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R-matrices for integrable $SU(2) \times U(1)$-symmetric $S = \frac{1}{2}$ spin-orbital chains

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Abstract

The Yang–Baxter equation for an $SU(2) \times U(1)$-symmetric $S = \frac{1}{2}$ spin-orbital chain was solved using the special computer algorithm developed by the author. The seven new R-matrices separated into four groups are presented. Among the obtained integrable models there are special cases related to 1D ferromagnet TDAE $-$ C_{60}, 1D superconductors AC_{60} (A $=$ K, Cs, Rb), the quarter-filled ladder compound NaV_2O_5 and the model of correlated electrons on a chain of Berry phase molecules.

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1. Introduction

At the beginning of the 1970s Kugel and Khomskii [1] and, independently, Inagaki [2] suggested two various models to describe magnetic properties of solids with orbital degeneracy in electron systems of atoms. Starting from the two-band Hubbard model [3] they obtained low-energy Hamiltonians depending on both spin and pseudospin (orbital) operators. Kugel and Khomskii took into account geometry of d-orbitals entailing asymmetry of hopping integrals and obtained a general but realistic Hamiltonian. In contrast, Inagaki postulating the symmetric hopping distinguished between the Coulomb repulsions on the same and different orbitals. It was suggested in [1–3] that a non-trivial coupling between spin and orbital terms would result in a complex magnetic behaviour such as a ferromagnetism induced by orbital ordering.

While the spin dependence of the Hamiltonians [1, 2] has purely an $SU(2)$-invariant Heisenberg form, its dependence upon pseudospin is more complicated and in the simplest case possess only the $U(1)$ symmetry related to rotations along the z axis in the pseudospin space.

After the works [1, 2] some new applications of $SU(2) \times U(1)$-invariant spin models were suggested in a number of papers [4–10]. Ground state and excitations of some $SU(2) \times U(1)$-invariant spin chains were studied in [11, 12].

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The most elaborated approach for exact detailed analysis of a one-dimensional integrable spin chain was suggested by Faddeev and his school Quantum Inverse Scattering Method (Algebraic Bethe Ansatze) [13–15]. The latter is described by a Hamiltonian

$$\hat{H} = \sum_{n=1}^{N} H_{n,n+1}, \tag{1}$$

acting on the finite-dimensional space $(\mathbb{C}^M)^{\otimes N}$ $(M = 2, 3, 4, \ldots)$. Each term $H_{n,n+1}$ acts nontrivially as an $M^2 \times M^2$-matrix H only on the tensor product of two neighbour spaces $\mathbb{C}_n^M \otimes \mathbb{C}_{n+1}^M$.

The keystone of this approach is the Yang–Baxter equation

$$R_{12}(\lambda - \mu)R_{23}(\lambda)R_{12}(\mu) = R_{23}(\mu)R_{12}(\lambda)R_{23}(\lambda - \mu), \tag{2}$$

with the initial regularity condition

$$R(0) = cI. \tag{3}$$

Here $R(\lambda)$ is an $M^2 \times M^2$ matrix, I is the matrix unity while c is an arbitrary non-zero constant.

If the Hamiltonian density matrix H relates to $R(\lambda)$ by the following formula:

$$H = \left.\frac{\partial R(\lambda)}{\partial \lambda}\right|_{\lambda=0}, \tag{4}$$

then the system (1) is integrable.

In [16], a new method was suggested for solving equations (2) and (3). It is based on the series expansion for R-matrix:

$$R(\lambda) = \sum_{n=0}^{\infty} \frac{1}{n!} R^{(n)} \lambda^n, \tag{5}$$

where

$$\begin{aligned}
R^{(1)} &= H, \\
R^{(2)} &= H^2, \\
R^{(3)} &= H^3 + K, \\
R^{(4)} &= H^4 + 2(HK + KH), \\
R^{(5)} &= H^5 + L + 2(KH^2 + H^2K) + 6HKH, \\
R^{(6)} &= H^6 + KH^3 + H^3K + 9(H^2KH + HKH^2) + 10K^2 + 3(HL + LH).
\end{aligned} \tag{6}$$

The matrices K and L may be obtained from the following integrability conditions [13, 16, 17]:

$$\begin{aligned}
&K_{23} - K_{12} = [H_{12} + H_{23}, [H_{12}, H_{23}]], \\
&L_{23} - L_{12} = \left[H_{12}^3 + H_{23}^3 + 3(K_{12} + K_{23}), J\right] + 3(H_{12}[J, H_{12}]H_{12} + H_{23}[J, H_{23}]H_{23}) \\
&\qquad + (H_{12}H_{23} + H_{23}H_{12})(K_{23} - K_{12}) + (K_{23} - K_{12})(H_{12}H_{23} + H_{23}H_{12}) \\
&\qquad - 2(H_{12}(K_{23} - K_{12})H_{23} + H_{23}(K_{23} - K_{12})H_{12}),
\end{aligned} \tag{7}$$

where $J = [H_{12}, H_{23}]$.

