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Extended Watson Integral について

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積分

$$I_s(a;l,m,n)=\frac{1}{\pi^3}\iiint_0^\pi \frac{\cos lx\cos my\cos nz\,dx\,dy\,dz}{a+i\epsilon-\cos x-\cos y-\cos z} \quad (0)$$

(ϵは正の無限小)を考える.(0)は単純立方格子に対するGreen関数であって格子振動の振動数分布,強磁性のHeisenberg模型,其他多くの物性物理学上の応用をもつ積分である.体心立方格子,面心立方格子に対しては

$$I_b(a;l,m,n)=\frac{1}{\pi^3}\iiint_0^\pi \frac{\cos 2lx\cos 2my\cos 2nz\,dx\,dy\,dz}{a+i\epsilon-\cos x\cos y\cos z}$$

$$I_f(a;l,m,n)=\frac{1}{\pi^3}\iiint_0^\pi \frac{\cos 2lx\cos 2my\cos 2nz\,dx\,dy\,dz}{a+i\epsilon-\cos x\cos y-\cos y\cos z-\cos z\cos x}$$

という積分があらわれるが ここでは $l=m=n=0$ の場合の単

純立方格子を問題とする。

$I_s(3;0,0,0)$, $I_b(1;0,0,0)$, $I_f(3;0,0,0)$ は Watson[1] により求められて居りその巧妙さによって(0)に Extended Watson Integral の名が冠せられた。

$I_s(a;0,0,0)$ は $a>3$ に対して実数, $0<a<3$ に対しては複素数で $a=1$ と $a=3$ が特異点になっている。$I_s(a>3,0,0,0)$ の $1/a^2$ による展開係数の数値は Tickson[2] により求められ, $a>3$ に対する数表が与えられた。Maradudin, Montroll[3] 等は $I_s(a>3;l,m,n)$ の $(a-3)$ による展開係数の最初の数項を求め $a=3$ $(a>3)$ における leading term が $O((a-3)^{1/2})$ であることを示し、$I_s(a>3;l,m,n)$ の数表を与えた。Mannari and Kawabata[4] は $I_s(a>3;0,0,0)$, $I_b(a>1;0,0,0)$, $I_f(a>3;0,0,0)$ を楕円積分およびその定積分であらわし, 数値積分により詳細な数表を与えた。Yussouff and Mahanty[5] は後にのべる(2)の実数部および虚数部を個々に Simpson 法で数値積分することにより, また Vashishta and Yussouff[6] は Fourier 級数による展開により $I_s(a;l,m,n)$, $I_b(a;l,m,n)$, $I_f(a;l,m,n)$ の数表を与えたが Ref. 5 と Ref. 6 との結果の差も

大きく相対誤差は10〜20%に達する所もあると思われる.

本積分は応用上多大の興味が持たれているに拘らず[2] 解析的及び数値的に知られていることは十分ではない. 本論文第1部では $I_s(a; 0,0,0)$ を Mellin-Barnes 型積分に変換し, その解析接続により $a>3$ (real part) 及び $0<a<1$ (real part 及び imaginary part) の級数表示を求める方法をのべる. $1<a<3$ については第3部以下にゆずる. 第2部においては $I_s(a; 0,0,0)$ が $0<a<1$, $1<a<3$ の場合にも楕円積分の定積分で与えられることを示し, これにより $I_s(a)$ を計算する. 第1部の方法は関数の解析的性質が見易いこと, 分子に $\cos lx$ 等の項のある一般形に拡張し易いことの特徴を有し, 第2部の方法は体心立方格子, 面心立方格子に拡張し易いという特徴を有する. これ等については第3部以下にのべる予定である.

1) G. N. Watson, Quart. J. Math. (Oxford) 10. (1939) 266.

2) M. Tickson, J. Res. Natl. Bur. Stds. 50 (1953) 177.

3) A. A. Maradudin, E. W. Montroll, G. H. Weiss, R. Herman and H. W. Milnes, Memoires Acad. Royale de Belgique (Science) 14 (1960)

4) I. Mannari and C. Kawabata, Research Notes of Dept. Phys. Okayma Univ. No. 15 (1964).

5) M. Yussouff and J. Mahanty, Proc. Phys. Soc. 85 1223 (1965)

6) P. Vashishta and M. Yussouff, Tech. Rep. No. 12/66, Dept. Phys. Indian Inst. Technology, Kanpur.

7) L. Van Hove, Phys. Rev. 89 1189 (1953)
E. W. Montroll, Berkeley Symposium on Mathematical Statistics and Probability, Vol. 3 (1956) 209.
G. F. Newell, J. Chem. Phys. 21 (1953) 1877.

