MFRG STUDY OF SPIN-1 ISING MODELS: EFFECTS OF A TRANSVERSE FIELD AND RANDOMNESS IN THE CRYSTAL-FIELD COUPLING

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ABSTRACT — The mean-field renormalization group method is used to study the effect of the transverse field on the quantum Blume-Capel model; the critical surface in the temperature — crystal field coupling — transverse field space is obtained. The same method is applied to the Blume-Capel model with random crystal field interactions. Comparison is made with the results obtained by other methods.

1 — INTRODUCTION

Spin-1 models with crystal and biquadratic interactions were firstly introduced by Blume, Emery and Griffiths [1] to describe phase separation and superfluid ordering in He^3-He^4 mixtures, and have since been applied to order-disorder phenomena in adsorbed monolayers, multicomponent fluids and magnetic systems. Despite its simplicity the Blume-Emergy-Griffiths (BEG) model presents a complex phase diagram with first and second-order transition lines and tricritical points. Starting with the conventional mean-field aproximation used in the original paper [1], the model has since been investigated by diferent methods ranging from improved mean-field like approximations [2, 3, 4] to different RG versions [5, 6, 7]; as a result, rather accurate estimates for the location of tricritical points and tricritical exponents are now available.

Alternatively some authors have studied the (d-1)-dim model in a transverse field Γ at $T = 0$ as an equivalent system to the d-dim classical BEG model [8, 9, 10, 11, 12]. However, as far as we know, no study of the classical-to-quantum crossover which arises by switching on the transverse field at $T \neq 0$ has been presented: In this work we make use of MFRG (mean-field renormalization group), a technique which has previously been applied to the transverse spin-1/2 Ising model [13] and to the Potts model in a transverse field [14]. This same method has already been applied to the study of classical spin-1 Ising model [15, 16] and provides a reasonably accurate description of the phase diagram, namely the location of second-order phase transitions and tricritical points. The method is not entirely justified for first-order phase transitions, however its estimates of the first-order critical coupling are in some cases [17] better than those obtained by mean-field. This stands as one of the limitations of MFRG; on the other hand, the method has the advantage of enabling the calculation of the entire T-Γ phase diagram.

2.1 — *MFRG for the quantum Blume-Capel model*

We start with an hamiltonian of the form

$$H = -J \sum_{<ij>} S_i^z S_j^z + \sum_i [D(S_i^z)^2 + \Gamma S_i^x]$$

where S_i^x, S_i^z are the corresponding spin-1 matrices. When $\Gamma = 0$ this reduces to the classical Blume-Capel model. At $T = 0$, $\Gamma \neq 0$ this model is equivalent to the classical $(d + 1)$ Blume-Capel model [9].

MFRG is a model based on the comparison of two clusters of different size; the interactions within the clusters are treated exactly and the effect of the other spins is represented by a mean-field b which is assumed to scale like the order parameter itself.

We have chosen to compare one-spin and two-spin clusters, the main advantage being that calculations can then be done analytically.

The hamiltonian for the one-spin cluster is then

$$H_I = \Gamma' \, S_1^x + D' \, (S_1^z)^2 - C_I \, S_1^z$$

where $C_I = zJ'b'$ represents the surrounding mean-field, and z is the number of nearest neighbours to one spin.

If we assume b' to be small (which is true in the vicinity of a second-order transition) we can work out a perturbation expansion for $<S^z>$ in powers of b' and keep only the lienar term. This is done in the Appendix following the method of ref. [14]; one gets

$$m_I = <S^z>_I = \frac{2}{\beta \, C_I} \cdot \frac{Z_\uparrow^{(2)}}{Z_\uparrow^{(0)}} + 0\,(b'^2)$$

The hamiltonian for the two-spin cluster is

$$H_{II} = \Gamma \, (S_1^x + S_2^x) + D \, [\, (S_1^z)^2 + \, (S_2^z)^2 \,] - \\ - J \, S_1^z S_2^z - C_{II} \, (S_1^z + S_2^z)$$

Where $C_{II} = (z-1)\,Jb$; and

$$m_{II} = < \frac{S_1^z + S_2^z}{2} >_{II} = \frac{1}{\beta \, C_{II}} \cdot \frac{Z_{II}^{(2)}}{Z_{II}^{(0)}} + 0\,(b^2) \quad \text{(see Apendix)}$$

The MFRG assumption is that b' and b must scale like m_I and m_{II}; imposing this scaling relation for b' and b, we arrive at the renormalization recursive relation for $K' \, (= J' \beta')$, $\Delta' \, (= D' \beta')$, $\alpha' \, (= \Gamma' \beta')$ and K, Δ, α (defined analogously).

