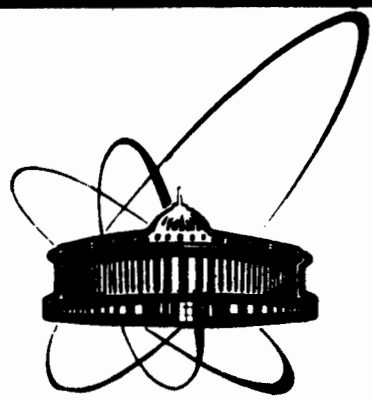


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ОБЪЕДИНЕННЫЙ
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EXACT FORMULATION OF PARTICLE-HOLE
STATE DENSITIES IN THE EQUIDISTANT
SPACING MODEL WITH PAULI
AND PAIRING CORRECTIONS

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I. Introduction

Meeting the nuclear data needs of the fission and fusion technology requires a wide use of theories and phenomenological models. One of the most important elements in these theories is often the nuclear state density. In the study of precompound reactions development of exciton and hybrid models [1-4] has introduced requirements for an accurate knowledge of the average densities of nuclear excitation states with a fixed number of excited particles and holes. Quite recently, a fast development of multistep compound (MSC) and multistep direct (MSD) theories [5-7] and semiphenomenological models [8] has enhanced the role of particle-hole state densities.

Several authors have given formulae for these densities without incorporating the Pauli exclusion principle [1,9,10] or approximately involving it based on statistical [11,12] and group theoretical method [13]. An advanced pairing correction for a most common William's formula was formulated in Fu's [14] and Kalbach's [15] works, but as was pointed out by Kalbach, "remaining discrepancies between the simple state densities and the results of a detailed pairing calculation are attributable to deficiencies in the original ESM state density formula".

Last year a new approach based on group theoretical methods has been proposed [16], and new numerical values of Pauli corrections, and also formulae for particle-hole state density in ESM were obtained. Although these results are very useful it seems reasonable to derive analytical formulation of particle-hole state density by a long time used statistical method without any approximation, because two main problems still remain: First, there is no way to check the obtained results [16] because we haven't any other exact approach to the problem of partial state densities. Second, it is impossible to take into account pairing corrections by the Kalbach-Fu method [14,15] in the formulae of Ref.[16].

Owing to the great importance of the exact formula for particle-hole state density for precompound models we will try to obtain them by another method, to implement an advanced pairing correction in this formula and, finally, to compare new formula with the results of Ref.[16]. That is the purpose of this paper.

II. Particle-hole state density derivation

Our initial suppositions follow William's model [11]. The single

particle levels are non-degenerate with a constant spacing d . The one-particle density of states is $g=1/d$. For convenience of calculations, units are chosen so that $d=1$. As has been proposed by Kalbach [12], energies are measured from the Fermi energy taken to be halfway between the last filled and first vacant single particle level in the ground state of the nucleus. This condition guarantees particle-hole symmetry in all theory.

As has been shown by William [11], we can write the particle-hole state density in the form,

$$\omega(p,h,U) = \frac{1}{2\pi i} \int_{\sigma-i\infty}^{\sigma+i\infty} dz \frac{\exp[(U - E_p(p,h)) z]}{\prod_{k=1}^p (1-\exp(-kz)) \prod_{j=1}^h (1-\exp(-jz))}, \quad (1)$$

where U is the excitation energy and $E_p(p,h)$ is the Pauli energy, which have in William's work [11] the following value:

$$E_p(p,h) = 1/2 [p(p+1) + h(h-1)]. \quad (2)$$

In our case, we change the Fermi level, i.e we take $E_p(p,h)$ as

$$E_p(p,h) = 1/2 [p^2 + h^2]. \quad (3)$$

To calculate the partial state density from (1), one can use the Cauchy residue theorem, as was suggested by William. First, let us analyze the case $h=0$ (or $p=0$); thus only a pure particle (hole) state density will be obtained.

