Applications of Mellin Transforms to Some Problems of Statistical Mechanics II

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(Received April 10, 1971)

§1. Introduction

The usefulness of Mellin transforms for evaluating some integrals in statistical mechanical problems was shown ten years ago in a paper[1]. An essential virtue of the use of Mellin transforms is to make a parameter conspicuous that plays the role of an expansion parameter. A Mellin type integral may be expanded in powers of that parameter when the parameter is either large or small, by translating the line of integration to the right or to the left. Another virtue is to make feasible otherwise complicated integration or summation. To furnish further examples, the technique of Mellin transform will be applied to two problems treated by A. Wasserman and others[2].

§2. The exchange integral

The exchange integral with the Coulomb interaction

$$J_{ex}(\alpha)=\frac{1}{\pi^3}\int d\mathbf{x}\int d\mathbf{y}\,\frac{f^-(\mathbf{x}^2)f^-(\mathbf{y}^2)}{|\mathbf{x}-\mathbf{y}|^2}, \quad f^-(z)=(e^{z-\alpha}+1)^{-1}$$

was evaluated by Wasserman and others to be

$$J_{ex}(\alpha)=C_1\alpha^2+C_2\log\alpha+C_3+O(\alpha^{-2})$$

where

$$C_1=4/\pi, \qquad C_2=2\pi/3$$

and

$$C_3=2\pi-\frac{4}{3}\pi\log 2-\frac{2}{3}\pi\gamma+\frac{4}{\pi}\zeta'(2)$$

Elementary integrations simplify the integral to

$$J_{ex}(\alpha)=\frac{8}{\pi}\int_0^\infty dx\,x\,f^-(x^2)\int_0^\infty dy\,y\,f^-(y^2)\log\left|\frac{x+y}{x-y}\right|$$

with $x=|\mathbf{x}|$ and $y=|\mathbf{y}|$.

A formula of Mellin transform[3]

$$\frac{1}{1+x}=\frac{1}{2\pi i}\int_{\sigma-i\infty}^{\sigma+i\infty}\frac{\pi}{\sin\pi s}x^{-s}ds\,,\quad 0<\mathcal{R}s\equiv\sigma<1$$

may be advantageously employed to give

$$\frac{\pi}{8}J_{ex}(\alpha)=\frac{1}{(2\pi i)^2}\iint\frac{\pi}{\sin\pi s}\frac{\pi}{\sin\pi t}e^{\alpha s+\alpha t}ds\,dt\,J,\quad 0<\mathcal{R}s,\,\mathcal{R}t<1$$

where

$$J=\int_0^\infty\int_0^\infty\exp(-sx^2-ty^2)\,x\,dx\,y\,dy\,\log\left|\frac{x+y}{x-y}\right|.$$

To evaluate J, a formula of Mellin transform[4)]

$$\log\left|\frac{1+x}{1-x}\right|=\frac{1}{2\pi i}\int_{\sigma-i\infty}^{\sigma+i\infty}\frac{\pi}{s}\tan\frac{1}{2}\pi s\cdot x^{-s}ds\,,\quad -1<\sigma<0$$

is evoked to give

$$\begin{aligned}J&=\frac{1}{2\pi i}\int\frac{\pi}{z}\tan\frac{1}{2}\pi z\cdot dz\int_0^\infty\int_0^\infty\exp(-sx^2-ty^2)(y/x)^{-z}x\,y\,dx\,dy\\&=\frac{1}{2\pi i}\int\frac{\pi}{z}\tan\frac{1}{2}\pi z\,dz\cdot\int_0^\infty\exp(-sx^2)\,x^{z+1}\,dx\int_0^\infty\exp(-ty^2)\,y^{1-z}\,dy\\&=\frac{1}{2\pi i}\int\frac{\pi}{\cos\pi\zeta}\frac{d\zeta}{s^{1+\zeta}t^{1-\zeta}}\frac{\pi}{4},\quad \zeta=z/2\\&=\frac{1}{2\pi i}\int\frac{\pi}{\sin\pi\eta}\left(\frac{s}{t}\right)^{-\eta}d\eta\cdot s^{-1/2}t^{-3/2}\pi/4\,,\quad \eta=\zeta+1/2\\&=\frac{1}{s^{1/2}t^{1/2}(s+t)}\cdot\frac{\pi}{4}\end{aligned}$$

where use of a functional relation of gamma functions $\Gamma(1+x)\Gamma(1-x)=\pi x/\sin\pi x$ and the formula of Mellin transform concerning $1/(1+x)$ mentioned above is made.