As equation (2), equations (6) and (7) are invariant under the following $Q \in SL(M)$ action:

$$X \to Q^{-1}\otimes Q^{-1} X Q \otimes Q, \tag{8}$$

$Q \in SL(M)$, $X = H, K, R(\lambda)$.

In [16], it was shown that a detailed analysis of series expansions applied to quotients of the R-matrix entries gives possibility of guessing right the whole R-matrix. An alternative approach for solving systems (2) and (3) is given in the recent paper [19].

In the following sections, we shall present the R-matrices obtained by our approach related to the general $SU(2)\times U(1)$-symmetric spin–orbit Hamiltonian

$$\begin{aligned} H_{n,n+1} = (s_n s_{n+1})\big(a_1 + a_2\big(\tau_n^x\tau_{n+1}^x + \tau_n^y\tau_{n+1}^y\big) + a_3\tau_n^z\tau_{n+1}^z + \tfrac{1}{2}a_6\big(\tau_n^z + \tau_{n+1}^z\big)\big) \\ + a_4\big(\tau_n^x\tau_{n+1}^x + \tau_n^y\tau_{n+1}^y\big) + a_5\tau_n^z\tau_{n+1}^z + \tfrac{1}{2}a_7\big(\tau_n^z + \tau_{n+1}^z\big), \end{aligned} \tag{9}$$

which may be parameterized by the set of coefficients $S = \{a_1, a_2, \ldots, a_7\}$. Here in (9) the spin and pseudospin operators are expressed from the Pauli matrices

$$s^k = \tfrac{1}{2}\sigma^k \otimes I_2, \qquad \tau^k = \tfrac{1}{2}I_2 \otimes \sigma^k, \qquad k = x, y, z. \tag{10}$$

The following change of coefficients

$$\{a_1, a_2, a_3, a_4, a_5, a_6, a_7\} \to \{a_1, a_2, a_3, a_4, a_5, -a_6, -a_7\} \tag{11}$$

does not destroy an integrability or change the spectrum of Hamiltonian because it corresponds to the transformation (8) with $Q = I_2 \otimes \sigma^x$.

For a chain with even numbers of sites the same is true for the following change of variables:

$$\{a_1, a_2, a_3, a_4, a_5, a_6, a_7\} \to \{a_1, -a_2, a_3, -a_4, a_5, a_6, a_7\}, \tag{12}$$

which corresponds to the graduated version of (8).

$$H_{2n,2n+1} \to 4\tau_{2n}^z H_{2n,2n+1}\tau_{2n}^z, \qquad H_{2n-1,2n} \to 4\tau_{2n}^z H_{2n-1,2n}\tau_{2n}^z. \tag{13}$$

The case

$$S^{\mathrm{KH}} = \{1-\alpha, 0, 4(1+\alpha), 0, 1+\alpha, 4, -1\} \tag{14}$$

corresponds to the Kugel–Khomskii model of 1D perovskite [1].

The case

$$S^I = \left\{\tfrac{1}{2}(\alpha-\beta)+\gamma, 2(\alpha+\beta), 2(2\gamma+\beta-\alpha), \tfrac{1}{2}(3\beta-\alpha), \tfrac{1}{2}(3\beta+\alpha-2\gamma), 0, 0\right\}, \tag{15}$$

(where the unphysical region $\alpha \approx \beta \approx \gamma$, but $\beta > \alpha$ and $\beta > \gamma$) corresponds to Inagaki's model [2]. In [4], it was also applied to organic 1D ferromagnet TDAE $-$ C_{60} and in [5] to the family of 1D superconductors AC_{60} (A = K, Cs, Rb) (with $T_c > 30$ K).

The special case of (15) with

$$\alpha = 1 - \delta, \qquad \beta = 1 + \delta, \qquad \gamma = 1 - \delta^2, \tag{16}$$

(where in the physical region $0 < \delta < 1$) was studied in [6].

The two cases

$$S_1^{\mathrm{NaV_2O_5}} = \{\alpha, 8\beta, 4\alpha, 2\beta, 4\beta - \alpha, 0, 0\}, \tag{17}$$

$$S_2^{\mathrm{NaV_2O_5}} = \{-\alpha, 4\alpha, 4\alpha, 3\alpha, 3\alpha, -4\beta, \beta\}, \tag{18}$$

correspond to limiting cases of the model describing the quarter-filled ladder compound $\alpha' - \mathrm{NaV_2O_5}$ [7].

