Pramāṇa – J. Phys., Vol. 27, No. 5, November 1986, pp. 685–692. © Printed in India.

Theoretical study of the satellites and hypersatellites in the K-LL Auger spectrum of magnesium

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MS received 16 April 1986

Abstract. This paper reports calculations of the energies of the satellite and hypersatellite lines in the K-LL Auger spectrum of magnesium. The results show that it may be possible to observe many more satellite and hypersatellite lines in the Auger spectrum which have not been hitherto reported experimentally.

Keywords. Auger spectra; satellite lines; hypersatellite lines; defect-electron configurations.

PACS No. 32·80

1. Introduction

In the last few years the subject of multiple innershell ionization of light elements as studied using accelerated ion-atom collisions has aroused considerable interest (Åberg and Suvanen 1982; Crasemann 1984; Mirakhmedov and Parilis 1984). Information on the multiply ionized states of atoms is obtained by studying the satellites and hypersatellites in x-ray and Auger spectra. In an earlier paper (Lakshmi Natarajan *et al* 1986) hereafter called paper I, we reported our theoretical calculations of the x-ray satellite and hypersatellite lines of magnesium arising out of transitions between different defect electron configurations. In the present paper, we report similar calculations of the K-LL Auger satellite and hypersatellite lines of magnesium. The x-ray satellite and hypersatellite lines, which usually lie on the high energy side of the prominent diagram lines, occur due to radiative transitions between different multiply ionized atomic configurations. On the other hand, the competing non-radiative transitions between such states give rise to satellites and hypersatellites in Auger spectrum, which are generally observed on the low energy side of the diagram Auger line.

Experimental work on Auger satellites of some light elements like Ne, Al and Si has been carried out by Matthews *et al* (1973), Woods *et al* (1975) and Whaley and Thomas (1984) while theoretical calculations using HFS wave functions have been carried out by Bhalla *et al* (1973) for the elements Ne and Ar.

The only work on Auger satellites of Mg was reported by Breuckmann and Schmidt (1974) and Breuckmann (1979). They have, however, considered configurations having a single hole either in the 3*s* shell or in the 2*p* shell. Thus no detailed theoretical calculations are available for the transition energies of the Auger satellites and hypersatellites of magnesium arising from different defect atomic configurations. Hence it was considered worthwhile to undertake the present calculations.

2. Procedure for calculations

The average energies of an atom in various defect configurations are needed for calculating the energies of the satellite and hypersatellite lines. We have calculated these values for magnesium making use of screened hydrogenic wavefunctions developed earlier (Tankhiwale and Mande 1970; Lakshmi Natarajan *et al* 1986) neglecting exchange and configuration interactions and many-body effects (Kelly 1975; Chattarji *et al* 1978). We have earlier shown (Tankhiwale *et al* 1971) that these screened hydrogenic wavefunctions agree very closely with the HFS wavefunctions for the inner orbitals like 1*s*, 2*s*, 2*p* etc though they show some deviation for the outer orbitals. In the present calculations which involve the inner shells, the integrals involved come in a closed form due to the analytical nature of the wavefunctions and thus give a better picture of the actual physical processes. The effective charges for the orbitals 1*s*, 2*s*, 2*p* and 3*s* were taken to be 11·52, 9·25, 8·48 and 4·95 respectively as shown in paper I. The screening of a K electron by the other electron from the same shell comes out as 0·48, while the screening for an L electron by a single K electron and a single L electron is 0·75 and 0·30 respectively. The screening for an M electron by a single K electron and a single L electron is 0·80 and 0·60 respectively. The average energies of the different defect configurations were calculated using Slater's (1960) expression given in paper I.

Since the Auger transitions are governed only by parity conservation considerations (Burhop and Asaad 1972), for a given initial state there are many more Auger transitions as compared to the corresponding radiative x-ray transitions. We classify these transitions as (i) 2*p*-2*p* meaning a 2*p* electron jumps to an initially vacant 1*s* shell and the other 2*p* electron goes to the continuum; (ii) 2*s*-2*p* and (iii) 2*s*-2*s* with similar meanings. Double ionization of the K shell in the initial state gives rise to Auger hypersatellites. The energies of the above Auger satellite and hypersatellite lines are given by the following expressions which are simply the differences of the initial and final state average energies.

