**Chapter 11S**
**Poisson summation formula**
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Poisson summation formula
Fourier series
Convolution
Random walk
Diffusion
Magnetization
Gaussian distribution function

## 11S.1 Poisson summataion formula

For appropriate functions $f(x)$, the Poisson summation formula may be stated as

$$\sum_{n=-\infty}^{\infty} f(x=n) = \sqrt{2\pi} \sum_{m=-\infty}^{\infty} F(k=m), \qquad (1)$$

where $m$ and $n$ are integers, and $F(k)$ is the Fourier transform of $f(x)$ and is defined by

$$F(k) = \mathbf{F}[f(x)] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ikx} f(x) dx .$$

Note that the inverse Fourier transform is given by

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ikx} F(k) dk .$$

The factor of the right hand side of Eq.(1) arises from the definition of the Fourier transform.

((**Proof**)) The proof of Eq.(1) is given as follows.

$$\sum_{n=-\infty}^{\infty} f(x=n) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(k) dk \sum_{n=-\infty}^{\infty} e^{ikn}$$

We evaluate the factor

$$I = \sum_{n=-\infty}^{\infty} e^{ikn} .$$

It is evident that *I* is not equal to zero only when $k = 2\pi m$ (*m*; integer). Therefore *I* can be expressed by

$$I = A\sum_{m=-\infty}^{\infty} \delta(k - 2\pi m) ,$$

where *A* is the normalization factor. Then

$$\begin{aligned}
\sum_{n=-\infty}^{\infty} f(x=n) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(k)dk[A\sum_{m=-\infty}^{\infty}\delta(k-2\pi m)] \\
&= \frac{A}{\sqrt{2\pi}} \sum_{m=-\infty}^{\infty} \int_{-\infty}^{\infty} F(k)\delta(k-2\pi m)dk \\
&= \frac{A}{\sqrt{2\pi}} \sum_{m=-\infty}^{\infty} F(k=2\pi m) \\
&= \frac{A}{\sqrt{2\pi}} \sum_{n=-\infty}^{\infty} F(k=2\pi n)
\end{aligned}$$

The normalization factor, *A*, is readily shown to be $2\pi$ by considering the symmetrical case

$$f(x=n) = e^{-\pi n^2} ,$$

$$F(k=2\pi n) = \frac{1}{\sqrt{2\pi}} e^{-\pi n^2}$$

---

((**Mathematica**))

```
f[x_] = Exp[-π x^2];
FourierTransform[f[x], x, k,
 FourierParameters → {0, -1}]
```

$$\frac{e^{-\frac{k^2}{4\pi}}}{\sqrt{2\pi}}$$

---

Since

$$A = \frac{\sqrt{2\pi}\, f(x=n)}{F(k=2\pi m)} = 2\pi\ .$$

or

$$I = \sum_{n=-\infty}^{\infty} e^{ikn} = 2\pi \sum_{m=-\infty}^{\infty} \delta(k-2\pi m)\ . \qquad (2)$$

Using this formula, we have

$$\sum_{n=-\infty}^{\infty} f(x=n) = \sqrt{2\pi} \sum_{n=-\infty}^{\infty} F(k=2\pi n). \qquad \text{(Poisson sum formula)}$$

## 11S.2 Summary

When we put $k = 2\pi x$ in $I$ of Eq.(2)

$$\begin{aligned}\sum_{n=-\infty}^{\infty} e^{2\pi i x n} &= 2\pi \sum_{m=-\infty}^{\infty} \delta(2\pi x - 2\pi m) \\ &= \frac{2\pi}{2\pi} \sum_{m=-\infty}^{\infty} \delta(x-m) \\ &= \sum_{m=-\infty}^{\infty} \delta(x-m)\end{aligned}$$

or

$$\sum_{n=-\infty}^{\infty} e^{2\pi i x n} = \sum_{m=-\infty}^{\infty} \delta(x-m). \tag{3}$$

## 11S.3. Convolution of Dirac comb: another method in the derivation of Poisson sum formula

The convolution of functions *f*(*x*) and *g*(*x*) is defined by

$$f * g = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x-\xi) g(\xi) d\xi = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(\xi) g(x-\xi) d\xi$$

The Fourier transform of the convolution is given by

$$\mathbf{F}[f * g] = \mathbf{F}[f]\mathbf{F}[g].$$

Here we assume that

$$g(x) = \sum_{n=-\infty}^{\infty} \delta(x-na). \qquad \text{(Dirac comb)}$$

The Fourier transform of *g*(*x*) is

$$G(k) = \mathbf{F}[g(x)] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ikx} \sum_{n=-\infty}^{\infty} \delta(x-na) dx = \frac{1}{\sqrt{2\pi}} \sum_{n=-\infty}^{\infty} e^{-ikna}.$$

The convolution *f***g* is obtained as

$$f * g = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x-\xi) \sum_{n=-\infty}^{\infty} \delta(\xi-na) d\xi = \frac{1}{\sqrt{2\pi}} \sum_{n=-\infty}^{\infty} f(x-na). \tag{4}$$

The Fourier transform of the convolution is

$$\mathbf{F}[f * g] = F(k)G(k) = \frac{1}{\sqrt{2\pi}} F(k) \sum_{n=-\infty}^{\infty} e^{-ikna}.$$

We use the Poisson summation formula;

$$\sum_{n=-\infty}^{\infty} e^{-ikna} = \sum_{n=-\infty}^{\infty} e^{ikna} = \sum_{m=-\infty}^{\infty} \delta(\frac{ka}{2\pi} - m)$$
$$= \sum_{m=-\infty}^{\infty} \delta[\frac{a}{2\pi}(k - \frac{2\pi m}{a})]$$
$$= \frac{2\pi}{a} \sum_{m=-\infty}^{\infty} \delta(k - \frac{2\pi m}{a})$$

where

$$\sum_{n=-\infty}^{\infty} e^{2\pi i x n} = \sum_{m=-\infty}^{\infty} \delta(x - m) .$$

with $x = \frac{ka}{2\pi}$. Then we get

$$\mathbf{F}[f * g] = \frac{1}{\sqrt{2\pi}} F(k) \sum_{n=-\infty}^{\infty} e^{-ikna} = \frac{1}{\sqrt{2\pi}} F(k) \sum_{n=-\infty}^{\infty} e^{ikna}$$
$$= \frac{1}{\sqrt{2\pi}} \frac{2\pi}{a} \sum_{m=-\infty}^{\infty} \delta(k - \frac{2\pi m}{a}) F(k)$$
$$= \frac{1}{\sqrt{2\pi}} \frac{2\pi}{a} \sum_{m=-\infty}^{\infty} \delta(k - \frac{2\pi m}{a}) F(k = \frac{2\pi m}{a})$$

