§1. Introduction

After Blackman's elaborate numerical works, Montroll made a series of elegant calculations based on the general method of the moment problem of statistics. As is pointed out by Houston, Montroll's trace-moment method appears to have a poor convergence property, and if, for instance, we want to get some detailed information about the behavior of distribution function $g(v)$ at smaller frequency region, his method would supply rather poor approximation compared to Houston's method or Montroll's another rigorous one performed for a square lattice.

However, when we actually attempt to get better approximation by Houston's method, we shall find it difficult to go further on. The same will be said for Montroll's rigorous one. On the other hand, it seems that we might be allowed to keep some hopes to improve this trace-moment method for low frequency regions.

Now, we shall start to examine the essential character of Montroll's method rather carefully. Above all, the symmetrical property of the frequency distribution in his papers

$$ g(v) = g(-v) \quad (1.1) $$

must be reexamined. We consider that it is not an essential property of the distribution function, but rather an arbitrary one; and in our calculation it is not taken into account.
Mathematically, the Montroll's method is an example of the well-known program of the moment problem in statistics, so if we want to have a desired distribution function, it is necessary to calculate all its moments. In our present subject, we must notice the very fact that it is the only Born-von Kármán matrix that is actually given to us, and its eigenvalues are \( \lambda \)'s (which are equal to \( n^2 \)'s), not \( n \)'s themselves. As for \( V \), we may imagine the square root matrix of B.-K. matrix \( M \), but its actual form cannot be known, and then, using the trace of \( M^2 \), we are only able to evaluate the even moments of \( g(V) \). Now, it seems to us reasonable to interpret (1.1) as to give the property for \( g(V) \) to overcome the above-mentioned unfavourable situation.

Now, it is interesting to consider a simple example of Fourier expansion for the function \( f(x) = x \) in the closed interval \( 0 \leq x \leq \pi \). If we assume \( f(x) = f(-x) \), we should have a cosine series expansion, while if \( f(x) = -f(-x) \), we should have a sine series expansion. The frequency distribution function \( g(V) \) is also defined only for positive values of \( V \). If we should actually know the square root matrix of \( M \), then we might be able to obtain an odd function-like expansion for \( g(V) \) together with the definition \( g(V) = -g(-V) \). For the above example, both cosine and sine series expansions are of course equivalent when we take infinite terms, but, if we confine ourselves for a finite number of terms for approximation, they are not equivalent. For example, at smaller values of variable, sine expansion should be better than cosine expansion. In the latter case, a finite constant term would remain, when \( x \) tends to zero. In Montroll's
approximation, just the same situation can be seen. 
[see Fig. 1 of his first paper]. That is to say, it will 
be supposed that the property (1.1) itself makes the 
approximation poor in the neighbourhood of the origin, 
then it is natural for us to have some hopes to improve 
the approximation by deriving an odd-function-like 
expansion for \( g(\nu) \).

Now, remembering that Born-von Kármán matrix \( M \) 
gives us the eigenvalues of \( \lambda = \nu^2 \), not of \( \nu \) itself, 
it is very natural that we attempt to calculate at first 
the distribution function \( D(\lambda) \) for the eigenvalue \( \lambda \) of 
\( M \) in the region \( 0 < \lambda \leq \lambda_c \). Then, from \( D(\lambda) \), we can 
transfer to \( g(\nu) \), our desired frequency distribution 
function, by a change of valuable, just like as treated 
in statistics under the subject, “problem of dist-
ribution”.

In this manner, we can actually obtain an odd 
function-like expansion for \( g(\nu) \), and, at the same 
time, remove some ambiguity of explanations, one 
might feel in the original papers of Montroll.

In spite of lacking the property like (1.1) for our 
\( D(\lambda) \), our results are simple and compact enough for ac-
tual numerical calculations.

§ 2. Expansion of \( D(\lambda) \) by Legendre polynomials.

In the following analysis, we shall be concerned 
only with Born-von Kármán matrix \( M \) itself.

Denoting the \( i \)-th eigenvalue of \( M \) by \( \lambda_i = \nu_i^2 \), then

\[
M \psi_i = \lambda_i \psi_i ,
\]

and in general

\[
M^k \psi_i = \lambda_i^k \psi_i ,
\]
and

\[ \text{Trace } M^k = \sum \lambda_i^k . \]  

(2.3)

Since the total number of eigenvalues is equal to the order of matrix, we can now define the distribution function \( D(\lambda) \) for the distribution of eigenvalue \( \lambda \) as follows:

\[ \int_{\lambda_s}^{\lambda_L} D(\lambda) d\lambda = m, \]  

(2.4)

where \( m \) denotes the order of the matrix.

