Magnetic-field control of electric polarization in coupled spin chains with three-site interactions

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The linear perturbation renormalization group (LPRG) is used to study coupled XY chains with Dzyaloshinskii-Moriya (DM) and three-spin interactions in a magnetic field. Starting with a minimal model exhibiting the magnetoelectric effect, a spin-$\frac{1}{2}$ XY chain with nearest, next-nearest (J_2^x), and DM (D_1^y) interactions in a magnetic field, the recursion relations for all effective interactions generated by the LPRG transformation are found. The evaluation of these relations allows us to analyze, among others, the influence of J_2^x, D_1^y, three-spin ($S_i^x S_{i+1}^y S_{i+2}^z - S_i^y S_{i+1}^x S_{i+2}^z$), and interchain interactions on the thermodynamic properties. The field and temperature dependences of the polarization, specific heat, and correlation functions are found. It is shown that an interchain coupling triggers a phase transition indicated by the divergence of the renormalized coupling parameters.

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I. INTRODUCTION

The interest in the magnetoelectric effect (MEE), the mutual influence of magnetic and electric properties, dates back to the 19th century [1,2]. However, recently a surge in interest in multiferroic materials caused studies of MEE to be intensified [2–6]. There are several mechanisms which lead to the effect of induction of polarization by a magnetic field or magnetization by an electric field, one of which was described by Katsura, Nagaosa, and Balatsky [7] (called the KNB mechanism). In this mechanism the spin-current-induced electric polarization is given by

$$\mathbf{P} \propto \sum_i \mathbf{e}_\beta \times (\mathbf{S}_i \times \mathbf{S}_{i+\beta}), \tag{1}$$

where $\mathbf{e}_\beta$ is the unit vector in the β direction. According to the KNB scenario the local electric polarization is connected to the noncollinear ordering of the neighboring spins, and the polarization operator is related to the Dzyaloshinskii-Moriya (DM) interaction. So the minimal model exhibiting the magnetoelectric effect in the spirit of the KNB mechanism is the XY spin chain with nearest-neighbor (J_1), next-nearest-neighbor (J_2), and DM interactions [5,8]:

$$\mathcal{H} = \sum_n \left[J_1 \left(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y \right) + J_2 \left(S_n^x S_{n+2}^x + S_n^y S_{n+2}^y \right) + D_1^y \left(S_n^x S_{n+1}^y - S_n^y S_{n+1}^x \right) - H_z S_n^z \right]. \tag{2}$$

D_1^y denotes the strength of the DM coupling, which is interpreted as an external electric field coupled to the electric polarization. Brockman *et al.* [5] studied the integrable part of the Hamiltonian (2) without the next-nearest-neighbor interaction ($J_2 = 0$) and showed that in such a model the polarization can be controlled by a magnetic field only if the DM interaction parameter D_1^y is finite. Recently, Menchyshyn *et al.* [6] additionally included three-spin interactions in the form

$$E \sum_n \left(S_n^x S_{n+1}^z S_{n+2}^y - S_n^y S_{n+1}^z S_{n+2}^x \right) + K \sum_n \left(S_n^x S_{n+1}^z S_{n+2}^x - S_n^y S_{n+1}^z S_{n+2}^y \right). \tag{3}$$

The model is still integrable (if $J_2 = 0$), and as the authors have shown rigorously it allows us to get finite magnetic-field-dependent polarization also in the absence of the electric field ($D_1^y = 0$), provided E is different from zero.

Exactly solvable models are fundamental, enabling better understanding of the main feature of a phenomenon, and they are reference points for more realistic cases. However, in order to consider real materials one should have methods which allow one to study more complicated models, foregoing rigor. In this paper we consider the full chain Hamiltonian (2) with weak interchain coupling at finite temperature by using the linear perturbation renormalization group (LPRG) [9]. As usual, even in one dimension, the RG transformation generates all interactions admitted by the symmetry of the problem. Consequently, for one chain, in addition to the four original coupling parameters (J_1, J_2, D_1^y, and H_z) of the Hamiltonian (2) we have to consider eight others.

II. THE RG TRANSFORMATION

Let us start with a one-chain Hamiltonian

$$\mathcal{H}_1(\hat{S}) = \sum_n \mathcal{H}_1^n \tag{4}$$

and

$$\mathcal{H}_1^n = k_1^x \left(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y \right) + k_2^x \left(S_n^x S_{n+2}^x + S_n^y S_{n+2}^y \right) + d_1^y \left(S_n^x S_{n+1}^y - S_n^y S_{n+1}^x \right) - h_z S_n^z, \tag{5}$$

where the operators S_n^α obey the commutation relations $[S_n^x, S_n^y] = 2i S_n^z$, etc.; $k_i = J_i/T$; $d_i^y = D_i^y/T$; $h_z = H_z/T$; and a factor $-\beta = -1/k_\beta T$ has been absorbed in the Hamiltonian (4).

The RG transformation of the Hamiltonian (4) is defined by

$$e^{\mathcal{H}_1'(\hat{\sigma})} = \mathrm{Tr}_S P(\hat{\sigma}, \hat{S}) e^{\mathcal{H}_1(\hat{S})}, \tag{6}$$

with a linear weight operator $P(\hat{\sigma}, \hat{S})$, which projects the original spin space S onto the space of new spins σ. Tr_S denotes the partial trace over S space. In the LPRG transformation one divides the chain into m-spin blocks, and the first step in the

procedure is the choice of the block size. It is obvious that a renormalization-group transformation should preserve all symmetries of the original problem. This determines, to some extent, the choice of the block size. So if one wants to consider nearest-neighbor and next-nearest-neighbor interactions and admit the possibility of the existence of a phase transition to the two-sublattice phase, one should use blocks with the following numbers of sites: 7, 11, 15, ... For a quantum system, because of the noncummativity of several terms of the Hamiltonian, the renormalization transformation cannot be carried out exactly even for one chain, and the results of the transformation depend on the block size. The advantage of using a larger block was discussed in our previous article [10], where an XY chain with nearest-neighbor interactions was considered by using four-, six-, and eight-spin blocks. For not very low temperatures all three approximations are in quite good agreement with the exact result. In this paper, taking into account a number of degrees of freedom of the considered model, we will confine ourselves to the smallest acceptable and tractable block without extended numerics, which is a seven-site one $(S_1,S_2,S_3,S_4,S_5,S_6,S_7)$. For such a block

$$P(\hat{\sigma},\hat{S}) = \tfrac{1}{128}\big(1+\tfrac{1}{3}\hat{S}_1\hat{\sigma}_1\big)\big(1+\tfrac{1}{3}\hat{S}_4\hat{\sigma}_2\big)\big(1+\tfrac{1}{3}\hat{S}_7\hat{\sigma}_3\big), \quad (7)$$

and $\hat{S}_i\hat{\sigma}_j = S_i^x\sigma_j^x + S_i^y\sigma_j^y + S_i^z\sigma_j^z$. The RG transformation (6)–(7) applied to the Hamiltonian (4) generates all terms acceptable by the symmetry, namely, in addition to the four original terms (5), three two-spin terms,

$$\mathcal{H}_2^n = k_1^z S_n^z S_{n+1}^z + k_2^z S_n^z S_{n+2}^z + d_2^y\big(S_n^x S_{n+2}^y - S_n^y S_{n+2}^x\big), \quad (8)$$

and five three-spin interactions,

$$\begin{aligned}\mathcal{H}_3^n = {} & k_{xxz}\big(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y\big)S_{n+2}^z + k_{xzx}\big(S_n^x S_{n+1}^z S_{n+2}^x \\ & + S_n^y S_{n+1}^z S_{n+2}^y\big) + k_{xyz}\big(S_n^x S_{n+1}^y - S_n^y S_{n+1}^x\big)S_{n+2}^z \\ & + k_{xzy}\big(S_n^x S_{n+1}^z S_{n+2}^y - S_n^y S_{n+1}^z S_{n+2}^x\big) \\ & + d_z S_n^z S_{n+1}^z S_{n+2}^z. \end{aligned} \quad (9)$$

