Integrable models of interacting quantum spins with competing interactions

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Abstract  
We present a class of exactly solvable quantum spin models which consist of two Heisenberg-subsystems coupled via a long-range Lieb-Mattis interaction. The total system is exactly solvable whenever the individual subsystems are solvable and allows to study the effects of frustration. We consider (i) the antiferromagnetic linear chain and (ii) the Lieb-Mattis antiferromagnet for the subsystem-Hamiltonians and present (i) the complete ground-state phase diagram and (ii) the full thermodynamic phase diagram. We find a novel phase which exhibits order from disorder phenomena.  
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Introduction. – The properties of interacting quantum spins have been studied intensively over a long period. Some selected model Hamiltonians, which typically describe homogeneous collections of interacting spins, can be solved exactly. Examples are (i) models in one dimension solvable by Bethe-Ansatz [1], (ii) a one-dimensional model with long-range inverse-square exchange [2], (iii) valence-bond models [3] and (iv) models with long-range interaction of constant magnitude (Lieb-Mattis type models [4] which have recently been used to discuss spontaneous symmetry breaking in spin systems [5]). Our understanding of interacting quantum spins has benefited greatly from these studies.

On the other hand, in experimental applications we have to deal sometimes with situations where two subsystems of spins interact mutually. One example is the garnet, Mn$_3$Cr$_2$Ge$_3$O$_{12}$, in which the Mn and Cr moments are located on two disjunct, interpenetrating sublattices [6, 7], with the intra-sublattice couplings dominating over the inter-sublattice coupling due to frustration effects [8, 9]. Another example is the two-layer structure in certain high-$T_c$ compounds, like YBa$_2$Cu$_3$O$_6$ [10], where the competition between the inter-layer and the intra-layer couplings might lead to a spin-gap [10].

Here we present a class of exactly solvable models which consist of two subsystems coupled via a long-range Lieb-Mattis [4] interaction. The total system is exactly solvable whenever the solutions of the individual subsystems are known and it allows to investigate the effects of competing interactions. We consider two different types of subsystems, the linear chain and the Lieb-Mattis model, and present the ground-state (GS) phase diagrams. In addition we present for the case of two coupled Lieb-Mattis subsystems the full thermodynamic phase diagram. We find a novel phase which exhibits order from disorder phenomena [13, 5].

Model. – We consider a system of $N = N_1 + N_2$ interacting quantum spins ($s = 1/2$) made up of two mutually interacting subsets described by the Hamiltonian

$$H = \alpha_1 H_1\{s_i\} + \alpha_2 H_2\{s_i\} + \alpha H_{\text{int}}\{s_i, s_i\}$$

with $\alpha, \alpha_1, \alpha_2 > 0$. Here $H_1\{s_i\}$ ($i = 1, \ldots, N_1$) and $H_2\{s_i\}$ ($l = N_1 + 1, \ldots, N$) contain the interactions within the first and the second subset of $N_1$ and $N_2$ spins respectively. The antiferromagnetic ($\alpha > 0$) interaction between the two subsets of spins is taken to be of the Lieb-Mattis form [4]. $H_{\text{int}}\{s_i, s_i\} = S_1 \cdot S_2/(N_1 N_2)$ with $S_1 = \sum_{i=1}^{N_1} s_i$ and $S_2 = \sum_{i=N_1+1}^{N} s_i$. We assume $H_1$ and $H_2$ to be spin-rotationally invariant. Then the operators $S^2 = (S_1^2 + S_2^2)$, $S_1^2$, $S_2^2$, $H$, $H_1$ and $H_2$ all commute with each other. The eigenvalues of Eq. (1) are given by $E_{S, S_1, S_2} = [\alpha/(2N_1 N_2)] [S(S + 1) - S_1(S_1 + 1) - S_2(S_2 + 1)] + \alpha_1 E_1 + \alpha_2 E_2$, where $S_1$, $S_2$, $E_1$, $E_2$ and $S$ denote the quantum numbers of $S^2_1$, $S^2_2$, $H_1$, $H_2$ and $S^2$ respectively with $S \in \{|S_2 - S_1|, S_2 + S_1\}$. We consider the thermodynamic limit, $N_1, N_2 \to \infty$, and define the normalized quantum numbers $x_\gamma = 2S_\gamma/N_\gamma$ ($0 \leq x_\gamma \leq 1$, $\gamma = 1, 2$). The GS energy which is realized for $S = |S_2 - S_1|$, can then be written as $E_0 = -\alpha x_1 x_2/4 + \alpha_1 E_1(x_1) + \alpha_2 E_2(x_2)$, where $E_1(x_1)$ and $E_2(x_2)$ are the lowest eigenvalues of $H_1$ and $H_2$ within the subspace of a given magnetisation $x_1$ and $x_2$. For a large class of antiferromagnetic Hamiltonians $H_\gamma$ a level ordering $E_\gamma(x) \geq E_\gamma(x')$ is valid for $x > x'$ [4]. Then a competition arises in $E_0$ between the term proportional to $\alpha$ which tends to maximize $x_\gamma$ and the terms proportional to $\alpha_\gamma$ which tend to minimize $x_\gamma$, giving rise to frustration effects.

