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Evaluation of the Watson Integral of a Face-centered Lattice

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Along the general line of Watson, the Watson integral of a face-centered lattice is shown to be expressible in terms of complete elliptic integrals.

§ 1. Introduction

In 1939, G. N. Watson[1] evaluated the following integrals

$$I_1=\frac{1}{\pi^3}\iiint\frac{du\cdot dv\cdot dw}{z-\cos u\cdot\cos v\cdot\cos w},$$

$$I_2=\frac{1}{\pi^3}\iiint\frac{du\cdot dv\cdot dw}{z-\cos u\cdot\cos v-\cos v\cdot\cos w-\cos u\cdot\cos w},$$

$$I_3=\frac{1}{\pi^3}\iiint\frac{du\cdot dv\cdot dw}{z-\cos u-\cos v-\cos w}$$

for special values of z, ($z=1$ for I_1, $z=3$ for I_2 and I_3) in terms of complete elliptic integrals. Numerical values of these integrals have been tabulated extensively by Mannari and Kawabata.[2]

The first integral is related to a body-centered lattice, the second to a face-centered lattice, and the third to a simple cubic lattice. The first integral is expressible as the square of a complete elliptic integral, that is,

$$I_1=\frac{1}{z}\cdot\frac{4}{\pi^2}K^2(k),\qquad k=\frac{1}{2}\left(1-\sqrt{1-\frac{1}{z^2}}\right)$$

as is shown in Reference 2.

So far the second and third integrals seem to lack such expression. The second integral will be shown here to be expressible as the product of two complete elliptic integrals, for case 1, $z\geqq 3$ as well as for case 2, $z<-1$.

§ 2. Case 1, $z \geqq 3$

A Watson integral in a face-centered lattice takes the following form

$$I_2 = \frac{1}{\pi^3}\iiint_0^\pi \frac{du \cdot dv \cdot dw}{z - \cos u \cdot \cos v - \cos v \cdot \cos w - \cos w \cdot \cos u}$$

for $z \geqq 3$. Preliminary integrations with respect to w and $x = \cos v$ give

$$I_2 = \frac{1}{\pi^2}\iint_0^\pi \frac{du \cdot dv}{\sqrt{(z - \cos u \cdot \cos v)^2 - (\cos u + \cos v)^2}}$$

$$= \frac{1}{\pi^2}\int_0^\pi du \int_{-1}^1 \frac{1}{\sqrt{(z+\cos u) + (1-\cos u)x}\sqrt{(z-\cos u) - (1+\cos u)x}} \frac{dx}{\sqrt{1-x^2}}$$

$$= \frac{1}{\pi^2}\int_0^\pi \frac{du}{\sin u} \cdot \frac{2\sin u}{z+1} \cdot K\left(\frac{2\sqrt{z+\cos^2 u}}{z+1}\right)$$

$$= \frac{2}{\pi^2(z+1)}\int_0^\pi K\left(\frac{2\sqrt{z+\cos^2 u}}{z+1}\right) du$$

where K is a complete elliptic integral.

The modulus of K may be put in a more convenient form

$$\frac{2\sqrt{z+\cos^2 u}}{z+1} = \sqrt{a^2 \cos^2 u + b^2 \sin^2 u}$$

where $a = 2\sqrt{z+1}/(z+1)$, and $b = 2\sqrt{z}/(z+1)$.

Further the expression under the sign of square root is transformed as follows

$$a^2 \cos^2 u + b^2 \sin^2 u = \frac{a^2+b^2}{2} + \frac{a^2-b^2}{2}\cos 2u$$

$$= A(1+\rho e^{2iu})(1+\rho e^{-2iu})$$

where $A = [(a+b)/2]^2$, $\rho = (a-b)/(a+b)$. Since z is assumed to be greater than 3, it follows that $A < 1$ and $\rho < 1$.

We have then

$$\int_0^\pi K(\sqrt{a^2 \cos^2 u + b^2 \sin^2 u})\, du$$

$$= \int_0^\pi \frac{\pi}{2}\sum_{l=0}^\infty \left(\frac{\left(\frac{1}{2}\right)_l}{l\,!}\right)^2 (a^2\cos^2 u + b^2 \sin^2 u)^l du$$

$$((\alpha)_l = \alpha(\alpha+1)\cdots(\alpha+l-1),\ (\alpha)_0 = 1)$$

$$=\frac{\pi}{2}\sum_{l=0}^{\infty}\left(\frac{\left(\frac{1}{2}\right)_l}{l\,!}\right)^2\int_0^{\pi}A^l(1+\rho e^{2iu})^l(1+\rho e^{-2iu})^l du$$