Now $J_{ex}(\alpha)$ is expressed as

$$J_{ex}(\alpha)=\frac{2}{(2\pi i)^2}\iint\frac{e^{\alpha(s+t)}}{s+t}\frac{\pi}{\sin\pi s}\frac{\pi}{\sin\pi t}\frac{ds\,dt}{\sqrt{st}}.$$

To make the parameter α stand out, variables are changed from s, t to u, v through the relations

$$s+t=u\,,\quad s-t=v$$

or

$$s=(u+v)/2\,,\quad t=(u-v)/2$$

under the restriction that

$$-1<\mathcal{R}v<\mathcal{R}u<2$$

to get

$$J_{ex}(\alpha)=\frac{1}{2\pi i}\int e^{\alpha u}\frac{du}{u}J_0(u)$$

$$J_0(u)=\frac{1}{2\pi i}\int\frac{\pi^2}{\sin\frac{\pi}{2}(u+v)\sin\frac{\pi}{2}(u-v)}\cdot\frac{2dv}{\sqrt{(u^2-v^2)}}.$$

An approximate evaluation of $J_{ex}(\alpha)$ for large α depends on the behaviour of $J_0(u)$ in the right neighbourhood of the origin $u=0$, $\mathcal{R}u>0$.

By taking as the path of integration with respect to v the imaginary axis, and setting $v=ix$, J_0 is changed into

$$J_0(u)=\frac{8\pi}{2i\sin\pi u}\int_0^\infty\left(\frac{1}{e^{\pi(x-iu)}-1}-\frac{1}{e^{\pi(x+iu)}-1}\right)\frac{dx}{\sqrt{u^2+x^2}},$$

The variable u is restricted to be real for the present and use is made of the formula of Mellin transform[5)]

$$\frac{1}{e^x-1}=\frac{1}{2\pi i}\int\Gamma(s)\zeta(s)x^{-s}ds\,,\quad \mathcal{R}s>1,\ \mathcal{R}x>0$$

to derive

$$J_0(u)=\frac{8\pi}{\sin\pi u}\cdot\frac{1}{2\pi i}\int\Gamma(s)\zeta(s)\varphi(s)(\pi u)^{-s}ds$$

where

$$\varphi(s)=\frac{1}{2i}\int_0^\infty\{(y-i)^{-s}-(y+i)^{-s}\}\frac{dy}{\sqrt{1+y^2}},\quad \mathcal{R}s>1\,,\ y=x/u\,.$$

The change of the path of integration from the one of $0\to\infty$ on the real axis to the one of $0\to i\to i\infty$ on the imaginary axis leads to

$$\int_0^\infty(y+i)^{-s}\frac{dy}{\sqrt{1+y^2}}=i\exp\left(-\frac{1}{2}\pi si\right)\int_0^1\frac{(w+1)^{-s}}{\sqrt{1-w^2}}dw$$
$$+\exp\left(-\frac{1}{2}\pi si\right)\frac{2^{-s}\Gamma(1/2)\Gamma(s)}{\Gamma(s+1/2)}.$$

