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Critical temperature of an anisotropic two-dimensional Potts model

Kaoru Yasumura

Department of Physics, Tokyo Institute of Technology, Oh-okayama, Meguro-ku, Tokyo 152, Japan

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Abstract. The phase transition temperature T_c of the q -state Potts model with ferromagnetic interactions J_x and antiferromagnetic ones J_y in the two respective directions of a 2D lattice is calculated by the high-temperature series expansion (HTSE) of the appropriate staggered susceptibility as well as by the cluster variate approximation (CVA). For $q=3$ the HTSE result in the range of $|J_x|/J_y \leq 1.5$ shows a good coincidence with the Kosterlitz-Thouless-type phase transition temperature calculated on the prescription by Ostlund which is given by $1/16\pi = \exp(-2\beta_c J_x) \coth(-\beta_c J_y/2)$, $\beta = 1/kT_c$. The CVA result shows similar behaviour of T_c to that of the Migdal-Kadanoff renormalisation group method obtained by Kinzel *et al*, but it is considered to be less reliable than the HTSE result.

1. Introduction

The ordered phase of the q -state antiferromagnetic Potts model (AFPM) has been found to have interesting features caused by its infinitely degenerate ground state with the zero-point entropy of the order of N (the number of the Potts spins). On the cubic lattice, $q=3$ and 4, AFPM reveals a continuous phase transition, which is shown by the Monte Carlo simulation (Banavar *et al* 1980), and the transition temperature is calculated by the high-temperature series expansion (Yasumura and Oguchi 1984). For the model of $q=3$, simulations performed by Banavar *et al* and by Ono (1986) suggest that the low-temperature phase is a floating phase in which the correlations decay algebraically with the distance of the spins.

On the square lattice, on the other hand, $q \geq 3$, AFPM has been shown to reveal no phase transition at non-zero temperatures (Baxter 1982, Yasumura and Oguchi 1984). Kinzel *et al* (1981) introduced a q -state Potts model on an anisotropic two-dimensional (2D) lattice with ferromagnetic interactions $J_x (>0)$ in the x direction and antiferromagnetic ones $J_y (<0)$ in the y direction. In this paper I report the results of some estimates of the phase transition temperature of this system.

The Hamiltonian of this system is written as

$$\mathcal{H} = -J_x \sum_{\langle i,j \rangle_x} \delta(\sigma_i, \sigma_j) - J_y \sum_{\langle i,j \rangle_y} \delta(\sigma_i, \sigma_j) \quad (1)$$

where $\sigma_i (=0, 1, \dots, q-1)$ is the Potts spin on the lattice site i , δ is the Kronecker delta and $\langle \rangle_\xi$ ($\xi = x, y$) represents the nearest-neighbour (NN) pairs in the ξ direction. This model has also an infinitely degenerate ground state, but its zero-point entropy is of the order of \sqrt{N} (the number of the rows in the lattice), which is much smaller than that of the isotropic AFPM.

Kinzel *et al* showed that this system has an ordered phase and gave a conjectural expression of the critical temperature T_c by the method of the Migdal-Kadanoff renormalisation (MKR), which is given by

$$[1 + \exp(\beta_c J_x)][1 - \exp(\beta_c J_y)] = q \quad (2)$$

where $\beta_c = 1/kT_c$ and k is the Boltzmann constant.

In the case of $q = 3$ another conjectured expression of T_c is given by Truong (1984) by considering the symmetry properties of the partition function, which is written as

$$\exp(\beta_c J_x) - 2 \exp(\beta_c J_y) - \exp[\beta_c (J_x + J_y)] = 1. \quad (3)$$

Computer analysis has also been done for the model of $q = 3$ (Houlik *et al* 1983, Selke and Wu 1987), but gives rather lower T_c than that obtained by (2) or (3).

Another result for this problem is given by Ostlund (1981) who investigated the asymmetric clock model by the method of the free-fermion approximation (FFA) which is a technique introduced by Villain and Bak (1981) to investigate the phase transition of the ANNNI model. Ostlund showed that his model reveals a phase transition of the Kosterlitz-Thouless (1973) type and the low-temperature phase is a floating phase with algebraic decay of correlations. Our model in the case of $q = 3$ is included in Ostlund's investigations, and we can obtain an estimation of its T_c by the method of FFA according to the Ostlund-Villain-Bak prescription.