The fixed point equation associated with it

$$\frac{1}{z-1} \cdot \frac{Z_{II}^{(2)}}{Z_{II}^{(0)}} \Bigg|_{(K^*,\, \Delta^*,\, \alpha^*)} = \frac{2}{z} \cdot \frac{Z_I^{(0)}}{Z_I^{(2)}} \Bigg|_{(K^*,\, \Delta^*,\, \alpha^*)} \qquad (1)$$

yields the phase diagram in the transverse field-temperature space.

2.2 – *Results*

The phase diagram obtained from equation [1] for a square lattice ($z = 4$) is chown in Fig. 1. For $\Gamma = 0$ the model reduces to the situation treated by de Alcantara Bonfim [15], i. e. the classical Blume-Capel model. This author has associated the tricritical coordinate, Δ_t, to the maximum value taken by Δ in the

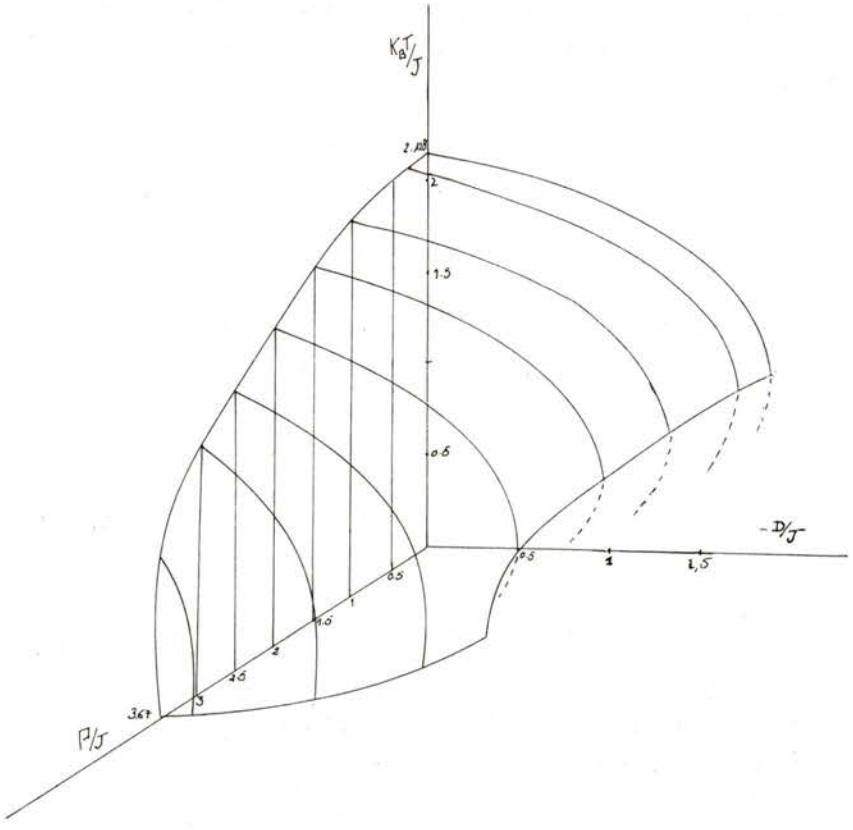

Fig. 1 — Phase diagram of the quantum Blume-Capel model in the T-D-Γ space

———— second-order transition

– – – – – – – first-order transition

curve obtained from MFRG. This method does not envolve a calculation of the free energy necessary to locate the first-order line. However a study of this model by means of the linear chain approximation [4] has shown that in the Δ region where a pair of solutions exists, the upper branch of the curve can be interpreted as giving the Curie temperature of a second-order phase transition, the tricritical point Δ_t within 0.2 % of the maximum value taken by Δ in that curve. We take this argument to support the, otherwise unjustified, assumption of de Alcantara Bonfim and associate the tricritical point with the point beyond which no solution exists to equation (1). The lower branch of the curve (shown in dash) represents an unstable solution. One knows from ground state energy considerations that the first-order line must cut the $T = 0$ axis at $2D/zJ = 1$, so at low temperatures the first-order line is certainly not well represented by the dashed line.