In this case, from (1)

$$\omega(p,h=0,U) = \frac{1}{2\pi i} \int_{\sigma-i\infty}^{\sigma+i\infty} dz \frac{\exp[(U-E_p(p,h)) z]}{\prod_{k=1}^p (1-\exp(-kz))} = \frac{1}{2\pi i} \int_{\sigma-i\infty}^{\sigma+i\infty} dz f(z). \quad (4)$$

Using the Cauchy residue theorem we get

$$\omega(p,h=0,U) = \text{Res}[f(z)]_{z=0} = \frac{1}{(p-1)!} \lim_{z \rightarrow 0} \frac{d^{p-1}}{dz^{p-1}} [z^p f(z)] \quad (5)$$

because at point $z=0$ the integrand in (4) has a pole of an order of p . Now we can make a Taylor expansion of $f(z)$'s denominator

$$\prod_{k=1}^p (1-\exp(-kz)) = \lim_{m \rightarrow \infty} \prod_{k=1}^p kz Q_{m-1}(kz) = p! z^p \lim_{m \rightarrow \infty} \prod_{k=1}^p Q_{m-1}(kz), \quad (6)$$

where a polynomial $Q_{m-1}(kz) = \sum_{i=1}^m (-kz)^{i-1}/i!$ of the $(m-1)^{\text{th}}$ order was defined.

From (5), substituting (6) we have

$$\omega(p, h=0, U) = \frac{1}{p!(p-1)!} \lim_{z \rightarrow 0} \frac{d^{p-1}}{dz^{p-1}} \left(\frac{\exp[(U - E_p(p, h))z]}{\lim_{m \rightarrow \infty} \prod_{k=1}^p Q_{m-1}(kz)} \right) \quad (7)$$

Allowing for the presence of limit ($z \rightarrow 0$) and the order $p-1$ of the derivative in expression (7), we require that the maximum order of polynomial in the denominator of (7) should be equal to $p-1$. Otherwise those terms, whose order is higher than $p-1$ will disappear when we take the limit at $z \rightarrow 0$. From the mentioned condition we can reduce the denominator to the following expression:

$$\lim_{m \rightarrow \infty} \prod_{k=1}^p Q_{m-1}(kz) \rightarrow \prod'_{k=1}^p Q_{p-1}(kz) \equiv R_{p-1}(z), \quad (8)$$

where by \prod' we denote that only those terms from the product are taken, whose order is equal to or less than $p-1$. The polynomial $R_{p-1}(z)$ can be written in the classical form as

$$R_{p-1}(z) = \sum_{k=0}^{p-1} \Phi_p(k) z^k, \quad (9)$$

when the coefficients $\Phi_p(k)$ are obtained directly from definition (8). Our problem is now reduced to calculation of the following expression:

$$\omega(p, h=0, U) = \frac{1}{p!(p-1)!} \lim_{z \rightarrow 0} \frac{d^{p-1}}{dz^{p-1}} \left(\frac{\exp[tz]}{R_{p-1}(z)} \right), \quad (10)$$

where $t = U - E_p(p, h)$.

Using Leibniz's formula for the $(p-1)^{\text{th}}$ derivative we can write the following expression:

$$[\exp(tz) R_{p-1}^{-1}(z)]^{(p-1)} = \sum_{k=0}^{p-1} \binom{p-1}{k} [\exp(tz)]^{(p-k-1)} [R_{p-1}^{-1}(z)]^{(k)}, \quad (11)$$

where $\binom{p-1}{k}$ denotes the binomial coefficient.

It is trivial that

$$\lim_{z \rightarrow 0} [\exp(tz)]^{(p-k-1)} = t^{p-k-1} \quad (12)$$

and if we suppose that

$$\lim_{z \rightarrow 0} [R_{p-1}^{-1}(z)]^{(k)} = F_p(k) k!, \quad (13)$$

the following expression for $F_p(k)$ can be obtained (see appendix A)

$$F_p(k) = \begin{cases} 1 & \text{if } k = 0 \\ (-1)^k \sum_{j=1}^k \bar{\Phi}_p(j) F_p(k-j) & \text{otherwise} \end{cases} \quad (14)$$

Finally, by using (10)-(14) the formula for pure particle state density can be written in the form:

$$\omega(p, h=0, U) = \frac{1}{p!} \sum_{k=0}^{p-1} [U - E_p(p, 0)]^{p-k-1} F_p(k) / (p-1-k)! \quad (15)$$

We can obtain the numerical value of the Pauli correction, as proposed in Ref. [16], from the following condition:

$$\omega(p, h=0, U_0) = 0 \Rightarrow A(p, h=0) = U_0 \quad (16)$$

$\omega(p, h=0, U) > 0$ for any energy $U > A(p, h=0)$.