In § 2 we estimate the second-order phase transition temperature T_c of the system represented by the Hamiltonian (1) by the calculation of a high-temperature series expansion (HTSE) of an appropriate staggered susceptibility. This T_c can be estimated also by the cluster variate approximation (CVA), which will be shown in § 3. The phase transition temperature to the floating phase in Ostlund's picture is also shown in § 4, where these results will be compared and discussed.

2. High-temperature series expansion (HTSE)

In this section we will calculate T_c of the system with the Hamiltonian (1) by the HTSE of the paramagnetic susceptibility to the staggered field applied in accordance with the correlations relevant to the low-temperature phase. Kinzel *et al* (1981) showed that these correlations should be those that are ferromagnetic along the x direction and antiferromagnetic (ferromagnetic) along the y direction with an odd (even) number of lattice spaces. We will calculate the staggered correlation along the sublattices A and B shown in figure 1.

Here we take the external staggered field \mathbf{H} as a q -component vector (H^1, H^2, \dots, H^q) , which gives a Zeeman energy term,

$$- \sum_{\alpha=1}^q H^\alpha \left(\sum_{i \in A}^{N/2} \delta(\alpha, \sigma_i) - \sum_{j \in B}^{N/2} \delta(\alpha, \sigma_j) \right) \quad (4)$$

to be added to (1) where $\sum_{i \in A} (\sum_{i \in B})$ represents the sum over the site i on the sublattice A(B). This type of Zeeman field is adopted by Yasumura and Oguchi (1984) in the calculation of HTSE of the isotropic AFPM, though the two sublattices A and B are determined differently there.

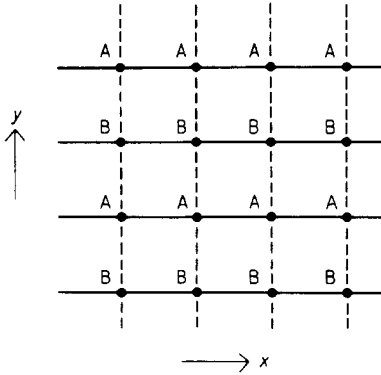


Figure 1. The two sublattices A and B. The full line shows the ferromagnetic bond and the broken line the antiferromagnetic one.

The components of \mathbf{H} must satisfy the following condition, because the perfectly disordered spin has zero Zeeman energy;

$$\sum_{\alpha=1}^q H^\alpha = 0. \tag{5}$$

The linear response of the free energy of the paramagnetic phase to this field is easily shown to be written as $\chi^{st} \mathbf{H}^2/2$, where

$$\chi^{st} = 2\beta \frac{q}{q-1} \left(\sum_{i \in A} \sum_{j \in A} \langle \hat{\delta}_i^1 \hat{\delta}_j^1 \rangle - \sum_{i \in A} \sum_{j \in B} \langle \hat{\delta}_i^1 \hat{\delta}_j^1 \rangle \right) \tag{6}$$

$$\hat{\delta}_i^1 = \delta(1, \sigma_i) - 1/q. \tag{7}$$

The method used to calculate the high-temperature series expansion of χ^{st} defined by (6) is similar to that of Yasumura and Oguchi (1984) and the details are not presented here. Now we expand χ^{st} as

$$\chi^{st} = \frac{\beta N}{q} \sum_{n=0} a_n (\beta J_x)^n. \tag{8}$$

I have calculated the coefficients a_n up to the seventh order which are shown in the appendix, where λ represents the absolute ratio of the interactions, $|J_y|/J_x$.

In order to determine T_c , I have applied the ratio method (RM) and the Padé approximation (PA) (Gaunt and Guttmann 1974). In RM, the ratio plot (a_n/a_{n-1} against $1/n$) is linearly extrapolated to $1/n \rightarrow 0$, and the limit $a_n/a_{n-1} \rightarrow kT_c/J_x$ gives the critical temperature. In PA, we have applied the $[p, p]$ approximation ($p = 2, 3$) to the logarithmic derivative of (8): $(d/d\beta) \log \chi^{st}$, whose pole β_c , if it exists, will be the inverse of the critical temperature.

Some of the results for the $q = 3$ model are shown in table 1. In the range of $\lambda \leq 1.5$, the Padé $[p, p]$ approximation ($p = 2, 3$) shows a good convergence. The RM result gives a little larger T_c , though it is considered to be consistent with the PA result. In the vicinity of $\lambda \approx 1.6$ and when T_c is small, PA does not converge well. When $\lambda \geq 1.7$, PA and RM give inconsistent values of T_c . In the range of larger λ , the ratio plot lies on a winding curve and does not fit a straight line. When $\lambda \geq 2$, therefore, the extrapolated value of RM is not considered to be reliable. I have shown the result of the Padé $[3, 3]$ approximation in figure 2.