The \( k \)-th moment of \( D(\lambda) \) is given by

\[ \langle \mu_k \rangle = \frac{1}{m} \int_{\lambda_s}^{\lambda_L} D(\lambda) \lambda^k d\lambda = \frac{\text{Trace } M^k}{m}, \]  

(2.5)

where \( \lambda_s, \lambda_L \) are smallest and largest eigenvalue respectively (\( 0 \leq \lambda_s < \lambda_L \)).

Suppose the distribution function is expanded as a linear combination of Legendre polynomials:

\[ D(\lambda) = \sum_{n=0}^{\infty} \alpha_n P_n \left( \frac{2\lambda - (\lambda_L + \lambda_s)}{\lambda_L - \lambda_s} \right), \]  

(2.6)

where

\[ P_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n} (x^2 - 1)^n. \]  

(2.7)

Putting \( x = (2\lambda - \lambda_L - \lambda_s)/(\lambda_L - \lambda_s) \), the coefficients \( \{ \alpha_n \} \) are

\[ \alpha_n = \frac{(2n+1)}{2} \int_{\lambda_s}^{\lambda_L} D \left( \frac{2x + (\lambda_L - \lambda_s)}{\lambda_L - \lambda_s} \right) P_n(x) dx \]  

(2.8)

Without loss of generality, we assume \( \lambda_s \) to be equal to zero. If it is not the case, we are only to put

\[ D(\lambda) = 0 \quad \text{for } 0 \leq \lambda < \lambda_s. \]  

Then putting

\[ \lambda_s = 0, \quad \lambda/\lambda_s = f, \quad \lambda = \lambda_L f, \quad d\lambda = \lambda_L df \]  

(2.9)

and \( x = 2(\lambda/\lambda_s) - 1 = 2f - 1, \quad dx = 2df. \)

and hence (2.6), (2.8) are transformed

\[ D(\lambda_L f) = \sum_{n=0}^{\infty} \alpha_n P_n(2f - 1), \]  

(2.6')

\[ \alpha_n = (2n+1) \int_{f}^{1} D(\lambda_L f) P_n(2f - 1) df. \]  

(2.8')
Further, using Rodrigues formula (2.7), it is easy to show that
\[ P_n(x) = \sum_{r=0}^{\infty} (-1)^r \frac{1}{(r)!^2} \frac{(n+r)!}{(n-r)!} \left( \frac{x}{2} \right)^r, \]  

(2.10)
then
\[ P_n(2f-1) = \sum_{r=0}^{\infty} (-1)^r \frac{1}{(r)!^2} \frac{(n+r)!}{(n-r)!} f^r, \]  

(2.11)
and substituting (2.11) into (2.6)
\[ D(\lambda) = \sum_{n=0}^{\infty} D_n \sum_{r=0}^{\infty} (-1)^r \frac{1}{(r)!^2} \frac{(n+r)!}{(n-r)!} f^r. \]

Therefore, if we define new coefficients \{b_r\} as follows
\[ D(\lambda f) = \sum_{r=0}^{\infty} b_r f^r \]  

(2.12)
then
\[ b_r = \sum_{n=0}^{\infty} (-1)^r \frac{1}{(r)!^2} \frac{(n+r)!}{(n-r)!} a_n \]  

(2.13)
In a similar manner, we get
\[ a_n = (2n+1) \sum_{r=0}^{\infty} (-1)^r \frac{1}{(r)!^2} \frac{(n+r)!}{(n-r)!} \int_0^1 D(\lambda f) f^r df. \]

Remembering (25).
\[ (\mu_k)_{\lambda} = \frac{1}{\lambda} \int_0^\lambda D(\lambda) \lambda^k d\lambda = \frac{\lambda^{k+1}}{\lambda^{k+1}} \int_0^1 D(\lambda f) f^k df = \frac{\text{Trace} M^k}{\lambda^{k+1}} \]
then, for the later convenience, we define \( \mu_k \) as follows:
\[ \int_0^1 D(\lambda f) f^k df = (\mu_k)_f = \mu_k. \]  

(2.14)
In this definition
\[ \mu_k = \frac{m}{\lambda_{k+1}} (\mu_k)_{\lambda} = \frac{\text{Trace} M^k}{\lambda_{k+1}}, \]  

(2.15)
therefore, we obtain for \( a_n \),
\[ a_n = (2n+1) \sum_{r=0}^{\infty} (-1)^r \frac{1}{(r)!^2} \frac{(n+r)!}{(n-r)!} \mu_r. \]  

