the transition observed at ~88°K (Figure 4). It is also interesting that the initial slope of α' is steeper than for the methacrylates, with the expansion coefficients somewhat larger. We recall in this connection that Crissman, Sauer, and Woodward[20] observed a fairly large mechanical relaxation at ~24°K (10 Hz) and much more pronounced than for PiBMA with its similar side group.

The results for the E–P copolymer (Figure 4) above 100°K are similar to those of Zakin, *et al.*[21] The decrease in α between 190 and 90°K could be indicative of an extremely broad relaxation region. It is also noteworthy that a slight plateau region appears around 140°K, similar to that in Figure 9 of ref 21 at approximately 133°K. On reducing the temperature further, the copolymer should exhibit an analogous relaxation, if the mechanism is indeed similar to that postulated for the polyethylene γ-transition. The observed transition lies considerably lower, ~56°K, and this may be related to the absence of crystallinity. Finally it may be worthy of note that infrared measurements of Shen and coworkers[22] indicate freezing out of $-CH_2-$ vibrations in polyethylene below 100°K.

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Matrix Method for Determining the Dimensions of Branched Random-Flight Chains[1]

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ABSTRACT: A new method is presented for mathematically characterizing branching in random-flight chains. The method is then used to calculate mean-square radii of gyration for a number of examples. For every mode of branching there can be defined a matrix, $[D]$, with eigenvalues that completely define the distribution of radii of gyration. The parameter g, the ratio of the mean-square radius of gyration of the branched chain to that of a linear chain with the same number of statistical segments t, is given by $g = (6/t^3)$ trace $[D]$. When applied to cruciform, star, and uniformly branched molecules the method gives values for g in agreement with those obtained previously by other investigators using entirely different mathematics.

Because of the effect of branching on many of the physical properties of polymers, there has been a continuing interest in the configurational statistics of branched-chain molecules.[2–8] We present here a new method of mathematically characterizing chain branching that is completely general and requires only matrix algebra.

It will be shown that a matrix, $[D]$, is associated with any random-flight chain, whether linear or with any mode of branching, and that this matrix determines many of the important statistical features of the chain. In particular, we will show that the distribution of radii of gyration is determined by its eigenvalues and that the mean-square radius of gyration is simply related to trace $[D]$. Mean-square radii for the examples treated in this paper are in agreement with those of previous investigators.

It is always possible that the matrix method may give reasonable closed-form expressions for chain dimensions for classes of branched chains other than those reported here. Of more interest, however, is that this new approach is especially suitable for digital computer calculations and could be applied to branched chains far more complex than those usually treated by analytical methods. Furthermore, since so much structural information is contained in $[D]$, it is tempting to imagine that this matrix might also be directly related to various types of chain behavior. For example, we have established a simple relationship between $[D]$ and chain dynamics that will be presented in a subsequent publication.

Since the calculations presented in this paper are based on random-flight statistics, the results are assumed to apply to real polymer molecules at the Flory Θ temperature. We also assume, as has been done previously,[4] that this work could be extended to include polymer–solvent interactions.

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Formulation of the Problem

The model describing unperturbed linear flexible polymer molecules as chains of t statistical segments was described previously.[9] In defining the relative positions of the $t + 1$ beads in the chain we consider $\mathbf{P}_i$, the vector from the center of mass of the chain to the ith bead; $\mathbf{P}_0$, the vector from the center of mass to the zeroth bead; $\mathbf{L}_i$, the vector from the zeroth bead to the ith bead; $\mathbf{L}_t$, the end-to-end distance vector; and the t vectors $\mathbf{T}_j$ connecting adjacent beads. These vectors are related by the equations

$$\mathbf{P}_i = \mathbf{L}_i + \mathbf{P}_0 \tag{1}$$

where

$$\mathbf{L}_i = \sum_{j=1}^{i} \mathbf{T}_j$$

The x component of this equation is written

$$x_i = x_0 + \sum_{j=1}^{i} \gamma_j \tag{2}$$

where x_i is the x coordinate of the ith bead (relative to the center of mass), and γ_j is the x component of the vector $\mathbf{T}_j$.