In polynomial zero calculations a FORTRAN program implementing the Müller method was employed. The major zero of the polynomial (15) was taken as $A(p, h=0)$; so the condition (16) has automatically been satisfied.

It is easy to show how our method can be generalized to the case when $p \neq 0$ and $h \neq 0$. By analogy with (10) we can write

$$\omega(p, h, U) = \frac{1}{p! h! (n-1)!} \lim_{z \rightarrow 0} \frac{d^{n-1}}{dz^{n-1}} \left(\frac{\exp[tz]}{R_{n-1}^{ph}(z)} \right), \quad (17)$$

where by definition $n=p+h$ and

$$R_{n-1}^{ph}(z) = \prod_{k=1}^p Q_{n-1}(kz) \prod_{j=1}^h Q_{n-1}(jz). \quad (18)$$

As has been pointed out before [see (8), (9)] the polynomial $R_{n-1}^{ph}(z)$ can be represented in a different way,

$$R_{n-1}^{ph}(z) = \sum_{k=0}^{n-1} \Lambda_{ph}(k) z^k, \quad (19)$$

where $\Lambda_{ph}(k)$ may be calculated directly from definition (18). In a similar way, it is easy to obtain, that the general particle-hole state density has the following formula:

$$\omega(p, h, U) = \frac{1}{p!h!} \sum_{k=0}^{n-1} [U - E_p(p, h)]^{n-k-1} G_{ph}(k) / (n-1-k)! \quad (20)$$

where we can obtain $G_{ph}(k)$ from the following recursive relation:

$$G_{ph}(k) = \begin{cases} 1 & \text{if } k = 0 \\ (-1)^k \sum_{j=1}^k \Lambda_{ph}(k) G_{ph}(k-j) & \text{otherwise} \end{cases} \quad (21)$$

The numerical value of the Pauli correction can be obtained from the following condition:

$$\omega(p, h, U_0) = 0 \Rightarrow A(p, h) = U_0 \quad (22)$$

$\omega(p, h, U) > 0$ for any energy $U > A(p, h)$.

We find all the zeros of the polynomial (20), and the biggest one was taken as $A(p, h)$, satisfying in this way condition (22).

III. Results

FORTTRAN expressions for pure particle (or hole) state density polynomials are shown in appendix B. The polynomial coefficients $C_{po}(k)$, which appear in this appendix were calculated exactly implementing formula (15) in REDUCE [17] code. Similar results for the particle-hole state density are shown in appendix C. The above mentioned density can be written as

$$\omega(p, h, U) = \sum_{k=0}^{n-1} c_{ph}(k) [U - E_p(p, h)]^{n-k-1} \quad \text{for } U > A(p, h) \quad (23)$$

The numerical values of the Pauli correction $A(p, h)$ are shown in tables 1 and 2 for the number of particles p and holes h less or equal to 5.

TABLE 1. Pauli corrections $A(p, h)$ for pure particle(hole) state density [$A(p=0, h)=A(p, h=0)$], $A_K(p, h)=1/4[p(p-1)+h(h-1)]$

p=	h=	E (p, h) Pauli energy	This work A(p, 0)	Ref. [16] A(p, 0)	Ref. [15] A _K (p, 0)
1	0	0.50000	0.00000	0.00	0.00
2	0	2.00000	0.50000	0.50	0.5
3	0	4.50000	2.58012	2.46	1.5
4	0	8.00000	5.73861	5.66	3.0
5	0	12.50000	9.96059	9.93	5.0
6	0	18.00000	15.23511	15.22	7.5
7	0	24.50000	21.55402	21.52	10.5
8	0	32.00000	28.91096	28.86	14.0
9	0	40.50000	37.30076	37.26	18.0
10	0	50.00000	46.71912	46.68	22.5

For comparison we also show the results of Ref.[16]. In the general case ($p \neq 0$ and $h \neq 0$) agreement between our results and the results of Ref.[16] is not good (see table 2). We checked out the calculations in Ref.[16] and found that an approximate expression for the trace in the case of the Exciton model was employed.

