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by

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§ 1. Summary.

This work originated in a metallurgical problem, treated in § 5, on the diffusion of electrons in a crystal structure. This problem is a special case of some general theory, developed in §§ 3, 4, on the asymptotic distribution of the sum of a large number of vectors selected from a fixed set of vectors by a Markovian process of finite order. This extends the work of Romanovsky, who treated the corresponding problem for scalars selected by a Markovian process of order unity. Some standard algebraic theory, required for § 3, appears in § 2.

§ 2. Properties of finite constant stochastic matrices.

A *finite constant stochastic matrix* (hereafter called simply a stochastic matrix) is a finite square matrix $\boldsymbol{P}$ with real constant elements p_{jk} $(j, k = 1, 2, \ldots, n)$ satisfying

$$p_{jk} \geqq 0; \sum_{k=1}^{n} p_{jk} = 1; \tag{2.1}$$

that is to say each row-sum of $\boldsymbol{P}$ is unity. A stochastic matrix is *simple* if it has a simple latent root $\lambda = 1$. A *rearrangement* of a matrix is a permutation of its rows accompanied by the *same* permutation of its columns.

THEOREM 2.1. *Let λ be any latent root of a square matrix with (perhaps complex) elements a_{jk} $(j, k = 1, 2, \ldots, n)$; let $\alpha_j = \sum_{k=1}^{n} |\, a_{jk} \,|$; let $\alpha = \max_{1 \leqq j \leqq n} \alpha_j$; and let $\mathfrak{J}$ be the (perhaps empty) set of all integers j such that $\alpha_j < \alpha$. Then $|\, \lambda \,| \leqq \alpha$; and $|\, \lambda \,| = \alpha$ implies the existence of a (possibly empty but otherwise proper) subset $\mathfrak{K}$ of the integers $1, 2, \ldots, n$ such that $\mathfrak{K} \supseteq \mathfrak{J}$ and $a_{jk} = 0$ whenever $j \notin \mathfrak{K}$ and $k \in \mathfrak{K}$.*

THEOREM 2.2. *Any stochastic matrix P has at least one latent root $\lambda = 1$, and all its latent roots satisfy $|\, \lambda \,| \leqq 1$.*

THEOREM 2.3. *If m is the multiplicity of the latent root $\lambda = 1$ of a stochastic matrix $\boldsymbol{P}$, then $\boldsymbol{P}$ can be rearranged into one of the alternative forms*

$$\begin{bmatrix} \boldsymbol{P}_{11} & \boldsymbol{O} & \dots & \boldsymbol{O} \\ \boldsymbol{O} & \boldsymbol{P}_{22} & \dots & \boldsymbol{O} \\ \dots & \dots & \dots & \dots \\ \boldsymbol{O} & \boldsymbol{O} & \dots & \boldsymbol{P}_{mm} \end{bmatrix} \quad \text{or} \quad \begin{bmatrix} \boldsymbol{P}_{11} & \boldsymbol{O} & \dots & \boldsymbol{O} & \boldsymbol{O} \\ \boldsymbol{O} & \boldsymbol{P}_{22} & \dots & \boldsymbol{O} & \boldsymbol{O} \\ \dots & \dots & \dots & \dots & \dots \\ \boldsymbol{O} & \boldsymbol{O} & \dots & \boldsymbol{P}_{mm} & \boldsymbol{O} \\ \boldsymbol{P}_{m+1,1} & \boldsymbol{P}_{m+1,2} & \dots & \boldsymbol{P}_{m+1,m} & \boldsymbol{P}_{m+1,m+1} \end{bmatrix} \tag{2.2}$$

where $\boldsymbol{P}_{jj}$ $(j = 1, 2, \dots, m)$ is a simple stochastic matrix, and the latent roots λ of $P_{m+1,m+1}$ satisfy $|\lambda| < 1$.

These results are standard, being either explicit or more or less implicit in the work of Frobenius [1], Romanovsky [2], and Brauer [3]. However to save the reader, who is not already familiar with these results, the trouble of extracting them from amongst the lengthier and more complete treatments cited above, we prove them here.

In Theorem 2.1, corresponding to the latent root λ there is a non-null row-vector $(x_1, x_2, \dots, x_n)$ such that

$$\lambda x_k = \sum_{j=1}^{n} x_j a_{jk}. \tag{2.3}$$

Hence

$$\begin{aligned} |\lambda| \sum_{j=1}^{n} |x_j| &= \sum_{k=1}^{n} |\lambda x_k| = \sum_{k=1}^{n} \Big| \sum_{j=1}^{n} x_j a_{jk} \Big| \\ \leqq \sum_{j=1}^{n} \sum_{k=1}^{n} |x_j|\,|a_{jk}| &= \sum_{j=1}^{n} |x_j| \alpha_j \leqq \alpha \sum_{j=1}^{n} |x_j|; \end{aligned} \tag{2.4}$$

and $|\lambda| \leqq \alpha$ follows from $\sum_{j=1}^{n} |x_j| > 0$. For the remainder of the theorem we may suppose that $\mathfrak{J}$ is not empty, else we could take $\mathfrak{K}$ empty too. Then $\alpha > 0$. If $|\lambda| = \alpha$, the quantities of (2.4) are equal; and the last two quantities show that $x_j = 0$ for $j \in J$. Take $\mathfrak{K}$ to be the set of all j such that $x_j = 0$. Then $\mathfrak{K} \supseteq \mathfrak{J}$ and is a proper subset of $1, 2, \dots, n$ because $(x_1, x_2, \dots, x_n)$ is non-null. Since $j \notin \mathfrak{K}$ implies $j \notin \mathfrak{J}$, it also implies $\alpha_j = \alpha$; and so (2.3) yields

$$\begin{aligned} \alpha \sum_{j \notin \mathfrak{K}} |x_j| &= \sum_{k \notin \mathfrak{K}} |\lambda x_k| = \sum_{k \notin \mathfrak{K}} \Big| \sum_{j=1}^{n} x_j a_{jk} \Big| = \sum_{k \notin \mathfrak{K}} \Big| \sum_{j \notin \mathfrak{J}} x_j a_{jk} \Big| \\ &\leqq \sum_{j \notin \mathfrak{K}} |x_j| \sum_{k \notin \mathfrak{K}} |a_{jk}| = \sum_{j \notin \mathfrak{K}} |x_j| \Big(\alpha_j - \sum_{k \in \mathfrak{K}} |a_{jk}|\Big) = \\ &\qquad \alpha \sum_{j \notin \mathfrak{K}} |x_j| - \sum_{j \notin \mathfrak{K}} \sum_{k \in \mathfrak{K}} |x_j|\,|a_{jk}|. \end{aligned}$$

This completes Theorem 2.1, since $|x_j| > 0$ for $j \notin \mathfrak{K}$. The last part of Theorem 2.2 is a particular case of the first part of Theorem

2.1, in view of (2.1); and the first part of Theorem 2.2 is obvious, since the row-sums of $I - P$ are zero.