Utilizing eq 1 and the relationship that Σx_i from $i = 0$ to $i = t$ equals 0, which defines the center of mass, we showed[9] that the x component of the radius of gyration, S_x, can be written as

$$(tS_x)^2 = [\gamma]^{\mathrm{T}}[a][\gamma] \tag{3}$$

The matrix $[\gamma]$ is the column vector of the γ_i coordinates and $[a]$ is the $t \times t$ symmetric matrix with elements

$$\begin{aligned} a_{ij} &= (t + 1 - i)j,\ i \geq j \\ &= (t + l - j)i,\ j \geq i \end{aligned} \tag{4}$$

Since $[a]$ is symmetric it is possible to effect an orthogonal transformation to a second set of coordinates $[\eta] = [b][\gamma]$ so that no cross terms appear in the quadratic form giving $(tS_x)^2$; that is

$$(tS_x)^2 = \sum_{i=1}^{t} \lambda_i \eta_i^2 \tag{5}$$

The same distribution function characterizes all of the η_i and γ_i. It follows that $\langle \eta_i^2 \rangle = \langle \gamma_i^2 \rangle$, or, since all the second moments are equal, we can write them without subscripts, *i.e.*, $\langle \eta^2 \rangle = \langle \gamma^2 \rangle$. Because of the equivalence of second moments we can write

$$t^2\langle S_x^2 \rangle = \langle \eta^2 \rangle \sum \lambda_i = \langle \gamma^2 \rangle \sum \lambda_i \tag{6}$$

But since the trace of a matrix is invariant to orthogonal transformation, we showed that

$$t^2\langle S_x^2 \rangle = \langle \gamma^2 \rangle \text{ trace } [a] \tag{7}$$

It is important to note that the development leading from eq 2 to eq 7 is dependent only on the functional form of eq 2 and on the fact the Σx_i from $i = 0$ to $i = t$ equals 0, and *not* on any features of the model. We will show in the following sections that it is possible to write an expression

$$x_i = x_0 + \sum_{j=1}^{i} \Gamma_j \tag{8}$$

for branched polymer chains where the Γ_j are linear combinations of the γ_i. It follows directly from eq 8 that

$$t^2\langle S_x^2 \rangle = [\Gamma]^{\mathrm{T}}[a][\Gamma] \tag{9}$$

We can then express the relationship between the Γ_i and γ_i in the matrix form

$$[\Gamma] = [C][\gamma] \tag{10}$$

We thus find then that

$$\begin{aligned} (tS_x)^2 &= [\gamma]^{\mathrm{T}}[C]^{\mathrm{T}}[a][C][\gamma] \\ &= [\gamma]^{\mathrm{T}}[D][\gamma] \end{aligned} \tag{11}$$

where

$$[D] = [C]^{\mathrm{T}}[a][C] \tag{12}$$

It was previously demonstrated[9,10] that the distribution of S_x for linear chains can be determined using eq 3 and the eigenvalues of $[a]$. By comparing eq 3 and 11, it is clear that the distribution of S_x for branched chains is, in a like manner, completely determined by the eigenvalues of $[D]$.

Since it can also be shown that $[D]$ is symmetric, the same arguments as those leading from eq 3 to eq 7 can be applied to lead from eq 11 to the expression

$$t^2\langle S_x^2 \rangle = \langle \gamma^2 \rangle \text{ trace } [D] \tag{13}$$

Following previous notation,[2] we define a parameter g which is the ratio of $\langle S_x^2 \rangle$ for a given branched chain to $\langle S_x^2 \rangle$ for the linear chain of the same number of statistical segments. Considering that $\langle S_x^2 \rangle = \langle S^2 \rangle/3$, the parameter g applies to the ratio of the mean-square radius of gyration itself as well as to the x component. The value of trace $[a]$ is $t^3/6$ if $t \gg 1$, the only case of interest here. For any mode of branching defined by $[C]$, or equivalently $[D]$, we find

$$g = (6/t^3) \text{ trace } [D] \tag{14}$$

In this work we find it convenient to write

$$[C] = [I] - [E] \tag{15}$$

where $[I]$ is the unit matrix and $[E]$ is a $t \times t$ matrix which we will show to have all elements equal either to zero or unity. We find

$$\begin{aligned} [D] &= \{[I] - [E]^{\mathrm{T}}\}[a]\{[I] - [E]\} \\ &= [a] - [E]^{\mathrm{T}}[a] - [a][E] + [E]^{\mathrm{T}}[a][E] \end{aligned} \tag{16}$$

$$g = 1 - (6/t^3) \text{ trace } \{[a][E] + [E]^{\mathrm{T}}[a] - [E]^{\mathrm{T}}[a][E]\} \tag{17}$$

Equation 17 can be simplified by noting that trace $[E]^{\mathrm{T}}[a]$ = trace $[a][E]$. By defining a matrix $[f]$, where

$$[f] = 2[a][E] - [E]^{\mathrm{T}}[a][E] \tag{18}$$

we can finally write

$$g = 1 - (6/t^3) \text{ trace } [f] \tag{19}$$

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(9) W. C. Forsman and R. E. Hughes, *J. Chem. Phys.*, **38**, 2118 (1963).