A. A. Maradudin, P. Mazur, E. W. Montroll and G. H. Weiss, Rev. Mod. Phys. 30 (1958) 175.

G. F. Koster and J. C. Slater, Phys. Rev. 95 (1954) 1167; 96 (1954) 1208.

T. Wolfram and J. Callaway, Phys. Rev. 130 (1963) 2207.

R. G. Boyd and J. Callaway, Phys. Rev. 138 (1965) A1621.

Extended Watson Integral

Part I

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$$I(a) = \frac{1}{\pi^3}\iiint_0^{\pi} \frac{dx\,dy\,dz}{a+i\epsilon - \cos x - \cos y - \cos z} \tag{1}$$

(1)は

$$= -\frac{i}{\pi^3}\int_0^{\infty} dt \int_0^{\pi} dx \int_0^{\pi} dy \int_0^{\pi} dz \times e^{i[(a+i\epsilon) - \cos x - \cos y - \cos z]t}$$

と書ける. $\int_0^{\pi} dx \int_0^{\pi} dy \int_0^{\pi} dz$ を先に行なうと

$$= -i\int_0^{\infty} e^{i(a+i\epsilon)t}\,[J_0(t)]^3\,dt \tag{2}$$

$[J_0(t)]^2$ の級数表示を Mellen-Barnes 型 積分表示になおすと

$$[J_0(t)]^2 = \sum_{m=0} \frac{(-)^m \left(\frac{t}{2}\right)^{2m} (m+1)_m}{m!\,[\Gamma(m+1)]^2}$$

$$= \frac{1}{\sqrt{\pi}}\,\frac{1}{2\pi i}\int_C ds\, \frac{\Gamma(-s)\,\Gamma(s+\frac{1}{2})\,t^{2s}}{[\Gamma(s+1)]^2} \tag{3}$$

C は $s = -\Delta$ $(\Delta \to +0)$ を通る虚軸に平行な直線である. (3) を (2) に入れ ds と dt の順序を交換すると

$$I(a) = \frac{-i}{\sqrt{\pi}}\,\frac{1}{2\pi i}\int_C ds\, \frac{\Gamma(-s)\,\Gamma(s+\frac{1}{2})}{[\Gamma(s+1)]^2}$$

$$\times \int_0^\infty e^{i(a+i\epsilon)t} \; J_0(t)\, t^{2s} dt \qquad (4)$$

$\int_0^\infty dt$ は $\epsilon > 0$, $2s+1>0$ なら収束して

$$\int_0^\infty dt = \frac{\Gamma(2s+1)}{(-ia)^{2s+1}} {}_2F_1\left(s+\frac{1}{2}, s+1; 1; \frac{1}{a^2}\right)$$

故に

$$I(a) = \frac{1}{\pi a} \frac{1}{2\pi i} \int ds \frac{\Gamma(-s)\left[\Gamma(s+\frac{1}{2})\right]^2}{\Gamma(s+1)} \left(-\frac{4}{a^2}\right)^s$$

$$\times {}_2F_1\left(s+\frac{1}{2}, s+1; 1; \frac{1}{a^2}\right) \qquad (5)$$

$|a|>1$ ならば ${}_2F_1$ をそのまま展開して積分と総和の順序を変更すると

$$I(a) = \frac{1}{\pi a} \sum_{n=0} \frac{1}{n!\,\Gamma(1+n)} \left(\frac{1}{a^2}\right)^n$$

$$\times \frac{1}{2\pi i} \int ds \left(-\frac{4}{a^2}\right)^s \frac{\Gamma(-s)\Gamma(s+\frac{1}{2})\Gamma(s+\frac{1}{2}+n)\Gamma(s+1+n)}{[\Gamma(s+1)]^2} \qquad (6)$$

$|\alpha|>2$ ならば積分路 を右半面に閉ぢる。このとき被積分関数の極は $s=0, 1, 2, \cdots m, \cdots$ のみである から

$$I(a) = \frac{1}{\pi a} \sum_{n=0}^\infty \sum_{m=0}^\infty \frac{\Gamma(m+\frac{1}{2})\Gamma(m+n+\frac{1}{2})\Gamma(m+n+1)\,4^m}{n!\,\Gamma(1+n)\, m!\,[\Gamma(1+m)]^2} \left(\frac{1}{a^2}\right)^{m+n} \qquad (7)$$

(7) を一般化した2重級数

$$I(x,y)=\frac{1}{\pi a}\sum_{n=0}^{\infty}\sum_{m=0}^{\infty}\frac{\Gamma(m+\frac{1}{2})\Gamma(m+n+\frac{1}{2})\Gamma(m+n+1)\,4^m}{n!\,\Gamma(n+1)\,m!\,[\Gamma(1+m)]^2}x^m y^n$$

$$\equiv\sum_n\sum_m A_{mn}x^m y^n \qquad (8)$$

の収束域をしらべて見る. $m=t\mu$, $n=t\nu$ とおいて

$$\frac{1}{r}\equiv\lim_{t\to\infty}\frac{A_{m+1,n}}{A_{mn}}=\frac{4(\mu+\nu)^2}{\mu^2}$$

$$\frac{1}{s}\equiv\lim_{t\to\infty}\frac{A_{m,n+1}}{A_{mn}}=\frac{(\mu+\nu)^2}{\nu^2}$$

