ON THE STOCHASTIC TYPES OF MOTION IN A SYSTEM OF COUPLED HARMONIC OSCILLATORS

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COTENTS

I. Preliminaries

Since the early works of Poincaré[1], Fermi[2], and others[3], it has been a long standing desire to unify particle mechanics and statistical mechanics by exhibiting a mechanical systsm, whose exact solution can be shown to yield an approach to thermodynamic equilibrium. Physicists now tend to believe that weakly coupled nonlinear systems will exhibit the ergodic behavior which is considered necessary for an approach to thermodynamic equilibrium. In accepting ergodicity, however, we should give up almost all hope making analytic solution of the system; for in that case, the equations of motion of the system would become so much complicated that we should be oblized to make computations by means of electronic computers[4][5].

To their surprise, Fermi and his collaborators[4] found that their nonlinear oscillator systems yielded very little energy sharing and did not exhibit ergodic behavior. And the result obtained by Ford and Waters[5] by means of computer also showed that their nonlinear systems have many features in common with linear systems. Particularly, after perturbation theory[6] their systems are not likely to be ergodic, although theirs are energy sharing oscillator systems.

On the other hand, according to studies by Debye[7] and Peierls[8] on the heat conduction in crystals, the existence of anharmonicities in the interatomic force could be necessary to yield a finite thermal conductivity in crystals. They introduced the concept of mean free path of phonons, as a measure of the strength of the coupling of normal modes brought about by the anharmonicity involved in the Hamiltonian of the system.

The nonlinear oscillator systems of Peierls[8] on lattice thermal conductivity, however, make us hesitate to believe that his systems do not exhibit an approach to thermodynamic equilibrium. Up to the present, we have had a growing amount of evidence showing that many physically interesting systems are not ergodic. For example, Resibois and Prigogine[9] have found constants of motion for gas systems, and Kolmogorov[10] has shown that his more general nonlinear systems are not ergodic.

Linear systems also have been investigated from the view-point of statistical dynamics of irreversible phenomena, especially in the fields of lattice vibrations and rheology. The statistical dynamical approach to the stationary state in the linear system gives much information and instructive fundamental concept on the irreversibility of a statistical ensemble.

If one gives up nonlinearity and, accordingly, ergodicity, then one can treat oscillator systems wholly analytically. The ensemble of harmonic oscillators seems to be the only one of the many-body systems with strong coupling between particles which admits of precisely analytical and statistical calculations.

Klein and Prigogine[11] took linear systems of harmonic oscillators, and calculated the correlation functions and showed that their systems approach finally to a stationary state, where the energy of the systems is a constant of motion. Hemmer[12], Teramoto[13], and Takizawa and Kobayasi[14], each made study of heat flow in a linear system of harmonically coupled oscillators. They all showed that the large system of oscillators approaches finally to a stationary state, but not to an equilibrium state. Starting from an ensemble half of whose system is at temperature zero, and the other half at temperature T, they showed that the average value of the potential energies and that of the kinetic energies of each particle in a large system approach to the same stationary value at the final state, *viz.* after infinitely long time. This means that the microscopic local tempertures of any particle in the system approach to the same stationary value and that there is no temperature gradient in the system at the final state. They also showed that the energy flow[14] still exists at every point of the system at the final state. According to the works[11][14] mentioned above, on the problems of energy flow in the one-dimensional harmonic lattice, it seems true that the harmonic model is incapable of discribing the phenomena of heat conduction in a system of coupled oscillators. However, it is not yet clear[15] how the anharmonic coupling plays an essential rôle in the fundamental molecular kinetic theory of heat conduction. Rubin[16] investigated the heat flow in a harmonic lattice with arbitrary distribution of two kinds of isotopes by means of the electronic computors.

Meixner[17], Kashiwamura and Teramoto[18], Hemmer[12], Turner[19], Rubin[20], and Mazur and Montroll[21], also investigated the model of linear chain with external force, or with a heavy mass. They treated the chain by means of normal modes or Laplace transform of the solutions of equations of motion of the system, with particular reference to thermal fluctuation, or heat conduction, or recurrence time. In the previous paper[14], Takizawa and Kobayasi took a one-dimensional harmonic lattice and investigated heat flow in the system by means of the Schrödinger coordinates[25]. They layed special emphasis on elucidating the superiority of using the Schrödinger coodinates; for by means of these coordinates one can take explicitly into account the initial conditions in the solutions of dynamical equation of the one-dimensional harmonic lattice.

In the present paper, the authors show that if we want to make a study of a one-dimensional lattice with isotopic impurities, we can also use the Schrödinger coordinates; by means of the coordinates the dynamical solutions with initial conditions can be easily obtained. And in these solutions the initial conditions can be seen explicitly. Whereas if we use, in stead, normal mode expressions[22] of the solutions of the dynamical system, the initial conditions can not be seen very explicitly in the expressions of the dynamical solutions. In this study statistics is introduced in the initial conditions, and the timal behavior thereafter of the system is persued. Here let us assume that we start with an initial ensemble corresponding to such a macroscopic state that half the system is at temperature zero, and the other half at temperature T. The timal evolution of this ensemble is determined purely by the law of classical dynamics. Mathematical formulation of the dynamical solution is given in Chapter II. The initial ensemble and the expressions of momentum-momentum correlation functions and position position correlation functions as well as momentum-position correlation functions are given in Chapter III.

By introducing the Schrödinger coordinates and by means of the solutions of the dynamical system expressed in Bessel functions[11][14], one can easily pursue the timal behavior of the correlation functions of the particles in the system. It should also be noted that the method used here is simpler by far than by means of the trigonometric eigenfunctions of the dynamical system.

From these correlation functions, the average kinetic and potential energies of each particle in the large system are derived, and the asymptotic behavior of these energies is examined in Chapters III and IV. The instantaneous energy flow is obtained from momentum-position correlation functions. In Chapter III, the authors show that the average kinetic and potential energies of each particle in a large system of perfect lattice approach to the same stationary value of $kT/4$ after infinitely long time. On the other hand, it is also shown that in such a system the momentum-position correlation functions do not vanish but remain finite even after infinitely long time. In other words, at the final state the instantaneous flow of energy still exists at every point in the system. And, the energy flow does not obey the classical Fourier's law, which states that the vector of heat flax is proportional to the negative gradient of temperature. This shows clearly that the final state thus obtained in our system is by no means the state of thermodynamic equilibrium, but a stationary state.

In Chapter IV, a study is made on the effect of an impurity atom in a large system of linear harmonic oscillators. There the dynamical solutions of the system are obtained in the expression of the Schrödinger coordinates, and then the initial canonical ensemble with temperature T is introduced, and the correlation functions of particles are calculated as functions of time. From these correlation functions, the authors show that the average kinetic and potential energies of each particle in a large system approach to stationary values, which are different, on either side of the impurity atom, in other words, the system approaches to a stationary state which has a gap of the energy distribution at the impurity site. And the energy flow still exists at every point of the system at the final state, though there is no temperature gradient at any point of the system except at the impurity site. As for the system having an isotopic impurity of small mass, there exist stationary and oscillating terms in the expressions of microscopic local temperatures. Aside from oscillating terms, the constant energy flow of the same magnitude also exists at every point of the system at the final state. Some discussions on the problems of flow of energy in the lattice system with isotopic impurities are also made in this chapter.

Lastly, in chapter V, the authors make mention of the existence of localized vibrations and discuss the localized vibration in an infinitely extended system of linear harmonic oscillators, especially in relation to the Schrödinger coordinates. In our opinion, a locally reduced mass, or local strong interactions between particles, or an applied external force of high frequency, forms the cause of the existence of the localized vibration in an infinitely extended system. The authors also make brief discussion on the range of extension of the localized vibration by means of the Schrödinger coordinates.

II. Solutions of the Equations of Motion of the Coupled Harmonic Oscillators in the Schrödinger Coordinates

In this chapter, various types of systems of one-dimensional harmonic lattice are treated by means of the Schrödinger coordinates, and the solutions of equations of motion are expressed by Bessel functions.

We shall take a system of one-dimensional harmonic lattice consisting of an infinite number of particles. Let the perticles of the system be located at integer sites numbered from $(-\infty)$ to $(+\infty)$ (from the left to the right side along the system) (cf. Fig. 1).

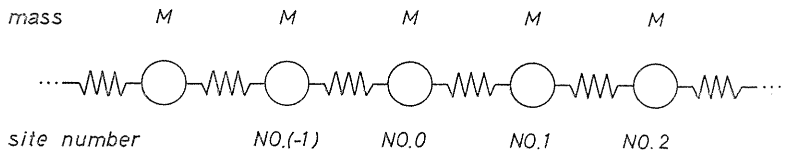

FIG. 1. Infinite linear lattice.

They interact each other with their two nearest neighbours which have the same lattice constant K. They have the same mass M. The displacement of the i-th particle from equilibrium position will be written as $x_i(t)$. Then the equations of motion will read as follows:

$$\frac{d^2}{dt^2}x_i(t) = \omega_0^2\{x_{i+1}(t) - 2x_i(t) + x_{i-1}(t)\}, \qquad \text{for } -\infty < i < +\infty \tag{2-1}$$

where $\omega_0 = \sqrt{K/M}$ and $t = \text{time}$.

Now, let us introduce the Schrödinger coordinates[25], which are defined by

$$\left.\begin{aligned} y_{2n}(\tau) &= \dot{x}_n(t)/(\sigma\omega_0), \\ y_{2n+1}(\tau) &= \{x_{n+1}(t) - x_n(t)\}/\sigma, \\ \text{and by} \qquad & \\ \tau &= 2\omega_0 t, \end{aligned}\right\} \tag{2-2}$$

where σ is a characteristic length, and $\dot{x}_n(t)$ is the velocity of the n-th particle. From definition (2–2), we can see that $y_{2m}(\tau)$ is the velocity of the m-th particle for any integers m and that $y_{2m+1}(\tau)$ is the relative displacement between the m-th and the $(m+1)$-th particles for any integers m. By means of the Schrödinger coordinates (2–2), the equations of motion (2–1) can be written as follws:

$$2\frac{d}{d\tau}y_n(\tau) = y_{n+1}(\tau) - y_{n-1}(\tau), \tag{2-3}$$

for any integers n. The solutions of the equations of motion (2–3) are given at once in the form:

$$y_n(\tau) = \sum_{\nu=-\infty}^{+\infty} a_\nu J_{\nu-n}(\tau), \qquad \text{for } -\infty < n < +\infty \tag{2-4}$$

where a_ν is the initial value of $y_\nu(\tau)$ and $J_m(\tau)$ the Bessel function of order m and of argument τ.

This expression, which was devised by Schrödinger[25] and adapted by Klein and Prigogine[11], and Hemmer[12], is more convenient than the one obtained by means of the trigonometric eigenfunctions of the system. In terms of solutions (2–4) expressed by Bessel functions, we can take explicitly into account the initial conditions of the system, and we can diagonalize covariance matrix[24] in the distribution function of the canonical ensemble, as and when we want to introduce the statistics at the initial instant of time.

Here, we can show the equations of the motion of finitely extended systems which have various end conditions, and we take their solutions expressed by Bessel functions.

a) For a linear lattice with both ends free (cf. Fig. 2), we have the equations of motion in the Schrödinger coordinates, *viz.*:

$$\left.\begin{aligned} &2\frac{d}{d\tau}y_l(\tau) = y_{l+1}(\tau) - y_{l-1}(\tau), \text{ for } l = 2n+1,\ 2n+2,\ \ldots,\ 2(n+m)-1 \\ &2\frac{d}{d\tau}y_{2n}(\tau) = y_{2n+1}(\tau), \\ &\text{and} \\ &2\frac{d}{d\tau}y_{2(n+m)}(\tau) = -y_{2(n+m)-1}(\tau). \end{aligned}\right\} \tag{2-5}$$

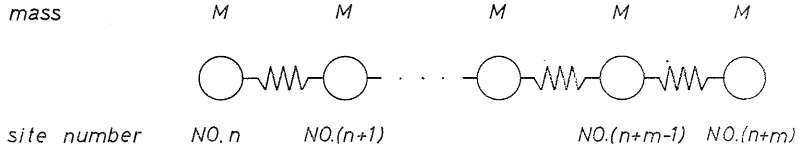

FIG. 2. Linear lattice with both ends free.

We shall take the solutions of equations (2–5):

$$y_l(\tau) = \sum_{\nu=-\infty}^{+\infty} a_\nu J_{\nu-l}(\tau). \tag{2-6}$$

The expression (2–6) satisfies the first equation of (2–5). We put (2–6) into the second equation of (2–5):

$$\sum_{\nu=-\infty}^{+\infty} a_\nu J_{\nu-2n+1}(\tau)=0,$$

i.e.

$$\sum_{\nu=-\infty}^{+\infty} a_{\nu+2n-1} J_\nu(\tau)=0.$$

$$\therefore\quad a_{2n-1}J_0(\tau)+\sum_{\nu=1}^{+\infty} a_{\nu+2n-1}J_\nu(\tau)+\sum_{\nu=1}^{+\infty} a_{-\nu+2n-1}J_{-\nu}(\tau)=0.$$

$$\therefore\quad a_{\nu+2n-1}=(-1)^{\nu+1}a_{-\nu+2n-1}. \tag{2-7}$$

Accordingly, the expression (2–7) is the necessary condition for establishing the second equation of (2–5).

In a similar manner, we shall obtain the condition between a's satisfying the third equation of (2–5):

$$a_{\nu+2(n+m)+1}=(-1)^{\nu+1}a_{-\nu+2(n+m)+1}. \tag{2-8}$$

From (2–7) and (2–8), we shall obtain

$$\left.\begin{aligned} &a_{\nu+2k\cdot 2(m+1)}=a_\nu,\\ \text{and}\quad &\\ &a_{\nu+(2k+1)\cdot 2(m+1)}=(-1)^\nu a_{4n+2m-\nu}.\end{aligned}\right\} \tag{2-9}$$

From (2–6) and (2–9), we shall finally obtain the solutions of equations (2–5):

$$y_l(\tau)=\sum_{\nu=2n}^{2(n+m)} a_\nu \sum_{k=-\infty}^{+\infty}\{J_{\nu+2k\cdot 2(m+1)-l}(\tau)+(-1)^\nu J_{4n+2m-\nu+(2k+1)\cdot 2(m+1)-l}(\tau)\}, \tag{2-10}$$

$$\text{for } l=2n,\ 2n+1,\ \dots,\ 2(n+m)$$

with a_ν the initial values of $y_\nu(\tau)$ (for $\nu=2n,\ 2n+1,\ \dots,\ 2(n+m)$).

b) For a linear lattice with both ends fixed (cf. Fig. 3), the equations of motion will be:

$$\left.\begin{aligned} &2\frac{d}{d\tau}y_l(\tau)=y_{l+1}(\tau)-y_{l-1}(\tau),\quad \text{for } l=2n+1,\ 2n+2,\ \dots,\ 2(n+m)-1\\ &y_{2n}(\tau)=0,\\ \text{and}\quad&\\ &y_{2(n+m)}(\tau)=0.\end{aligned}\right\} \tag{2-11}$$

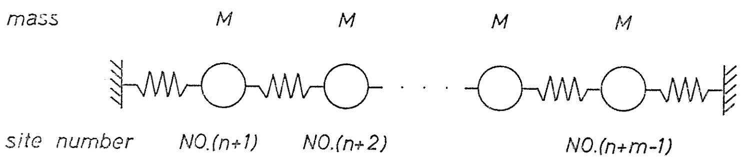

FIG. 3. Linear lattice with both ends fixed.

