha_r\alpha_s\rangle = (1/n^3)[2n(n+1)]^{L/2}. \tag{A18}$$

9. Calculation of $\langle \beta_r|\beta_s\rangle$ and $\langle 0|\beta_r\beta_s\rangle$ for $|r-s|>3$

As in Sec. A 7, comparison with the calculation of $\langle 0|\beta_r\rangle$ yields

$$\langle \beta_r|\beta_s\rangle = 4(n+1)^2[(n+1)^{L-4} + n^2 - 1]$$

$$\approx [2/(n+1)]^2\langle 0|0\rangle. \tag{A19}$$

10. Calculation of $\langle \beta_t|\beta_r\beta_s\rangle$ for $|r-s|>3, |r-t|>3, |s-t|>3$

Here $|\beta_r\beta_s\rangle$ is defined in the obvious way in Fig. 12. Comparison with the calculation of $\langle 0|\beta_r\rangle$ yields

$$\langle \beta_t|\beta_r\beta_s\rangle = 8(n+1)^3[(n+1)^{L-6} + n^2 - 1]. \tag{A20}$$

APPENDIX B: VARIATIONAL VERIFICATION OF TRUE GROUND STATE

We consider states of the form

$$|\psi_1\rangle = |0\rangle + a|\beta\rangle,$$

$$|\psi_2\rangle = |EO\rangle + b|\alpha\rangle, \tag{B1}$$

where

$$|\beta\rangle \equiv (1/L)\sum_r |\beta_r\rangle,$$

$$|\alpha\rangle \equiv [1/(2L)]\sum_r |\alpha_{2r}\rangle. \tag{B2}$$

We will see that variations in the parameters a and b do not affect the energies of the states at order $1/n$ thus verifying that the symmetric ground state is the true ground state (in the large n limit). Throughout this section, we will make the assumption that for large L, when the Hamiltonian acts on
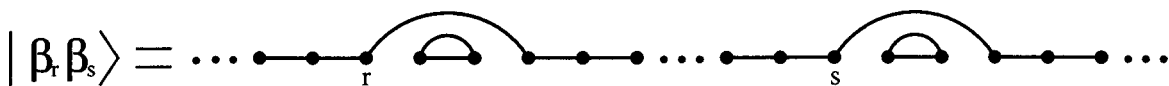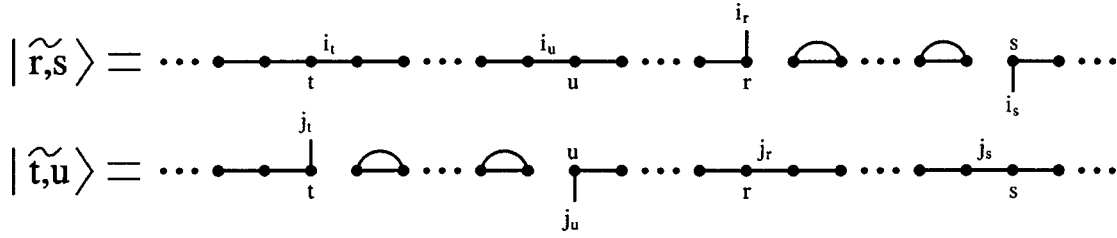

FIG. 12. Double beta state.

FIG. 13. Site and index labeling when $t < u \leqslant r < s$.

$|\alpha_r\rangle$ or $|\beta_r\rangle$, we can neglect the terms of the Hamiltonian acting on the five sites $r-1$ to $r+3$ since their effect is suppressed by a factor of L compared to the other sites (of which there are $L-5$).

For the symmetric ground state, we wish to calculate

$$E_1 = \langle \psi_1 | H | \psi_1 \rangle / \langle \psi_1 | \psi_1 \rangle. \tag{B3}$$

We already know $H|0\rangle$. Now, for $|r-s| > 3$,

$$H_s|\beta_r\rangle = -(1+2/n)|\beta_r\rangle - (1/n)|\beta_r\beta_s\rangle, \tag{B4}$$

where $|\beta_r\beta_s\rangle$ is defined in Appendix A. Thus, using our large L assumption,

$$H|\beta_r\rangle = -L(1+2/n)|\beta_r\rangle - (1/n)\sum_s |\beta_r\beta_s\rangle. \tag{B5}$$

Thus we see that the normalization conditions [(A7), (A13), and (A19)] and the action of H are consistent with

$$|\beta\rangle \approx [2/(n+1)]|0\rangle. \tag{B6}$$

Although this equation is not literally true, the variational calculations give the same result as if it were true. Therefore, $|\psi_1\rangle$ just acts as a scalar multiple of $|0\rangle$ and so

$$\langle \psi_1 | H | \psi_1 \rangle / \langle \psi_1 | \psi_1 \rangle = \langle 0|H|0\rangle / \langle 0|0\rangle = -L(1+2/n) \tag{B7}$$

to first order in $1/n$.

