数理解析研究所講究録
第130巻 1971年 78-132

Lattice Green's Function for the Tetragonal Lattice at Arbitrary Points

Yoshihiko Abe and Shigetoshi Katsura

Department of Applied Physics and Department of Physics
Tohoku University, Sendai

Synopsis

The lattice Green's function for the tetragonal lattice at an arbitrary point

$$I(\alpha;\ell,m,n;\gamma) = \frac{1}{\pi^3}\iiint_0^{\pi} \frac{\cos \ell x \ \cos my \ \cos nz}{\alpha - i\varepsilon - \gamma \cos x - \cos y - \cos z}\, dxdydz$$

is evaluated, assuming $\alpha \geqq 0$, $\gamma \geqq 0$ without loss of generality. The integral $I(\alpha;\ell,m,n;\gamma)$ which has singularities at $\alpha = \pm\gamma\pm1\pm1$, is expressed in all regions of (α, γ), i. e., for i) $\alpha > 2 + \gamma$, ii) $2 - \gamma > \alpha > \gamma (\gamma < 2)$, iii) $\alpha < \gamma - 2$ $(\gamma > 2)$, iv) $\alpha < 2 - \gamma$ $(1 < \gamma < 2)$ and $\gamma > \alpha$ $(0 < \gamma < 1)$, v) $|\alpha - \gamma| < 2$ and $\alpha + \gamma > 2$, in terms of Kampé de Fériet function by the method of the analytic continuation using the Mellin-Barnes type integral. The numerical values are listed in figures.

§1. Introduction

We consider the lattice Green's function (LGF) for the tetragonal lattice. As a general introduction of the lattice Green's function, see for example ref. 1. The lattice Green's function for the tetragonal lattice at an arbitrary point (ℓ, m, n) is given by

$$I \equiv I(\alpha;\ \ell,\ m,\ n;\ \gamma)$$

$$= \frac{1}{\pi^3}\iiint_0^{\pi} \frac{\cos \ell x \cos mx \cos nz \, dxdydz}{\alpha - i\varepsilon - \gamma\cos x - \cos y - \cos z}, \quad (1.\ 1)$$

where α is the negative of the nomalized energy, ε is a positive infinitesimal, and γ, 1, 1 are normalized force constants of the tetragonal lattice. The regions $|\alpha| > 2 + |\gamma|$ and $|\alpha| < 2 + |\gamma|$ corresponds to the outside and the inside of the band, respectively.

The integral (1. 1) is real for $|\alpha| > |\gamma| + 2$, and complex otherwise. It has singularities at $\alpha = \pm\gamma \pm 1 \pm 1 = \gamma + 2, \gamma, \gamma - 2, -\gamma, -\gamma + 2$, and $-\gamma - 2$.

The real part of $I(\alpha;\ \ell,\ m,\ n;\ \gamma)$ is an odd or even function of α and the imaginary part is an even or odd function, according as $\ell + m + n$ is even or odd. The real and the imaginary parts of $I(\alpha;\ \ell,\ m,\ n;\ \gamma)$ are even or odd functions of γ when ℓ is even or odd. We assume $\ell \geqq 0$, $m \geqq n \geqq 0$ and $\alpha \geqq 0$, $\gamma \geqq 0$ without loss of generality.

The value $I(2 + \gamma;\ 0,\ 0,\ 0;\ \gamma)$ is obtained by

Montroll[2] in terms of complete elliptic integral of the second kind. Maradudin, Montroll, Weiss, Herman and Milnes[3] (MMWHM) give series expansion of $I(\alpha >> 2 + \gamma, \ell, m, n; \gamma)$ in powers of $1/\alpha^2$ and a few terms of $I(\alpha \gtrsim 2 + \gamma, \ell, m, n; \gamma)$ in powers of $\alpha-2-\gamma$. They also give a table for $\ell^2 + m^2 + n^2 \leq 15$, $2 + \gamma < \alpha < \infty$. Mannari and Kawabe[4] expressed $I(\alpha > 2 + \gamma, 0, 0, 0; \gamma)$ as a single integral of the complete elliptic integrals.

In this paper the integral (1. 1) is evaluated for respective regions in (α, γ) plane by the method of the analytic continuation using the Mellin-Barnes type integral developed in the previous paper[5] of the evaluation of LGF of the simple cubic lattice at the origin. The integral in each region is evaluated in terms of Kampé de Fériet functions[6] and of modified Kampé de Fériet functions defined in this paper. Figure 1 shows the singular lines in (α, γ) plane and the correspondence between each region and each section in this paper. They provide simple and rapid subroutines for numerical calculations of the values of integrals and give insight on the analytical nature of the singularities. The results of the numerical calculations are shown in Fig. 2.

The results of the present paper reduce to those for the simple cubic lattice at the origin[5] ($\ell = m = n = 0$, $\gamma \doteq 1$), for the square lattice[7] ($\ell = 0$, $\gamma = 0$) and for the linear lattice[7] ($m = n = 0$, $\alpha \to \alpha\gamma$, $\gamma \to \infty$) as special cases. i. e.,

$$I_{sc}(\alpha) = I(\alpha;\ 0,\ 0,\ 0;\ 1),$$

$$I_{sq}(\alpha;\ m,\ n) = I(\alpha;\ 0,\ m,\ n;\ 0),$$

$$I_{lin}(\alpha;\ \ell) = \lim_{\gamma\to\infty} \gamma\, I(\gamma\alpha;\ \ell,\ 0,\ 0;\ \gamma).$$

Hereafter ref. 5 and ref. 7 are referred as KIA and KI, respectively.

§2. Mellin-Barnes Type Integral Representation

The integral (1. 1) is transformed into

$$I = i^{\ell+m+n+1} \int_0^\infty e^{-i(a-i\varepsilon)t} J_\ell(\gamma t)\, J_m(t)\, J_n(t)\, dt. \quad (2.\ 1)$$

The product of Bessel functions $J_m(t)J_n(t)$ is transformed into the Mellin-Barnes type integral representation by

$$J_m(z)J_n(z) = \frac{1}{m!n!} \left(\frac{z}{2}\right)^{m+n} {}_2F_3 \left[\begin{matrix} \frac{m+n+1}{2}, \frac{m+n}{2}+1; -z^2 \\ m+1, n+1, m+n+1 \end{matrix}\right]$$

$$= \left(\frac{z}{2}\right)^{m+n} \frac{1}{2\pi i} \int_C ds \frac{\Gamma(2s+m+n+1)\,\Gamma(-s)}{\Gamma(s+m+1)\,\Gamma(s+n+1)\,\Gamma(s+m+n+1)} \left(\frac{z^2}{4}\right)^s,$$

(2. 2)

where C is a straight line parallel to the imaginary axis crossing at the point $s = -\Delta$ $(\Delta \to +0)$. Substituting Eq. (2. 2) into Eq. (2. 1) and changing the order of integrations ds and dt, we have

$$I = i^{p+1} \left(\frac{1}{2}\right)^{m+n} \frac{1}{2\pi i} \int_C ds \frac{\Gamma(2s+m+n+1)\Gamma(-s)}{\Gamma(s+m+1)\Gamma(s+n+1)\Gamma(s+m+n+1)} \left(\frac{1}{4}\right)^s$$

$$\times \int_0^\infty dt\, e^{-i(a-i\varepsilon)t} J_\ell(\gamma t)\, t^{2s+m+n}. \quad (2.\ 3)$$

For $\varepsilon > 0$ and $\ell+m+n > 0$, the integral $\int dt$ containing a Bessel function converges and gives

$$\int_0^\infty dt \;\ldots = (\tfrac{\gamma}{2})^{\ell} (-\tfrac{i}{a})^{p+2s+1} \frac{\Gamma(2s+p+1)}{\ell\,!}$$

$$\times\; {}_2F_1\,(s + \tfrac{p+1}{2}\;,\; s + \tfrac{p}{2} + 1\;;\; \ell + 1\;; \tfrac{\gamma^2}{a^2}),$$

(2. 4)

where $p = \ell + m + n$. Then

$$I = \frac{1}{a}\,(\frac{1}{2a})^p\,\frac{\gamma^{\ell}}{\ell!}$$

$$\times\; \frac{1}{2\pi i}\int_C ds\; \frac{\Gamma(2s+p+1)\Gamma(2s+m+n+1)\Gamma(-s)}{\Gamma(s+m+1)\Gamma(s+n+1)\Gamma(s+m+n+1)}\;(-\frac{1}{4a^2})^s$$

$$\times\; {}_2F_1\,(s + \tfrac{p+1}{2}\;,\; s + \tfrac{p}{2} + 1\;;\; \ell + 1\;; \tfrac{\gamma^2}{a^2}). \qquad (2.\ 5)$$

We can obtain expressions for the tetragonal LGF in terms of Mellin-Barnes type integral. Later calculations are based on the integral representation (2. 5).

§3. $a > \gamma + 2$

For $a > \gamma$, expanding ${}_2F_1$ in Eq. (2. 5) and changing the order of the integration and summation, we obtain

$$I = \frac{2^{m+n}\gamma^{\ell}}{\pi a^{p+1}} \sum_k \frac{1}{k!\,\Gamma(k+\ell+1)} \left(\frac{\gamma^2}{a^2}\right)^k$$

$$\times \frac{1}{2\pi i}\int_C ds \frac{\Gamma(s+\frac{m+n+1}{2})\Gamma(s+\frac{m+n}{2}+1)}{\Gamma(s+m+1)\Gamma(s+n+1)\Gamma(s+m+n+1)}$$

$$\times \Gamma(s+k+\frac{p+1}{2})\Gamma(s+k+\frac{p}{2}+1)\Gamma(-s)\left(-\frac{4}{a^2}\right)^s. \quad (3.\ 1)$$

The abbreviation $\sum_k$ is used throughout the present paper when the upper and lower indices of summation are 0 and ∞. For $a > 2$, the path of the integration is closed with a semi-circle in the right half plane in the complex s-plane. The poles of the integrand in the right half plane are

$$s = j, \qquad j = 0, 1, 2, \ldots. \quad (3.\ 2)$$

The contribution of poles is denoted by I3. By calculating the residues, we have

$$I3 = \frac{\pm}{a}\left(\frac{1}{2a}\right)^p \gamma^{\ell} \sum_k \sum_j \frac{\Gamma(m+n+2j+1)\,\Gamma(p+2k+2j+1)}{k!j!\,\Gamma(\ell+k+1)\,\Gamma(m+j+1)}$$

$$\times \frac{\gamma^{2k}}{\Gamma(n+j+1)\,\Gamma(m+n+j+1)} \frac{1}{(4a^2)^{k+j}} \,. \tag{3. 3}$$

Using the Kampé de Fériet function (see Appendix), Eq. (3. 3) is represented by

$$I3 = \frac{1}{a} \frac{p!\gamma^{\ell}}{\ell!m!n!} \left(\frac{1}{2a}\right)^p$$

$$\times F \left[\begin{array}{c|l|c} 2 & \frac{p+1}{2}, \frac{p}{2}+1 & \\ 2 & \frac{m+n+1}{2}, \frac{m+n}{2}+1;\ \alpha,\ \alpha' & \frac{4}{a^2}, \frac{\gamma^2}{a^2} \\ 0 & & \\ 3 & m+1,\ n+1,\ m+n+1;\ \ell+1,\ \alpha,\ \alpha' & \end{array} \right] \tag{3. 4}$$

Equation (3. 3) converges for $a > 2 + \gamma$. Equation (3. 3) is transformed into

$$I3 = \frac{1}{a} \left(\frac{1}{2a}\right)^p \frac{\gamma^{\ell}}{m!n!} \sum_k \frac{\Gamma(p+2k+1)}{k!\,\Gamma(\ell+k+1)} \left(\frac{\gamma}{2a}\right)^{2k}$$

$$\times\ {}_4F_3 \left[\begin{array}{l} \frac{m+n+1}{2}, \frac{m+n}{2}+1, -k, -k-\ell;\ \frac{1}{\gamma^2} \\ m+1,\ n+1,\ m+n+1 \end{array} \right], \tag{3. 5}$$

which is a single series of γ^2/a^2 when the coefficients have been calculated by a finite series. The imaginary part of $I(a;\ \ell,\ m,\ n;\ \gamma)$ does not appear for $a > 2 + \gamma$.

For $\gamma = 1$ and $\ell = m = n = 0$, we have

$$I3 = \frac{1}{a} F \left[\begin{array}{c|ll|l} 2 & \frac{1}{2}, 1 & & \\ 1 & \frac{1}{2}; \alpha & & \frac{4}{a^2}, \frac{1}{a^2} \\ 0 & & & \\ 2 & 1, 1; & 1, \alpha & \end{array} \right] \qquad (3.\ 6)$$

in agreement with the LGF of the simple cubic lattice given in Eq. (7) in KIA.

For $\gamma = 0$ and $\ell = 0$, the LGF of the square lattice, Eq. (3. 2) in KI, is reproduced.

For $a \to \gamma a$ and $m = n = 0$, we have

$$\lim_{\gamma \to \infty} \gamma I(\gamma a; \ell, 0, 0; \gamma)$$

$$= \frac{1}{a} \left(\frac{1}{2a}\right)^{\ell} {}_2F_1 \left(\frac{\ell+1}{2}, \frac{\ell}{2} + 1; \ell+1; \frac{1}{a^2} \right)$$

$$= a(a^2 - 1)^{-1/2} [\, a - (a^2 - 1)^{1/2}]^{\ell} \qquad (3.\ 7)$$

which is the LGF of the linear lattice given in Eq. (A. 1) in KI.

§4. $2 - \gamma > \alpha > \gamma \quad (\gamma < 2)$

We start from Eq. (3. 1). For $\alpha < 2$, the path of integration in Eq. (3. 1) is closed with a semi-circle in the left half plane. The integrand has double poles at

$$s = -[\tfrac{p+1}{2}]-k-\tfrac{1}{2}-j, \quad j = 0, 1, 2, \dots, \tag{4. 1a}$$

and simple poles at

$$s = -[\tfrac{p}{2}]-k-1-j, \quad j = 0, 1, \dots, m-[\tfrac{p}{2}]-k-1, \tag{4. 1b}$$

and at

$$s = -[\tfrac{m+n+1}{2}]-\tfrac{1}{2}-j, \quad j = 0, 1, \dots, [\tfrac{p+1}{2}]-[\tfrac{m+n+1}{2}]+k-1. \tag{4. 1c}$$

where $[x]$ is the largest integer not exceeding x.
When $m - [\frac{p}{2}] - k - 1 < 0$, poles in (4. 1b) do not appear.
Similar situations are not notified hereafter.