Fig. 2 shows the phase diagram at $T = 0$, for a unidimensional lattce ($z = 2$), together with the predictions of mean-field and other RG methods [9, 11, 12] devised for the $T = 0$ case only. We can see that the curve obtained from equation (1) compares well with the estimates of the second-order lines as given by other RG techniques. However the intersection of the line of extremal points (T_f , D_t , Γ) with the $T = 0$ plane does not coincide with the tricritical point as predicted by the other RG methods. Whether this is due to a failure of the criterium used by the Alcantara Bonfim for the location of the tricritical point within MFRG, or whether it is a limitation of the other RG methods is not clear at the moment. The techniques used by other authors are essentially real-space block spin RG schemes by which a few neighbouring spins are grouped into blocks, the intrablock Hamiltonian is diagonalized and its three lowest levels retained to define the new single-spin variables; this truncation procedure is certainly a limitation of these methods. In the MFRG method the contributions of all the energy levels of the two-spin cluster are duly accounted for in the derivation of the RG recursion relation. On the other hand the MFRG procedure leads to just one equation relating K, α, Δ and K′, α', Δ', whereas a completely specified RG scheme requires more than one equation; thus, only

a few points in the critical surface obtained from equation (1) are actually fixed points of such a well specified procedure; in that respect, those other RG methods stand a better chance of

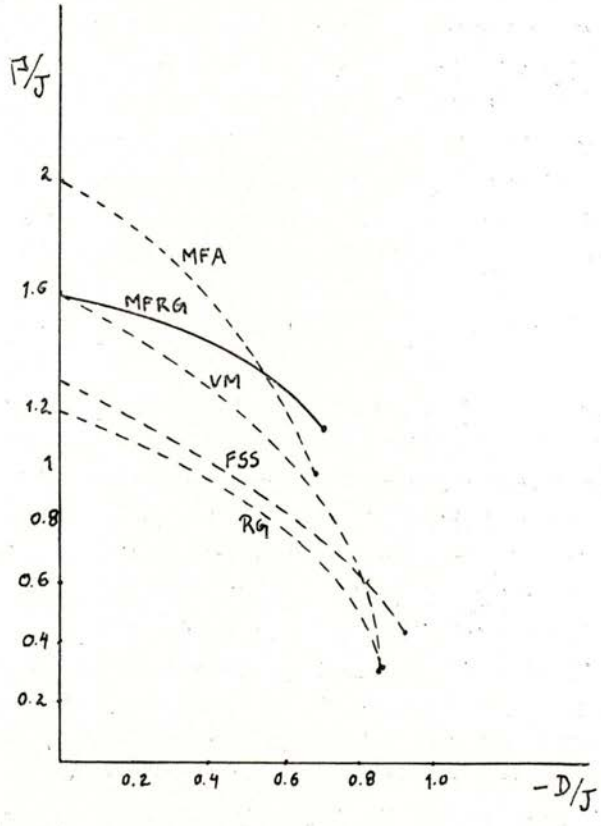

Fig. 2 — Transverse field (Γ) against crystal-field (D) for the quantum Blume-Capel model at $T = 0$; denotes the critical point (MFA — mean-field approximation; MFRG — mean-field renormalization group; VM — variational methods; FSS — finite size scaling; RG — block-spin renormalization group).

appropriately locating first-order phase transitions, since these are then associated with critical coupling lying in the domain of attraction of the so called 'discontinuity fixed points'.

3 – BLUME-CAPEL MODEL WITH RANDOM CRYSTAL-FIELD COUPLING

In this section we consider the effect of random crystal-field interactions on the phase diagram of the classical Blume-Capel system. A similar model has been studied by Kaneyoshi [18] by means of the differential operator technique.

