

**ON THE ENERGY SPECTRUM AND THERMODYNAMICS
OF ANISOTROPIC SPIN-1/2 TWO-LEG LADDER**

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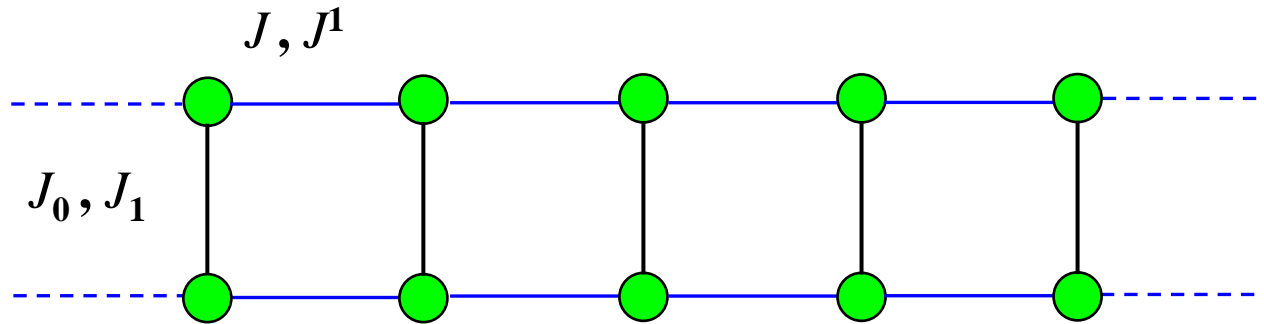
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Outlook

1. General properties of anisotropic spin-1/2 two-leg model (ASLM)
2. Two electron bound states of Hubbard model with spin dependent hopping (particular case of ASLM). The lowest state energy in $S^z=0$ subspace (ground state energy-?) from DMRG and “pair approximation”.
3. Bound states of several inverted spins in ASLM with XY interaction along the legs. The DMRG simulation
4. Strong coupling limit of ASLM. XXZ spin-1 model with single ion anisotropy as a particular case of ASLM. The ground state magnetization.
5. The temperature dependence of the spin part of ladder heat capacity. The effect of local states.

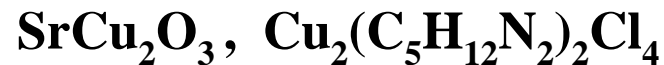
Anisotropic spin-1/2 2-leg ladder model



$$\hat{H} = -\sum_{\alpha=1}^2 \sum_{n=1}^N \left[J \left(S_{\alpha,n}^x S_{\alpha,n+1}^x + S_{\alpha,n}^y S_{\alpha,n+1}^y \right) + J' S_{\alpha,n}^z S_{\alpha,n+1}^z + h S_{\alpha,n}^z \right]$$

$$- \sum_{n=1}^N \left[J_0 S_{1,n}^z S_{2,n}^z + J_1 \left(S_{1,n}^x S_{2,n}^x + S_{1,n}^y S_{2,n}^y \right) \right]$$

$$\mathbf{S}_{\alpha,N+1} = \mathbf{S}_{\alpha,N}$$



Dagotto E. 1999 Prog. Phys. **62**, 1525

Tandon K, Lai S, Pati S K, Ramasesha S and Sen D 1999 *Phys. Rev. B* **59** 396

Hirikava T. and Furusaki A. 2001 *Phys. Rev. B* **63** 143438

Shiba H 1972 *Prog. Theor. Phys.* **48** 2171

$$\mathbf{H} = \mathbf{H}_1 - h (N - N_1 - N_2) - 0.25 J_0 (N - 2N_1 - 2N_2)$$

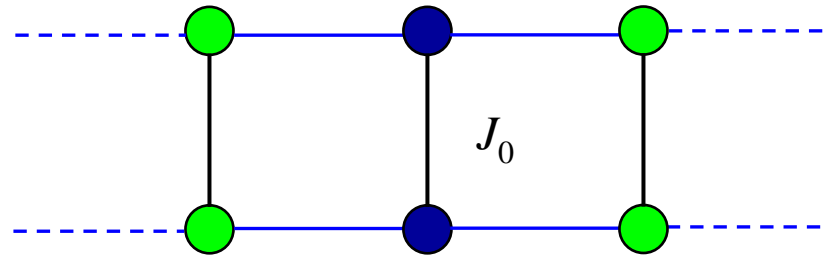
$$\mathbf{H}_1 = -\frac{1}{2} \left(\sum_{i=1}^{N-1} J_1 a_{i\alpha}^+ a_{i+1\alpha} + J_2 a_{i\beta}^+ a_{i+1\beta} + h.c. \right) - J_0 \sum_{i=1}^N a_{i\alpha}^+ a_{i\alpha} a_{i\beta}^+ a_{i\beta}$$