We denote the contributions from the first, the second and the third sets of poles by $I4_1$, $I4_2$ and $I4_3$, respectively. Then

$$I4_1 = \frac{(-\gamma)^{\ell}}{2\pi^{3/2}\ell!}\,\alpha^{2[\frac{p+1}{2}]-p}\,\frac{\Gamma([\frac{p+1}{2}]-m+\frac{1}{2})\Gamma([\frac{p+1}{2}]-n+\frac{1}{2})}{\Gamma([\frac{p+1}{2}]-[\frac{p}{2}]+\frac{1}{2})\Gamma(2[\frac{p+1}{2}]-m-n+1)}$$

$$\times\,\Gamma([\tfrac{p+1}{2}]-m-n+\tfrac{1}{2})\Gamma([\tfrac{p+1}{2}]+\tfrac{1}{2})$$

$$\times(F+i\tilde{F})\left[\begin{array}{c|l|c} 4 & [\frac{p+1}{2}]-m+\frac{1}{2},[\frac{p+1}{2}]-n+\frac{1}{2},[\frac{p+1}{2}]-m-n+\frac{1}{2},[\frac{p+1}{2}]+\frac{1}{2} & \\ 0 & & \\ 2 & [\frac{p+1}{2}]-\frac{m+n}{2}+1,[\frac{p+1}{2}]-\frac{m+n}{2}+\frac{1}{2} & \frac{\alpha^2}{4},\frac{\gamma^2}{4} \\ 1 & [\frac{p+1}{2}]-[\frac{p}{2}]+\frac{1}{2}\ ;\ \ell+1 & \end{array}\right], \quad (4.\ 2)$$

where $\tilde{F}$ is a modified Kampé de Fériet function defined in the Appendix, and

$$I4_2=\frac{\sqrt{\pi}(-)^{n+1+\ell}}{2\ell!}\gamma^{\ell}\alpha^{2[\frac{p}{2}]+1-p}\ \frac{\Gamma([\frac{p}{2}]+1)\Gamma([\frac{p}{2}]-n+1)}{\Gamma([\frac{p}{2}]-[\frac{p+1}{2}]+\frac{3}{2})\Gamma(2[\frac{p}{2}]-m-n+2)}$$

$$\times\frac{1}{\Gamma(m-[\frac{p}{2}])\Gamma(m+n-[\frac{p}{2}])}$$

$$\times F\left[\begin{array}{c|l|c} 4 & [\frac{p}{2}]+1,[\frac{p}{2}]-m+1,[\frac{p}{2}]-n+1,[\frac{p}{2}]-m-n+1 & \\ 0 & & \\ 2 & [\frac{p}{2}]-\frac{m+n}{2}+\frac{3}{2},[\frac{p}{2}]-\frac{m+n}{2}+1 & \frac{\alpha^2}{4},\frac{\gamma^2}{4} \\ 1 & [\frac{p}{2}]-[\frac{p+1}{2}]+\frac{3}{2}\ ;\ \ell+1 & \end{array}\right], \quad (4.\ 3)$$

and

$$I4_3=\frac{i(-)^{m+n}}{\pi^{5/2}}(\frac{\gamma}{2\alpha})^{\ell}\alpha^{2[\frac{m+n+1}{2}]-m-n}\sum_k\frac{1}{k!\Gamma(k+\ell+1)}(\frac{\gamma^2}{4\alpha^2})^k$$

$$\times\sum_{j=0}^{[\frac{p+1}{2}]-[\frac{m+n+1}{2}]+k-1}\frac{\Gamma(p+2k-2j-2[\frac{m+n+1}{2}])\Gamma(j+[\frac{m+n+1}{2}]-m-n+\frac{1}{2})}{j!\Gamma(j+[\frac{m+n+1}{2}]-[\frac{m+n}{2}]+\frac{1}{2})}$$

$$\times\,\Gamma\left(j+\left[\frac{m+n+1}{2}\right]-m+\frac{1}{2}\right)\Gamma\left(j+\left[\frac{m+n+1}{2}\right]-n+\frac{1}{2}\right)\Gamma\left(j+\left[\frac{m+n+1}{2}\right]+\frac{1}{2}\right)\alpha^{2j} \quad (4.\ 4)$$

$$=\frac{i(-)^{m+n}}{\pi^3}\,\gamma^{\ell}\,(2\alpha)^{2\left[\frac{p+1}{2}\right]-p-2}$$

$$\times\left\{\gamma^2\,\frac{\Gamma\left(\left[\frac{p+1}{2}\right]+\frac{1}{2}\right)\Gamma\left(\left[\frac{p+1}{2}\right]-m+\frac{1}{2}\right)\Gamma\left(\left[\frac{p+1}{2}\right]-n+\frac{1}{2}\right)\Gamma\left(\left[\frac{p+1}{2}\right]-m-n+\frac{1}{2}\right)}{\Gamma(\ell+2)\,\Gamma\left(2\left[\frac{p+1}{2}\right]-m-n+1\right)}\right.$$

$$\times\,F\left[\begin{array}{c|l|l} 0 & & \\ 5 & \left[\frac{p+1}{2}\right]+\frac{1}{2},\left[\frac{p+1}{2}\right]-m+\frac{1}{2},\left[\frac{p+1}{2}\right]-n+\frac{1}{2},\left[\frac{p+1}{2}\right]-m-n+\frac{1}{2},1; & \\ & \qquad\left[\frac{p}{2}\right]-\left[\frac{p+1}{2}\right]+\frac{3}{2},1,1,\alpha,\alpha' & \frac{\gamma^2}{4},\ \frac{\gamma^2}{\alpha^2} \\ 2 & 2,\ \ell+2 & \\ 2 & \left[\frac{p+1}{2}\right]-\frac{m+n}{2}+1,\left[\frac{p+1}{2}\right]-\frac{m+n}{2}+\frac{1}{2}\ ;\ \alpha,\ \alpha' & \end{array}\right].$$

$$+\,\frac{\Gamma\left(\left[\frac{p+1}{2}\right]-\frac{1}{2}\right)\Gamma\left(\left[\frac{p+1}{2}\right]-m-\frac{1}{2}\right)\Gamma\left(\left[\frac{p+1}{2}\right]-n-\frac{1}{2}\right)\Gamma\left(\left[\frac{p+1}{2}\right]-m-n-\frac{1}{2}\right)}{\ell!\,\Gamma\left(2\left[\frac{p+1}{2}\right]-m-n-1\right)}$$

$$\left.\times\,F\left[\begin{array}{c|l|l} 2 & 1,\ \left[\frac{p}{2}\right]-\left[\frac{p+1}{2}\right]+\frac{3}{2} & \\ 3 & \frac{m+n}{2}-\left[\frac{p+1}{2}\right]+1,\frac{m+n}{2}-\left[\frac{p+1}{2}\right]+\frac{3}{2},\ 1;\ \alpha,\ \alpha',\ \alpha'' & \\ 0 & & \frac{4}{\alpha^2},\frac{\gamma^2}{\alpha^2} \\ 4 & -\left[\frac{p+1}{2}\right]+\frac{3}{2},-\left[\frac{p+1}{2}\right]+m+\frac{3}{2},-\left[\frac{p+1}{2}\right]+n+\frac{3}{2},-\left[\frac{p+1}{2}\right]+m+n+\frac{3}{2};\ell+1,\alpha,\alpha',\alpha'' & \end{array}\right]\right\}.$$

(4. 4')

The common region of the convergence of $I4_1$, $I4_2$ and $I4_3$ is given by $2 - \gamma > \alpha > \gamma$ ($\gamma < 1$).

For $\ell = 0$ and $\gamma = 0$, $I4_1$ is reduced to Eqs. (4. 7a) and (4. 7b) in KI, and $I4_2$ to Eqs. (4. 6a) and (4. 6b) in KI. $I4_3$ does not contribute for $\ell = 0$ and $\gamma = 0$. These are LGF of the square lattice.

§5. $a < \gamma - 2 \quad (\gamma > 2)$

Transforming ${}_2F_1(\ ;\ ;\gamma^2/a^2)$ in Eq. (2. 5) into ${}_2F_1(\ ;\ ;a^2/\gamma^2)$ with use of the Kummer's relation, and expanding ${}_2F_1(\ ;\ ;a^2/\gamma^2)$ for $a < \gamma$ and changing the order of the summation and the integration, we have

$$I = \frac{i}{\gamma\pi}\left(\frac{a}{\gamma}\right)^{2[\frac{p+1}{2}]-p}\left(-\frac{2}{\gamma}\right)^{m+n}\sum_k \frac{1}{k!\Gamma([\frac{p+1}{2}]-[\frac{p}{2}]+k+\frac{1}{2})}\left(\frac{a^2}{\gamma^2}\right)^k$$

$$\times \frac{1}{2\pi i}\int_C ds \frac{\cos s\pi\ \Gamma(s+[\frac{m+n+1}{2}]+\frac{1}{2})\Gamma(s+[\frac{m+n}{2}]+1)}{\Gamma(s+m+1)\Gamma(s+n+1)\Gamma(s+m+n+1)}$$

$$\times \Gamma(s+[\tfrac{p+1}{2}]+k+\tfrac{1}{2})\Gamma(s+[\tfrac{p+1}{2}]+k-\ell+\tfrac{1}{2})\Gamma(-s)\left(\frac{4}{\gamma^2}\right)^s$$

$$+ \frac{-1}{\gamma\pi}\left(\frac{a}{\gamma}\right)^{2[\frac{p}{2}]+1-p}\left(-\frac{2}{\gamma}\right)^{m+n}\sum_k \frac{1}{k!\Gamma([\frac{p}{2}]-[\frac{p+1}{2}]+k+\frac{3}{2})}\left(\frac{a^2}{\gamma^2}\right)^k$$

$$\times \frac{1}{2\pi i}\int_C ds \frac{\sin s\pi\ \Gamma(s+[\frac{m+n+1}{2}]+\frac{1}{2})\Gamma(s+[\frac{m+n}{2}]+1)}{\Gamma(s+m+1)\Gamma(s+n+1)\Gamma(s+m+n+1)}$$

$$\times \Gamma(s+[\tfrac{p}{2}]+k+1)\Gamma(s+[\tfrac{p}{2}]+k-\ell+1)\Gamma(-s)\left(\frac{4}{\gamma^2}\right)^s. \qquad (5.\ 1)$$

The first and the second terms of Eq. (5. 1) correspond to the imaginary and the real parts of I, respectively. We consider the case for $\gamma > 2$ in this section and the case for $\gamma < 2$ in the next section. The path of integration in both terms in Eq. (5. 1) are closed with a semi-circle in the right half plane. In this region, the integrand of the first term in Eq. (5. 1) has poles at

$$s = j, \qquad j = 0, 1, 2, \ldots \qquad (5.\ 2)$$

The integrand of the second term in Eq. (5. 1) has poles at

$$s = j, \qquad j = 0, 1, \ldots, \ell-[\tfrac{p}{2}]-k-1. \qquad (5.\ 3)$$

The contribution of poles of the first and the second sets of poles are denoted by $I5_1$ and $I5_2$.

$$I5_1 = \frac{i}{\sqrt{\pi}\gamma m! n!}\left(\frac{\alpha}{\gamma}\right)^{2[\frac{p+1}{2}]-p}\left(-\frac{1}{\gamma}\right)^{m+n}\frac{\Gamma([\frac{p+1}{2}]+\frac{1}{2})\Gamma([\frac{p+1}{2}]-\ell+\frac{1}{2})}{\Gamma([\frac{p+1}{2}]-[\frac{p}{2}]+\frac{1}{2})}$$

$$\times F\left[\begin{array}{c|l|c} 2 & [\frac{p+1}{2}]+\frac{1}{2},\ [\frac{p+1}{2}]-\ell+\frac{1}{2} & \\ 2 & \frac{m+n}{2}+\frac{1}{2},\ \frac{m+n}{2}+1;\quad \alpha,\ \alpha' & \\ 0 & & \frac{4}{\gamma^2},\ \frac{\alpha^2}{\gamma^2} \\ 3 & m+1, n+1, m+n+1;\ [\frac{p+1}{2}]-[\frac{p}{2}]+\frac{1}{2},\ \alpha, \alpha' & \end{array}\right], \qquad (5.\ 4)$$

and

$$I5_2 = \frac{\sqrt{\pi}(-)^{[\frac{p}{2}]-p}}{m!n!}\left(\frac{\alpha}{\gamma}\right)^{2[\frac{p}{2}]+1-p}\left(\frac{1}{\gamma}\right)^{m+n+1}\frac{\Gamma([\frac{p}{2}]+1)}{\Gamma(\ell-[\frac{p}{2}])\Gamma([\frac{p}{2}]-[\frac{p+1}{2}]+\frac{3}{2})}$$

$$\times F\left[\begin{array}{c|l|l} 2 & [\frac{p}{2}]+1,\ [\frac{p}{2}]-\ell+1 & \\ 2 & \frac{m+n}{2}+\frac{1}{2},\ \frac{m+n}{2}+1;\ \alpha,\ \alpha' & \frac{4}{\gamma^2},\ \frac{\alpha^2}{\gamma^2} \\ 0 & & \\ 3 & m+1, n+1, m+n+1; [\frac{p}{2}]-[\frac{p+1}{2}]+\frac{3}{2},\ \alpha,\ \alpha' & \end{array}\right]. \qquad (5.\ 5)$$

$I5_1$ and $I5_2$ converge $\alpha < \gamma - 2$. The real part, $I5_2$, vanish for $\alpha < \gamma - 2$ when $\ell \leq [\frac{p}{2}]$.

The LGF of the linear lattice is obtained from the sum of $I5_1$ and $I5_2$ for $\gamma \to \infty$, $m = n = 0$:

$$\lim_{\gamma\to\infty} \gamma\, I(\alpha\gamma;\ \ell,\ 0,\ 0;\ \gamma)$$

$$= (-)^{\frac{\ell+1}{2}}\ {}_2F_1\left(\frac{\ell+1}{2},\ \frac{-\ell+1}{2};\ \frac{1}{2}\ ;\ \alpha^2\right)$$

$$+ (-)^{\frac{\ell}{2}}\ \alpha\ell\ {}_2F_1\left(\frac{\ell}{2}+1,\ -\frac{\ell}{2}+1;\ \frac{3}{2};\ \alpha^2\right). \qquad (5.\ 6)$$

The first term is equal to Eq. (A. 3) or Eq. (A. 4) in KI, when ℓ is even or odd, respectively. The second term is equal to Eq. (A. 4) or Eq. (A. 3) in KI, when ℓ is even or odd, respectively.

§6. $\alpha < 2 - \gamma$ $(1 < \gamma < 2)$ and $\gamma > \alpha$ $(0 < \gamma < 1)$

We start from the Eq. (5. 1) and consider the case for $\gamma < 2$ in this section. The paths of the integrations of Eq. (5. 1) are closed by a semi-circle in the left half plane.