The inverse Fourier transform of $\mathbf{F}[f * g]$ is obtained as

$$f * g = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathbf{F}[f * g] e^{ikx} dk = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ikx} dk \frac{1}{\sqrt{2\pi}} \frac{2\pi}{a} \sum_{m=-\infty}^{\infty} \delta(k - \frac{2\pi m}{a}) F(k = \frac{2\pi m}{a})$$
$$= \frac{1}{a} \sum_{m=-\infty}^{\infty} F(k = \frac{2\pi}{a} m) \int_{-\infty}^{\infty} e^{ikx} dk \delta(k - \frac{2\pi m}{a})$$
$$= \frac{1}{a} \sum_{m=-\infty}^{\infty} F(k = \frac{2\pi}{a} m) e^{i \frac{2\pi m}{a} x}$$

where

$$F(k=\frac{2\pi}{a}m)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}e^{-i\frac{2\pi}{a}mx}f(x)dx\,.$$

Finally we get

$$f*g=\frac{1}{\sqrt{2\pi}}\sum_{n=-\infty}^{\infty}f(x-na)=\frac{1}{a}\sum_{m=-\infty}^{\infty}F(k=\frac{2\pi m}{a})e^{i\frac{2\pi m}{a}x}\,. \qquad (5)$$

or

$$\sum_{n=-\infty}^{\infty}f(x-na)=\frac{\sqrt{2\pi}}{a}\sum_{m=-\infty}^{\infty}F(k=\frac{2\pi m}{a})e^{i\frac{2\pi m}{a}x}\,.$$

When $a = 1$, we get

$$\sum_{n=-\infty}^{\infty}f(x-n)=\sqrt{2\pi}\sum_{m=-\infty}^{\infty}F(k=2\pi m)e^{i2\pi mx}\,. \qquad (6)$$

When $x = 0$,

$$\sum_{n=-\infty}^{\infty}f(x=n)=\sqrt{2\pi}\sum_{m=-\infty}^{\infty}F(k=2\pi m)\,. \qquad (7)$$

This is the Poisson sum formula.

## 11S.3 Fourier transform of periodic function

We consider a periodic function $N(x)$;

$$N(x+a)=N(x)\,,$$

where $a$ is the periodicity. The function $N(x)$ can be described by

$$N(x)=\sum_{n=-\infty}^{\infty}f(x-na)=\frac{\sqrt{2\pi}}{a}\sum_{m=-\infty}^{\infty}F(k=\frac{2\pi m}{a})e^{i\frac{2\pi m}{a}x}$$
$$=\sum_{G}N_G e^{iGx}$$

Note that $f(x)$ is defined only in the limited region (for example, $-a/2 \le x \le a/2$). $G$ is the reciprocal lattice defined by

$$G = \frac{2\pi}{a} m .$$

The Fourier coefficient $N_G$ is given by

$$\begin{aligned} N_G &= \frac{\sqrt{2\pi}}{a} F(k = G) \\ &= \frac{1}{a} \int_{-\infty}^{\infty} e^{-iGx} f(x) dx = \frac{1}{a} \int_{-a/2}^{a/2} e^{-iGx} f(x) dx \end{aligned} .$$

where $f(x)$ is just like a Gaussian distribution function around $x = 0$.

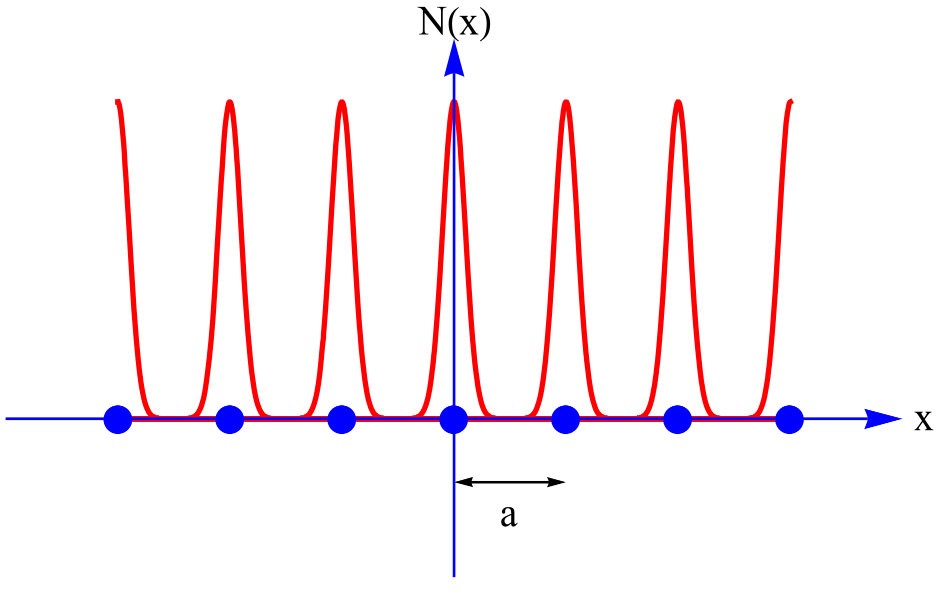



Fig. Plot of $N(x)$ as a function of $x$. $a$ is the lattice constant of the one-dimensional chain.