In the same manner as in the case of a), we shall obtain the solutions of equations (2-11):

$$y_l(\tau) = \sum_{\nu=2n+1}^{2(n+m)-1} a_\nu \sum_{k=-\infty}^{+\infty} \{ J_{\nu+2k\cdot 2m-l}(\tau) + (-1)^{\nu+1} J_{4n+2m-\nu+(2k+1)\cdot 2m-l}(\tau) \}. \tag{2-12}$$

for $l = 2n+1,\ 2n+2,\ \ldots,\ 2(n+m)-1$

with a_ν the initial values of $y_\nu(\tau)$ (for $\nu = 2n+1,\ 2n+2,\ \ldots,\ 2(n+m)-1$).

c) For a linear lattice with one end fixed and the other end free (cf. Fig. 4), the equations of motion will be:

$$\left.\begin{aligned} &2\frac{d}{d\tau} y_l(\tau) = y_{l+1}(\tau) - y_{l-1}(\tau), \quad \text{for } l = 2n+1,\ 2n+2,\ \ldots,\ 2(n+m)-1 \\ &y_{2n}(\tau) = 0, \\ &\text{and} \\ &2\frac{d}{d\tau} y_{2(n+m)}(\tau) = -y_{2(n+m)-1}(\tau). \end{aligned}\right\} \tag{2-13}$$

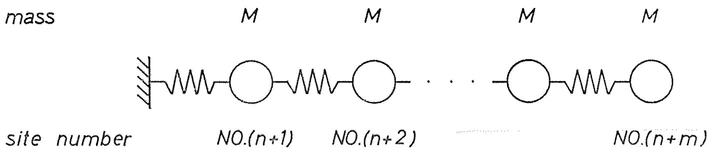

FIG. 4. Linear latttice with one end fixed and other end free.

The solutions of equations (2-13) will be given by:

$$\begin{aligned} y_l(\tau) = \sum_{\nu=2n+1}^{2(n+m)} a_\nu \sum_{k=-\infty}^{+\infty} \{ & J_{\nu+4k\cdot(2m+1)-l}(\tau) + (-1)^{\nu} J_{4n+2m+1-\nu+(4k+1)\cdot(2m+1)-l}(\tau) - \\ & - J_{\nu+(4k+2)\cdot(2m+1)-l}(\tau) + (-1)^{\nu+1} J_{4n+2m+1-\nu+(4k+3)\cdot(2m+1)-l}(\tau) \}, \end{aligned} \tag{2-14}$$

for $l = 2n+1,\ 2n+2,\ \ldots,\ 2(n+m)$

with a_ν the initial values of $y_\nu(\tau)$ (for $\nu = 2n+1,\ 2n+2,\ \ldots,\ 2(n+m)$).

d) For a ring consisting of $2N$ particles (cf. Fig. 5), the equations of motion will be:

$$\left.\begin{aligned} &2\frac{d}{d\tau} y_l(\tau) = y_{l+1}(\tau) - y_{l-1}(\tau), \quad \text{for any integers } l \\ &\text{and} \\ &y_\nu(\tau) = y_{\nu+4N}(\tau). \quad \text{for } -\infty < \nu < +\infty \end{aligned}\right\} \tag{2-15}$$

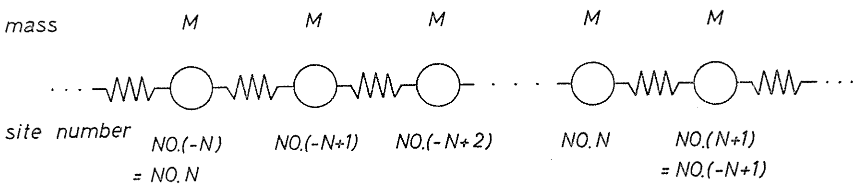

FIG. 5. Periodic lattice consisting of $2N$ particles.

The solutions of (2-15) will be given as follows:

$$y_l(\tau) = \sum_{\nu=-2N+2}^{2N+1} a_\nu \sum_{k=-\infty}^{+\infty} J_{\nu-4kN-l}(\tau), \tag{2-16}$$

with a_ν the initial values of $y_\nu(\tau)$ (for $\nu=-2N+2,\ -2N+3,\ \ldots,\ 2N+1$).

For a sufficiently long chain, however, by means of the following formula, *viz.*:

$$\begin{aligned}
\lim_{N\to+\infty} \sum_{k=-\infty}^{+\infty} J_{2kN+s}(z) &= \lim_{N\to+\infty} \frac{(-1)^s}{2N} \cdot \sum_{r=-N}^{N-1} \exp\Big[i\Big(\frac{rs\pi}{N} + z\sin\frac{r\pi}{N}\Big)\Big] \\
&= \frac{(-1)^s}{\pi}\int_{-\pi/2}^{\pi/2} \exp[i(2sx + z\sin 2x)]\,dx \\
&= \frac{(-1)^s}{2\pi}\int_{-\pi}^{\pi} \exp[i(sx + z\sin x)]\,dx \\
&= (-1)^s J_s(-z) = J_s(z), \quad \text{for any integers } s
\end{aligned} \tag{2-17}$$

we can express approximately solutions of equations of motion whatever boundary condition it may have, as follows:

$$y_n(\tau) = \sum_\nu a_\nu J_{\nu-n}(\tau), \tag{2-18}$$

where the summation with regard to ν covers the whole region of the lattice, and a_ν is the initial value of $y_\nu(\tau)$.

As mentioned above, the initial values appear explicitly in the solutions (2-4), (2-10), (2-12), (2-14) and (2-16). We can then easily introduce the statistics into the initial values and we calculate the covariance matrix.

We shall use the Schrödinger coordinates in the following investigation.

III. Energy Flow in a System of One-Dimensional Harmonic Oscillators

In this chapter, we shall consider the phenomenon of energy flow in the classical system of a linear lattice consisting of an infinite number of particles. Starting with an initial ensemble which corresponds to such a macroscopic state that half the system is at temperature T and the other half is at temperature zero, the correlation functions of particles are calculated explicitly as functions of time. The average values of kinetic and potential energies are essentially the same as those obtained by means of the solutions in trigonometric eigenfunctions[13]. However, the correlation functions between different positions and the momentum correlation functions between different particles vanish after a sufficiently long time; while the average kinetic and potential energies of each particle approach to the same stationary value of $kT/4$ after a sufficiently long time. On the other hand, the correlation functions between the momentum of a particle and the position of another particle do not vanish and remain finite, even after a long time. In other words, at the final state $\tau=+\infty$, the instantaneous flow of energy still exists at any point throughout the system.

§ 3.1 *Initial Ensemble*

We shall consider a system of harmonic lattice which consists of an infinite number of particles having the same mass M. Each particle is located at integer site from $-\infty$ to $+\infty$ (cf. Fig. 1). Assuming the interaction with their nearest neighbours with the same lattice constant K, we have the equations of motion (2–3) and their solutions (2–4) in the Schrödinger coordinates.

Now, let us introduce an initial ensemble in which particles located at the non-positive integer sites are fixed at their equilibrium positions, namely:

$$a_0 = a_{-1} = a_{-2} = \ \ldots \ = 0, \tag{3-1}$$

and particles at the positive integer sites are distributed with canonical distribution at temperature T. That is to say, we shall take the distribution function:

$$W(a_1, a_2, a_3, \ldots) = \prod_{p} \sqrt{\frac{\sigma^2 K}{2\pi kT}} \cdot \exp\left[-\frac{\sigma^2 K}{2kT} \cdot a_p^2 \right], \tag{3-2}$$

where k is the Boltzmann constant. The initial ensemble with (3–1) and (3–2) has the averages:

$$\left.\begin{aligned} \langle a_m \rangle_{Av} &= \int_{-\infty}^{+\infty}\cdots\int a_m W(a_1, a_2, a_3, \ldots) \prod_p da_p = 0, \qquad \text{for any integers } m \\ \langle a_m \cdot a_n \rangle_{Av} &= \int_{-\infty}^{+\infty}\cdots\int a_m \cdot a_n W(a_1, a_2, a_3 \ldots) \prod_p da_p \\ &= \begin{cases} \dfrac{kT}{2K}\delta_{m,n}, & \text{for } m \geq 1 \text{ and } n \geq 1 \\ 0, & \text{for } m \leq 0 \text{ or } n \leq 0 \end{cases} \end{aligned}\right\} \tag{3-3}$$

where $\delta_{\alpha,\beta}$ is Kronecker's delta.

§ *3. 2 Correlation Function*

Starting with the initial ensemble of (3–1) and (3–2), we shall consider the timal behavior of the system. Now, we define the correlation functions and the microscopic local temperature as follows:

$$C_{\alpha,\beta}(\tau) = \frac{\sigma^2 K}{2k} \langle y_\alpha(\tau) y_\beta(\tau) \rangle_{Av}, \qquad \text{for any integers } \alpha \text{ and } \beta \tag{3-4}$$

and

$$T_m(\tau) = C_{2m,2m}(\tau) + \frac{1}{2}\{C_{2m+1,2m+1}(\tau) + C_{2m-1,2m-1}(\tau)\}. \tag{3-5}$$

for any integers m

The expression (3–5) measures the average value of the thermal energy of the m-th particle and has a dimension of temperature. From (2–4) and (3–4), we shall have the following expressions of the correlation functions:

$$\begin{aligned} \Theta_{n,n+m}(\tau) \equiv C_{2n,2n+2m}(\tau) &= \frac{\sigma^2 K}{2k} \left\langle \sum_{\nu=1}^{+\infty} a_\nu J_{\nu-2n}(\tau) \cdot \sum_{\nu=1}^{+\infty} a_\nu J_{\nu-2n-2m}(\tau) \right\rangle_{Av} \\ &= \frac{\sigma^2 K}{2k} \cdot \left[\sum_{\nu,\mu=1}^{+\infty} \langle a_\nu a_\mu \rangle_{Av} \cdot J_{\nu-2n}(\tau) J_{\mu-2n-2m}(\tau) \right], \end{aligned} \tag{3-6}$$

for $\alpha = 2n$ and $\beta = 2n + 2m$, and

$$U_{n,n+m}(\tau) \equiv C_{2n+1,2n+2m+1}(\tau) = \frac{\sigma^2 K}{2k} \langle \sum_{\nu=1}^{+\infty} a_\nu J_{\nu-2n-1}(\tau) \cdot \sum_{\nu=1}^{+\infty} a_\nu J_{\nu-2n-2m-1}(\tau) \rangle_{Av}$$

$$= \frac{\sigma^2 K}{2k} \cdot [\sum_{\nu,\mu=1}^{+\infty} \langle a_\nu a_\mu \rangle_{Av} \cdot J_{\nu-2n-1}(\tau) J_{\mu-2n-2m-1}(\tau)], \qquad (3\text{-}7)$$

for $\alpha = 2n+1$ and $\beta = 2n+2m+1$.

By means of the averages of the initial values (3–3), we shall obtain the momentum-momentum correlation functions:

$$\Theta_{n,n+m}(\tau) = \frac{T}{2} \cdot \sum_{\nu=1}^{+\infty} J_{\nu-2n}(\tau) J_{\nu-2n-2m}(\tau)$$

$$= \frac{T}{2} \cdot \sum_{\nu=1-2n-m}^{+\infty} J_{\nu+m}(\tau) J_{\nu-m}(\tau), \qquad (3\text{-}8)$$

and we shall obtain the position-position correlation functions:

$$U_{n,n+m}(\tau) = \frac{T}{2} \cdot \sum_{\nu=1}^{+\infty} J_{\nu-2n-1}(\tau) J_{\nu-2n-2m-1}(\tau)$$

$$= \frac{T}{2} \cdot \sum_{\nu=-2n-m}^{+\infty} J_{\nu+m}(\tau) J_{\nu-m}(\tau). \qquad (3\text{-}9)$$

If we put $m=0$ in (3–8) and (3–9), then the average values of kinetic energy $K_n(\tau)$ and of potential energy $\Phi_n(\tau)$ of the n-th particle will be obtained as follows:

$$K_n(\tau) = k \cdot \Theta_{n,n}(\tau) = \frac{kT}{2} \cdot \sum_{\nu=1-2n}^{+\infty} J_\nu^2(\tau), \quad \text{for any integers } n \qquad (3\text{-}10)$$

and

$$\Phi_n(\tau) = \frac{k}{2} \cdot [U_{n,n}(\tau) + U_{n-1,n-1}(\tau)] = \frac{kT}{4} \cdot [\sum_{\nu=-2n}^{+\infty} J_\nu^2(\tau) + \sum_{\nu=-2n-2}^{+\infty} J_\nu^2(\tau)]. \qquad (3\text{-}11)$$

for any integers n

Moreover, from (3–4), (2–4), and (3–3), we shall obtain the momentum-position correlation functions at any instant of time:

$$V_{n,m}(\tau) \equiv C_{2n,2n+2m+1}(\tau) = \frac{\sigma^2 K}{2k} \langle \sum_{\nu=1}^{+\infty} a_\nu J_{\nu-2n}(\tau) \cdot \sum_{\nu=1}^{+\infty} a_\nu J_{\nu-2n-2m-1}(\tau) \rangle_{Av}$$

$$= \frac{\sigma^2 K}{2k} \cdot \sum_{\nu,\mu=1}^{+\infty} \langle a_\nu a_\mu \rangle_{Av} \cdot J_{\nu-2n}(\tau) J_{\mu-2n-2m-1}(\tau)$$

$$= \frac{T}{2} \cdot \sum_{\nu=1}^{+\infty} J_{\nu-2n}(\tau) J_{\nu-2n-2m-1}(\tau)$$

$$= \frac{T}{2} \cdot \sum_{\nu=1/2-2n-m}^{+\infty} J_{\nu+m+1/2}(\tau) J_{\nu-m-1/2}(\tau). \qquad (3\text{-}12)$$

Here, by means of the formula:

$$\sum_{\nu=-\infty}^{+\infty} J_{\nu+m}(\tau) J_{\nu-m}(\tau) = \delta_{m,0}, \qquad (3\text{-}13)$$

the expressions (3-8) and (3-9) can be written in the following form:

$$\Theta_{n,n+m}(\tau)=$$

$$=\begin{cases}\frac{T}{4}[\delta_{m,0}-(-1)^m J_m^2(\tau)+2\sum_{\nu=1-2n-m}^{0} J_{\nu+m}(\tau)J_{\nu-m}(\tau)], & \text{for } 2n>-m \quad (3\text{-}14)\\ \frac{T}{4}[\delta_{m,0}-(-1)^m J_m^2(\tau)], & \text{for } 2n=-m \quad (3\text{-}15)\\ \frac{T}{4}[\delta_{m,0}-(-1)^m J_m^2(\tau)-2\sum_{\nu=1}^{-2n-m} J_{\nu+m}(\tau)J_{\nu-m}(\tau)], & \text{for } 2n<-m \quad (3\text{-}16)\end{cases}$$

and

$$U_{n,n+m}(\tau)=$$

$$=\begin{cases}\frac{T}{4}[\delta_{m,0}-(-1)^m J_m^2(\tau)+2\sum_{\nu=-2n-m}^{0} J_{\nu+m}(\tau)J_{\nu-m}(\tau)], & \text{for } 2n>-m-1 \quad (3\text{-}17)\\ \frac{T}{4}[\delta_{m,0}-(-1)^m J_m^2(\tau)], & \text{for } 2n=-m-1 \quad (3\text{-}18)\\ \frac{T}{4}[\delta_{m,0}-(-1)^m J_m^2(\tau)-2\sum_{\nu=1}^{-1-2n-m} J_{\nu+m}(\tau)J_{\nu-m}(\tau)]. & \text{for } 2n<-m-1 \quad (3\text{-}19)\end{cases}$$

For $m=0$, we shall have:

$$\Theta_{n,n}(\tau)=\begin{cases}\frac{T}{4}[1+J_0^2(\tau)+2\sum_{\nu=1}^{2n-1} J_\nu^2(\tau)], & \text{for } n\geq 1 \quad (3\text{-}20)\\ \frac{T}{4}[1-J_0^2(\tau)], & \text{for } n=0 \quad (3\text{-}21)\\ \frac{T}{4}[1-J_0^2(\tau)-2\sum_{\nu=1}^{2|n|} J_\nu^2(\tau)], & \text{for } n\leq -1 \quad (3\text{-}22)\end{cases}$$

and

$$U_{n,n}(\tau)=\begin{cases}\frac{T}{4}[1+J_0^2(\tau)+2\sum_{\nu=1}^{2n} J_\nu^2(\tau)], & \text{for } n\geq 1 \quad (3\text{-}23)\\ \frac{T}{4}[1+J_0^2(\tau)], & \text{for } n=0 \quad (3\text{-}24)\\ \frac{T}{4}[1-J_0^2(\tau)-2\sum_{\nu=1}^{|2n+1|} J_\nu^2(\tau)]. & \text{for } n\leq -1 \quad (3\text{-}25)\end{cases}$$

Accordingly, from (3-20) ~ (3-25), the microscopic local temperatures (3-5) of the n-th particle will be obtained:

$$T_n(\tau)/T=\frac{1}{2}+\frac{J_0^2(\tau)}{2}+\sum_{\nu=1}^{2n-2} J_\nu^2(\tau)+\frac{3}{4}J_{2n-1}^2(\tau)+\frac{1}{4}J_{2n}^2(\tau), \quad \text{for } n\geq 1 \quad (3\text{-}26)$$

$$T_0(\tau)/T=\frac{1}{2}-\frac{J_0^2(\tau)}{4}-\frac{J_1^2(\tau)}{4}, \quad (3\text{-}27)$$

and

$$T_n(\tau)/T=\frac{1}{2}-\frac{J_0^2(\tau)}{2}-\sum_{\nu=1}^{-2n-1} J_\nu^2(\tau)-\frac{3}{4}J_{-2n}^2(\tau)-\frac{1}{4}J_{-2n+1}^2(\tau). \quad (3\text{-}28)$$

for $n\leq -1$

The expressions (3–20), (3–21), and (3–22), are essentitlly the same as those obtained by the solutions in trigonometric eigenfunctions.