The hamiltonian of the system is then given by

$$H = - \sum_{<ij>} J \, S_i^z S_j^z - \sum_i D_i (S_i^z)^2$$

where D_i has a probability distribution of the form

$$P (D_i) = x \, \delta (D_i - D) + (1 - x) \, \delta (D_i)$$

We get for the 1-spin and 2-spin clusters, after a configurational average has been performed:

$$m_I = <S^z>_I = \frac{2Z \, e^{\Delta'}}{2 \, e^{\Delta'} + 1} \, . \, x' \, k' \, b' + \frac{2Z}{3} (1 - x') \, k' \, b'$$

$$m_{II} = < \frac{S_1^z + S_2^z}{2} >_{II} = 2 (z - 1) \, . \, ((2 \, e^{2\Delta + k} + e^{\Delta}) /$$

$$(4 \, e^{2\Delta} \cosh k + 4 \, e^{\Delta} + 1)) \, . \, x^2 kb + 2 (z - 1) \frac{2 \, e^k + 1}{4 \cosh k + 5} \, .$$

$$(1 - x)^2 kb + 2 (z - 1) \, . \, ((4 \, e^{k + \Delta} + e^{\Delta} + 1) /$$

$$(4 \, e^{\Delta} \cosh k + 2 \, e^{\Delta} + 3)) \, . \, x (1 - x) \, kb$$

The critical lines derived from the MFRG fixed point equation are drawn in figures 3.1 and 3.2 for different values of the concentration and in the case $z = 3$ (honeycomb lattice).

The tricritical point disappears for $x = 0.745$; this differs from the value $x = 0.68$ obtained by Kaneyoshi.

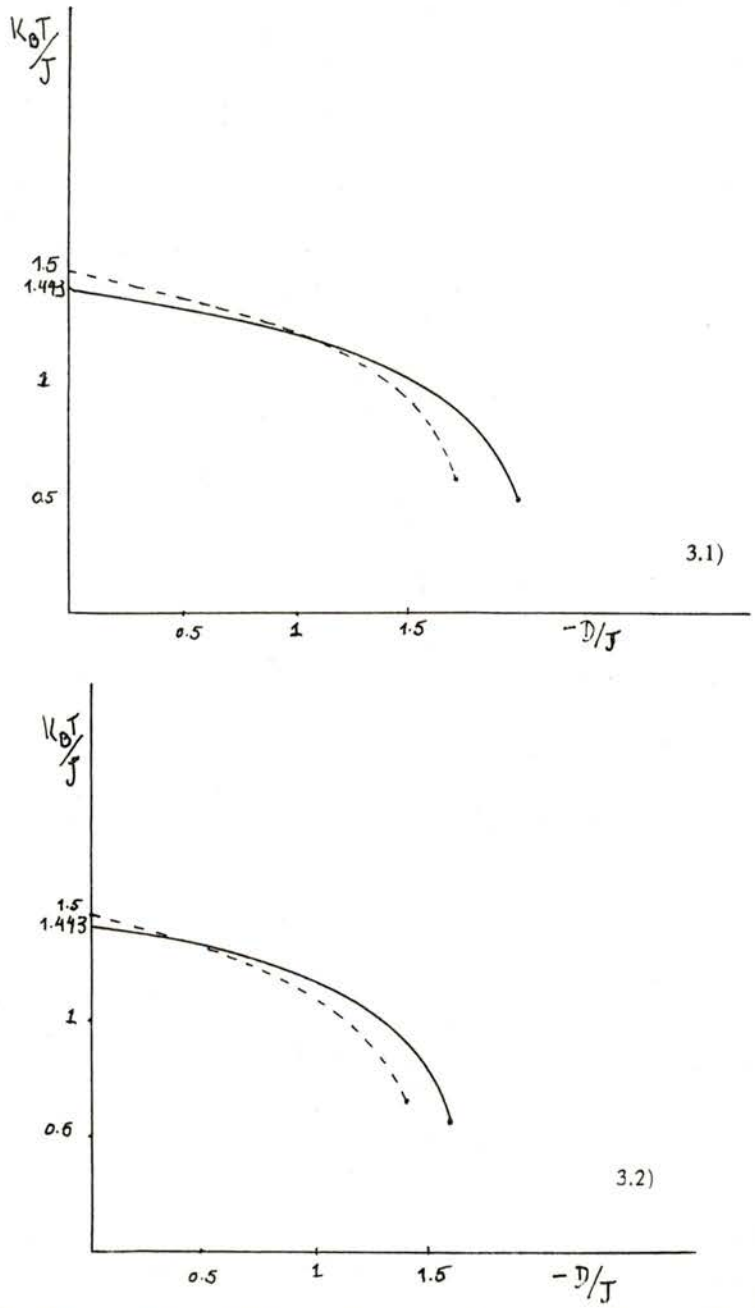

Fig. 3 — Temperature versus crystal field (D) for the classical Blume-Capel with random crystal field at two different concentrations — 3.1 — Pure case; 3.2 — x = 0.8.