((**Example**))

Suppose that $f(x)$ is given by a Gaussian distribution,

$$f(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp(-\frac{x^2}{2\sigma^2}) .$$

Then we get

$$N_G = \frac{1}{a} \int_{-a/2}^{a/2} e^{-iGx} f(x) dx = \frac{1}{2} \exp(-\frac{1}{2} G^2 \sigma^2)[erf(\frac{1-2iG\sigma^2}{2\sqrt{2}\sigma}) + erf(\frac{1+2iG\sigma^2}{2\sqrt{2}\sigma})] ,$$

where erf($x$) is the error function and is defined by

$$erf(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-t^2} dt$$

Figure shows the intensity $|N_G|^2$ vs $n$, where $G = \frac{2\pi}{a} n$ .

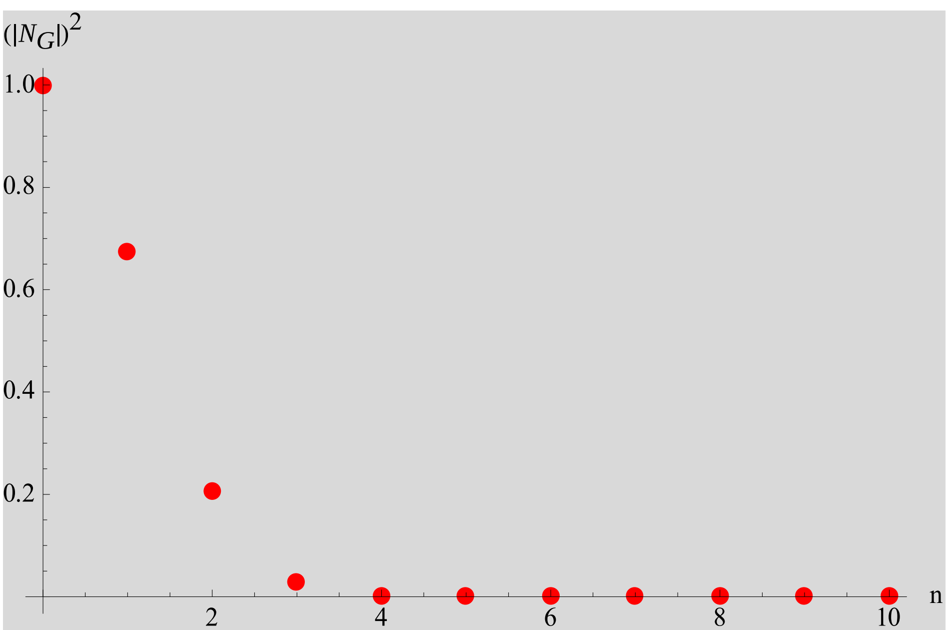



Fig. $a = 1$. $\sigma = 0.1$. $G = \frac{2\pi}{a} n$. The intensity $|N_G|^2$ vs $n$ (= integer).

## 11S.10 Fourier series

Suppose that the function $N(x)$ is a periodic function of $x$ with the periodicity $a$. Then we have

$$N(x) = \sum_{n=-\infty}^{\infty} f(x - na) = \frac{\sqrt{2\pi}}{a}\sum_{m=-\infty}^{\infty} F(k = \frac{2\pi m}{a})e^{i\frac{2\pi m}{a}x}$$
$$= \sum_G N_G e^{iGx}$$

where $G = \frac{2\pi}{a}m$ ($m$: integer).

((**Example-1**))

$f(x) = x$ for $|x|<a/2$, with $a = 2$

$$F(k = G = \pi n) = \frac{1}{\sqrt{2\pi}}\int_{-1}^{1} x\exp(-i\pi n x)dx = \frac{2i(-1)^n}{n\pi\sqrt{2\pi}} \qquad \text{for } n \neq 0.$$

$$F(k = G = 0) = \frac{1}{\sqrt{2\pi}}\int_{-1}^{1} xdx = 0 \qquad \text{for } n = 0.$$

$$N(x) = \frac{1}{\pi}\sum_{n=-\infty}^{\infty}\frac{i(-1)^n}{n}e^{i\pi n x} = \frac{1}{\pi}\sum_{\substack{n=-\infty \\ n\neq 0}}^{\infty}\frac{i(-1)^n}{n}e^{i\pi n x}$$

We make a plot of $N(x)$ as a function of x for the summation for $n = -n_{max}$ and $n_{max}$ with $n_{max} = 50$.

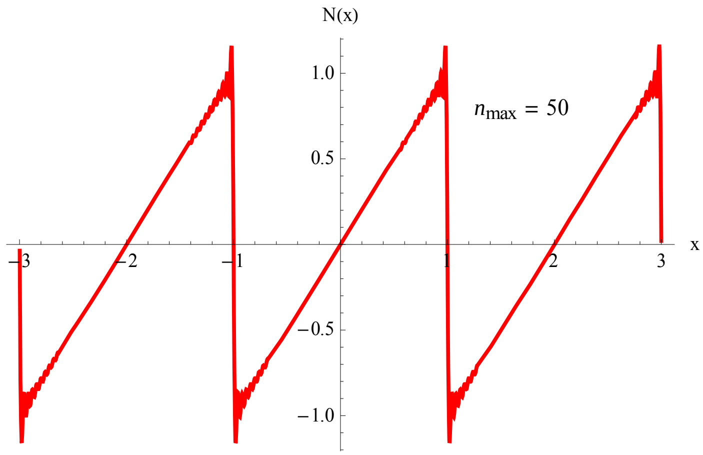



Fig. $n_{max}$ = 50. The Gibbs phenomenon is clearly seen.