Table 1. kT_c/J_x estimated by RM and PA ([2, 2] and [3, 3] approximation).

λ	RM	[3, 3]	[2, 2]
0.2	0.39 ± 0.02	0.38	0.18
0.4	0.47 ± 0.03	0.44	0.43
0.8	0.54 ± 0.03	0.48	0.47
1.2	0.53 ± 0.05	0.50	0.48
1.6	0.57 ± 0.05	0.36	0.46
2.0	0.60 ± 0.05	0.40	0.41
2.5	0.65 ± 0.07	0.13	0.31

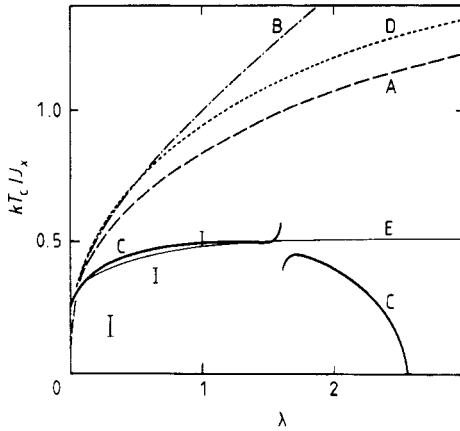


Figure 2. The phase boundary of the $q=3$ model, kT_c/J_x is drawn as a function of $\lambda = |J_y|/J_x$. A refers to the conjecture by the Migdal-Kadanoff renormalisation of Kinzel *et al* (1981), B to that of Truong (1984) by the symmetry considerations, C shows the present result of the high-temperature series expansion with Padé [3, 3] approximation, D shows that of the cluster variate approximation and E is drawn after the free-fermion approximation method of Ostlund (1981). Recent Monte Carlo data by Selke and Wu (1987) are also shown in the error bars.

For the $q \geq 4$ model, RM gives no trustworthy result of T_c , but PA shows good convergence except in the case that the solution of T_c is very small. The solution of the Padé [3, 3] approximation for the models of $q = 4, 5$ and 6 is shown in figure 3.

3. Cluster variate approximation (CVA)

In the previous section we determined the second-order phase transition temperature T_c of the system with the Hamiltonian (1) by HTSE. If this transition leads to a sublattice-type long-range ordered phase, its T_c can be estimated also by CVA as will be shown in this section.

The calculation follows the effective Hamiltonian method (Oguchi and Ono 1966) which is an improved version of the Bethe approximation method.

The sublattice-type order can be expressed by the effective internal field. Here the two sublattices A and B are taken in the same way as in § 2 (figure 1). The notation L_{AA} (L_{BB}) denotes the effective field acting on a spin belonging to the sublattice A(B)

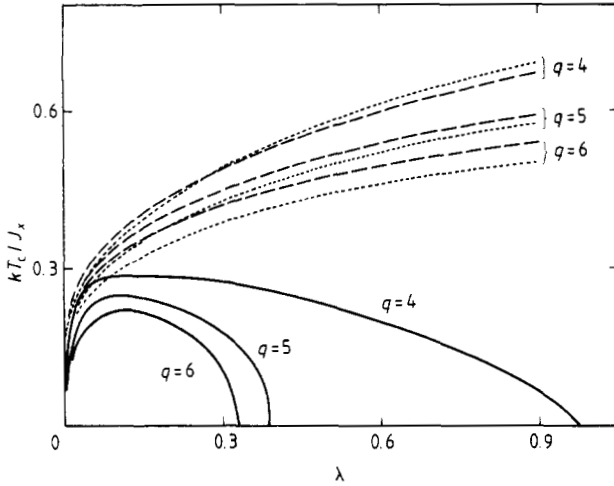


Figure 3. The phase boundary of the $q = 4, 5$ and 6 models. The full curves show the HTSE result (Padé [3, 3] approximation), while the dotted and broken lines refer to CVA and MKR results respectively.

through the ferromagnetic bond from one of its NN spins on the sublattice A(B), and L_{BA} (L_{AB}) shall denote that acting on a spin belonging to A(B) through the antiferromagnetic bond from one of its NN spins on B(A), where $L(=L_{AA}, L_{BB}, L_{AB}$ or $L_{BA})$ is a q -component vector (L^1, L^2, \dots, L^q) and it gives a Zeeman energy

$$- \sum_{\alpha=1}^q L^\alpha \delta_i^\alpha \tag{9}$$

for the Potts spin σ_i , where the Kronecker delta $\delta(\alpha, \sigma_i)$ is written as δ_i^α . The component of the effective field satisfies the condition similar to (5), that is $\sum_\alpha L^\alpha = 0$.