So to consider the model (4) in the frame of the RG one has to take into account 12 interaction parameters: the four original ones (k_1^x,k_2^x,d_1^y, and h_z) and the eight generated by RG transformation (k_1^z,k_2^z,d_2^y,k_{xxz},k_{xzx},k_{xyz},k_{xzy}, and d_z), and the final Hamiltonian of a seven-spin block reads [(4), (8), and (9)],

$$\mathcal{H}_0(\hat{S}) = \sum_{n=1}^{6}\mathcal{H}_1^n + \sum_{n=1}^{6}\mathcal{H}_2^n + \sum_{n=1}^{5}\mathcal{H}_3^n. \quad (10)$$

It is easy to find the renormalized Hamiltonian (5) in the form

$$\mathcal{H}_0'(\hat{\sigma}) = \ln \mathrm{Tr}_S P(\hat{\sigma},\hat{S})e^{\mathcal{H}_0(\hat{S})} = \ln \tilde{\mathcal{H}}_0(\hat{\sigma}), \quad (11)$$

where

$$\begin{aligned}\tilde{\mathcal{H}}_0(\hat{\sigma}) = {} & f_0 + f_1^x\big(\sigma_1^x\sigma_2^x + \sigma_2^x\sigma_3^x + \sigma_1^y\sigma_2^y + \sigma_2^y\sigma_3^y\big) \\ & + f_2^x\big(\sigma_1^x\sigma_3^x + \sigma_1^y\sigma_3^y\big) + f_1^{xy}\big(\sigma_1^x\sigma_2^y - \sigma_1^y\sigma_2^x \\ & + \sigma_2^x\sigma_3^y - \sigma_2^y\sigma_3^x\big) - f_z\big(\sigma_1^z + \sigma_3^z\big) - f_z'\sigma_2^z \\ & + f_1^z\big(\sigma_1^z\sigma_2^z + \sigma_2^z\sigma_3^z\big) + f_2^z\sigma_1^z\sigma_3^z \\ & + f_2^{xy}\big(\sigma_1^x\sigma_3^y - \sigma_1^y\sigma_3^x\big) + f_{xxz}\big(\sigma_1^x\sigma_2^x + \sigma_1^y\sigma_2^y\big)\sigma_3^z \\ & + f_{xzx}\big(\sigma_1^x\sigma_2^z\sigma_3^x + \sigma_1^y\sigma_2^z\sigma_3^y\big) + f_{xyz}\big(\sigma_1^x\sigma_2^y - \sigma_1^y\sigma_2^x\big) \\ & \times\sigma_3^z + f_{xzy}\big(\sigma_1^x\sigma_2^z\sigma_3^y - \sigma_1^y\sigma_2^z\sigma_3^x\big) + f_d\sigma_1^z\sigma_2^z\sigma_3^z, \end{aligned} \quad (12)$$

and for example,

$$\begin{aligned} f_0 &= \tfrac{1}{128}\mathrm{Tr}_S e^{\mathcal{H}_0(\hat{S})}, \\ f_1^x &= \tfrac{1}{128}\mathrm{Tr}_S S_1^x S_4^x e^{\mathcal{H}_0(\hat{S})}, \\ f_2^x &= \tfrac{1}{128}\mathrm{Tr}_S S_1^x S_7^x e^{\mathcal{H}_0(\hat{S})}, \end{aligned} \quad (13)$$

and so on. Now the point is to find $\mathcal{H}_0'(\hat{\sigma})$ [Eq. (11)] in the same form as the original Hamiltonian $\mathcal{H}_0(\hat{S})$ [Eq. (10)]. The task is not trivial because of the noncommutativity of several terms in the Hamiltonian, but it can be done by using the formula

$$\ln\tilde{\mathcal{H}}_0(\hat{\sigma}) = \sum_{i=1}^{8}\ln\lambda_i\prod_{j\neq i}\frac{\tilde{\mathcal{H}}_0(\hat{\sigma}) - \lambda_j\mathcal{I}_8}{\lambda_i - \lambda_j}, \quad (14)$$

where λ_i are eigenvalues of the Hamiltonian $\mathcal{H}_0(\hat{\sigma})$ and $\mathcal{I}_8$ is the unity matrix.

We can factor the eight-dimensional space of three spins into four subspaces (two one-dimensional and two three-dimensional), which allows us to find analytical formulas for eigenvalues of the Hamiltonian $\tilde{\mathcal{H}}_0(\hat{\sigma})$ [Eq. (12)], so

$$\begin{aligned} &\lambda_1 = f_0 + f_d + f_z + f_z' + f_2^z + 2f_1^z, \quad \lambda_8 = f_0 - f_d - f_z - f_z' + f_2^z + 2f_1^z, \\ &\lambda_2 = \frac{1}{3}C_q + \frac{2^{1/3}B_q}{3A_q} - \frac{A_q}{2^{2/3}3}, \quad \lambda_{3,4} = \frac{1}{3}C_q - \frac{(1\pm\imath\sqrt{3})B_q}{2^{2/3}3A_q} + \frac{(1\mp\imath\sqrt{3})A_q}{2^{1/3}6}, \\ &\lambda_5 = \frac{1}{3}C_Q + \frac{2^{1/3}B_Q}{3A_Q} - \frac{A_Q}{2^{2/3}3}, \quad \lambda_{6,7} = \frac{1}{3}C_Q - \frac{(1\pm\imath\sqrt{3})B_Q}{2^{2/3}3A_Q} + \frac{(1\mp\imath\sqrt{3})A_Q}{2^{1/3}6}, \end{aligned} \quad (15)$$

where the coefficients A_i,B_i,C_i $(i=q,Q)$ are defined in Appendix A. Using formula (14), one can find the renormalized Hamiltonian in the same form as the original one [(10), (5), (8), and (9)] with new effective interaction parameters:

$$\big(f_0\ ,\ k_1^x\ ,\ k_2^x\ ,\ d_1^y\ \ ,\ h_z\ ,\ k_1^z\ ,\ k_2^z\ ,\ d_2^y\ ,\ k_{xxz}\ ,\ k_{xzx}\ ,\ k_{xyz}\ ,\ k_{xzy}\ ,\ d_z\big) \quad (16)$$

$$\downarrow$$

$$\big(Z_0\ ,\ K_1^x\ ,\ K_2^x\ ,\ D_1^y\ \ ,\ H_z\ ,\ K_1^z\ ,\ K_2^z\ ,\ D_2^y\ ,\ K_{xxz}\ ,\ K_{xzx}\ ,\ K_{xyz}\ ,\ K_{xzy}\ ,\ D_z\big). \quad (17)$$

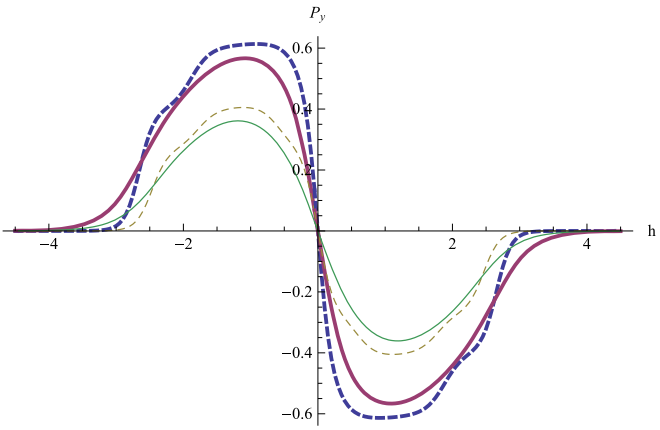


FIG. 1. Field dependences of polarization for $k_{xyz} = 0.5, k_{xzy} = 0$ (thick lines) and $k_{xyz} = 0, k_{xzy} = 0.5$ (thin lines) at reduced temperature $t = 0.5$ (solid lines) and $t = 0.2$ (dashed lines).