For $0 \leq \forall\tau < +\infty$, we can see, from (3–20)～(3–25), the following relations:

(a) if $1 \leq l \leq n$,

$$\frac{T}{4} \leq \Theta_{l,l}(\tau) \leq \Theta_{n,n}(\tau) \leq \frac{T}{2}, \tag{3-29}$$

(b) if $n \leq l \leq 0$,

$$0 \leq \Theta_{n,n}(\tau) \leq \Theta_{l,l}(\tau) \leq \frac{T}{4}, \tag{3-30}$$

(c) if $0 \leq l \leq n$,

$$\frac{T}{4} \leq U_{l,l}(\tau) \leq U_{n,n}(\tau) \leq \frac{T}{2}, \tag{3-31}$$

(d) if $n \leq l \leq -1$,

$$0 \leq U_{n,n}(\tau) \leq U_{l,l}(\tau) \leq \frac{T}{4}. \tag{3-32}$$

In the case of $\tau \to +\infty$, the expressions (3–14)～(3–25) approach to the same stationary value of $(T/4)\delta_{m,0}$. In other words, the covariance matrices $\|\Theta_{n,n+m}(\tau)\|$ and $\|U_{n,n+m}(\tau)\|$ have vanishing off-diagonal elements at the final state: $\tau \to +\infty$; while their diagonal elements $\Theta_{n,n}(\tau)$ and $U_{n,n}(\tau)$ remain constant $T/4$ at $\tau = +\infty$.

From (3–10), (3–11), and (3–20)～(3–25), the kinetic and the potential energies of each particle approach to the same stationary value of $kT/4$ when τ goes to infinity.

As for the microscopic local temperature, we shall have the following results, after differentiating $T_n(\tau)$ with regard to τ:

$$\frac{d}{d\tau}T_n(\tau) = -\frac{T}{2}\left\{\frac{(2n-1)}{\tau}J^2_{2n-1}(\tau) + \frac{2n}{\tau}J^2_{2n}(\tau)\right\}, \quad \text{for } n \geq 1 \tag{3-33}$$

$$\left.\begin{aligned} &\frac{d}{d\tau}T_0(\tau) = \frac{T}{2\tau}J^2_1(\tau), \\ \text{and} \\ &\frac{d}{d\tau}T_n(\tau) = \frac{T}{2}\left\{\frac{(-2n)}{\tau}J^2_{-2n}(\tau) + \frac{(-2n+1)}{\tau}J^2_{-2n+1}(\tau)\right\}. \quad \text{for } n \leq -1 \end{aligned}\right\} \tag{3-34}$$

The right-hand side of (3–33) is always negative for positive τ, and the right-hand sides of (3–34) are positive for positive τ. Accordingly, we see that the terms $T_n(\tau)$ for any positive n are monotonously decreasing with increasing positive τ, while the expressions $T_n(\tau)$ for any non-positive n are monotonously increasing with increasing positive τ. In other words, the microscopic local temperature $T_n(\tau)$ of any particles at the positive sites are steadily decreasing with increasing positive τ, while the microscopic local temperature at the non-positive sites are steadily increasing with increasing positive τ.

For a sufficiently large τ, we can see from (3–26)～(3–28), (3–33) and (3–34):

$$\lim_{\tau \to +\infty} T_n(\tau) = \frac{T}{2}. \tag{3-35}$$

for any integers n. That is to say, the microscopic local temperature of each particle approaches to the same stationary value $T/2$ at $\tau=+\infty$.

In Fig. 6, the numerical values of $T_n(\tau)$ versus τ are plotted for some values of n.

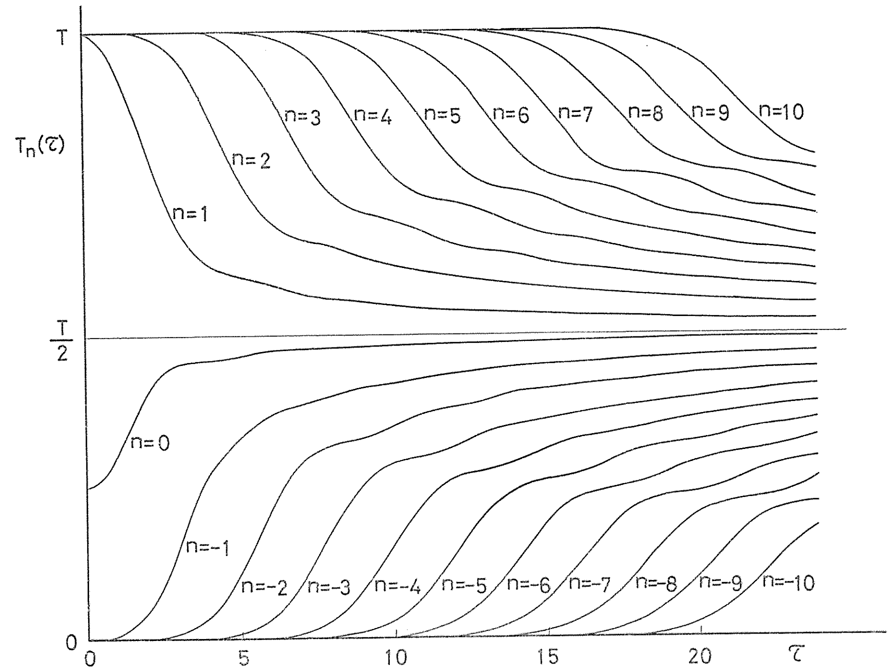

FIG. 6. Average value of microscopic local temperature versus time τ.

It is worth while remarking here that our results (3–20) ~ (3–22), (3–23) ~ (3–25) and (3–26) ~ (3–28) have similar properties to the solution:

$$\Theta(x,t)=\frac{T}{2}\left\{1+\frac{1}{a\sqrt{\pi t}}\int_0^x \exp[-x^2/(4a^2t)]dx\right\}, \tag{3-36}$$

of the classical equation of heat flow in an infinite rod:

$$\frac{\partial\Theta}{\partial t}=a^2\frac{\partial^2\Theta}{\partial x^2}, \tag{3-37}$$

with the initial condition:

$$\Theta(x,t=0)=\begin{cases}T, & \text{for } x>0\\ 0. & \text{for } x\leq 0\end{cases} \tag{3-38}$$

The expressions (3–20) ~ (3–22), (3–23) ~ (3–25), (3–26) ~ (3–28) and (3–36), represent the process of thermal conduction to establish a uniform temperature in the system. The solution (3–36) for $x<0$ increases monotonously and the solution (3–36) for $x>0$ decreases monotonously, with increasing time. From

(3–33) and (3–34), the microscopic local temperatures $T_n(\tau)$ also change monotonously, with increasing time, while, the energies (3–20) ~ (3–22) and (3–23) ~ (3–25) oscillate with increasing time (cf. Fig. 7). In brief, all the expressions mentioned above approach to the stationary value after a sufficiently long time. It should be added, however, that the timal behavior of (3–20) ~ (3–22) and (3–23) ~ (3–25) is essentially different from the process of thermal diffusion in a rod given by (3–36),

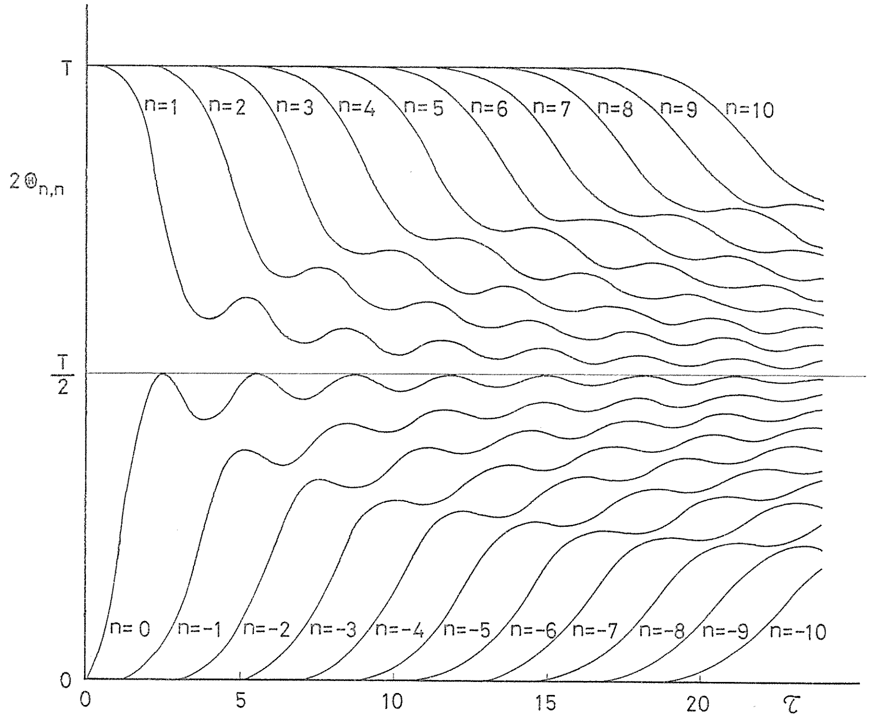

FIG. 7. Average value of thermal energy versus time τ.

while, the timal behavior of (3–26) ~ (3–28) is very simillar to the process of thermal diffusion in a rod. As shown in (3–33) and (3–34), the microscopic local temperatures $T_n(\tau)$ decrease monotonously for $n \geq 1$ and increase monotonously for $n \leq 0$, with increasing time (cf. Fig. 6). In this respect, the timal behavior of (3–28) is more similar to the process of thermal diffusion in a rod (3–36) than to that of (3–20) ~ (3–25).

§ 3.3 *Energy Flow in the System*

From the expression (3–12) and the following formula (cf. appendix 1), *viz.*:

$$\lim_{\tau \to +\infty} \sum_{k=1/2}^{+\infty+1/2} J_{k+\alpha}(\tau) J_{k-\alpha}(\tau) = \frac{\sin \pi\alpha}{2\pi\alpha}, \qquad (3\text{–}39)$$

$$k \in \{(\frac{1}{2} + \text{non-negative integers})\}$$

we find

$$\lim_{\tau\to+\infty} V_{n,m}(\tau) = T\cdot\frac{(-1)^m}{2\pi(2m+1)}. \tag{3-40}$$

In the case of $m=0$ and $m=-1$, we shall obtain:

$$\lim_{\tau\to+\infty} V_{n,0}(\tau) = \lim_{\tau\to+\infty} V_{n,-1}(\tau) = \frac{T}{2\pi}. \tag{3-41}$$

The energy flow from the n-th particle to the $(n-1)$-th particle is given by the rate of change of total energy contained in the system of particles in the right-hand side (in the positive side) of the n-th particle. Let us indicate the total energy in the positive side of the n-th particle with $E_n(\tau)$. Then we shall obtain,

$$E_n(\tau) = M\cdot\sum_{s=n}^{+\infty}\left\{\frac{1}{2}\dot{x}_s^2+\frac{\omega^2}{2}(x_{s+1}-x_s)^2\right\}. \tag{3-42}$$

Differentiating the expression (3–42) with regard to τ, we shall obtain:

$$\begin{aligned}-\frac{dE_n(\tau)}{d\tau} &= \frac{\sigma^2K}{2}\cdot\sum_{s=n}^{+\infty}\{y_{2s-1}(\tau)y_{2s}(\tau)-y_{2s+1}(\tau)y_{2s+2}(\tau)\}\\ &= \frac{\sigma^2K}{2}\cdot y_{2n-1}(\tau)y_{2n}(\tau).\end{aligned} \tag{3-43}$$

The above expression corresponds to the energy flow from the right-hand side of the n-th particle to the left-hand side of the $(n-1)$-th particle, and corresponds physically to the work done by the n-th particle upon the $(n-1)$-th particle. Calculating the average value of (3–43), we shall obtain:

$$\left\langle-\frac{dE_n(\tau)}{d\tau}\right\rangle_{Av} = kV_{n,-1}(\tau). \tag{3-44}$$

At the final state: $\tau=+\infty$, we shall obtain from (3–41) and (3–44),

$$\lim_{\tau\to+\infty}\left\langle-\frac{dE_n(\tau)}{d\tau}\right\rangle_{Av} = \frac{kT}{2\pi}. \tag{3-45}$$

This result serves to prove the existence of the instantaneous flow of energy $\lim_{t\to+\infty}\left\langle-\frac{dE_n(\tau)}{dt}\right\rangle_{Av}=\frac{k\omega T}{\pi}$ from the right-hand side to the left-hand side at every point of the system.

In brief, the kinetic and potential energies at every point of the system approach to the same stationary value of $kT/4$, while there exists the instantaneous flow of energy at every point throughout the system, at the final state: $\tau=+\infty$. That is to say, our system attains by no means to the thermodynamic equilibrium at $\tau=+\infty$.

IV. Effect of an Isotopic Impurity on the Energy Flow in a System of One-Dimensional Coupled Harmonic Oscillators

In this chapter, the authors investigate the effect of an impurity atom on the energy transport in a one-dimensional linear system of coupled harmonic oscillators. Let us assume an initial canonical ensemble of which half the system is at temperature T and other half at temperature zero, and calculate the correlation functions of particles in the system as functions of time. Thus, it is shown that the average kinetic and potential energies of each particle in the infinitely large system approach to stationary values, which are different, on either side of the impurity atom, and that the system approaches to a stationary state with a gap of energy distribution along the system at the impurity site. This result, it is to be noted, is essentially the same with that obtained by Kashiwamura and Teramoto[15] by means of the trigonometric eigenfunctions of the dynamical system.

Momentum-position correlation functions are also calculated. And from these the energy flow in the large system is derived, and it is also proved that after a sufficiently long time the finite energy flow still exists at every site in the system though there is no temperature gradient at that site.

A comparison is made in the following two cases:

a) oscillator system with an isotopic impurity of large mass,

b) oscillator system with an isotopic impurity of small mass.

The similarity and difference between the two systems at the final state are also discussed.

§ *4.1 Dynamical System*

We shall consider again the same model as we dealt with in the last chapter. Let us assume that only 0-th particle has mass M' (cf. Fig. 8), which is different from the mass M of the other particles, *viz.* the mother crystal.

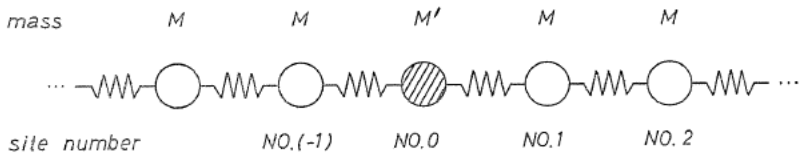

FIG. 8. Linear lattice with one impurity atom.

The equations of motion will be

$$\frac{d^2}{dt^2} x_i(t) = \omega_0^2\Big(1-\frac{Q}{1+Q}\delta_{i,0}\Big)\cdot\{x_{i+1}(t)-2x_i(t)+x_{i-1}(t)\}, \tag{4-1}$$

with the displacement of the i-th particle $x_i(t)$ and $Q=\frac{M'}{M}-1$. By means of the Schrödinger coordinates defined by (2–2), the equations (4–1) can be rewritten in the form:

$$2\frac{d}{d\tau}y_n(\tau) = \Big(1-\frac{Q}{1+Q}\delta_{n,0}\Big)\{y_{n+1}(\tau)-y_{n-1}(\tau)\}, \tag{4-2}$$

for any integers n.