(10) R. F. Hoffman, Ph.D. Thesis, University of Pennsylvania 1967.

$$\begin{bmatrix} \gamma_1 \\ \gamma_2 \\ \cdots \\ \gamma_{m+n} \\ \gamma_{m+n+1} - \gamma_m - \gamma_{m-1} - \cdots - \gamma_{m+n} \\ \gamma_{m+n+2} \\ \cdots \\ \gamma_{m+n+p} \\ \gamma_{m+n+p+1} - \gamma_{m+n+1} - \gamma_{m+n+2} - \cdots - \gamma_{m+n+p} \\ \gamma_{m+n+p+2} \\ \cdots \\ \gamma_t \end{bmatrix}$$

Figure 1. The [Γ] matrix for the cruciform molecule

Cruciform Molecules

As before, we assume a total of t segments and $t + 1$ beads. In this case, the four branches of the molecule originate from a common point and are made up of m, n, p, and q segments where, of course

$$m + n + p + q = t$$

To find the matrix [Γ] that satisfies eq 10, we consider the relationship between the x_i and various γ_i; this relationship is shown in eq A-1 of the Appendix and the appropriate matrix [Γ] is shown in Figure 1. The corresponding $[E]$ matrix is shown in Figure 2.

In order to handle this problem more easily, we introduce a new function, $\Delta_{i,j,k}$

$$\begin{aligned} \Delta_{i,j,k} &= 1 \text{ if } i \leqslant j \leqslant k \qquad (20) \\ &= 0 \text{ otherwise} \end{aligned}$$

Note that the $\Delta_{i,j,k}$ are defined only for $k \geqslant i$.

In the case of the cruciform molecule we can write

$$E_{ij} = \delta_{i,m+n+1}\Delta_{m+1,j,m+n} + \delta_{i,m+n+p-1}\Delta_{m+n+1,j,m+n+p} \qquad (21)$$

Applying eq 18 to the cruciform molecule then yields trace $[f]$ given by eq A-2 in the Appendix. We can now write eq A-2 explicitly by using the matrix elements defined in eq 4 with the result

$$\text{trace}\,[f] = 2[(t - m - n) \sum_{i=m+1}^{m+n} i + (t + m - n - p) \sum_{i=m+n+1}^{m+n+p} i] - [n(t - m - n)(m + n) + p(t - m - n - p)(m + n + p)] = [nmp + nmq + pqm + pqn] \qquad (22)$$

If we define the fraction of segments in each branch of the molecule as

$$\begin{aligned} \alpha &= (n/t) \\ \beta &= (m/t) \\ \gamma &= (p/t) \\ \delta &= (q/t) \qquad (23) \end{aligned}$$

the expression for g for the cruciform molecule becomes

$$g = 1 - 6(\alpha\beta\gamma + \alpha\beta\delta + \alpha\delta\gamma + \beta\gamma\delta) \qquad (24)$$

Although the above expression for g has been obtained previously by entirely different techniques,[2] it was apparently never recognized that it could be expressed as simply and symmetrically.

If one of the branches has zero segments, say $\delta = 0$, the equation for g becomes simply

$$g = 1 - 6\alpha\beta\gamma \qquad (25)$$

Uniformly Branched Molecules

We define the uniformly branched, or comb, molecule as one having n branches of b segments on a linear backbone, each branch being separated from its nearest neighbors by m backbone segments. For this example the total number of segments is given by