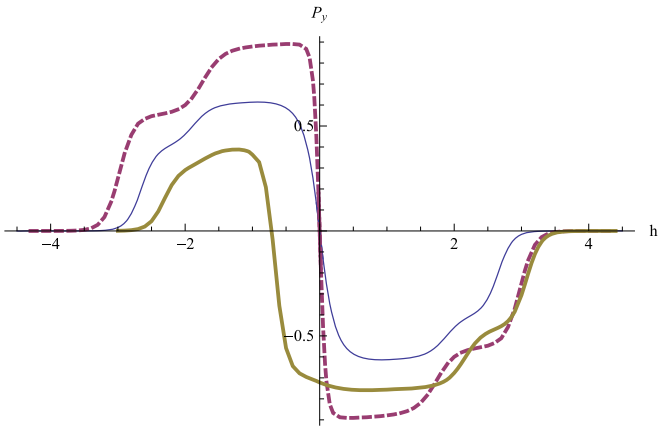


FIG. 3. Field dependences of polarization for three models: (i) $k_{xyz} = 0.5, k_2^x = 0, d_1^0 = 0$ (thin solid line), (ii) $k_{xyz} = 0.5, k_2^x = -0.5, d_1^y = 0$ (dashed line), and (iii) $k_{xyz} = 0.5, k_2^x = 0, d_1^y = 0.3$ (thick solid line) at $t = 0.2$.

The formulas for the effective parameters as functions of the original ones generated by the RG transformation have a rather complicated but closed form and are presented in Appendix B. We are now able to evaluate numerically the renormalization transformation which allows us to find the thermodynamic properties of the system. In each step of the transformation, in addition to the spin-dependent terms (couplings) a constant Z_0 (independent of effective spins $\hat{\sigma}$) is generated. This constant, presented in Appendix B [Eq. (B4)], can be used to calculate the free energy per site according to the following formula:

$$f = \sum_{n=1}^{\infty} \frac{Z_0^{(n)}}{3^n}, \tag{18}$$

where n indicates the numbers of RG steps.

Evaluating the RG recursion relations, we can find the field and temperature dependences of the polarization defined by

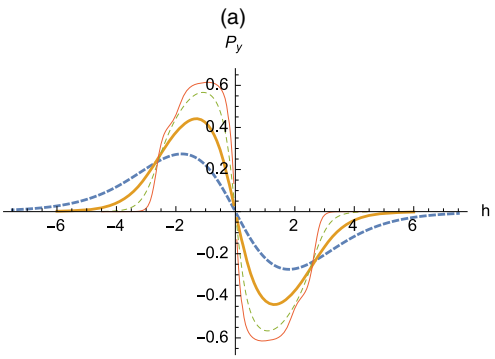
$$P_y = \frac{1}{N} \sum_n \langle S_n^x S_{n+1}^y - S_n^y S_{n+1}^x \rangle, \tag{19}$$

specific heat C_h, and the nearest-neighbor correlation function

$$G_{xx} = \frac{1}{2N} \sum_n \langle S_n^x S_{n+1}^x + S_n^y S_{n+1}^y \rangle, \tag{20}$$

where the angle brackets denote the thermal average.

As shown in Fig. 1, the three-spin interactions k_{xyz} and k_{xzy} [Eq. (9)] induce the magnetic-field-dependent polarization even if $d_i^y = 0$ for a certain range of the field [6]. At any temperature the effect is larger for the model with $k_{xyz} \neq 0, k_{xyz} = 0$ (thick lines) than for the opposite case $k_{xyz} = 0, k_{xyz} \neq 0$ (considered in Ref. [6]). The remaining three-spin interactions of Eq. (9) cannot lead to a finite polarization for $d_i^y = 0$. Hereafter, we take $J_1^x = 1$ and assume that only three original couplings, J_2^x, D_1^y, and $J_{xyz} = k_{xyz} T$, can be different from zero. The possible origin of the latter one has been discussed in several papers [11]. Figure 2 shows the field dependence of the polarization for several values of temperature [Fig. 2(a)] and for several values of d_1^y [Fig. 2(b)] at temperature $t = 0.5$. As can be seen, the external electric field through the effective Dzyaloshinskii-Moriya interactions d_1^y introduces asymmetry with respect to $h \to -h$ and $P_y \to -P_y$. For d_1^y large enough, $d_1^y \geqslant d_g \approx 0.8$, the polarization is negative for negative and positive magnetic fields [Fig. 2(b)]. At lower temperature $t = 0.2$ (Fig. 3) the polarization exhibits a broad, flat maximum (plateau) that is clearly visible for two cases: (i) $k_{xyz} = 0.5, k_2^x = 0, d_1^0 = 0$ and (ii) $k_{xyz} = 0.5, k_2^x = -0.5, d_1^y = 0$. For the third case $k_{xyz} = 0.5, k_2^x = 0, d_1^y = 0.3$, the shape of the polarization curve strongly



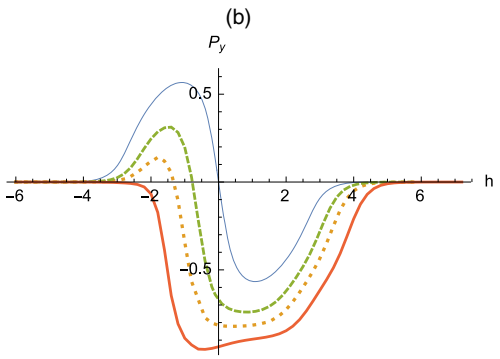


FIG. 2. Field dependences of polarization for $k_{xyz} = 0.5, k_{xzy} = 0$ (a) for several values of temperature, $t = 2$ (thick dashed line), 1 (thick solid line), 0.5 (thin dashed line), and 0.2 (thin solid line), and (b) for several values of the electric field, $d_1^y = 0$ (thin solid line), 0.3 (thick dashed line), 0.5 (dotted line), and 0.8 (thick solid line), at $t = 0.5$.

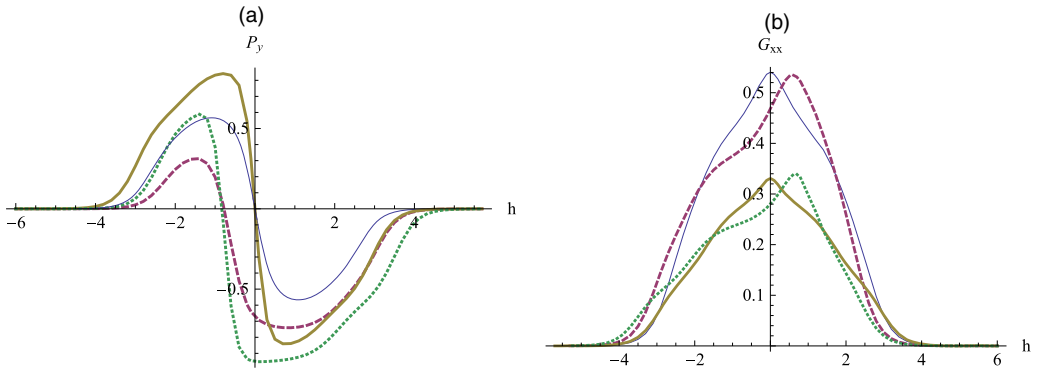


FIG. 4. Field dependences of (a) polarization P_y and (b) nearest-neighbor correlation function G_{xx} for (i) $k_{xyz} = 0.5, k_2^x = 0.0, d_1^y = 0.0$ (thin solid line), (ii) $k_{xyz} = 0.5, k_2^x = -0.5, d_1^y = 0.0$ (thick solid line), (iii) $k_{xyz} = 0.5, k_2^x = 0.0, d_1^y = 0.3$ (dashed line), and (iv) $k_{xyz} = 0.5, k_2^x = -0.5, d_1^y = 0.3$ (dotted line) at $t = 2$.

depends on the sign of the field, and the plateau is not so pronounced.

Figure 4 illustrates the effect of the next-nearest-neighbor (k_2^x) interaction and the electric field d_1^y on the polarization P_y and the correlation function G_{xx} [Eq. (20)]. There are field dependences of P_y and G_{xx} for the three cases mentioned above plus another case where $k_{xyz} = 0.5, k_2^x = -0.5, d_1^y = 0.3$. As can be seen, a negative value for k_2^x ($k_2^x = -0.5$) reduces the correlation function, whereas such an interaction increases the polarization. A positive value for d_1^y ($d_1^y = 0.3$) shifts the maximum of G_{xx} from $h = 0$ towards positive fields and the point $P_y = 0$ towards negative fields. Figure 5 shows the polarization and specific heat of model (i) as functions of temperature. For some range of the field (around $h = 2$) the polarization exhibits a maximum related to the low-temperature maximum of the specific heat. A second peak structure in the specific heat at low temperature has also been observed for the model with three-spin interaction at $h = 0$ when $J_1^x / J_{xzy} > \alpha_c$ (some critical value) [12]. The existence of the three-spin interaction is not, of course, a necessary condition to get the two-maximum structure of the specific heat, which can be expected if there are at least two mechanisms of local orderings. However, in the present model the second peak of the specific heat is accompanied by a maximum of the polarization. In Fig. 6 the polarization maxima and the low-temperature peaks of the specific heat for $k_{xyz} = 0.2, 0.5$, and 0.8 and relevant values of the magnetic field (from the range in which such maxima occur) are compared.