We consider two models for the Heisenberg Hamiltonians $H_1\{s_i\}$ and $H_2\{s_i\}$ entering Eq. (1) and set $\alpha = 1$ for the rest of this paper. The two models are the antiferromagnetic linear chain (LC), $H_{LC}^\gamma = (1/N_\gamma) \sum_i s_i s_{i+1}$, and the Lieb-Mattis (LM) model, $H_{LM}^\gamma = (2/N_\gamma)^2 S^A_\gamma S^B_\gamma$, with $S^A_\gamma = \sum_{i \in A \in \gamma} s_i$ and $S^B_\gamma = \sum_{i \in B \in \gamma} s_i$ being the total-spin
operators of the $A$, $B$ sublattice of the respective subsystem ($\gamma = 1, 2$). The scalings with $N_s$ are chosen such that (i) all energies become intensive in the thermodynamic limit $N_1, N_2 \to \infty$ and (ii) that for the fully polarized state ($x_\gamma = 1$) the energies are $E^{LC}_\gamma(1) = E^{LM}_\gamma(1) = 1/4$. Both models can be solved exactly. For the LM model in addition to $S_2^\gamma$ also the respective sublattice spin-operators, $(S^{A,B}_\gamma)^2$, commute with the Hamiltonian and the corresponding (normalized) quantum numbers, $x^{A,B}_\gamma = (4/N_s)S^{A,B}_\gamma$ ($0 \leq x^{A,B}_\gamma \leq 1$) are separately conserved.

For the LM model, mean-field theory becomes exact and quantum fluctuations vanish identically in the thermodynamic limit. The energy $E_\gamma(x_\gamma)$ can be calculated as $E^{LM}_\gamma = x_\gamma^2/2 - 1/4$. On the other side, quantum fluctuations are maximal for the antiferromagnetic LC. We computed $E^{LC}_\gamma(x_\gamma)$ by numerically solving the Bethe-Ansatz equations for finite magnetisation $x_\gamma$.

**Ground-state phase diagram.** – The knowledge of $E_\gamma(x_\gamma)$ ($\gamma = 1, 2$) allows to determine the GS phase diagram, which we present in Fig.1. The phase diagram is symmetric under $\alpha_1 \leftrightarrow \alpha_2$ and the GS has minimal total spin $S = |S_2 - S_1|$. For small $\alpha_1$ and $\alpha_2$ the antiferromagnetic inter-subsystem interaction dominates and the subsystems are saturated ferromagnets ($x_1 = x_2 = 1$) with parallel sublattice magnetisations. For large $\alpha_1$ and $\alpha_2$ the antiferromagnetic intra-subsystem interaction dominates and two subsystems effectively decouple into their individual singlets ($x_1 = x_2 = 0$). A line of first-order phase transitions separates the spin-singlet region from a region near the axis where one of the subsystems is partially magnetized and the other one is fully magnetized. The states with partial magnetisation are connected to the fully polarized state by a second-order phase transition.