In proving Theorem 2.3, we neglect the trivial case $m = 1$. Then $n \geqq m \geqq 2$; and adj $(\lambda I - P)$ exists. Let $f_{jk}(\lambda)$ be the (j, k)-element of adj $(\lambda I - P)$, and let $f(\lambda) = |\lambda I - P|$. Since $f_{jj}(\lambda)$ is a real continuous function of real λ which is positive for large positive λ we have

$$f_{jj}(\lambda) \geqq 0, \quad \lambda \geqq 1; \tag{2.5}$$

for otherwise, in contradiction of Theorem 2.1, the complementary minor of p_{jj} in P would have a latent root $\lambda > 1$. On the other hand, since $m \geqq 2$,

$$\sum_{j=1}^{n} f_{jj}(1) = \left[\frac{\partial f(\lambda)}{\partial \lambda}\right]_{\lambda=1} = 0. \tag{2.6}$$

Combining this with (2.5) we have $f_{jj}(1) = 0$, $j = 1, 2, \ldots, n$. We assert that for $\lambda = 1$ we can find a latent column-vector $\{x_1, x_2, \ldots, x_n\}$ of P, whose elements x_j are real and not all equal. This is obvious if the rank of $I - P$ is less than $n - 1$. Since $|I - P| = 0$, there only remains the case in which the rank of $I - P$ is $n - 1$, i.e. when there is some non-zero element $f_{j'k'}(1)$. In this case we may take $x_k = f_{j'k}(1)$, $k = 1, 2, \ldots, n$, according to the rule of false cofactors; and we shall ensure $0 = x_{j'} \neq x_{k'}$. Therefore in any case we may divide the integers $1, 2, \ldots, n$ into two *non-empty* classes $j \in \mathfrak{J}$ if $x_j = \min_{1 \leqq j \leqq n} x_j$ and $j \in \mathfrak{K}$ if $x_j > \min_{1 \leqq j \leqq n} x_j$. Then by (2.1)

$$0 = x_j - \sum_{k=1}^{n} p_{jk} x_k = \sum_{k=1}^{n} p_{jk}(x_j - x_k) = \sum_{k \in \mathfrak{K}} p_{jk}(x_j - x_k), \quad j \in \mathfrak{J};$$

and therefore, because $x_j - x_k < 0$ for $j \in \mathfrak{J}$, $k \in \mathfrak{K}$, (2.1) yields

$$p_{jk} = 0, \quad j \in \mathfrak{J}, \quad k \in \mathfrak{K}. \tag{2.7}$$

Now let i be the maximum integer such that P can be written in the form

$$\begin{bmatrix} Q_{11} & O & \ldots & O \\ Q_{21} & Q_{22} & \ldots & O \\ \ldots & \ldots & \ldots & \ldots \\ Q_{i1} & Q_{i2} & \ldots & Q_{ii} \end{bmatrix}, \tag{2.8}$$

where the partitioning of rows is the same as the partitioning of columns in (2.8), and all possible rearrangements of P are considered in arriving at (2.8). We have $i \geqq 2$, by (2.7). We assert that, if Q_{jj} has a latent root λ satisfying $|\lambda| = 1$, then $Q_{jk} = 0$ for $k = 1, 2, \ldots, j - 1$. For the row sums of Q_{jj} cannot exceed unity;

and hence, by Theorem 2.1, there exists a maximal non-empty set $\mathfrak{L}$ of the rows of $\boldsymbol{Q}_{jj}$ such that the elements of each member of $\mathfrak{L}$ sum to unity. Let $\mathfrak{J}'$ be the set of rows of $\boldsymbol{Q}_{jj}$ which do not belong to $\mathfrak{L}$. Suppose (for the sake of a contradiction) that $\mathfrak{J}'$ is not empty. Then, by Theorem 2.1, there exists a proper subset $\mathfrak{K}'$ of the rows of $\boldsymbol{Q}_{jj}$ such that $\mathfrak{K}' \supseteq \mathfrak{J}'$ and the elements q_{jk} of $\boldsymbol{Q}_{jj}$ satisfy $q_{jk} = 0$ for $j \notin \mathfrak{K}'$, $k \in \mathfrak{K}'$; whereupon we can rearrange $\boldsymbol{P}$ by permuting those rows which intersect $\boldsymbol{Q}_{jj}$, and thereby increase i to $i + 1$. This is a contradiction because i is maximal. Thus $\mathfrak{J}'$ is empty, and the assertion follows from (2.1). Hence $\boldsymbol{Q}_{jj}$ is a stochastic matrix if it has a latent root $|\lambda| = 1$; and it must also be a simple stochastic matrix, otherwise (2.7) would operate to show that i was not maximal. Now rearrange the partitional blocks of (2.8) so that rows which intersect a $\boldsymbol{Q}_{jj}$ having $|\lambda| = 1$ precede all other rows (if any). Then $\boldsymbol{P}$ takes one of the forms (2.2); and the theorem is complete because rearrangement will not alter the multiplicity of the latent root $\lambda = 1$.

§ 3. Markovian interstate distributions.

Suppose that a system is restricted to a finite number of states $S_0, S_1, \ldots, S_{t-1}$, that it passes from state to state at consecutive instants, and that, N being a fixed integer, there is a constant probability $p_{j_1 j_2 \ldots j_N k}$ that the system will pass into S_k when it is known to have just occupied $S_{j_1}, S_{j_2}, \ldots, S_{j_N}$ in that order. The system is then said to follow an N-th *order finite constant Markovian process*, hereafter denoted by $\mathfrak{M}_N$. Let ν_j denote the number of instants at which the system occupies S_j, when a total of $\nu = \sum_{j=1}^{n} \nu_j$ consecutive instants are considered. The joint distribution of the random variables ν_j is termed the *interstate distribution* of the $\mathfrak{M}_N$; and we shall determine it asymptotically for large ν. With $\mathfrak{M}_N$ we associate a stochastic matrix $\boldsymbol{P}$, whose rows and columns are numbered in t-ary digit scale from 0 to $n - 1 = t^N - 1$. The element p_{jk} of $\boldsymbol{P}$ is

$$p_{jk} = \begin{cases} p_{j_1 j_2 \ldots j_N k_N} & \text{if } [j_2 j_3 \ldots j_N] = [k_1 k_2 \ldots k_{N-1}] \\ 0 & \text{otherwise} \end{cases} \tag{3.1}$$

where $j = [j_1 j_2 \ldots j_N]$, $k = [k_1 k_2 \ldots k_N]$ are the expressions of j and k in the scale of t. We say that $\mathfrak{M}_N$ is *simple* if $\boldsymbol{P}$ is a simple stochastic matrix.