より

$$4r+s+\sqrt{16rs}=1 \qquad (9)$$

$r=s$ とおけば $r=\frac{1}{9}$ となる. 即ち (7) は $a>3$ で収束する. $m+n=p$ とおくと (7) は

$$I(a)=\frac{1}{\pi a}\sum_{p=0}^{\infty}\Gamma(p+\tfrac{1}{2})\Gamma(p+1)\left(\frac{1}{a^2}\right)^p$$

$$\times\sum_{m=0}^{p}\frac{\Gamma(m+\frac{1}{2})\,4^m}{(m!)^3[(p-m)!]^2} \qquad (10)$$

となる. これは $\left(\frac{1}{a^2}\right)$ のべき級数で $\left(\frac{1}{a^2}\right)^p$ の係数は有限級数である. 数値計算には (10) を用いる. $a>3$ では虚数部は消える.

(7)は a が大きい場合の展開であったが積分表示(5)を解析接続することにより a が小さい場合の展開を求めよう. 超幾何関数の変換公式により ${}_2F_1(\;;\;;1/a^2)$ を ${}_2F_1(\;;\;;a^2)$ にかえると

$$I(a)=\frac{1}{\pi a}\frac{1}{2\pi i}\int ds\,\frac{\Gamma(-s)[\Gamma(s+\frac{1}{2})]^2}{\Gamma(s+1)}\left(-\frac{4}{a^2}\right)^s$$

$$\times\left[\frac{\Gamma(\frac{1}{2})}{\Gamma(s+1)\Gamma(-s+\frac{1}{2})}\left(-\frac{1}{a^2}\right)^{-s-\frac{1}{2}}{}_2F_1\left(s+\frac{1}{2},s+\frac{1}{2};\frac{1}{2};a^2\right)\right.$$

$$\left.+\frac{\Gamma(-\frac{1}{2})}{\Gamma(s+\frac{1}{2})\Gamma(-s)}\left(-\frac{1}{a^2}\right)^{-s-1}{}_2F_1\left(s+1,s+1;\frac{3}{2};a^2\right)\right] \quad (11)$$

[ ]内第1項は imaginary part, 第2項は real part を与える. これを $I(a)=I_R(a)+I_I(a)$ と記すこととする.

Real part: (11)の第2項の ${}_2F_1$ を展開し級数の和と積分の順序を変更すると

$$I_R(a)=a\sum_{n=0}\frac{a^{2n}}{n!\,\Gamma(n+\frac{3}{2})}$$

$$\times\frac{1}{2\pi i}\int ds\,\frac{\Gamma(s+\frac{1}{2})[\Gamma(s+1+n)]^2 4^s}{[\Gamma(s+1)]^3} \quad (12)$$

$\int ds$ の中が 4^s であるので積分路は左半円で閉じなければならない。分子の pole は $s+\frac{1}{2}=0,-1,-2,\cdots$ (simple pole) と $s+1+n=0,-1,-2,\cdots$ (double pole) であるが後者は分母の pole により相殺されるから前者のみを考えればよい。留数を求めると

$$I_R(a)=\frac{a}{2\pi}\sum_n\sum_m\frac{\left[\Gamma(\frac{1}{2}+m)\right]^3\left(\frac{1}{4}\right)^m(a^2)^n}{n!\,m!\,\Gamma(\frac{3}{2}+n)\left[\Gamma(\frac{1}{2}-n+m)\right]^2} \tag{13}$$

(13) を一般化した二重級数 $\sum A_{mn}x^m y^n$ について収束域を求めると (9) を求めたときと同様にして

$$\frac{1}{r}=\frac{\mu^2}{(\mu-\nu)^2}\,,\qquad \frac{1}{s}=\frac{(\mu-\nu)^2}{\nu^2}$$

より

$$\frac{1}{\sqrt{r}}-\sqrt{s}=1 \tag{14}$$

故に (13) は $x=\frac{1}{4}$ に対しては $y\,(=a^2)=1$ が収束半径を与える。従って (13) は $a<1$ で用いられる。

$a<1$ における imaginary part : (11) の [ ] 内第1項の寄与は

$$I_I(a)=\frac{-i}{\sqrt{\pi}}\frac{1}{2\pi i}\int ds\,4^s\frac{\Gamma(-s)\left[\Gamma(s+\frac{1}{2})\right]^2}{\left[\Gamma(s+1)\right]^2\Gamma(-s+\frac{1}{2})}$$

$$\times\,{}_2F_1\left(s+\tfrac{1}{2},s+\tfrac{1}{2};\tfrac{1}{2};a^2\right) \tag{15}$$