In Fig.2 we have plotted the GS expectation values of the inter-subsystem correlation function, $\langle s_i s_l \rangle_{1,2}$ ($i$ and $l$ are in the first and second subsystem, respectively), and the intra-subsystem correlation function $\langle s_i s_j \rangle_{1,1}$ of the first subsystem (for the LC case $j = i + 1$, for the LM case $i \in A$ and $j \in B$) as a function of $\alpha_1$ for fixed $\alpha_2 = 0.075$. For small $\alpha_1$ saturated ferromagnetic long-range order within the subsystems ($\langle s_i s_j \rangle_{1,1} = +1/4$ but $\langle s_i s_l \rangle_{1,2} = -1/4$) is present up to $\alpha_1^* = 1/4$ for both the LC and the LM case. At this point a second-order phase transition leads to the non-saturated magnetic structure. For the case of two coupled LM systems we have that $\langle s_i s_j \rangle_{1,1} - 1/4 \sim (\alpha_1 - 1/4)$ while for the case of two coupled LC’s $\langle s_i s_j \rangle_{1,1} - 1/4 \sim \sqrt{\alpha_1 - 1/4}$, both for small $\alpha_1 - 1/4$. The latter result can be rigorously established from the analytic expression $E^{LC}_\gamma(x_\gamma) - 1/4 = -1(x_\gamma) + \ln 2\alpha_1(1) + (\pi^2/48)(1 - x_\gamma)^3 + O((1-x_\gamma)^5)$ for the energy of the antiferromagnetic LC near maximal polarization, $x_\gamma$, which can be extracted from the Bethe-Ansatz.

The first- and second-order phase boundaries shown in Fig.1 meet in tricritical points at $(\alpha_1, \alpha_2) = 1/4 (1, -1 + \frac{1}{\ln 2})$ and at $(\alpha_1, \alpha_2) = 1/4 (-1 + \frac{1}{\ln 2}, 1)$ for the LC case and in a tricritical point at $(1/4, 1)$ for the LM case. The line of the first-order transition is the result of a numerical solution of the Bethe-Ansatz for the LC system, whereas for two coupled LM systems it is given by $16\alpha_1 \alpha_2 = 1$. Finally we note that the straight first-order line between the two tricritical points in Fig.1(a) separates the state with classical ferromagnetic long-range order within the subsystems ($x_\gamma = 1, \gamma = 1, 2$) from the quantum disordered state without long-range order (Bethe singlet).

**Thermodynamics.** – For the Lieb-Mattis model the saddle-point approximation becomes exact, i.e. the partition function is given in the thermodynamic limit by its largest term. The same statement holds also for the model of coupled Lieb-Mattis subsystems considered here and all thermodynamic potentials can be determined. The quantum
numbers of the largest term in the partition function depend on both \( \alpha_1, \alpha_2 \) and the temperature \( T \). For the Lieb-Mattis model the four (normalized) quantum numbers \( x^{A,B}_\gamma \) of the total spin operators \( (S^{A,B}_\gamma)^2 \) of the respective sublattices are independently conserved. Due to symmetry we have \( x^{A}_\gamma = x^{B}_\gamma \equiv y_\gamma \ (\gamma = 1, 2) \) and the total subsystem magnetisation \( x_\gamma \in [0, y_\gamma] \). The subsystem magnetisations \( x_\gamma = 2S_\gamma/N_\gamma \) are always antiparallel and \( S = |S_2 - S_1| \). We can define three independent order parameters \( \psi_1, \psi_2 \) and \( \psi_3 \) by

\[
\psi_1 = y_1^2 - x_1^2 \ ; \ \psi_2 = y_2^2 - x_2^2 \ ; \ \psi_3 = x_1^2 + x_2^2 .
\]

The parameters \( \psi_1 \) and \( \psi_2 \) are proportional to the antiferromagnetic order parameter, \( \psi_\gamma = 4(1/N_\gamma^2)\langle (S^{A}_\gamma - S^{B}_\gamma)^2 \rangle \), of the respective subsystems \( (\gamma = 1, 2) \) and \( \psi_3 \) is proportional to the order parameter for ferromagnetism in the individual subsystems, \( \psi_3 = 4[(1/N_1^2)\langle S_1^2 \rangle + (1/N_2^2)\langle S_2^2 \rangle] \). Though there are \( 2^3 = 8 \) possible phases, one of them, \( \psi_i > 0, \ i = 1, 2, 3 \), is found to be thermodynamically never stable. In the table we list the stable phases and illustrate in Fig.3 the phase diagram as a function of \( \alpha_1 \) and \( \alpha_2 \) for a constant \( \alpha_2 = 0.075 \). The high-temperature paramagnetic P-phase has the highest symmetry. For small \( \alpha_\gamma \ (\gamma = 1, 2) \) the inter-sublattice exchange dominates and both the first and the second subsystem are ferromagnetic. We call the resulting phase the ferromagnetic, or F-phase. For large \( \alpha_\gamma \ (\gamma = 1, 2) \) the intra-sublattice couplings dominate, leading to a singlet state in both subsystems, corresponding to the collinear antiferromagnetic AF-phase. The low temperature AF-phase gives way to the AF\(_1\)-phase at higher temperature when the second subsystem becomes paramagnetic, \( x_2 = 0 \) (the AF\(_2\) phase is realized for certain \( \alpha_1 < \alpha_2 \)).