With a simple stochastic matrix $\boldsymbol{P}$ we associate a column vector $\boldsymbol{m}$ and a square matrix $\boldsymbol{M}$ as follows:— Let π_{jk} denote the value

of the determinant obtained by deleting from $\boldsymbol{I} - \boldsymbol{P}$ its jth and kth rows and its jth and kth columns. In case this process breaks down because there are no surviving rows and columns, we define $\pi_{jk} = 1$. Now set

$$m_{jk} = \pi_{jk} \Big| \sum_{j=1}^{n} \pi_{jj}. \tag{3.2}$$

This formula is not nugatory, because, $\boldsymbol{P}$ being simple, (2.6) cannot apply. We take $\boldsymbol{m} = \{m_{11}, m_{22}, \ldots, m_{nn}\}$, and $\boldsymbol{M}$ for the matrix with elements m_{jk} $(j, k = 1, 2, \ldots, n)$. Let $\boldsymbol{u}$ be the n-rowed column vector $\{1, 1, \ldots, 1\}$; and let $\boldsymbol{K}$ be the $(t \times n)$-matrix $(\boldsymbol{I}, \boldsymbol{I}, \ldots, \boldsymbol{I})$. Write $\boldsymbol{v} = \boldsymbol{Km}$, and $\boldsymbol{V} = (\boldsymbol{K} - \boldsymbol{vu}')\boldsymbol{M}(\boldsymbol{uv}' - \boldsymbol{K}')$.

THEOREM 3.1. *The interstate distribution of a simple $\mathfrak{M}_N$ with stochastic matrix $\boldsymbol{P}$ is asymptotically normal as $v \to \infty$, having mean $v\boldsymbol{v}$ and variance-covariance $v\boldsymbol{V}$, independently of the initial state.*

The transformation (3.1) takes the given $\mathfrak{M}_N$ with states $S_0, S_1, \ldots, S_{t-1}$ into an $\mathfrak{M}_1$ with states $\mathfrak{S}_0, \mathfrak{S}_1, \mathfrak{S}_{n-1}$. Let p_{j_0} denote the probability that this $\mathfrak{M}_1$ is in $\mathfrak{S}_{j_0}$ after the first N instants. The probability that it then passes successively through $\mathfrak{S}_{j_0} \to \mathfrak{S}_{j_1} \to \ldots \to \mathfrak{S}_{j_v}$ is $p_{j_0}p_{j_0j_1}p_{j_1j_2}\ldots p_{j_{v-1}j_v}$; and hence the joint characteristic function of the variates v_j of $\mathfrak{M}_1(\mathfrak{S}_j)$ is

$$\phi_v(t) = \phi_v(t_0, t_1, \ldots, t_{n-1}) = \Sigma p_{j_0}p_{j_0j_1}p_{j_1j_2}\ldots p_{j_{v-1}j_v} \exp\{i(t_{j_0} + t_{j_1} + \ldots + t_{j_v})\},$$

where the sum is taken over all $j_0, j_1, \ldots, j_v = 0, 1, \ldots, n-1$. Define $\boldsymbol{Q}(t)$ to be the matrix with elements $q_{jk} = p_{jk}\exp(it_k)$, $(j, k = 0, 1, \ldots, n-1)$, and $\boldsymbol{q}(t)$ be the column-vector with elements $p_j\exp(it_j)$. Then

$$\phi_v(t) = [\boldsymbol{q}(t)]'\,[\boldsymbol{Q}(t)]^v\boldsymbol{u}. \tag{3.3}$$

Hereafter we suppose throughout that t is a real vector.

Let $\boldsymbol{x} = \{x_0, x_1, \ldots, x_{n-1}\}$ be an arbitrary column-vector, and write $\| \boldsymbol{x} \|$ for the non-negative square root of $\sum_{j=0}^{n-1} | x_j |^2$. Since $| x_j |^2 \leqq \| x \|^2$, $p_{jk} \geqq 0$ and $\sum_{k=0}^{n-1} p_{jk} = 1$, we have for any positive integer v

$$\begin{aligned}
\big\| [\boldsymbol{Q}(t)]^v \boldsymbol{x} \big\|^2 &= \sum_{j=0}^{n-1} \big| \Sigma' p_{jk_1}p_{k_1k_2}\ldots p_{k_{v-1}k_v}x_{k_v} \exp\{i(t_{k_1} + t_{k_2} + \ldots + t_{k_v})\} \big|^2 \\
&\leqq \sum_{j=0}^{n-1} (\Sigma' p_{jk_1}p_{k_1k_2}\ldots p_{k_{v-1}k_v} \mid x_{k_v} |)^2 \\
&\leqq \| x \|^2 \sum_{j=0}^{n-1} (\Sigma' p_{jk_1}p_{k_1k_2}\ldots p_{k_{v-1}k_v})^2 = \| x \|^2 \sum_{j=0}^{n-1} 1^2 = n \| x \|^2,
\end{aligned}$$

in which Σ' denotes summation over $k_1, k_2, \ldots, k_v = 0, 1, \ldots,$

$n - 1$. Thus

$$|| [Q(t)]^\nu x || \leqq n^{\frac{1}{2}} || x ||. \tag{3.4}$$

As a matter of passing interest, this is a best possible inequality.

Let $\lambda_j^*(t)$ denote the latent roots of $Q(t)$ with due regard to multiplicity. By Theorem 2.1, $| \lambda_j^*(t) | \leqq 1$; and so each $\lambda_j^*(t)$ is a bounded root of a polynomial equation, whose coefficients are continuous functions of t. Therefore there exists a set of n one-valued continuous functions $\lambda_j(t)$ such that, for each fixed t, the numbers λ_j^* are a permutation of the numbers λ_j. Thus $\lim_{t \to 0} \lambda_j(t) = \lambda_j$ are the latent roots of P; and, since P is simple, there is precisely one of these functions, which without loss of generality we denote by $\lambda_0(t)$, such that

$$\lim_{t \to 0} \lambda_0(t) = 1; \quad \lambda_j(t) \neq \lambda_0(t), \quad j \neq 0, \quad t \in \mathfrak{T} \tag{3.5}$$

for some sufficiently small open neighbourhood $\mathfrak{T}$ of $t = O$. Now (3.5) shows that the rank of $(Q(t) - \lambda_0(t)I)$ is precisely $n - 1$ for $t \in \mathfrak{T}$; and therefore there exists a unique continuous column-vector $u_0(t)$ satisfying

$$\left.\begin{aligned} [Q(t) - \lambda_0(t)I]\, u_0(t) = O, \ t \in \mathfrak{T} \\ \lim_{t \to 0} u_0(t) = u \end{aligned}\right\}, \tag{3.6}$$

for $Pu = u$. Thus (3.4) and (3.6) yield for any fixed t

$$0 \leqq \limsup_{\nu \to \infty} \left\| [Q(\nu^{-\frac{1}{2}}t)]^\nu [u_0(\nu^{-\frac{1}{2}}t) - u] \right\| \leqq \limsup_{\nu \to \infty} n^{\frac{1}{2}} \left\| u_0(\nu^{-\frac{1}{2}}t) - u \right\| = 0;$$

whereupon

$$\begin{aligned} O &= \lim_{\nu \to \infty} [Q(\nu^{-\frac{1}{2}}t)]^\nu [u_0(\nu^{-\frac{1}{2}}t) - u] = \\ &= \lim_{\nu \to \infty} \{[\lambda_0(\nu^{-\frac{1}{2}}t)]^\nu u_0(\nu^{-\frac{1}{2}}t) - [Q(\nu^{-\frac{1}{2}}t)]^\nu u\} = \\ &= \lim_{\nu \to \infty} \{[\lambda_0(\nu^{-\frac{1}{2}}t)]^\nu u - [Q(\nu^{-\frac{1}{2}}t)]^\nu u\}. \end{aligned}$$

