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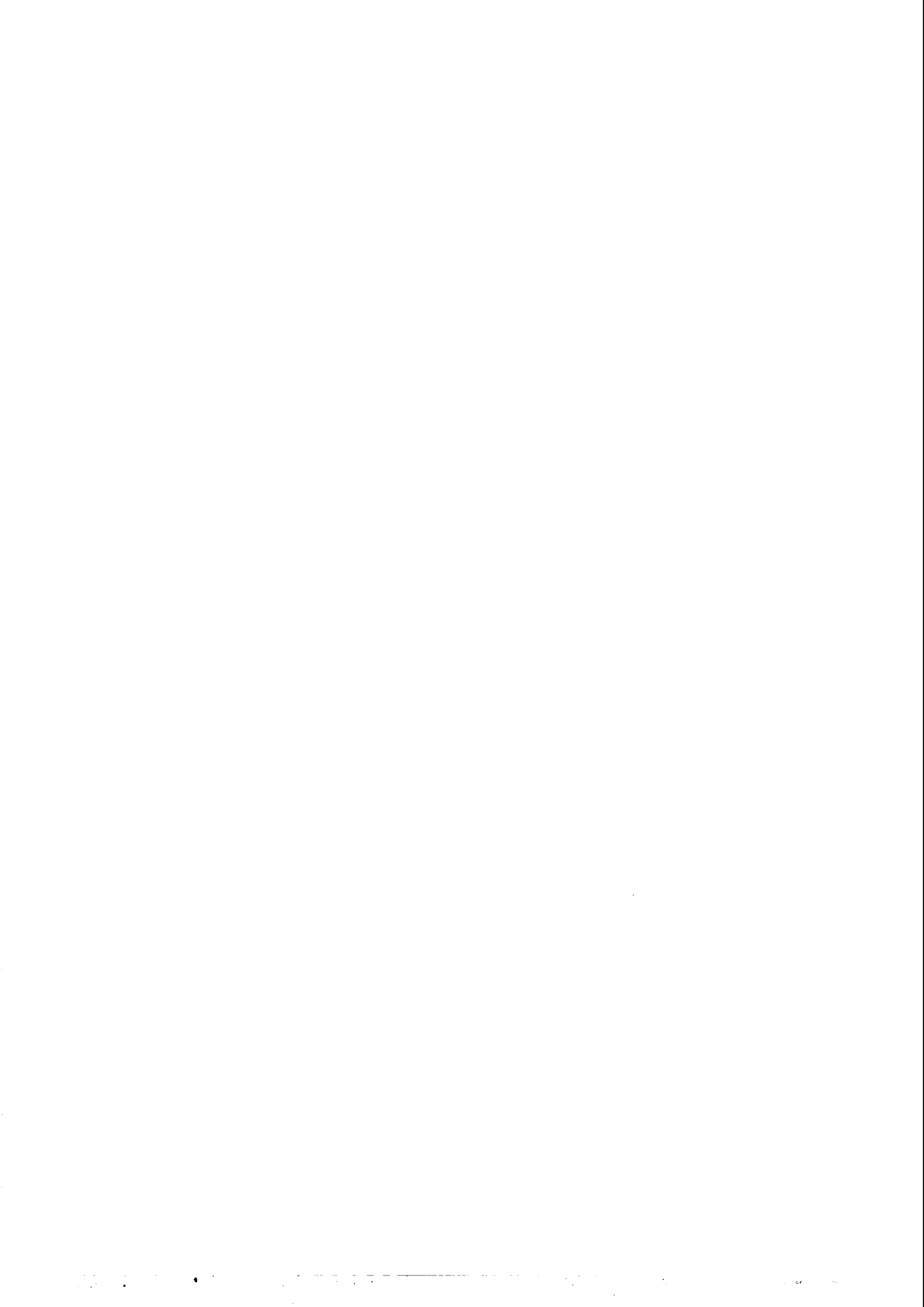
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ABSTRACT

An $L \times \infty$ system of odd number of coupled Heisenberg spin chains is studied using a degenerate perturbation theory, where L is the number of coupled chains. An effective chain Hamiltonian is derived explicitly in terms of two spin half degrees of freedom of a closed chain of L sites, valid in the regime the inter-chain coupling is stronger than the intra-chain coupling. The spin gap has been calculated numerically using the effective Hamiltonian for $L = 3, 5, 7, 9$ for a finite chain up to ten sites. It is suggested that the ground state of the effective Hamiltonian is correlated, by examining various variational trial states for the effective-spin chain Hamiltonian.