(2.16)
From (2.16) and (2.13).
Therefore, if we introduce new coefficients $C_{rs}$,

$$b_r = \sum_{s} C_{rs} \mu_s,$$  \hspace{1cm} (2.18)

then finally

$$
\begin{align*}
&b_r = \sum_{r=s}^{\infty} (-1)^{r-s} \frac{1}{r!} \frac{1}{(r-s)!} \sum_{s=0}^{\infty} \frac{(-1)^s}{(s)!} \frac{(n+r)!}{(n-r)!} \frac{(n+s)!}{(n-s)!} \mu_s \\
&\text{Further more, if we cut the summation in (2.19) at \(k\)-th term, we could perform the summation actually. The result is}
\end{align*}
$$

$$
\begin{align*}
C_{rs} &= \sum_{m=r}^{\infty} \frac{1}{m!} \frac{1}{(m-s)!} \sum_{n=r}^{\infty} \frac{(-1)^n}{n!} \frac{(m+r)!}{(m-r)!} \frac{(m+s)!}{(m-s)!} \\
&= (-1)^{r-s} \frac{1}{r!} \frac{1}{(r-s)!} \frac{1}{r+s+1} \frac{(k+r+1)!}{(k-r)!} \frac{(k+s+1)!}{(k-s)!} \\
&\text{Once } C_{rs} \text{'s are obtained, } b_r \text{ can be expressed as a linear combination of } \mu_s \text{'s, then if we know the numerical values of } \mu_s \text{'s for each case, we shall be able to reach the approximate expansion of } D(\lambda) \text{ by means of (2.12).}
\end{align*}
$$

Above results are general ones and applicable to any lattice type and dimension in principle.

§3. Power Series Approximation by Direct Application of the Method of Least Squares.

This section will be devoted to formulate the method described in Montroll's second paper, for our case. But the following method will prove identical in its final result with the one given in the preceding section.

Let us suppose to try to approximate $D(\lambda)$ by a function $U(\lambda) = U(\lambda; V)$ of a set of parameters $\{\lambda_r\}$, chosen in such a manner that
to be a minimum. According to the calculus of variations, the necessary condition for $I(\mathbf{a})$ to be a minimum is

$$\frac{\partial I(\mathbf{a})}{\partial a_n} = 0 \quad n = 0, 1, \ldots, k.$$  

Now, if we take the following power series as $U(\mathbf{a}; \lambda)$,

$$U(\mathbf{a}; \lambda) = \sum_{n=0}^{k} a_n \left( \frac{\lambda}{k+1} \right)^n = \sum_{n=0}^{k} a_n f^n,$$

then, from (3.2), we finally reach to

$$\mu_n - \sum_{n=0}^{k} a_n \left( \frac{1}{(m+n)+1} \right) = 0,$$

($n = 0, 1, \ldots, k$).

These are the $k+1$ equations determining $\{a_n\}$. Explicitly,

$$\begin{align*}
a_0/1 + a_1/2 + \cdots + a_k/(k+1) &= \mu_0, \\
a_0/2 + a_1/3 + \cdots + a_k/(k+2) &= \mu_1, \\
&\vdots \\
a_0/(k+1) + a_1/(k+2) + \cdots + a_k/(2k+1) &= \mu_k.
\end{align*}$$  

Or, if we define the following three matrix,

$$A(k) = \begin{bmatrix} 1, 1/2, 1/3, \ldots, 1/(k+1) \\ \vdots \\ 1/(k+1), \ldots, 1/(2k+1) \end{bmatrix},$$

$$\mathbf{a}(k) = (a_0, a_1, a_2, \ldots, a_k),$$

$$\mu(k) = (\mu_0, \mu_1, \mu_2, \ldots, \mu_k),$$

our set of linear equations (3.5) becomes the matrix equation

$$A(k) \cdot \mathbf{a}(k) = \mu(k).$$

Now suppose $A^{-1}(k)$ is the inverse of $A(k)$. Then

$$A^{-1}(k) = \mu(k) \cdot A^{-1}(k).$$

Here, we must notice that, $(A(k))_i = a_{i-1}$, $(\mu(k))_i = \mu_{i-1}$.