III. COUPLED CHAINS

For higher dimensions the LPRG approach starts with a renormalization of one chain [(6) and (7)]. Then, on the basis of this renormalization, the interchain interaction $\mathcal{H}_I$ is renormalized in a perturbative way [9]. The renormalization transformation for the system made of the coupled chains can be written as

$$\mathcal{H}'(\hat{\sigma}) = \mathcal{H}'_0(\hat{\sigma}) + \ln\langle e^{\mathcal{H}_I}\rangle_{\mathcal{H}_0(\hat{S})}, \tag{21}$$

with the standard cumulant expansion for $\ln\langle e^{\mathcal{H}_I}\rangle_{\mathcal{H}_0(\hat{S})}$, where $\mathcal{H}'_0(\hat{\sigma})$ is the effective chain Hamiltonian (11) and $\mathcal{H}_0(\hat{S})$ is the original chain Hamiltonian (10). An average of an operator $\hat{A}$ is defined as

$$\langle \hat{A}\rangle = \tfrac{1}{4}\{\mathrm{Tr}\{\hat{A}, Pe^{\mathcal{H}_0(\hat{S})}\}, [\mathcal{H}'_0(\hat{\sigma})]^{-1}\}, \tag{22}$$

where the curly brackets denote anticommutators.

Now, in the frame of LPRG [9] we consider the weak interchain interactions in the form

$$\mathcal{H}_{I1} = j_1^x \sum_n \left(S_{n,m}^x S_{n,m+1}^x + S_{n,m}^y S_{n,m+1}^y\right), \tag{23}$$

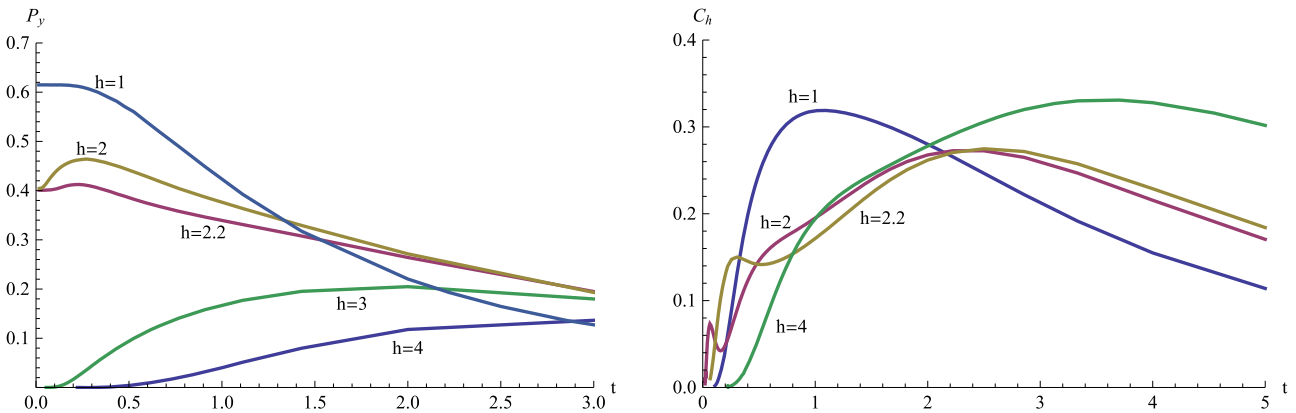


FIG. 5. Temperature dependences of polarization P_y and specific heat C_h for $k_{xyz} = 0.5, k_2^x = 0.0, d_1^y = 0.0$, and several values of magnetic field.

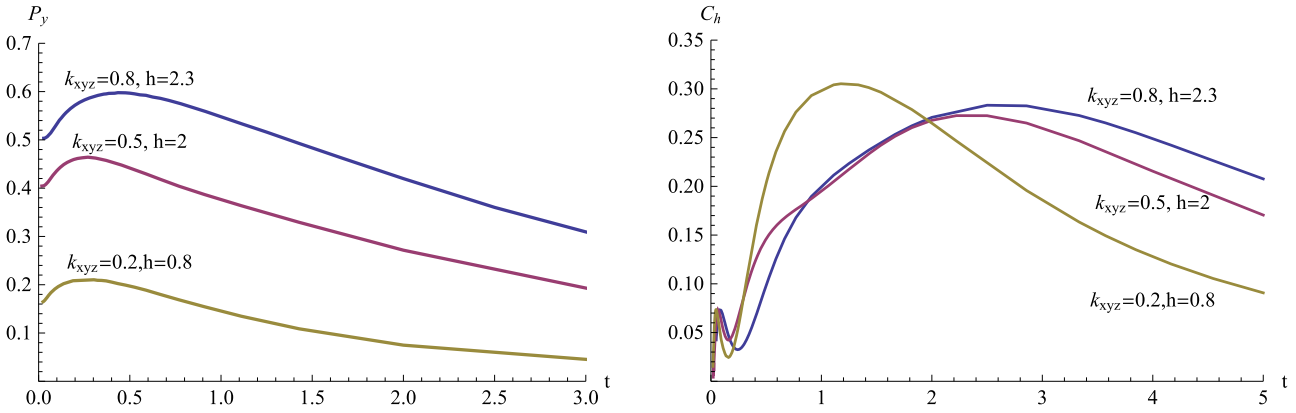


FIG. 6. Temperature dependences of polarization P_y and specific heat C_h for several values of k_{xyz} and magnetic field.

where the label n refers to chains (rows) and m refers to columns.

The LPRG transformation [9,13] when applied on an infinite system generates an infinite number of new interactions already in the second-order cumulant expansion which is the lowest nontrivial case for the present system. Thus, in order to find the LPRG recursion relations we have to confine ourselves to a finite cluster. In a second-order calculation we have to consider three chains (rows). Until now, considering the one-dimensional (1D) system we have used seven spin blocks to find RG recursion relations. In order to study the interchain interaction we apply a (4-6-4) cluster with four, six, and again four spins for the first, second, and third chains, respectively. In addition for simplification we confine ourselves to only two-site interactions between chains. Under these assumptions the LPRG transformation generates only two new couplings, j_2^x and d_2^y,

$$\mathcal{H}_{I2} = j_2^x \sum_n \left(S_{n,m}^x S_{n+1,m+1}^x + S_{n,m}^y S_{n+1,m+1}^y\right) + d_2^y \sum_n \left(S_{n,m}^x S_{n+1,m+1}^y - S_{n,m}^y S_{n+1,m+1}^x\right). \quad (24)$$

Finally, the interchain Hamiltonian is given by

$$\mathcal{H}_I = \mathcal{H}_{I1} + \mathcal{H}_{I2}. \quad (25)$$

To evaluate the transformation (21) we have to know the averages of the spin components and their products. They can be easily found but have rather complicated, although closed, expressions, for example,

$$\langle S_1^x \rangle = x_{11}\sigma_1^x + x_{12}\sigma_2^x + y_{11}\sigma_1^y + y_{12}\sigma_2^y + x_z\sigma_1^x\sigma_2^z + z_x\sigma_1^z\sigma_2^x + z_y\sigma_1^z\sigma_2^y, \quad (26)$$

where coefficients are expanded functions of all interaction parameters.