Premultiply this last relationship by $\lim_{\nu \to \infty} [q(\nu^{-\frac{1}{2}}t)]' = (p_0, p_1, \ldots, p_{n-1}) = p'$, notice that $p'u = 1$, use (3.3), and deduce

$$\lim_{\nu \to \infty} \{\phi_\nu(\nu^{-\frac{1}{2}}t) - [\lambda_0(\nu^{-\frac{1}{2}}t)]^\nu\} = 0. \tag{3.7}$$

Setting D for the diagonal matrix with elements e^{-it_j}, $(j = 0, 1, \ldots, n - 1)$, we can write the characteristic equation of $Q(t)$ in the form

$$\dot{0}=g=|I-Q(t)||D|=\begin{vmatrix} \lambda e^{-it_0}-p_{00} & -p_{01}\cdots & -p_{0,n-1} \\ -p_{10} & \lambda e^{it_1}-p_{11}\cdots & -p_{1,n-1} \\ \cdots\cdots & \cdots\cdots & \cdots\cdots \\ -p_{n-1,0} & -p_{n-1,1}\cdots & \lambda e^{-it_{n-1}}-p_{n-1,n-1} \end{vmatrix} \tag{3.8}$$

Row-by-row differentiation of (3.8) yields

$$g_j=\left[\frac{\partial g}{\partial t_j}\right]_{\substack{t=0\\ \lambda=1}}=-i\pi_{jj};\quad g_\lambda=\left[\frac{\partial g}{\partial \lambda}\right]_{\substack{t=0\\ \lambda=1}}=\sum_{j=0}^{n-1}\pi_{jj};$$

$$g_{jk}=\left[\frac{\partial^2 g}{\partial t_j \partial t_k}\right]_{\substack{t=0\\ \lambda=1}}=-\pi_{jk};\quad g_{\lambda j}=\left[\frac{\partial^2 g}{\partial \lambda \partial t_j}\right]_{\substack{t=0\\ \lambda=1}}=-i\sum_{k=0}^{n-1}\pi_{jk};$$

$$g_{\lambda\lambda}=\left[\frac{\partial^2 g}{\partial \lambda^2}\right]_{\substack{t=0\\ \lambda=1}}=\sum_{j,k=0}^{n-1}\pi_{jk}-\sum_{j=0}^{n-1}\pi_{jj}.$$

Since g is differentiable as many times as we please and $\partial g/\partial\lambda \neq 0$ for $t \in \mathfrak{T}$, we may appeal to the implicit function theorem to obtain

$$\lambda_0(t)=1+\sum_{j=0}^{n-1}\left(-\frac{g_j}{g_\lambda}\right)t_j+\frac{1}{2}\sum_{j,k=0}^{n-1}\left(-\frac{g_{\lambda\lambda}g_jg_k}{g_\lambda^3}+\frac{g_{\lambda j}g_k+g_{\lambda k}g_j}{g_\lambda^2}-\frac{g_{jk}}{g_\lambda}\right)t_jt_k+0(||t||^3)$$

$$=1+i\sum_{j=0}^{n-1}m_{jj}t_j+\frac{1}{2}\sum_{j,k=0}^{n-1}t_jt_k\left\{m_{jk}-\sum_{\alpha=0}^{n-1}(m_{jj}m_{k\alpha}+m_{kk}m_{j\alpha})\right.$$

$$\left.-\left(1-\sum_{\alpha,\beta=0}^{n-1}m_{\alpha\beta}\right)m_{jj}m_{kk}\right\}+O(||t||^3),\ t\in\mathfrak{T}.$$

Then (3.7) provides

$$\lim_{\nu\to\infty}e^{-im't\sqrt{\nu}}\emptyset_\nu(\nu^{-\frac{1}{2}}t)=\lim_{\nu\to\infty}\left\{1-\frac{1}{2\nu}\sum_{j,k=0}^{n-1}t_jt_k\left[\sum_{\alpha=0}^{n-1}(m_{jj}m_{k\alpha}+m_{kk}m_{j\alpha})\right.\right.$$

$$\left.\left.-m_{jk}-m_{jj}m_{kk}\sum_{\alpha,\beta=0}^{n-1}m_{\alpha\beta}\right]+0(\nu^{-3/2})\right\}^\nu$$

$$=\exp\{-\tfrac{1}{2}t'(I-mu')M(um'-I)t\}.$$

The theorem is now completed by taking the inverse Fourier transform of this last relation and then by means of the transformation K, condensing the states $\mathfrak{S}_j$ to S_j by enumerating the former in terms of the last t-ary digit of their suffices. In the course of the foregoing proof we have been entitled to make no distinction between ν and $\nu+N$, since these quantities are asymptotically equivalent. The normal distribution just obtained is singular, because $\nu=\Sigma\nu_j$: this we may see otherwise in terms of the identities $m'u=1$, $(I-mu')M(um'-I)u=O$.

Turning now to the case when $\mathfrak{M}_N$ is not simple, we first permute the suffices of $\mathfrak{S}_j$ and thereby rearrange P into the form

(2.2). Let $\mathfrak{S}_j^*$ $(j = 1, 2, \ldots, m)$ denote the aggregate of states $\mathfrak{S}_j$ which correspond to rows of $\boldsymbol{P}_{jj}$ in the rearrangement; and let $\mathfrak{S}_j^{**}$ $(j = 1, 2, \ldots, 1)$ denote the remaining $\mathfrak{S}_j$ (if any) corresponding to the rows of $\boldsymbol{P}_{m+1,\,m+1}$. Then the transition matrix for the states $\mathfrak{S}^*$ and $\mathfrak{S}^{**}$ is

$$\boldsymbol{P}^* = \begin{pmatrix} 1 & 0 & 0 & \ldots & 0 & \boldsymbol{O} \\ 0 & 1 & 0 & \ldots & 0 & \boldsymbol{O} \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & 0 & \ldots & 1 & \boldsymbol{O} \\ \boldsymbol{r}_1 & \boldsymbol{r}_2 & \boldsymbol{r}_3 & \ldots & \boldsymbol{r}_m & \boldsymbol{R} \end{pmatrix}$$

in which $\boldsymbol{R} = \boldsymbol{P}_{m+1,\,m+1}$ and $\boldsymbol{r}_j$ is a column-vector composed of the row-sums of $\boldsymbol{P}_{m+1,\,j}$. (In case $\boldsymbol{P}_{m+1,\,m+1}$ does not exist, we take $\boldsymbol{R} = \boldsymbol{O}$, $\boldsymbol{r}_j = \boldsymbol{O}$). Let p_j^* denote the probability that the system starts in $\mathfrak{S}_j^*$ and p_j^{**} the probability that the system starts in $\mathfrak{S}_j^{**}$ (In case $\boldsymbol{P}_{m+1,\,m+1}$ does not exist, we take $p_j^{**} = 0$). The corresponding probabilities after ν steps are

$$p_{j\nu}^* = p_{j,\,\nu-1}^* + \boldsymbol{q}_{\nu-1}'\boldsymbol{r}_j;\ \boldsymbol{q}_\nu' = \boldsymbol{q}_{\nu-1}'\boldsymbol{R};\ \boldsymbol{q}_\nu = \{p_{1\nu}^{**}, p_{2\nu}^{**}, \ldots, p_{1\nu}^{**}\};$$

whence

$$\boldsymbol{q}_\nu' = \boldsymbol{q}'\boldsymbol{R}^\nu;\ p_{j\nu}^* = p_j^* + \boldsymbol{q}'(\boldsymbol{R}^{\nu-1} + \boldsymbol{R}^{\nu-2} + \ldots + \boldsymbol{I})\boldsymbol{r}_j.$$