The case

$$S^{\mathrm{st}} = \{1, 2, 0, 0, 0, 0, 0\} \tag{19}$$

corresponds the effective spin-tube Hamiltonian suggested in [8].

Let us also mention the paper [9] where the spin-orbital Hamiltonian was applied to arrays of quantum dots.

In the special $SU(4)$-symmetric point

$$S^{SU(4)} = \{1, 4, 4, 1, 1, 0, 0\}, \tag{20}$$

the model (20) was solved in [18] ($R(\lambda) = \eta I + \lambda \mathcal{P}$). This point corresponds to degenerative cases of (15) ($\alpha = \beta = \gamma$) (or $\delta = 0$). Using the transformations (12) and (13), we may obtain the R-matrix for the model with

$$\tilde{S}^{SU(4)} = \{1, -4, 4, -1, 1, 0, 0\}. \tag{21}$$

In the special $Sp(4)$-symmetric point

$$S^{Sp(4)} = \{1, 4, 8, 2, 1, 0, 0\}, \tag{22}$$

(equivalent to $\tilde{S}^{Sp(4)} = \{1, -4, 8, -2, 1, 0, 0\}$) related to $3\alpha = \beta = \gamma$ in (17) the R-matrix was presented in [20].

Except (20) and (22) no integrable cases of the Hamiltonian (9) were studied up to now. In order to start this process we have solved systems (2), (3) related to (9). The calculations were performed by two steps. In the first, using the Gröbner package of the computer algebra system MAPLE 7 we have found seven new solutions of system (7). In the second, we derived the corresponding R-matrices using the approach suggested in [16, 19].

For convenience of representation the obtained R-matrices are separated into four groups. In each one all R-matrices have similar positions of non-zero entries, therefore they may be presented in a unique form.

Everywhere below $\varepsilon = \pm 1$.

2. The group 1

In this group, the R-matrix corresponds to

$$S^{(1)} = \{0, 4, 0, 1, 0, 4\varepsilon, \varepsilon\}, \tag{23}$$

and has the following form:

$$R^{(1)}(\lambda) = \begin{pmatrix}
f_+ & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \eta & 0 & 0 & g_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \eta & 0 & 0 & 0 & 0 & 0 & g_2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \eta & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & g_1 & 0 & 0 & 0 \\
0 & g_1 & 0 & 0 & \eta & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & f_- & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \eta & 0 & 0 & g_1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \eta & 0 & 0 & 0 & 0 & 0 & g_3 & 0 & 0 \\
0 & 0 & g_2 & 0 & 0 & 0 & 0 & 0 & \eta & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & g_1 & 0 & 0 & \eta & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & f_+ & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \eta & 0 & 0 & g_1 & 0 \\
0 & 0 & 0 & g_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \eta & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & g_3 & 0 & 0 & 0 & 0 & 0 & \eta & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & g_1 & 0 & 0 & \eta & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & f_-
\end{pmatrix}, \tag{24}$$

where $f_\pm = \pm\varepsilon\lambda + \eta$, $g_1 = \lambda$, $g_2 = -g_3 = \varepsilon\lambda$.

3. The group 2

This group consists of two related subgroups. For the first one the R-matrix is the following:

$$R^{(2a)}(\lambda) = \begin{pmatrix}
f_+ & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \eta & 0 & 0 & g_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \eta & 0 & 0 & 0 & 0 & 0 & g_2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \eta & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & g_1 & 0 & 0 & 0 \\
0 & g_1 & 0 & 0 & \eta & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & f_- & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \eta & 0 & 0 & g_1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & f_- & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & g_2 & 0 & 0 & 0 & 0 & 0 & \eta & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & g_1 & 0 & 0 & \eta & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & f_+ & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \eta & 0 & 0 & g_1 & 0 \\
0 & 0 & 0 & g_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \eta & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & f_- & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & g_1 & 0 & 0 & \eta & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & f_-
\end{pmatrix}, \tag{25}$$

and there are two solutions. The first one

$$S^{(2a,1)} = \{1, 8\varepsilon, 4, 2\varepsilon, 3, 4, -1\} \tag{26}$$

corresponds to $f_+ = f_- = \lambda + \eta$, $g_1 = -g_2 = \varepsilon\lambda$. The second

$$S^{(2a,2)} = \{1, 8\varepsilon, 4, 2\varepsilon, -1, 4, 3\} \tag{27}$$

corresponds to $f_\pm = \eta \pm \lambda$, $\varepsilon g_1 = g_2 = \lambda$.