$$nb + (n + 1)m = t \qquad (26)$$

The relationships between the various x_i and γ_i are

$$\begin{array}{l|cccccccccccccccccc|} & & & & & \text{column } m+1 & & & & \text{column } m+n & \text{column } m+n+1 & & & & \text{column } m+n+p & & & & \\ & 0 & 0 & \cdots & & & & \cdots & & & & & & \cdots & & & & 0 & 0 \\ & 0 & 0 & \cdots & & & & \cdots & & & & & & \cdots & & & & 0 & 0 \\ & \cdot & \cdot & \cdots & & & & \cdots & & & & & & \cdots & & & & \cdot & \cdot \\ & \cdot & \cdot & \cdots & & & & \cdots & & & & & & \cdots & & & & \cdot & \cdot \\ \text{row } m+n+1 & 0 & 0 & \cdots & 0 & 1 & 1 & \cdots & 1 & 1 & 0 & & & \cdots & & & & 0 & 0 \\ & \cdot & \cdot & \cdots & & & & \cdots & & & & & & \cdots & & & & \cdot & \cdot \\ & \cdot & \cdot & \cdots & & & & \cdots & & & & & & \cdots & & & & \cdot & \cdot \\ \text{row } m+n+p+1 & \cdot & \cdot & \cdots & & & & \cdots & & 0 & 1 & 1 & \cdots & 1 & 1 & 0 & \cdots & 0 & 0 \\ & 0 & 0 & \cdots & & & & \cdots & & & & & & \cdots & & & & 0 & 0 \\ & \cdot & \cdot & \cdots & & & & \cdots & & & & & & \cdots & & & & \cdot & \cdot \\ & \cdot & \cdot & \cdots & & & & \cdots & & & & & & \cdots & & & & \cdot & \cdot \\ & 0 & 0 & \cdots & & & & \cdots & & & & & & \cdots & & & & 0 & 0 \\ & 0 & 0 & \cdots & & & & \cdots & & & & & & \cdots & & & & 0 & 0 \end{array}$$

Figure 2. The $[E]$ matrix for the cruciform molecule.

$$\begin{array}{l|cccccccccccccc|c}
 & & & \text{column } m+1 & & \text{column } m+b & & \text{column } 2m+b+1 & & \text{column } 2m+2b & & \text{column } nm+(n-1)b+1 & & \text{column } nm+nb & & \\
 & 0\;0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0\;0 \\
 & 0\;0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0\;0 \\
 & \vdots & & & & & & & & & & & & & & \vdots \\
\text{row } m+b+1 & 0\;0 & \cdots & 0\;1\;1 & \cdots & 1\;1\;0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0\;0 \\
 & 0\;0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0\;0 \\
 & \vdots & & & & & & & & & & & & & & \vdots \\
\text{row } 2m+2b+1 & 0\;0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0\;1\;1 & \cdots & 1\;1\;0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0\;0 \\
 & 0\;0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0\;0 \\
 & \vdots & & & & & & & & & & & & & & \vdots \\
\text{row } nm+nb+1 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0\;1\;1 & \cdots & 1\;1\;0 & \cdots & 0\;0 \\
 & 0\;0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0\;0 \\
 & \vdots & & & & & & & & & & & & & & \vdots \\
 & 0\;0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0\;0
\end{array}$$

Figure 3. The $[E]$ matrix for the uniformly branched, or comb, molecule.

given in eq A-3 and the appropriate matrix $[E]$ is shown in Figure 3. The elements of $[E]$ are given by

$$E_{ij} = \sum_{k=1}^{n} \delta_{i,k(m+b)+1}\Delta_{km+(k-1)b+1,j,k(m+b)} \qquad (27)$$

and the trace of $[f]$ by eq A-4. We then write λ for the fraction of segments in the branches and r for the ratio of the number of segments in each branch to the number of backbone segments separating each branch, *i.e.*

$$\begin{aligned} \lambda &= nb/t = nr/[nr + (n+1)] \\ r &= b/m \end{aligned} \qquad (28)$$

The equation for g for the uniformly branched molecule becomes

$$g = 1 - \lambda^3[1 + 2r^{-1} + r^{-2} - n^{-1}(3 - 3r^{-2}) + n^{-2}(2 - 2r^{-1} + 2r^{-2})] \qquad (29)$$

It can be shown that eq 29 is identical with an expression obtained for g for uniformly branched molecules by different mathematical techniques.[5]

A limiting case of interest is the regular star molecule, a chain with all its branches originating from a common point. For this case $r = \infty$ and $\lambda = 1$ or

$$g = (3/n) - (2/n^2) \qquad (30)$$

If $n = 3$, this model represents a cruciform molecule with three equal branches and one "branch" of zero segments. Both eq 25 and 30 predict $g = {}^7/_9$. If $n = 4$ in this case, the molecule corresponds to a cruciform with four equal branches. Equations 24 and 30 are in agreement, as they must be, both giving $g = {}^5/_8$.