Since all the latent roots of $\boldsymbol{R}$ are less than unity in modulus, we have

$$\lim_{\nu\to\infty} p_{j\nu}^* = p_j^* + \boldsymbol{q}'(\boldsymbol{I} - \boldsymbol{R})^{-1}\boldsymbol{r}_j,\ \lim_{\nu\to\infty} \boldsymbol{q}_\nu' = \boldsymbol{O}.$$

Let $\boldsymbol{m}_j$, $\boldsymbol{u}_j$, $\boldsymbol{M}_j$ denote the values of $\boldsymbol{m}$, $\boldsymbol{u}$, $\boldsymbol{M}$ for $\boldsymbol{P}_{jj}$. Then in the rearrangement of $\mathfrak{S}_j$ the interstate distribution is the weighted mean of m normal distributions, the jth distribution having mean $\nu\boldsymbol{m}_j$, variance $\nu(\boldsymbol{I} - \boldsymbol{m}_j\boldsymbol{u}_j')\boldsymbol{M}_j(\boldsymbol{u}_j\boldsymbol{m}_j' - \boldsymbol{I})$, and weight $p_j^* + \boldsymbol{q}'(\boldsymbol{I} - \boldsymbol{R})^{-1}\boldsymbol{r}_j$. To obtain the required interstate distribution we must transform this by $\boldsymbol{K}^*$, the column permutation of $\boldsymbol{K}$ corresponding to the rearrangement of $\boldsymbol{P}$. We obtain

THEOREM 3.2. *The interstate distribution of a general $\mathfrak{M}_N$, as $\nu \to \infty$, is asymptotically the weighted mean of a finite number of normal distributions specified above.*

§ 4. Abstract crystals.

This section consists largely of definitions. They are framed to give, on the one hand, sufficient generality to deal with most applied mathematical problems, which may fall within the present subject matter; but, on the other hand, they avoid the pathological difficulties which would be the result of a completely general pure mathematical approach.

A *directed linear graph* (hereafter called simply a graph) is a countable (i.e. finite or enumerably infinite) aggregate of *points* and *bonds*: the points are points $P_1, P_2, \ldots$ of an abstract space $\mathfrak{S}$, and the bonds are directed paths joining certain pairs of (not necessarily distinct) points. If there is a bond from P_j to P_k, we denote it by P_jP_k and say that P_jP_k exists. The existence of P_jP_k does not necessarily imply the existence of P_kP_j. We write $\mathfrak{G} = \mathfrak{G}(P_j, \mathfrak{S})$ for such a graph.

A random walk on a graph $\mathfrak{G}$ is the motion of a particle which, at each of a sequence of discrete instants, steps in a random fashion from point to point of $\mathfrak{G}$ along the directed bonds of $\mathfrak{G}$. We write $\mathfrak{W}[\mathfrak{G}(P_j, \mathfrak{S})]$ for such a walk. We also write $\pi_K\{\mathfrak{P}_j \to \mathfrak{P}_k \mid \mathfrak{W}[\mathfrak{G}(P_j, \mathfrak{S})]\}$ for the probability that at the Kth instant of $\mathfrak{W}[\mathfrak{G}(P_j, \mathfrak{S})]$ the particle steps from some point of the set $\mathfrak{P}_j$ to some point of the set $\mathfrak{P}_k$.

A graph $\mathfrak{G}^*(P_j^*, \mathfrak{S}^*)$ is called a *homomorph* of $\mathfrak{G}(P_j, \mathfrak{S})$ if there exists a one-valued transformation $H(P_j) = P_j^*$ such that the existence of $P_j^*P_k^*$ implies the existence of P_jP_k. We then write $H(\mathfrak{G}) = \mathfrak{G}^*$. We also write $H^{-1}(\mathfrak{P}^*)$ for the set of all points P of $\mathfrak{S}$ which map into a given set $\mathfrak{P}^*$ of $\mathfrak{S}^*$ under H. The random walk $\mathfrak{W}^*(\mathfrak{G}^*)$ on $\mathfrak{G}^* = H(\mathfrak{G})$ is called a *probability homomorph* of $\mathfrak{W}(\mathfrak{G})$, written $\mathfrak{W}^* = H(\mathfrak{W})$, if and only if

$$\pi_K\{H^{-1}(\mathfrak{P}_j^*) \to H^{-1}(P_k^*) \mid \mathfrak{W}[\mathfrak{G}(P_j, \mathfrak{S})]\} = \\ = \pi_K\{\mathfrak{P}_j^* \to \mathfrak{P}_k^* \mid \mathfrak{W}^*[\mathfrak{G}^*(P_j^*, \mathfrak{S}^*)]\}$$

for all K, $\mathfrak{P}_j$, $\mathfrak{P}_k$.

Let $\mathfrak{S}$ be a vector space with a vector basis $\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots$; so that with $\boldsymbol{x} = \Sigma_j \alpha_j \boldsymbol{x}_j$ the scalar coordinates of a general point $\boldsymbol{x}$ are $\alpha_1, \alpha_2, \ldots$ For any arbitrary set of (positive, negative, or zero) integers $\beta_1, \beta_2, \ldots$, the transformation $\Sigma_j \alpha_j \boldsymbol{x}_j \to \Sigma_j(\alpha_j + \beta_j)\boldsymbol{x}_j$ is called an integral shift. Points of $\mathfrak{S}$ which can be transformed into each other by suitable integral shifts are called congruent. The set of all points $\boldsymbol{x} = \Sigma_j \alpha_j \boldsymbol{x}_j$, $0 \leqq \alpha_j < 1$ is called the fundamental cell of $\mathfrak{S}$. A *lattice* $\mathfrak{L}$ is a graph of $\mathfrak{S}$ with the three properties

(i) $\mathfrak{L}$ is invariant under all integral shifts as regards both its points and its bonds,

(ii) the set $\mathfrak{B}$ of all points of $\mathfrak{L}$ in the fundamental cell is finite, and

(iii) the set $\mathfrak{V}$ of all bonds of $\mathfrak{L}$ directed *from* points of the fundamental cell is finite.