Now let us try to solve the equations (4–2). Introducing the generating function:

$$F(z\,;\,\tau) = \sum_{n=-\infty}^{+\infty} y_n(\tau)\cdot z^n, \tag{4-3}$$

and applying the operation: $\sum_{n=-\infty}^{+\infty} z^n$ to the equations (4–2), we shall obtain

$$2\frac{d}{d\tau}F(z\,;\,\tau) = \left(\frac{1}{z} - z\right)\cdot F(z\,;\,\tau) - 2\,Q\cdot\frac{d}{d\tau}y_0(\tau). \tag{4-4}$$

The differential equation (4–4) will lead us to:

$$F(z\,;\,\tau) = \sum_{n,\,\mu=-\infty}^{+\infty} z^n J_{\mu-n}(\tau)\Big[a_\mu - Q\int_0^\tau J_\mu(x)\cdot\frac{d}{dx}y_0(x)\cdot dx\Big]. \tag{4-5}$$

where a_ν is the initial values of $y_\nu(\tau)$, and $J_k(\tau)$ is Bessel function of order k and argument τ.

Comparing (4–3) with (4–5), we shall have

$$y_n(\tau) = \sum_{\mu=-\infty}^{+\infty} J_{\mu-n}(\tau)\cdot\Big[a_\mu - Q\int_0^\tau J_\mu(x)\cdot\frac{d}{dx}y_0(x)\cdot dx\Big]. \tag{4-6}$$

By partial integration and by exchanging integration and summation in (4–6), we shall obtain

$$y_n(\tau)\cdot(1+Q\delta_{n,0}) = \sum_{\mu=-\infty}^{+\infty} a_\mu J_{\mu-n}(\tau)\cdot(1+Q\delta_{\mu,0}) + Q\int_0^\tau y_0(x)\cdot\frac{d}{dx}J_n(x-\tau)\cdot dx, \tag{4-7}$$

where the following formula is used:

$$J_k(y+z) = \sum_{m=-\infty}^{+\infty} J_m(y)\cdot J_{k-m}(z).$$

Put $n=0$ in (4–7), and we shall obtain:

$$y_0(\tau) - \frac{Q}{1+Q}\int_0^\tau y_0(x)\cdot J_1(\tau-x)\cdot dx = \frac{1}{1+Q}\cdot\sum_{\mu=-\infty}^{+\infty} a_\mu J_\mu(\tau)(1+Q\delta_{\mu,0}), \tag{4-8}$$

The integral equation (4–8) can be solved and we shall have its solution as follows (cf. Appendix 2):

$$\begin{aligned} y_0(\tau) = \frac{1}{1+Q}\cdot\sum_{\mu=-\infty}^{+\infty}(1+Q\delta_{\mu,0})\cdot a_\mu\cdot\Big\{J_\mu(\tau) + \\ + (-1)^{\mu\varepsilon(-\mu)}\cdot\sum_{m=1}^{+\infty}\Big(\frac{2\,Q}{1+Q}\Big)^m\cdot\sum_{k_i=0}^{+\infty}(-1)^{k_1+k_2+\,\dots\,+k_m} J_{|\mu|+2m+2(k_1+\,\dots\,+k_m)}(\tau)\Big\}. \end{aligned} \tag{4-9}$$

where

$$\varepsilon(k) = \begin{cases} 1, & \text{for } k \geq 1 \\ 0. & \text{for } k \leq 0 \end{cases}$$

Substituting (4–9) for (4–7), we shall obtain the final solutions of the difference-differential equations (4–2) in the following form (cf. Appendix 3):

$$y_n(\tau) = \frac{1}{1+Q\delta_{n,0}} \cdot \sum_{\mu=-\infty}^{+\infty} (1+Q\delta_{\mu,0}) \cdot a_\mu \cdot \Big[J_{\mu-n}(\tau) + (-1)^{(n+1)\varepsilon(n)+\mu\varepsilon(-\mu)} \times$$

$$\times \frac{Q}{1+Q} \cdot \sum_{p=1}^{+\infty} \left(\frac{Q-1}{Q+1}\right)^{p-1} \cdot \{ J_{|n-1|+|\mu|+2p-1}(\tau) - (-1)^{\delta_{n,0}} \cdot J_{|n+1|+|\mu|+2p-1}(\tau) \} \Big], \quad (4\text{-}10)$$

$$\text{for } -\infty < n < +\infty$$

with initial values a_ν of $y_\nu(\tau)$.

The series appearing in p-summation in (4–10) are essentially the same as Lommel's functions[28] of two variables $U_n(w, z)$ and $V_n(w, z)$, which are defined by:

$$U_n(w, z) = \sum_{m=0}^{+\infty} (-1)^m \left(\frac{w}{z}\right)^{n+2m} J_{n+2m}(z),$$

and

$$V_n(w, z) = \sum_{m=0}^{+\infty} (-1)^m \left(\frac{w}{z}\right)^{-n-2m} J_{-n-2m}(z),$$

with $w = cz$.

If the mass M' of the isotopic impurity particle at site No. 0 is greater than the mass M of other particles, *i.e.* if $Q>0$, then we can easily see that the functions expressed in p-summation in (4–10) are convergent and that we can calculate correlation functions by means of (4–10).

While, if M' is smaller than M, *i.e.* if $-1<Q<0$ and accordingly

$$\sqrt{\frac{1-Q}{1+Q}} > 1,$$

then Lommel's function of two variables appearing in p-summation in (4–10):

$$U_n(cz, z) = \sum_{p=0}^{+\infty} (-1)^p \cdot \left(\frac{cz}{z}\right)^{2p+n} J_{2p+n}(z),$$

is convergent, and for $c>1$ it is oscillatory at $z=+\infty$. Accordingly we should treat the term more carefully.

Using the formula (cf. Appendix 4):

$$\sum_{p=1}^{+\infty} \sqrt{r}^{\,2p} J_{2p+s}(z) = \frac{1}{2\sqrt{r}^{\,s}} \Big[\exp\Big\{ \frac{z}{2}\Big(\sqrt{r} - \frac{1}{\sqrt{r}}\Big)\Big\} +$$

$$+ (-1)^s \exp\Big\{ -\frac{z}{2}\Big(\sqrt{r} - \frac{1}{\sqrt{r}}\Big)\Big\} \Big] - \sum_{p=0}^{+\infty} \sqrt{r}^{\,-2p} J_{s-2p}(z), \quad (4\text{-}11)$$

for any integers s, we can rewrite (4–10) as follows:

$$y_n(\tau) = \frac{1}{1+Q\delta_{n,0}} \cdot \sum_{\mu=-\infty}^{+\infty} (1+Q\delta_{\mu,0}) a_\mu \Big[J_{\mu-n}(\tau) +$$

$$+ (-1)^{(n+1)\varepsilon(n)+\mu\varepsilon(-\mu)} \cdot \frac{Q}{1+Q} \Big[\frac{1}{2} \Big\{ \exp\Big(\frac{i\tau}{\sqrt{1-Q^2}}\Big) + (-1)^{n+\mu} \cdot \exp\Big(\frac{-i\tau}{\sqrt{1-Q^2}}\Big) \Big\} \times$$

$$\times \Big\{ \Big(\frac{Q+1}{Q-1}\Big)^{(|n-1|+|\mu|+1)/2} - (-1)^{\delta_{n,0}} \cdot \Big(\frac{Q+1}{Q-1}\Big)^{(|n+1|+|\mu|+1)/2} \Big\} -$$

$$- \sum_{p=0}^{+\infty} \Big(\frac{Q+1}{Q-1}\Big)^{p+1} \cdot \{ J_{|n-1|+|\mu|-2p-1}(\tau) - (-1)^{\delta_{n,0}} \cdot J_{|n+1|+|\mu|-2p-1}(\tau) \} \Big] \Big]. \quad (4\text{-}12)$$

After simple calculation, we shall find that the expressions (4–10) and (4–12) coincide completely with the results obtained by Kashiwamura[23], which are derived by means of the trigonometric eigenfunctions (normal modes) of the dynamical system for the perfect lattice. But the method used in the present paper is simpler and easier to understand than that by means of the trigonometric eigenfunctions of the system.

§ 4. 2 *Correlation Functions*

Now, we shall take again the initial ensemble (3–1) and (3–2), *i.e.*

$$a_0 = a_{-1} = a_{-2} = \cdots = 0, \tag{3-1}$$

and

$$W(a_1, a_2, a_3, \ldots) = \prod_{\nu} \sqrt{\frac{\sigma^2 K}{2\pi kT}} \cdot \exp\left[-\frac{\sigma^2 K}{2kT} a_\nu^2\right]. \tag{3-2}$$

Accordingly, we shall have

$$\langle a_m \cdot a_n \rangle_{Av} = \left\{ \begin{array}{ll} \dfrac{kT}{\sigma^2 K}\delta_{m,n}, & \text{for } m \geq 1 \text{ and } n \geq 1 \\ 0. & \text{for } m \leq 0 \text{ or } n \leq 0 \end{array} \right\} \tag{3-3}$$

The correlation functions can be calculated from (3–3), (4–10), and (4–12).

Case of an Isotopic Impurity of Large Mass

The mass M' of the isotopic impurity particle is greater than the mass M of the other particles, *i.e.* $Q>0$. In this case, from (3–3) and (4–10), we shall obtain the correlation functions as follows:

$$\begin{aligned} C_{m,n}(\tau) = &\frac{T}{2} \cdot \frac{1}{(1+Q\delta_{m,0})(1+Q\delta_{n,0})} \cdot \sum_{\nu=1}^{+\infty}\Big[J_{\nu-m}J_{\nu-n} + \\ &+(-1)^{(n+1)\varepsilon(n)} \cdot \frac{Q}{Q+1} \cdot \sum_{p=1}^{+\infty}\left(\frac{Q-1}{Q+1}\right)^{p-1} J_{\nu-m}\{J_{\nu+|n-1|+2p-1} - (-1)^{\delta_{n,0}} J_{\nu+|n+1|+2p-1}\} + \\ &+(-1)^{(m+1)\varepsilon(m)} \cdot \frac{Q}{Q+1} \cdot \sum_{p=1}^{+\infty}\left(\frac{Q-1}{Q+1}\right)^{p-1} J_{\nu-n}\{J_{\nu+|m-1|+2p-1} - (-1)^{\delta_{m,0}} J_{\nu+|m+1|+2p-1}\} + \\ &+(-1)^{(m+1)\varepsilon(m)+(n+1)\varepsilon(n)} \cdot \left(\frac{Q}{Q+1}\right)^2 \cdot \sum_{p,q=1}^{+\infty}\left(\frac{Q-1}{Q+1}\right)^{p+q-2} \{J_{\nu+|m-1|+2p-1}J_{\nu+|n-1|+2q-1} - \\ &-(-1)^{\delta_{m,0}} J_{\nu+|m+1|+2p-1}J_{\nu+|n-1|+2q-1} - (-1)^{\delta_{n,0}} J_{\nu+|m-1|+2p-1}J_{\nu+|n+1|+2q-1} + \\ &+(-1)^{\delta_{m,0}+\delta_{n,0}} J_{\nu+|m+1|+2p-1}J_{\nu+|n+1|+2q-1}\}\Big], \end{aligned} \tag{4-13}$$

and

$$\begin{aligned} C_{n,n}(\tau) = &\frac{T}{2} \cdot \frac{1}{(1+Q\delta_{n,0})^2} \cdot \sum_{\nu=1}^{+\infty}\Big[J_{\nu-n}^2 + \left(\frac{Q}{Q+1}\right)^2 \sum_{p,q=1}^{+\infty}\left(\frac{Q-1}{Q+1}\right)^{p+q-2} \{J_{\nu+|n-1|+2p-1} \times \\ &\times J_{\nu+|n-1|+2q-1} - 2(-1)^{\delta_{n,0}} J_{\nu+|n+1|+2p-1}J_{\nu+|n-1|+2q-1} + J_{\nu+|n+1|+2p-1}J_{\nu+|n+1|+2q-1}\} + \\ &+(-1)^{(n+1)\varepsilon(n)} \cdot \frac{2Q}{Q+1} \cdot J_{\nu-n} \cdot \sum_{p=1}^{+\infty}\left(\frac{Q-1}{Q+1}\right)^{p-1} \{J_{\nu+|n-1|+2p-1} - (-1)^{\delta_{n,0}} J_{\nu+|n+1|+2p-1}\}\Big]. \end{aligned} \tag{4-13'}$$

for any integers m and n, with $J_\alpha = J_\alpha(\tau)$.
We shall obtain:

(i) for $n \geq 1$,

$$C_{n,n} = \frac{T}{2} \cdot \sum_{\nu=1}^{+\infty} \Big[J_{\nu-n}^2 + \Big(\frac{Q}{Q+1}\Big)^2 \cdot \sum_{p,q=1}^{+\infty} \Big(\frac{Q-1}{Q+1}\Big)^{p+q-2} \{J_{\nu+n+2p-2} J_{\nu+n+2q-2} - - 2 J_{\nu+n+2p} J_{\nu+n+2q-2} + J_{\nu+n+2p} J_{\nu+n+2q}\} + + (-1)^{n+1} \cdot \frac{2Q}{Q+1} \cdot J_{\nu-n} \cdot \sum_{p=1}^{+\infty} \Big(\frac{Q-1}{Q+1}\Big)^{p-1} \{J_{\nu+n+2p-2} - J_{\nu+n+2p}\} \Big], \tag{4-14}$$

(ii) for $n = 0$,

$$C_{0,0}(\tau) = \frac{T}{2} \cdot \frac{1}{(1+Q)^2} \cdot \sum_{\nu=1}^{+\infty} \Big[J_\nu^2 + 4\Big(\frac{Q}{Q+1}\Big)^2 \cdot \sum_{p,q=1}^{+\infty} \Big(\frac{Q-1}{Q+1}\Big)^{p+q-2} J_{\nu+2p} J_{\nu+2q} + + \frac{4Q}{Q+1} \cdot J_\nu \cdot \sum_{p=1}^{+\infty} \Big(\frac{Q-1}{Q+1}\Big)^{p-1} J_{\nu+2p} \Big], \tag{4-15}$$

(iii) for $n \leq -1$,

$$C_{n,n}(\tau) = \frac{T}{2} \cdot \sum_{\nu=1}^{+\infty} \Big[J_{\nu-n}^2 + \Big(\frac{Q}{Q+1}\Big)^2 \cdot \sum_{p,q=1}^{+\infty} \Big(\frac{Q-1}{Q+1}\Big)^{p+q-2} \{J_{\nu-n+2p} J_{\nu-n+2q} - - 2 J_{\nu-n+2p-2} J_{\nu-n+2q} + J_{\nu-n+2p-2} J_{\nu-n+2q-2}\} + + \frac{2Q}{Q+1} \cdot J_{\nu-n} \cdot \sum_{p=1}^{+\infty} \Big(\frac{Q-1}{Q+1}\Big)^{p-1} \{J_{\nu-n+2p} - J_{\nu-n+2p-2}\} \Big]. \tag{4-16}$$