${}_2F_1$ を a^2 で展開して

$$I_I(a) = -i\sum_{n=0}\frac{a^{2n}}{n!\,\Gamma(-\frac{1}{2}+n)}\frac{1}{2\pi i}\int ds\,\frac{\Gamma(-s)\left[\Gamma(s+n+\frac{1}{2})\right]^2}{\left[\Gamma(s+1)\right]^2\Gamma(-s+\frac{1}{2})}4^s \qquad (16)$$

積分路を左半面で閉じなければならない。$s=-\frac{1}{2}-n-m$, $m=0,1,2,\cdots$ が double pole である。留数を計算すると

$$\frac{1}{2\pi i}\int ds\,4^s\frac{\Gamma(-s)\left[\Gamma(s+n+\frac{1}{2})\right]^2}{\left[\Gamma(s+1)\right]^2\Gamma(-s+\frac{1}{2})}$$

$$=\sum_{m=0}\left[\frac{d}{ds}\left(s+\frac{1}{2}+n+m\right)^2\frac{\left[\Gamma(s+n+\frac{1}{2})\right]^2\Gamma(-s)\,4^s}{\left[\Gamma(s+1)\right]^2\Gamma(-s+\frac{1}{2})}\right]_{s=-\frac{1}{2}-n-m}$$

$$=\sum_{m=0}\left[\frac{d}{ds}\frac{\pi^2\left(s+\frac{1}{2}+n+m\right)^2}{\sin^2\left[\pi\left(-s-n-\frac{1}{2}\right)\right]}\frac{\Gamma(-s)\,4^s}{\left[\Gamma(1-s-n-\frac{1}{2})\right]^2\left[\Gamma(s+1)\right]^2\Gamma(-s+\frac{1}{2})}\right]$$

$$=\sum_{m=0}\frac{\Gamma(\frac{1}{2}+m+n)\,4^{-\frac{1}{2}-n-m}}{\left[\Gamma(1+m)\right]^2\left[\Gamma(\frac{1}{2}-m-n)\right]^2\Gamma(1+n+m)}$$

$$\times\left\{-\psi(\tfrac{1}{2}+m+n)+2\psi(1+m)-2\psi(\tfrac{1}{2}-m-n)+\psi(1+n+m)+\log 4\right\} \qquad (17)$$

故に

$$I_I(a) = i\,\frac{1}{2\pi^2}\sum_{n=0}\sum_{m=0}\frac{\left(\frac{a^2}{2^2}\right)^n\left(\frac{1}{4}\right)^m\left[\Gamma(\frac{1}{2}+m+n)\right]^3}{n!\,\Gamma(\frac{1}{2}+n)\left[\Gamma(1+m)\right]^2\Gamma(1+m+n)}$$

$$\times\left\{3\psi(\tfrac{1}{2}+m+n)-2\psi(1+m)-\psi(1+n+m)-\log 4\right\} \qquad (18)$$

(18)の収束半径も $a<1$ である.

$I_R(a)$ の $a=1$ における値は正確に求めることが出来る. すなわち (13) より $\sum_n$ を先に行うと

$$I_R(a)=\frac{a}{\pi^{3/2}}\sum_{m=0}\frac{\Gamma(m+\frac{1}{2})}{m!}\left(\frac{1}{4}\right)^m {}_2F_1\left(\frac{1}{2}-m,\frac{1}{2}-m;\frac{3}{2};a^2\right)$$

$a=1$ を入れ ${}_2F_1(\ ;\ ;1)$ の公式を用いると

$$I_R(1)=\frac{\Gamma(\frac{3}{2})}{\pi^{3/2}}\sum_{m=0}\frac{(\frac{1}{4})^m\,\Gamma(\frac{1}{2}+m)\,\Gamma(\frac{1}{2}+2m)}{m!\,[\Gamma(1+m)]^2}$$

$\Gamma(\frac{1}{2}+2m)$ を倍角公式で分解すると $\sum_m$ は ${}_3F_2$ となり, ${}_3F_2(\ ;\ ;1)$ の公式より

$$I_R(1)=\frac{\Gamma(\frac{1}{2})\Gamma(\frac{1}{4})\Gamma(\frac{3}{4})}{\pi^{3/2}\,2^{3/2}}\,{}_3F_2\left(\frac{1}{4},\frac{1}{2},\frac{3}{4};1,1;1\right)$$

$$=\frac{\pi}{2}\frac{1}{[\Gamma(\frac{5}{8})]^2[\Gamma(\frac{7}{8})]^2}$$

$$=0.6428822$$

${}_2F_1(\ ;\ ;a^2)$ は ${}_2F_1(\ ;\ ;1-a^2)$ および ${}_2F_1(\ ;\ ;1-\frac{1}{a^2})$ に変換し得るからこれより $I_R(a)$ および $I_I(a)$ の $1-a^2$ による展開, $1-\frac{1}{a^2}$ による展開を求めることが出来る. 前者は $a\lesssim 1$ で, 後者