$$=\frac{\pi}{2}\sum_{l=0}^{\infty}\left(\frac{\left(\frac{1}{2}\right)_l}{l\,!}\right)^2 A^l\pi\sum_{m=0}^{l}\left(\frac{l\,!}{m\,!\,(l-m)\,!}\right)^2\rho^{2m}$$

$$=\frac{\pi^2}{2}\sum_{n=0}^{\infty}\sum_{m=0}^{\infty}\left(\frac{\left(\frac{1}{2}\right)_{m+n}}{m\,!\,n\,!}\right)^2(A\rho^2)^m A^n \qquad (l=m+n)$$

$$=\frac{\pi^2}{2}F_4\left(\frac{1}{2},\ \frac{1}{2};\ 1,\ 1;\ A\rho^2,\ A\right)$$

where F_4 denotes the fourth kind of Appell's hypergeometric function of two variables, or

$$F_4(\alpha,\beta\,;\gamma,\gamma'\,;x,y)=\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{(\alpha)_{m+n}(\beta)_{m+n}}{(\gamma)_m(\gamma')_n\,m\,!\,n\,!}x^m y^n\,.$$

We now avail ourselves of Bailey's equality that

$$F_4(\alpha,\beta\,;\gamma,\alpha+\beta-\gamma+1\,;\xi(1-\eta),\eta(1-\xi))$$
$$={}_2F_1(\alpha,\beta\,;\gamma\,;\xi)\cdot{}_2F_1(\alpha,\beta\,;\alpha+\beta-\gamma+1\,;\eta)$$

which is valid inside simply connected regions surrounding $\xi=0$, $\eta=0$ for which

$$|\xi(1-\eta)|^{1/2}+|\eta(1-\xi)|^{1/2}<1\,.$$

In a special case $\alpha=\beta=1/2$, $\gamma=1$, the equality yields

$$F_4\left(\frac{1}{2},\frac{1}{2},1,1\,;\xi(1-\eta),\eta(1-\xi)\right)$$

$$={}_2F_1\left(\frac{1}{2},\frac{1}{2}\,;1\,;\xi\right)\cdot{}_2F_1\left(\frac{1}{2},\frac{1}{2}\,;1\,;\eta\right)$$

$$=\frac{2}{\pi}K(\sqrt{\xi}\,)\cdot\frac{2}{\pi}K(\sqrt{\eta}\,)\,.$$

For any positive values of a and b less than one, we see that

$$A<1,\ \rho<1 \qquad \text{and} \qquad (A\rho^2)^{1/2}+A^{1/2}=A^{1/2}(1+\rho)=a<1\,.$$

Therefore we have

$$\int_0^{\pi}K(\sqrt{a^2\cos^2 u+b^2\sin^2 u})\,du=2K(\sqrt{\xi}\,)\cdot K(\sqrt{\eta}\,)$$

where ξ and η are determined by the relations $\xi(1-\eta)=A\rho^2$ and $\eta(1-\xi)=A$ to be

$$\xi=\frac{1}{2}\{1+ab-\sqrt{(1-a^2)(1-b^2)}\}$$

$$=\frac{(\sqrt{1-a^2}-\sqrt{1-b^2})^2+(a+b)^2}{4}$$

and

$$\eta=\frac{1}{2}\{1-ab-\sqrt{(1-a^2)(1-b^2)}\}$$

$$=\frac{(\sqrt{1-a^2}-\sqrt{1-b^2})^2+(a-b)^2}{4}$$

respectively. Special values of a and b corresponding to the Watson integral give the desired result that

$$I_2=\frac{4}{\pi^2(z+1)}K(\sqrt{\xi})\cdot K(\sqrt{\eta})$$

$$\xi=\frac{1}{2}\left\{1+\frac{4\sqrt{z}\sqrt{z+1}}{(z+1)^2}-\frac{(z-1)\sqrt{(z+1)(z-3)}}{(z+1)^2}\right\}$$

$$=\frac{1}{(z+1)^2}\left\{\left(\frac{\sqrt{z+1}-\sqrt{z-3}}{2}\right)^4+(\sqrt{z+1}+\sqrt{z})^2\right\}$$

$$\eta=\frac{1}{2}\left\{1-\frac{4\sqrt{z}\sqrt{z+1}}{(z+1)^2}-\frac{(z-1)\sqrt{(z+1)(z-3)}}{(z+1)^2}\right\}$$

$$=\frac{1}{(z+1)^2}\left\{\left(\frac{\sqrt{z+1}-\sqrt{z-3}}{2}\right)^4+(\sqrt{z+1}-\sqrt{z})^2\right\}$$

The expansion of the above I_2 in powers of $\frac{1}{z}$ gives coefficients that are obtained by averaging the expansion of $1/(z-\cos u\cdot\cos v-\cos v\cdot\cos w-\cos w\cdot\cos u)$ in powers of $\frac{1}{z}$.