Case of an Isotopic Impurity of Small Mass

For $M'<M$, *i.e.* for $-1<Q<0$, we obtain, from (3–3) and (4–12),

$$\begin{aligned} C_{m,n}(\tau) = {} & \frac{T}{2} \cdot \frac{1}{(1+Q\delta_{m,0})(1+Q\delta_{n,0})} \cdot \sum_{\nu=1}^{+\infty} \Big[J_{\nu-m} J_{\nu-n} + \\ & + \frac{Q^2(-1)^{(m+1)\delta(m)+(n+1)\delta(n)}}{4(1+Q)^2} \cdot \gamma(m) \cdot \gamma(n) \cdot \{[\exp(+)]^2 + (-1)^{m+n} \times \\ & \qquad \times [\exp(-)]^2\} \cdot \Big(\frac{Q+1}{Q-1}\Big)^\nu + \\ & + \frac{Q^2(-1)^{\nu+(m+1)\delta(m)+(n+1)\delta(n)}}{4(1+Q)^2} \cdot \{(-1)^m + (-1)^n\} \cdot \gamma(m) \cdot \gamma(n) \cdot \Big(\frac{Q+1}{Q-1}\Big)^\nu + \\ & + \frac{Q(-1)^{(n+1)\delta(n)}}{2(1+Q)} \cdot \gamma(n) \cdot \exp(+) \cdot \Big(\frac{Q+1}{Q-1}\Big)^{\nu/2} \cdot J_{\nu-m} \\ & + \frac{Q(-1)^{(m+1)\delta(m)}}{2(1+Q)} \cdot \gamma(m) \cdot \exp(+) \cdot \Big(\frac{Q+1}{Q-1}\Big)^{\nu/2} \cdot J_{\nu-m} \\ & + \frac{Q(-1)^{\nu+n+(n+1)\delta(n)}}{2(1+Q)} \cdot \gamma(n) \cdot \exp(-) \cdot \Big(\frac{Q+1}{Q-1}\Big)^{\nu/2} \cdot J_{\nu-m} \\ & + \frac{Q(-1)^{\nu+m+(m+1)\delta(m)}}{2(1+Q)} \cdot \gamma(m) \cdot \exp(-) \cdot \Big(\frac{Q+1}{Q-1}\Big)^{\nu/2} \cdot J_{\nu-n} \\ & - \frac{Q(-1)^{(n+1)\delta(n)}}{1+Q} \cdot \xi(1, \nu+|n-1|-1) \cdot J_{\nu-m} - \frac{Q(-1)^{(m+1)\delta(m)}}{1+Q} \times \\ & \qquad \times \xi(1, \nu+|m-1|-1) \cdot J_{\nu-n} \end{aligned}$$

$$+\frac{Q(-1)^{\delta_{n,0}+(n+1)\delta(n)}}{1+Q}\cdot\xi(1,\nu+|n+1|-1)\cdot J_{\nu-m}+\frac{Q(-1)^{\delta_{m,0}+(m+1)\delta(m)}}{1+Q}\times$$

$$\times\xi(1,\nu+|m+1|-1)\cdot J_{\nu-n}$$

$$-\frac{Q^2(-1)^{(m+1)\delta(m)+(n+1)\delta(n)}}{2(1+Q)^2}\cdot\gamma(m)\cdot\exp(+)\cdot\xi\left(\frac{\nu}{2}+1,\nu+|n-1|-1\right)$$

$$+\frac{Q^2(-1)^{\delta_{n,0}+(m+1)\delta(m)+(n+1)\delta(n)}}{2(1+Q)^2}\cdot\gamma(m)\cdot\exp(+)\cdot\xi\left(\frac{\nu}{2}+1,\nu+|n+1|-1\right)$$

$$-\frac{Q^2(-1)^{(m+1)\delta(m)+(n+1)\delta(n)}}{2(1+Q)^2}\cdot\gamma(n)\cdot\exp(+)\cdot\xi\left(\frac{\nu}{2}+1,\nu+|m-1|-1\right)$$

$$+\frac{Q^2(-1)^{\delta_{m,0}+(m+1)\delta(m)+(n+1)\delta(n)}}{2(1+Q)^2}\cdot\gamma(n)\cdot\exp(+)\cdot\xi\left(\frac{\nu}{2}+1,\nu+|m+1|-1\right)$$

$$-\frac{Q^2(-1)^{\nu+m+(m+1)\delta(m)+(n+1)\delta(n)}}{2(1+Q)^2}\cdot\gamma(m)\cdot\exp(-)\cdot\xi\left(\frac{\nu}{2}+1,\nu+|n-1|-1\right)$$

$$+\frac{Q^2(-1)^{\nu+m+\delta_{n,0}+(m+1)\delta(m)+(n+1)\delta(n)}}{2(1+Q)^2}\cdot\gamma(m)\cdot\exp(-)\cdot\xi\left(\frac{\nu}{2}+1,\nu+|n+1|-1\right)$$

$$-\frac{Q^2(-1)^{\nu+n+(m+1)\delta(m)+(n+1)\delta(n)}}{2(1+Q)^2}\cdot\gamma(n)\cdot\exp(-)\cdot\xi\left(\frac{\nu}{2}+1,\nu+|m-1|-1\right)$$

$$+\frac{Q^2(-1)^{\nu+n+\delta_{m,0}+(m+1)\delta(m)+(n+1)\delta(n)}}{2(1+Q)^2}\cdot\gamma(n)\cdot\exp(-)\cdot\xi\left(\frac{\nu}{2}+1,\nu+|m+1|-1\right)$$

$$+\frac{Q^2(-1)^{(m+1)\delta(m)+(n+1)\delta(n)}}{(1+Q)^2}\cdot\xi(1,\nu+|n-1|-1)\cdot\xi(1,\nu+|m-1|-1)$$

$$-\frac{Q^2(-1)^{\delta_{n,0}+(m+1)\delta(m)+(n+1)\delta(n)}}{(1+Q)^2}\cdot\xi(1,\nu+|n+1|-1)\cdot\xi(1,\nu+|m-1|-1)$$

$$-\frac{Q^2(-1)^{\delta_{m,0}+(m+1)\delta(m)+(n+1)\delta(n)}}{(1+Q)^2}\cdot\xi(1,\nu+|n-1|-1)\cdot\xi(1,\nu+|m+1|-1)$$

$$+\frac{Q^2(-1)^{\delta_{m,0}+\delta_{n,0}+(m+1)\delta(m)+(n+1)\delta(n)}}{(1+Q)^2}\cdot\xi(1,\nu+|n+1|-1)\cdot\xi(1,\nu+|m+1|-1)\Bigg].\tag{4-17}$$

and

$$C_{n,n}(\tau)=\frac{T}{2}\cdot\frac{1}{(1+Q\delta_{n,0})^2}\cdot\sum_{\nu=1}^{+\infty}\Bigg[J_{\nu-n}^2+\frac{Q^2}{2(1+Q)^2}\cdot\{\gamma(n)\}^2\cdot\cos\frac{2\tau}{\sqrt{1-Q^2}}\cdot\left(\frac{Q+1}{Q-1}\right)^{\nu}$$

$$+\frac{Q^2(-1)^{\nu+n}}{2(1+Q)^2}\cdot\{\gamma(n)\}^2\cdot\left(\frac{Q+1}{Q-1}\right)^{\nu}+\frac{Q(-1)^{(n+1)\delta(n)}}{1+Q}\cdot\gamma(n)\cdot\exp(+)\cdot\left(\frac{Q+1}{Q-1}\right)^{\nu/2}\cdot J_{\nu-n}$$

$$+\frac{Q(-1)^{\nu+n+(n+1)\delta(n)}}{1+Q}\cdot\gamma(n)\cdot\exp(-)\cdot\left(\frac{Q+1}{Q-1}\right)^{\nu/2}\cdot J_{\nu-n}-\frac{2Q(-1)^{(n+1)\delta(n)}}{1+Q}\times$$

$$\times\xi(1,\nu+|n-1|-1)\cdot J_{\nu-n}$$

$$+\frac{2Q(-1)^{\delta_{n,0}+(n+1)\delta(n)}}{1+Q}\cdot\xi(1,\nu+|n+1|-1)\cdot J_{\nu-n}-\frac{Q^2}{(1+Q)^2}\cdot\gamma(n)\cdot\exp(+)\times$$

$$\times\xi\left(\frac{\nu}{2}+1,\nu+|n-1|-1\right)$$

$$+\frac{Q^2(-1)^{\delta_{n,0}}}{(1+Q)^2}\cdot\gamma(n)\cdot\exp(+)\cdot\xi\left(\frac{\nu}{2}+1,\nu+|n+1|-1\right)$$

$$- \frac{Q^2(-1)^{\nu+n}}{(1+Q)^2} \cdot \gamma(n) \cdot \exp(-) \cdot \xi\Big(\frac{\nu}{2}+1, \nu+|n-1|-1\Big)$$

$$+ \frac{Q^2(-1)^{\nu+n+\delta_{n,0}}}{(1+Q)^2} \cdot \gamma(n) \cdot \exp(-) \cdot \xi\Big(\frac{\nu}{2}+1, \nu+|n+1|-1\Big)$$

$$+ \frac{Q^2}{(1+Q)^2} \cdot \{\xi(1, \nu+|n-1|-1\}^2 - \frac{2Q^2(-1)^{\delta_{n,0}}}{(1+Q)^2} \cdot \xi(1, \nu+|n-1|-1) \times \xi(1, \nu+|n+1|-1)$$

$$+ \frac{Q^2}{(1+Q)^2} \cdot \{\xi(1, \nu+|n+1|-1)\}^2\Big]. \qquad (4\text{-}18)$$

for any integers m and n, with

$$\gamma(m) = \gamma^{(|m-1|+1)/2} - (-1)^{\delta_{m,0}} \cdot \gamma^{(|m+1|+1)/2},$$

$$\exp(\pm) = \exp\Big(\frac{\pm i\tau}{\sqrt{1-Q^2}}\Big),$$

$$\xi(\alpha, \beta) = \sum_{p=0}^{+\infty} \Big(\frac{Q+1}{Q-1}\Big)^{p+\alpha} J_{\beta-2p}, \qquad J_s = J_s(\tau),$$

and

$$\delta(m) = \begin{cases} 1, & \text{for} \quad m \geq 1 \\ 0. & \text{for} \quad m \leq 0 \end{cases}$$

We shall obtain:

(i) for $n \geq 1$,

$$C_{n,n}(\tau) = \frac{T}{2} \cdot \sum_{\nu=1}^{+\infty} \Big[J_{\nu-n}^2 + \frac{2Q^2}{(1-Q^2)^2} \cdot \Big(\frac{Q+1}{Q-1}\Big)^{\nu+n} \cdot \cos\frac{2\tau}{\sqrt{1-Q^2}} + \frac{2Q^2(-1)^{\nu+n}}{(1-Q^2)^2} \cdot \Big(\frac{Q+1}{Q-1}\Big)^{\nu+n}$$

$$+ \frac{2Q(-1)^{n+1}}{1-Q^2} \cdot \Big(\frac{Q+1}{Q-1}\Big)^{(\nu+n)/2} \cdot \exp\Big(\frac{i\tau}{\sqrt{1-Q^2}}\Big) \cdot J_{\nu-n} - \frac{2Q(-1)^{\nu}}{1-Q^2} \cdot \Big(\frac{Q+1}{Q-1}\Big)^{(\nu+n)/2} \times \exp\Big(\frac{-i\tau}{\sqrt{1-Q^2}}\Big) \cdot J_{\nu-n}$$

$$- \frac{2Q(-1)^{n+1}}{1+Q} \cdot \sum_{p=0}^{+\infty} \Big(\frac{Q+1}{Q-1}\Big)^{p+1} J_{\nu-2p+n-2} J_{\nu-n} + \frac{2Q(-1)^{n+1}}{1+Q} \cdot \sum_{p=0}^{+\infty} \Big(\frac{Q+1}{Q-1}\Big)^{p+1} J_{\nu-2p+n} J_{\nu-n}$$

$$- \frac{2Q^2}{(1-Q)(1+Q)^2} \cdot \Big(\frac{Q+1}{Q-1}\Big)^{(\nu+n)/2} \cdot \exp\Big(\frac{i\tau}{\sqrt{1-Q^2}}\Big) \cdot \sum_{p=0}^{+\infty} \Big(\frac{Q+1}{Q-1}\Big)^{p+1} J_{\nu-2p+n-2}$$

$$+ \frac{2Q^2}{(1-Q)(1+Q)^2} \cdot \Big(\frac{Q+1}{Q-1}\Big)^{(\nu+n)/2} \cdot \exp\Big(\frac{i\tau}{\sqrt{1-Q^2}}\Big) \cdot \sum_{p=0}^{+\infty} \Big(\frac{Q+1}{Q-1}\Big)^{p+1} J_{\nu-2p+n}$$

$$- \frac{2Q^2(-1)^{\nu+n}}{(1-Q)(1+Q)^2} \cdot \Big(\frac{Q+1}{Q-1}\Big)^{(\nu+n)/2} \cdot \exp\Big(\frac{i\tau}{\sqrt{1-Q^2}}\Big) \cdot \sum_{p=0}^{+\infty} \Big(\frac{Q+1}{Q-1}\Big)^{p+1} J_{\nu-2p+n-2}$$

$$+ \frac{2Q^2(-1)^{\nu+n}}{(1-Q)(1+Q)^2} \cdot \Big(\frac{Q+1}{Q-1}\Big)^{(\nu+n)/2} \cdot \exp\Big(\frac{-i\tau}{\sqrt{1-Q^2}}\Big) \cdot \sum_{p=0}^{+\infty} \Big(\frac{Q+1}{Q-1}\Big)^{p+1} J_{\nu-2p+n}$$

$$+ \frac{Q^2}{(1+Q)^2} \cdot \sum_{p,q=0}^{+\infty} \Big(\frac{Q+1}{Q-1}\Big)^{p+q+2} J_{\nu-2p+n-2} J_{\nu-2q+n-2}$$

$$- \frac{2Q^2}{(1+Q)^2} \cdot \sum_{p,q=0}^{+\infty} \Big(\frac{Q+1}{Q-1}\Big)^{p+q+2} J_{\nu-2p+n-2} J_{\nu-2q+n}$$

$$+ \frac{Q^2}{(1+Q)^2} \cdot \sum_{p,q=0}^{+\infty} \Big(\frac{Q+1}{Q-1}\Big)^{p+q+2} J_{\nu-2p+n} J_{\nu-2q+n} \Big], \qquad (4\text{-}19)$$

(ii) for $n = 0$,

$$C_{0,0}(\tau) = \frac{T}{2}\cdot\frac{1}{(1+Q)^2}\cdot\sum_{\nu=1}^{+\infty}\Big[J_\nu^2 + \frac{2Q^2}{(1+Q)^2}\cdot\Big(\frac{Q+1}{Q-1}\Big)^{\nu+2}\cdot\cos\frac{2\tau}{\sqrt{1-Q^2}} + \frac{2Q^2(-1)^\nu}{(1+Q)^2}\cdot\Big(\frac{Q+1}{Q-1}\Big)^{\nu+2}$$

$$+\frac{2Q}{1+Q}\cdot\Big(\frac{Q+1}{Q-1}\Big)^{(\nu/2)+2}\cdot\exp\Big(\frac{i\tau}{\sqrt{1-Q^2}}\Big)\cdot J_{\nu-n} + \frac{2Q(-1)^\nu}{1+Q}\cdot\Big(\frac{Q+1}{Q-1}\Big)^{(\nu/2)+2}\cdot\exp\Big(\frac{-i\tau}{\sqrt{1-Q^2}}\Big)\cdot J_{\nu-n}$$

$$-\frac{4Q}{1+Q}\cdot\sum_{p=0}^{+\infty}\Big(\frac{Q+1}{Q-1}\Big)^{p+1}J_{\nu-2p}J_\nu - \frac{4Q^2}{(1+Q)^2}\cdot\Big(\frac{Q+1}{Q-1}\Big)^{(\nu/2)+2}\cdot\exp\Big(\frac{i\tau}{\sqrt{1-Q^2}}\Big)\cdot\sum_{p=0}^{+\infty}\Big(\frac{Q+1}{Q-1}\Big)^{p+1}J_{\nu-2p}$$

$$-\frac{4Q^2(-1)^\nu}{(1+Q)^2}\cdot\Big(\frac{Q+1}{Q-1}\Big)^{(\nu/2)+2}\cdot\exp\Big(\frac{-i\tau}{\sqrt{1-Q^2}}\Big)\cdot\sum_{p=0}^{+\infty}\Big(\frac{Q+1}{Q-1}\Big)^{p+1}J_{\nu-2p} + \frac{4Q^2}{(1+Q)^2}\times$$

$$\times\sum_{p,q=0}^{+\infty}\Big(\frac{Q+1}{Q-1}\Big)^{p+q+2}\cdot J_{\nu-2p}J_{\nu-2q}\Big], \qquad (4\text{-}20)$$