は $1 \lesssim a < 3$ で用いることが出来る．特にこれより

$$\begin{matrix} I_R(1) \\ I_I(1) \end{matrix} = \mp \frac{1}{8} \frac{\left[\Gamma\left(\frac{3}{4}\right)\right]^2}{\left[\Gamma\left(\frac{7}{8}\right)\right]^4} + \frac{1}{4} \frac{\left[\Gamma\left(\frac{1}{4}\right)\right]^2}{\left[\Gamma\left(\frac{5}{8}\right)\right]^4}$$

$$= \begin{matrix} 0.6428822 \\ 0.9091728 \end{matrix}$$

が得られる．詳細については数値計算の結果とともに第3報以下にゆずる．

Extended Watson Integral. Part II

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1. Introduction

In this paper we present numerical values of the integral:

$$G(s) = \frac{1}{\pi^3}\int_0^\pi dx \int_0^\pi dy \int_0^\pi dz \frac{1}{s+i\epsilon - \cos x - \cos y - \cos z} \quad (1)$$

where s takes onè real values and ϵ is an infinitesimal positive number. Watson[1] expressed the value for s=3 in terms of the complete elliptic integral of the first kind.

The function G(s) has an imaginary part when $-3 < s < 3$. It is related with the level density of vibrational mode of harmonic simple cubic lattice. The function as a function of s was given in a numeber of works presented in the past.[2] But no table of the values is available.

The function G(s) for $s > 3$ is real and appears when one considers the localized mode of oscillation when one defect is imbedded in a simple cubic harmonic lattice. A short table was given by Mar ıdudin et al.[3] and a detailed table was presented by Mannari and Kawabata.[4] Moreover a Chebyshev interpolation formula was prepared by Mannari and Kageyama.[5]

In evaluating G(s) for $s > 3$, Mannari and Kawabata startє with its expression $G(s)=G_R(s)$ where

$$G_R(s) = \frac{1}{\pi^2}\int_0^{\pi/2} dx\; k\,K(k), \quad (2)$$

where

$$K(k) = \int_0^{\pi/2} \frac{d\theta}{\sqrt{1-k^2\sin^2\theta}}, \quad (3)$$

$$k = 2/(s-\cos x). \quad (4)$$

This expression was obtained by introducing the variable θ by

$$\frac{2 - k(1 + \cos y)}{2 + k(1 - \cos y)} = \frac{1 - k^2 \sin^2\theta}{1 + k} \qquad (5)$$

after the integration over z. In the present paper, we consider the real as well as the imaginary part of G(s) for $s < 3$. For each part, we introduce a variable θ by a relation similar to (5) and express the integral as an integral of the elliptic function, similar to (2). Then a numerical computation of the integral is attempted.

In §2, the formulas by which numerical calculation is performed are derived. The numerical calculation is discussed in §3.

2. Results of integration over z

The integration over z for fixed values of x and y is performed as usual. The result is real or pure imaginary according as the absolute value of

$$D \equiv s - \cos x - \cos y \tag{6}$$

is more or less than unity. More explicitly one has

$$G(s) = G_R(s) + i\, G_I(s), \tag{7}$$

$$G_R(s) = \frac{1}{\pi^2}\int_0^\pi dx \int_0^\pi dy \frac{1}{\sqrt{(s-\cos x-\cos y)^2-1}} \quad (s-\cos x-\cos y > 1)$$

$$-\frac{1}{\pi^2}\int_0^\pi dx \int_0^\pi dy \frac{1}{\sqrt{(s-\cos x-\cos y)^2-1}} \quad (s-\cos x-\cos y < -1). \tag{8}$$

and

$$G_I(s) = -\frac{1}{\pi^2}\int_0^\pi dx \int_0^\pi dy \frac{1}{\sqrt{1-(s-\cos x-\cos y)^2}} \quad (-1 < s-\cos x-\cos y < 1). \tag{9}$$

It is straightforward to see that $G_R(s)$ is an odd function and $G_I(s)$ is an even function of s:

$$G_R(-s) = -G_R(s) \tag{10}$$

$$G_I(-s) = G_I(s) \tag{11}$$

Hence in the following we consider $G_R(s)$ and $G_I(s)$ only for positive s.

The expressions (8) and (9) are investigated separately for three cases of positive s:

I: $3 < s$,

II: $1 < s < 3$,

III: $0 < s < 1$.