((**Example-2**))

$f(x) = 0$ for $-1<x<0$ and 1 for $0<x<1$. $a = 2$

$$F(k=G=\pi n)=\frac{1}{\sqrt{2\pi}}\int_0^1 \exp(-i\pi nx)dx=-\frac{i(-1)^n[-1+(-1)^n]}{n\pi\sqrt{2\pi}} \qquad \text{for } n\neq 0.$$

$$F(k=G=0)=\frac{1}{\sqrt{2\pi}}\int_0^1 dx=\frac{1}{\sqrt{2\pi}}, \qquad \text{for } n=0.$$

$$N(x)=\frac{1}{2}-\frac{1}{\pi}\sum_{\substack{n=-\infty \\ n\neq 0}}^{\infty}\frac{i(-1)^n[-1+(-1)^n]}{2n}e^{i\pi nx}$$

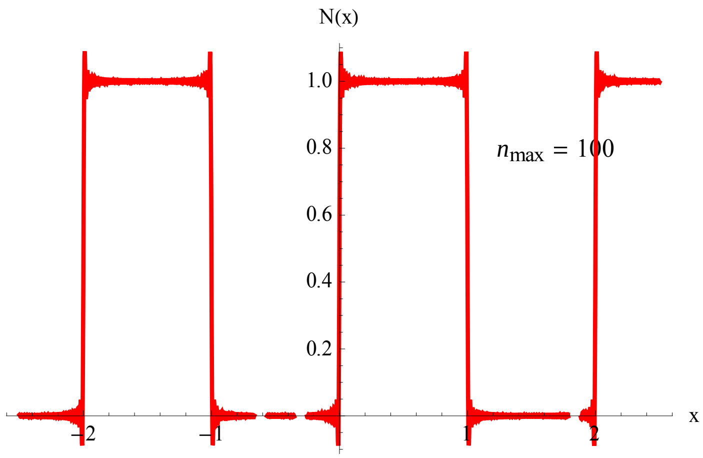



Fig. $n_{max}$ = 100. The Gibbs phenomenon is clearly seen.

## 11S.11 Fourier transform of function having values at inetger x-value

We consider a function defined by

$$f(x) = \sum_{m=-\infty}^{\infty} f(m)\delta(x-m). \qquad (8)$$

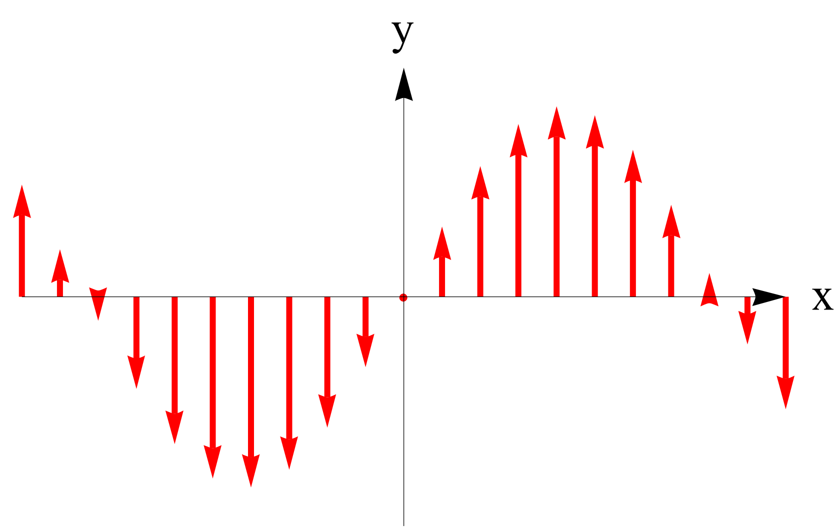



Fig. Plot of $f(x)$ which is described by a combination of the Dirac delta function with $f(m)$ at $x = m$.

The Fourier transform of $f(x)$ is given by

$$
\begin{aligned}
F(k) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} dx \\
&= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \sum_{m=-\infty}^{\infty} f(m)\delta(x-m) e^{-ikx} dx \\
&= \frac{1}{\sqrt{2\pi}} \sum_{m=-\infty}^{\infty} f(m) \int_{-\infty}^{\infty} \delta(x-m) e^{-ikx} dx \\
&= \frac{1}{\sqrt{2\pi}} \sum_{m=-\infty}^{\infty} e^{-ikm} f(m)
\end{aligned}
$$

We note that

$$
F(k+2\pi) = \frac{1}{\sqrt{2\pi}} \sum_{m=-\infty}^{\infty} e^{-i(k+2\pi)m} f(m) = \frac{1}{\sqrt{2\pi}} \sum_{m=-\infty}^{\infty} e^{-ikm} f(m) = F(k),
$$

In other words, $F(k)$ is a periodic function of $k$ with a periodicity $2\pi$. We can also show that

$$
f(m) = \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} F(k) e^{ikm} dk, \qquad (9)
$$

where

$$
\int_{-\pi}^{\pi} e^{ik(m-m')} dk = 2\pi\delta_{m,m'}, \qquad (10)
$$

since

$$
\begin{aligned}
\frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} F(k) e^{ikm} dk &= \frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{2\pi}} \sum_{m'=-\infty}^{\infty} f(m') \int_{-\pi}^{\pi} e^{ik(m-m')} dk \\
&= \frac{1}{2\pi} \sum_{m'=-\infty}^{\infty} f(m') 2\pi\delta_{m,m'} \\
&= f(m)
\end{aligned}
$$

Note that the inverse Fourier transform of $F(k)$ is obtained as

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(k) e^{ikx} dk = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk e^{ikx} \frac{1}{\sqrt{2\pi}} \sum_{m=-\infty}^{\infty} e^{-ikm} f(m)$$

$$= \frac{1}{2\pi} \sum_{m=-\infty}^{\infty} f(m) \int_{-\infty}^{\infty} dk e^{ik(x-m)}$$

$$= \frac{1}{2\pi} \sum_{m=-\infty}^{\infty} f(m) 2\pi \delta(x-m)$$

$$= \sum_{m=-\infty}^{\infty} f(m) \delta(x-m)$$

((**Note**)) The proof where the Poisson summation formula is used.