(i) For the 2*p*-2*p* Auger lines

$$E_A\,(2p\text{-}2p) = E_i\,(1s^1 2s^m 2p^n 3s^2) - E_f\,(1s^{l+1} 2s^m 2p^{n-2} 3s^2)$$

where l, m and n denote the occupation numbers of electrons in the 1*s*, 2*s* and 2*p* shells respectively. Here if $m = 0$ and 1, n takes the values 1 to 6 while for $m = 2$, n takes the values 1 to 5.

(ii) For the 2*s*-2*p* Auger lines

$$E_A\,(2s\text{-}2p) = E_i\,(1s^l 2s^m 2p^n 3s^2) - E_f\,(1s^{l+1} 2s^{m-1} 2p^{n-1} 3s^2).$$

For $m = 1$, n takes the values 1 to 6 and for $m = 2$, n takes the values 1 to 5.

(iii) For the 2*s*-2*s* Auger lines

$$E_A\,(2s\text{-}2s) = E_i\,(1s^l 2s^m 2p^n 3s^2) - E_f\,(1s^{l+1} 2s^{m-2} 2p^n 3s^2).$$

Here for $m = 2$, n varies from 1 to 5.

In all the above cases for the satellites $l = 1$, while for the hypersatellites $l = 0$.

3. Results and discussion

Using the procedure described above we have calculated the transition energies of the Auger satellite and hypersatellite lines arising from the various defect electron configurations as initial states. These are tabulated in tables 1a, 1b and 1c for the transitions $2p$-$2p$, $2s$-$2p$ and $2s$-$2s$ respectively. In the same table are given the experimental values of the transition energies for the few transitions reported by Breuckmann (1979). The positions of the various K-LL satellite and hypersatellite lines

Table 1a. Energies (in eV) of the K-LL Auger satellite and hypersatellite lines of magnesium for different defect-configurations ($2p$-$2p$ transitions).

Initial configuration	Present calculations	Value due to Breuckmann (1979)
$1s^1 2s^2 2p^6 3s^2$	1170	1161·9
		1167·1
		1171·0
Satellites		
$1s^1 2s^2 2p^5 3s^2$	1145·3	1145·5
		1148·5
		1151·9
$1s^1 2s^2 2p^4 3s^2$	1118·2	
$1s^1 2s^2 2p^3 3s^2$	1084·2	
$1s^1 2s^2 2p^2 3s^2$	1051·5	
$1s^1 2s^1 2p^6 3s^2$	1147·1	
$1s^1 2s^1 2p^5 3s^2$	1117·2	
$1s^1 2s^1 2p^4 3s^2$	1086·8	
$1s^1 2s^1 2p^3 3s^2$	1053·5	
$1s^1 2s^1 2p^2 3s^2$	1019·0	
$1s^1 2s^0 2p^6 3s^2$	1122·0	
$1s^1 2s^0 2p^5 3s^2$	1092·1	
$1s^1 2s^0 2p^4 3s^2$	1060·8	
$1s^1 2s^0 2p^3 3s^2$	1030·2	
$1s^1 2s^0 2p^2 3s^2$	998·2	
Hypersatellites		
$1s^0 2s^2 2p^6 3s^2$	1231·6	
$1s^0 2s^2 2p^5 3s^2$	1202·7	
$1s^0 2s^2 2p^4 3s^2$	1172·8	
$1s^0 2s^2 2p^3 3s^2$	1140·0	
$1s^0 2s^2 2p^2 3s^2$	1104·9	
$1s^0 2s^1 2p^6 3s^2$	1206·9	
$1s^0 2s^1 2p^5 3s^2$	1179·6	
$1s^0 2s^1 2p^4 3s^2$	1148·8	
$1s^0 2s^1 2p^3 3s^2$	1114·9	
$1s^0 2s^1 2p^2 3s^2$	1086·2	
$1s^0 2s^0 2p^6 3s^2$	1196·8	
$1s^0 2s^0 2p^5 3s^2$	1162·8	
$1s^0 2s^0 2p^4 3s^2$	1130·2	
$1s^0 2s^0 2p^3 3s^2$	1095·5	
$1s^0 2s^0 2p^2 3s^2$	1058·2	

Table 1b. Energies (in eV) of the K-LL Auger satellite and hypersatellite lines of magnesium for different defect configurations (2*s*-2*p* transitions).