Let $B_0, B_1, \ldots, B_{t-1}$ be the points of $\mathfrak{B}$ and $\boldsymbol{v}_0, \boldsymbol{v}_1, \ldots, \boldsymbol{v}_{s-1}$ be the distinct displacement vectors representing the directed bonds of $\mathfrak{V}$. The set of all points congruent to B_j is denoted by S_j, called

the jth *point-state* of the lattice. A walk $\mathfrak{W}[\mathfrak{L}]$ is called Markovian and denoted by $\mathfrak{M}_N[\mathfrak{L}]$ if it is an $\mathfrak{M}_N$ on the S_j.

A homomorph of a lattice is called a *crystal*. A *Markovian walk on a crystal* $\mathfrak{C} = H(\mathfrak{L})$, denoted by $\mathfrak{M}_N[\mathfrak{C}]$, is any $H(\mathfrak{M}_N[\mathfrak{L}])$. The problem is to determine the asymptotic distribution of the point reached by an $\mathfrak{M}_N(\mathfrak{C})$ after a large number ν of steps.

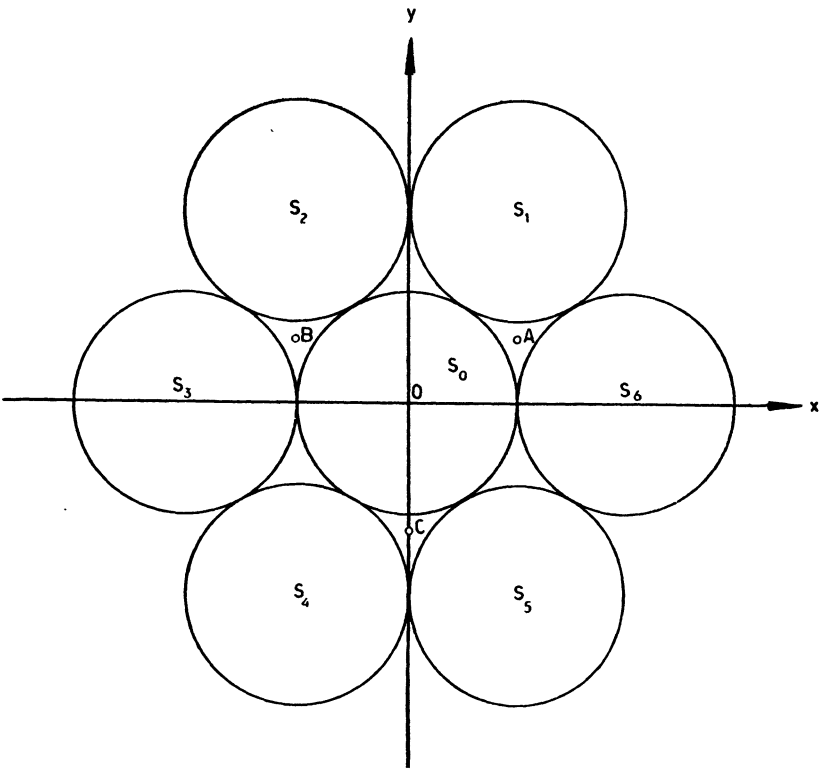
If $\mathfrak{X}$ and $\mathfrak{Y}$ are finite sets of objects x_j and y_k respectively, their direct product set $\mathfrak{X} \times \mathfrak{Y}$ is the set of all pairs (x_j, y_k). We also define $\mathfrak{X}^{(l)} = \mathfrak{X} \times \mathfrak{X}^{(l-1)}$, $\mathfrak{X}^{(1)} = \mathfrak{X}$. In place of $\mathfrak{M}_N[\mathfrak{C}]$ consider an $\mathfrak{M}_1$ on $\mathfrak{T} = \mathfrak{S}^{(N)} \times \mathfrak{V}$, where $\mathfrak{S}$ is the set of S_j for an $\mathfrak{L}$ such that $\mathfrak{C} = H(\mathfrak{L})$. By admitting zero probabilities wherever necessary we can obviously choose this $\mathfrak{M}_1$ so that it is homomorphic in probability with the $\mathfrak{M}_N[\mathfrak{L}]$ satisfying $H(\mathfrak{M}_N[\mathfrak{L}]) = \mathfrak{M}_N[\mathfrak{C}]$; for $\mathfrak{T}$ exhausts all states of the $\mathfrak{M}_N[\mathfrak{L}]$. According to § 3 we can find the asymptotic interstate distribution of $\mathfrak{T}$; and then condense $\mathfrak{T}$ onto $\mathfrak{V}$. This will give the interstate distribution on $\mathfrak{V}$; and hence, since $\mathfrak{L}$ is a lattice, the asymptotic distribution of terminal position on $\mathfrak{L}$. The required result then follows by mapping this distribution under H.

We illustrate this theory with a simple example.

§ 5. Practical application.

In a certain metallic structure the atoms may be considered as contiguous spheres all of equal radius. These spheres lie in layers as shown in the diagram. In a given layer, a given atom S_0 is touched by six neighbours S_j ($j = 1, 2, \ldots, 6$) as shown, the centres lying in the plane $0xy$. The layer which lies above this layer is similar in structure and orientation, but has suffered a displacement in the $0y$ direction, so that the centres of three of its spheres lie above the points A, B, C in such a way that the sphere (centred above A for example) touches the spheres S_0, S_1, S_6. The layer in the $0xy$ plane may be termed an even layer, and the one above it an odd layer. The complete three-dimensional structure then consists of even and odd layers stacked alternately. A particle starts at one atom and moves from atom to atom in a sequence of steps. At any step it may move to a contiguous sphere, so that it has 12 available possibilities for each step. The probability that it will make a step to any one of the six atoms in the same layer is $p/6$, and the probability that it will step to any one of the six atoms in the layers above and below is $q/6$, where p and q are given and $p + q = 1$. The probabilities of successive choices amongst the 12 available are independent. The problem is to determine the distribution of the final position after a large number ν of steps.

Taking right-handed axes as shown in the diagram the steps and their probabilities may be represented by the following displacement vectors (where we take the radius of a sphere to be 3):—