Hubert L. and Caille A. 1991 *Phys.Rev. B* **43** 13187

Cheranovskii V.O., Ezerskaya E.V. and Ozkan I. 2001 *J.Phys.: Condens.Matter* **13** 4525

Vekua T., Japaridze G.I., and Mikeska H.-J. *cond-mat/0401301*

$$\Delta E = E_2 - 2 * \min(E_1)$$



Pair approximation:
$$- \varepsilon_0 = \frac{1}{\pi} \sqrt{J_0^2 + (J_1 + J_2)^2} E \left(\frac{2 \sqrt{J_1 J_2}}{\sqrt{J_0^2 + (J_1 + J_2)^2}} \right)$$

Lieb E.H., Wu F.Y. 1968, *Phys.Rev.Lett.* **20**, 1445.

$$\varepsilon(N_1, N_2, |J_0|) = |J_0| N_1 + \varepsilon(N_1, N - N_2, -|J_0|)$$

Kocharyan A.N., Yang C., and Chang Y.L. 1999, *Phys.Rev. B* **59**, 7458

Marsiglio F. 1977, *Phys.Rev. B* **55**, 575

$$\varepsilon_0 = -\frac{2}{\pi} \sqrt{I^2 + \Delta^2} E\left(\frac{I}{\sqrt{I^2 + \Delta^2}}\right) - \frac{J_0}{4} + \frac{\Delta^2}{J_0}$$

$$I = \frac{1}{2}(J_1 + J_2) \quad K\left(\frac{I}{\sqrt{I^2 + \Delta^2}}\right) = \frac{\pi\sqrt{I^2 + \Delta^2}}{J}$$

$$E(J_1, J_2) = E(J'_1, J'_2), \quad \text{if } J_1 + J_2 = J'_1 + J'_2$$

Cheranovskii V.O., Ezerskaya E.V. and Ozkan I. 2002 *Int.Journ.Quant.Chem.* **88**, 398

Exact energy spectrum of the states with one and two inverted spins

$$(\hat{H} - E_0)|n\rangle = \varepsilon|n\rangle \quad |n\rangle = \sum_{\substack{\alpha_1 \dots \alpha_n, \\ m_1 \dots m_n}} A_{m_1 \dots m_n}^{\alpha_1 \dots \alpha_n} S_{\alpha_1 m_1}^- \dots S_{\alpha_n m_n}^- |0\rangle$$

where $E_0 = -\left(h + \frac{J_0 + 2J'}{4}\right)N$ is the energy of “ferromagnetic” state