Initial configuration	Present calculations	Values due to Breuckmann (1979)
		1121·5
$1s^1 2s^2 2p^6 3s^2$	1132·0	1135·4
Satellites		
		1098·3
$1s^1 2s^2 2p^5 3s^2$	1110·2	1104·2
		1110·7
$1s^1 2s^2 2p^4 3s^2$	1085·2	
$1s^1 2s^2 2p^3 3s^2$	1056·3	
$1s^1 2s^2 2p^2 3s^2$	1028·3	
$1s^1 2s^2 2p^1 3s^2$	1000·2	
$1s^1 2s^1 2p^6 3s^2$	1108·4	
$1s^1 2s^1 2p^5 3s^2$	1081·2	
$1s^1 2s^1 2p^4 3s^2$	1054·0	
$1s^1 2s^1 2p^3 3s^2$	1026·1	
$1s^1 2s^1 2p^2 3s^2$	1001·9	
$1s^1 2s^1 2p^1 3s^2$	971·1	
Hypersatellites		
$1s^0 2s^2 2p^6 3s^2$	1190·0	
$1s^0 2s^2 2p^5 3s^2$	1158·7	
$1s^0 2s^2 2p^4 3s^2$	1134·9	
$1s^0 2s^2 2p^3 3s^2$	1105·7	
$1s^0 2s^2 2p^2 3s^2$	1074·4	
$1s^0 2s^2 2p^1 3s^2$	1043·4	
$1s^0 2s^1 2p^6 3s^2$	1181·8	
$1s^0 2s^1 2p^5 3s^2$	1153·7	
$1s^0 2s^1 2p^4 3s^2$	1122·0	
$1s^0 2s^1 2p^3 3s^2$	1093·7	
$1s^0 2s^1 2p^2 3s^2$	1062·1	
$1s^0 2s^1 2p^1 3s^2$	1031·1	

of magnesium have been shown in figure 1A on energy scale. The three diagram lines arising due to the transitions—

(a) $1s^1 2s^2 2p^6 3s^2$ $\quad 1s^2 2p^6 3s^2 (1s\text{-}2s2s)$,
(b) $1s^1 2s^2 2p^6 3s^2$ $\quad 1s^2 2s^1 2p^5 3s^2 (1s\text{-}2s2p)$ and
(c) $1s^1 2s^2 2p^6 3s^2$ $\quad 1s^2 2s^2 2p^4 3s^2 (1s\text{-}2p2p)$

are shown by thick lines. Their satellites and hypersatellites are shown respectively by thin and dotted lines. Most of them lie on the low energy side except for a few hypersatellite lines.

It may be mentioned here that Breuckmann and Schmidt (1974) and Breuckmann (1979) have made theoretical calculations using HFS wavefunctions for the few satellite lines arising from the initial configurations having just one hole in the 2*p* shell and also with a single hole in the 3*s* shell. They have further considered the multiplet structure of the initial and final configurations for these lines. The positions of these lines are shown

Table 1c. Energies (in eV) of the K-LL Auger satellite and hypersatellite lines of magnesium for different defect configurations (2*s*-2*s* transitions).

Initial configuration	Present calculations	Values due to Breuckmann (1979)
$1s^1 2s^2 2p^6 3s^2$	1099·7	1087·5
Satellites		
$1s^1 2s^2 2p^5 3s^2$	1079·0	1064·9 1071·3
$1s^1 2s^2 2p^4 3s^2$	1053·2	
$1s^1 2s^2 2p^3 3s^2$	1028·7	
$1s^1 2s^2 2p^2 3s^2$	1002·9	
$1s^1 2s^2 2p^1 3s^2$	981·1	
Hypersatellites		
$1s^0 2s^2 2p^6 3s^2$	1156·0	
$1s^0 2s^2 2p^5 3s^2$	1132·9	
$1s^0 2s^2 2p^4 3s^2$	1105·3	
$1s^0 2s^2 2p^3 3s^2$	1075·7	
$1s^0 2s^2 2p^2 3s^2$	1046·1	
$1s^0 2s^2 2p^1 3s^2$	1020·0	