The integrand of the first term of Eq. (5. 1) in the left half plane has double poles at

$$s = -\left[\frac{p+1}{2}\right] - k - j - \frac{1}{2}, \qquad j = 0, 1, 2, \ldots \tag{6. 1a}$$

and simple poles at

$$s = \ell - \left[\frac{p+1}{2}\right] - k - j - \frac{1}{2}, \qquad j = \max\left(0, \ell + \left[\frac{m+n+1}{2}\right] - \left[\frac{p+1}{2}\right] - k\right), \ldots, \ell - 1. \tag{6. 1b}$$

We denote the contribution from the first and that from the second sets of poles by $I6_{1-1}$ and $I6_{1-2}$, respectively. Then

$$I6_{1-1} = \frac{i}{2\pi^{3/2}\ell!}(-\gamma)^{\ell}\,\alpha^{2[\frac{p+1}{2}] - p}$$

$$\times \frac{\Gamma([\frac{p+1}{2}]-m+\frac{1}{2})\Gamma([\frac{p+1}{2}]-n+\frac{1}{2})\Gamma([\frac{p+1}{2}]-m-n+\frac{1}{2})\Gamma([\frac{p+1}{2}]+\frac{1}{2})}{\Gamma(2[\frac{p+1}{2}]-m-n+1)\Gamma([\frac{p+1}{2}]-[\frac{p}{2}]+\frac{1}{2})}$$

$$\times \tilde{F}\left[\begin{array}{c|l} 4 & [\frac{p+1}{2}]-m+\frac{1}{2},[\frac{p+1}{2}]-n+\frac{1}{2},[\frac{p+1}{2}]-m-n+\frac{1}{2},[\frac{p+1}{2}]+\frac{1}{2} \\ 0 & \\ 2 & [\frac{p+1}{2}]-\frac{m+n}{2}+\frac{1}{2},\ [\frac{p+1}{2}]-\frac{m+n}{2}+1 \\ 1 & \ell+1\ ;\ [\frac{p+1}{2}]-[\frac{p}{2}]+\frac{1}{2} \end{array}\middle| \frac{\gamma^2}{4},\frac{a^2}{4}\right], \quad (6.\ 2)$$

and

$$I6_{1-2} = \frac{i}{2\pi^{5/2}}\frac{a^{2[\frac{p+1}{2}]-p}}{\gamma^{\ell}}\sum_k \frac{1}{k!\Gamma(k+[\frac{p+1}{2}]-[\frac{p}{2}]+\frac{1}{2})}(\frac{a^2}{4})^k$$

$$\times \sum_{j=\max(0,\ell+[\frac{m+n+1}{2}]-[\frac{p+1}{2}]-k)}^{\ell-1}\frac{\Gamma(j+k+[\frac{p+1}{2}]-\ell+\frac{1}{2})}{j!\Gamma(2j+2k+2[\frac{p+1}{2}]-p-\ell+1)}$$

$$\times \Gamma(j+k+[\frac{p+1}{2}]-\ell-m+\frac{1}{2})\Gamma(j+k+[\frac{p+1}{2}]-\ell-n+\frac{1}{2})$$

$$\times \Gamma(j+k+[\frac{p+1}{2}]-p+\frac{1}{2})\Gamma(\ell-j)(-\frac{\gamma^2}{4})^j \quad (6.\ 3)$$

$$= \frac{i}{2\pi^{5/2}}\frac{a^{2[\frac{p+1}{2}]-p}}{\gamma^{\ell}}(-\frac{\gamma^2}{4})^{\ell-1}$$

$$\times \left\{\frac{a^2}{4}\times\frac{\Gamma([\frac{p+1}{2}]-m+\frac{1}{2})\Gamma([\frac{p+1}{2}]-n+\frac{1}{2})\Gamma([\frac{p+1}{2}]-m-n+\frac{1}{2})\Gamma([\frac{p+1}{2}]+\frac{1}{2})}{\Gamma([\frac{p+1}{2}]-[\frac{p}{2}]+\frac{3}{2})\Gamma(\ell)\Gamma(2[\frac{p+1}{2}]-m-n+1)}\right.$$

$$\times F\left[\begin{array}{c|c|c} 0 & & \\ 5 & [\frac{p+1}{2}]+\frac{1}{2},[\frac{p+1}{2}]-m+\frac{1}{2},[\frac{p+1}{2}]-n+\frac{1}{2},[\frac{p+1}{2}]-m-n+\frac{1}{2},1; & \\ & 1-\ell,\ 1,\ 1,\ \alpha,\ \alpha' & \frac{a^2}{4},\frac{a^2}{\gamma^2} \\ 2 & 2,\ [\frac{p+1}{2}]-[\frac{p}{2}]+\frac{3}{2} & \\ 2 & [\frac{p+1}{2}]-\frac{m+n}{2}+\frac{1}{2},\ [\frac{p+1}{2}]-\frac{m+n}{2}+1;\ \alpha,\ \alpha' & \end{array}\right]$$

$$+\frac{\Gamma([\frac{p+1}{2}]-\frac{1}{2})\Gamma([\frac{p+1}{2}]-m-\frac{1}{2})\Gamma([\frac{p+1}{2}]-n-\frac{1}{2})\Gamma([\frac{p+1}{2}]-m-n-\frac{1}{2})}{\Gamma([\frac{p+1}{2}]-[\frac{p}{2}]+\frac{1}{2})\Gamma(\ell)\Gamma(2[\frac{p+1}{2}]-m-n-1)}$$

$$\times\frac{\Gamma([\frac{p+1}{2}]-\frac{1}{2})\Gamma([\frac{p+1}{2}]-m-\frac{1}{2})\Gamma([\frac{p+1}{2}]-n-\frac{1}{2})\Gamma([\frac{p+1}{2}]-m-n-\frac{1}{2})}{\Gamma([\frac{p+1}{2}]-[\frac{p}{2}]+\frac{1}{2})\Gamma(\ell)\Gamma(2[\frac{p+1}{2}]-m-n-1)}$$

$$\times F\left[\begin{array}{c|c|c} 2 & 1,\ 1-\ell & \\ 3 & \frac{m+n}{2}-[\frac{p+1}{2}]+1,\ \frac{m+n}{2}-[\frac{p+1}{2}]+\frac{3}{2},\ 1;\ \alpha,\alpha',\alpha'' & \\ 0 & & \frac{4}{\gamma^2},\ \frac{a^2}{\gamma^2} \\ 4 & -[\frac{p+1}{2}]+\frac{3}{2},m-[\frac{p+1}{2}]+\frac{3}{2},n-[\frac{p+1}{2}]+\frac{3}{2},m+n-[\frac{p+1}{2}]+\frac{3}{2}; & \\ & [\frac{p+1}{2}]-[\frac{p}{2}]+\frac{1}{2},\ \alpha,\alpha',\alpha'' & \end{array}\right]\Bigg\}. \qquad (6.\ 3')$$

The integrand of the second term in Eq. (5. 1) has poles at

$$s = -[\frac{m+n+1}{2}] - j - \frac{1}{2}\ , \quad j = 0, 1, 2, \ldots \qquad (6.\ 4a)$$

and at

$$s = -[\tfrac{p}{2}] - k - j - 1, \qquad j = 0, 1, \ldots, m-[\tfrac{p}{2}]-k-1 . \tag{6. 4b}$$

The contribution of the former and the latter are denoted by $I6_{2-1}$ and $I6_{2-2}$, respectively. Then

$$I6_{2-1} = \frac{1}{2\pi^3} (\tfrac{\alpha}{\gamma})^{2[\frac{p}{2}]+1-p} (\tfrac{\gamma}{2})^{2[\frac{m+n+1}{2}]-m-n}$$

$$\left\{ \frac{\Gamma([\frac{m+n+1}{2}]-m-n+\frac{1}{2})\Gamma([\frac{m+n+1}{2}]-m+\frac{1}{2})\Gamma([\frac{m+n+1}{2}]-n+\frac{1}{2})}{\Gamma([\frac{m+n+1}{2}]-[\frac{m+n}{2}]+\frac{1}{2})\Gamma([\frac{p}{2}]-[\frac{p+1}{2}]+\frac{3}{2})} \right.$$

$$\times \Gamma([\tfrac{m+n+1}{2}]+\tfrac{1}{2})\Gamma([\tfrac{p}{2}]-[\tfrac{m+n+1}{2}]+\tfrac{1}{2})\Gamma([\tfrac{p}{2}]-[\tfrac{m+n+1}{2}]-\ell+\tfrac{1}{2})$$

$$\times F\left[\begin{matrix} 0 \\ 4 \\ \\ 2 \\ 1 \end{matrix}\left|\begin{matrix} \\ [\frac{m+n+1}{2}]-m-n+\frac{1}{2},[\frac{m+n+1}{2}]-m+\frac{1}{2},[\frac{m+n+1}{2}]-n+\frac{1}{2},[\frac{m+n+1}{2}]+\frac{1}{2}; \\ [\frac{p}{2}]-[\frac{m+n+1}{2}]+\frac{1}{2},[\frac{p}{2}]-[\frac{m+n+1}{2}]-\ell+\frac{1}{2},\ 1,\ \alpha \\ [\frac{p}{2}]-[\frac{p+1}{2}]+\frac{3}{2},\ 1 \\ [\frac{m+n+1}{2}]-[\frac{m+n}{2}]+\frac{1}{2}\ ;\alpha \end{matrix}\right| \frac{\alpha^2}{4},\frac{\alpha^2}{\gamma^2}\right]$$

$$+ \frac{\gamma^2}{4} \frac{\Gamma([\frac{m+n+1}{2}]-m-n+\frac{3}{2})\Gamma([\frac{m+n+1}{2}]-m+\frac{3}{2})\Gamma([\frac{m+n+1}{2}]-n+\frac{3}{2})}{\Gamma([\frac{m+n+1}{2}]-[\frac{m+n}{2}]+\frac{3}{2})\Gamma([\frac{p}{2}]-[\frac{p+1}{2}]+\frac{3}{2})}$$

$$\times\ \Gamma([\tfrac{m+n+1}{2}]+\tfrac{3}{2})\Gamma([\tfrac{p}{2}]-[\tfrac{m+n+1}{2}]-\tfrac{1}{2})\Gamma([\tfrac{p}{2}]-[\tfrac{m+n+1}{2}]-\ell-\tfrac{1}{2})$$

$$\times\ F\left[\begin{array}{c|l|l} 4 & [\frac{m+n+1}{2}]-m-n+\frac{3}{2}, [\frac{m+n+1}{2}]-m+\frac{3}{2}, [\frac{m+n+1}{2}]-n+\frac{3}{2}, [\frac{m+n+1}{2}]+\frac{3}{2} & \\ 1 & 1\ ;\ \alpha & \\ 2 & [\frac{m+n+1}{2}]-[\frac{m+n}{2}]+\frac{3}{2},\ 2 & \frac{\gamma^2}{4}, \frac{a^2}{4} \\ 2 & [\frac{m+n+1}{2}]-[\frac{p}{2}]+\frac{3}{2}, [\frac{m+n+1}{2}]-[\frac{\gamma}{2}]+\ell+\frac{3}{2}; [\frac{p}{2}]-[\frac{p+1}{2}]+\frac{3}{2},\ \alpha & \end{array}\right]\Bigg\}$$

(6. 5)

$$I6_{2-2} = (-)^{\ell+n+1}\frac{\sqrt{\pi}}{2\ell!}\,a^{2[\frac{p}{2}]+1-p}\,\gamma^{\ell}$$

$$\times\ \frac{\Gamma([\frac{p}{2}]+1)\Gamma([\frac{p}{2}]-n+1)}{\Gamma([\frac{p}{2}]-[\frac{p+1}{2}]+\frac{3}{2})\Gamma(2[\frac{p}{2}]-m-n+2)} \times \frac{1}{\Gamma(m-[\frac{p}{2}])\Gamma(m+n-[\frac{p}{2}])}$$

$$\times\ F\left[\begin{array}{c|l|l} 4 & [\frac{p}{2}]+1,\ [\frac{p}{2}]-m+1,\ [\frac{p}{2}]-n+1,\ [\frac{p}{2}]-m-n+1 & \\ 0 & & \\ 2 & [\frac{p}{2}]-\frac{m+n}{2}+\frac{3}{2},\ [\frac{p}{2}]-\frac{m+n}{2}+1 & \frac{\gamma^2}{4}, \frac{a^2}{4} \\ 1 & \ell+1;\ [\frac{p}{2}]-[\frac{p+1}{2}]+\frac{3}{2} & \end{array}\right].$$

(6. 6)

Notice that $I6_{1-2}$ appears only when $\ell \geqq 1$ and $I6_{2-2}$ appears only when $m-[\frac{p}{2}] > 0$.

The common region of the convergence of $I6_{1-1}$, $I6_{1-2}$, $I6_{2-1}$, $I6_{2-2}$ is given by $a < \gamma$ $(\gamma < 1)$ and $a < 2 - \gamma$ $(1 < \gamma < 2)$.

For $\gamma = 1$ and $\ell = m = n = 0$, we have

$$I6_{1-1} = \frac{i}{2}\,\tilde{F}\left[\begin{array}{c|l|l} 3 & \frac{1}{2}\,,\ \frac{1}{2}\,,\ \frac{1}{2} & \\ 0 & & \frac{1}{4}\,,\ \frac{a^2}{4} \\ 1 & 1 & \\ 1 & 1\,;\ \frac{1}{2} & \end{array}\right], \qquad (6.\ 7)$$

and

$$I6_{2-1} = \frac{a}{\pi}\,F\left[\begin{array}{c|l|l} 0 & & \\ 3 & \frac{1}{2}\,,\ \frac{1}{2}\,,\ \frac{1}{2}\,;\ \frac{1}{2}\,,\ \frac{1}{2}\,,\ 1 & \frac{a^2}{4}\,,\ a^2 \\ 2 & \frac{3}{2}\,,\ 1 & \\ 0 & & \end{array}\right]$$

$$+\ \frac{a}{8\pi}\,F\left[\begin{array}{c|l|l} 3 & \frac{3}{2}\,,\ \frac{3}{2}\,,\ \frac{3}{2} & \\ 1 & \alpha\,;\ 1 & \frac{a^2}{4}\,,\ \frac{1}{4} \\ 1 & 2 & \\ 2 & \frac{3}{2}\,,\ \alpha\,;\ \frac{3}{2}\,,\ \frac{3}{2} & \end{array}\right]. \qquad (6.\ 8)$$

Equation (6. 7) is equivalent to Eq. (18) in KIA, the imaginary part of the LGF of the simple cubic lattice. Equation (6. 8) is equivalent to Eq. (13) in KIA, the real part of the LGF of the simple cubic lattice. $I6_{1-2}$ and $I6_{2-2}$ do not contribute to the case for $\ell = m = n = 0$.

§7. $|\alpha - \gamma| < 2$ and $\alpha + \gamma > 2$

Quadratic transformation is useful to obtain the series expansion in terms of $\alpha - \gamma$, and the hypergeometric function in Eq. (2. 5) is transformed into

$$ {}_2F_1(s+\tfrac{1}{2}p+\tfrac{1}{2}, s+\tfrac{1}{2}p+1; \ell+1; \frac{\gamma^2}{\alpha^2}) $$

$$ = (\frac{\alpha}{\alpha+\gamma})^{2s+p+1} {}_2F_1(2s+p+1, \ell+\tfrac{1}{2}; 2\ell+1; \frac{2\gamma}{\alpha+\gamma}) . \qquad (7.\ 1) $$

We again apply the Kummer's relation which transforms ${}_2F_1(\ ;\ ;z)$ into ${}_2F_1(\ ;\ ;1-z)$ to the hypergeometric function of Eq. (7.1). Expanding the hypergeometric function and changing the order of the summation and the integration, we obtain

$$ I = I7_1 + I7_2 $$

$$ I7_1 = \frac{\sqrt{\pi}\ (-)^{m+n+1}}{\alpha+\gamma} \left(\frac{1}{2(\alpha+\gamma)}\right)^p (4\gamma)^\ell \frac{1}{\Gamma(\ell+\frac{1}{2})} $$

$$ \times \sum_k \frac{\Gamma(k+\ell+\frac{1}{2})}{k!} \left(\frac{\alpha-\gamma}{\alpha+\gamma}\right)^k $$

$$ \times \frac{1}{2\pi i} \int_C ds \frac{\Gamma(2s+p+k+1)\Gamma(2s+m+n+1)\Gamma(-s)}{\Gamma(s+m+1)\Gamma(s+n+1)\Gamma(s+m+n+1)} $$

$$ \times \frac{1}{\Gamma(-2s-p+2\ell)\Gamma(2s+m+n+k+\frac{3}{2}) \cos 2s\pi} (-\tfrac{1}{4})^s \left(\frac{1}{\alpha+\gamma}\right)^{2s}, \qquad (7.\ 2) $$

and

$$I7_2 = \frac{1}{\sqrt{\pi}\sqrt{\alpha^2-\gamma^2}} \left(\frac{1}{2(\alpha-\gamma)}\right)^{m+n} \left(\frac{2\gamma}{\alpha+\gamma}\right)^{\ell} \frac{1}{\Gamma(\ell+\frac{1}{2})}$$

$$\times \sum_k \frac{\Gamma(k+\ell+\frac{1}{2})}{k!} \left(\frac{\alpha-\gamma}{\alpha+\gamma}\right)^k$$

$$\times \frac{1}{2\pi i}\int_C ds \frac{\Gamma(2s+m+n+1)\Gamma(2s+m+n+\frac{1}{2})\Gamma(-2s-m-n+\frac{1}{2})}{\Gamma(s+m+1)\Gamma(s+n+1)\Gamma(s+m+n+1)\Gamma(-2s+\ell-m-n)}$$

$$\times \frac{\Gamma(-2s+\ell-m-n+k)\Gamma(-s)}{\Gamma(-2s-m-n+k+\frac{1}{2})} \left(-\frac{1}{4}\right)^s \left(\frac{1}{\alpha-\gamma}\right)^{2s}. \qquad (7.\ 3)$$