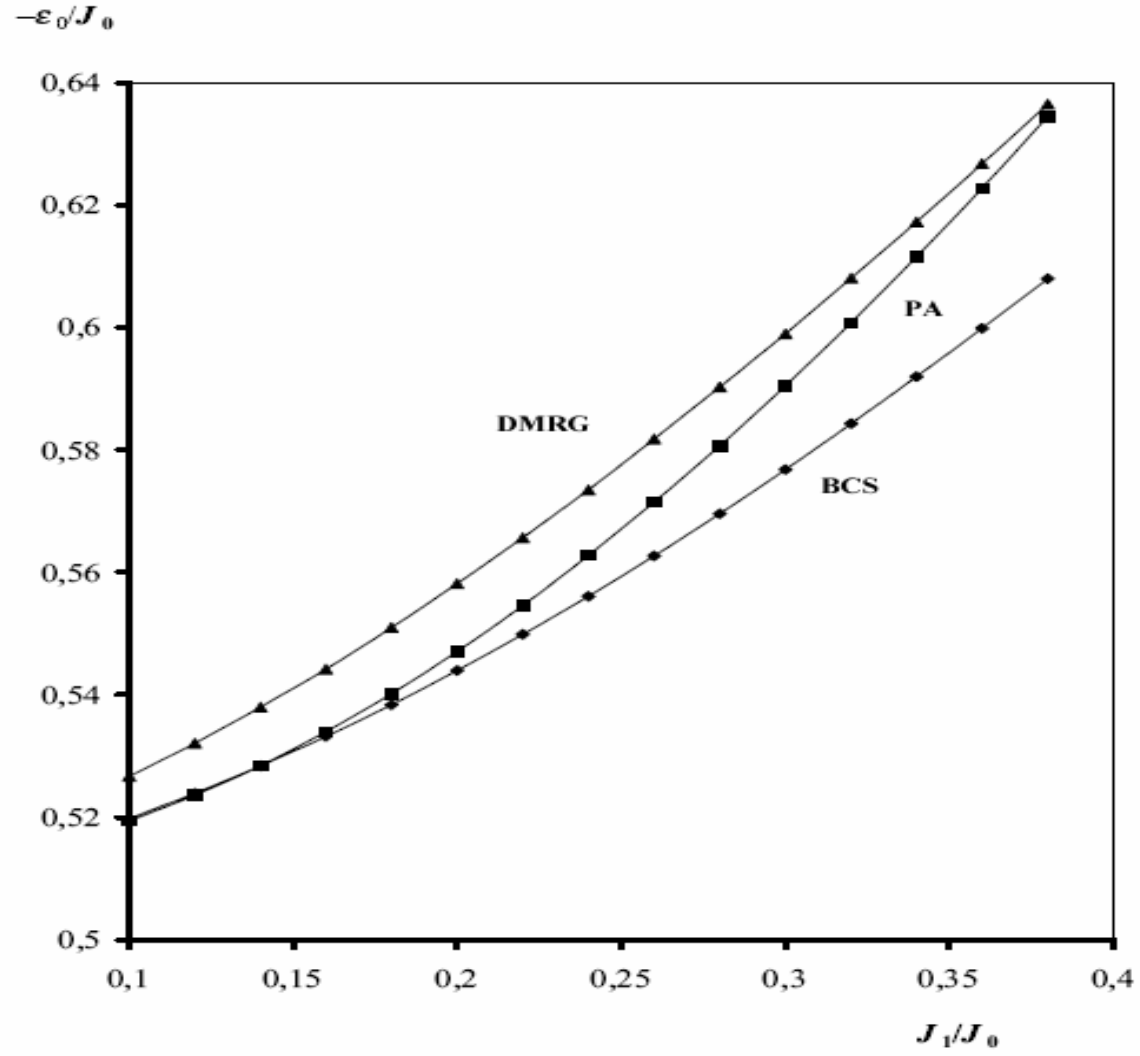
$$\mathbf{n=1:} \quad \varepsilon_{1,2k} = h + \frac{J_0}{2} \pm \frac{J_1}{2} + J' - J \cos k$$

$$\mathbf{n=2:} \quad \varepsilon = 2h + J_0 \left(1 - \sqrt{1 + \frac{4J^2 \cos^2(k/2)}{J_0^2 - J_1^2}} \right), \quad \cos(k/2) \leq \frac{|J_0^2 - J_1^2|}{2J_1 J}$$

$$E(J_0, J_1 J, J') = E(J_0, -J_1 J, J'),$$

$$E(J_0, J_1 J, J') = E(J_0, J_1 - J, J')$$

Lowest energies per rung of infinite ladder with $N_1=N_2=0.5N$ and $J_2=1$ as a function of J_1 (In DMRG simulation we kept 32- 80 optimized states).



The case of strong coupling in ladder rungs

$$E_1 = \frac{J_0}{4} + \frac{J_1}{2}, \quad \varphi_1 = \frac{1}{\sqrt{2}}(S_{1,1}^- - S_{2,1}^-)|0\rangle \quad E_2 = -\frac{J_0}{4} - h, \quad \varphi_2 = |0\rangle$$

$$E_3 = -\frac{J_0}{4} + h, \quad \varphi_3 = S_{1,1}^- S_{2,1}^- |0\rangle \quad E_4 = \frac{J_0}{4} - \frac{J_1}{2}, \quad \varphi_4 = \frac{1}{\sqrt{2}}(S_{1,1}^- + S_{1,2}^-)|0\rangle$$