For the nonsymmetric ground state, we need to calculate

$$E_2 = \langle \psi_2 | H | \psi_2 \rangle / \langle \psi_2 | \psi_2 \rangle. \tag{B8}$$

Calculations analogous to those for the symmetric yield ground state demonstrate that the normalization conditions [(A9), (A16), and (A17)] and the action of H are consistent with

$$|\alpha\rangle \approx (1/n)|EO\rangle. \tag{B9}$$

Again, this equation is not literally true; the variational calculations just give the same result as if it were true. Therefore, $|\psi_2\rangle$ just acts as a scalar multiple of $|EO\rangle$ and so

$$\langle \psi_2 | H | \psi_2 \rangle / \langle \psi_2 | \psi_2 \rangle = \langle EO|H|EO\rangle / \langle EO|EO\rangle$$
$$= -L(1+1/n) \tag{B10}$$

to first order in $1/n$.

Thus, variations in a and b do not affect the energies of the states $|\psi_1\rangle$ and $|\psi_2\rangle$ at order $1/n$ as claimed.

APPENDIX C: CALCULATION OF OVERLAPS FOR SOLITON-ANTISOLITON STATES

In this section, we will only consider states in which the soliton is to the left of the antisoliton (that is, $|\widetilde{r,s}\rangle$ for which $s > r$). The other cases are easily seen to produce analogous results. In the forthcoming calculations, we will find the overlap of 2-site wave functions, one corresponding to a single bond and the other to a double bond, to be useful. This is just

$$\langle {}^{i_1 i_2}, {}_{i_1 i_2} | {}_{j_1 j_2}, {}^{j_2 j_3}\rangle = (\delta^{i_1}_{j_1}\delta^{i_2}_{j_2} + \delta^{i_1}_{j_2}\delta^{i_2}_{j_1})(\delta^{j_2}_{i_1}\delta^{j_3}_{i_2} + \delta^{j_2}_{i_2}\delta^{j_3}_{i_1})$$
$$= 2(n+1)\delta^{j_3}_{j_1}. \tag{C1}$$

This result can obviously be extended to longer chains:

$$\langle {}^{i_1 i_2}, {}_{i_1 i_2} \ldots {}^{i_{x-2} i_{x-1}}, {}_{i_{x-2} i_{x-1}} | {}_{j_1 j_2}, {}^{j_2 j_3} \ldots {}_{j_{x-2} j_{x-1}}, {}^{j_{x-1} j_x}\rangle$$
$$= [2(n+1)]^{(x-1)/2}\delta^{j_x}_{j_1}, \tag{C2}$$

where we note that in the above, x must be odd.

Let us first calculate the overlap $\langle \widetilde{r,s} | \widetilde{t,u}\rangle$ when $t < u \leqslant r < s$. We label indices as in Fig. 13. We define $x' = u-t$, $x = s-r$ and $d = r-u+1$. From Eq. (C2), the overlap for sites $t+1$ through $u-1$ is

$$[2(n+1)]^{(x'-1)/2}\delta^{i_u}_{i_t}. \tag{C3}$$

Similarly, the overlap for sites $r+1$ through $s-1$ is

$$[2(n+1)]^{(x-1)/2}\delta^{j_r}_{j_s}. \tag{C4}$$

From Appendix A we know that the overlap for sites u through r,

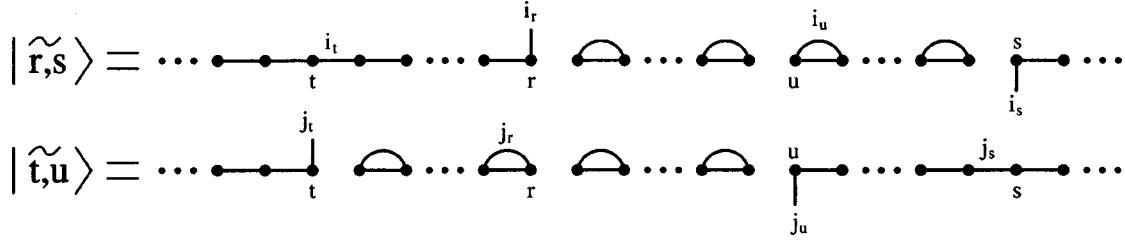$$[((n+1)^d-1)/n]\delta^{j_u}_{i_u}\delta^{i_r}_{j_r} + \delta^{j_u}_{j_r}\delta^{i_r}_{i_u} \tag{C5}$$