The path of the integration in $I7_1$ is closed with a semi-circle in the right half plane. The integrand has poles at

$$2s = j + \frac{1}{2}, \qquad j = 0, 1, 2, \ldots, \qquad (7.\ 4a)$$

and at

$$s = j, \qquad j = 0, 1, \ldots, \ell - [\tfrac{p}{2}] - 1. \qquad (7.\ 4b)$$

The contribution of those residues are denoted by $I7_{1-1}$ and $I7_{1-2}$. Then

$$I7_{1-1} = \frac{(1-i)(-)^{m+n+1}}{\sqrt{2\pi}} \left(\frac{1}{2(a+\gamma)}\right)^{p+\frac{3}{2}} (4\gamma)^{\ell} \frac{1}{\Gamma(\ell+\frac{1}{2})} \sum_k \frac{\Gamma(k+\ell+\frac{1}{2})}{k!} \left(\frac{a-\gamma}{a+\gamma}\right)^k$$

$$\times \sum_j \frac{\Gamma(j+p+k+\frac{3}{2})\Gamma(j+m+n+\frac{3}{2})\Gamma(-\frac{j}{2}-\frac{1}{4})}{\Gamma(\frac{j}{2}+m+\frac{5}{4})\Gamma(\frac{j}{2}+n+\frac{5}{4})\Gamma(\frac{j}{2}+m+n+\frac{5}{4})\Gamma(-j-p+2\ell-\frac{1}{2})\Gamma(j+m+n+2)} \left(\frac{-i}{2(a+\gamma)}\right)^j, \tag{7. 5}$$

and

$$I7_{1-2} = 2\sqrt{\pi}(-)^{m+n+1} \frac{(4\gamma)^{\ell}}{(2(a+\gamma))^{p+1}} \frac{1}{\Gamma(\ell+\frac{1}{2})\Gamma(2\ell-p)m!n!}$$

$$\times \sum_k \frac{\Gamma(k+\ell+\frac{1}{2})\Gamma(p+k+1)}{k!\Gamma(m+n+k+\frac{3}{2})} \left(\frac{a-\gamma}{a+\gamma}\right)^k$$

$$\times {}_6F_5\left[\begin{matrix}\frac{p+k}{2}+\frac{1}{2}, \frac{p+k}{2}+1, \frac{m+n}{2}+\frac{1}{2}, \frac{m+n}{2}+1, \frac{p}{2}-\ell+\frac{1}{2}, \frac{p}{2}-\ell+1; \left(\frac{2}{a+\gamma}\right)^2 \\ \\ m+1, n+1, m+n+1, \frac{m+n+k}{2}+\frac{3}{4}, \frac{m+n+k}{2}+\frac{5}{4}\end{matrix}\right]. \tag{7. 6}$$

The path of the integration is closed with a semicircle in the left half plane.

no 91 The integrand of $I7_2$ has poles at

$$s = -[\frac{m+n+1}{2}]-\frac{1}{2}-j, \quad j = 0, 1, 2, \dots, \tag{7. 7a}$$

and

$$2s = -\frac{1}{2}-j, \quad j = \max(0, m+n-k), \dots . \tag{7. 7b}$$

The contribution of these poles are denoted by $I7_{2-1}$ and $I7_{2-2}$, respectively. Parity of m+n is denoted by σ (= 0 for even m+n, = 1 for odd m+n). Then

$$I7_{2-1} = \frac{-i}{\pi^2}\left(\frac{\alpha-\gamma}{\alpha+\gamma}\right)^{1/2}(\alpha-\gamma)^{\sigma}\left(\frac{2\gamma}{\alpha+\gamma}\right)^{\ell}\Gamma\left(\left[\frac{m+n+1}{2}\right]-m-n+\frac{1}{2}\right)$$

$$\times\frac{\Gamma\left(\left[\frac{m+n+1}{2}\right]+\frac{1}{2}\right)\Gamma\left(\left[\frac{m+n+1}{2}\right]-m+\frac{1}{2}\right)\Gamma\left(\left[\frac{m+n+1}{2}\right]-n+\frac{1}{2}\right)}{\Gamma(\sigma+\ell+1)\Gamma(\ell+\frac{1}{2})\Gamma(\sigma+\frac{1}{2})}$$

$$\times\sum_k\frac{\Gamma(k+\ell+\frac{1}{2})\Gamma(\sigma+\ell+k+1)}{k!\,\Gamma(\sigma+k+\frac{3}{2})}\left(\frac{\alpha-\gamma}{\alpha+\gamma}\right)^k$$

$$\times{}_6F_5\left[\begin{matrix}\sigma+\frac{\ell+k+1}{2},\frac{\ell+k}{2}+1,\left[\frac{m+n+1}{2}\right]-m-n+\frac{1}{2},\left[\frac{m+n+1}{2}\right]-m+\frac{1}{2},\left[\frac{m+n+1}{2}\right]-n+\frac{1}{2},\left[\frac{m+n+1}{2}\right]+\frac{1}{2};\ \left(\frac{\alpha-\gamma}{2}\right)^2\\ \sigma+\frac{\ell+1}{2},\frac{\ell}{2}+1,\sigma+\frac{k}{2}+\frac{3}{4},\frac{k}{2}+\frac{5}{4},\sigma+\frac{1}{2}\end{matrix}\right] \tag{7. 8}$$

and

$$I7_{2-2} = \frac{1+i}{2\sqrt{\pi}(\alpha+\gamma)^{1/2}}\left(\frac{-1}{2(\alpha-\gamma)}\right)^{m+n}\left(\frac{2\gamma}{\alpha+\gamma}\right)^{\ell}\frac{1}{\Gamma(\ell+\frac{1}{2})}\sum_k\frac{\Gamma(k+\ell+\frac{1}{2})}{k!}\left(\frac{\alpha-\gamma}{\alpha+\gamma}\right)^k$$

$$\times\sum_{j=\max(0,m+n-k)}^{\infty}\frac{\Gamma(-j+m+n+\frac{1}{2})\Gamma(j+\ell-m-n+k+\frac{1}{2})\Gamma(\frac{j}{2}+\frac{1}{4})(2i(\alpha-\gamma))^j}{\Gamma(-\frac{j}{2}+m+\frac{3}{4})\Gamma(-\frac{j}{2}+n+\frac{3}{4})\Gamma(-\frac{j}{2}+m+n+\frac{3}{4})\Gamma(j+\ell-m-n+\frac{1}{2})\Gamma(j-m-n+k+1)}. \tag{7. 9}$$

The common region of convergence of double series $I7_{1-1}$, $I7_{1-2}$, $I7_{2-1}$ and $I7_{2-2}$ are given by

$$2 < \alpha + \gamma \text{ and } |\alpha - \gamma| < 2.$$

The right hand sides of $I7_{1-1}$, $I7_{1-2}$, $I7_{2-2}$ are analytic at $\alpha = \gamma$. The leading term of $I7_{2-1}$ is $(\alpha - \gamma)^{1/2}$ when m+n is even and $(\alpha - \gamma)^{3/2}$ when m+n is odd. Hence it is to be noted that the singularity $(\alpha - \gamma)^{1/2}$ vanishes when m+n is odd. Similar situation has been found in the square lattice.[7]

For $\ell = m = n = 0$ and $\alpha = \gamma = 1$, $I7_{1-1}$ for even j gives $\frac{-1+i}{8} \frac{[\Gamma(\frac{3}{4})]^2}{[\Gamma(\frac{7}{8})]^4}$, $I7_{1-1}$ for odd j gives $\frac{1+i}{4} \frac{[\Gamma(\frac{1}{4})]^2}{[\Gamma(\frac{5}{8})]^4} - \frac{(1+i)\pi}{2[\Gamma(\frac{3}{4})]^4}$, $I7_{2-2}$ gives $\frac{(1+i)\pi}{2[\Gamma(\frac{3}{4})]^4}$, $I7_{1-2}$ and $I7_{2-1}$ give no contributions, and the sum reproduces the value of Re $I_{sc}(1)$ and Im $I_{sc}(1)$ given in Eq. (33) in KIA.

The expressions for the results in this section in terms of Kampé de Fériet function are omitted.

§8. Conclusion

The lattice Green's function of the tetragonal lattice, $I(\alpha;\ \ell,\ m,\ n;\ \gamma)$ given in Eq. (1. 1), was evaluated. It has singularities at $\alpha = \pm1\pm1\pm\gamma$ and $(\alpha,\ \gamma)$ plane is divided in several regions by these singular lines. The integral $I(\alpha;\ \ell,\ m,\ n;\ \gamma)$ is expressed in terms of Kampé de Fériet functions in the respective regions in $(\alpha,\ \gamma)$ plane. These expressions supplies simple and rapid subroutines for the numerical calculations. The results for $\gamma = 0,\ 1$, and ∞ agrees analytically with the LGF of the square lattice, simple cubic lattice, and the linear lattice, respectively, derived in the previous papers.[5, 7] The values of $I(\alpha;\ \ell,\ m,\ n;\ \gamma)$ were calculated for $\gamma = 0.5$, 1.5 and 2.5. Those values for $\ell + m + n \leqq 3$ were shown in Fig. 2. The values for $\gamma = 1$ agree with those by Horiguchi[8] who calculated them by the method of the integration of the complete elliptic integral and the use of the recurrence relations. The leading term of $I(\alpha;\ \ell,\ m,\ n;\ \gamma)$ at the singularities is generally[9, 10] $C_0 + C_1(\alpha-\alpha_0)^{1/2}$. However, C_1 vanishes when $\alpha_0 = \gamma$ and m+n is odd.

In the calculation of the lattice vibration of the diatomic lattice and impurity mode of the antiferromagnet one encounters the modified LGF which can be reduced to the ordinary LGF of the pure imaginary argument.[11, 12] The present method can be be applied also to such cases. Details will be given in another occasion.

Acknowledgments

The authors thank Dr. S. Inawashiro for valuable discussions. The numerical calculation was carried out using NEAC 2200/500 TSS and 2200/700 in the Computer Center in Tohoku University.

Appendix. Kampé de Fériet Function and Modified Kampé de Fériet Function

The Kampé de Fériet function F, which is a generalized hypergeometric function of two variables, is defined by[6]

$$F\left[\begin{array}{c|l|c} \mu & \alpha_1, \alpha_2, \ldots, \alpha_\mu & \\ \nu & \beta_1, \beta_2, \ldots, \beta_\nu; \ \beta'_1, \beta'_2, \ldots, \beta'_\nu & \\ \rho & \gamma_1, \gamma_2, \ldots, \gamma_\rho & x, y \\ \sigma & \delta_1, \delta_2, \ldots, \delta_\sigma; \ \delta'_1, \delta'_2, \ldots, \delta'_\sigma & \end{array}\right]$$

$$= \sum_{j=0}^{\infty} \sum_{k=0}^{\infty} \frac{(\alpha_1)_{j+k} \cdots (\alpha_\mu)_{j+k} (\beta_1)_j \cdots (\beta_\nu)_j (\beta'_1)_k \cdots (\beta'_\nu)_j \, x^j y^k}{j!k!(\gamma_1)_{j+k} \cdots (\gamma_\rho)_{j+k} (\delta_1)_j \cdots (\delta_\sigma)_j (\delta'_1)_k \cdots (\delta'_\sigma)_k} \tag{A1}$$

When one of α_i, β_i, or β'_i is a negative integer or zero, the corresponding upper limit of the summation becomes finite. Some of β's and δ's (β's and δ's) may take redundant values which is not equal to zero and negative integers (like α and α' in Eq. (3. 4)). When $\mu+\nu-\rho-\sigma-1 > 0$, F in (A1) diverges except $x = y = 0$. When $\mu+\nu-\rho-\sigma-1 < 0$, F converges for all values of x and y. When $\mu+\nu-\rho-\sigma-1 = 0$, the region of the convergence of F is given by

$$|x| < \min(r, 1), \quad |y| < \min(s, 1)$$

where r and s are shown to be determined by

$$r^{1/(\mu-\rho)} + s^{1/(\mu-\rho)} = 1 . \qquad \text{(A1')}$$

We also define here a modified function $\tilde{F}$.

$$\tilde{F}\left[\begin{array}{c|l|c} \mu & \alpha_1, \alpha_2, \ldots, \alpha_\mu & \\ \nu & \beta_1, \beta_2, \ldots, \beta_\nu; \quad \beta'_1, \beta'_2, \ldots, \beta'_\nu & x, y \\ \rho & \gamma_1, \gamma_2, \ldots, \gamma_\rho & \\ \sigma & \delta_1, \delta_2, \ldots, \delta_\sigma; \quad \delta'_1, \delta'_2, \ldots, \delta'_\sigma & \end{array}\right]$$

$$\equiv \frac{1}{\pi} \sum_{j=0}^{\infty} \sum_{k=0}^{\infty} \frac{(\alpha_1)_{j+k} \ldots (\alpha_\mu)_{j+k} (\beta_1)_j \ldots (\beta_\nu)_j (\beta'_1)_k \ldots (\beta'_\nu)_k x^j y^k}{j!k!(\gamma_1)_{j+k} \ldots (\gamma_\rho)_{j+k} (\delta_1)_j \ldots (\delta_\sigma)_j (\delta'_1)_k \ldots (\delta'_\sigma)_k}$$

$$\times \{-\psi(\alpha_1 + j + k) \ldots -\psi(\alpha_\mu + j + k) - \psi(\beta_1 + j) \ldots -\psi(\beta_\nu + j)$$

$$+ \psi(\gamma_1 + j + k) \ldots +\psi(\gamma_\rho + j + k) + \psi(\delta_1 + j) \ldots +\psi(\delta_\sigma + j)$$

$$+ \psi(j + 1) - \log |x| \} \qquad \text{(A2)}$$

Some formulas on Kampé de Fériet function are summarized.