The effective low-energy Hamiltonians

$$1. \quad |h - \Delta| \sim |J|, |J'|, \quad \Delta = \frac{1}{2}(J_1 - J_0)$$

$$H = -\sum_{i=1}^N \left[J(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) + \frac{J'}{2} \left(S_i^z + \frac{1}{2} \right) \left(S_i^z + \frac{1}{2} \right) \right]$$

$$- (h - \Delta) \sum_{i=1}^N \left(S_i^z + \frac{1}{2} \right) + \frac{N}{4} (J_0 - 2J_1)$$

$$S_i^z \varphi_2 = \frac{1}{2} \varphi_2, \quad S_i^z \varphi_4 = -\frac{1}{2} \varphi_4$$

$$2. \quad (J_0 - J_1) \sim J, J', h$$

$$H = -\left(\frac{J_0}{4} + \Delta\right)N - \sum_{i=1}^N \left[\frac{J'}{2} T_i^z T_{i+1}^z + \frac{J}{2} (T_i^+ T_{i+1}^- + T_{i+1}^+ T_i^-) + h T_i^z - \Delta (T_i^z)^2 \right]$$

$$T_i^z = S_{1,i}^z + S_{2,i}^z, \quad T_i^\pm = \frac{1}{\sqrt{2}} (S_{1,i}^\pm + S_{2,i}^\pm)$$

Schulz J., *Phys. Rev. B* **1986**. 34, 6372

Vekua T., Japaridze G.I., and Mikeska H.-J., cond-mat/0401301

Chen W., Hida K., Sanctuary B.C. 2003 *Phys.Rev. B* **67**, 104401

Dmitriev D.V., Krivnov V.Ya, A.A.Ovchinnikov, 1997 *Phys.Rev. B* **56**, 5985

Cheranovskii V.O., Pamuk H.O., and Esenturk O. 1998 *Phys.Rev. B* **58**, 12260

Lieb E.H., Shultz T., and Mattis D 1961 *Ann.Phys.* **3** 407

The lowest energy levels for N=6 ladder (exact diagonalization)

$J' \setminus S^z$	0	1	2	3	4	5	6
0.3090	-2.6548	-2.6334	-2.6516	-2.6205	-2.6482	-2.6030	-2.6545
0.3100	-2.6547	-2.6333	-2.6516	-2.6206	-2.6484	-2.6033	-2.6550

$$J_0=10\text{K}, J_1=8\text{K}, J = 1\text{K}$$

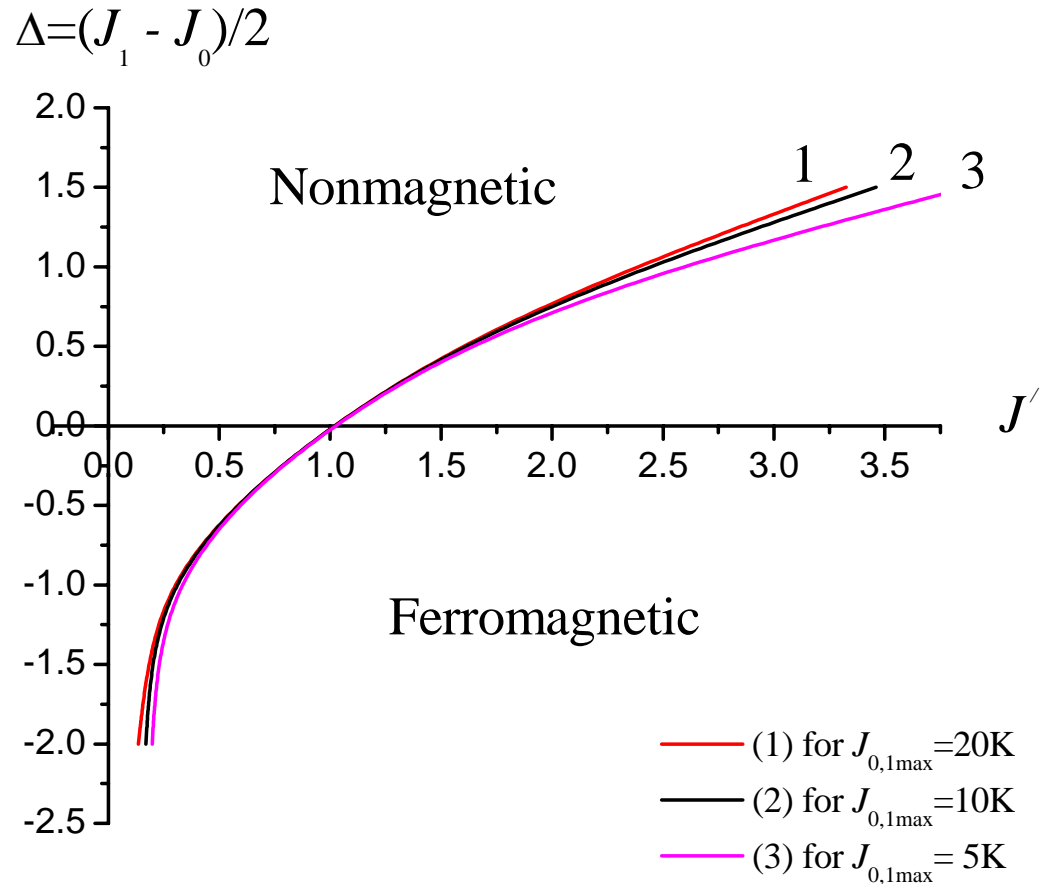
$J' \setminus S^z$	0	1	2	3	4	5	6
2.4130	-3.2069	-3.1542	-3.1187	-3.1034	-3.1079	- 3.1377	-3.2065
2.4140	-3.2069	-3.1542	-3.1187	-3.1034	-3.1081	-3.1380	-3.2070