For the second subgroup, the corresponding Hamiltonians may be obtained from (26), (27) by the transformation (11), while the R-matrices may be obtained by transposition with respect to the second diagonal.

4. The group 3

In this group, R-matrices have the form

$$R^{(3)}(\lambda) = \begin{pmatrix}
f_+ & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & h & 0 & 0 & g & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & f_+ & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & h & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & g & 0 & 0 & 0 \\
0 & g & 0 & 0 & h & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & f_- & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & h & 0 & 0 & g & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & f_- & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & f_+ & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & g & 0 & 0 & h & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & f_+ & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & h & 0 & 0 & g & 0 \\
0 & 0 & 0 & g & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & h & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & f_- & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & g & 0 & 0 & h & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & f_-
\end{pmatrix}. \tag{28}$$

There are two solutions. The first one corresponds to

$$S^{(3,1)} = \{0, 4, 0, 1, \theta, 0, 0\}. \tag{29}$$

Here $f_+ = f_- = \sinh(\lambda + \eta)$ for $\theta = 2\cosh\eta > 2$, $f_+ = f_- = \sin(\lambda + \eta)$ for $\theta = 2\cos\eta < 2$ and $f_+ = f_- = \lambda + \eta$ for $\theta = 2$. The latter solution is related to the special case of (15) with $\alpha = \beta$ and $\gamma = 0$ as well to the special case of (17) with $\alpha = 0$.

The second solution corresponds to

$$S^{(3,2)} = \{0, 4, 0, 1, 0, 0, \theta\}. \tag{30}$$

Here $f_\pm = \sinh(\eta \pm \lambda)$ for $\theta = 2\cosh\eta > 2$, $f_\pm = \sin(\eta \pm \lambda)$ for $\theta = 2\cos\eta < 2$ and $f_\pm = \eta \pm \lambda$ for $\theta = 2$. In both the cases $g = \sinh\lambda$, $h = \sinh\eta$ for $\theta > 2$, $g = \sin\lambda$, $h = \sin\eta$ for $\theta < 2$, and $g = \lambda$, $h = \eta$ for $\theta = 2$.

5. The group 4

In this group, R-matrices have the form

$$R^{(4)}(\lambda)=\begin{pmatrix}
f_1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&f_2&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&f_1&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&f_3&0&0&-g_1&0&0&g_2&0&0&g_1&0&0&0\\
0&0&0&0&f_2&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&f_1&0&0&0&0&0&0&0&0&0&0\\
0&0&0&-g_1&0&0&f_3&0&0&g_1&0&0&g_2&0&0&0\\
0&0&0&0&0&0&0&f_1&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&f_1&0&0&0&0&0&0&0\\
0&0&0&g_2&0&0&g_1&0&0&f_3&0&0&-g_1&0&0&0\\
0&0&0&0&0&0&0&0&0&0&f_1&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&f_2&0&0&0&0\\
0&0&0&g_1&0&0&g_2&0&0&-g_1&0&0&f_3&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&f_1&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&f_2&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&f_1
\end{pmatrix}, \tag{31}$$

where $g_2=f_2-f_3$.

There are two solutions. The first one corresponds to

$$S^{(4,1)}=\{1,4\varepsilon,-4,-\varepsilon,1,0,0\}, \tag{32}$$

where $f_1=f_2=\sinh(\lambda+\eta)$, $\varepsilon g_1=g_2=\sinh\lambda$, $f_3=\sinh(\lambda+\eta)-\sinh\lambda$, $\sinh\eta=\sqrt{3}$. For $\varepsilon=1$, this model is the special case of (15) with $\beta=\gamma=0$. For $\varepsilon=-1$, it is $SU(2)\times SU(2)$-symmetric (in fact $SU(4)$-symmetric [21]), and as was mentioned in [11] it corresponds to the four-critical point in the phase diagram of the ferromagnetic $SU(2)\times U(1)$-symmetric spin-orbital model. This model was also suggested in [10] as a model of correlated electrons in a lattice of Berry phase molecules. It was also shown in [19] that it is a Temperly–Lieb system [22].

The second solution corresponds to

$$S^{(4,2)}=\{2,4\varepsilon,-8,-\varepsilon,5,0,0\}, \tag{33}$$

where $f_1=f_2\mathrm{e}^{\lambda}=4e^{2\lambda}-1,\quad f_3=2e^{\lambda}+e^{-\lambda},\quad g_1=\varepsilon(1-e^{-2\lambda}),\quad g_2=4\sinh\lambda.$

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