We have another method for the derivation of Eq.(9):

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(k) e^{ikx} dk = \frac{1}{\sqrt{2\pi}} \sum_{n=-\infty}^{\infty} \int_{(2n-1)\pi}^{(2n+1)\pi} F(k) e^{ikx} dk$$

We put

$$k' = k - 2n\pi$$

Then we have

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(k) e^{ikx} dk = \frac{1}{\sqrt{2\pi}} \sum_{n=-\infty}^{\infty} \int_{-\pi}^{\pi} F(k'+2n\pi) e^{i(k'+2n\pi)x} dk'$$

$$= \sum_{n=-\infty}^{\infty} e^{i2\pi nx} \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} F(k') e^{ik'x} dk'$$

$$= \sum_{m=-\infty}^{\infty} \delta(x-m) \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} F(k) e^{ikx} dk$$

$$= \frac{1}{\sqrt{2\pi}} \sum_{m=-\infty}^{\infty} \delta(x-m) \int_{-\pi}^{\pi} F(k) e^{ikm} dk$$

$$= \sum_{m=-\infty}^{\infty} \delta(x-m) f(m)$$

Here we use the Poisson summation formula

$$\sum_{n=-\infty}^{\infty} e^{i2\pi xn} = \sum_{m=-\infty}^{\infty} \delta(x-m).$$

## 11S.11 Random walk in the one-dimensional chain

We consider the case when a particle moves on the one dimensional chain. The particle can be located only on a discrete position [$x = m$ ($m$; integer)]. the particle starts from the origin $x = 0$. The particle can move from x = m to $x = m+1$, or from $x = m$ to x = $m$-1 for each jump. We assume that the probability $W(m, N)$ such that the particle reaches at the position $x = m$ after jumps with $N$ times. The probability $W(m, N+1)$ can be described by

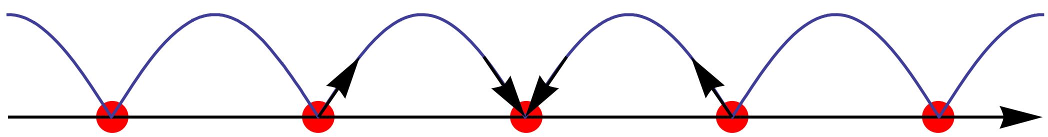



Fig. Random walk model.

$$W(m, N+1) = \frac{1}{2} W(m-1, N) + \frac{1}{2} W(m+1, N),$$

where one is a jump from $\boldsymbol{x} = m$-1 to $x = m$ for the ($N$+1)-th jump, and the another is a jump from $x = m$+1 to $x = m$ for the ($N$+1)-th jump. The probability for these jumps is 1/2.

In order to find the expression of $W(m, N)$ we define the Fourier transform

$$\Phi(k, N) = \frac{1}{\sqrt{2\pi}} \sum_{m=-\infty}^{\infty} e^{-ikm} W(m, N).$$

Note that $\Phi(k, N)$ is a periodic function of $k$ with a periodicity $2\pi$, and

$$\begin{aligned} \frac{1}{\sqrt{2\pi}} \sum_{m=-\infty}^{\infty} e^{-ikm} W(m-1, N) &= \frac{1}{\sqrt{2\pi}} e^{-ik} \sum_{m=-\infty}^{\infty} e^{-ik(m-1)} W(m-1, N) \\ &= e^{-ik} \Phi(k, N) \end{aligned},$$

$$\frac{1}{\sqrt{2\pi}}\sum_{m=-\infty}^{\infty}e^{-ikm}W(m+1,N)=\frac{1}{\sqrt{2\pi}}e^{ik}\sum_{m=-\infty}^{\infty}e^{-ik(m+1)}W(m+1,N)$$
$$=e^{ik}\Phi(k,N)$$

Then we have

$$\Phi(k,N+1)=\frac{1}{\sqrt{2\pi}}\sum_{m=-\infty}^{\infty}e^{-ikm}W(m,N+1)$$
$$=\frac{1}{2}(e^{-ik}+e^{-ik})\Phi(k,N)$$
$$=(\cos k)\Phi(k,N)$$

or

$$\Phi(k,N)=(\cos k)^{N}\Phi(k,N=0)\,.$$

We use the initial condition that the particle is located at $x = 0$ at the probability of 1;

$$W(m,N=0)=\delta_{m,0}\,.$$

or

$$\Phi(k,N=0)=\frac{1}{\sqrt{2\pi}}\sum_{m=-\infty}^{\infty}e^{-ikm}W(m,N=0)=\frac{1}{\sqrt{2\pi}}\sum_{m=-\infty}^{\infty}e^{-ikm}\delta_{m,0}=\frac{1}{\sqrt{2\pi}}\,.$$

So we get

$$\Phi(k,N)=\frac{1}{\sqrt{2\pi}}(\cos k)^{N}\,.$$

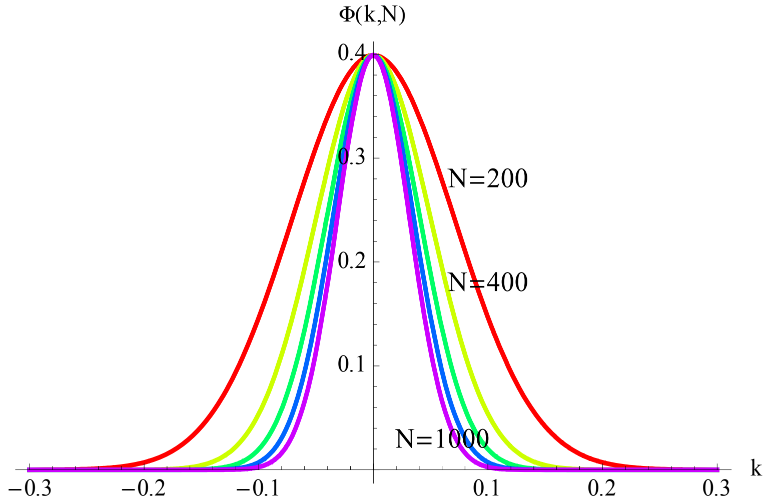



Fig. Plot of $\Phi(k,N)$ vs $k$, where $N$ = 200, 400, 600, 800, and 1000. In the large limit of N, $\Phi(k,N)$ approaches a Gaussian distribution.