and the overlap for sites s through t (periodic boundary conditions) is

$$[((n+1)^{L-d-x-x'+2}-1)/n]\delta^{j_s}_{i_s}\delta^{i_t}_{j_t} + \delta^{j_s}_{j_t}\delta^{i_t}_{i_s}. \tag{C6}$$

Therefore, the entire overlap is

$$[2(n+1)]^{(x+x'-2)/2}\delta^{i_u}_{i_t}\delta^{j_r}_{j_s}$$

$$\times [([(n+1)^d-1]/n)\delta^{j_u}_{i_u}\delta^{i_r}_{j_r} + \delta^{j_u}_{j_r}\delta^{i_r}_{i_u}]$$

$$\times [([(n+1)^{L-d-x-x'+2}-1]/n)\delta^{j_s}_{i_s}\delta^{i_t}_{j_t} + \delta^{j_s}_{j_t}\delta^{i_t}_{i_s}]. \tag{C7}$$

Now, for our purposes, $i_r = j_t$ and $i_s = j_u$ since the two states considered here are intended to be the same state either trans-

FIG. 14. Site and index labeling when $t<r\leqslant u<s$.

lated or acted on by our Hamiltonian (or both) and both of these operations preserve the value of the free index. Now, in order to avoid mixing with the singlet states, we also assume $i_r\neq i_s$ and $j_t\neq j_u$. Thus, after expanding and contracting indices, the above expression reduces to

$$[2(n+1)]^{(x+x'-2)/2}[((n+1)^d-1)/n$$
$$+((n+1)^{L-d-x-x'+2}-1)/n]. \quad \text{(C8)}$$

In the large L and large n limits (taking L large first as usual), this reduces to

$$2^{(x+x'-2)/2}n^{L-d-(x+x')/2}. \quad \text{(C9)}$$

We now consider the case in which $t<r\leqslant u<s$. We label the sites and indices as in Fig. 14. We define $x'=u-t$, $x=s-r$ and $d=u-r-1$. Routine calculations similar to those above demonstrate that the overlap is equal to

$$[2(n+1)]^{(x+x'-2)/2-d}\delta^{i_r}_{i_t}\delta^{j_u}_{j_s}[2n(n+1)]^{d/2}$$
$$\times[([(n+1)^{L-x-x'+d+2}-1]/n)\delta^{j_s}_{i_s}\delta^{i_t}_{j_t}+\delta^{j_s}_{j_t}\delta^{i_t}_{i_s}].$$
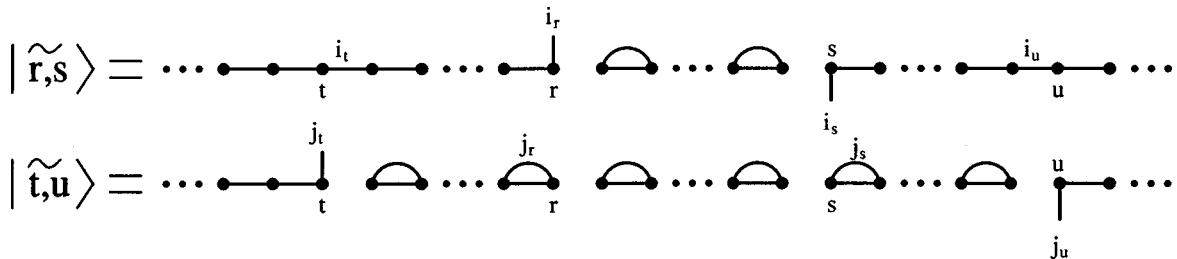$$\text{(C10)}$$

Using the same conditions on the indices as above, the overlap reduces to

$$[2(n+1)]^{(x+x'-2)/2-d}[2n(n+1)]^{d/2}$$
$$\times[((n+1)^{L-x-x'+d+2}-1)/n]. \quad \text{(C11)}$$

In the large L and large n limits (taking L large first as usual), the overlap reduces to

$$2^{(x+x'-d-2)/2}n^{L+d-(x+x')/2}. \quad \text{(C12)}$$

Lastly, we must consider the case where $t<r\leqslant s<u$. We label the indices as in Fig. 15.