The effective density matrix of the spin σ_i on the sublattice A is written in terms of L in the following form:

$$\rho_i^I = \exp\left(2\beta \sum_\alpha (L_{AA}^\alpha + L_{BA}^\alpha) \delta_i^\alpha\right) \tag{10}$$

as well as in the form of the partial trace of the density matrix of the Bethe cluster centred on the site i :

$$\rho_i^{II} = \text{Tr}_1 \text{Tr}_2 \text{Tr}_3 \text{Tr}_4 \exp\left(\beta \sum_\alpha \{ \delta_i^\alpha [J_x(\delta_1^\alpha + \delta_3^\alpha) + J_y(\delta_2^\alpha + \delta_4^\alpha)] + (L_{AA}^\alpha + 2L_{BA}^\alpha)(\delta_1^\alpha + \delta_3^\alpha) + (L_{AB}^\alpha + 2L_{BB}^\alpha)(\delta_2^\alpha + \delta_4^\alpha) \}\right) \tag{11}$$

where the site 1 and 3 is the i NN site located on the sublattice A and the site 2 and 4 is that on the sublattice B, and $\text{Tr}_j = \sum_{\sigma_j=1}^q$ ($j = 1, 2, 3, 4$) is the trace over the Potts spin σ_j .

Since two expressions (10) and (11) must be equivalent under this approximation, we put

$$\frac{\rho_i^I}{\text{Tr}_i \rho_i^I} = \frac{\rho_i^{II}}{\text{Tr}_i \rho_i^{II}} \tag{12}$$

which gives a self-consistent equation for L .

Equation (12) has a trivial solution $L_{AA} = L_{BB} = L_{AB} = L_{BA} = 0$ which represents the paramagnetic phase. A non-zero solution for L will represent the ordered phase. The linear approximation in L is applied near the second-order phase transition temperature, where we can put $L_{AB} = -\lambda L_{AA}$ and $L_{BA} = -\lambda L_{BB}$; $\lambda = -J_y/J_x$. Then we get

$$\lim_{T \rightarrow T_c - 0} \frac{L_{BB}}{L_{AA}} = \frac{X(q+y) - \lambda Y(q+X) - (q+X)(q+Y)}{2\lambda X(q+Y) - 2Y(q+X) - \lambda(q+X)(q+Y)} \quad (13)$$

where

$$X = \exp(\beta_c J_x) - 1 \quad (13a)$$

$$Y = \exp(\beta_c J_y) - 1 \quad (13b)$$

which gives $T_c = 1/k\beta_c$.

Taking the central site i of the Bethe cluster on sublattice B, we get a similar equation to (13) where A and B are substituted with each other. Hence the LHS of (13) equals 1 or -1 . Taking the former limit of $L_{BB}/L_{AA} \rightarrow 1$, we obtain an equation for the second-order critical temperature from the paramagnetic phase to the ferromagnetic one. Putting $\lambda = -1$, we get an equation for the isotropic ferromagnetic Potts model that has been given in Wang and Wu (1976).

In our model where λ is positive, we should take the limit $L_{BB}/L_{AA} \rightarrow -1$ in order to detect the sublattice-type staggered order. Equation (13) yields

$$(1+2\lambda) \frac{X}{q+X} - (2+\lambda) \frac{Y}{q+Y} = 1 + \lambda. \quad (14)$$

The solution of (14) is shown in figures 2 and 3. We can see that this result has almost the same character as the MKR result given by (2). In the limit of large λ , both the estimation of T_c given here and that given by MKR tend to the same constant: $J_x/[k \log(q-1)]$. In the case of $q=2$ (Ising model), the solution of (2) gives the rigorous T_c ; nevertheless, that of (14) with finite λ does not.