Particle stepping from even layer				Particle stepping from odd layer			
	Vector		Probability		Vector		Probability
v_1	$(+6, 0, 0)$		$p/6$	v_7	$(+6, 0, 0)$		$p/6$
v_2	$(+3, +3\sqrt{3}, 0)$		$p/6$	v_8	$(+3, +3\sqrt{3}, 0)$		$p/6$
v_3	$(-3, +3\sqrt{3}, 0)$		$p/6$	v_9	$(-3, +3\sqrt{3}, 0)$		$p/6$
v_4	$(-6, 0, 0)$		$p/6$	v_{10}	$(-6, 0, 0)$		$p/6$
v_5	$(-3, -3\sqrt{3}, 0)$		$p/6$	v_{11}	$(-3, -3\sqrt{3}, 0)$		$p/6$
v_6	$(+3, -3\sqrt{3}, 0)$		$p/6$	v_{12}	$(+3, -3\sqrt{3}, 0)$		$p/6$
v_{13}	$(+3, +\sqrt{3}, +2\sqrt{6})$		$q/6$	v_{19}	$(-3, -\sqrt{3}, -2\sqrt{6})$		$q/6$
v_{14}	$(-3, +\sqrt{3}, +2\sqrt{6})$		$q/6$	v_{20}	$(+3, -\sqrt{3}, -2\sqrt{6})$		$q/6$
v_{15}	$(0, -2\sqrt{3}, +2\sqrt{6})$		$q/6$	v_{21}	$(0, +2\sqrt{3}, -2\sqrt{6})$		$q/6$
v_{16}	$(+3, +\sqrt{3}, -2\sqrt{6})$		$q/6$	v_{22}	$(-3, -\sqrt{3}, +2\sqrt{6})$		$q/6$
v_{17}	$(-3, +\sqrt{3}, -2\sqrt{6})$		$q/6$	v_{23}	$(+3, -\sqrt{3}, +2\sqrt{6})$		$q/6$
v_{18}	$(0, -2\sqrt{3}, -2\sqrt{6})$		$q/6$	v_{24}	$(0, +2\sqrt{3}, +2\sqrt{6})$		$q/6$

A little reflection will show that the steps $v_1, v_2, \ldots, v_6$ cannot follow immediately after the steps $v_7, v_8, \ldots, v_{18}$. This together with 7 similar considerations shows that the stochastic matrix of the transitions amongst the 24 displacement vectors is

$$\boldsymbol{P} = \begin{bmatrix} -\pi\boldsymbol{U} & \boldsymbol{O} & -\tilde{\omega}\boldsymbol{U} & \boldsymbol{O} \\ \boldsymbol{O} & -\pi\boldsymbol{U} & \boldsymbol{O} & -\tilde{\omega}\boldsymbol{U} \\ \boldsymbol{O} & -\pi\boldsymbol{U} & \boldsymbol{O} & -\tilde{\omega}\boldsymbol{U} \\ -\pi\boldsymbol{U} & \boldsymbol{O} & -\tilde{\omega}\boldsymbol{U} & \boldsymbol{O} \end{bmatrix} \tag{5.1}$$

where $\pi = -p/6$, $\tilde{\omega} = -q/6$, and $\boldsymbol{U}$ and $\boldsymbol{O}$ are 6×6 matrices whose elements are all unities and zeros respectively. To get the joint interstate distribution we have to evaluate the principal minors of $\boldsymbol{I} - \boldsymbol{P}$ obtained by omitting one or two rows and the same one or two columns. Let $\mu_j = 0, 1, 2$ $(j = 1, 2, 3, 4)$ be the number of rows omitted from the jth block of $\boldsymbol{I} - \boldsymbol{P}$ when partitioned in the same way as (5.1). To evaluate the resulting determinant carry out the following operations successively:—

(i) In each block, subtract the first row of the block from each of the remaining rows of the block;

(ii) In each block, add to the first column of the block the sum of the remaining columns of the block;

(iii) Subtract the first row of the fourth row-block from the first row of the first row-block, and subtract the first row of the third row-block from the first row of the second row-block;

(iv) Add the first column of the first column-block to the first column of the fourth column-block, and add the first column of the second column-block to the first column of the third column-block.

The resulting determinant is identical with a unit determinant except in two rows (namely the first rows of the third and fourth row-blocks); and hence on evaluating it by these rows and the corresponding columns, we find as its value

$$\begin{vmatrix} 1+(6-\mu_2)\pi & (6-\mu_4)\tilde{\omega} \\ (6-\mu_3)\tilde{\omega} & 1+(6-\mu_1)\pi \end{vmatrix} = (q+p\mu_1/6)(q+p\mu_2/6) - (q-q\mu_3/6)(q-q\mu_4/6) \tag{5.2}$$

This vanishes, as it should, when $\mu_1 = \mu_2 = \mu_3 = \mu_4 = 0$. Inserting into (5.2) the appropriate values of μ_j, we find, in the notation preceding (3.1),

$\pi_{jj} = pq/6,\ (j = 1, 2, \ldots, 12);\ \pi_{jj} = q^2/6,\ (j = 13, 14, \ldots, 24)$

$$\pi_{jk} = \begin{cases} pq/3 & \begin{cases} (j, k = 1, 2, \ldots, 6;\ j \neq k) \\ (j, k = 7, 8, \ldots, 12;\ j \neq k) \end{cases} \\ pq/3 + p^2/36 & \begin{cases} (j = 1, 2, \ldots, 6;\ k = 7, 8, \ldots, 12) \\ (j = 7, 8, \ldots, 12;\ k = 1, 2, \ldots, 6\ ) \end{cases} \\ q^2/3 & \begin{cases} (j, k = 13, 14, \ldots, 18;\ j \neq k) \\ (j, k = 19, 20, \ldots, 24;\ j \neq k) \end{cases} \\ 11q^2/36 & \begin{cases} (j = 13, 14, \ldots, 18;\ k = 19, 20, \ldots, 24) \\ (j = 19, 20, \ldots, 24;\ k = 13, 14, \ldots, 18) \end{cases} \\ 1/6 & \begin{cases} (j = 1, 2, \ldots, 12;\ k = 13, 14, \ldots, 24) \\ (j = 13, 14, \ldots, 24;\ k = 1, 2, \ldots, 12) \end{cases} \end{cases}$$

Since $\sum_{j=1}^{24} \pi_{jj} = 2q$, the latent root $\lambda = 1$ is simple whenever $q \neq 0$. [If $q = 0$, the walk is confined almost certainly to a single layer of atoms, and can be treated separately in a much simpler fashion; so we may suppose $q \neq 0$.] It follows that

$$\boldsymbol{M} = \begin{bmatrix} \frac{p}{6}\boldsymbol{U} - \frac{p}{12}\boldsymbol{I} & \left(\frac{p}{6} + \frac{p^2}{72q}\right)\boldsymbol{U} & \frac{1}{12q}\boldsymbol{U} & \frac{1}{12q}\boldsymbol{U} \\ \left(\frac{p}{6} + \frac{p^2}{72q}\right)\boldsymbol{U} & \frac{p}{6}\boldsymbol{U} - \frac{p}{12}\boldsymbol{I} & \frac{1}{12q}\boldsymbol{U} & \frac{1}{12q}\boldsymbol{U} \\ \frac{1}{12q}\boldsymbol{U} & \frac{1}{12q}\boldsymbol{U} & \frac{q}{6}\boldsymbol{U} - \frac{q}{12}\boldsymbol{I} & \frac{11q}{72}\boldsymbol{U} \\ \frac{1}{12q}\boldsymbol{U} & \frac{1}{12q}\boldsymbol{U} & \frac{11q}{72}\boldsymbol{U} & \frac{q}{6}\boldsymbol{U} - \frac{q}{12}\boldsymbol{I} \end{bmatrix}$$

$$= \begin{bmatrix} \frac{p}{6}\boldsymbol{U}_1 + \boldsymbol{A} & \frac{1}{12q}\boldsymbol{U}_1 \\ \frac{1}{12q}\boldsymbol{U}_1 & \frac{q}{6}\boldsymbol{U}_1 + \boldsymbol{B} \end{bmatrix} \tag{5.2}$$

where $\boldsymbol{U}_1$ is a 12×12 matrix of unities; and

$$\boldsymbol{A} = \begin{bmatrix} -\frac{p}{12}\boldsymbol{I} & \frac{p^2}{72q}\boldsymbol{U} \\ \frac{p^2}{72q}\boldsymbol{U} - \frac{p}{12}\boldsymbol{I} \end{bmatrix}, \quad \boldsymbol{B} = \begin{bmatrix} -\frac{q}{12}\boldsymbol{I} & -\frac{q}{72}\boldsymbol{U} \\ -\frac{q}{72}\boldsymbol{U} - \frac{q}{12}\boldsymbol{I} \end{bmatrix} \tag{5.3}$$