Case I.

For case I, there exist no region of integral for the integral (9) and the second integral of (8). The inequality $D \equiv s-\cos x-\cos y > 1$ is satisfied for all values of x and y between 0 and π. Hence

$$G_R(s) = \frac{1}{\pi^2} \int_0^{\pi} dx \int_0^{\pi} dy \frac{1}{\sqrt{(s-\cos x-\cos y)^2-1}} , \qquad (12)$$

$$G_I(s) = 0 \qquad (13)$$

By introducing k and θ by (4) and (5), one can write (12) as (2)-(4).

Case II.

In Fig. 1, the region of integral is shown by taking cosx and cosy as abscissa and ordinate. The integral is taken in the square restriced by the lines cos $x=\pm 1$ and cos $y=\pm 1$. The region is divided by the line $D \equiv s-\cos x-\cos y = 1$, which cuts the abscidda at $\cos x=s-1$. For the present case s-1 is between 0 and 2. In the right-top region, $-1 < D < 1$ and $G_I(s)$ has a contribution from this region. In the left-bottom region, $D > 1$ and the first terms of (8) is contributed from this region.

The second term of (8) is zero.

Fig. 1

In the evaluation of $G_I(s)$, the variable k_1 and θ are introduced by

$$k_1 = \frac{s - \cos x}{2} \tag{14}$$

$$\frac{-2k_1 + (1+\cos y)}{2k_1 + (1-\cos y)} = \frac{(1-k_1)\cos^2\theta}{k_1} . \tag{15}$$

Then one finds

$$G_I(s) = -\frac{1}{\pi^2}\int_0^{\cos^{-1}(s-2)} dx \; K(k_2) , \tag{16}$$

where

$$k_2 = \frac{1}{2}\sqrt{4 - (s - \cos x)^2} . \tag{17}$$

In evaluating $G_R(s)$, one separates the region of integral by whether cosx is less or more than s. For the latter region, the variable k_1 and θ are introduced by (14) and

$$\frac{2k_1 - (1+\cos y)}{2k_1 + (1-\cos y)} = \frac{k_1 \cos^2\theta}{1+k_1} . \tag{18}$$

For the latter region, k and θ introduced for the case I are used. Then one gets

$$G_R(s) = \frac{1}{\pi^2}\int_0^{\cos^{-1}(s-2)} dx\; K(k_1)$$

$$+ \frac{1}{\pi^2}\int_{\cos^{-1}(s-2)}^{\pi} dx\; k\,K(k), \qquad (19)$$

where k is given by (4).

Case III.

The region of integral is shown in Fig. 2, where the lines D=1 and D=-1 are drawn . The region in between these two lines contributes to $G_I(s)$. This region is devided by whether cosx is more or less than s. For the former region, variable k'_1 and θ are introduced by

$$k'_1 = \frac{\cos x - s}{2} \equiv -k_1 \qquad (20)$$

$$\frac{-2k'_1 + (1-\cos y)}{2k'_1 + (1+\cos y)} = \frac{(1-k'_1)\cos^2\theta}{k'_1} \qquad (21)$$

The calculation for the former region is similar to the one for region II. $G_I(s)$ obtained is summed up, giving the result:

$$G_I(s) = -\frac{1}{\pi^2}\int_0^{\pi} dx\; K(k_2) \qquad (22)$$

where k_2 is given by (17) .

Fig. 2

The right-top region is the region of integral for the second term of (8). For its evaluation, θ is introduced by

$$\frac{-2k_1' + (1-\cos y)}{-2k_1' - (1+\cos y)} = \frac{k_1' \cos^2\theta}{1+k_1'}, \tag{23}$$

where k'_1 is given by (14). The left-bottom region is the region of integral for the first term of (8). Its evaluation is done in a similar way to the contribution of $G_R(s)$ from $s-2 < \cos x$ in the case II. The result we obtain is

$$G_R(s) = \frac{1}{\pi^2}\int_{\cos^{-1}s}^{\pi} dx \; K(k_1) - \frac{1}{\pi^2}\int_0^{\cos^{-1}s} dx \; K(k_1'), \tag{24}$$

where k_1 and k'_1 are given by (14) and (20), respectively.

3. Numerical calculation

The calculation of the functions $G_R(s)$ and $G_I(s)$ is performed with the aid of (16) and (19) for $1 < s < 3$ and (22) and (24) for $0 < s < 1$. The integration is performed by the Sympson formula. The complete elliptic function appearing in the integrand is evaluated by the method of arithmetic-geometric means.[6)]

For the b. c. c. and f. c. c. lattices, the corresponding formulas of calculating the real and imaginary parts of the extended Watson integral. The numerical calculation is in progress with the aid of the computer of the computer center of Tohoku University.