4 – CONCLUSIONS

The use of MFRG has enabled us to treat the quantum Blume-Capel model at all temperatures and spatial dimensionality. In the limits $T = 0$ or $\Gamma = 0$ the results of the present work reasonably agree with those presented by other authors in what concerns the location of the line of second-order phase transitions. The tricritical point is also approximately located. The method is not appropriate to study first-order phase transitions and some of its assumptions are less justified at low temperatures when certain relevant correlations are not accounted for; these two limitations affect more critically the location of the tricritical point at low temperatures and this may be the reason for certain discrepancies with the results of other authors at $T = 0$.

We have also applied MFRG to the Blume-Capel model with random crystal-field coupling. The results compare well with those obtained by other methods; this is probably due to the fact that dilution of the crystal-field coupling does not bring the tricriticral point to a low temperature range, as in the former case.

Better accuracy can be achieved by considering bigger clusters which means however that the fixed point equation no longer can be analytically obtained.

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APPENDIX

The eigenvalues and eigenvectors of the isolated one-spin cluster

$$H_I^0 = \Gamma' \, S_1^x + D' \, (S_1^z)^2$$

are the following

$$E_1 = D' \; ; \; |U_1> = \frac{1}{\sqrt{2}} \; (|\uparrow> - |\uparrow>)$$

$$E_2 = (D' + A)/2; \; |U_2> = \frac{D' + A}{\sqrt{2\,(D' + A)^2 + 8\,\Gamma'^2}} \cdot (|\uparrow> +$$

$$+ \frac{2\sqrt{2}\,\Gamma'}{D' + A} \cdot |\rightarrow> + |\uparrow>)$$

$$E_3 = (D' - A/2; \; |U_3> = \frac{D' - A}{\sqrt{2\,(D' - A)^2 + 8\,\Gamma'^2}} \cdot (|\uparrow> +$$

$$+ \frac{2\sqrt{2}\,\Gamma'}{D' - A} \cdot |\rightarrow> + |\downarrow>)$$

where $A = \sqrt{D'^2 + 4\,\Gamma'^2}$

The partition function Z_I which corresponds to the hamiltonian H_I can then be [14]

$$Z_I = Z_I^{(0)} + Z_I^{(2)} + O(b'^3)$$

where $Z_I^{(0)} = e^{-\beta D'} + e^{-\beta/2(D'+A)} + e^{-\beta/2(D'-A)}$ is the unperturbated partition function and

$$Z_I^{(2)} = \beta C_I^2 \left[\frac{(D' + A)^2}{(D' + A)^2 + 4\,\Gamma'^2} \cdot \frac{2}{A - D'} \cdot \right.$$

$$(e^{-\beta D'} - e^{-\beta/2(D'+A)}) + \frac{(D' - A)^2}{(D' - A)^2 + 4\,\Gamma'^2}$$

$$\left. \cdot \frac{2}{D' + A} \; (e^{-\beta/2(D'-A)} - e^{-\beta D'}) \right]$$

One then gets

$$\beta < S_1^z >_I = \frac{d\ln Z_I}{dC_I} = \frac{1}{Z_I^{(0)}} \cdot \frac{dZ_I^{(2)}}{dC_I} + O(b'^2) =$$

$$= \frac{2}{C_I} \cdot \frac{Z_I^{(2)}}{Z_I^{(0)}} + O(b'^2)$$

The hamiltonian for the isolated two-spin clusters is

$$H_{II}^{0} = \Gamma (S_1^x + S_2^x) + D [(S_1^z)^2 + (S_2^z)^2] - J \, S_1^z S_2^z$$