The symmetry group of the noncollinear "order-from-disorder" OD\(_1\)-phase (the OD\(_2\)-phase is realized for certain \( \alpha_1 < \alpha_2 \)) is a subgroup of the symmetry groups of both the F-phase and AF\(_1\)-phase (compare the table), which in turn are subgroups of the fully symmetric P-phase. These relations are consistent with general requirements for the tetracritical point given by \( \alpha_1 = \sqrt{(1/4)\alpha_2^2 + 1/8 - (1/2)\alpha_2} \) and \( k_B T = (1/2)\alpha_1 \), in which these four phases meet [12]. All phase transitions shown in Fig.3 are of second order (with the characteristic jump in the specific heat), besides the transition from the OD\(_1\)-phase to the AF-phase. The symmetry group of neither the OD\(_1\)-phase nor of the AF-phase is a subgroup of the other (see the table) and the transition is consequently of first-order.

For every region of the phase diagram a distinct set of self-consistency equations determines the free energy and the correlation functions. E.g., the subsystem magnetisations \( x_1 = x_2/(4\alpha_1) \) and \( x_2 \equiv y_2 \) as well as the sublattice magnetisations of the first subsystem, \( y_1 \), in this OD\(_1\)-phase are determined via the equations

\[
y_1 = \tanh \left[ \alpha_1 y_1/(2k_B T) \right] \ ; \ x_2 = \tanh \left[ (1/\alpha_1 - 8\alpha_2) x_2/(16k_B T) \right] .
\]

The inter- and intra-subsystem correlation functions for the OD\(_1\)-phase are given by

\[
\langle s_i s_l \rangle_{1,2} = -x_2^2/(16\alpha_1) \ ; \ \langle s_i s_m \rangle_{2,2} = x_2^2/4 \ ; \ \langle s_i s_j \rangle_{1,1} = x_2^2/(32\alpha_1^2) - y_1^2/4 .
\]

where \( i, l \in A \) and \( j, m \in B \) in \( \langle s_i s_j \rangle_{1,1} \) and \( \langle s_i s_m \rangle_{2,2} \). The transition from the OD\(_1\)-phase to the AF\(_1\)-phase takes place when \( x_2 = 0 \) in Eq. [3] and the transition to the F-phase takes place when \( y_1 = x_1 = x_2/(4\alpha_1) \).

In the OD\(_1\)-phase the sublattice magnetisations in the first subsystem are neither parallel nor anti-parallel, one might call the OD\(_1\)-phase also a "twist"-phase. The temperature dependence of the inter-sublattice correlation functions in the first subsystem, \( \langle s_i s_j \rangle_{1,1} \),
are presented in Fig.4 for some selected values of $\alpha_1$ and $\alpha_2 = 0.075$. In the OD$_1$-phase ($1/4 < \alpha_1 < 1/(16\alpha_2)$ at $T = 0$) the correlation function $\langle s_is_j \rangle_{1,1}$ increases in magnitude as a function of temperature. This effect is particulary pronounced for $\alpha_1 = 1/\sqrt{8}$. For $\alpha_1 = 1/\sqrt{8}$ the A- and the B- sublattices of the first subsystem are completely uncorrelated at zero temperature (see Eq. (3)) and become more and more correlated with increasing temperature, as long as we remain in the OD$_1$-phase. This phenomenon is called order from disorder \cite{13, 14}, and is due to the interplay between different competing energy scales govering the correlations (compare Eq. (3) and Eq. (4)) of the individual subsystems. The disappearance of $\langle s_is_j \rangle_{1,1}$ at zero temperature for $\alpha_1 = 1/\sqrt{8}$ and the increase of magnetic order by fluctuations is related to the maximum in the GS energy $E_0(\alpha_1)$ which signals maximal frustration. On the other hand, the correlations decrease in the usual way with increasing temperature within the ferromagnetic phase or the antiferromagnetic phase.