$$J_0=8\text{K}, J_1=10\text{K}, J = 1\text{K}$$

DMRG for infinite systems

Nit = 500, m = 10-40

$$J' = -(4 \Delta)^{-1}$$



Low temperature thermodynamics

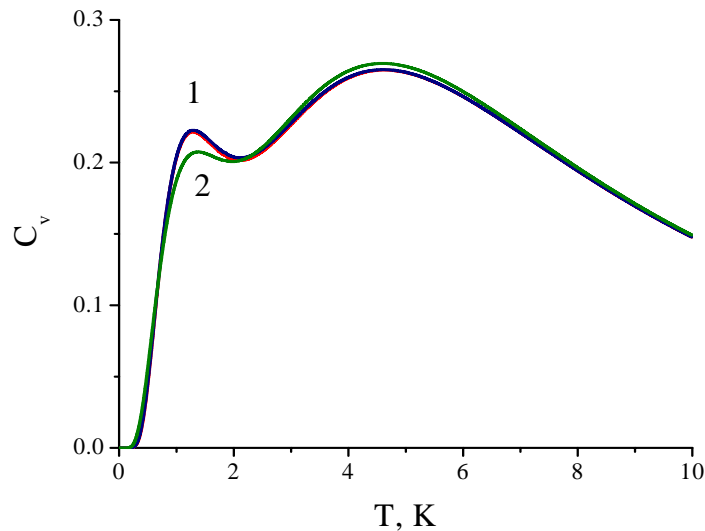
$$|J_0^2 - J_1^2| \gg 4J^2, \quad J' = 0, \quad J_1 > 2J$$

For statistical sum evaluation we will take into account only exact energies of low lying stationary states with one inverted spin (3) and approximate energy of bound states with two inverted spins.

$$F = E_0 - T \sum_k \ln \left(1 + \exp\left(\frac{-\varepsilon_{1k}}{T}\right) + \exp\left(\frac{-\varepsilon_{2k}}{T}\right) + \exp\left(\frac{-2h}{T}\right) \right)$$

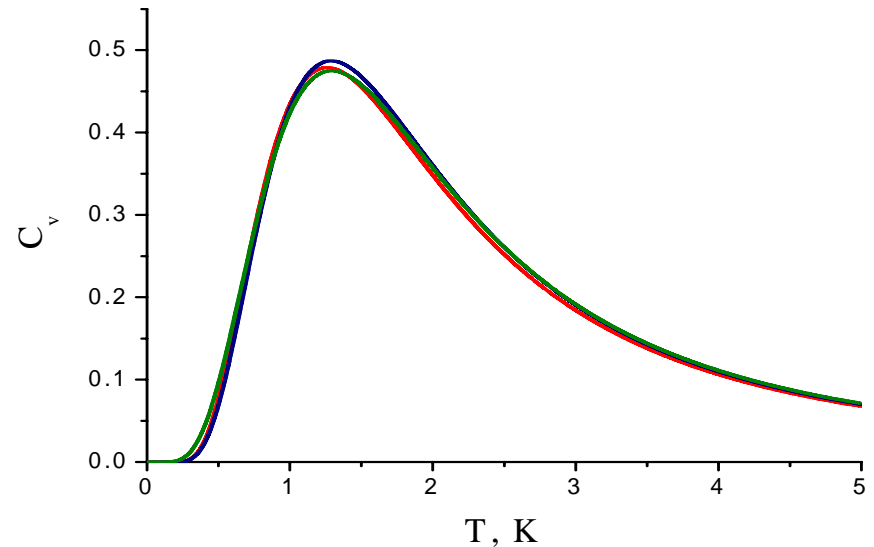
$$C_v = \frac{1}{T^2} \frac{1}{\pi} \int_0^\pi \frac{\left[\varepsilon_{1k}^2 e^{-\varepsilon_{1k}/T} + \varepsilon_{2k}^2 e^{-\varepsilon_{2k}/T} + \frac{J_1^2}{2} e^{-(\varepsilon_{1k} + \varepsilon_{2k})/T} \right]}{\left(2 + e^{-\varepsilon_{1k}/T} + e^{-\varepsilon_{2k}/T} \right)^2} dk,$$