Now our next task is to find $A^{-1}(k)$, and it can be obtained in a general form. Denoting the $(i,j)$ element of $A^{-1}(k)$ as $A^{-1}_{ij}$, then
Fron example, in case of small \( k \),

\[
A_{ik}(k) = \frac{(-1)^{i+k}}{(i+k-1)! (k-1)!} \left[ (i) \cdots (i+k) \right] \left[ (j) \cdots (j+k) \right] \frac{(i-k)}{(i-j+1)} \frac{(i)}{(i-j+1)}
\]

or

\[
A_{ik}(k) = A_{ik}(k) = \frac{(-1)^{i+k}}{(i+k-1)! (k-1)!} \left[ (i-1)! \right] \left[ (i-1)! \right] \frac{(i)}{(i-j+1)} \frac{(i)}{(i-j+1)} \frac{(i-1)}{(i-j+1)} \frac{(i-1)}{(i-j+1)}
\]

\[i = 1, 2, \ldots, k+1, \quad j = 1, 2, \ldots, k+1, \quad k = 0, 1, 2, \ldots\]

For example, in case of small \( k \),

\[
A^{-1}(1) = 1, \quad A^{-1}(1) = \begin{bmatrix} 4 & -6 \\ -6 & 12 \end{bmatrix} = \begin{bmatrix} (1.2)(1.2)/1 & (1.2)(2.3)/2 \\ (1.2)(2.3)/2 & (2.3)(2.3)/3 \end{bmatrix}
\]

Therefore from (3.9),

\[
(A(k))_{i} = \sum_{j=1}^{k+1} (\mu(k))_{i} A_{ik}(k)
\]

\[
= \frac{(-1)^{i+k}}{(i+k-1)! (k-1)!} \sum_{j=1}^{k+1} (-1)^{i+j} \left[ (i+j) \right] \left[ (i+j) \right] \frac{(i-j)}{(i-j+1)} \frac{(i)}{(i-j+1)} \frac{(i-j)}{(i-j+1)} \frac{(i-j)}{(i-j+1)}
\]

If, one expresses (3.11), using \( a_{0}, a_{1}, \ldots, a_{k} \), and \( \mu_{0}, \mu_{1}, \ldots, \mu_{k} \),

\[
A_{i} = \sum_{j=0}^{k+1} \frac{(-1)^{i+j}}{(i+j)! (j+1)!} \frac{(i+j+1)}{(i-j)! (i-j)!}
\]

Comparing this result with (2.20), one sees that these two methods, described above, give exactly the same result – the same approximation. This fact might appear surprising at first glance, but it is self-evident if we consider rather carefully the meaning of the process adopted in this section.

\section{Relation between \( D(\lambda) \) and \( g(V) \)}

Once we obtain \( D(\lambda) \), using the results of preceding section, it is easy to derive the frequency distribution function \( g(V) \), through the change of variable \( \lambda \rightarrow V \), just like in “Problem of Distribution” of statistics. Now we see
\[
D(\lambda) \, d\lambda = 2 \nu D(\nu^2) \, d\nu, \quad (4.1)
\]

then
\[
\tilde{g}(\nu) = 2 \nu D(\nu^2), \quad (4.2)
\]

More explicitly, remembering the definition of \( \mu_i \) and the formula (2.15), it is written as
\[
\frac{\nu}{m} \tilde{g}(\nu) = \sum_{n=0}^{\infty} 2a_n \left( \frac{\nu}{\nu_c} \right)^{2n+1} \quad (4.3)
\]

where \( \{ a_n \} \) are given as numerical coefficients and \( m \) is the order of Born-von Karman matrix which is equal to the total number of vibrational freedoms of interested system.

\section{Results and Discussion}

To compare with Montroll's result, numerical calculation was performed for the same square lattice as in Montroll's first paper.

For \( \nu = 5 \),
\[
\frac{\nu}{m} g(\nu) = 2 \left( \frac{\nu}{\nu_c} \right) \left\{ 1.38 + 1.04 \left( \frac{\nu}{\nu_c} \right)^2 - 17.39 \left( \frac{\nu}{\nu_c} \right)^4 + 30.98 \left( \frac{\nu}{\nu_c} \right)^6 
- 12.55 \left( \frac{\nu}{\nu_c} \right)^8 - 2.11 \left( \frac{\nu}{\nu_c} \right)^{10} \right\} \quad (5.1)
\]

This function is plotted in Fig.1. Qualitatively, it appears almost the same nature as Montroll's result except in the vicinity of origin. At \( \nu = 0 \), in Montroll's case, a constant term survives, but in ours \( g(0) = 0 \), of course.

Judging from these results, it seems that the Montroll's even function-like approximation and our odd function-like approximation are almost the same degree of efficiency as a whole, but we are hoping that our method has improved the trace-moment method in some degree for the smaller frequency region.
We have still much to be discussed in detail about these points and another. But there is no space enough to present them here, and then we shall discuss them in another place. (5)

Fig. 1

Reference.
(5) This journal p. 117.