**Summary.** – We have discussed quantum spin Heisenberg systems built of two coupled subsystems. If the individual subsystems are integrable on their part, the whole system is solvable for a long-ranged inter-subsystem coupling of constant magnitude. The three antiferromagnetic exchange integrals, namely the two intra-subsystem couplings and the inter-subsystem exchange parameter compete with each other. This competition gives rise to interesting frustration effects. Varying the strength of the three couplings we can tune the magnetic ordering of the individual subsystems between ferromagnetic and antiferromagnetic. In the limit of maximal competition between different exchange couplings neither ferromagnetic nor antiferromagnetic correlations dominate in the ground state. However, additional thermal fluctuations change the interplay between the competing energy scales and lead to an increase of magnetic order with temperature. This mechanism driving the order from disorder scenario seems to be not restricted on the special Lieb-Mattis coupling and we argue that the same phenomenon should be present in systems with more realistic couplings.

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Table 1: The seven thermodynamically stable phases for two coupled Lieb-Mattis antiferromagnets. $y_\gamma = (4/N_\gamma)S_\gamma^{A,B}$ $(0 \leq y_\gamma \leq 1, \gamma = 1, 2)$ are the relative magnetisations of the A,B-sublattice of the first/second subsystem and $x_\gamma = (2/N_\gamma)S_\gamma$ $(0 \leq y_\gamma \leq 1)$ $x_\gamma \in [0, y_\gamma]$ are the magnetisations of the respective $(\gamma = 1, 2)$ subsystem. The paramagnetic (P), ferromagnetic (F), the three antiferromagnetic phases (AF$_1$, (AF)$_2$, (AF) and the order from disorder phases (OD$_1$) and (OD$_2$) are characterized by the order parameters $\psi_1 = y_1^2 - x_1^2$, $\psi_2 = y_2^2 - x_2^2$ and $\psi_3 = x_1^2 + x_2^2$.

| Phase | $y_1$ | $y_2$ | $x_1$ | $x_2$ | $\psi_1$ | $\psi_2$ | $\psi_3$ |
|-------|-------|-------|-------|-------|----------|----------|----------|
| P     | 0     | 0     | 0     | 0     | 0        | 0        | 0        |
| F     | +     | +     | $y_1$ | $y_2$ | 0        | 0        | +        |
| AF$_1$| +     | 0     | 0     | 0     | +        | 0        | 0        |
| AF$_2$| 0     | +     | 0     | 0     | 0        | +        | 0        |
| AF    | +     | +     | 0     | 0     | +        | +        | 0        |
| OD$_1$| +     | +     | $\frac{y_2}{4\alpha_1}$ | $y_2$ | +        | 0        | +        |
| OD$_2$| +     | +     | $y_1$ | $\frac{y_2}{4\alpha_2}$ | 0 | +        | +        |

Figure 1: The ground-state phase diagram of a) two coupled antiferromagnetic linear chains and b) two coupled Lieb-Mattis antiferromagnets, as a function of the intrasubsystem couplings $\alpha_1$ and $\alpha_2$. The inter-subsystem coupling is $\alpha = 1$. The phases are characterized by the magnetisations $x_1$ and $x_2$ of the subsystems. The dashed/full lines denote phase transitions of first/second order.

Figure 2: The ground-state inter-subsystem $\langle s_is_j \rangle_{1,2}$ and the intra-subsystem $\langle s_is_j \rangle_{1,1}$ correlation function for two coupled linear chains (LC, dashed lines) and two coupled Lieb-Mattis antiferromagnets (LM, full lines), as a function of $\alpha_1$. The intra-subsystem coupling $\alpha_2 = 0.075$ and the inter-subsystem coupling $\alpha = 1$. At $\alpha_1 = 1/4$ a phase transition of second-order occurs for both systems and the correlation functions have a square-root singularity (kink) for the case of two LC’s (LM’s).

Figure 3: Phase diagram of two coupled Lieb-Mattis antiferromagnets, as a function of temperature $T$ and the intra-subsystem coupling $\alpha_1$, for $\alpha_2 = 0.075$ and the inter-subsystem coupling $\alpha = 1$. The phases are labelled with respect to the values of the correlation functions within the first subsystem.

Figure 4: The intra-subsystem correlation function $\langle s_is_j \rangle_{1,1}$ $(i \in A, j \in B)$ for two coupled Lieb-Mattis antiferromagnets, as a function of temperature $T$ for some selected $\alpha_1$’s, and fixed $\alpha_2 = 0.075$, $\alpha = 1$. The kinks in $\langle s_is_j \rangle_{1,1}$ correspond to phase transitions of second order. Note the particular strong “order from disorder” phenomenon for $\alpha_1 = 8^{-1/2}$. 

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