Specific heat vs temperature



1) Formula (1) and exact diagonalization for $J_0 = -25$ K, $J_1 = 3$ K, $J = 1$ K, $J' = 0$ (two curves almost coincide);

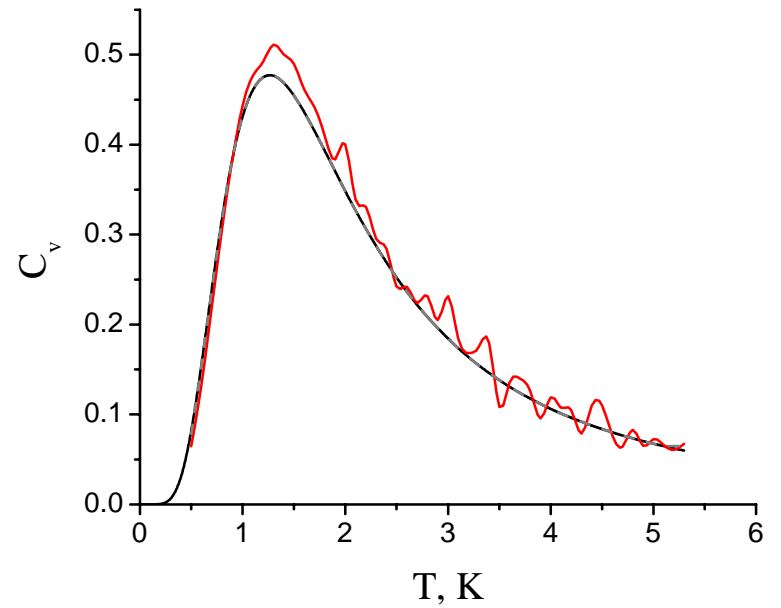
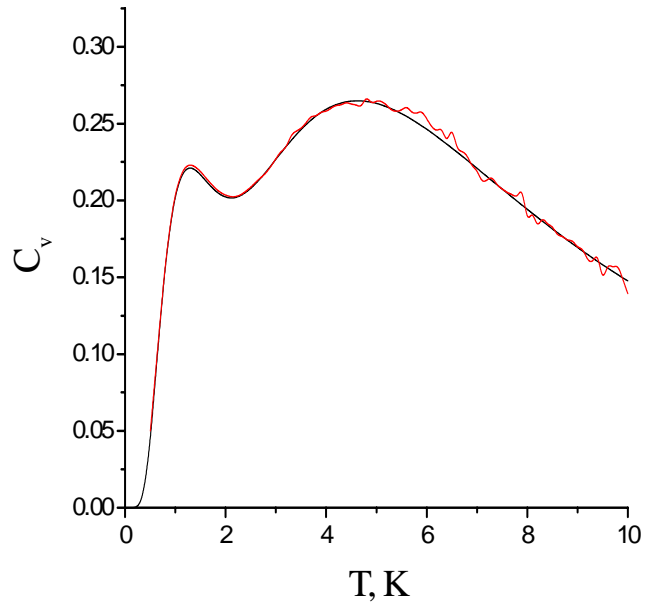
2) The exact diagonalization for $J_0 = -25$ K, $J_1 = 3$ K, $J = J' = 1$ K