There is a growing interest in coupled chains of Hubbard-Heisenberg spin systems, following the experimental realization of coupled arrays of metal-oxide-metal ladder systems [1, 2]. A number of investigations [3, 4, 5, 6, 7] of weakly-coupled Heisenberg spin chains have been carried out, in which the coupling between the chains is weaker than intra-chain coupling, and have provided a strong indication that a system of even number of chains can be understood in terms of a short-range resonating valence bond (RVB) picture, with spin gap and a finite spin-spin correlation length. Whereas a system of odd number of chains is gapless with power-law spin correlations, indicating that it is in the same universality class as a single spin chain. The framework for understanding the difference between even and odd numbered chains is the RVB picture[6, 8], which suggests that an even-numbered coupled chain system can be thought of as an integer spin chain exhibiting a Haldane spin gap, and an odd-numbered coupled system maps onto a half-odd integer spin chain. Below we will construct an effective spin Hamiltonian for odd-numbered coupled system, which is cast explcitily in terms of spin half degrees of freedom. This can be done staightforwardly in the regime the coupling along the chain is weaker than the coupling between the chains. complementary to the earlier studies.

We consider the Heisenberg Hamiltonian given as

$$ H = J \sum_{l,n} \vec{s}_{l,n} \vec{s}_{l+1,n} + J' \sum_{l,n} \vec{s}_{l,n} \vec{s}_{l,n+1} - h \sum_{l,n} s^z_{l,n} \qquad (1) $$

defined on an $L \times N$ lattice where $l = 1, 2, ..L$ and $n = 1, 2, ...N$, and $\vec{s}_{l,n}$ is a spin-1/2 operator at site (l, n). The intra-chain exchange coupling constant is J' and the interchain coupling constant is J, and h is a magnetic field. We use periodic boundary conditions in both directions, and as we see below it makes a big difference. We are interested in regime where $J' < J$, and the case of odd-numbered coupled chains, $L = 3, 5..$ We can think of the system as consisting of N sites with 2^L degrees of freedom at each site, and a complicated bond interaction between the sites mediated by the J' bonds in the Hamiltonian given above.. Starting with an unperturbed system with $J' = 0$, we proceed to include the effect of a non-zero J' within a perturbation theory. This is achieved by identifying the most relevent degrees of freedom for a given site, and projecting out the not so important degrees of freedom. Below we explicit show an analytical construction of the effective-spin chain Hamiltonian for the case of $L = 3$, and 5, and for a larger L one can a similar procedure can be implemented numerically.

Let us consider the case of $J' = 0$, and $h = 0$. The ground state of the system is direct product of N copies of the ground state of a closed chain with L sites. The ground state of Heisenberg Hamiltonian of a closed chain with an odd number of sites is in sector with total spin $S = \frac{1}{2}$ and $S^z = \pm\frac{1}{2}$, implying at least a two-fold Kramers degeneracy. As a matter of fact the ground state is four-fold degenerate. This extra degeneracy arises from chirality. This can be viewed as an unpaired spin in an otherwise singlet ground state. i.e. a spinon which is forced to be there in the ground state[9]. In addition to the spin, the spinon carries a finite ground state momentum $\pm 4\pi/L$ (orbital angular momentum about the center of the closed chain). In the case of an open chain the chiral degeneracy disappears, and we will be left with a two-fold Kramers-degenerate ground state with $S^z = \pm 1/2$. The

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two ground states in $S^z = \frac{1}{2}$ sector can be written as $\phi^L_{\frac{1}{2},\pm} = \sum a^L_\pm(\{n_i\})|\{n_i\} >$, where n_i refer to locations of down spins ($n_1 < n_2...$). Similarly the ground states in $S^z = -\frac{1}{2}$ sector cab be written (here n_i refer to the up spins). The amplitudes $a^L_\pm$ are found using Bethe anstaz[10]; for $L = 3$ the amplitudes are given by (there is only one down spin in this case) $a^3_\pm(n_1) = exp(\pm i2\pi n_1/3)$, and for $L = 5$ the amplitudes are given by (there are two down spins in this case)

$$a^5_\pm(n_1, n_2) = \exp \pm 2ik(n_1 + n_2)\cos((k - \eta/5)(n_2 - n_1) + \eta/2), \qquad (2)$$