References

1) G. N. Watson, Quart. J. Math. 10 (1939) 266.

2)

3) A. A. Maradudin et al., Acad. Roy. Belgique, Classe des Sciences, Mémoires in 4°-2^{e} Serie, Tome XIV (1960).

4) I. Mannari and C. Kawabata, Res. Notes Dept. Phys. of Okayama University, No. 15 (1964).

5) I. Mannari and H. Kageyama, Prog. Theor. Phys. Suppl. Extra Number (1968) 269.

6) M. Abramowitz and I. A. Stegun (ed.), Handbook of Mathematical Functions, AMS 55 (Natl. Bur. Stds.) (1964).

Captions

Fig. 1. The regions of integrations (8) and (9) for $G_R(s)$ and $G_I(s)$, respectively, when $1 < s < 3$. The regions hatched by horizontal and vertical lines are for the integral (9) and the first term of (8), respectively. When $k=1$, $k_1=1$ also and both integrands of (19) for $G_R(s)$ are singular. The integrand of (16) for $G_I(s)$ is singular at $k_2=1$. The latter singularity is important only when $s \gtrsim 1$.

Fig. 2. The regions of integrations (8) and (9) for $G_R(s)$ and $G_I(s)$, respectively, when $0 < s < 1$. The region hatched by horizontal lines is for (9). There are two regions hatched vertically. The right-top one is for the second term of (8) and the left-bottom region is for the first term. When $k_2=1$, the integrand of (22) for $G_I(s)$ is singular. Both integrands of (24) for $G_R(s)$ are singular at $k_1=1$ where $k'_1=1$ also. The latter singularity is important only when $s \lesssim 1$.