$$F\left[\begin{array}{c|l|c} \mu & \alpha_1, \ldots \alpha_\mu & \\ \nu & \beta_1, \ldots \beta_\nu; \quad \beta'_1, \ldots \beta'_\nu & x, y \\ \rho & \gamma_1, \ldots \gamma_\rho & \\ \sigma & \delta_1, \ldots \delta_\sigma; \quad \delta'_1, \ldots \delta'_\sigma & \end{array}\right]$$

$$= \sum_m \frac{(\alpha_1)_m \ldots (\alpha_\mu)_m (\beta_1)_m \ldots (\beta_\nu)_m \, x^m}{m!(\gamma_1)_m \ldots (\gamma_\rho)_m (\delta_1)_m \ldots (\delta_\sigma)_m}$$

$$\times \; {}_{\mu+\nu}F_{\rho+\sigma} \left[\begin{matrix} \alpha_1 + m, \ldots \alpha_\mu + m, \beta_1', \ldots \beta_\nu'; & y \\ \gamma_1 + m, \ldots \gamma_\rho + m, \delta_1', \ldots \delta_\sigma' & \end{matrix} \right] \qquad (A3)$$

$$= \sum_n \frac{(\alpha_1)_n \ldots (\alpha_\mu)_n (\beta_1')_n \ldots (\beta_\nu')_n \, y^n}{n!(\gamma_1)_n \ldots (\gamma_\rho)_n (\delta_1')_n \ldots (\delta_\sigma')_n}$$

$$\times \; {}_{\mu+\nu}F_{\rho+\sigma} \left[\begin{matrix} \alpha_1 + n, \ldots \alpha_\mu + n, \beta_1, \ldots \beta_\nu; & x \\ \gamma_1 + n, \ldots \gamma_\rho + n, \delta_1, \ldots \delta_\sigma & \end{matrix} \right] \qquad (A4)$$

$$F \left[\begin{array}{c|c|c} \mu & \alpha_1, \ldots \alpha_\mu & \\ \nu & \beta_1, \ldots \beta_\nu; \;\; \beta_1', \ldots \beta_\nu' & x, 0 \\ \rho & \gamma_1, \ldots \gamma_\rho & \\ \sigma & \delta_1, \ldots \delta_\sigma; \;\; \delta_1', \ldots \delta_\sigma' & \end{array} \right]$$

$$= {}_{\mu+\nu}F_{\rho+\sigma} \left[\begin{matrix} \alpha_1, \ldots, \alpha_\mu, \beta_1, \ldots \beta_\nu; & x \\ \gamma_1, \ldots, \gamma_\rho, \delta_1, \ldots \delta_\sigma & \end{matrix} \right] \qquad (A5)$$

$$\tilde{F} \left[\begin{array}{c|c|c} \mu & \alpha_1, \ldots \alpha_\mu & \\ \nu & \beta_1, \ldots \beta_\nu; \;\; \beta_1', \ldots \beta_\nu' & x, 0 \\ \rho & \gamma_1, \ldots \gamma_\rho & \\ \sigma & \delta_1, \ldots \delta_\sigma; \;\; \delta_1', \ldots \delta_\sigma' & \end{array} \right]$$

$$= {}_{\mu+\nu}\tilde{F}_{\rho+\sigma}\left[\begin{matrix}\alpha_1, \ldots, \alpha_\mu, \beta_1, \ldots \beta_\nu; x\\ \gamma_1, \ldots, \gamma_\rho, \delta_1, \ldots \delta_\sigma\end{matrix}\right] \tag{A6}$$

$$\tilde{F}\left[\begin{array}{c|c|c}\mu & \alpha_1, \ldots \alpha_\mu & \\ \nu & \beta_1, \ldots \beta_\nu; \quad \beta_1', \ldots \beta_\nu' & 0, x\\ \rho & \gamma_1, \ldots \gamma_\rho & \\ \sigma & \delta_1, \ldots \delta_\sigma; \quad \delta_1', \ldots \delta_\sigma' & \end{array}\right]$$

$$= {}_{\mu+\nu}F_{\rho+\sigma}\left[\begin{matrix}\alpha_1, \ldots \alpha_\mu, \beta_1', \ldots \beta_\nu'; \quad x\\ \gamma_1, \ldots \gamma_\rho, \delta_1', \ldots \delta_\sigma'\end{matrix}\right] \tag{A7}$$

where the modified hypergeometric function ${}_p\tilde{F}_q$ is defined in ref. 7.

When m is a positive integer or zero,

$${}_{q+1}F_q\left[\begin{matrix}\alpha_1, \alpha_2, \ldots \alpha_q, -m; z\\ \beta_1, \beta_2, \ldots \beta_q\end{matrix}\right]$$

$$= \frac{(\alpha_1)_m(\alpha_2)_m \ldots (\alpha_q)_m(-z)^m}{(\beta_1)_m(\beta_2)_m \ldots (\beta_q)_m}$$

$$\times {}_{q+1}F_q\left[\begin{matrix}1-\beta_1-m, 1-\beta_2-m, \ldots 1-\beta_q-m, -m; \frac{1}{z}\\ 1-\alpha_1-m, 1-\alpha_2-m, \ldots 1-\alpha_q-m,\end{matrix}\right] \tag{A8}$$

$$F\left[\begin{array}{c|cc|c} \mu & \alpha_1,\dots\ \alpha_\mu & & \\ \nu & \beta_1,\dots\ \beta_\nu; & \beta_1',\dots\ \beta_\nu' & \\ \rho & \gamma_1,\dots\ \gamma_\rho & & ax,\ bx \\ \sigma & \delta_1,\dots\ \delta_\sigma; & \delta_1',\dots\ \delta_\sigma' & \end{array}\right]$$

$$= \sum_{p=0}^{\infty} \frac{(\alpha_1)_p \ \dots\ (\alpha_\mu)_p (\beta_1)_p \ \dots (\beta_\nu)_p (ax)^p}{p!(\gamma_1)_p \ \dots (\gamma_\rho)_p (\delta_1)_p \ \dots\ (\delta_\sigma)_p}$$

$$\times\ {}_{\sigma+\nu+1}F_{\sigma+\nu} \left[\begin{array}{l} 1-\delta_1-p,\ \dots\ 1-\delta_\sigma-p,\ \beta_1',\dots\ \beta_\nu',\ -p;\ (-)^{\nu-\sigma+1}\ b/a \\ 1-\beta_1-p,\ \dots\ 1-\beta_\nu-p,\ \delta_1',\dots\ \delta_\nu', \end{array}\right]$$

(A9)

Notation $(F+i\tilde{F})\left[\ \Big|\ \ \Big|\ \right]$ means $F\left[\ \Big|\ \ \Big|\ \right]$ + $i\tilde{F}\left[\ \Big|\ \ \Big|\ \right]$ with the same parameters and arguments.

References

1) S. Katsura, T. Morita, S. Inawashiro, T. Horiguchi and Y. Abe: J. math. Phys. 12 (1971) 892.

2) E. W. Montroll: in *Proceedings of the Third Berkeley Symposium on Mathematical Statistics and Probability*, edited by J. Neyman (U. of California Press. Berkeley, Calif. 1955). Vol. 3. p. 209.

3) A. A. Maradudin, E. W. Montroll, G. H. Weiss, R. Herman and H. W. Milnes: Acad. roy. Belg. Classe Sci., Mem: Collection in 4°, 14 (1960).

4) I. Mannari and T. Kawabe: Prog. theor. Phys. 44 (1970) 359.

5) S. Katsura, S. Inawashiro and Y. Abe: J. math. Phys. 12 (1971) 895.

6) P. Appell and M. J. Kampé de Fériet: *Fonctions hypergeometrique et hyperspherique — Polynomes d'Hermite*, (Gauthier-Villars, Paris 1926). The notation in the present paper is slightly changed from ref. 6.

7) S. Katsura and S. Inawashiro: J. math. Phys. 12 (1971) in press.

8) T. Horiguchi: J. Phys. Soc. Japan 30 (1971) 1261.

9) L. van Hove: Phys. Rev. 89 (1953) 1189.

10) T. Morita and T. Horiguchi: J. Phys. A. submitted.

11) S. Takeno: in *Proceedings of the International Conference on Lattice Dynamics*, edited by R. F. Wallis,

(Copenhagen, 1963) p. 497. Y. Mitani and S. Takeno, Prog. theor. Phys. 33 (1965) 779.

12) T. Tonegawa: Prog. theor. Phys. 40 (1968) 1195. S. Watarai and T. Kawasaki, preprint.

Fig. 1. The location of the singularities of the lattice Green's function of the tetragonal lattice in (α, γ) plane. The number denote the section where the LGF in that region is discussed.

Fig. 2. The lattice Green's function of the tetragonal lattice. The numbers in parentheses denote ℓ, m, and n.