where $k = 2\pi/5$ and the phase shift $\eta = 2.243...$ These two different states have spin currents going in two different directions. We refer to these two states as having chirality by defining $\chi^z|\phi^L_\pm >= \pm\frac{1}{2}|\phi^L_\pm >$, and the associated raising and lowering operators through $\chi^\pm|\pm >= 0, \chi^\pm|\mp >= |\pm >$. The chirality operator χ can be written in terms of the original spin operators. Following [11], we define a permutation operator P_l at a site l which permutes the spin labels such that $l + m \to N + l - m$. This is equivalent to doing a reflection on a regular polygon with L sites, around a straightline bisecting the angle at site l. The P operators can be readily constructed from the spin operators, as each of them involve $(L - 1)/2$ pair-wise permutations, as $P_l = 2^{\frac{N-1}{2}} \prod_{m=1}^{\frac{N-1}{2}} (s_{l+m} \cdot s_{N+l-m} + \frac{1}{4})$. Also, P_l can be expressed in terms of chiral lowering and raising operators as $P_l = A^*_l\chi^+ + A_l\chi^-$, where $A_l = \exp(i2\pi l/L)$. The chirality operator is now related to the original spin operators through $[P_l, P_{l+m}] = 4i\chi^z \sin 2\pi m/L$, and $\chi^z = P_1/2$.

If we denote the gap in the spectrum for this L-site closed chain by δ_L (see Table 1 for the acutal values of the gap for $L = 3,5,7,9$), for $J' < \delta_L$ it is a good approximation to just keep the ground state manifold. 4^N-fold degenerate for $J' = 0$, and dropping the excited states. This is expected to suffice for understanding the low-energy behaviour of the system described by the Hamiltonian given in Eq. ??, as the excitation processes to includd the the states dropped have high energy. The ground state subspace we keep, belonging to spin-1/2 sector of each site (of 2^L states), is identified as the most relevent degrees of freedom. For $L = 3$, this procedure keeps all the spin-1/2 at each site. However, for larger $L > 3$, there are also spin-1/2 excited states with large energy which are eliminated in our procedure. This approximation is not so good for $L = 9$ or more, as the the range of J' for validity of our procedure becomes very restricted, viz. $J' < 0.8612$ for $L = 9$. The ground-state subspace for $J' = 0$, is only 2^N dimensional if we use open boundary conditions for the L-site chain, in contrast for periodic boundary conditions we get a much larger Hilbert space, rendering the perturbation theory to be valid in a smaller regime of J' as the gap for the L-site open chain is smaller than that of a closed chain. Each of the basis states v_i for the full system is a direct product of N ground state eigenfunctions of close chain of L sites, $v_i = \phi^1_{l_1} \times \phi^2_{l_2}... \times \phi^N_{l_N}$, where $l_i = 1,4$. To find the effective Hamiltonian within this subspace, we compute the matrix elements $< v_i|H'|v_j >$, and use them to construct an effective Hamiltonian. The prime denotes that only J'bonds are included. The evaluation of the matrix elements reduces to a two-site problem (actually two closed chains of length L connexted by L bonds of strength J') problem as we have pair-wise interactions only.

Let us use two spin-$\frac{1}{2}$ effective degrees of freedom for constructing an effective Hamil-

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tonian, the spin and the chiral quantum numbers $\vec{S}_i$ and the chirality $\vec{\chi}_i$ of the L-site closed chains. An explicit calculation shows that the effective interaction strength $\tilde{A}_{i,j}$ between two closed chains connected by a J' bond (the corresponding operator is $\vec{s}_{i,1}.\vec{s}_{j,2}$) at sites i and j is given in terms of the total spins of the two closed chains and the permutation operators, which we discussed above, at sites i and j respectively of two chains as

$$\tilde{A}_{i,j} = J'\alpha_L \quad \vec{S}_1.\vec{S}_2 \ (\gamma_L + \frac{P_i(1)}{2}) \ (\gamma_L + \frac{P_j(2)}{2}). \tag{3}$$

Here for $L = 3$, $\alpha_3 = 16/9, \gamma_3 = 1/4$, and for $L = 5$ $\alpha_5 = 16\beta, \gamma_5 = 1/20\sqrt{\beta}$. The parameter β is given in terms of $x_1 = \cos k - \eta/5 + \eta/2$, and $x_2 = \cos 2(k - \eta/5) + \eta/2$ as

$$\beta = \frac{2}{5} \frac{(1 + \cos 2k)x_1^4 + (1 + \cos k)x_2^4 - x_1^2 x_2^2}{x_1^2 + x_2^2}. \tag{4}$$

For $L > 5$, the wave-function renormalization constants α_L and γ_L are difficult to calculate analytically, as the number of s^z-basis states in $S^Z = 1/2$ becomes very large. However, the constants can be calculated numerically, and the form of the interaction remains valid. Numerically computed values of the constants are given in Table 1 for up to $L = 9$.