TABLE 2. Pauli corrections $A(p,h)$ for particle-hole state density [$A(p,h)=A(p,h)$], $A_K(p,h)=1/4[p(p-1)+h(h-1)]$.

p=	h=	E (p,h) Pauli energy	This work A(p,h)	Ref.[16] A(p,h)	Ref.[15] A _K (p,h)
1	1	1.00000	0.00000	0.00	0.00
2	1	2.50000	1.20711	1.00	0.50
2	2	4.00000	2.58114	2.37	1.00
3	1	5.00000	3.43649	3.28	1.50
3	2	6.50000	4.91595	4.81	2.00
3	3	9.00000	7.29761	7.29	3.00
4	1	8.50000	6.72016	6.65	3.00
4	2	10.00000	8.28818	8.24	3.50
4	3	12.50000	10.70100	10.69	4.50
4	4	16.00000	14.10874	14.04	6.00
5	1	13.00000	11.05272	11.00	5.00
5	2	14.50000	12.70203	12.62	5.50
5	3	17.00000	15.14627	15.05	6.50
5	4	20.50000	18.55385	18.40	8.00
5	5	25.00000	22.98945	23.95	10.00

Taking into account that the distance between levels in the ESM is constant and equal to $1/g$, we can rewrite (3.1) of Ref.[16] in the following form

$$\text{tr} \left\{ \exp(-l\beta\mathcal{K}) \right\} = \sum_{\mu} \langle \mu | \exp(-l\beta\mathcal{K}) | \mu \rangle = \sum_{n=0}^{\infty} \exp \left\{ -(2n+1)l\beta/(2g) \right\}. \quad (24)$$

This trace can be calculated exactly

$$\text{tr} \left\{ \exp(-l\beta\mathcal{K}) \right\} = \left\{ 2 \text{sh} \left[\beta l / (2g) \right] \right\}^{-1}. \quad (25)$$

In Ref.[16] only the first term in the Taylor expansion for hyperbolic sinus has been taken, thus resulting for the trace in

$$\text{tr} \left\{ \exp(-l\beta\mathcal{K}) \right\} \approx gl/\beta. \quad (26)$$

Using the method proposed in Ref.[16], but taking the exact expression for Exciton model's trace (25), we obtained for the state density polynomial (23) and for the Pauli correction term $A(p,h)$ the same results of the present work.

IV. Pairing corrections

It is well known that the pairing effect plays an important role in partial state density. In our method we have a very simple way to implement realistic pairing corrections in exact particle-hole state density. This simplicity can be explained by the existence of the explicit dependence of the Pauli energy $E_p(p,h)$ in the partial state density formula [see (23)]. As has been pointed out by Kalbach [15], we can implement pairing corrections just substituting the Pauli energy $E_p(p,h)$ by the threshold energy for the pairing states E_{thresh} . From Fu's [14] and Kalbach's [15] works we can write

$$E_{\text{thresh}} = g \frac{\Delta_0^2 - \Delta^2}{4} + (n/2) \left[(n/(2g))^2 + \Delta^2 \right]^{1/2}, \quad (27)$$

where $n=p+h$ is the total exciton number, $\Delta_0 = 2 [P/g]^{1/2}$ is the condensation energy and P is the pairing constant obtained by fitting experimental level density data.

Pairing gap Δ can be taken from Fu's [14] and Kalbach's work [15] as

$$\begin{aligned} \Delta/\Delta_0 &= .996 - 1.76(n/n_c)^{1.6} (E/P)^{-.68} & \text{if } E > E_{\text{phase}} \\ &= 0 & \text{if } E < E_{\text{phase}}, \end{aligned} \quad (28)$$

where the quantity E_{phase} is the energy of the pairing phase transition given by

$$\begin{aligned} E_{\text{phase}} &= P [0.716 + 2.44(n/n_c)^{2.17}] & \text{if } n/n_c > 0.446 \\ &= 0 & \text{otherwise} \end{aligned} \quad (29)$$

and $n_c = 0.792 g \Delta_0$ is the critical number of excitons.

Now to take into account pairing correlations we only need to replace $E_p(p,h)$ by E_{thresh} [formula (27)] in all formulae of Section II.