(iii) for $n \leq -1$,

$$C_{n,n}(\tau) = \frac{T}{2}\cdot\sum_{\nu=1}^{+\infty}\Big[J_{\nu-n}^2 + \frac{2Q^2}{(1-Q^2)^2}\cdot\Big(\frac{Q+1}{Q-1}\Big)^{\nu-n}\cdot\cos\frac{2\tau}{\sqrt{1-Q^2}} + \frac{2Q^2(-1)^{\nu+n}}{(1-Q^2)^2}\cdot\Big(\frac{Q+1}{Q-1}\Big)^{\nu-n}$$

$$-\frac{2Q}{1-Q^2}\cdot\Big(\frac{Q+1}{Q-1}\Big)^{(\nu-n)/2}\cdot\exp\Big(\frac{i\tau}{\sqrt{1-Q^2}}\Big)\cdot J_{\nu-n} - \frac{2Q(-1)^{\nu+n}}{1-Q^2}\cdot\Big(\frac{Q+1}{Q-1}\Big)^{(\nu-n)/2}\times$$

$$\times\exp\Big(\frac{-i\tau}{\sqrt{1-Q^2}}\Big)\cdot J_{\nu-n}$$

$$-\frac{2Q}{1+Q}\cdot\sum_{p=0}^{+\infty}\Big(\frac{Q+1}{Q-1}\Big)^{p+1}J_{\nu-2p-n}J_{\nu-n} + \frac{2Q}{1+Q}\cdot\sum_{p=0}^{+\infty}\Big(\frac{Q+1}{Q-1}\Big)^{p+1}J_{\nu-2p-n-2}J_{\nu-n}$$

$$+\frac{2Q^2}{(1-Q)(1+Q)^2}\cdot\Big(\frac{Q+1}{Q-1}\Big)^{(\nu-n)/2}\cdot\exp\Big(\frac{i\tau}{\sqrt{1-Q^2}}\Big)\cdot\sum_{p=0}^{+\infty}\Big(\frac{Q+1}{Q-1}\Big)^{p+1}J_{\nu-2p-n}$$

$$-\frac{2Q^2}{(1-Q)(1+Q)^2}\cdot\Big(\frac{Q+1}{Q-1}\Big)^{(\nu-n)/2}\cdot\exp\Big(\frac{i\tau}{\sqrt{1-Q^2}}\Big)\cdot\sum_{p=0}^{+\infty}\Big(\frac{Q+1}{Q-1}\Big)^{p+1}J_{\nu-2p-n-2}$$

$$+\frac{2Q^2(-1)^{\nu+n}}{(1-Q)(1+Q)^2}\cdot\Big(\frac{Q+1}{Q-1}\Big)^{(\nu-n)/2}\cdot\exp\Big(\frac{-i\tau}{\sqrt{1-Q^2}}\Big)\cdot\sum_{p=0}^{+\infty}\Big(\frac{Q+1}{Q-1}\Big)^{p+1}J_{\nu-2p-n}$$

$$-\frac{2Q^2(-1)^{\nu+n}}{(1-Q)(1+Q)^2}\cdot\Big(\frac{Q+1}{Q-1}\Big)^{(\nu-n)/2}\cdot\exp\Big(\frac{-i\tau}{\sqrt{1-Q^2}}\Big)\cdot\sum_{p=0}^{+\infty}\Big(\frac{Q+1}{Q-1}\Big)^{p+1}J_{\nu-2p-n-2}$$

$$+\frac{Q^2}{(1+Q)^2}\cdot\sum_{p,q=0}^{+\infty}\Big(\frac{Q+1}{Q-1}\Big)^{p+q+2}J_{\nu-2p-n}J_{\nu-2q-n}$$

$$-\frac{2Q^2}{(1+Q)^2}\cdot\sum_{p,q=0}^{+\infty}\Big(\frac{Q+1}{Q-1}\Big)^{p+q+2}J_{\nu-2p-n}J_{\nu-2q-n-2}$$

$$+\frac{Q^2}{(1+Q)^2}\cdot\sum_{p,q=0}^{+\infty}\Big(\frac{Q+1}{Q-1}\Big)^{p+q+2}J_{\nu-2p-n-2}J_{\nu-2q-n-2}\Big]. \qquad (4\text{-}21)$$

§ 4.3 *Asymptotic Behavior of Correlation Functions and Thermal Energy*

The probability distribution function of our total system is seen not to approach to a Gaussian distribution function with diagonal covariance matrix. Accordingly our total system is seen never to approach to a thermodynamic equilibrium. Therefore, we can say nothing about the timal change in the macroscopic temperature in the strict sence, except for the temperature at the initial instant of time. In this case, the statistical quantities of the individual particles seem to be physically more concrete than those of the total system. Therefore, in the statistical treatment of energy flow in the lattice system, we should take the microscopic local temperature at any point of the system.

From (4–14) ~ (4–16) and (4–19) ~ (4–21), we shall find

(i) for $m \geq 1$ and for $Q > 0$,

$$\lim_{\tau \to +\infty} C_{m,m}(\tau) = \frac{1+2Q}{4(1+Q)} T, \tag{4-22}$$

(ii) for $m = 0$ and for $Q > 0$,

$$\lim_{\tau \to +\infty} C_{0,0}(\tau) = \frac{1}{4(1+Q)} T, \tag{4-23}$$

(iii) for $m \leq -1$ and for $Q > 0$,

$$\lim_{\tau \to +\infty} C_{m,m}(\tau) = \frac{1}{4(1+Q)} T, \tag{4-24}$$

(iv) for $m \geq 1$ and for $-1 < Q < 0$,

$$\lim_{\tau \to +\infty} C_{m,m}(\tau) = \frac{T}{2}\left[\frac{1-2Q}{2(1-Q)} - \frac{(Q+1)^{m-1}Q}{(Q-1)^{m+2}}\left\{((-1)^m(2Q-1)+Q)\cdot\cos^2\frac{\tau}{\sqrt{1-Q^2}} + \right.\right.$$
$$\left.\left. + ((-1)^m(2Q-1)-Q)\cdot\sin^2\frac{\tau}{\sqrt{1-Q^2}}\right\}\right], \tag{4-25}$$

(v) for $m = 0$ and for $-1 < Q < 0$,

$$\lim_{\tau \to +\infty} C_{0,0}(\tau) = \frac{T}{2}\left[\frac{1}{2(1-Q)} - \frac{Q}{(1-Q)^2}\left\{\cos^2\frac{\tau}{\sqrt{1-Q^2}} + \frac{1-Q}{1+Q}\cdot\sin^2\frac{\tau}{\sqrt{1-Q^2}}\right\}\right], \tag{4-26}$$

(vi) for $m \leq -1$ and for $-1 < Q < 0$,

$$\lim_{\tau \to +\infty} C_{m,m}(\tau) = \frac{T}{2}\left[\frac{1}{2(1-Q)} + \frac{(Q-1)^{m-2}Q\{(-1)^{m+1}+Q\}}{(Q+1)^{m+1}}\left\{\frac{(-1)^{m+1}-Q}{(-1)^{m+1}+Q} \times \right.\right.$$
$$\left.\left. \times \cos^2\frac{\tau}{\sqrt{1-Q^2}} + \sin^2\frac{\tau}{\sqrt{1-Q^2}}\right\}\right]. \tag{4-27}$$

Accordingly, from (4–22) ~ (4–27) we shall obtain the microscopic local temperatures which have the initial value T at the positive sites, $T/4$ at the 0-th site, and zero at the negative sites, for any positive integers n:

$$\lim_{\tau \to +\infty} T_n(\tau) = \frac{1+2Q}{2(1+Q)} T, \quad \text{for } Q \geq 0 \tag{4-28}$$

$$\lim_{\tau \to +\infty} T_0(\tau) = \frac{2+Q}{4(1+Q)} T, \quad \text{for } Q \geq 0 \tag{4-29}$$

$$\lim_{\tau \to +\infty} T_{-n}(\tau) = \frac{1}{2(1+Q)} T, \quad \text{for } Q \geq 0 \tag{4-30}$$

$$\lim_{\tau \to +\infty} T_n(\tau) = \frac{1-2Q}{2(1-Q)} T + (\text{Oscillating term } B_n), \quad \text{for } -1 < Q < 0 \tag{4-31}$$

$$\lim_{\tau\to+\infty} T_0(\tau) = \frac{2-Q}{4(1-Q)}T + (\text{Oscillating term } B_0), \quad \text{for } -1<Q<0 \qquad (4\text{-}32)$$

and

$$\lim_{\tau\to+\infty} T_{-n}(\tau) = \frac{1}{2(1-Q)}T + (\text{Oscillating term } B_{-n}), \quad \text{for } -1<Q<0 \qquad (4\text{-}33)$$

where

$$(\text{Oscillating term } B_n) = $$
$$= \frac{Q(Q+1)^{2n-2}}{(Q-1)^{2n+3}}\left\{(Q^3+2Q-1)\cdot\sin^2\frac{\tau}{\sqrt{1-Q^2}} - (Q^3-2Q+1)\cdot\cos^2\frac{\tau}{\sqrt{1-Q^2}}\right\}, \qquad (4\text{-}34)$$

$$(\text{Oscillating term } B_0) = $$
$$= \frac{Q}{2(Q-1)^3(Q+1)}\left\{(3Q^2+1)\cdot\sin^2\frac{\tau}{\sqrt{1-Q^2}} - (Q^2-1)\cdot\cos^2\frac{\tau}{\sqrt{1-Q^2}}\right\}, \qquad (4\text{-}35)$$

and

$$(\text{Oscillating term } B_{-n}) = $$
$$= \frac{Q(Q+1(^{2n-2}}{(Q-1)^{2n+3}}\left\{(Q^3+1)\cdot\sin^2\frac{\tau}{\sqrt{1-Q^2}} - (Q^3-1)\cdot\cos^2\frac{\tau}{\sqrt{1-Q^2}}\right\}. \qquad (4\text{-}36)$$

Aside from the oscillating terms, we can unify the results (4-28) ~ (4-30) and (4-31) ~ (4-33) into the following forms:

$$\lim_{\tau\to+\infty} T_n(\tau) = \frac{1+2|Q|}{2(1+|Q|)}T, \qquad (4\text{-}37)$$

$$\lim_{\tau\to+\infty} T_0(\tau) = \frac{2+|Q|}{4(1+|Q|)}T, \qquad (4\text{-}38)$$

and

$$\lim_{\tau\to+\infty} T_{-n}(\tau) = \frac{1}{2(1+|Q|)}T, \qquad (4\text{-}39)$$

for any positive integers n.

From (4-37) ~ (4-39), we can see that, without the oscillating terms, the macroscopic local temperatures in positive sites and in negative sites, approach to different stationary values, with a gap of the energy distribution remaining at the impurity site. The height of the gap of the microscopic local temperature at the impurity site is:

$$\frac{|Q|}{1+|Q|}T. \qquad (4\text{-}40)$$

The expression (4-40) has a limiting value T as Q goes to infinity, which corresponds to the case of the impurity atom of an infinite mass ($M'\to+\infty$). In other words, the impurity atom plays the rôle of a fixed wall, and prevents the flow of energy across that point. For a perfect lattice, *i.e.* in the case of $Q=0$, the stationary state in the system with a uniform microscopic local temperature, *viz.*:

$$\lim_{\tau\to+\infty} T_n(\tau) = \frac{1}{2}T, \qquad \text{(for any integers } n\text{)}$$

is established, as we expected. For $-1<Q<0$, the local temperatures have the oscillating terms, which proves the existence of the localized vibration in the system. Finally, for $Q\to-1$, *i.e.* $M'\to 0$, the height of the gap of microscopic local temperature (4–40) has the value of $T/2$.

§ 4.4 *Energy Flow in the System*

In the previous section, we have seen that, aside from the oscillating terms, the microscopic local temperatures approach to stationary values at the final state: $\tau=+\infty$. However, this does not mean that our system approaches to the thermodynamic equilibrium at $\tau=+\infty$. In fact, the correlation matrix $\|V_{n,m}\|$ $(\equiv\|C_{2n,2n+2m+1}\|)$ has non-vanishing elements at the final state: $\tau=+\infty$, and we can show that the energy flow still exists at every point of the system even at $\tau=+\infty$.

Let us indicate the total energy in the positive side of the n-th particle with $E_n^*(\tau)$. Then we shall obtain

$$E_n^*(\tau) = M\sum_{s=n}^{+\infty}\left\{\frac{1}{2}(1+Q\delta_{s,0})\dot{x}_s^2+\frac{\omega^2}{2}(x_{s+1}-x_s)^2\right\}. \tag{4-41}$$

Accordingly, we shall obtain

$$-\frac{dE_n^*(\tau)}{d\tau} = -\frac{\sigma^2K}{2}\cdot\sum_{s=n}^{+\infty}\Big[(1+Q\delta_{s,0})\Big(1-\frac{Q}{1+Q}\delta_{s,0}\Big)y_{2s}(\tau)\{y_{2s+1}(\tau)-y_{2s-1}(\tau)\}+ \\ +y_{2s+1}(\tau)\{y_{2s+2}(\tau)-y_{2s}(\tau)\}\Big]. \tag{4-42}$$

In a special case, *i.e.* if we take $n=0$ in (4–42), we shall obtain

$$-\frac{dE_0^*(\tau)}{d\tau} = \frac{\sigma^2K}{2}\cdot y_0(\tau)y_{-1}(\tau). \tag{4-43}$$

This corresponds to the energy flow from the right-hand side of the zero-th particle to the left-hand side of the (-1)-th particle, or in other words, the expression (4–43) corresponds physically to the work done by the zero-th particle upon the (-1)-th particle.

Calculating the average value of (4–43) and taking the limit: $\tau\to+\infty$, we shall obtain the following results:

$$\lim_{\tau\to+\infty}\left\langle-\frac{dE_0^*(\tau)}{d\tau}\right\rangle_{Av} =$$

$$=\frac{kT}{2\pi(1+Q)^2}\cdot\left\{\frac{4Q^2}{(1+Q)^2}\cdot\left(\frac{Q+1}{Q-1}\right)^{3/2}\cdot\text{arctg}\left(\frac{Q-1}{Q+1}\right)^{1/2}+\frac{Q^2}{\sqrt{Q^2-1}}\cdot\text{arctg}\sqrt{Q^2-1}-\frac{Q+1}{Q-1}\right\}, \quad \text{for } 1<Q \tag{4-44}$$

$$=\frac{kT}{3\pi}, \quad \text{for } Q=1 \tag{4-45}$$

$$= \frac{kT}{2\pi(1+Q)^2}\cdot\left\{\frac{1+Q}{1-Q} - \frac{Q^2}{1+Q}\cdot\left(\frac{1+Q}{1-Q}\right)^{3/2}\cdot\log\frac{1+\sqrt{1-Q^2}}{Q}\right\}, \qquad \text{for } 0<Q<1 \qquad (4\text{-}46)$$

$$= \frac{kT}{2\pi}, \qquad \text{for } Q=0 \qquad (4\text{-}47)$$

$$= \frac{kT}{2\pi(1+Q)}\cdot\left\{\frac{1}{1-Q} - \frac{Q^2}{(1-Q)\sqrt{1-Q^2}}\cdot\log\frac{1+\sqrt{1-Q^2}}{-Q}\right\} + \frac{kTQ^2}{2(1-Q)^2\sqrt{1-Q^2}}\cdot\sin\frac{2\tau}{\sqrt{1-Q^2}}.$$
$$\text{for } -1<Q<0 \qquad (4\text{-}48)$$

It is worth while remarking that our results have very similar qualitative properties to the change of temperature in a perfect lattice. We can also compare the flow of energy in our system which contains an impurity atom, with the flow of heat in an infinite rod. In our system, however, Fourier's law that the vector of heat flax is proportional to the negative gradient of temperature, does not hold true at every point of the system, even at $\tau=+\infty$. We have seen in Chapter III and we can also derive from our present results, that even in a perfect lattice $(M'=M)$ of infinite length, there exists a constant energy flow of $kT\omega_0/\pi$ at every point throughout the system, though the whole system attains uniform distribution of microscopic local temperature $T/2$ at $\tau=+\infty$. Also in our present system, the constant flow of energy exists throughout the system from the right side to the left side at the final state: $\tau=+\infty$, while the uniform local temperature is attained on both sides of the impurity atom. In this respect, energy flow in the harmonic lattice is essentially different from heat flow in a classical system.

From these results, it would be possible for us to explain the effect of many number of isotopic impurity atoms in a one-dimensional or in a three-dimensional lattice. It would also be possible to explain the existence of stationary values of the microscopic local temperatures in one-dimensional and in three-dimensional lattices, and also the existence of gaps of energy distribution at the impurity sites and the existence of the energy flow which does not obey the classical Fourier's law.

V. Localized Vibration

The existence of localized vibrations in a system of coupled harmonic oscillators has been mentioned by many investigators[26] in relation to the reduced mass or random external force of high frequency. The localized vibrations occur in the vicinity of a particle, when the mass of the particle is reduced, or when the particle has harder springs than the other ones, or when the external force is applied whose frequency is higher than the maximum frequency of the system. In the present chapter, we shall show explicitly the existence of such localized vibrations and make clear some dynamical aspects.