In a one-dimensional system (one chain) the RG transformation from the original set of coupling parameters to the set of renormalized ones [(16) and (17)] exhibits only one stable fixed point at $T = \infty$ ($K_\alpha = 0, D_\alpha = 0$). In a two-dimensional (2D) system evaluating the LPRG recursion relations with interchain interactions (25), we have found two stable fixed points at $T = \infty$ and $T = 0$ and the critical surface in the space of the 15 parameters: 12 from Eq. (16) and three interchain interactions, j_1^x, j_2^x, and d_2^y [(23) and (24)]. This means that the interchain interactions (23) trigger a phase transition indicated by divergences of the coupling parameters. Unfortunately, this method does not allow us to decide the character of the phase transition and the nature of a low-temperature phase. However, we can determine the location of the singularity (critical) point. In Fig. 6 the critical temperatures as functions of external field for several coupled chains are displayed. Only in the case with $j_1^x = 0.9, k_{xyz} = 0$, and $d_1^y = 0$ close to the spatially isotropic XY model ($j_1^x = 1$) can the critical temperature be satisfactory fitted for small fields to a single power (parabolic) law, $t_c(h) = 0.498 - 0.067h^2$. In other cases the dependences are more complicated. Figure 7 shows the field dependences of the polarization for temperatures above and below the zero-field critical temperature $t_c(0)$. For $t > t_c(0)$ the appropriate curves are close to that for a single chain, whereas for $t < t_c(0)$ the polarization increases near the critical point $t \to t_c(h)$ because of divergences of the coupling parameters. For the model with $j_1^x = 0.1, k_2^x = -0.5$ at low temperature (but still higher than the critical one), the polarization displays a broad, flat maximum like in the 1D case. Such a maximum has been observed, for example, in $Ba_2Mg_2Fe_{12}O_{22}$ [14]. The critical temperature is accompanied by the divergence of the

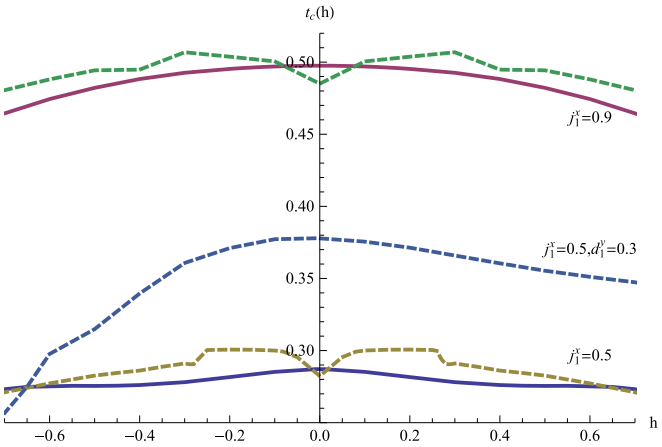


FIG. 7. Critical temperature as a function of magnetic field for $k_{xyz} = 0$ (solid lines) and $k_{xyz} = 0.5$ (dashed lines), $j_1^x = 0.5$ or 0.9, and $d_1^y = 0$ (bottom and top curves) or $d_1^y = 0.3$ (middle curve).

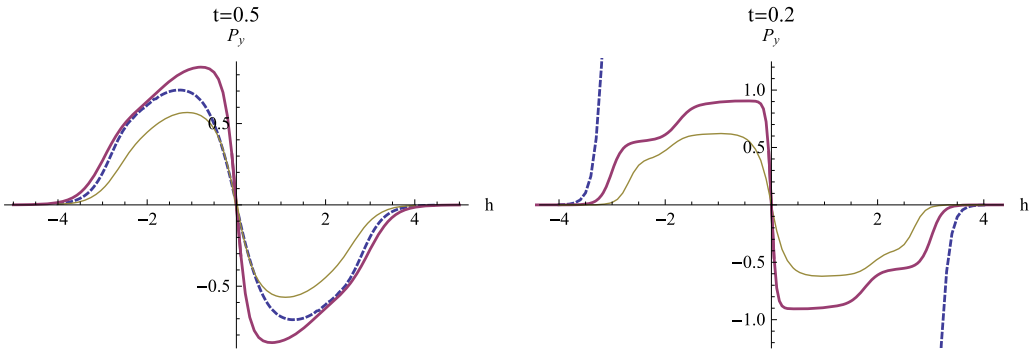


FIG. 8. Field dependences of polarization for 2D ($k_{xyz} = 0.5$) and $j_1^x = 0.5, k_2^x = 0$ (dashed lines), $j_1^x = 0.1, k_2^x = 0$ (thin solid line), and $j_1^x = 0.1, k_2^x = -0.5$ (thick solid line) at temperature $t = 0.5$ and 0.2.

specific heat (Fig. 8), but in the frame of the LPRG method we are not able to determine the character of this singularity (critical index) reliably.

IV. CONCLUSIONS

Admittedly, there is no universal generally accepted mechanism of the magnetoelectric effect, but the KNB mechanism may be regarded as a plausible explanation in several quasi-one-dimensional magnetic materials such as spin-$\frac{1}{2}$ chain cuprates $LiCu_2O_2$ [15,16] and $LiCuVO_4$ [17], the frustrated magnet $MnWO_4$ [18], cupric chloride ($CuCl_2$) [19], and a number of others [4]. The fundamental properties of the models based on the KNB mechanism have been analyzed for exactly solvable spin chains in Refs. [5,6]. The authors of those papers, in order to preserve system integrability, confined themselves to the nearest-neighbor XY model with DM interaction in a magnetic field [5], supplemented alternatively with three-spin interaction (3) [6]. At the expense of giving up exact solvability one can, of course, consider more realistic or at least more complex models. The main point is the possibility of taking into account the next-nearest-neighbor interaction J_2^x. Moreover, although the compounds mentioned above may be regarded as one-dimensional, it is known that they undergo a phase transition triggered by some interchain coupling. So we have used the method that allows us to consider both next-nearest-neighbor and interchain interactions in a reasonable approximation.

The linear RG transformation applied to the Hamiltonian of a J_1^x-J_2^x chain with DM interaction in a magnetic field generates eight new effective interactions, three two-spin and five three-spin ones, which have to be considered in an analysis of the RG recursion relations, although their original values (16) can be zero. In the present paper we have focused on the influence of the next-nearest-neighbor (NNN) k_2^x, three-spin k_{xyz} [Eq. (9)], and interchain j_1^x [Eq. (23)] interactions and an external electric field d_1^y (5) on the polarization, the nearest-neighbor correlation function, and the specific heat. As already shown [6], the three-spin interaction k_{xzy} [Eq. (9)] triggers the polarization and is influenced by the magnetic field even in the absence of the electric field. Similarly, the polarization can be controlled solely by the three-spin interaction k_{xyz} [Eq. (9)], and the effect is larger in the latter case. The polarization as a function of magnetic field is, of course, impacted by an electric field d_1^y [Fig. 2(b)] and also by NNN interaction [Fig. 4(a)]. A sufficiently large electric field ensures that the polarization does not change sign for any value or sign of the magnetic field. The electric field also shifts the maximum of the correlation function G_{xx} from the point $h = 0$ [Fig. 4(b)]. The negative NNN interaction reduces G_{xx} but increases the polarization. The temperature dependences of the polarization and the specific heat have also been studied for several values of the magnetic field (Fig. 9). It has been shown

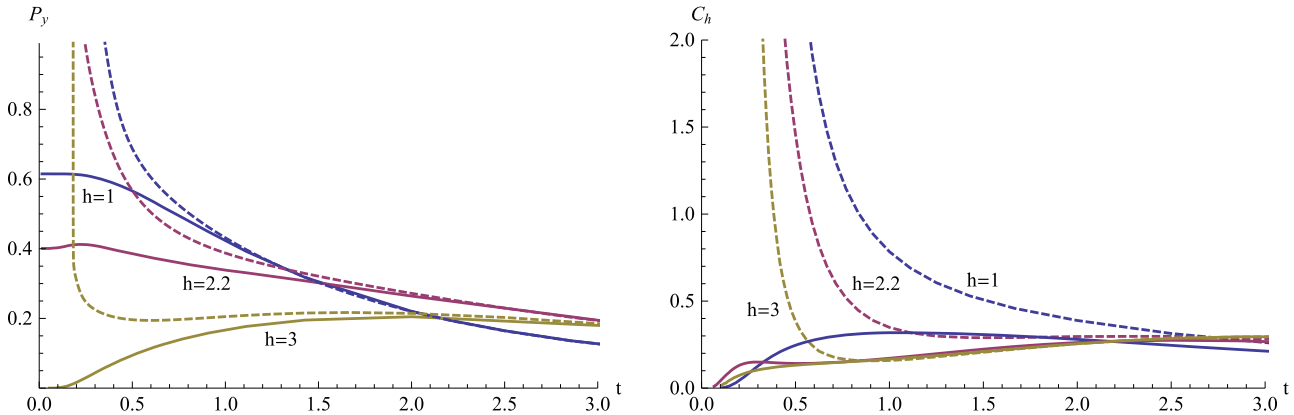


FIG. 9. Temperature dependences of polarization P_y and specific heat C_h for $k_{xyz} = 0.5$ and $j_1^x = 0$ (solid lines) and $j_1^x = 0.5$ (dashed lines) at several values of field.