The other integral in φ is complex conjugate to the above integral, so that one gets

$$\varphi(s)=\sin\frac{1}{2}\pi s\cdot\frac{2^{-s}\Gamma(1/2)\Gamma(s)}{\Gamma(s+1/2)}-\cos\frac{1}{2}\pi s\cdot\psi(s)\,,$$

$$\psi(s)=\int_0^1\frac{(w+1)^{-s}}{\sqrt{1-w^2}}dw\,.$$

Since the function $\psi(s)$ is regular everywhere in s except $s=\infty$, singular points of the function $\varphi(s)$ are only poles of the first order at $s=-1,\ -3,\ -5,\ \cdots$. One gets then

$$J_0(u)=\frac{8\pi}{\sin \pi u}\left(\frac{1}{\pi u}+\frac{\zeta(2)}{2\pi}\left(1-2\log 2+\frac{\zeta'(2)}{\zeta(2)}+\log u\right)u+\cdots\right)$$

summing up the residues, or

$$\frac{J_0(u)}{u}=8\left\{\frac{1}{\pi u^3}+\frac{\zeta(2)}{2\pi}\frac{\log u}{u}\right.$$
$$\left.+\left(2\pi-\frac{4\pi}{3}\log 2+\frac{4}{\pi}\zeta'(2)\right)\frac{1}{u}+\cdots\right\}$$

where use is made of the well known functional relation of the Riemann Zeta function $\Gamma(s)\cos\frac{1}{2}\pi s\cdot\zeta(s)=2^{-s}\pi^s\zeta(1-s)$.

Expanding $J_0(u)/u$ in powers of u, one gets the result of Wasserman and others mentioned at the beginning of this section.

§ 3. The free energy integral

The free energy integral of an electron gas in a magnetic field H can be written

$$F=\zeta N-\mathcal{D}(\beta,\omega,\zeta)$$

where

$$\mathcal{D}(\beta,\omega,\zeta)=\frac{m\omega}{2\pi^2\beta h}\int_{-\infty}^{\infty}dk_z\sum_{\eta=0}^{\infty}\log(1+\exp\beta[\zeta-\varepsilon])$$

ζ being the chemical potential, N the average number of particles in the system, $\omega=eH/mc$, and

$$\varepsilon=\mathrm{h}\omega\left(\eta+\frac{1}{2}\right)+\frac{\mathrm{h}^2k_z^2}{2m}.$$

Use of a formula of Mellin transform[6)]

$$\log(1+x)=\frac{1}{2\pi i}\int\frac{\pi}{s\sin\pi s}x^s\,ds\,,\quad 0<\mathcal{R}s<1$$

leads to the representation of $\mathcal{D}$

$$\mathcal{D}=\frac{m\omega}{2\pi^2\beta h}\sqrt{\frac{2\pi m}{h^2\beta}}J$$

where

$$J=\frac{1}{2\pi i}\int\frac{\pi e^{\alpha s}}{s^{3/2}\sin\pi s\,\mathrm{Sin}\,\lambda s}ds\,,\quad 0<\mathcal{R}s<1$$

and $\lambda=\beta\mathrm{h}\omega/2$, $\alpha=\beta\zeta$.

To get an asymptotic expansion of J in α, it suffices to expand $1/\sin\pi s\cdot\mathrm{Sin}\,\lambda s$ in powers of s and to integrate termwise. As is obvious

$$\frac{1}{\sin \pi s \operatorname{Sin} \lambda s} = \frac{1}{\pi\lambda}\frac{1}{s^2} + \frac{1}{6}\left(\frac{\pi}{\lambda} - \frac{\lambda}{\pi}\right) + \left(\frac{7}{360}\frac{\lambda^3}{\pi} - \frac{1}{36}\pi\lambda + \frac{7}{360}\frac{\pi^3}{\lambda}\right)s^2 + \cdots .$$

Hence one gets

$$J = \frac{1}{\lambda}\frac{\alpha^{5/2}}{\Gamma(7/2)} + \frac{\pi}{6}\left(\frac{\pi}{\lambda} - \frac{\lambda}{\pi}\right)\frac{\alpha^{1/2}}{\Gamma(3/2)} + O(\alpha^{-3/2}) .$$