4. Results and discussions

In this paper we have calculated the second-order phase transition temperature T_c of the q -state Potts model on the anisotropic 2D lattice where ferromagnetic interactions J_x and antiferromagnetic ones J_y are arranged in the x and y direction respectively. We have calculated it by HTSE in § 2 and by CVA in § 3. These results are shown in figures 2 and 3 as a function of the absolute ratio of the interactions $\lambda = |J_y|/J_x$. In these figures the full curve shows the result of the Padé [3, 3] approximation of the HTSE and the dotted curve shows the CVA result; the MKR result obtained by equation (2) is also shown by the broken curve.

The CVA result shows almost the same behaviour as the MKR one and has the same limit of T_c tending to $J_x/[k \log(q-1)]$ as $\lambda \rightarrow \infty$. On the other hand T_c given by HTSE has a maximum value which is about a third of the value of the large- λ limit of the former approximations. The T_c estimated by PA of HTSE vanishes when λ grows large, where, however, the result of RM does not converge well and we cannot conclude that the PA result gives the true T_c . In the case of $q=3$ (figure 2) the result of the Padé

[3, 3] approximation shows a quite irregular behaviour in the neighbourhood of $\lambda = 1.6$. This irregularity is due to the truncation of the series of (8). Similar irregularities are observed also in other calculations using the Padé approximation (Obokata *et al* 1967).

In the case of $q = 3$, Truong's conjectured critical temperature given by (3) is shown in the same figure by dotted and broken curves. It is close to the CVA line when λ is not so large, but in the limit of $\lambda \rightarrow \infty$ Truong's T_c grows infinitely large. This asymptotic behaviour is similar to that of the critical temperature of the $q = 2$ (Ising) model whose ground state does not degenerate infinitely.

Ostlund's (1981) arguments are also available to obtain an estimation of T_c of our system in the case of $q = 3$. In his theory the partition function at low temperatures is approximately represented by the transfer matrix of a one-dimensional massless free-fermion system when the vortex-type excitations are neglected. These excitations destabilise the free-fermion state and cause the Kosterlitz-Thouless-type phase transition. This transition temperature $T_c = 1/\beta_c$ is given by the celebrated equation of Kosterlitz (1974) which is written as

$$\frac{1}{2\pi}(\pi\beta_c J_{\text{eff}} - 1) = \exp(-2\beta_c J_x) \coth(-\frac{1}{2}\beta_c J_y) \quad (15)$$

where $J_{\text{eff}} = 9/8\pi\beta_c$ is the effective exchange interaction of the corresponding XY model, and the LHS of this equation reduces to $(16\pi)^{-1}$. The RHS of (15) is the sum of the fugacities of the vortices. The derivation of (15) is similar to those performed by Villain and Bak (1981) to derive T_c of the ANNNI model and details are not shown here. The solution of (15) is also shown in figure 2 by a thin line.

This solution based on the free-fermion approximation (FFA) indicates the existence of a Kosterlitz-Thouless phase transition and suggests that the low-temperature phase is a floating phase with algebraic decay of correlations (Ostlund 1981). This suggestion is supported by the numerical calculation of the transfer matrix of the quantum version of this model (Herrmann and Martin 1984) as well as by the Monte Carlo study on the clock-model version (Selke and Yeomans 1982).

For $\lambda \leq 1.5$, T_c obtained by the HTSE (Padé [3, 3] approximation) and the FFA coincides very well. Therefore we consider that the T_c of these calculations gives a good estimation in this range of λ and that Ostlund's suggestion for the low-temperature phase is valid. It should be noted that the HTSE gives a lower limit of T_c at which the fluctuation in the paramagnetic phase diverges while the FFA gives an upper limit of T_c at which the postulated low-temperature phase with a topological order becomes unstable against the free vortex excitations.

When $\lambda \geq 1.5$, the HTSE gives no conclusive result for T_c . The PA curve is located much lower than the FFA curve while the RM result seems to support the FFA in $1.5 \leq \lambda \leq 1.8$. In the range of larger λ ($\lambda \geq 2$) the fit of the ratio plot to a straight line is not good and we cannot estimate T_c by RM. On the other hand, equation (15) is considered to become more accurate as λ grows larger and non-topological excitations omitted in Ostlund's theory increase in energy. In the limit of large λ , this equation gives $kT_c/J_x = 1/\log(4\sqrt{\pi}) \approx 0.51$ which is much smaller than the similar limit of the CVA and MKR result $kT_c/J_x = 1/\log 2 \approx 1.44$. For the estimation of the phase transition temperature to the floating phase, a calculation based on the assumption of long-range order such as CVA will not hold good.