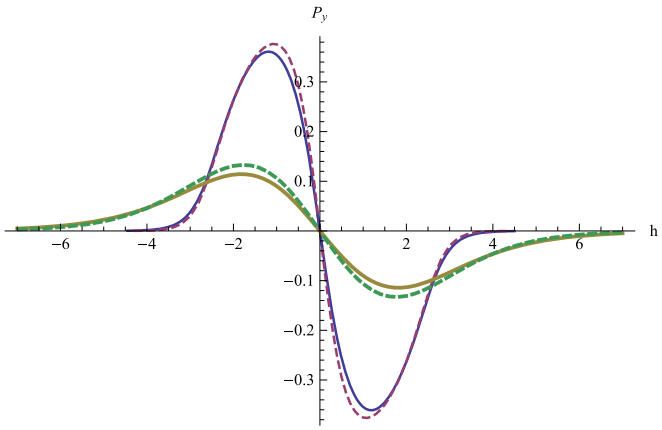


FIG. 10. Comparison of the polarization found in this paper (solid lines) with the exact results [6] (dashed lines) for the model (2)–(3) with $J_1 = 1, J_2 = 0, D_1^y = 0, K = 0$, and $E = 0.5$ at reduced temperatures $t = 0.5$ (thin lines) and 2 (thick lines).

that for some range of the field the polarization as a function of temperature exhibits a maximum. For the same values of the field a two-peak structure of the specific heat is observed.

Most of the compounds showing the magnetoelectric effect and treated as one-dimensional undergo a phase transition. For this reason we have taken into account weak interchain interactions (23) between the chains defined by the Hamiltonian (10). As one would expect, such an interaction can lead to a phase transition indicated by the divergence of the interaction parameters in the RG recursion relation iteration. The applied method does not allow us to recognize the nature of the transition, only its location as a function of couplings and strength of the magnetic field.

In contrast to the Ising model for the quantum system the linear renormalization-group transformation (6)–(7) cannot be carried out exactly even in 1D case because of the noncommutativity of several parts of the Hamiltonian. Thus, the approximation takes the quantum effect into account only within a single seven-spin block. Such an approximation is, of course, better at higher temperatures [20]. In Fig. 10 the polarization found in this paper is compared with the exact result obtained by Menchyshyn *et al.* [6] for the model (2)–(3) with $J_1 = 1, J_2 = 0, D_1^y = 0, K = 0$, and $E = 0.5$ at reduced temperatures $t = 0.5$ and 2. To make the comparison we used Eq. (3.5) of Ref. [6], taking into account that in our case $S^z = \pm 1$ instead of $S^z = \pm\frac{1}{2}$. As seen for both small and large magnetic fields, our RG approximation is in good agreement with the exact result. However, there is a visible deviation from the exact result around the field of the polarization maximum. As one would expect, the agreement with the exact result is better at higher temperature, where the location of the polarization maximum is correctly found. For coupled chains (2D system) the LPRG transformation is obtained by two additional approximations: (i) the abbreviation of the cumulant expansion, which is reasonable if the intrachain interaction is weaker than the interchain one, and (ii) the truncation of the interchain interaction generated by the transformation (21). As mentioned above, the number of different interactions generated by LPRG transformation already in the second-order cumulant expansion is infinite for an infinite system. Thus, in order to evaluate the LPRG transformation we have had to confine ourselves to a finite cluster, which is justified again only if the temperature is not too low. So the LPRG method can be used to locate a critical point for a system with a weak interchain interaction that is not too weak because in the latter case the critical temperature is shifted to very low temperatures.

APPENDIX A

Coefficients in the expressions for the eigenvalues of the Hamiltonian (12) are

$$\begin{aligned} A_q &= \big(2q_1^3 - 27o_1q_2^2 - 18o_1q_1q_3 + 18q_1q_2r_1 - 27q_3r_1^2 - 6q_1^2r_2 + 18o_1q_3r_2 - 18q_2r_1r_2 \\ &\quad + 6q_1r_2^2 - 2r_2^3 + \big\{\big[4(-q_1^2 - 3o_1q_3 - 6q_2r_1 + 2q_1r_2 - r_2^2)^3 + \big(2q_1^3 - 27o_1q_2^2 - 18o_1q_1q_3 \\ &\quad + 18q_1q_2r_1 - 27q_3r_1^2 - 6q_1^2r_2 + 18o_1q_3r_2 - 18q_2r_1r_2 + 6q_1r_2^2 - 2r_2^3\big)^2\big]^{1/2}\big\}^{1/3}, \\ B_q &= q_1^2 - 3o_1q_3 - 6q_2r_1 + 2q_1r_2 - r_2^2, \quad C_q = 2q_1 + r_2. \end{aligned} \tag{A1}$$

The coefficients A_Q, B_Q, C_Q are the same functions of Q_1, Q_2, Q_3, R_1, R_2, and O_1 as coefficients A_q, B_q, C_q of q_1, q_2, q_3, r_1, r_2, and o_1, and

$$\begin{aligned} q_1 &= f_0 - f_d + f_z' - f_2^z, \quad q_2 = 2\big(\imath f^{xy} + f_1^x + f_{xxz} + \imath f_{xyz}\big), \\ q_3 &= 2\big(\imath f_2^{xy} + f_2^x + f_{xzx} + \imath f_{xzy}\big), \quad r_1 = 2\big(-\imath f^{xy} + f_1^x + f_{xxz} - \imath f_{xyz}\big), \\ r_2 &= f_0 - f_d + f_z - f_z' + f_2^z - 2f_1^z, \quad o_1 = 2\big(-\imath f_2^{xy} + f_2^x + f_{xzx} - \imath f_{xzy}\big), \\ Q_1 &= f_0 + f_d - f_z' - f_2^z, \quad Q_2 = 2\big(\imath f^{xy} + f_1^x - f_{xxz} - \imath f_{xyz}\big), \\ Q_3 &= 2\big(\imath f_2^{xy} + f_2^x - f_{xzx} - \imath f_{xzy}\big), \quad R_1 = 2\big(-\imath f^{xy} + f_1^x - f_{xxz} + \imath f_{xyz}\big), \\ R_2 &= f_0 + f_d - f_z + f_z' + f_2^z - 2f_1^z, \quad O_1 = 2\big(-\imath f_2^{xy} + f_2^x - f_{xzx} + \imath f_{xzy}\big). \end{aligned} \tag{A2}$$