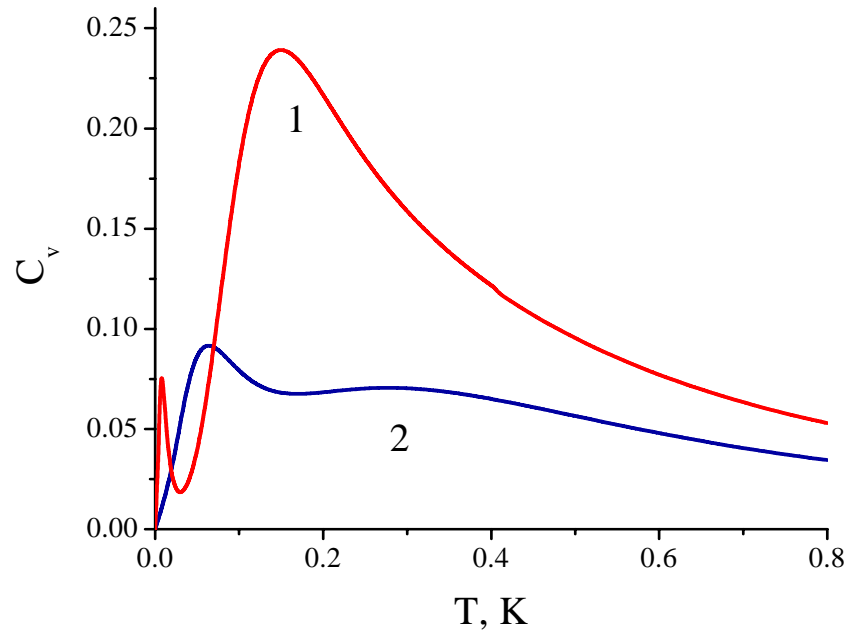


($J_0 = -5$ K, $J_1 = 3$ K, $J = 1$ K
 $J' = 0$).

The exact diagonalization, formula (1) and single rung calculations give almost coincident curves.

Specific heat vs temperature (symmetric variant of TDMRG, 4 optimized states for above values of parameters)

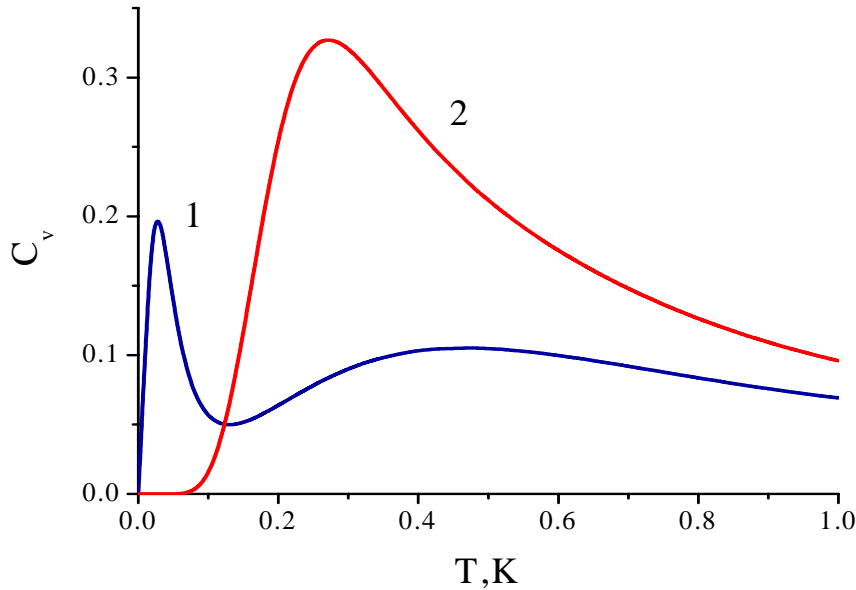




First two peaks of C_v as a function of temperature for $J_0 = 10$ K, $J_1 = 9.2$ K, $J = 0.6$ K): 1) exact diagonalization, 2) formula (1).

	Sum of exact lowest energies	Lowesy energy from DMRG
2	-0.45825	-0.45824
3	-0.65825	-0.66714
4	-0.91650	-0.91650

(In DMRG calculations we used 500 iterations and 10 optimized states).