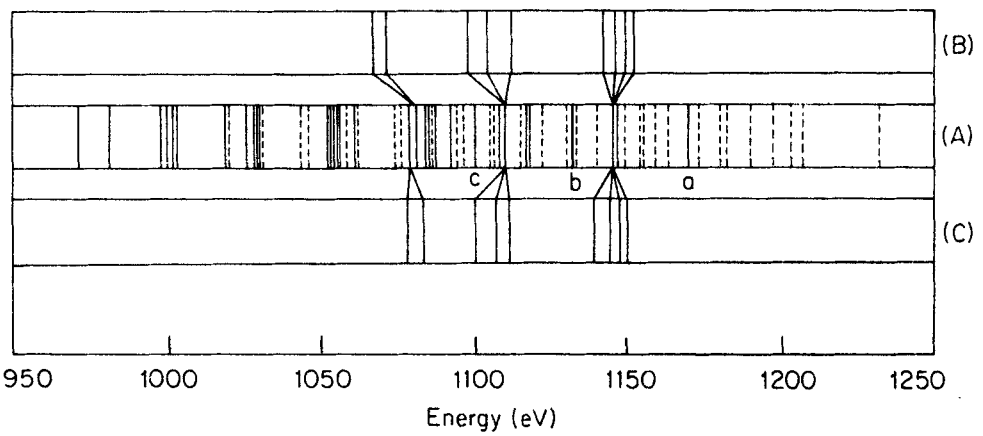

Figure 1. Positions of the satellites (thin lines) and hypersatellites (dotted lines) in the K-LL Auger spectrum of magnesium. Thick lines a, b and c represent the diagram lines corresponding to the (2*p*-2*p*), (2*s*-2*p*), and (2*s*-2*s*) transitions respectively. **A.** Our calculated values based on gross configurational energies. **B.** Values reported by Breuckmann invoking multiplet structure. **C.** Our corresponding values invoking multiplet structure.

in figure 1B. In order to compare the values we have also invoked the multiplet structure for the same configurations and calculated (using our method) the positions of these lines. The energies of these multiplet lines obtained by us are tabulated in table 2. For comparison of the energies of our multiplets with those of Breuckmann and Schmidt, we have shown them in figure 1C. Our calculated positions agree fairly well with those of Breuckmann and Schmidt for these lines. However, as figure 1A shows, we obtain

Table 2. Energies (in eV) of the K-LL Auger satellite lines of magnesium for the initial configurations $1s^1 2s^2 2p^5(^{1,3}P)3s^2$ and $1s^1 2s^2 2p^6 3s^1$ invoking multiplet structure.

Initial State	Final State	Present calculations	Values due to Breuckmann (1979)
$1s^1 2s^2 2p^5(^3P)3s^2$	$1s^2 2s^0 2p^5(^2P)3s^2$	1077·5	1064·9
$1s^1 2s^2 2p^5(^1P)3s^2$	$1s^2 2s^0 2p^5(^2P)3s^2$	1083·4	1071·3
$1s^1 2s^2 2p^5(^3P)3s^2$	$1s^2 2s^1 2p^4(^2P)3s^2$	1100·1	1098·3
$1s^1 2s^2 2p^5(^1P)3s^2$	$1s^2 2s^1 2p^4(^2P)3s^2$	1107·0	1104·3
$1s^1 2s^2 2p^5(^3P)3s^2$	$1s^2 2s^1 2p^4(^2D)3s^2$	1111·2	1110·7
$1s^1 2s^2 2p^5(^3P)3s^2$	$1s^2 2s^2 2p^3(^2P)3s^2$	1139·4	1142·1
$1s^1 2s^2 2p^5(^3P)3s^2$	$1s^2 2s^2 2p^3(^2D)3s^2$	1144·0	1145·5
$1s^1 2s^2 2p^5(^1P)3s^2$	$1s^2 2s^2 2p^3(^2P)3s^2$	1147·1	1148·5
$1s^1 2s^2 2p^5(^1P)3s^2$	$1s^2 2s^2 2p^2(^2D)3s^2$	1149·8	1151·9
$1s^1 2s^2 2p^6 3s^1$	$1s^2 2s^0 2p^6(^1S)3s^1\ ^2S$	1088·0	1075·8
	$1s^2 2s^1 2p^5(^1P)3s^1\ ^2P$	1111·7	1109·5
	$1s^2 2s^1 2p^5(^3P)3s^1\ ^4P$	1128·1	1123·3
	$1s^2 2s^2 2p^4(^1S)3s^1\ ^2S$	1151·5	1149·9
	$1s^2 2s^2 2p^4(^1D)3s^1\ ^2S$	1158·9	1155·1