The inverse Fourier transform of $\Phi(k,N)$ is

$$W(m,N) = \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} \Phi(k,N) e^{ikm} dk = \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} dk e^{ikm} \frac{1}{\sqrt{2\pi}} (\cos k)^N$$
$$= \frac{1}{2\pi} \int_{-\pi}^{\pi} dk e^{ikm} (\cos k)^N$$

Here we use the binomial theorem to get

$$(\cos k)^N = \left(\frac{1}{2}\right)^N (e^{ik} + e^{-ik})^N$$
$$= \left(\frac{1}{2}\right)^N \sum_{l=0}^{N} \frac{N!}{(N-l)!l!} e^{ik(2l-N)}$$

Then we have

$$
\begin{aligned}
W(m,N) &= \frac{1}{2\pi}\int_{-\pi}^{\pi} dke^{ikm}\left(\frac{1}{2}\right)^N \sum_{l=0}^{N}\frac{N!}{(N-l)!l!}e^{ik(2l-N)} \\
&= \left(\frac{1}{2}\right)^N \sum_{l=0}^{N}\frac{N!}{(N-l)!l!}\frac{1}{2\pi}\int_{-\pi}^{\pi} dke^{ik(m+2l-N)} \\
&= \left(\frac{1}{2}\right)^N \sum_{l=0}^{N}\frac{N!}{(N-l)!l!}\frac{1}{2\pi}(2\pi)\delta_{m+2l-N,0} \\
&= \left(\frac{1}{2}\right)^N \sum_{l=0}^{N}\frac{N!}{(N-l)!l!}\delta_{m+2l-N,0} \\
&= \left(\frac{1}{2}\right)^N \sum_{l=0}^{N}\frac{N!}{(N-l)!l!}\delta_{m+2l-N,0} \\
&= \frac{1}{2^N}\frac{N!}{(\frac{N+m}{2})!\left(\frac{N-m}{2}\right)!}
\end{aligned}
$$

where

$$
m = N - 2l, \qquad \text{or} \qquad l = \frac{N-m}{2}.
$$

This implies that for $N$ = even, $m$ should be even. In other words, $W(N = \text{even}, m = \text{odd}) = 0$. For $N$ = odd, $m$ should be odd. In other words, $W(N = \text{odd}, m = \text{even}) = 0$.

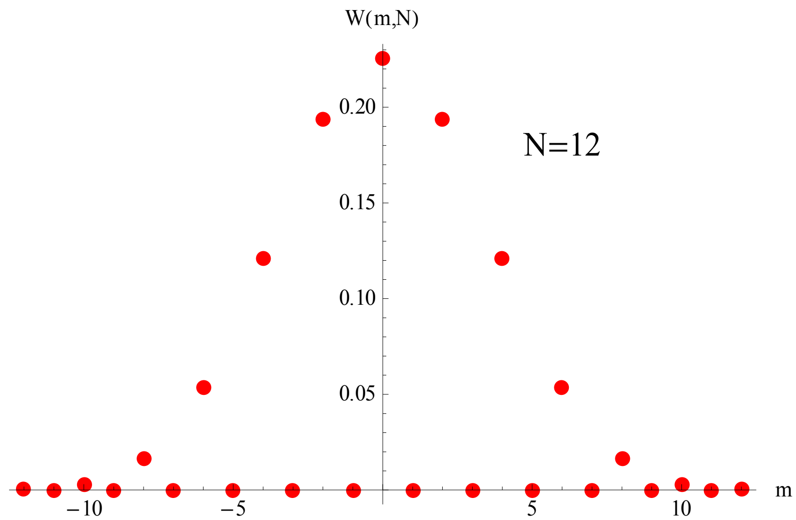
## 11S.13 Numerical calculation of *W*(*m, N*)

Using the Mathematica, we calculate numerically the value of $W(m,N)$ given by

$$
W(m,N) = \frac{1}{2\pi}\int_{-\pi}^{\pi} dke^{ikm}(\cos k)^N = \frac{1}{\pi}\int_{0}^{\pi} dk\cos(km)(\cos k)^N ,
$$

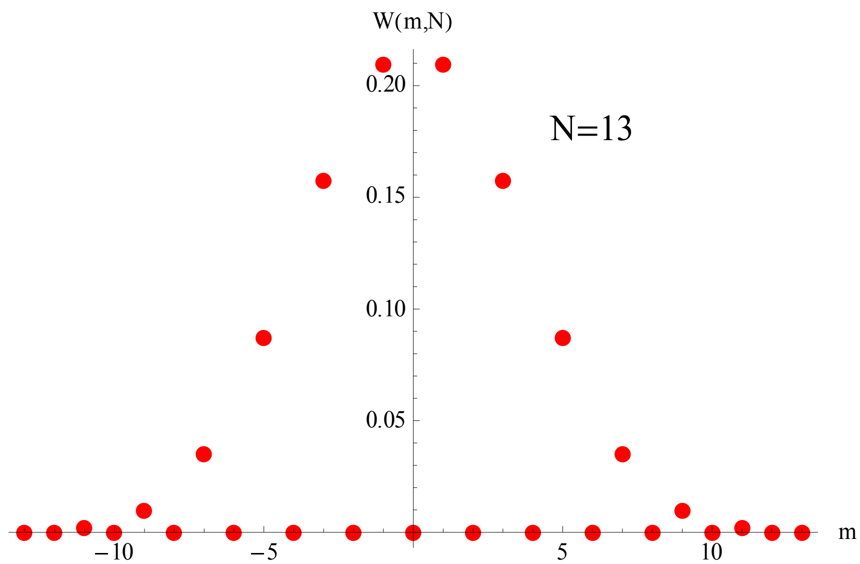
for the cases with $N = 12$ (even) and $N = 13$ (odd).

(i) $N = 12$.




This figure clearly shows that $W(m, N = 12) = 0$ for $m$ = -11, -9, -7, -5, -3, -1, 1, 3, 5, 7, 9, and 11 ($m$ = odd).

(ii) $N = 13$.