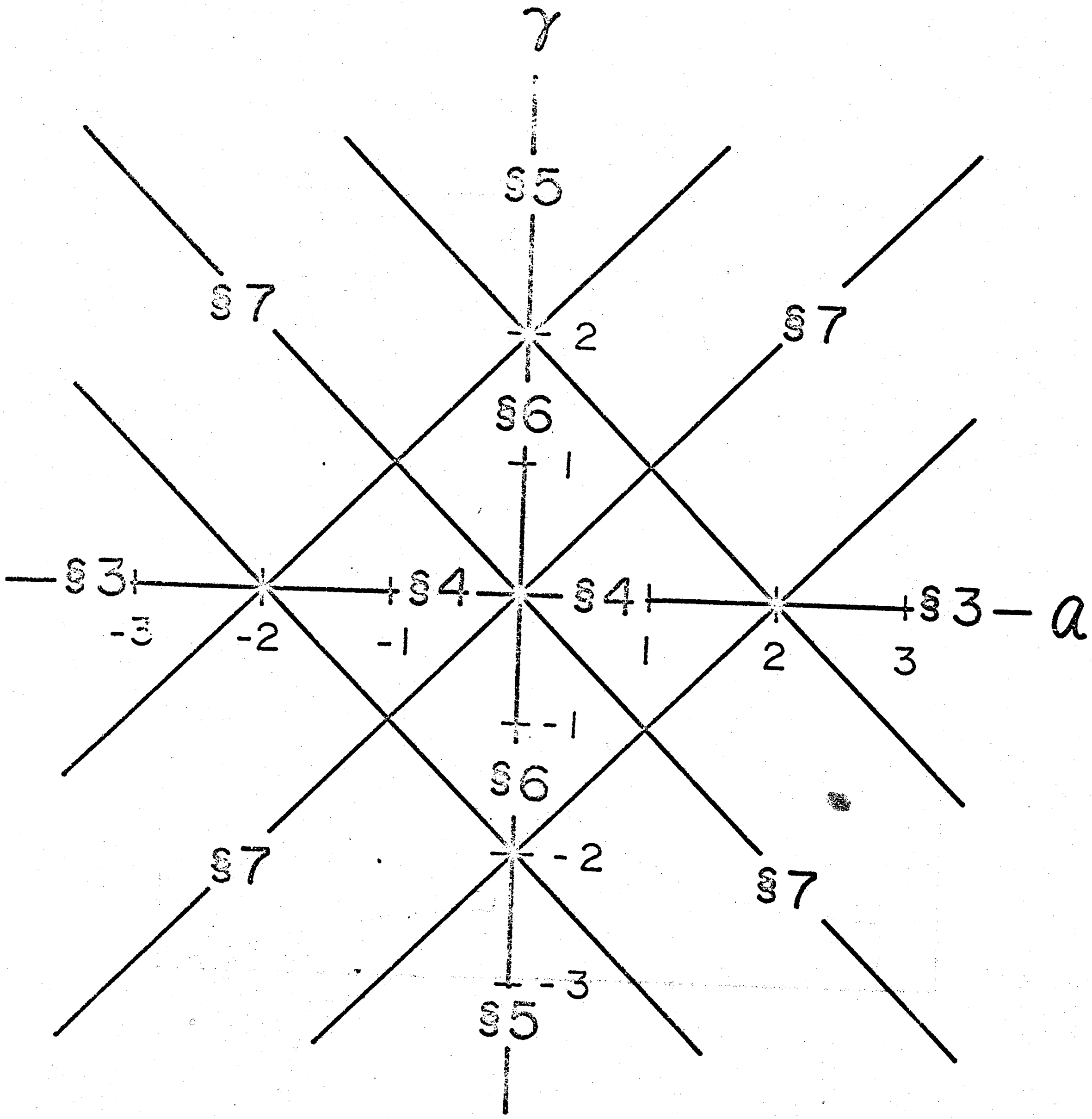

Fig. 1

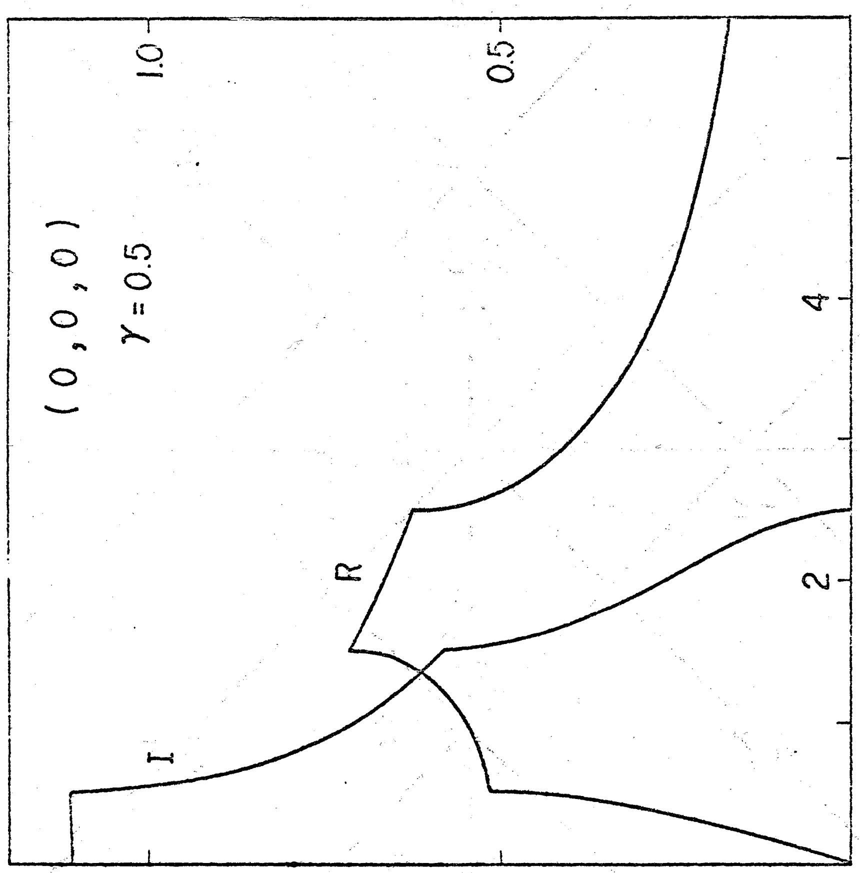

Fig. 2-1

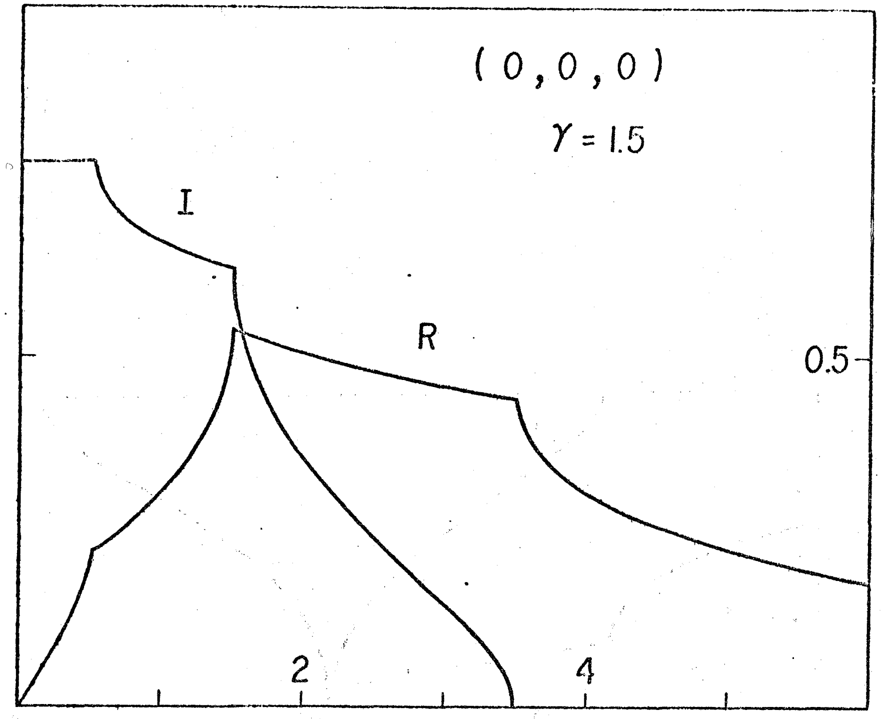

Fig. 2-2

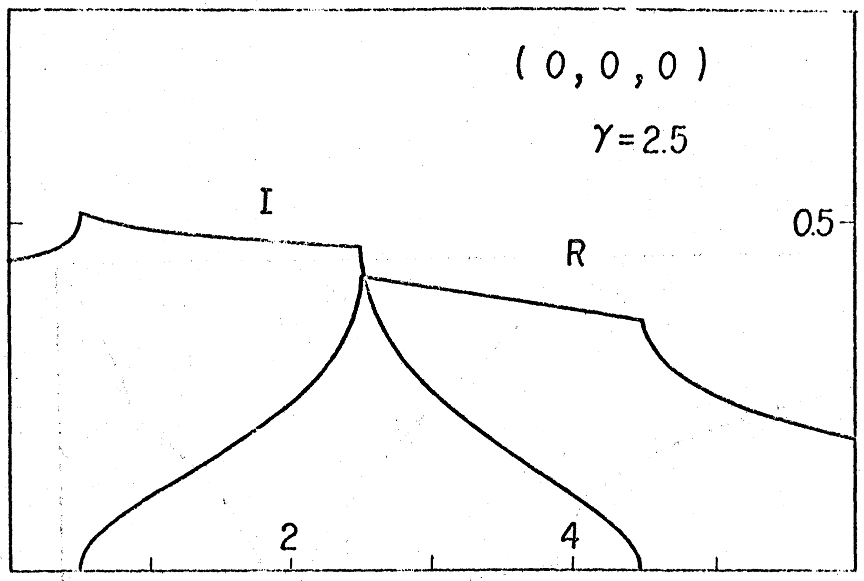

Fig. 7-3

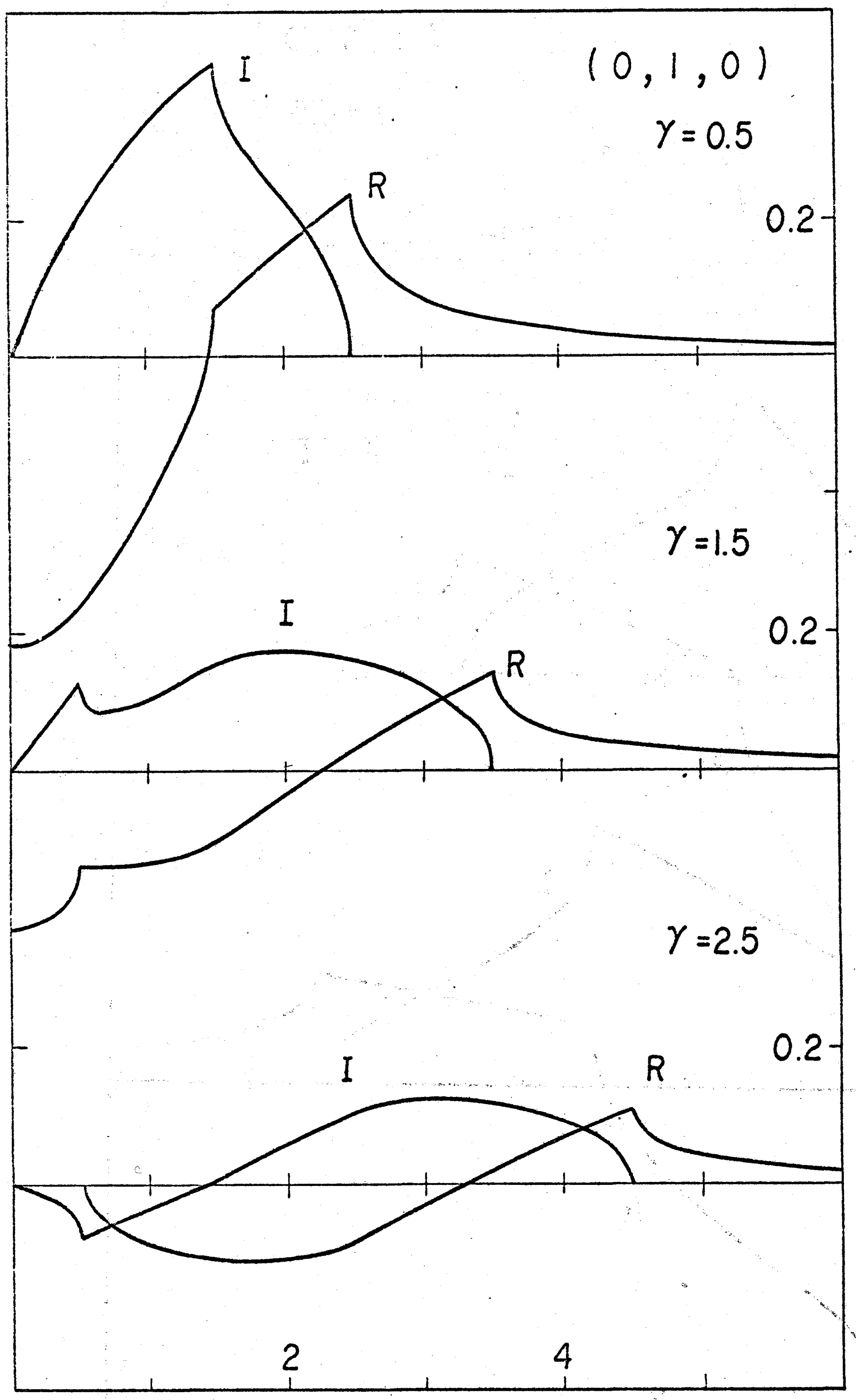

Fig 2-4