We define $x'=u-t$, $x=s-r$ and $d=u-s$. Routine calculations similar to those shown above demonstrate that the overlap is equal to

$$[2(n+1)]^{(x'-x)/2}\delta^{i_r}_{i_t}\delta^{i_u}_{i_s}[2n(n+1)]^{(x-1)/2}$$
$$\times[([(n+1)^{L-x'}-1]/n)\delta^{j_u}_{i_u}\delta^{i_t}_{j_t}+\delta^{j_u}_{j_t}\delta^{i_t}_{i_u}].$$
$$\text{(C13)}$$

Using the same conditions on the indices as above, this reduces to

$$[2(n+1)]^{(x'-x)/2}[2n(n+1)]^{(x-1)/2}[([(n+1)^{L-x'}-1]/n)].$$
$$\text{(C14)}$$

In the large L and large n limits (taking L large first as usual), the overlap reduces to

$$2^{(x'-1)/2}n^{L+(x-x')/2-1}. \quad \text{(C15)}$$

Thus, we see that the overlap $\langle\widetilde{r,s}|\widetilde{t,u}\rangle$ is order n^{L-1} if $r=t,s=u$ and higher order in $1/n$ in every other case. Although, we have only dealt with the cases in which $s>r$ and $u>t$, it can easily be seen that the other cases yield the same conclusion.

APPENDIX D: POSITIVITY OF $\psi_0(x)$

We will now prove that $\psi_0(x)$ is positive for all odd x. Since we know $\psi_0(x)$ is an even function of x, we need only prove the result for $x\geqslant 1$. In order for ψ_0 to be normalizable, $\psi_0(x)$ must converge to zero. Now, by construction, $\psi_0(1)>0$. Assume $\psi_0(x)>0$ $\forall x$ such that $1\leqslant x\leqslant X$, with x,X odd. We will demonstrate that $\psi(X+2)>0$ by contradiction. Thus, by induction, $\psi_0(x)>0$ $\forall x$ odd.

Assume $\psi(X+2)<0$. Then, by Eq. (2.39)

FIG. 15. Site and index labeling when $t<r\leqslant s<u$.

$$\psi_0(X+4) = [(X+2-n\,\delta E-1)/(2\sqrt{2})]\psi_0(X+2) - \psi_0(X)$$

$$\Rightarrow \psi_0(X+4) - \psi_0(X+2)$$

$$= [(X+1-2\sqrt{2}-n\,\delta E)/(2\sqrt{2})]\psi_0(X+2)$$
$$- \psi_0(X) < 0$$

$$\Rightarrow \psi(X+4) < \psi(X+2) < 0. \tag{D1}$$

Since $X+1-2\sqrt{2}-n\,\delta E > 2-2\sqrt{2}-n\,\delta E > 0$, $\psi_0(X+2)\psi_0(X+2) < 0$ and $\psi_0(X) > 0$. Now, if $\psi_0(x+2) < \psi_0(x) < 0$ for $x \geq 3$, then

$$\psi_0(x+4) = [(x+2-n\,\delta E-1)/(2\sqrt{2})]\psi_0(x+2) - \psi_0(x)$$

$$\Rightarrow \psi_0(x+4) - \psi_0(x+2)$$

$$= [(x+1-2\sqrt{2}-n\,\delta E)/(2\sqrt{2})]\psi_0(x+2) - \psi_0(x)$$

$$\Rightarrow \psi_0(x+4) - \psi_0(x+2) \leq \psi_0(x+2) - \psi_0(x) < 0$$

$$\Rightarrow \psi(x+4) < \psi(x+2) < 0. \tag{D2}$$

Since $x+1-2\sqrt{2}-n\,\delta E > 4-2\sqrt{2}-n\,\delta E > 2\sqrt{2}$. Thus, by induction, $\psi_0(x) \leq \psi_0(X+2) < 0$ $\forall x \geq X+2$ which contradicts the fact that $\psi_0(x) \to 0$ as $x \to \infty$. Therefore, we must have that $\psi_0(X+2) > 0$ which completes our initial induction and so $\psi_0(x) > 0$ for all x. Here we have used the numerically determined value of $n\,\delta E \approx -3.747$. Higher energy eigenfunctions will not be positive.

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