By letting $n = 1$, eq 29 yields

$$g = 1 - {}^3/_2\lambda + 3\lambda^2 - {}^3/_2\lambda^3 \qquad (31)$$

which is again a special case of the cruciform molecule, in this example where γ from eq 24 is equivalent to λ and $\alpha = \beta$.

The most intriguing feature of eq 29 becomes apparent, however, when we consider chains with enough branches to allow us to assume $n \cong n + 1$. If this be true, then

$$g \cong 1 - (1 + n^{-1} - n^{-2})\lambda + 2(2n^{-1} - n^{-2})\lambda^2 - n^{-2}\lambda^3 \qquad (32)$$

Finally, if n is sufficiently large, we obtain the exceedingly simple expression

$$g = 1 - \lambda \qquad (33)$$

Remembering that λ is the fraction of segments in the branches, we can say that for this case g is simply equal to the fraction of segments in the backbone.

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Appendix

Relationships between x_i and γ_i and Expressions for Trace $[f]$. For Cruciform Molecules

$$\begin{aligned}
x_1 &= x_0 + \gamma_1 \\
x_2 &= x_0 + \gamma_1 + \gamma_2 \\
\ldots &\quad \ldots\ldots\ldots \\
x_{m+n} &= x_0 + \gamma_1 + \ldots + \gamma_{m+n} \\
x_{m+n+1} &= x_0 + \gamma_1 + \ldots + \gamma_{m+n} + (\gamma_{n+m+1} - \gamma_{m+1} - \ldots - \gamma_{m+n})
\end{aligned}$$

$$\begin{aligned}
x_{m+n+2} &= x_0 + \gamma_1 + \ldots + \gamma_{m+n} + (\gamma_{n+m+1} - \gamma_{m+1} - \ldots - \gamma_{m+n}) + \gamma_{m+n+2} \\
\ldots \quad & \ldots\ldots\ldots \\
x_{m+n+p} &= x_0 + \gamma_1 + \ldots + \gamma_{m+n} + (\gamma_{n+m+1} - \gamma_{m+1} - \ldots - \gamma_{m+n}) + \gamma_{m+n+2} + \ldots + \gamma_{m+n+p} \\
x_{m+n+p+1} &= x_0 + \gamma_1 + \ldots + \gamma_{m+n} + (\gamma_{n+m+1} - \gamma_{m+1} - \ldots - \gamma_{m+n}) + \gamma_{m+n-2} + \ldots + \gamma_{m+n+p} + (\gamma_{m+n+p+1} - \gamma_{m+n+1} - \ldots - \gamma_{m+n+p}) \\
x_{m+n+p+2} &= x_0 + \gamma_1 + \ldots + \gamma_{m+n} + (\gamma_{n+m+1} - \gamma_{m+1} - \ldots - \gamma_{m+n}) + \gamma_{m+n+2} + \ldots + \gamma_{m+n+p} + (\gamma_{m+n+p+1} - \gamma_{m+n+1} - \ldots - \gamma_{m+n+p}) + \gamma_{m+n+p+2} \\
\ldots \quad & \ldots\ldots\ldots \\
x_t &= x_0 + \gamma_1 + \ldots + \gamma_{m+n} + (\gamma_{n+m+1} - \gamma_{m+1} - \ldots - \gamma_{m+n}) + \gamma_{m+n+2} + \ldots + \gamma_{m+n+p} + (\gamma_{m+n+p+1} - \gamma_{m+n+1} - \ldots - \gamma_{m+n+p}) + \gamma_{m+n+p+2} + \ldots + \gamma_t
\end{aligned} \qquad \text{(A-1)}$$

$$\begin{aligned}
\text{trace } [f] = {} & 2 \sum_i \sum_j a_{ij}[\delta_{j,m+n+1}\Delta_{m+1,i,m+n} + \delta_{j,m+n+p+1}\Delta_{m+n+1,i,m+n+p}] - \sum_{i=1}^{t}\sum_{j=1}^{t}\sum_{k=1}^{t} \\
& [\delta_{i,m+n+1}\Delta_{m+1,j,m+n} + \delta_{i,m+n+p+1}\Delta_{m+n+1,j,m+n+p}]a_{ik} \times \\
& [\delta_{k,m+n+1}\Delta_{m+1,j,m+n} + \delta_{k,m+n+p+1}\Delta_{m+n+1,j,m+n+p}] = \\
& 2\sum_{i=m+1}^{m+n} a_{i,m+n+1} + 2\sum_{i=m+n+1}^{m+n+p} a_{i,m+n+p+1} - na_{m+n+1,m+n+1} - pa_{m+n+p+1,m+n+p+1}
\end{aligned} \qquad \text{(A-2)}$$