APPENDIX B

The RG transformation (6)–(7) for the Hamiltonian (10) has the form of 12 recursion relations for the renormalized coupling parameters as functions of the original ones (16):

$$
\begin{aligned}
K_1^x &= \sum_{i\neq j\neq k=2,3,4} N_q^x \ln\lambda_k + \sum_{i\neq j\neq k=5,6,7} N_Q^x \ln\lambda_k - \left(N_{qa}^x + N_{Qa}^x\right)\ln a,\\
K_1^z &= \sum_{i\neq j\neq k=2,3,4} N_q^z \ln\lambda_k + \sum_{i\neq j\neq k=5,6,7} N_Q^z \ln\lambda_k - \left(N_{qa}^z + N_{Qa}^z\right)\ln a + \frac{1}{8}(\ln\lambda_1 + \ln\lambda_8 - 2\ln a),\\
H_z &= \frac{1}{2}\left(\sum_{i\neq j\neq k=2,3,4} N_q^z \ln\lambda_k + \sum_{i\neq j\neq k=5,6,7} N_Q^z \ln\lambda_k - \left(N_{qa}^z + N_{Qa}^z\right)\ln a\right) + \frac{1}{4}(\ln\lambda_1 - \ln\lambda_8),\\
K_2^x &= \sum_{i\neq j\neq k=2,3,4} N_q^{2x} \ln\lambda_i + \sum_{i\neq j\neq k=5,6,7} N_Q^{2x} \ln\lambda_i - \left(N_{qa}^{2x} + N_{Qa}^{2x}\right)\ln a,\\
K_2^z &= -\sum_{i\neq j\neq k=2,3,4} N_q^{2z} \ln\lambda_i - \sum_{i\neq j\neq k=5,6,7} N_Q^{2z} \ln\lambda_i + \left(N_{qa}^{2z} + N_{Qa}^{2z}\right)\ln a + \frac{1}{8}(\ln\lambda_1 + \ln\lambda_8 - 2\ln a),\\
D_z &= -\sum_{i\neq j\neq k=2,3,4} N_q^{d} \ln\lambda_i - \sum_{i\neq j\neq k=5,6,7} N_Q^{d} \ln\lambda_i + \left(N_{qa}^{d} + N_{Qa}^{d}\right)\ln a + \frac{1}{8}(\ln\lambda_1 - \ln\lambda_8),\\
D_1^y &= i\sum_{i\neq j\neq k=2,3,4} N_q^{1y} \ln\lambda_i + i\sum_{i\neq j\neq k=5,6,7} N_Q^{1y} \ln\lambda_i - i\left(N_{qa}^{1y} + N_{Qa}^{1y}\right)\ln a,\\
D_2^y &= -i\sum_{i\neq j\neq k=2,3,4} N_q^{2y} \ln\lambda_i - i\sum_{i\neq j\neq k=5,6,7} N_Q^{2y} \ln\lambda_i + i\left(N_{qa}^{2y} + N_{Qa}^{2y}\right)\ln a,\\
K_{xxz} &= -\sum_{i\neq j\neq k=2,3,4} N_q^{xxz} \ln\lambda_i - \sum_{i\neq j\neq k=5,6,7} N_Q^{xxz} \ln\lambda_i + \left(N_{qa}^{xxz} + N_{Qa}^{xxz}\right)\ln a,\\
K_{xzx} &= -\sum_{i\neq j\neq k=2,3,4} N_q^{xzx} \ln\lambda_i - \sum_{i\neq j\neq k=5,6,7} N_Q^{xzx} \ln\lambda_i + \left(N_{qa}^{xzx} + N_{Qa}^{xzx}\right)\ln a,\\
K_{xyz} &= i\sum_{i\neq j\neq k=2,3,4} N_q^{xyz} \ln\lambda_i + i\sum_{i\neq j\neq k=5,6,7} N_Q^{xyz} \ln\lambda_i - i\left(N_{qa}^{xyz} + N_{Qa}^{xyz}\right)\ln a,\\
K_{xzy} &= -i\sum_{i\neq j\neq k=2,3,4} N_q^{xzy} \ln\lambda_i - i\sum_{i\neq j\neq k=5,6,7} N_Q^{xzy} \ln\lambda_i + i\left(N_{qa}^{xzy} + N_{Qa}^{xzy}\right)\ln a,
\end{aligned}
\tag{B1}
$$

where

$$
\begin{aligned}
N_q^\alpha &= \frac{W_{q1}^\alpha + (\lambda_i+\lambda_j)W_{q2}^\alpha + \lambda_i\lambda_j W_{q3}^\alpha}{8(a-\lambda_k)(\lambda_k-\lambda_i)(\lambda_k-\lambda_j)},\\
N_{qa}^\alpha &= \frac{w_{q0}^\alpha + (\lambda_2+\lambda_3+\lambda_4)w_{q1}^\alpha + (\lambda_2\lambda_3+\lambda_2\lambda_4+\lambda_3\lambda_4)w_{q2}^\alpha}{8(a-\lambda_2)(a-\lambda_3)(a-\lambda_4)},\\
w_{q0}^x &= 2q_2^2 r1 + 2q_2 r_1^2 + q_1^2(q_2+r_1) + q_3 r_1 r_2 + q_2 r_2^2 + r_1 r_2^2 + q_1[2q_3 r_1 + (q_2+r_1)r_2]\\
&\quad + o_1[2q_1q_2 + q_3 r_1 + q_2(q_3+r_2)],\\
w_{q1}^x &= -[o_1 q_2 + q_3 r_1 + q_1(q_2+r_1) + q_2 r_2 + r_1 r_2],\quad w_{q2}^x = q_2 + r_1,\\
W_{q1}^x &= q_1^2 q_2 + q_1^2 r_1 + 2q_2^2 r_1 + 2q_1 q_3 r_1 + 2q_2 r_1^2 + q_1 q_2 r_2 + q_3 r_1 r_2 + q_2 r_2^2\\
&\quad - a[o_1 q_2 + q_3 r_1 + q_1(q_2+r_1) + q_2 r_2 + r_1 r_2] + o_1[2q_1 q_2 + q_3 r_1 + q_2(q_3+r_2)],\\
W_{q2}^x &= -[o_1 q_2 + q_1 q_2 + q_1 r_1 + q_3 r_1 - a(q_2+r_1) + q_2 r_2 + r_1 r_2],\\
w_{q0}^z &= a^3 - o_1 q_2^2 - 2q_1 q_2 r_1 - q_3 r_1^2 - 4q_2 r_1 r_2 - r_2^3,\quad w_{q1}^z = -a^2 + 2q_2 r_1 + r_2^2,\\
W_{q1}^z &= -o_1 q_2^2 - 2q_1 q_2 r_1 - q_3 r_1^2 - 4q_2 r_1 r_2 - r_2^3 + a\left(2q_2 r_1 + r_2^2\right),\\
w_{q2}^z &= a - r_2,\quad W_{q2}^z = 2q_2 r_1 + r_2(r_2 - a),
\end{aligned}
$$

$$
\begin{aligned}
N_q^{2z} &= \frac{n_{q0}^{2z} + n_{q1}^{2z}(a+\lambda_j+\lambda_k) + n_{q2}^{2z}[a(\lambda_j+\lambda_k)+\lambda_j\lambda_k - a^2(\lambda_j+\lambda_k]}{8(a-\lambda_i)(\lambda_i-\lambda_j)(\lambda_i-\lambda_k)},\\
N_{qa}^{2z} &= \frac{a^3 + n_{q0}^{2z} + \left(n_{q1}^{2z}-a^2\right)(\lambda_2+\lambda_3+\lambda_4) + n_{q2}^{2z}(\lambda_2\lambda_3+\lambda_2\lambda_4+\lambda_3\lambda_4)}{8(a-\lambda_2)(a-\lambda_3)(a-\lambda_4)},\\
n_{q0}^{2z} &= -2q_1^3 - o_1q_2^2 - q_3r_1^2 - 2q_1(3o_1q_3+q_2r_1) + 2q_2r_1r_2 + r_2^2,\\
n_{q1}^{2z} &= 2q_1^2 + 2o_1q_3^2 - r_2^2, \quad n_{q2}^{2z} = a - 2q_1 + r_2,\\
N_q^d &= \frac{n_{q0}^d + n_{q1}^d(a+\lambda_j+\lambda_k) + n_{q2}^d[a(\lambda_j+\lambda_k)+\lambda_j\lambda_k] + 3a\lambda_j\lambda_k}{8(a-\lambda_i)(\lambda_i-\lambda_j)(\lambda_i-\lambda_k)},\\
N_{qa}^d &= \frac{n_{q0}^d + 3a^3 + \left(n_{q1}^d - 3a^2\right)(\lambda_i+\lambda_j+\lambda_k) + \left(n_{q2}^d+3a\right)(\lambda_2\lambda_3+\lambda_2\lambda_4+\lambda_3\lambda_4)}{8(a-\lambda_i)(\lambda_i-\lambda_j)(\lambda_i-\lambda_k)},\\
n_{q0}^d &= -2q_1^3 - 3o_1q_2^2 - 3q_3r_1^2 - 6q_1(o_1q_3+q_2r_1) - 6q_2r_1r_2 - r_2^3,\\
n_{q1}^d &= 2q_1^2 + 2o_1q_3 + 4q_2r_1 + r_2^2, \quad n_{q2}^d = -(2q_1+r_2),
\end{aligned}
\tag{B2}
$$