The interaction H'_{12} between two closed chains is mediated by L bonds of strength J'. $H' + 12 = J'\sum_i \vec{s}_{i,1}.\vec{s}_{i,2}$. which in terms of the effective degrees of freedom is obtained by $\sum_{i=} \tilde{A}_{i,i}$. Now it is strightforwad to write the effective Hamiltonian for the full system within the closed chain ground state subspace as

$$H_{eff} = K_L \sum_{i=1}^{N} \vec{S}_i.\vec{S}_{i+1}(b_L + \chi_i^x \chi_{i+1}^x + \chi_i^y \chi_{i+1}^y). \tag{5}$$

where $K_L = J'\alpha_L L/2$. and $b_L = 2\gamma_L^2$ ($K_3 = 8J'/3, b_3 = 1/8$, and $K_5 \approx 2.845J', b_5 \approx 0.06528$, see Table 1). It is interesting to note that only xy-component of the chiral interaction enters the effective Hamiltonian leaving only a two-fold up-down symmetry for the chiral variables. The rotational invariant for the total spin is expected as we started with a fully rotational invariant interaction and we did not break the symmetry by restricting the Hilbert space to the spin-1/2 sector of every closed chain. Just by looking at the form of the effective interaction we learn that on a pair of neighbouring sites the spins and chiral variables are strongly correlated. If we try to lower the spin energy by forcing a singlet state between a pair of neighbouring sites, the chiral variables go into a triplet state (with $\chi^z = 0$). However, because of the additive constant b_L in front of the chirality interaction. spin triplet and a chiral singlet is not favored.

Let us try some variational ansatz. A simple variational state of spin singlets and chiral triplets on nearest neighbours. $\psi_{ST} = \prod_{i odd} v_i^S v_i^T$. where v_i^S is a spin singlet between sites i and $i + 1$ and v_i^T is a chiral triplet state with $\chi^z = 0$. gives an upperbound on the ground state energy of the effective Hamiltonian given above $E_{eff}^G/K_L \leq E_{ST}(2)/K_L = -\frac{3}{4}(b_L + \frac{1}{2})\frac{N}{2}$ (=-0.9375$N/4$. for $L = 3$). The factor -3/4 is the spin singlet energy, one half is the chiral triplet energy and $N/2$ is due to the fact that only half the bonds have spin singlets and chiral triplets. This state is of course too simple to give us any insight about the

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structure of the actual ground state. However, as we will see below, it is doing better than expected. Let us use Jordon-Wigner fermion language for the chirality terms. The xy-term translates into a simple spinless fermion hopping. Now it is tempting to try a free fermion ground state for chirality variables, with an average value of $\frac{1}{\pi}$ for the xy chiral interaction. In this case, we would be left with a Bethe ansatz ground state for the spins, giving an energy estimate $E_{BF}/K_L = -(\log 2 - \frac{1}{4})(b_L + \frac{1}{\pi})N(\approx -0.786N/4$ for $L = 3)$. Compared to the singlet-triplet valnece bond variational state the Bethe Free-Fermion variational state has 20% larger energy, indicating that a correlated state with spin singlets and chiral triplets with longer-ranged valence bonds would do much better. Let us consider a four-site system and construct valence-bond state space. We form two orthogonal states for a four-site system (the sector with $S = 0$ has only two states in this case) from the valence bond states, viz. $A = (12)(34), B = \{(23)(41) - \frac{1}{2}(12)(34)\}2/\sqrt{3}$, where (12) stands for a spin singlet between the two sites. Similarly we construct the chiral states A' and B' where (12) denotes a chiral triplet with $\chi^z = 0$. Diagonalizing the effective Hamiltonian given in Eq. 5, with this four-fold spin-chiral valence bond subspace yields a variational energy of $E_{ST}(4)/K_L \approx -0.9695N/4$ for $L = 3$. This is a 3% lowering of energy compared to the nearest-neighbour valence bond state we considered above. The probability amplitude for a valence bond configuration with a bond occupied by a spin singlet and chiral triplet is more than the other configurations, implying strong correlations between the spin and chiral degrees of freedom. It is interesting to note that this further neighbor valence bond variational state has an energy very close to the exact ground state energy by less than three percent (the indication from numerical diagonalization of the effective Hamiltonian on a finite site system up to $N = 10$ is that the ground state enegy tends to $-NK_L/4$ for $L = 3$, as we discuss below).