This hamiltonian comutes with the site interchange operator and the «reflexion» operator $\hat{P} \mid m_1 m_2 > = \mid - m_1 - m_2 >$; we can therefore search for the eigenvectors of H_{II}^{0} among the eigenvectors of these operators. One obtains

$$\mid V_1 > = \frac{J + D + B}{\sqrt{(J + D + B)^2 + 4\Gamma^2}} \cdot \left[\frac{2\Gamma}{J + D + B} \cdot \mid U_1 > + \mid U_2 > \right] \qquad E_1 = \frac{J + 3D - B}{2}$$

$$\mid V_2 > = \frac{J + D - B}{\sqrt{(J + D + B)^2 + 4\Gamma^2}} \cdot \left[\frac{2\Gamma}{J + D - B} \cdot \mid U_1 > + \mid U_2 > \right] \qquad E_2 = \frac{J + 3D + B}{2}$$

$$\mid V_3 > = \mid U_3 > \qquad E_3 = D$$

$$\mid V_8 > = \frac{D - J - C}{\sqrt{(D - J - C)^2 + 4\Gamma^2}} \cdot \left[\frac{2\Gamma}{D - J - C} \mid U_8 > - U_9 > \right] \qquad E_8 = \frac{3D - J + C}{2}$$

$$\mid V_9 > = \frac{D - J + C}{\sqrt{(D - J + C)^2 + 4\Gamma^2}} \cdot \left[\frac{2\Gamma}{D - J + C} \mid U_8 > - U_9 > \right] \qquad E_9 = \frac{3D - J - C}{2}$$

where $B = \sqrt{4\Gamma^2 + (J + D)^2}$, $\quad C = \sqrt{4\Gamma^2 + (J - D)^2}$ and

$$f(J, D, \Gamma, E_k) = (E_k (-J + 2D - E_k)(J + 2D - E_k)) / \sqrt[\Gamma]{F}$$

$$F = E_k^2 (J + 2D - E_k)^2 + 2(-J + 2D - E_k)^2 (J + 2D - E_k^2) + \\ + E_k^2 (-J + 2D - E_k)^2 + E_k^2 (-J + 2D - E_k)^2 (J + 2D - E_k^2)/\Gamma^2$$

$$|V_k> = \frac{\Gamma}{J-2D+E_k} \cdot f(J,D,\Gamma,E_k) \cdot |U_4> + \frac{\sqrt{2}\,\Gamma}{E_k} \cdot$$

$$f(J,D,\Gamma,E_k)\,|U_6> - \frac{\Gamma}{J+2D-E_k}\, f(J,D,\Gamma,E_k) \cdot$$

$$\cdot\, |U_7> + f(J,D,\Gamma,E_k)\,|U_5> \qquad E_k\,,\ k=4,5,6,7$$

The E_k's are the solutions of equation

$$[(2D-E_k)^2 - J^2]\ [E_k(E_k-D) - 2\Gamma^2] + 2\Gamma^2 E_k(2D-E_k) = 0$$

A perturbation expansion of $<S_1^z + S_2^z>$ requires the calculation of matrix elements $<V_j|\, S_1^z + S_2^z\,|V_j>$, of which only a few are nonzero.

Following the same procedure as above we get

$$1/2\,<S_1^z + S_2^z>_{II} = \frac{C_{II}}{Z_{II}^{(0)}} \sum_{i=1}^{7} e^{-\beta E_i} \sum_j \frac{A_{ji}}{E_j - E_i}$$

where the coefficients A_{ij} are defined as $|\,<V_j|\, S_1^z + S_2^z\,|\,V_i>\,|^2$. The expressions for the nonvanishing elements are

$$A_{31} = A_{13} = \frac{4\Gamma^2}{4\Gamma^2 + (J+D+B)^2}$$

$$A_{32} = A_{23} = \frac{4\Gamma^2}{4\Gamma^2 + (J+D-B)^2}$$

$$A_{8k} = A_{k8} = \frac{(D-J-C)^2}{4\Gamma^2 + (D-J-C)^2} \cdot f^2(J,D,\Gamma,E_k) \cdot$$

$$\left[\frac{4\Gamma^2}{(D-J-C)\,(J-2D+E_k)} - 1\right]^2;\ k=4,5,6,7$$

$$A_{9k} = A_{k9} = \frac{(D-J+C)^2}{4\Gamma^2 + (D-J+C)^2} \cdot f^2(J,D,\Gamma,E_k)$$

$$\left[\frac{4\Gamma^2}{(D-J+C)\,(J-2D+E_k)} - 1\right]^2;\ k=4,5,6,7$$

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