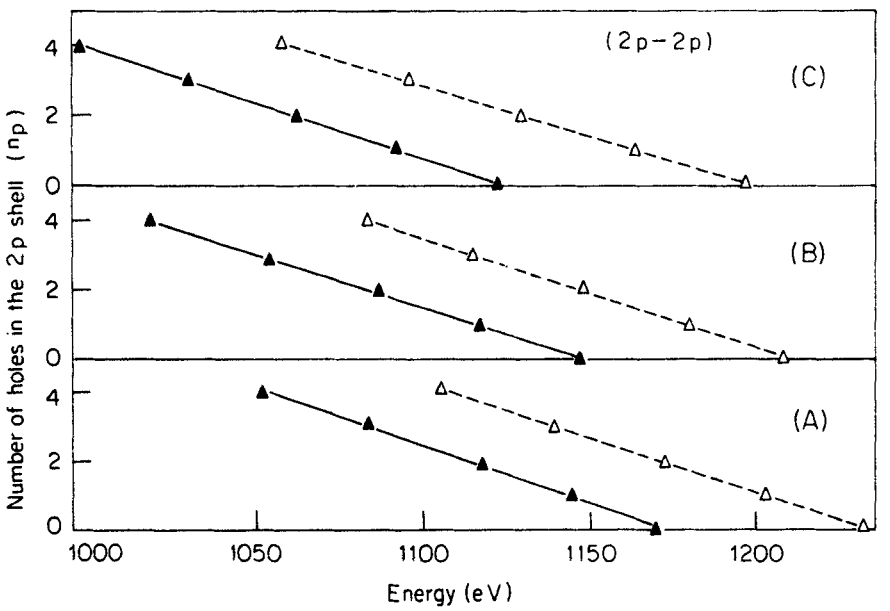

Figure 2. Variation of the energies of magnesium Auger satellite (continuous curves) and hypersatellite lines (broken curves) with n_p, the number of holes in the $2p$ shell for the $2p$-$2p$ transitions. A, B, C represent atoms with no permanent holes one and two permanent holes respectively in the $2s$ shell.

many more Auger satellite and hypersatellite lines with our calculations which are based on gross configurational energies without invoking the multiplet structure. As is obvious in figure 1 all the lines reported by Breuckmann and Schmidt can be simply explained as arising due to transitions between one gross configurational level to

another. For example, the three central lines 1098·3 eV, 1104·2 eV and 1110·7 eV, observed by Breuckmann and Schmidt, may very well be taken as arising due to transitions from the initial configurations $1s^02s^02p^33s^2$, $1s^02s^22p^33s^2$ and $1s^12s^22p^53s^2$ to the final configurations $1s^12s^02p^13s^2$, $1s^12s^22p^13s^2$ and $1s^22s^22p^33s^2$ respectively. On the basis of such considerations we have been able to account for the observed x-ray satellite and hyper-satellites of magnesium (paper I). The same concept of average energies has been used by Richard *et al* (1972) in their work on the transition energies of the x-ray satellite and hypersatellite lines of magnesium. Bhalla *et al* (1973) also based their extensive theoretical study on x-ray and Auger satellites and hypersatellites of the light elements like Ne and Ar making use of the gross configurational average energies. Similarly Matthews *et al* (1973) used the same concept as the basis to account for their experimentally observed Auger satellite and hypersatellite lines of neon. These earlier studies lend support to our work on transition energies using average energies, without any necessity to invoke multiplet structure.

In figures 2, 3 and 4 we have shown the energies of the Auger satellite and hypersatellite lines against n_p, the number of holes in the 2*p* shell. In these figures A, B and C correspond respectively to the cases of zero, one and two permanent holes in the 2*s* shell. The Auger satellite energy decreases regularly with progressive increase in the number of holes in the 2*p* shell. For the hypersatellites, with the 2*p* holes having a value one or two there is first an increase in energy, but with further increase in the number of holes the energy decreases. In all cases, a striking parallelism in the E vs n_p curves is observed for the Auger satellites and hypersatellites, as in the case of x-ray satellites and hypersatellites (paper I).