V. Summary and conclusions

We have obtained an exact analytical formula for particle-hole state density (20) as polynomial of $(U - E_p(p,h))$, where U is the excitation energy and $E_p(p,h)$ is the Pauli energy of the system. The numerical values of the polynomial coefficients are tabulated using REDUCE code for analytical calculations. The Pauli corrections $A(p,0)$ and $A(p,h)$ are calculated and tabulated, these results agree satisfactorily with the results of Ref.[16]. For practical calculations formula (23) can be used. FORTRAN expressions for exact state density polynomials are given in appendix B and C.

Pairing effects in exact partial state density calculations can be taken into account substituting everywhere $E_p(p,h)$ by E_{thresh} [see (27)]. Threshold energy can be calculated by the method proposed by Fu and Kalbach in earlier works [14,15].

Finally, we need to comment on state densities calculations. As was pointed out in several works, the sum of partial state density must agree with the total state density and experimental level density data. To reach this purpose, we can use in all state density calculations a new set of parameters a, D obtained by fitting experimental level density data with one-component total state density [18]. This is the simplest way to achieve consistency between calculated partial and total state density, and therefore between preequilibrium and equilibrium parts of spectra in Exciton model calculations. These comments remain important for the proposed method to calculate partial state density exactly. Further investigations to apply the obtained formulae to Exciton Model calculations will be carried out.

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APPENDIX.

A.-We should obtain the value of $\lim_{z \rightarrow 0} [R_{p-1}^{-1}(z)]^{(k)}$.

To obtain the k^{th} derivative for an inverse of polynomial, we first calculate polynomial derivative $R_{p-1}^{(n)}(z)$. From definition we have

$$R_{p-1}(z) \equiv \prod_{k=1}^p Q_{p-1}(kz) = \sum_{i=0}^{p-1} \phi_p(i) z^i ; \quad R_{p-1}(z=0) \equiv 1 \quad (\text{A1})$$

We can write polynomial derivative as

$$R_{p-1}^{(m)}(z) = \sum_{i=0}^{p-1} i(i-1)\dots(i-m+1) \phi_p(i) z^{i-m} . \quad (\text{A2})$$

Taking the limit,

$$\lim_{z \rightarrow 0} R_{p-1}^{(m)}(z) = m! \phi_p(m) . \quad (\text{A3})$$

Denoting $g(z) \equiv R_{p-1}^{-1}(z)$, we should obtain the derivative $g^{(k)}(z)$.

We have the following identity:

$$[g(z) R_{p-1}(z)]^{(k)} = 0. \quad (A4)$$

The l.h.s. of identity (A4) may be expanded using the Leibniz formula

$$\sum_{i=0}^{p-1} \binom{k}{i} [g(z)]^{(k-i)} [R_{p-1}(z)]^{(i)} = 0. \quad (A5)$$

By isolating the first term the following recursive relation can be obtained

$$[g(z)]^{(k)} R_{p-1}(z) = (-1) \sum_{i=1}^k \binom{k}{i} [g(z)]^{(k-i)} [R_{p-1}(z)]^{(i)}. \quad (A6)$$

Taking the limit as $z \rightarrow 0$ in (A6), substituting (A1), (A3) & (13) and simplifying combinatorial factor we can obtain the recursive relation (14).

B.-FORTRAN expressions for pure particle state density polynomials $\omega(p, h, Z)$ with coefficients $C_{p0}(k)$; $k \in [1, p-1]$, where $Z = U - E_p(p, h)$; U - excitation energy.

$$\omega(2, 0, Z) = 1./2.*Z + 3./4.$$

$$\omega(3, 0, Z) = 1./12.*Z**2 + 1./2.*Z + 47./72.$$

$$\omega(4, 0, Z) = 1./144.*Z**3 + 5./48.*Z**2 + 15./32.*Z + 175./288.$$

$$\omega(5, 0, Z) = 1./2880.*Z**4 + 1./96.*Z**3 + 31./288.*Z**2 + 85./192.*Z + 50651./86400.$$

$$\omega(6, 0, Z) = 1./86400.*Z**5 + 7./11520.*Z**4 + 77./6480.*Z**3 + 245./2304.*Z**2 + 43981./103680.*Z + 199577./345600.$$

$$\omega(7, 0, Z) = 1./3628800.*Z**6 + 1./43200.*Z**5 + 79./103680.*Z**4 + 161./12960.*Z**3 + 3991./38400.*Z**2 + 21343./51840.*Z + 87797891./152409600.$$