The Monte Carlo renormalisation result ($kT_c/J_x = 0.53 \pm 0.3$ for $q = 3$, $\lambda = 1$ in our notation) by Houlrik *et al* (1983) and the recent data of the Monte Carlo study by Selke and Wu (1987) shown in figure 2 with error bars are favourable to the HTSE and

FFA result at $\lambda = 1.0$. But for other values of λ we need more precise numerical estimations.

For the $q \geq 4$ model the HTSE result gives a lower bound of T_c . Figure 3 affirms the existence of the low-temperature phase in the models of $q = 4, 5$ and 6, but no convincing estimate of T_c has been obtained. A method to apply FFA to the $q = 4$ model with further approximations and to determine T_c taking account of the vortex-type excitations will be reported in a subsequent paper by Yasumura and Ueno.

The phase transition of the Potts model with additional next-nearest-neighbour interactions in the y direction of this model is being investigated analytically as well as by the Monte Carlo simulation by Yasumura and Ono and will be reported soon.

Appendix

The coefficients a_n of the high-temperature series expansion of the staggered susceptibility (8) are calculated to have the following form:

$$a_0 = 1 \quad a_1 = 2(\lambda + 1)/q$$

$$a_2 = 4\lambda(\lambda + 2)/q^2 + (-\lambda^2 + 1)/q$$

$$a_3 = 8\lambda(\lambda^2 + 3\lambda + 1)/q^3 + 4\lambda(-\lambda^2 - \lambda + 1)/q^2 + (\lambda^3 + 1)/3q$$

$$a_4 = 16\lambda^2(\lambda^2 + 4\lambda + 3)/q^4 + 4\lambda(-3\lambda^3 - 6\lambda^2 + \lambda + 2)/q^3 \\ + \lambda(7\lambda^3 + 4\lambda^2 - 6\lambda + 4)/3q^2 + (-\lambda^4 + 1)/12q$$

$$a_5 = 32\lambda^2(\lambda^3 + 5\lambda^2 + 6\lambda + 1)/q^5 + 4\lambda^2(-8\lambda^3 - 24\lambda^2 - 9\lambda + 11)/q^4 \\ + 2\lambda(15\lambda^4 + 21\lambda^3 - 10\lambda^2 - 6\lambda + 7)/3q^3 \\ + \lambda(-3\lambda^4 - \lambda^3 + 2\lambda^2 - 2\lambda + 1)/3q^2 + (\lambda^5 + 1)/60q$$

$$a_6 = 8\lambda^3(8\lambda^3 + 48\lambda^2 + 79\lambda + 32)/q^6 + 2\lambda^2(-40\lambda^4 - 160\lambda^3 - 139\lambda^2 + 56\lambda + 23)/q^5 \\ + 2\lambda^2(52\lambda^4 + 120\lambda^3 + 15\lambda^2 - 80\lambda + 33)/3q^4 \\ + \lambda(-18\lambda^5 - 18\lambda^4 + 13\lambda^3 + 4\lambda^2 - 11\lambda + 6)/3q^3 \\ + \lambda(31\lambda^5 + 6\lambda^4 - 15\lambda^3 + 20\lambda^2 - 15\lambda + 6)/90q^2 + (-\lambda^6 + 1)/360q$$

$$a_7 = 16\lambda^3(8\lambda^4 + 56\lambda^3 + 116\lambda^2 + 18\lambda + 8)/q^7 \\ + 4\lambda^2(-48\lambda^5 - 240\lambda^4 - 319\lambda^3 - 7\lambda^2 + 83\lambda + 1)/q^6 \\ + 4\lambda^2(80\lambda^5 + 260\lambda^4 + 165\lambda^3 - 182\lambda^2 + 27)/3q^5 \\ + \lambda^2(-80\lambda^5 - 144\lambda^4 + 9\lambda^3 + 119\lambda^2 - 93\lambda + 21)/3q^4 \\ + \lambda(129\lambda^6 + 93\lambda^5 - 87\lambda^4 - 15\lambda^3 + 95\lambda^2 - 81\lambda + 31)/45q^3 \\ + \lambda(-9\lambda^6 - \lambda^5 + 3\lambda^4 - 5\lambda^3 + 5\lambda^2 - 3\lambda + 1)/90q^2 + (\lambda^7 + 1)/2520q$$

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