The integrand of J has poles of first order at $s = \pm 1, \pm 2, \cdots$. The origin $s=0$ is a branch point, so that the path of integration cannot be shifted to the left beyond the origin. However the path of integration may be deformed to a contour L starting from $-i\infty$, encircling the origin counterclockwise, extending to $-i\infty$ again. Residues at points $s = in\pi/\lambda$, $n = 1, 2, 3, \cdots, -1, -2, -3, \cdots$.

$$(-)^{n+1}\frac{\lambda^{1/2}}{\pi^{1/2}} \cdot \frac{e^{i(n\pi\alpha/\lambda - \pi/4)}}{n^{3/2}\operatorname{Sin}(n\pi^2/\lambda)}$$

being taken into account, J will be written

$$J = \text{the expression obtained above} + \sqrt{\frac{\lambda}{\pi}}\sum_{n=1}^{\infty}\frac{(-)^{n+1}\, 2\cos(n\pi\alpha/\lambda - \pi/4)}{n^{3/2}\operatorname{Sin}(n\pi^2/\lambda)} .$$

Our result differs from that of Wasserman and others. One reason is some typographical errors commited in their paper, and another reason seems to lie in the functional relation

$$\sum_{n=1}^{\infty}\frac{(-)^{n-1}}{n}\left(\frac{1}{\operatorname{Sin} n\lambda} - \frac{1}{\operatorname{Sin}(n\pi^2/\lambda)}\right) = \frac{\pi^2}{12\lambda} - \frac{\lambda}{12} .$$

This functional relation may be proved as follows. A formula of Mellin transform[7] gives

$$\sum_{n=1}^{\infty}\frac{(-)^{n-1}}{n \operatorname{Sin} n\lambda} = \frac{1}{2\pi i}\sum_{n=1}^{\infty}\frac{(-)^{n-1}}{n}\int 2(1-2^{-s})\Gamma(s)\zeta(s)(n\lambda)^{-s}ds , \quad \mathscr{R}s > 1$$

$$= \frac{1}{2\pi i}\int 2(1-2^{-s})^2\Gamma(s)\zeta(s)\zeta(s+1)\lambda^{-s}ds , \quad \mathscr{R}s > 1 .$$

Shift of the path of integration to the position $-2 < \mathscr{R}s < -1$ leads to

$$\text{The right member} = \frac{\pi^2}{12\lambda} - \frac{\lambda}{12} + \frac{1}{2\pi i}\int 2(1-2^{-s})^2\Gamma(s)\zeta(s)\zeta(s+1)\lambda^{-s}ds , \quad -2 < \mathscr{R}s < -1 .$$

The change of variable $s \to s'$ and use of the functional relation

$$\Gamma(s)\zeta(s)\zeta(s+1) = (2\pi)^{2s}\Gamma(-s)\zeta(-s)\zeta(1-s)$$

give

$$\frac{1}{2\pi i}\int 2(1-2^{-s})^2\Gamma(s)\zeta(s)\zeta(s+1)\lambda^{-s}ds, \qquad -2<\mathcal{R}s<-1$$

$$=\frac{1}{2\pi i}\int 2(1-2^{s'})^2\Gamma(-s')\zeta(-s')\zeta(1-s')\lambda^{s'}ds', \qquad 1<\mathcal{R}s'<2$$

$$=\frac{1}{2\pi i}\int 2(1-2^{-s'})^2\Gamma(s')\zeta(s')\zeta(s'+1)(\pi^2/\lambda)^{-s'}ds', \quad 1<\mathcal{R}s'<2$$

$$=\sum_{n=1}^{\infty}\frac{(-)^{n-1}}{n\,\mathrm{Sin}(n\pi^2/\lambda)}.$$

The above functional relation can be easily derived from the well known functional relation mentioned at the end of § 2.

References

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2) A. Wasserman, T.J. Buckholtz and H.E. Dewitt: Journ. Math. Phys. 11 (1970), 477.
3) A. Erdélyi: Tables of Integral Transforms, vol. 1, New York, 1954, p. 308, (3).
4) Ibidem: p. 316, (24).
5) Ibidem: p. 312, (7).
6) Ibidem: p. 315, (15).
7) Ibidem: p. 323, (2).