$$\omega(8, 0, Z) = 1./203212800.*Z**7 + 1./1612800.*Z**6 + 307./9676800.*Z**5 + 13./15360.*Z**4 + 728681./58060800.*Z**3 + 15599./153600.*Z**2 + 2812349./6967296.*Z + 39226571./67737600.$$

$$\omega(9, 0, Z) = 1./14631321600.*Z**8 + 1./81285120.*Z**7 + 193./209018880.*Z**6 + 29./774144.*Z**5 + 464921./522547200.*Z**4 + 290309./23224320.*Z**3 + 873824279./8778792960.*Z**2 + 5557231./13934592.*Z + 256697834389./438939648000.$$

$$\omega(10, 0, Z) = 1./1316818944000.*Z**9 + 11./58525286400.*Z**8 + 869./43893964800.*Z**7 + 121./104509440.*Z**6 + 3222263./78382080000.*Z**5 + 7607149./8360755200.*Z**4 + 362312621./29262643200.*Z**3 + 859801921./8778792960.*Z**2 + 745508886881./1881169920000.*Z + 1039519669529./1755758592000.$$

C.-FORTRAN expressions for particle-hole state density polynomials $\omega(p,h,Z)$ with coefficients $C_{ph}(k)$; $k \in [1, p+h-1]$, where $Z=U-E_p(p,h)$; U-excitation energy

$$\omega(1,1,Z)=Z+1.$$

$$\omega(2,1,Z)=1./4.*Z**2+Z+7./8.$$

$$\omega(3,1,Z)=1./36.*Z**3+7./24.*Z**2+11./12.*Z+119./144.$$

$$\omega(4,1,Z)=1./576.*Z**4+11./288.*Z**3+83./288.*Z**2+55./64.*Z+2815./3456.$$

$$\omega(5,1,Z)=1./14400.*Z**5+1./360.*Z**4+89./2160.*Z**3+5./18.*Z**2+317./384.*Z+8861./10800.$$

$$\omega(2,2,Z)=1./24.*Z**3+3./8.*Z**2+49./48.*Z+13./16.$$

$$\omega(3,2,Z)=1./288.*Z**4+1./16.*Z**3+7./18.*Z**2+31./32.*Z+1357./1728.$$

$$\omega(4,2,Z)=1./5760.*Z**5+13./2304.*Z**4+59./864.*Z**3+871./2304.*Z**2+3581./3840.*Z+10855./13824.$$

$$\omega(5,2,Z)=1./172800.*Z**6+1./3200.*Z**5+19./2880.*Z**4+11./160.*Z**3+42143./115200.*Z**2+1171./1280.*Z+413989./518400.$$

$$\omega(3,3,Z)=1./4320.*Z**5+1./144.*Z**4+101./1296.*Z**3+29./72.*Z**2+24299./25920.*Z+655./864.$$

$$\omega(4,3,Z)=1./103680.*Z**6+1./2160.*Z**5+181./20736.*Z**4+53./648.*Z**3+9107./23040.*Z**2+11819./12960.*Z+93877./124416.$$

$$\omega(5,3,Z)=1./3628800.*Z**7+7./345600.*Z**6+209./345600.*Z**5+217./23040.*Z**4+21149./259200.*Z**3+88991./230400.*Z**2+7843667./8709120.*Z+1582631./2073600.$$

$$\omega(4,4,Z)=1./2903040.*Z**7+1./41472.*Z**6+19./27648.*Z**5+425./41472.*Z**4+23603./276480.*Z**3+1201./3072.*Z**2+3099547./3483648.*Z+185705./248832.$$

$$\omega(5,4,Z)=1./116121600.*Z**8+1./1161216.*Z**7+179./4976640.*Z**6+5./6144.*Z**5+134513./12441600.*Z**4+28309./331776.*Z**3+2973431./7741440.*Z**2+6124385./6967296.*Z+1120716881./1492992000.$$

$$\omega(5,5,Z)=(1./362880.*Z**9+1./2688.*Z**8+37./1728.*Z**7+395./576.*Z**6+12037./900.*Z**5+15671./96.*Z**4+9933611./8064.*Z**3+4881655./896.*Z**2+6474529381./518400.*Z+374216881./34560.)/(120.*120.)$$

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