	Sum of exact lowest energies	Lowesy energy from DMRG
2	-0.13794	-0.13793
3	0.36206	0.35637
4	-0.27588	-0.27587

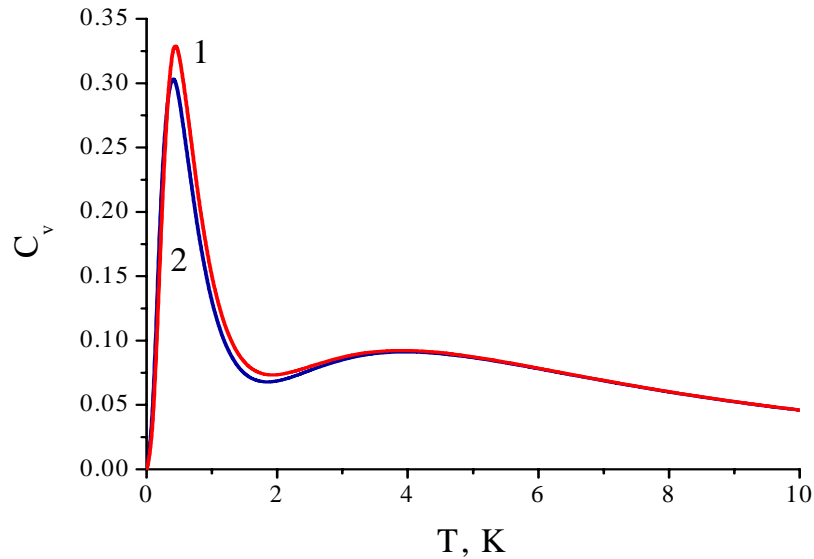
The exact diagonalization for $N=6$:

1) $J_0 = 10$ K, $J_1 = 8$ K, $J = 0.5$ K,

2) $J_0 = 10$ K, $J_1 = 8$ K, $J = 0.5$ K,

$J' = 0.5$ K

(For $J' = 0.5$ K DMRG gives positive energies: 0.71372 for $n=2$ and 1.50227 for $n=3$)



$J_0 = 8 \text{ K}, J_1 = 10 \text{ K}, J = 0.5 \text{ K},$

1) The exact diagonalization

2) Formula (1)

	Sum of exact lowest energies	Lowesy energy from DMRG
2	-3	-2.9999
3	-4.5	-4.49997
4	-6	-5.99872

$(\epsilon_{\text{loc}} = 0.111896 \text{ K})$

The positions of $C_v(T)$ maxima for finite lattice clusters (the exact diagonalization)

	$N=4$	$N=5$	$N=6$	Isolated rung
C_v	0.3304	0.3317	0.3307	0.3809
T, K	0.45	0.43	0.43	0.37
C_v	0.0929	0.0924	0.0924	0.0903
T, K	3.89	3.90	3.90	4.00

$$J_0=8\text{K}, J_1=10\text{K}, J=1, J' = 0\text{K}$$

	$N=4$	$N=5$	$N=6$	Isolated rung
C_v	0.2396	0.1892	0.2014	-
T, K	0.03	0.03	0.03	
C_v	0.1051	0.1052	0.1051	0.1204
T, K	0.47	0.47	0.47	0.44
C_v	0.0915	0.0915	0.0915	0.0901
T, K	3.70	3.71	3.70	3.75

$$J_0=10\text{K}, J_1=8\text{K}, J=0.5, J' = 0\text{K}$$

	$N = 4$	$N = 5$	$N = 6$	Isolated rung
C_v	0.0957	0.00755	0.0627	-
T, K	0.04	0.04	0.04	
C_v	0.2848	0.3048	0.3151	-
T, K	0.46	0.42	0.40	
C_v	0.0888	0.0887	0.0887	0.0832
T, K	4.36	4.36	4.37	4.62

$$J_0=10K, J_1=10K, J=1, J' = 0K$$

	$N = 4$	$N = 5$	$N = 6$	Isolated rung
C_v	-	0.7516	0.7371	-
T, K		0.08	0.03	
C_v	0.2246	0.2387	0.2544	0.1203
T, K	0.15	0.15	0.14	0.17
C_v	0.0861	0.0861	0.0861	0.0841
T, K	4.2	4.25	4.25	4.33

$$J_0=10K, J_1=9.2K, J=0.6, J' = 0K$$

Summary

1. Simple approximate formula for the ground state energy of uniform Hubbard model chain with spin dependent hopping was given.
2. The transition between lowest states with marginal values of S_z for ASLM with ferromagnetic interactions in rung is similar to corresponding transition in XXZ spin-1 model with single ion anisotropy
3. The temperature dependence of the specific heat of ASLM may have up to three maxima in zero magnetic field.
4. Simple approximate formula for specific heat was derived. It was shown that the adequacy of this approximation depends strongly on the existence of low-energy bound states.