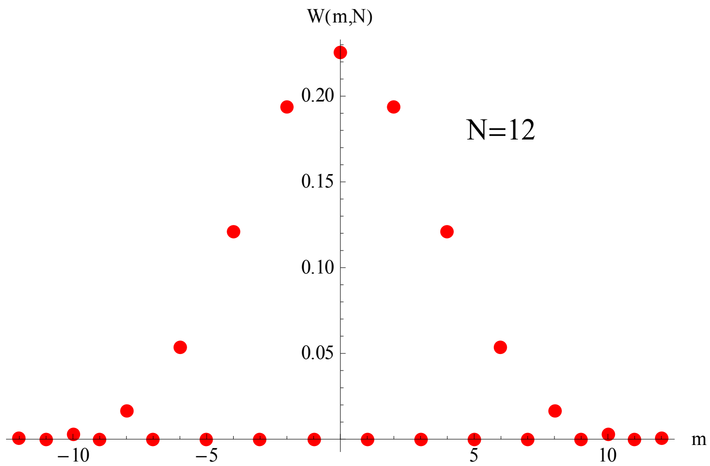

This figure clearly shows that $W(m, N = 13) = 0$ for $m$ = -12, -10, -8, -6, -4, -2, 0, 2, 4, 6, 8, 10, and 12 ($m$ = even).

((**Mathematica**))

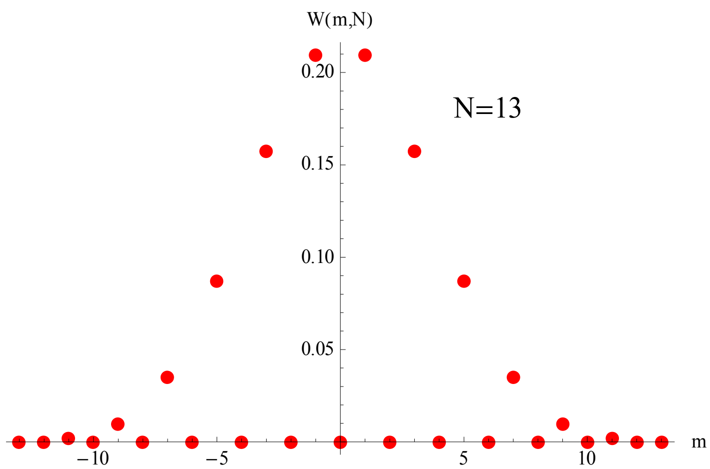
```
Clear["Gobal`"];

J1[m_, N1_] := 1/π ∫_0^π Cos[k m] Cos[k]^N1 ⅆk

d12 = Table[{m, J1[m, 12]}, {m, -12, 12, 1}];
f1 = ListPlot[d12, PlotStyle → {Red, PointSize[0.02]}, AxesLabel → {"m", "W(m,N)"}];
f2 = Graphics[{Text[Style["N=12", Black, 15], {6, 0.18}]}];
Show[f1, f2]
```




```
d13 = Table[{m, J1[m, 13]}, {m, -13, 13, 1}];
g1 = ListPlot[d13, PlotStyle → {Red, PointSize[0.02]}, AxesLabel → {"m", "W(m,N)"}];
g2 = Graphics[{Text[Style["N=13", Black, 15], {6, 0.18}]}];
Show[g1, g2]
```




## 11S.14 Limit of long distance and long time

Using the Stirling's formula,

$$\ln(x!) = \frac{1}{2}\ln(2\pi) + (x + \frac{1}{2})\ln(x) - x \qquad \text{for large } x,$$

and the Mathematica, we have the series expansion to the order of $(m/N)^8$,

$$\begin{aligned}
\ln W(m,N) &= -N\ln(2) + \ln(N!) - \ln(\frac{N+m}{2})! - \ln(\frac{N-m}{2})! \\
&\approx -\frac{1}{2}\ln(\frac{\pi N}{2}) + \frac{1}{2}(1-N)\left(\frac{m}{N}\right)^2 + \frac{1}{12}(3-N)\left(\frac{m}{N}\right)^4 \\
&\quad + \frac{1}{30}(5-N)\left(\frac{m}{N}\right)^6 + \frac{1}{56}(7-N)\left(\frac{m}{N}\right)^8 + \ldots \\
&\approx -\frac{1}{2}\ln(\frac{\pi N}{2}) - \frac{1}{2}\frac{m^2}{N}
\end{aligned}$$

or

$$\begin{aligned}
W(m,N) &= \exp[-\frac{1}{2}\ln(\frac{\pi N}{2}) - \frac{1}{2}\frac{m^2}{N}] \\
&= \exp[\ln(\frac{\pi N}{2})^{-\frac{1}{2}} - \frac{1}{2}\frac{m^2}{N}] \\
&= (\frac{\pi N}{2})^{-\frac{1}{2}} \exp(-\frac{1}{2}\frac{m^2}{N}) \\
&= \left(\frac{2}{\pi N}\right)^{\frac{1}{2}} \exp(-\frac{1}{2}\frac{m^2}{N})
\end{aligned}$$

((**Mathematica**))

```
Clear["Gobal`"];

f1[x_] := 1/2 Log[2 π] + (x + 1/2) Log[x] - x;

g1 = -N Log[2] + f1[N] - f1[(N + m)/2] - f1[(N - m)/2];

rule1 = {m → N x};

g11 = g1 /. rule1; Series[g11, {x, 0, 8}] // Simplify //
 Normal
```

$$\frac{1}{2}(1-N)x^2+\frac{1}{12}(3-N)x^4+\frac{1}{30}(5-N)x^6+\frac{1}{56}(7-N)x^8-\frac{1}{2}\mathrm{Log}\left[\frac{N\pi}{2}\right]$$

## 11S.15 Diffusion

We assume that the distance between the nearest neighbor lattices is $\Delta x$ and the time taken for each jump is $\Delta t$. Then we have

$$t = N\Delta t, \qquad x = m\Delta x.$$

The probability of finding particle between $x$ and $x + dx$ is

$$P(x,t)dx = W\left(\frac{x}{\Delta x},\frac{t}{\Delta t}\right)\frac{dx}{2\Delta x} = dx\left(\frac{1}{4\frac{(\Delta x)^2}{2\Delta t}\pi t}\right)^{\frac{1}{2}}\exp\left(-\frac{1}{4t}\frac{x^2}{\frac{(\Delta x)^2}{2\Delta t}}\right)$$

$$= dx\frac{1}{\sqrt{4D\pi t}}\exp\left(-\frac{x^2}{4Dt}\right)$$

where $D$ is the diffusion constant and is defined by

$$D = \frac{(\Delta x)^2}{2\Delta t}.$$

Here we note that the factor $2\Delta x$ of the $W(\frac{x}{\Delta x},\frac{t}{\Delta t})\frac{dx}{2\Delta x}$ arises from the fact that (i) for every jump ($N$ = even), the probability of finding the particle at the sites with even $m$ is zero, and that (ii) for every jump ($N$ = odd), the probability of finding the particle at the sites with odd $m$ is zero. The distance for the jump is $2\Delta x$, but not $\Delta x$.