Further

$$\boldsymbol{I} - \boldsymbol{m}\boldsymbol{u}' = \begin{bmatrix} \boldsymbol{I} - \frac{p}{12}\boldsymbol{U}_1 & -\frac{p}{12}\boldsymbol{U}_1 \\ -\frac{q}{12}\boldsymbol{U}_1 & \boldsymbol{I} - \frac{q}{12}\boldsymbol{U}_1 \end{bmatrix} \tag{5.4}$$

Thus, using the relations $U^2 = 6U$, $U_1^2 = 12U_1$, we find

$$(I - mu')M(um' - I) =$$

$$\begin{pmatrix} -A + \frac{p}{12}[U_1A + AU_1] - \frac{p^2}{144}U_1[A+B]U_1 + \frac{p^2}{6}U_1, & \frac{q}{12}AU_1 + \frac{p}{12}U_1B - \frac{pq}{144}U_1[A+B]U_1 - \frac{p^2}{6}U_1 \\ \frac{q}{12}U_1A + \frac{p}{12}BU_1 - \frac{pq}{144}U_1[A+B]U_1 - \frac{p^2}{6}U_1, & -B + \frac{q}{12}[U_1B + BU_1] - \frac{q^2}{144}U_1[A+B]U_1 + \frac{p^2}{6}U_1 \end{pmatrix}$$

$$= \begin{pmatrix} -A + \left[\frac{p^2}{6} + \frac{p^3}{144q}\right]U_1, & -\left[\frac{p^2}{6} + \frac{pq}{144}\right]U_1 \\ -\left[\frac{p^2}{6} + \frac{pq}{144}\right]U_1, & -B + \left[\frac{p^2}{6} - \frac{q(q+1)}{144}\right]U_1 \end{pmatrix}$$

$$= \begin{pmatrix} \frac{p}{12}I + \left[\frac{p^2}{6} + \frac{p^3}{144q}\right]U, & -\left[\frac{p^2}{6} + \frac{pq}{144}\right]U, \\ \left[\frac{p^2}{6} - \frac{p^2(q+1)}{144q}\right]U, & -\left[\frac{p^2}{6} + \frac{pq}{144}\right]U, \\ -\left[\frac{p^2}{6} + \frac{pq}{144}\right]U, & \frac{q}{12}I + \left[\frac{p^2}{6} - \frac{q(q+1)}{144}\right]U, \\ -\left[\frac{p^2}{6} + \frac{pq}{144}\right]U, & \left[\frac{p^2}{6} + \frac{pq}{144}\right]U \end{pmatrix}$$

$$\begin{pmatrix} \frac{p}{12}I + \left[\frac{p^2}{6} + \frac{p^3}{144q}\right]U, & -\left[\frac{p^2}{6} + \frac{pq}{144}\right]U, \\ \left[\frac{p^2}{6} - \frac{p^2(q+1)}{144q}\right]U, & -\left[\frac{p^2}{6} + \frac{pq}{144}\right]U, \\ -\left[\frac{p^2}{6} + \frac{pq}{144}\right]U, & \frac{q}{12}I + \left[\frac{p^2}{6} - \frac{q(q+1)}{144}\right]U, \\ -\left[\frac{p^2}{6} + \frac{pq}{144}\right]U, & \left[\frac{p^2}{6} + \frac{pq}{144}\right]U \end{pmatrix}$$

This last matrix is puzzling. I cannot interpret physically what happens as $q \to 0+$: yet I can detect no fault in the steps leading to this matrix, which moreover leads to the physically reasonable final result (5.5).

The diffusion matrix is now

$$\boldsymbol{D} = \boldsymbol{T}(\boldsymbol{I} - \boldsymbol{mu}')\boldsymbol{M}(\boldsymbol{um}' - \boldsymbol{I})\boldsymbol{T}'$$

where

$$\boldsymbol{T} = (\boldsymbol{T}_1, \boldsymbol{T}_1, \boldsymbol{T}_2, -\boldsymbol{T}_2)$$

$$\boldsymbol{T}_1 = \begin{pmatrix} +6 & +3 & -3 & -6 & -3 & +3 \\ 0 & +3\sqrt{3} & +3\sqrt{3} & 0 & -3\sqrt{3} & -3\sqrt{3} \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

$$\boldsymbol{T}_2 = \begin{pmatrix} +3 & -3 & 0 & +3 & -3 & 0 \\ +\sqrt{3} & +\sqrt{3} & -2\sqrt{3} & +\sqrt{3} & +\sqrt{3} & +2\sqrt{3} \\ +2\sqrt{6} & +2\sqrt{6} & +2\sqrt{6} & -2\sqrt{6} & -2\sqrt{6} & -2\sqrt{6} \end{pmatrix}$$

This yields

$$\boldsymbol{D} = \frac{p}{6}\boldsymbol{T}_1\boldsymbol{T}_1' + \frac{q}{6}\boldsymbol{T}_2\boldsymbol{T}_2' + \frac{23p^2}{36}\boldsymbol{T}_1\boldsymbol{U}\boldsymbol{T}_1' - \frac{q}{36}\boldsymbol{T}_2\boldsymbol{U}\boldsymbol{T}_2' =$$

$$= \frac{p}{3}\boldsymbol{S}_1\boldsymbol{S}_1' + \frac{q}{3}\boldsymbol{S}_2\boldsymbol{S}_2'$$

where

$$\boldsymbol{S}_1 = \begin{pmatrix} +6 & +3 & -3 \\ 0 & +3\sqrt{3} & +3\sqrt{3} \\ 0 & 0 & 0 \end{pmatrix}, \quad \boldsymbol{S}_2 = \begin{pmatrix} +3 & -3 & 0 \\ +\sqrt{3} & +\sqrt{3} & -2\sqrt{3} \\ +2\sqrt{6} & +2\sqrt{6} & +2\sqrt{6} \end{pmatrix}$$

and so finally

$$\boldsymbol{D} = \begin{pmatrix} 18p + 6q & 0 & 0 \\ 0 & 18p + 6q & 0 \\ 0 & 0 & 24q \end{pmatrix}. \tag{5.5}$$

§ 6. Acknowledgements.

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