We shall consider an infinitely extended lattice with one-isotopic impurity. Let us assume that the initial velocity of the 0-th particle a_0 is finite, and all the other particles are at rest at the initial time $\tau=0$, namely $a_\nu=\delta_{\nu,0}$. From (4-6) above, we shall have, in the Schrödinger coordinates:

$$y_n(\tau) = J_{-n}(\tau) - Q\int_0^\tau dx\cdot J_n(x-\tau)\frac{d}{dx}y_0(x), \qquad (5\text{-}1)$$

for $-\infty<n<\infty$. In order to take out the localized vibration which remains for infinitely large τ, let us assume:

$$\lim_{\tau\to+\infty} y_n(\tau) = A_n\cdot e^{i\omega\tau}, \qquad (5\text{-}2)$$

where A_n is independent of τ, and ω is the frequency of localized vibration. Inserting (5-2) into (5-1), we obtain:

$$A_n = (-1)^{n+n\varepsilon(-n)+1} Q A_0 \omega(\omega^2-1)^{-1/2}(\omega+\sqrt{\omega^2-1})^{-|n|}\cdot e^{-i(|n|\pi)/2}, \qquad (5-3)$$
$$\text{for } -\infty<n<\infty$$

where

$$\varepsilon(n) = \begin{cases} 0, & \text{for } n\geq 0 \\ 1. & \text{for } n<0 \end{cases}$$

In order to obtain the expression of ω in terms of Q, let us put $n=0$ in (5-3), and we shall get

$$\omega = \frac{1}{\sqrt{1-Q^2}}. \qquad \text{for } -1<Q<0 \qquad (5\text{-}4)$$

Accordingly, the expression (5-2) will become:

$$\lim_{\tau\to+\infty} y_n(\tau) = (-1)^{n+n\varepsilon(-n)} A_0 \left(\frac{1+Q}{1-Q}\right)^{|n|/2} \cdot \exp\left[i\left(\frac{\tau}{\sqrt{1-Q^2}} - \frac{|n|\pi}{2}\right)\right], \qquad (5\text{-}5)$$

for $-\infty<n<\infty$ and $-1<Q<0$.

From (5-5), we can see that the amplitude of y_n decreases in the powers of $|n|$ for infinitely large τ. That is, the vibrations do not propagate through the system but localize around the impurity particle when the mass of the impurity atom is smaller than that of the other particles. We can also explain the existence of localized vibrations in a lattice system where a spring is harder than the others. The maximum frequency of the perfect lattice is represented by the square root of the ratio of its spring constant to the mass of the particle. Therefor, the harder a spring is, the higher is the frequency, and the smaller a mass is, the higher is the frequency.

(i) External force acting on the 0-th particle

We shall consider the one-dimensional perfect lattice, consisting of infinite number of particles, with an external force $f(\tau)$ acting on the 0-th particle. The equations of motion can be written in the Schrödinger coordinates:

$$2\frac{d}{d\tau}y_n(\tau) = y_{n+1}(\tau) - y_{n-1}(\tau) + f(\tau)\delta_{n,0}. \qquad \text{for } -\infty<n<\infty \qquad (5\text{-}6)$$

The solutions of the equations (5-6) can be obtained:

$$y_n(\tau) = \sum_{\nu=-\infty}^{+\infty} a_\nu J_{\nu-n}(\tau) + \frac{1}{2}\int_0^\tau dx\cdot f(x) J_n(x-\tau), \qquad \text{for } -\infty<n<\infty \qquad (5\text{-}7)$$

with a_ν the initial value of $y_\nu(\tau)$ $(\nu = \ldots, -2, -1, 0, 1, 2, \ldots)$.

If we assume as follows, for the external force $f(\tau)$ and initial values a_ν, *viz.*:

$$\left.\begin{aligned} & f(\tau) = F\sin\frac{\omega}{\omega_0}\tau, \\ \text{and} & \\ & a_\nu = 0, \quad \text{for } \nu = \ldots, -2, -1, 0, 1, 2, \ldots \end{aligned}\right\} \tag{5-8}$$

with constant F, and ω_0 for the maximum frequency of the system, then we shall have

$$\begin{aligned} y_n(\tau) &= \frac{F}{2}\int_0^\tau dx\cdot J_n(x-\tau)\sin\frac{\omega}{\omega_0}x \\ &= (-1)^{n\varepsilon(-n)}\frac{F}{2}\int_0^\tau dz\cdot J_{|n|}(z)\sin\frac{\omega}{\omega_0}(\tau - z), \qquad (5\text{-}9) \\ &= (-1)^{n\varepsilon(-n)}\frac{F}{2}\left\{\sin\frac{\omega}{\omega_0}\tau\cdot\int_0^\tau dz\cdot J_{|n|}(z)\cos\frac{\omega}{\omega_0}z - \cos\frac{\omega}{\omega_0}\tau\cdot\int_0^\tau dz\cdot J_{|n|}(z)\sin\frac{\omega}{\omega_0}z\right\}. \\ &\qquad \text{for } -\infty < n < \infty \qquad (5\text{-}10) \end{aligned}$$

Using the formula:

$$\int_0^{+\infty} dz\cdot J_{|n|}e^{i(\omega/\omega_0)z} = \begin{cases} = \left(1 - \frac{\omega^2}{\omega_0^2}\right)^{-1/2} e^{i|n|\varphi}, & \text{for } \omega < \omega_0 \\ = i\left(\frac{\omega^2}{\omega_0^2} - 1\right)^{-1/2}\left(\frac{\omega}{\omega_0} + \sqrt{\frac{\omega^2}{\omega_0^2} - 1}\right)^{-|n|} e^{-i(|n|\pi)/2}, & \text{for } \omega > \omega_0 \end{cases}$$

where $\varphi = \arcsin(\omega/\omega_0)$, we shall obtain at the final state $\tau = +\infty$,

$$\lim_{\tau\to+\infty} y_n(\tau) = (-1)^{n\varepsilon(-n)}\frac{F}{2}\left(1 - \frac{\omega^2}{\omega_0^2}\right)^{-1/2}\sin\left(\frac{\omega}{\omega_0}\tau - |n|\varphi\right). \quad \text{for } \omega < \omega_0 \tag{5-11}$$

and

$$\lim_{\tau\to+\infty} y_n(\tau) = (-1)^{n\varepsilon(-n)}\frac{F}{2}\left(\frac{\omega^2}{\omega_0^2} - 1\right)^{-1/2}\left(\frac{\omega}{\omega_0} + \sqrt{\frac{\omega^2}{\omega_0^2} - 1}\right)^{-|n|}\cos\left(\frac{\omega}{\omega_0}\tau + \frac{|n|\pi}{2}\right). \tag{5-12}$$

From the expression (5-11) for $\omega < \omega_0$, it will be seen that $y_n(\tau)$ oscillates as $|n|$ increases, and that from (5-12) for $\omega > \omega_0$, $y_n(\tau)$ vanishes for $\tau \to +\infty$ and $|n| \to +\infty$. This means that the localized vibration exists in the vicinity of the 0-th particle, when ω is higher than ω_0. The expressions (5-11) and (5-12) are essentially the same with the results obtained by Kashiwamura, Takeno and Teramoto[26].

In our method by means of the Schrödinger coordinates, unlike in the case of the method in trigonometric eigenfunction, there does not appear the term that corresponds to the translation of the system as a whole at $\tau = +\infty$. Therefore, we find that the Schrödinger coordinates are very convenient in investigating the problems of vibrations in individual particles in the lattice system.

(ii) White noise acting at site No. 0

For external force $f(\tau)$ and initial values a_ν of $y_\nu(\tau)$, we shall assume:

$$\langle f(\tau)\rangle_{Av} = 0, \tag{5-13}$$

$$\langle f(\tau_1)f(\tau_2)\rangle_{Av} = \delta(\tau_1 - \tau_2), \tag{5-14}$$

and

$$a_\nu = 0. \quad \text{for } \nu = \ldots, -2, -1, 0, 1, 2, \ldots \tag{5-15}$$

The expression (5–14) means that the random force $f(\tau)$ has a white spectrum.

In this case, the correlation function can be calculated from (5–7), (5–13), (5–14) and (5–15) as follows:

$$\begin{aligned}
C_{m,n}(\tau)\Big/\frac{\sigma^2 K}{2k} &= \langle y_m(\tau)y_n(\tau)\rangle_{Av} \\
&= \frac{1}{4}\int_0^\tau\int_0^\tau dxdy \cdot \langle f(x)f(y)\rangle_{Av} \cdot J_m(x-\tau)J_n(y-\tau) \\
&= \frac{1}{4}\int_0^\tau\int_0^\tau dxdy \cdot \delta(x-y)J_m(x-\tau)J_n(y-\tau) \\
&= \frac{1}{4}\int_0^\tau dx \cdot J_m(x-\tau)J_n(x-\tau) \\
&= \frac{(-1)^{m+n}}{4}\int_0^\tau dz \cdot J_m(z)J_n(z). \quad \text{for any integers } m \text{ and } n
\end{aligned} \tag{5-16}$$

In the case of $\tau \to +\infty$, the correlation function (5–16) will become

$$C_{m,n}(\tau)\Big/\frac{\sigma^2 K}{2k} =$$

$$\begin{cases} = \dfrac{(-1)}{4\pi}^{m+n)\varepsilon(m+n)+(m-n)/2+m+n+1}\left\{2\displaystyle\sum_{r=0}^{\left|\frac{m-n}{2}-1\right|}\frac{1}{|m-n|-(2r+1)} - \left[\operatorname{logtan}\left(\frac{\pi}{4}+\frac{\phi}{2}\right)\right]_{\phi=0}^{\pi/2}\right\}, \\ \qquad\qquad \text{for even integers } (m-n) \qquad (5\text{-}17) \\ = \dfrac{(-1)}{8}^{(m+n)\varepsilon(m+n)+(m-n-1)/2+m+n}, \quad \text{for odd integers } (m-n) \qquad (5\text{-}18) \end{cases}$$

From (5–17), the momentum-momentum correlation functions and the position-position correlation functions do diverge at $\tau = +\infty$. In the case of $m = n$, the expression (5–17) above shows that the kinetic and potential energies diverge at the final state: $\tau = \infty$. On the other hand, from (5–18), momentum-position correlation functions remain finite. This means that there exists the instantaneous flow of energy at every point throughout the system.

(iii) External forces acting on the particles No. 0 and No. *m*

Let us take a perfect lattice of infinite length, with an external force $f(\tau)$ acting on the 0-th particle and with another external force $g(\tau)$ acting on the m-th ($m > 0$) particle (cf. Fig. 9), then we shall obtain the following results.

The equations of motion will be:

$$2\frac{d}{d\tau}y_n(\tau) = y_{n+1}(\tau) - y_{n-1}(\tau) + f(\tau)\delta_{n,0} + g(\tau)\delta_{n,2m}. \tag{5-19}$$

$$\text{for } -\infty < n < \infty$$

The solutions of (5–19) will read:

$$y_n(\tau) = \sum_{\nu=-\infty}^{+\infty} a_\nu J_{\nu-n}(\tau) + \frac{1}{2}\int_0^\tau dx \cdot \{f(x)J_n(x-\tau) + g(x)J_{n-2m}(x-\tau)\}. \qquad (5\text{–}20)$$

$$\text{for } -\infty < n < \infty$$

Now, let us take two cases for $g(\tau)$, namely:

a) $g(\tau) = f(\tau)$,

b) $g(\tau) = -f(\tau)$.

From (5–20), we shall have, for case a):

$$y_n(\tau) = \sum_{\nu=-\infty}^{+\infty} a_\nu J_{\nu-n}(\tau) + \frac{1}{2}\int_0^\tau dx \cdot f(x)\{J_n(x-\tau) + J_{n-2m}(x-\tau)\}, \qquad (5\text{–}21)$$

$$\text{for } -\infty < n < \infty$$

and for case b):

$$y_n(\tau) = \sum_{\nu=-\infty}^{+\infty} a_\nu J_{\nu-n}(\tau) + \frac{1}{2}\int_0^\tau dx \cdot f(x)\{J_n(x-\tau) - J_{n-2m}(x-\tau)\}. \qquad (5\text{–}22)$$

$$\text{for } -\infty < n < \infty$$

If we assume (5–13), (5–14) for $f(\tau)$, and (5–15) for a_ν, the correlation functions $C_{\alpha,\beta}(\tau)\Big/\frac{\sigma^2 K}{2k}$ can be calculated from (5–21) and (5–22) as follows: for the case a)

$$C_{\alpha,\beta}(\tau)\Big/\frac{\sigma^2 K}{2k} = \frac{1}{4}\int_0^\tau dz \cdot \{J_\alpha(z) + J_{\alpha-2m}(z)\}\{J_\beta(z) + J_{\beta-2m}(z)\},$$

for the case b)

$$C_{\alpha,\beta}(\tau)\Big/\frac{\sigma^2 K}{2k} = \frac{1}{4}\int_0^\tau dz \cdot \{J_\alpha(z) - J_{\alpha-2m}(z)\}\{J_\beta(z) - J_{\beta-2m}(z)\}.$$

As a special case $\alpha = \beta$, we shall obtain for the case a) above:

$$C_{\alpha,\alpha}(\tau)\Big/\frac{\sigma^2 K}{2k} = \langle y_\alpha^2(\tau)\rangle_{Av} = \frac{1}{4}\int_0^\tau dz \cdot \{J(z) + J_{\alpha-2m}(z)\}^2, \qquad (5\text{–}23)$$

and for the case b) above:

$$C_{\alpha,\alpha}(\tau)\Big/\frac{\sigma^2 K}{2k} = \langle y_\alpha^2(\tau)\rangle_{Av} = \frac{1}{4}\int_0^\tau dz \cdot \{J_\alpha(z) - J_{\alpha-2m}(z)\}^2. \qquad (5\text{–}24)$$

Using recurrence formula of Bessel functions, we shall obtain from (5–23) and (5–24),

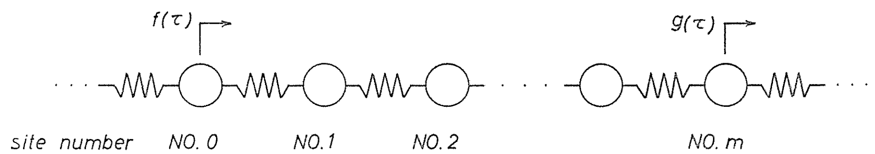

FIG. 9. Linear lattice with external forces $f(\tau)$ and $g(\tau)$ acting on the 0-th and m-th particles, respectively.

1) for the case a) and odd integers m,

$$\langle (y_n(\tau)-\langle y_n(\tau)\rangle_{Av})^2\rangle_{Av}=\langle y_n^2(\tau)\rangle_{Av}=\frac{1}{4}\int_0^{\tau}dz\cdot\{\sum_{\nu=0}^{m-1}(-1)^{\nu}(J_{n-2\nu}(z)+J_{n-2(\nu+1)}(z))\}^2$$
$$=\int_0^{\tau}dz\cdot\frac{1}{z^2}\{\sum_{\nu=0}^{m-1}(-1)^{\nu}(n-2\nu-1)J_{n-2\nu-1}(z)\}^2$$
$$=\sum_{\nu,\mu=0}^{m-1}(-1)^{\mu+\nu}(n-2\nu-1)(n-2\mu-1)\int_0^{\tau}dz\cdot\frac{J_{n-2\nu-1}(z)J_{n-2\mu-1}(z)}{z^2}, \tag{5-25}$$

and

2) for the case b) and even integers m,

$$\langle (y_n(\tau)-\langle y_n(\tau)\rangle_{Av})^2\rangle_{Av}=\langle y_n^2(\tau)\rangle_{Av}$$
$$=\sum_{\nu,\mu=0}^{m=1}(-1)^{\mu+\nu}(n-2\nu-1)(n-2\mu-1)\int_0^{\tau}dz\cdot\frac{J_{n-2\nu-1}(z)J_{n-2\mu-1}(z)}{z^2}. \tag{5-26}$$

From the formula:

$$\int_0^{\infty}dz\cdot\frac{J_{n-2\nu-1}(z)J_{n-2\mu-1}(z)}{z^2}=\frac{\Gamma\left(n-\nu-\mu-2+\frac{1}{2}\right)}{4\Gamma\left(\mu-\nu+1+\frac{1}{2}\right)\Gamma\left(\nu-\mu+1+\frac{1}{2}\right)\Gamma\left(n-\mu-\nu+\frac{1}{2}\right)},$$

the correlation functions (5–25) and (5–26) converge at the final state $\tau=+\infty$, while the correlation function (5–23) or (5–24) diverges at $\tau=+\infty$ for m even or odd integers, respectively. In brief, for sufficiently large τ, the mean square value of y_n remains finite, either when two external forces act in the same direction and m is odd integer, or when two external forces act in the opposite direction and m is even integer. For $\tau=+\infty$, the mean square value of y_n diverges, either when two external forces act in the same direction and m is even integer, or when two external forces act in the opposite direction and m is odd integer.