§ 3. Case 2, $z<-1$

For the sake of distinction we put

$$J_2=\frac{1}{\pi^3}\iiint_0^\pi\frac{du\cdot dv\cdot dw}{x+\cos u\cdot\cos v+\cos v\cdot\cos w+\cos w\cdot\cos u}$$

Preliminary integrations with respect to v and w yield

$$J_2=\frac{1}{\pi^2}\iint_0^\pi\frac{du}{\sqrt{\left(\frac{x+1}{2}\right)^2-\cos^2 u}}\cdot K\left(\sqrt{\frac{4x-4\cos^2 u}{(x+1)^2-4\cos^2 u}}\right)$$

$$=\frac{2}{x-1}\cdot\frac{1}{\pi^2}\int_0^{\pi}\frac{du}{\sqrt{a^2\cos^2 u+b^2\sin^2 u}}K'\left(\sqrt{\frac{1}{a^2\cos^2 u+b^2\sin^2 u}}\right)$$

where

$$a=\sqrt{\frac{(x+1)^2-4}{(x-1)^2}}, \qquad b=\frac{x+1}{x-1}$$

and

$$K(k')=K'(k), \qquad k'=(1-k^2)^{1/2}.$$

This is the same expression as the reduced form of I_3 in Watson's paper. Following the steps of Watson step by step we arrive at the formula

$$\int_0^{\pi}\frac{1}{\sqrt{a^2\cos^2 u+b^2\sin^2 u}}K'\left(\frac{1}{\sqrt{a^2\cos^2 u+b^2\sin^2 u}}\right)du$$

$$=\frac{4}{a+b}K(k_1)\cdot K(k_2)$$

k_1 and k_2 being given by

$$k_1=\left|\frac{\sqrt{a^2-1}-\sqrt{b^2-1}}{a+b}\right|, \qquad k_2=\frac{\sqrt{a^2-1}+\sqrt{b^2-1}}{a+b}.$$

We have then

$$J_2=\frac{2}{x-1}\cdot\frac{1}{\pi^2}\cdot\frac{4}{a+b}K(k_1)\cdot K(k_2)$$

where

$$k_1=\frac{2\sqrt{x}-2\sqrt{x-1}}{\sqrt{(x+3)(x-1)}+x+1}, \qquad k_2=\frac{2\sqrt{x}+2\sqrt{x-1}}{\sqrt{(x+3)(x-1)}+x+1}$$

and

$$\frac{1}{a+b}=\frac{x-1}{\sqrt{(x+3)(x-1)}+x+1}.$$

§ 4. Verification of the formula for I_2

To verify the formula for I_2 obtained in § 2, the values of I_2 given by the formula will be compared with those of the Table of Mannari and Kawabata for $z=3$, 4 and 6. It is to be noted that the Watson integral $I(3/z)$ in their table is equal to $3I_2(z)$.

For $z=3$, the formula gives precisely Watson's result

$$I_2(3)=\frac{1}{\pi^2}K\left(\sqrt{\frac{2-\sqrt{3}}{4}}\right)K\left(\sqrt{\frac{2+\sqrt{3}}{4}}\right)$$

$$=\frac{1}{\pi^2}K(\sin 15^{\circ})K(\sin 75^{\circ}).$$

For $z=4$ and 6, it gives

$$I_2(4)=\frac{4}{5\pi^2}K\left(\sqrt{\frac{25-11\sqrt{5}}{50}}\right)K\left(\sqrt{\frac{25+5\sqrt{5}}{50}}\right)$$

$$I_2(6)=\frac{4}{7\pi^2}K\left(\sqrt{\frac{49-4\sqrt{42}-5\sqrt{21}}{98}}\right)K\left(\sqrt{\frac{49+4\sqrt{42}-5\sqrt{21}}{98}}\right).$$

A complete elliptic integral $K(k)$ may be easily computed by the formula

$$K(k)=\pi/(2M(1,\sqrt{1-k^2}))$$

where $M(a, b)$ denotes the arithmetic-geometrical mean of a and b. One gets then

$$3I_2(4)=0.80824\ 87016\ 029$$

$$3I_2(6)=0.51342\ 43776\ 053$$

while Mannari and Kawabata give

$$I(3/4)=3I_2(4)=0.8082\ 4871$$

$$I(3/6)=3I_2(6)=0.5134\ 2438$$

Their values confirm the formula for I_2 beyond doubt.

The Watson integral I_3 may have a similar expression. However it remains to be seen.

References

1) G.N. Watson: Quart. Journ. Math. 10 (1939) 266.
2) I. Mannari and C. Kawabata: Extended Watson Integrals and Their Derivatives, 1964, Okayama University, Japan.