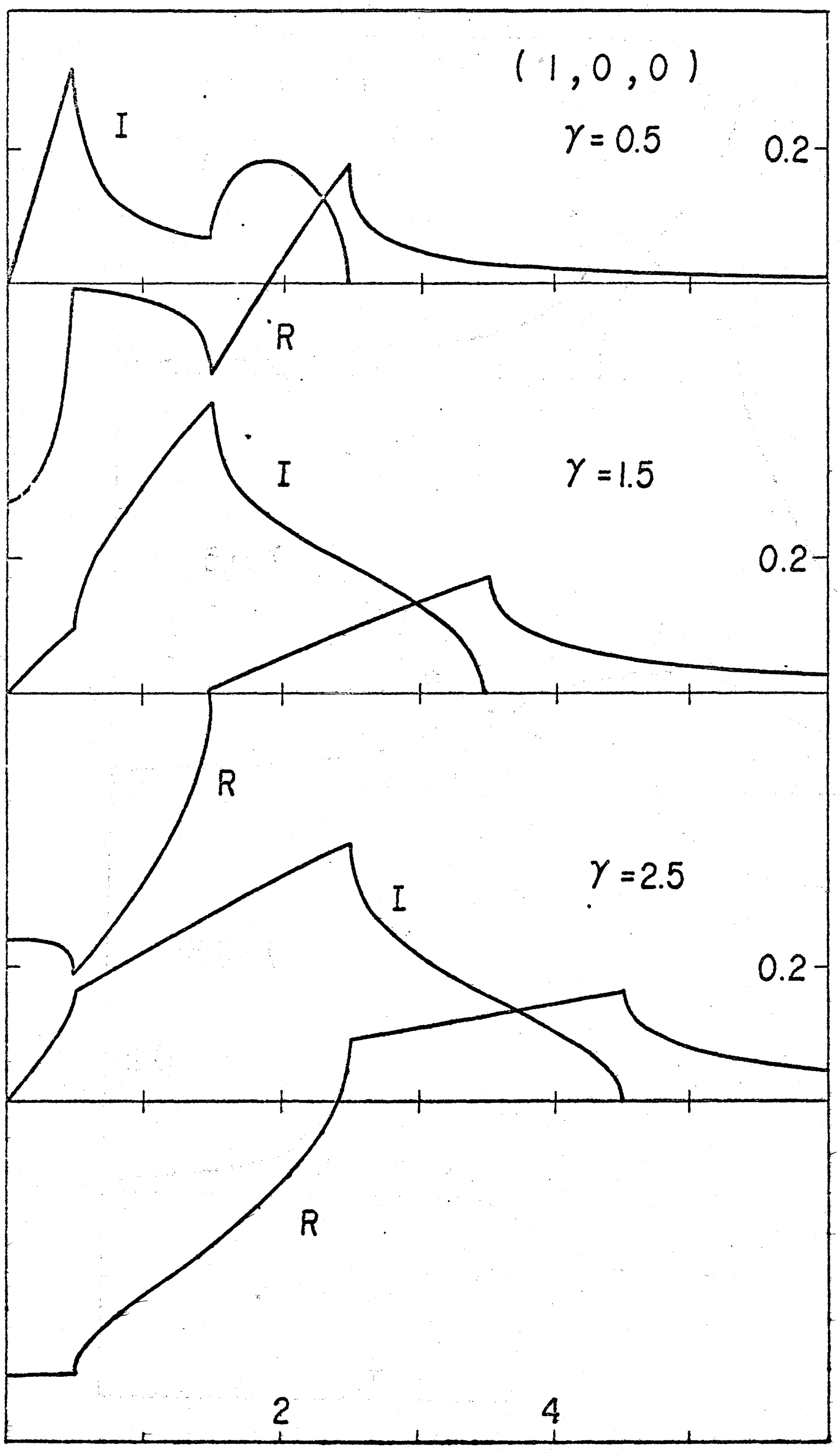

Fig. 2—5

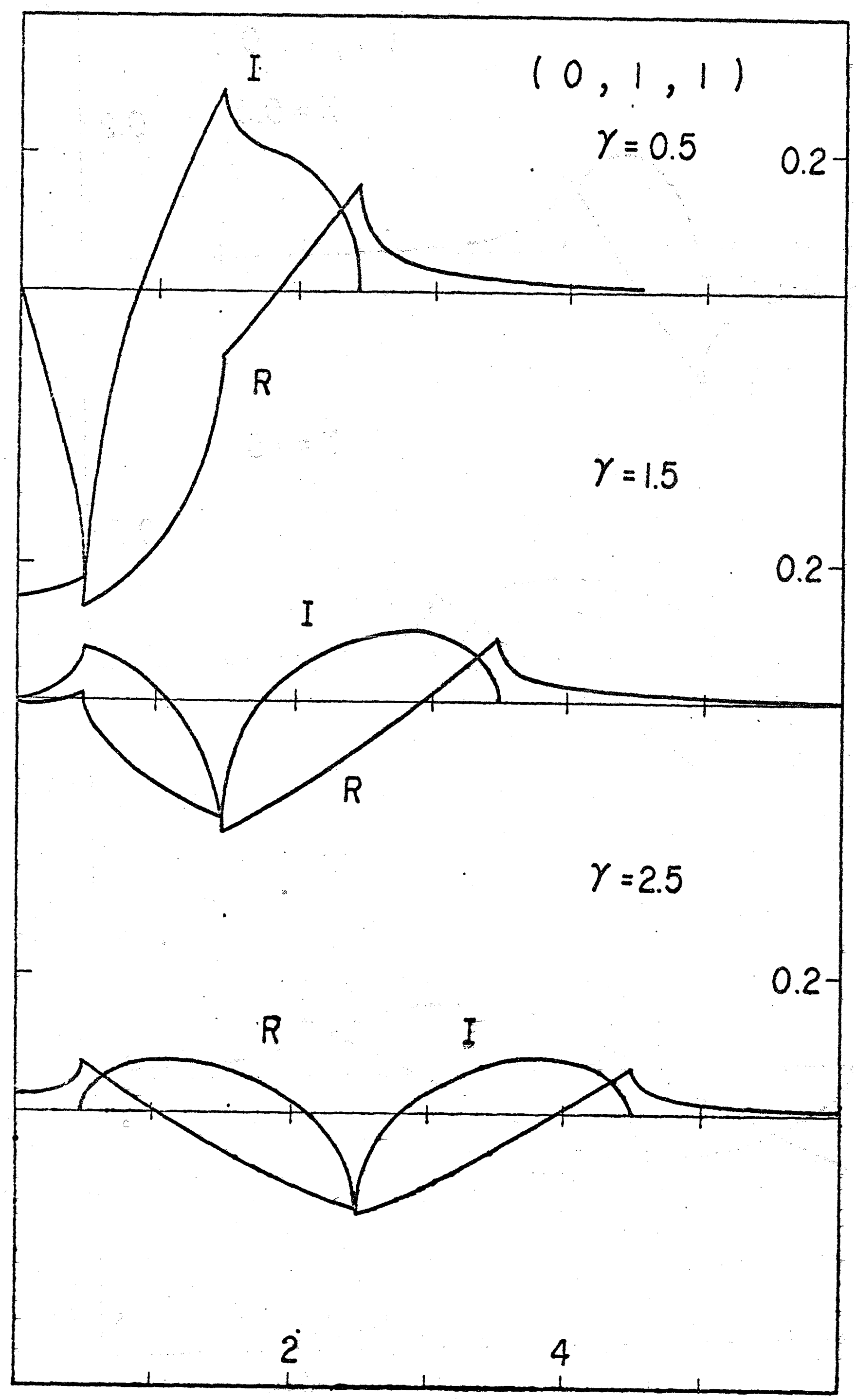

Fig. 2-6

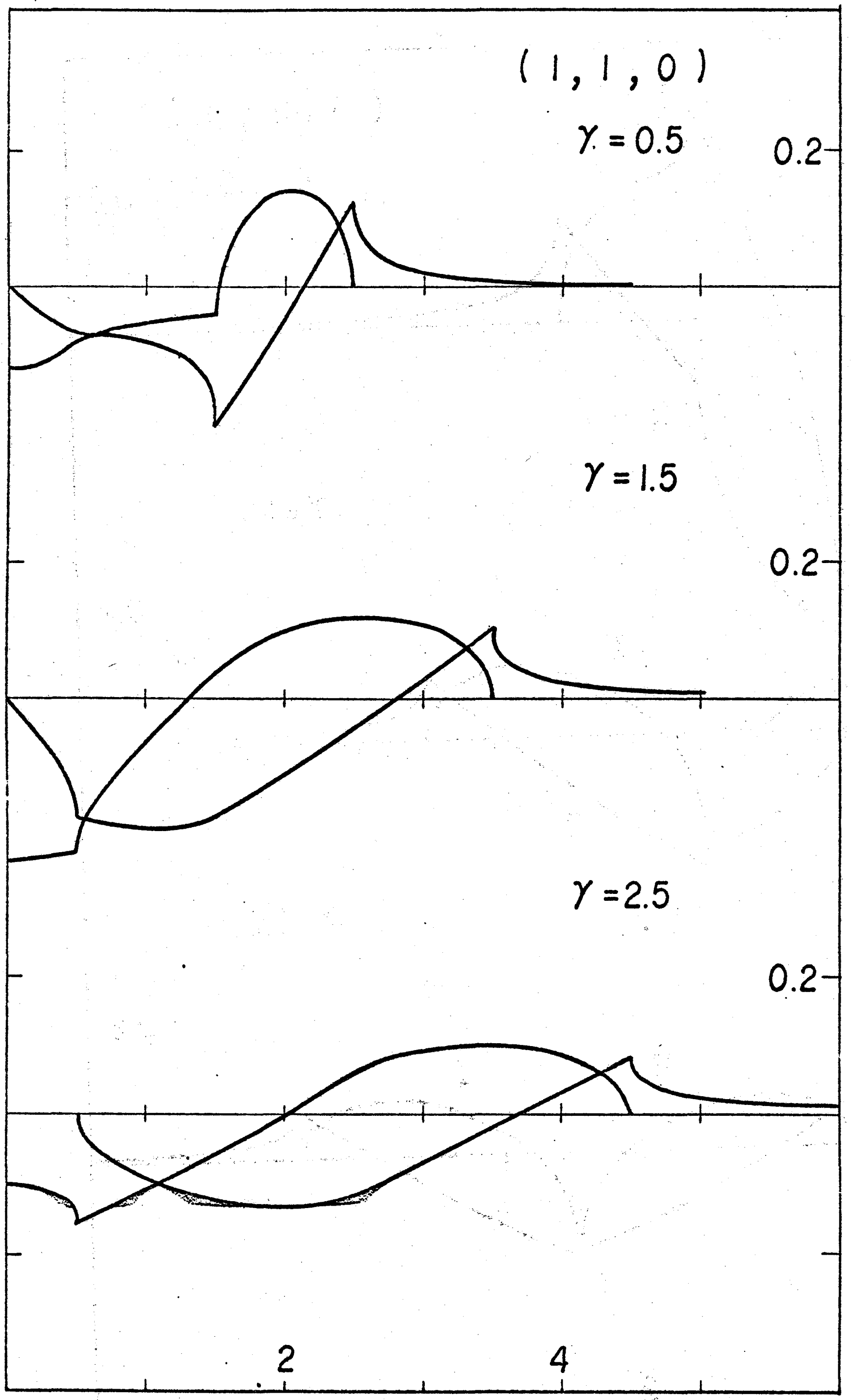

Fig. 2-7

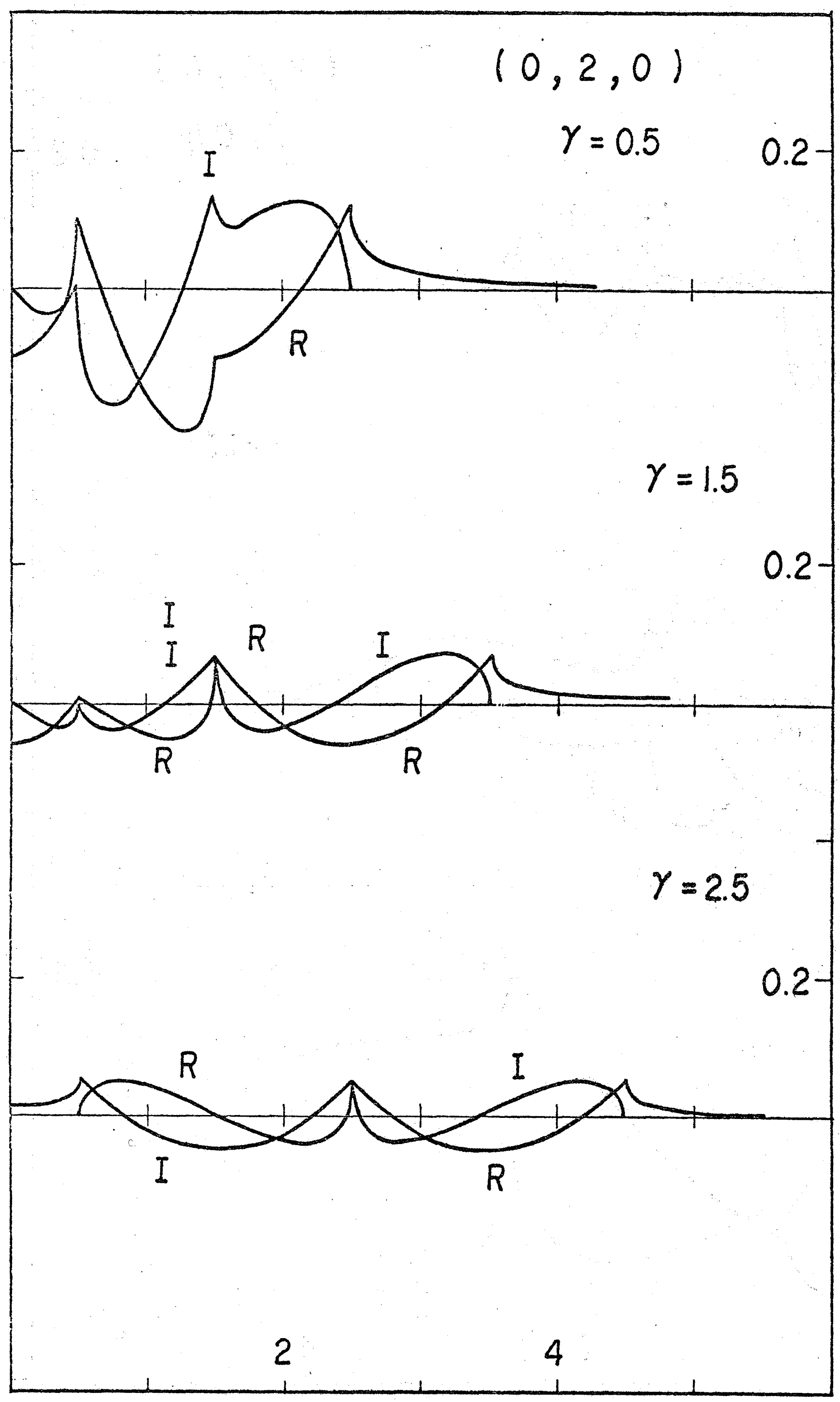

Fig 2-8

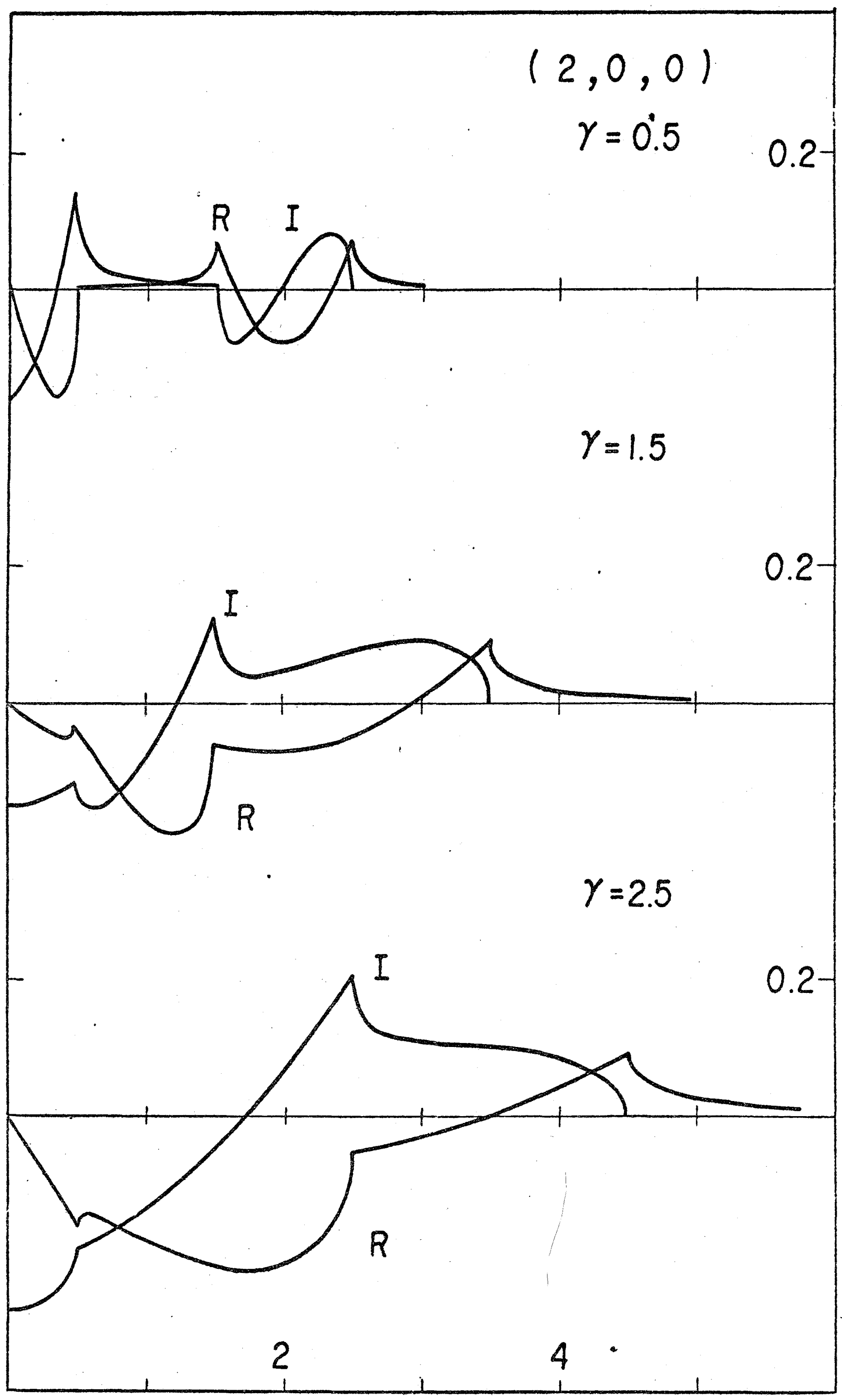

Fig 2

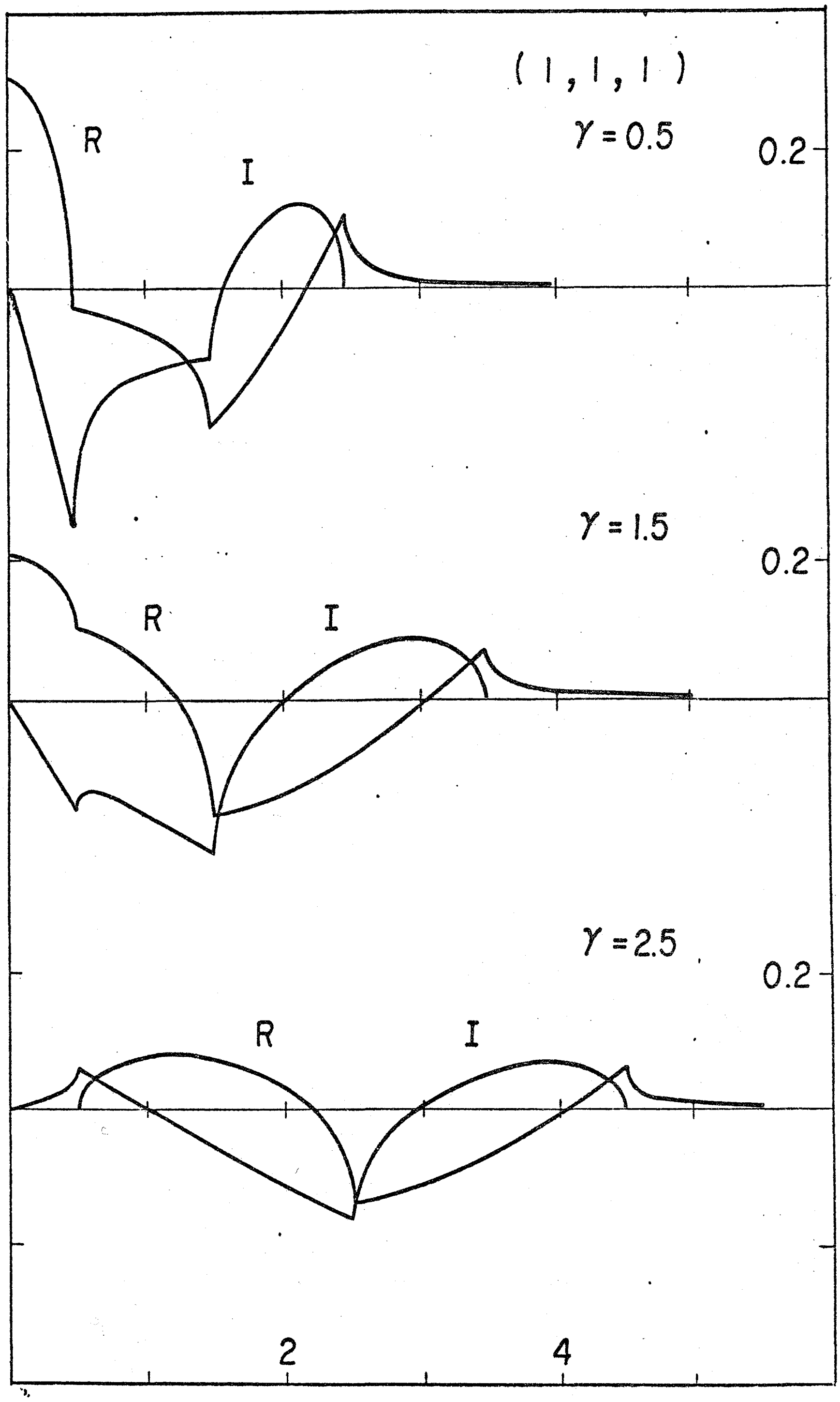