An effective way of constructing a convergent series of upper bounds on the exact ground state energy is by calculating the ground state energy $E(n)$ of a finite open chain of $n - even$ sites, giving rise a variational ineuality $E_G/N \le E(n)/n$. The best bound is obtained from the biggest open chain that can be numerically diagonalized. Since the number of states per site is 4, we are able diagonalize only up to ten sites. This gives us a bound for $L = 3$

$$E_{GS}/NK_3 \le E(10)/10 \approx -0.9932/4 \qquad (6)$$

From this calculation it seems that the ground state energy is tending towards $-NK_L/4$ from above. Similarly one can construct a sequence of lower bounds variationally from $l-$site chain energy through $E_G/N \ge E(n)/(n - 1)$. However, this sequence is seen to be not as converget as the sequence of upper bounds. A better convergent sequence of lower bounds can be constructed by varying the bond strengths for a given $n-$site chain, which becomes very complicated for even $n = 6$, and we will not present the details here. The ground state is seen to be in a sector with $S = 0$ and $\chi^z = 0$, in all the finite chain diagonalisations we have done up to $N = 10$. The spin gap, defined as the difference between the engergies of the lowest energy states of the sector $S = 1, \chi^z = 0$, and $S = 0, \chi^z = 0$, is seen to fall of as the number of sites is increased, as shown in Figure 1, for different values of L. However, the data at hand is insufficient to fit the finite-N scaling of the gap. The gap seems to be non-monotonic as a function of L for a given value of N, as it can be seen from the figure for $L = 9$ the gap is larger than for $L = 3$. This could be an artifact of our approximation,

implying the perturbation theory in conjunction with the truncation we have implemented may not be valid for larger L. We have studied the spin-spin correlation function also for the ten-site chain and is seen to be slowly decaying as in the case of $L = 1$. But the characterization of the long-distance behaviour needs an investigation of larger chains. The density matrix renormalization approach [?] can be used for this; currently an investigation is in progress icorporating this scheme for the finite-size spectrum and thermodynamics of larger chains ($N > 10$) for the effective Hamiltonian.

Now we consider the case of a non-zero magnetic field in the Hamiltonian given in Eq. 1. It is easy to see that the effective Hamiltonian given in Eq. 5 will have an additional piece, $viz.$ $-h \sum S_i^z$. Let us focus on the case of $L = 3$. The effective Hamiltonian is valid in the regime $h < 3J/4$, for $L = 3$, to ensure that the ground state subspace be composed of $S^z = \pm 1/2$ states of the L−site chains. Now, if the magnetic field is strong enough to polarise the spins in the effective Hamiltonian, the ground state would be just a polarised spins and a free fermion state for the chiral degrees of freedom. The range of h for which this state has lower energy than $S = 0$ state works out to be for $0.75J > h > (7\pi - 8)J'/6\pi \approx 0.74225J'$. The free fermion chiral state has low-lying excited states with a gap of $\Delta = (7\pi - 8)K_3/4N$. This should be contrasted with the case of $L = 1$, where there are no low-lying states if the magnetic field is of the order of the exchange coupling constants.

In conclusion, we have established an effective spin-chiral chain Hamiltonian for a system of odd-numbered coupled Heisenberg spin chains. The effective interaction has a product form, $viz.$ isotropic Heisenberg for spins and only xy interaction for chiral spins. The spin gap studied numerically using the effective Hamiltonian for $L = 3, 5, 7, 9$ falls off as the number of sites i increases. Indications from a finite-size study are that long-ranged resonating valence bond variational states (with spin singlets and chiral triplets) are suited to study the behaviour of the effective Hamiltonian.