and

$$
\begin{aligned}
N_q^\beta &= \frac{n_{q0}^\beta + n_{q1}^\beta(a+\lambda_j+\lambda_k) + n_{q2}^\beta[a(\lambda_j+\lambda_k)+\lambda_j\lambda_k]}{8(a-\lambda_i)(\lambda_i-\lambda_j)(\lambda_i-\lambda_k)}\ln\lambda_i,\\
N_{qa}^\beta &= \frac{n_{q0}^\beta + n_{q1}^\beta(\lambda_2+\lambda_3+\lambda_4) + n_{q2}^\beta(\lambda_2\lambda_3+\lambda_2\lambda_3+\lambda_3\lambda_4)}{8(a-\lambda_2)(a-\lambda_3)(a-\lambda_4)},\\
\beta &= 2x, 1y, 2y, xxz, xzx, xzy, xyz,\\
n_{q0}^{2x} &= o_1^2q3 + 3q_1^2q_3 + 2q_2Q_3r_1 + o_1\left(3q_1^2+q_3^2+2q_2r_1\right) + 2q_1\left(q_2^2+r_1^2\right) + q_2^2r_2 + r_1^2r_2,\\
n_{q1}^{2x} &= -\left(2o_1q_1 + q_2^2 + 2q_1q_3 + r_1^2\right), \quad n_{q2}^{2x} = o_1 + q_3,\\
n_{q0}^{1y} &= q_1^2(q_2-r_1) + 2q_2^2r_1 - 2q_2r_1^2 + q_3r_1r_2 + q_2r_2^2 - r_1r_2^2\\
&\quad - o_1(2q_1q_2 - q_2q_3 + q_3r_1 + q_2r_2) + q_1(2q_3r_1 + q - 2r_2 - r_1r_2),\\
n_{q1}^{1y} &= o_1q_2 - q_3r_1 + q_1(r_1-q_2) - q_2r_2 + r_1r_2, \quad n_{q2}^{1y} = q_2 - r_1,\\
n_{q0}^{2y} &= -2q_1q_2^2 + o_1^2q_3 - 3q_1^2q_3 - 2q_2q_3r_1 + 2q_1r_1^2\\
&\quad + o_1\left(3q_1^2 - q_3^2 + 2q_2r_1\right) - q_2^2r_2 + r_1^2r_2,\\
n_{q1}^{2y} &= -2o_1q_1 + q_2^2 + 2q_1q_3 - r_1^2, \quad n_{q2}^{2y} = o_1 - q_3,\\
n_{q0}^{xxz} &= 2q_2^2r_1 + 2q_2r_1^2 + q_1^2(q_2+r_1) + q_3r_1r_2 + q_2r_2^2 + r_1r_2^2\\
&\quad + q_1[2q_3r_1 + (q_2+r_1)r_2] + o_1[2q_1q_2 + q_3r_1 + q_2(q_3+r_2)],\\
n_{q1}^{xxz} &= -[o_1q_2 + q_3r_1 + q_1(q_2+r_1) + q_2r_2 + r_1r_2], \quad n_{q2}^{xxz} = q_2 + r_1,\\
n_{q0}^{xzx} &= o_1^2q_3 + 3q_1^2q_3 + 2q_2q_3r_1 + o_1\left(3q_1^2 + q_3^2 + 2q_2r_1\right)\\
&\quad + 2q_1\left(q_2^2 + r_1^2\right) + q_2^2r_2 + r_1^2r_2,\\
n_{q1}^{xzx} &= -\left(2o_1q_1 + q_2^2 + 2q_1q_3 + r_1^2\right), \quad n_{q2}^{xzx} = o_1 + q_3,\\
n_{q0}^{xyz} &= q_1^2(q_2 - r1) + 2q_2^2r_1 - 2q_2r_1^2 + q_3r_1r_2 + q_2r_2^2 - r_1r_2^2\\
&\quad - o_1(2q_1q_2 - q_2q_3 + q_3r_1 + q_2r_2) + q_1(2q_3r_1 + q_2r_2 - r_1r_2),\\
n_{q1}^{xyz} &= o_1q_2 - q_3r_1 + q_1(r_1-q_2) - q_2r_2 + r_1r_2, \quad n_{q2}^{xyz} = q_2 - r_1,\\
n_{q0}^{xzy} &= -2q_1q_2^2 + o_1^2q_3 - 3q_1^2q_3 - 2q_2q_3r_1 + o_1\left(3q_1^2 - q_3^2 + 2q_2r_1\right) - q_2^2r_2 + r_1^2r_2,\\
n_{q1}^{xzy} &= \left(-2o_1q_1 + q_2^2 + 2q_1q_3 - r_1^2\right), \quad n_{q2}^{xzy} = o_1 - q_3.
\end{aligned}
\tag{B3}
$$

A constant term appearing in each step of the transformation reads

$$
\begin{aligned}
Z_0 = \frac{1}{8}(\ln\lambda_1 + \ln\lambda_8) &+ \sum_{i\neq j\neq n=2,3,4} \frac{W_{q1} + (\lambda_i+\lambda_j)W_{q2} + \lambda_i\lambda_j W_{q3}}{8(a-\lambda_k)(\lambda_k-\lambda_i)(\lambda_k-\lambda_j)} \ln\lambda_k \\
&+ \sum_{i\neq j\neq n=5,6,7} \frac{W_{Q1} + (\lambda_i+\lambda_j)W_{Q2} + \lambda_i\lambda_j W_{Q3}}{8(a-\lambda_k)(\lambda_k-\lambda_i)(\lambda_k-\lambda_j)} \ln\lambda_k \\
&+ \left(\frac{7}{4} + \frac{-8\lambda_2\lambda_3\lambda_4 + (\lambda_2\lambda_3+\lambda_2\lambda_4+\lambda_3\lambda_4)w_{q2} - (\lambda_2+\lambda_3+\lambda_4)w_{q1} + w_{q0}}{8(a-\lambda_2)(a-\lambda_3)(a-\lambda_4)}\right. \\
&+ \left.\frac{-8\lambda_5\lambda_6\lambda_7 + (\lambda_5\lambda_6+\lambda_5\lambda_7+\lambda_6\lambda_7)w_{Q2} - (\lambda_5+\lambda_6+\lambda_7)w_{Q1} + w_{Q0}}{8(a-\lambda_5)(a-\lambda_6)(a-\lambda_7)}\right) \ln a, \qquad \text{(B4)}
\end{aligned}
$$

where

$$
\begin{aligned}
W_{q1} &= -2q_1^3 - 3o_1q_2^2 - 3q_3r_1^2 - 6q_1(o_1q_3 + q_2r_1) - 6q_2r_1r_2 - r_2^3 + a\left(2q_1^2 + 2o_1q_3 + 4q_2r_1 + r_2^2\right), \\
W_{q2} &= 2q_1^2 + 2o_1q_3 + 4q_2r_1 + r_2^2 - a(2q_1 + r_2), \quad W_{q3} = 3a - 2q_1 - r_2, \\
w_{q0} &= 5a^3 + 2q_1^3 + 3o_1q_2^2 + 6o_1q_1q_3 + 6q_1q_2r_1 + 3q_3r_1^2 + 6q_2r_1r_2 + r_2^3, \\
w_{q1} &= 5a^2 + 2q_1^2 + 2o_1q_3 + 4q_2r_1 + r_2^2, \quad w_{q2} = 5a2q_1 + r_2. \qquad \text{(B5)}
\end{aligned}
$$

Just as before the coefficients $n_{Qi}, W_{Qi}, w_{Qi}, W^{\alpha}_{Qi}, w^{\alpha}_{Qi}$ are the same functions of Q_1, Q_2, Q_3, R_1, R_2, and O_1 as coefficients $n_{qi}, W_{qi}, w_{qi}, W^{\alpha}_{qi}, w^{\alpha}_{qi}$ of q_1, q_2, q_3, r_1, r_2, and o_1 (22).

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