For Uniformly Branched Molecules

$$\begin{aligned}
x_1 &= x_0 + \gamma_1 \\
x_2 &= x_0 + \gamma_1 + \gamma_2 \\
\ldots \quad & \ldots\ldots\ldots \\
x_{m+b} &= x_0 + \gamma_1 + \gamma_2 + \ldots + \gamma_m + \gamma_{m+1} + \gamma_{m+2} + \ldots + \gamma_{m+b} \\
x_{m+b+1} &= x_0 + \gamma_1 + \ldots + \gamma_{m+b} + (\gamma_{m+b+1} - \gamma_{m+1} - \ldots - \gamma_{m+b}) \\
x_{m+b+2} &= x_0 + \gamma_1 + \ldots + \gamma_{m+b} + (\gamma_{m+b+1} - \gamma_{m+1} - \ldots - \gamma_{m+b}) + \gamma_{m+b+2} \\
\ldots \quad & \ldots\ldots\ldots \\
x_{2m+b} &= x_0 + \gamma_1 + \ldots + \gamma_{m+b} + (\gamma_{m+b+1} - \gamma_{m+1} - \gamma_{m+2} - \ldots - \gamma_{m+b}) + \gamma_{m+b+2} + \ldots + \gamma_{2m+b} \\
\ldots \quad & \ldots\ldots\ldots \\
x_{2(m+b)} &= x_0 + \gamma_1 + \ldots + \gamma_{m+b} + (\gamma_{m+b+1} - \gamma_{m+1} - \gamma_{m+2} - \ldots - \gamma_{m+b}) + \gamma_{m+b+2} + \ldots + \gamma_{2(m+b)} \\
x_{2(m+b)+1} &= x_0 + \gamma_1 + \ldots + \gamma_{m+b} + (\gamma_{m+b+1} - \gamma_{m+1} - \gamma_{m+2} - \ldots - \gamma_{m+b}) + \gamma_{m+b+2} + \ldots + \gamma_{2(m+b)} + (\gamma_{2(m+b)+1} - \gamma_{2m+b+1} - \gamma_{2m+b+2} - \ldots - \gamma_{2(m+b)}) \\
\ldots \quad & \ldots\ldots\ldots \\
x_{(n+1)m+nb} &= x_0 + \gamma_1 + \ldots + \gamma_{m+b} + (\gamma_{m+b+1} - \gamma_{m+1} - \gamma_{m+2} - \ldots - \gamma_{m+b}) + \gamma_{m+b+2} + \ldots + \gamma_{2(m+b)} + (\gamma_{2(m+b)+1} - \gamma_{2m+b+1} - \gamma_{2m+b+2} - \ldots - \gamma_{2(m+b)}) + \ldots + \gamma_{(n+1)m+nb}
\end{aligned} \qquad \text{(A-3)}$$

$$\begin{aligned}
\text{trace } [f] = {} & 2\sum_{i=1}^{t}\sum_{j=1}^{t}\sum_{k=1}^{n} a_{ij}\delta_{j,k(m+b)+1}\Delta_{k(m+b)-b+1,i,k(m+b)} - \sum_{i=1}^{t}\sum_{j=1}^{t}\sum_{k=1}^{t} \\
& \left\{\left[\sum_{p=1}^{n} \delta_{j,p(m+b)+1}\Delta_{p(m+b)-b+1,i,p(m+b)}\right]a_{jk} \times \left[\sum_{q=1}^{n} \delta_{k,q(m+b)+1}\Delta_{q(m+b)-b+1,i,q(m+b)}\right]\right\} = \\
= {} & \sum_{k=1}^{n} [t - k(m+b)][k(m+b)(b-2) - b(b-2) - 2]
\end{aligned} \qquad \text{(A-4)}$$