Fig. 2-10

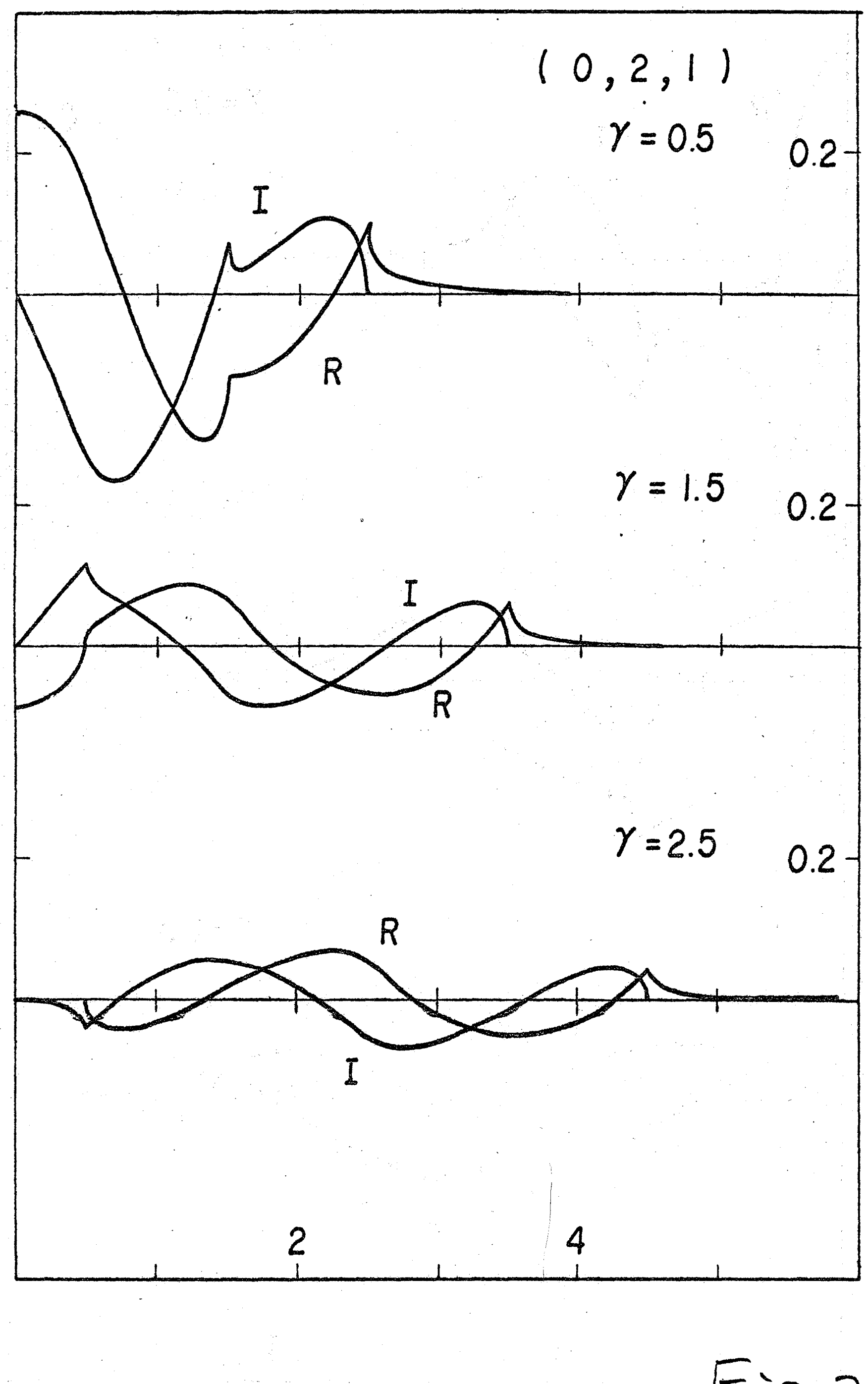

Fig. 2-11

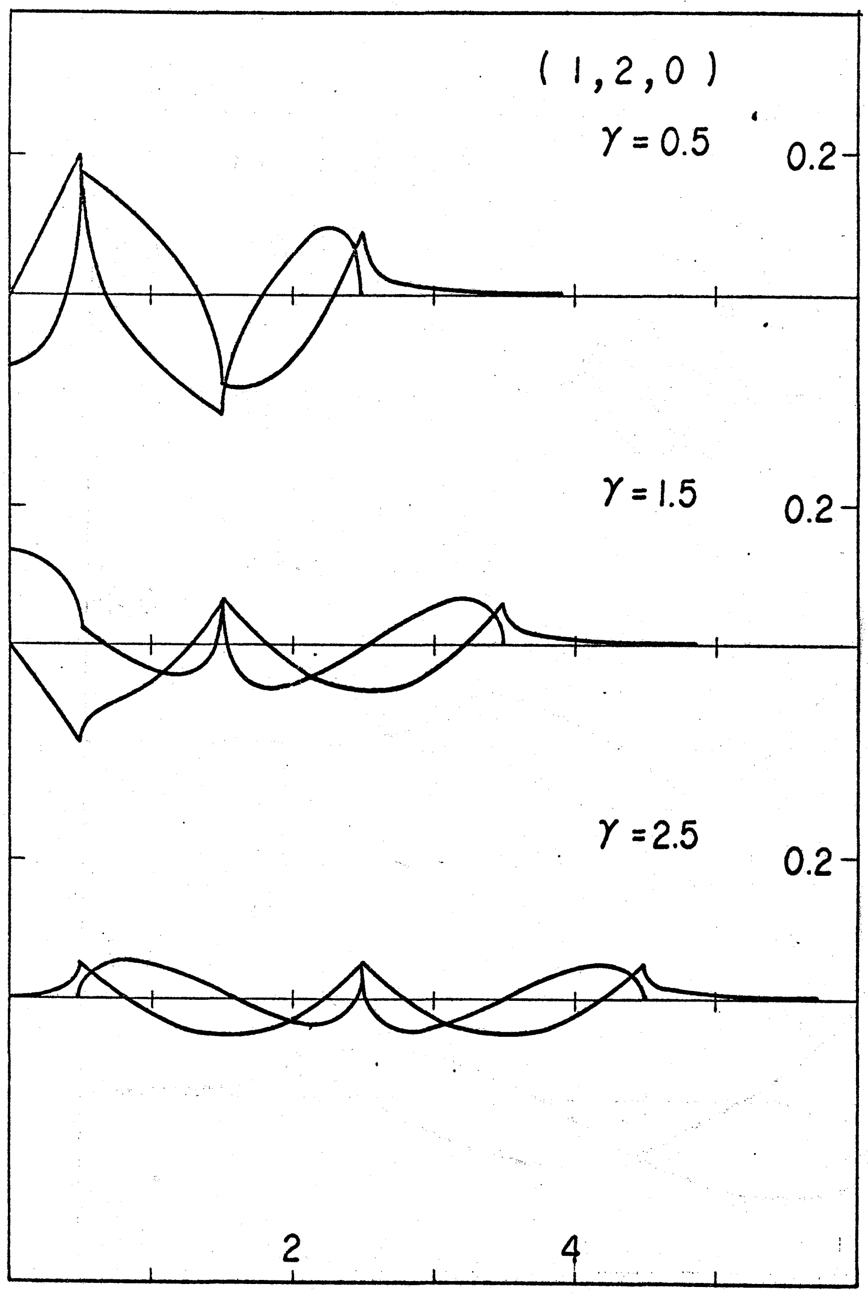

Fig. 2-12

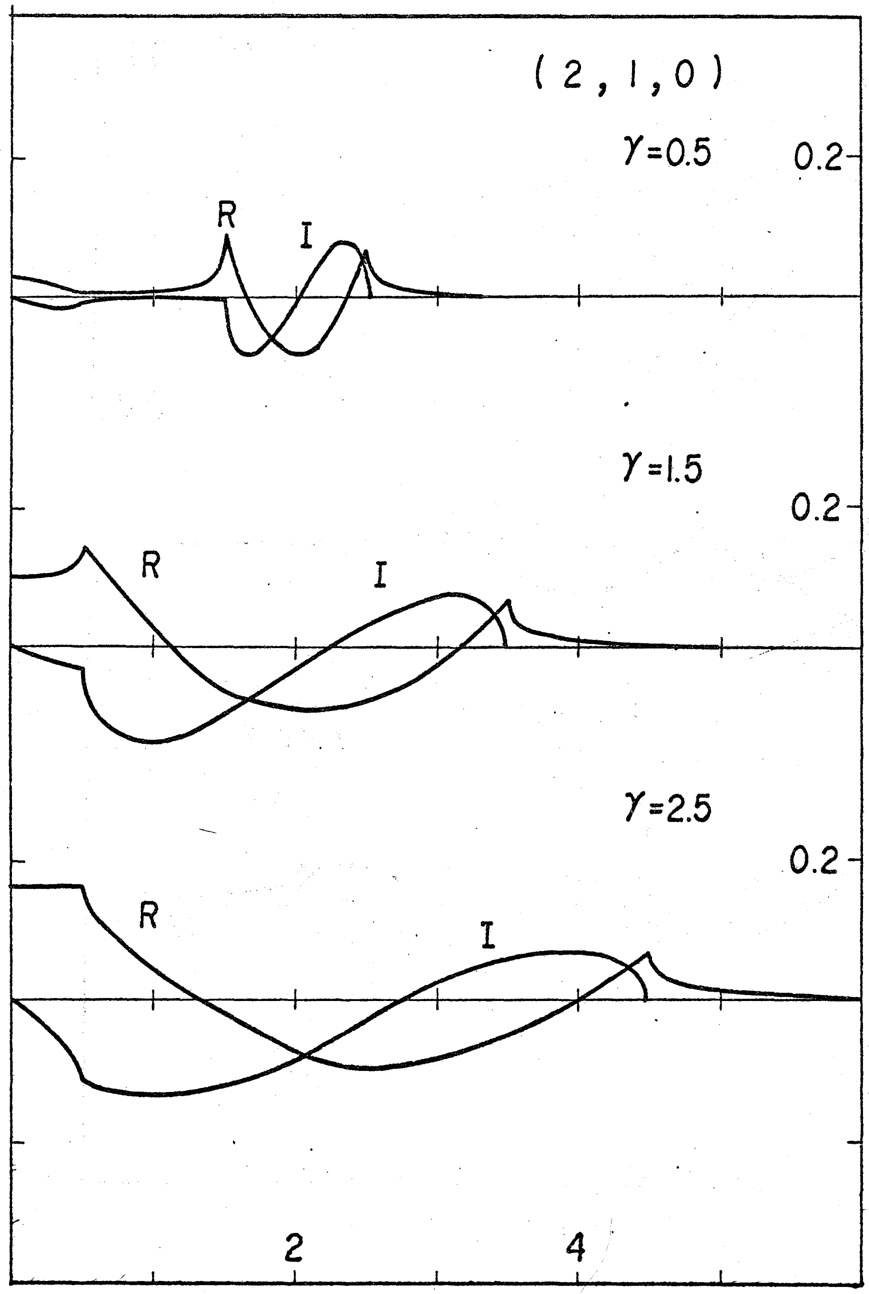

Fig 2-13

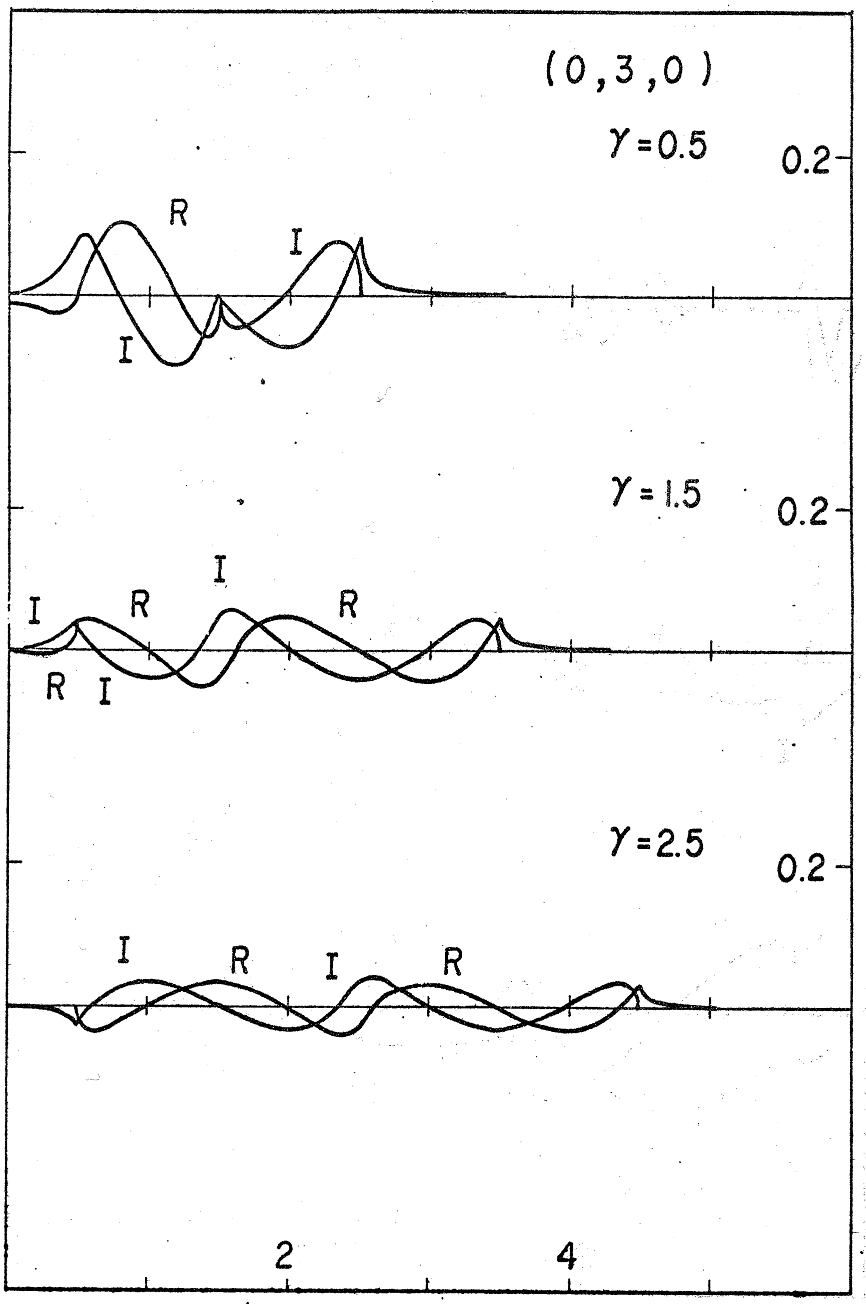

Fig. 2-14

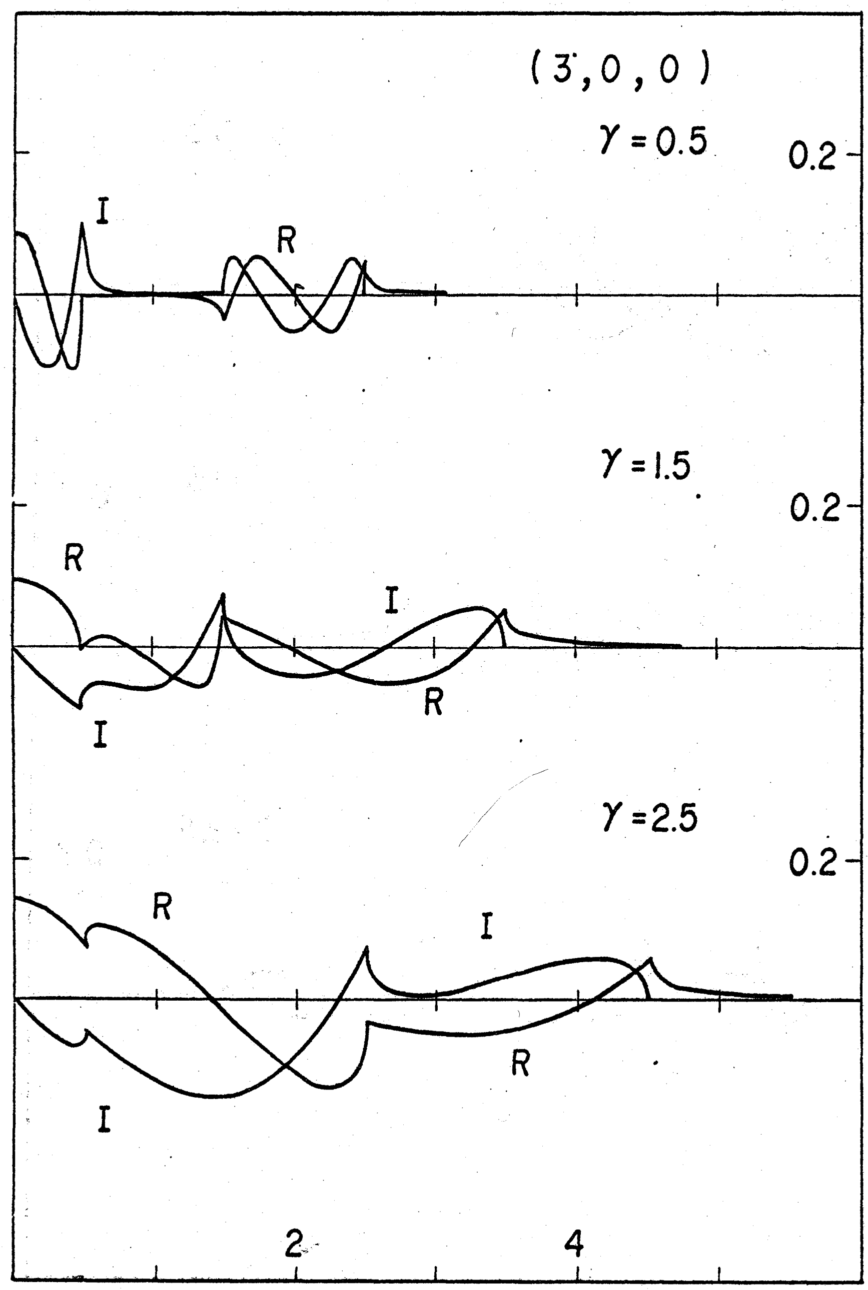

Fig. 2-15