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L	δ_L/J	b_L	K_L/J'
3	3/2	1/8	8/3
5	1.1180	0.0697	2.8685
7	1.0489	0.0436	3.2765
9	0.8612	0.0230	4.8275

Table 1: The energy gap of a $L-$site ring, and the wave-function renormalization constants that appear in the effective Hamiltonian given in Eq. 5 for various values of L.
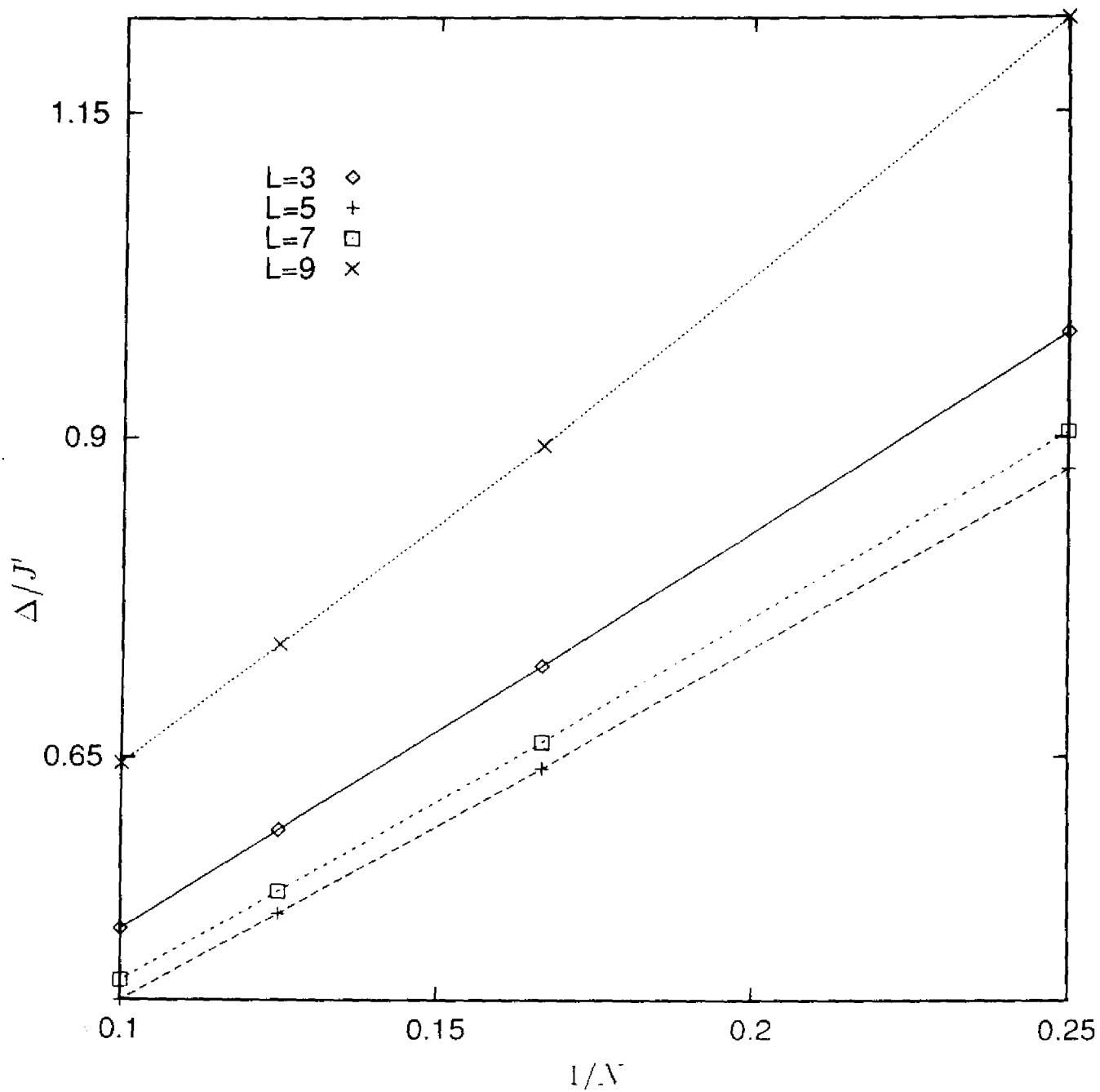
Fig.1

The spin gap of an $L \times N$ system as a function of $1/N$ for various number of coupled chains. $L = 3, 5, 7, 9$. The gap is calculated numerically from the effective Hamiltonian given in $Eq.$??.