If we put

$$\lim_{\tau\to+\infty}\langle y_n^2(\tau)\rangle_{Av}\equiv D_n,$$

the following relations will be obtained for converging cases:

$$\left.\begin{array}{l} D_0>D_{-1}>D_{-2}>\cdots>D_{-\infty},\\ D_0>D_1>D_2>\cdots>D_{m-1}>D_m,\\ D_{2m}>D_{2m-1}>D_{2m-2}>\cdots>D_{m+1}>D_m,\\ \text{and}\\ D_{2m}>D_{2m+1}>D_{2m+2}>\cdots>D_{+\infty}.\quad\text{for positive integers } m \end{array}\right\} \tag{5-27}$$

D_n has the maximum values at $n=0$ or at $n=2m$ (namely, the kinetic energy of the particle on which the external force acts is maximum after a sufficiently long time) and $D_{|n|}$ approaches to $4/(3\pi)$ when $|n|$ is infinitely large. From

(5–27) above, we can see that the localized vibrations exist in the vicinity of the 0-th and m-th particles and that the vibrations do not propagate through the system. The results mentioned above come from the fact that in the random force $f(\tau)$ there exist some components of vibrations with higher frequency than the maximum frequency of the system, while, from (5–17), we can see that the momentum-momentum correlation functions and the position-position correlation functions do diverge at $\tau=+\infty$, when the external random force acts merely on a lattice point. That is to say, the mean total energy at every site of the system goes to infinity after a sufficiently long time[27].

In two-dimensional and three-dimensional lattices, we may also expect such localized vibrations to occur under somewhat restricted conitions.

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Appendix 1

Using the formula[28]:

$$J_{\nu+\alpha}(z)\cdot J_{\nu-\alpha}(z)=\frac{2}{\pi}\int_0^{\pi/2} J_{2\nu}(2z\cos\theta)\cdot\cos(2\alpha\theta)\cdot d\theta, \tag{A-1}$$

for complex numbers ν and α, with $\Re_e(2\nu)>-1$, we shall have:

$$\begin{aligned}\sum_{k=1/2}^{+\infty} J_{k+\alpha}(\tau)\cdot J_{k-\alpha}(\tau) &= \frac{2}{\pi}\int_0^{\pi/2} d\theta\cdot\cos(2\alpha\theta)\cdot\sum_{k=1/2}^{+\infty} J_{2k}(2\tau\cos\theta)\\ &= \frac{2}{\pi}\int_0^{\pi/2} d\theta\cdot\cos(2\alpha\theta)\cdot\sum_{k=0}^{+\infty} J_{2k+1}(2\tau\cos\theta)\\ &= \frac{1}{\pi}\int_0^{2/\pi} d\theta\cdot\cos(2\alpha\theta)\cdot\int_0^{2\tau\cos\theta} d\xi\cdot J_0(\xi).\end{aligned} \tag{A-2}$$

Taking the limit: $\tau\to+\infty$ in (A–2), we shall obtain the formula (3–39):

$$\begin{aligned}\lim_{\tau\to+\infty}\sum_{k=1/2}^{+\infty} J_{k+\alpha}(\tau)\cdot J_{k-\alpha}(\tau) &= \frac{1}{\pi}\int_0^{\pi/2} d\theta\cdot\cos(2\alpha\theta)\cdot\int_0^{+\infty} d\xi\cdot J_0(\xi)\\ &= \frac{1}{\pi}\int_0^{\pi/2} d\theta\cdot\cos(2\alpha\theta)\\ &= \frac{\sin(\pi\alpha)}{2\pi\alpha}.\end{aligned}$$

Appendix 2

The solution of integral equation (4–8) is expressed by:

$$\begin{aligned}y_0(\tau) &= \frac{1}{1+Q}\cdot\sum_{\mu=-\infty}^{+\infty} a_\mu\cdot J_\mu(\tau)\cdot(1+Q\delta_{\mu,0})+\\ &+\frac{1}{1+Q}\cdot\sum_{\mu=-\infty}^{+\infty} a_\mu(1+Q\delta_{\mu,0})\cdot\sum_{m=1}^{+\infty}\left(\frac{Q}{1+Q}\right)^m\cdot\int_0^{\tau} K_m(\tau,z)\cdot J_\mu(z)dz,\end{aligned} \tag{A-3}$$

where

$$K_m(x,y)=\int_0^{x-y}\int_0^{z_{m-1}}\int_0^{z_{m-2}}\cdots\int_0^{z_2}J_1(x-y-z_{m-1})J_1(z_{m-1}-z_{m-2})J_1(z_{m-2}-z_{m-3})$$
$$\cdots J_1(z_2-z_1)J_1(z_1)dz_1dz_2\cdots dz_{m-1}.$$

By means of the formula:

$$\int_0^z J_\mu(t)\cdot J_\nu(z-t)dt=2\sum_{n=0}^{+\infty}(-1)^n J_{\mu+\nu+2n+1}(z), \qquad \text{(A-4)}$$
$$\text{for } \Re_e(\mu)>-1 \text{ and } \Re_e(\nu)>-1$$

we shall get at once:

$$K_m(x,y)=2^{m-1}\cdot\sum_{k_1,k_2,\dots,k_{m-1}=0}^{+\infty}(-1)^{k_1+\dots+k_{m-1}}\cdot J_{2m-1+2(k_1+k_2+\dots+k_{m-1})}(x-y). \quad \text{(A-5)}$$

Putting (A–5) into (A–3), we shall obtain (4–9).

Appendix 3

Inserting (4–9) into (4–7), we shall obtain

$$(1+Q\delta_{n,0})\cdot y_n(\tau)=\sum_{\mu=-\infty}^{+\infty}a_\mu\cdot(1+Q\delta_{\mu,0})\cdot J_{\mu-n}(\tau)+$$
$$+\frac{Q}{2(1+Q)}\cdot\sum_{\mu=-\infty}^{+\infty}(-1)^{(n+1)\varepsilon(n)+\mu\varepsilon(-\mu)}\cdot(1+Q\delta_{\mu,0})\cdot a_\mu\cdot\int_0^\tau\Big\{J_\mu(z)+\sum_{m=1}^{+\infty}\Big(\frac{2Q}{1+Q}\Big)^m\times$$
$$\times\sum_{k_1,k_2,\dots,k_m=0}^{+\infty}(-1)^{k_1+k_2+\dots+k_m}\cdot J_{|\mu|+2m+2(k_1+k_2+\dots+k_m)}(z)\cdot\{J_{|n-1|}(\tau-z)-(-1)^{\delta_{n,0}}$$
$$\times J_{|n+1|}(\tau-z)\}dz. \qquad \text{(A-6)}$$

If we put:

$$I\equiv\frac{1}{2}\int_0^\tau\Big\{J_{|\mu|}(z)+\sum_{m=1}^{+\infty}\Big(\frac{2Q}{1+Q}\Big)^m\cdot\sum_{k_1,k_2,\dots,k_m=0}^{+\infty}(-1)^{k_1+\dots+k_m}\cdot J_{|\mu|+2m+2(k_1+\dots+k_m)}(z)\Big\}\times$$
$$\times\{J_{|n+1|}(\tau-z)-(-1)^{\delta_{n,0}}\cdot J_{|n+1|}(\tau-z)\}dz,$$

and evaluate the integral by means of (A–4), we shall have:

$$I=\sum_{s=0}^{+\infty}(-1)^s\cdot J_{|n-1|+|\mu|+2s+1}(\tau)-(-1)^{\delta_{n,0}}\cdot\sum_{s=0}^{+\infty}(-1)^s\cdot J_{|n+1|+|\mu|+2s+1}(\tau)+$$
$$+\sum_{m=1}^{+\infty}\Big(\frac{2Q}{1+Q}\Big)^m\cdot\sum_{k_1,k_2,\dots,k_{m+1}=0}^{+\infty}(-1)^{k_1+\dots+k_{m+1}}\cdot J_{|n-1|+|\mu|+2m+2(k_1+\dots+k_{m+1})+1}(\tau)-$$
$$-(-1)^{\delta_{n,0}}\cdot\sum_{m=1}^{+\infty}\Big(\frac{2Q}{1+Q}\Big)^m\cdot\sum_{k_1,k_2,\dots,k_{m+1}=0}^{+\infty}(-1)^{k_1+\dots+k_{m+1}}\cdot J_{|m+1|+|\mu|+2m+2(k_1+\dots+k_{m+1})+1}(\tau)$$
$$=\sum_{m=0}^{+\infty}\Big(\frac{2Q}{1+Q}\Big)^m\cdot\sum_{k_1,k_2,\dots,k_{m+1}=0}^{+\infty}(-1)^{k_1+k_2+\dots+k_{m+1}}\cdot\{J_{|n-1|+|\mu|+2m+2(k_1+\dots+k_{m+1})+1}(\tau)-$$
$$-(-1)^{\delta_{n,0}}\cdot J_{|n+1|+|\mu|+2m+2(k_1+k_2+\dots k_{m+1})+1}(\tau)\}.$$

The multiple summation appearing in the above expression can be reduced to the following simple form:

$$\sum_{k_1=0}^{+\infty}\sum_{k_2=0}^{+\infty}\cdots\sum_{k_n=0}^{+\infty}F(k_1+k_2+\cdots+k_n+\alpha)$$
$$=\sum_{p=0}^{+\infty}\binom{p+n-1}{n-1}\cdot F(p+\alpha).$$

And we shall obtain:

$$I=\sum_{m=0}^{+\infty}\left(\frac{2Q}{1+Q}\right)^m\cdot\sum_{p=0}^{+\infty}(-1)^p\cdot\binom{p+m}{m}\cdot\{J_{|n-1|+|\mu|+2m+2p+1}(\tau)-$$
$$-(-1)^{\delta_{n,0}}\cdot J_{|n+1|+|\mu|+2m+2p+1}(\tau)\}.$$

If we put $r=p+m+1$, we shall have:

$$I=\sum_{r=1}^{+\infty}\sum_{p=0}^{r-1}(-1)^p\cdot\left(\frac{2Q}{1+Q}\right)^{r-1-p}\cdot\binom{r-1}{p}\cdot\{J_{|n-1|+|\mu|+2r-1}(\tau)-$$
$$-(-1)^{\delta_{n,0}}\cdot J_{|n+1|+|\mu|+2r-1}(\tau)\}$$
$$=\sum_{r=1}^{+\infty}\left(\frac{Q-1}{Q-1}\right)^{r-1}\cdot\{J_{|n-1|+|\mu|+2r-1}(\tau)-(-1)^{\delta_{n,0}}\cdot J_{|n+1|+|\mu|+2r-1}(\tau)\}. \quad \text{(A-7)}$$

Inserting (A-7) into (A-6), we shall obtain the solutions (4-10).

Appendix 4

Let us prove the following formula:

$$\sum_{r=-\infty}^{+\infty}p^{rN}\cdot J_{rN+s}(z)=\frac{1}{|N|p^s}\cdot\sum_{k=0}^{|N|-1}\exp\left[\frac{z}{2}(pe^{i(2k\pi)/|N|}-p^{-1}e^{-i(2k\pi)/|N|})\right]\cdot e^{-i(2k\pi/|N|)s}, \quad \text{(A-8)}$$

with integers N and s, where $J_\nu(z)$ is Bessel function of order ν and argument z.

Proof. In the first place, we shall prove the formula (A-8) for any positive integer N.

From the generating function of Bessel functions, we have

$$\sum_{r=0}^{+\infty}p^{rN+s}J_{rN+s}(z)=\frac{1}{2\pi i}\int^{(0+)}dt\cdot\exp\left[\frac{z}{2}\left(t-\frac{1}{t}\right)\right]\cdot t^{-s-1}\cdot p^s\cdot\sum_{r=0}^{+\infty}p^{rN}t^{-rN}$$
$$=\frac{1}{2\pi i}\int_c^{(0+)}dt\cdot\exp\left[\frac{z}{2}\left(t-\frac{1}{t}\right)\right]\cdot\frac{t^{-s-1+N}\cdot p^s}{t^N-p^N}, \quad \text{(A-9)}$$

where the path of integration is to be taken in such a way that the integration over C runs counterclockwise around the origin $t=0$ and that the closed curve C entirely contains the circle $|t|=|p|$.

The integrand of (A-9) has an essential singularity at the origin $t=0$, and also N simple-poles at points $t=q\cdot\exp\left[i\left(\delta+\frac{2k\pi}{N}\right)\right]$ $(k=0, 1, 2, \ldots, N-1)$, whose residues are respectively.

$$\frac{1}{N}\cdot\exp\left[\frac{z}{2}(qe^{i(\delta+(2k\pi)/N)}-q^{-1}e^{-i(\delta+(2k\pi)/N)})\right]\cdot e^{-i(2k\pi/N)s}, \quad \text{(A-10)}$$
$$(k=0, 1, 2, \ldots, N-1)$$

where $p=q\cdot\exp[i\delta]$, with real positive q and $0\leq\delta<2\pi$.

If we deform the curve C into a closed curve C_1 which lies inside the circle $|t|=|p|$ (cf. Fig. 10), then we shall obtain from (A–9) and (A–10) above:

$$\sum_{r=0}^{+\infty} p^{rN+s}\cdot J_{rN+s}(z)=\frac{1}{N}\cdot\sum_{k=0}^{N-1}\exp\left[\frac{z}{2}\{qe^{i(\delta+(2k\pi/N))}-q^{-1}e^{-i(\delta+(2k\pi/N))}\}\right]\cdot e^{-i(2k\pi/N)s}+$$
$$+\frac{1}{2\pi i}\int_{C_1}^{(0+)}dt\cdot\exp\left[\frac{z}{2}\left(t-\frac{1}{t}\right)\right]\cdot\frac{t^{-s-1+N}p^s}{t^N-p^N}. \qquad \text{(A-11)}$$

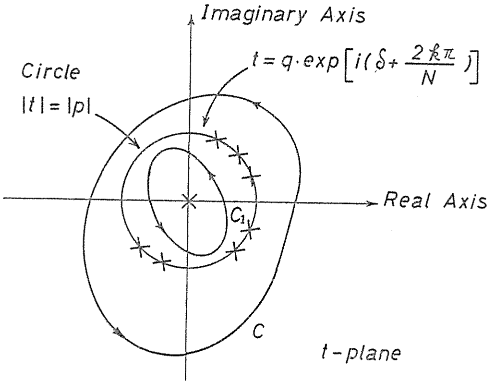

FIG. 10. Path of integration in (A–9) and (A–11).

Here the integration over C_1 is to be taken in such a way that it runs couter-clockwise around the origin $t=0$.

The second term in the right-hand side of (A–11) will become

$$\frac{1}{2\pi i}\int_{C_1}^{(0+)}dt\cdot\exp\left[\frac{z}{2}\left(t-\frac{1}{t}\right)\right]\cdot\frac{t^{-s-1+N}p^s}{t^N-p^N}$$
$$=-\frac{1}{2\pi i}\int_{C_1}^{(0+)}dt\cdot\exp\left[\frac{z}{2}\left(t-\frac{1}{t}\right)\right]\cdot\sum_{r=1}^{+\infty}p^{s-rN}\cdot t^{-s-1+rN}$$
$$=-\sum_{r=-\infty}^{-1}p^{rN+s}\cdot J_{rN+s}(z). \qquad \text{(A-12)}$$

The expressions (A–11) and (A–12) prove the formula (A–8) for any positive integer N.

From the proof given above, it is quite obvious that the formula (A–8) holds also for any negative integer N.

If we take $N=2$ in the formula (A–8), we shall obtain (4–11).

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