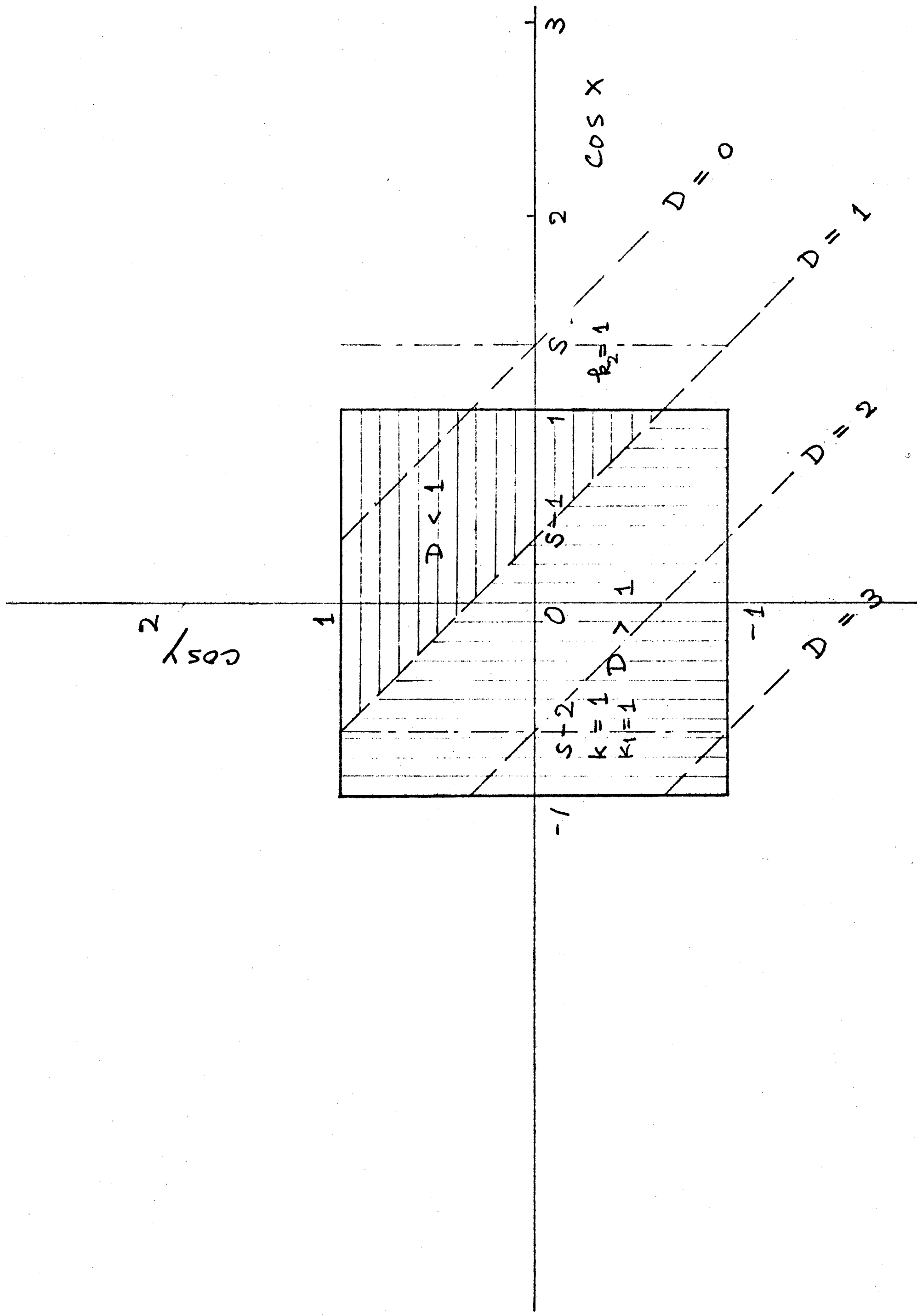

Fig. 1

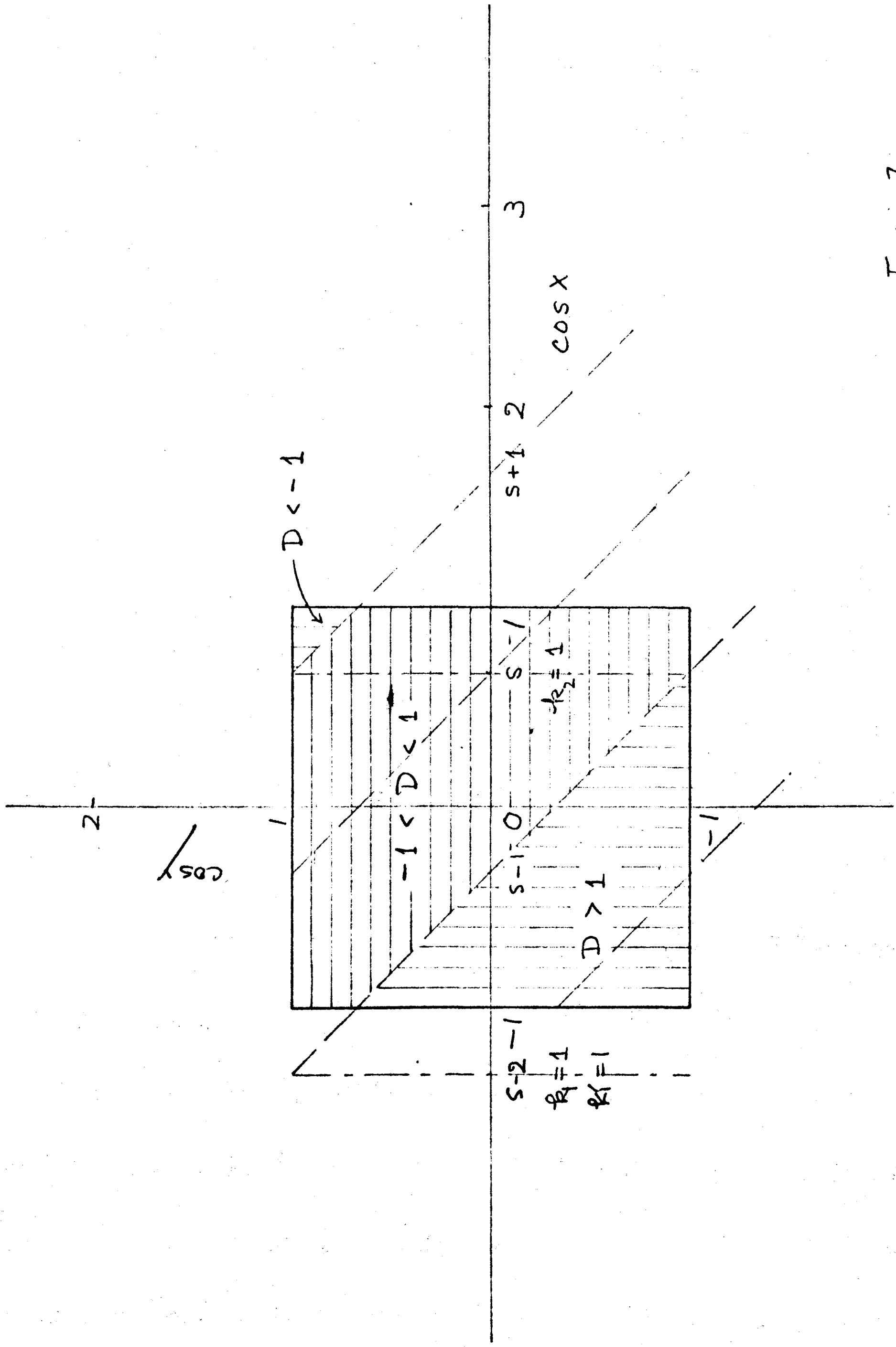

Fig. 2