It may not be out of place to comment on the possibility of Coster-Kronig transitions in the case of magnesium. Coster-Kronig transitions are Auger transitions between a higher sub-shell to an inner sub-shell of the same major shell of an atom. For

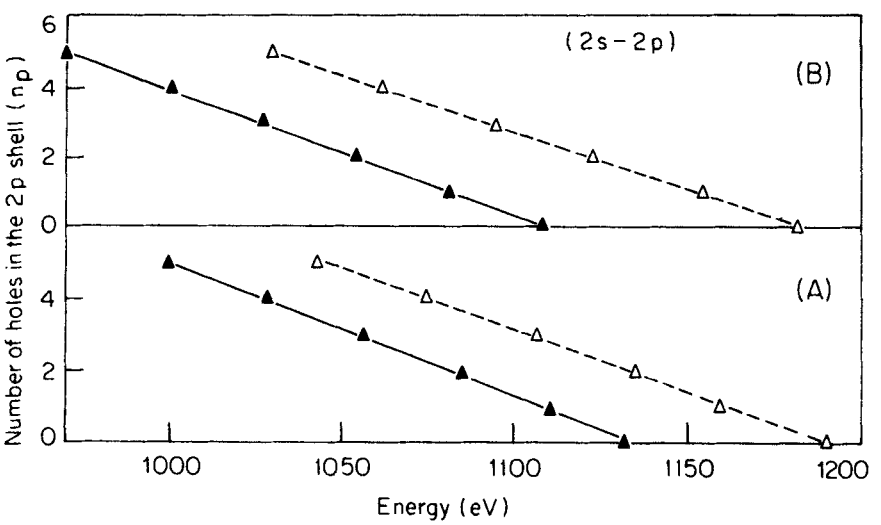

Figure 3. Variation of the energies of magnesium Auger satellite (continuous curves) and hypersatellite lines (broken curves) with n_p, the number of holes in the 2*p* shell for the 2*s*-2*p* transitions. A, B represent atoms with no permanent and one permanent hole respectively in the 2*s* shell.

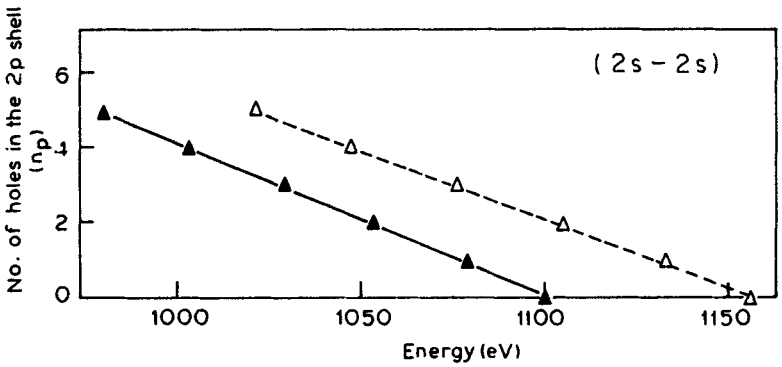

Figure 4. Variation of the energies of magnesium Auger satellite (continuous curves) and hypersatellite lines (broken curves) with n_p, the number of holes in the $2p$ shell for the $2s$-$2s$ transitions.

magnesium, they would arise due to transitions between the configurations $1s^l2s^m2p^n3s^2$ and $1s^l2s^{m+1}2p^{n-2}3s^2$, where l takes values from 0 to 2, m takes values 0 and 1 and n any value between 2 and 6. From our calculations, we conclude that the C-K transitions are energetically not possible in magnesium, since the energies of the final configurations are higher than those of the corresponding initial ones.

In their experiments Breuckmann and Schmidt have not been able to obtain the large number of expected Auger lines, probably because they have used electrons with energies of the order of a few keVs as projectiles. With new experimental facilities now available, if collision experiments are performed with high energy ($\sim$ few MeV) heavy ion projectiles, it may be possible to obtain many more Auger satellite and hypersatellite lines as shown by our theoretical calculations. Such experiments on the dynamics of inner shell processes are likely to elucidate the basic unity of the excitation and de-excitation phases of atoms and call for the elaboration of new, comprehensive theoretical approaches as mentioned by Crasemann (1984).

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