The final form of $P(x, t)$ is obtained as

$$P(x,t)=\frac{1}{\sqrt{4D\pi t}}\exp(-\frac{x^2}{4Dt}).$$

We note that $P(x, t)$ satisfies the diffusion equation given by

$$\frac{\partial P(x,t)}{\partial t}=D\frac{\partial^2 P(x,t)}{\partial x^2},$$

with the initial condition

$$P(x,t=0)=\delta(x).$$

## 11.S16 Gaussian distribution in magnetization; analogy of random walk

We consider a system consisting of $N$ independent spins. Each spin has a magnetic moment $\mu$. In the absence of an external magnetic field, each spin has the magnetic moment ($\pm\mu$) along the z axis. We assume that the number of spins having the $z$ component magnetic moment ($+\mu$) is $N_\uparrow$ and the number of spins having the $z$-component magnetic moment ($-\mu$):

$$N_\uparrow=\frac{1}{2}(N+n), \qquad N_\downarrow=\frac{1}{2}(N-n)$$

where

$$N=N_\uparrow+N_\downarrow.$$

Here we discuss the probability distribution of total magnetic moment, $M$, which is given by

$$M = \mu(N_\uparrow - N_\downarrow) = n\mu \ .$$

The probability that the total magnetization has $M = n\mu$ is obtained as

$$W(M) = \frac{1}{2^N}\frac{N!}{N_\uparrow!N_\downarrow!} = \frac{1}{2^N}\frac{N!}{[\frac{1}{2}(N+n)]![(\frac{1}{2}(N-n)]!}$$

Using the Stirling's formula, we have

$$\ln W(M) = -\frac{1}{2}\ln(\frac{\pi N}{2}) - \frac{n^2}{2N}$$

for $n<<N$. Then we get the probability as

$$W(M) = (\frac{2}{\pi N})^{1/2}\exp(-\frac{n^2}{2N}).$$

where $M = \mu n$. The average of magnetization is equal to zero.

$$< M >= \mu < n >= \mu \int_{-\infty}^{\infty} nW(M)dn = 0 \ .$$

Since

$$< M^2 >= \mu^2 < n >= \mu^2 \int_{-\infty}^{\infty} n^2 W(M)dn = 2\mu^2 N \ ,$$

the standard deviation is obtained as

$$\Delta M = \sqrt{< M^2 > - < M >^2} = \sqrt{2N}\mu \ .$$

Since

$$\frac{\Delta M}{2N\mu} = \frac{\sqrt{2N}}{2N} = \frac{1}{\sqrt{2N}}$$

the relative width of the Gaussian distribution becomes sharp as $N$ increases. We make a plot of $W(M = n\mu)$ as a function of $N$, where $N = 100$.

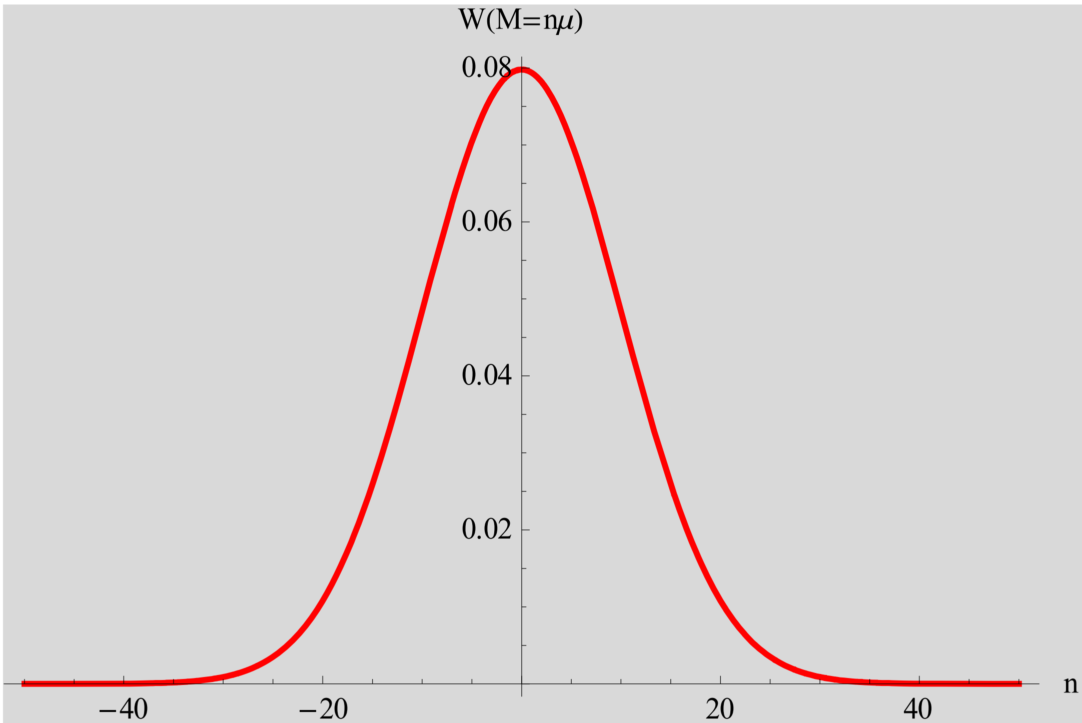



Fig. Plot of $W(M)$ vs $n$. $M = 2\mu n$. $N = 100$.

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K. Kitahara, Nonequilibrium Statistical Physics, 2nd edition (Iwanami, Tokyo, 1998). [in Japanese].

R. Reif, Statistical Thermal Physics, McGraw-Hill, New York, 1965).

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