Density of States and Partition function: Laplace transform

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(Date: September 08, 2018)

1. Laplace transformation

The partition function of a system is given by

$$Z(\beta) = \int_0^\infty dE\, e^{-\beta E}\Omega(E) \qquad \text{(Laplace transformation)}$$

The density of states satisfies the conditions

$$\Omega(\varepsilon) \geq 0, \qquad \lim_{E\to\infty} \Omega(E)e^{-\alpha E} = 0 \qquad (\alpha > 0)$$

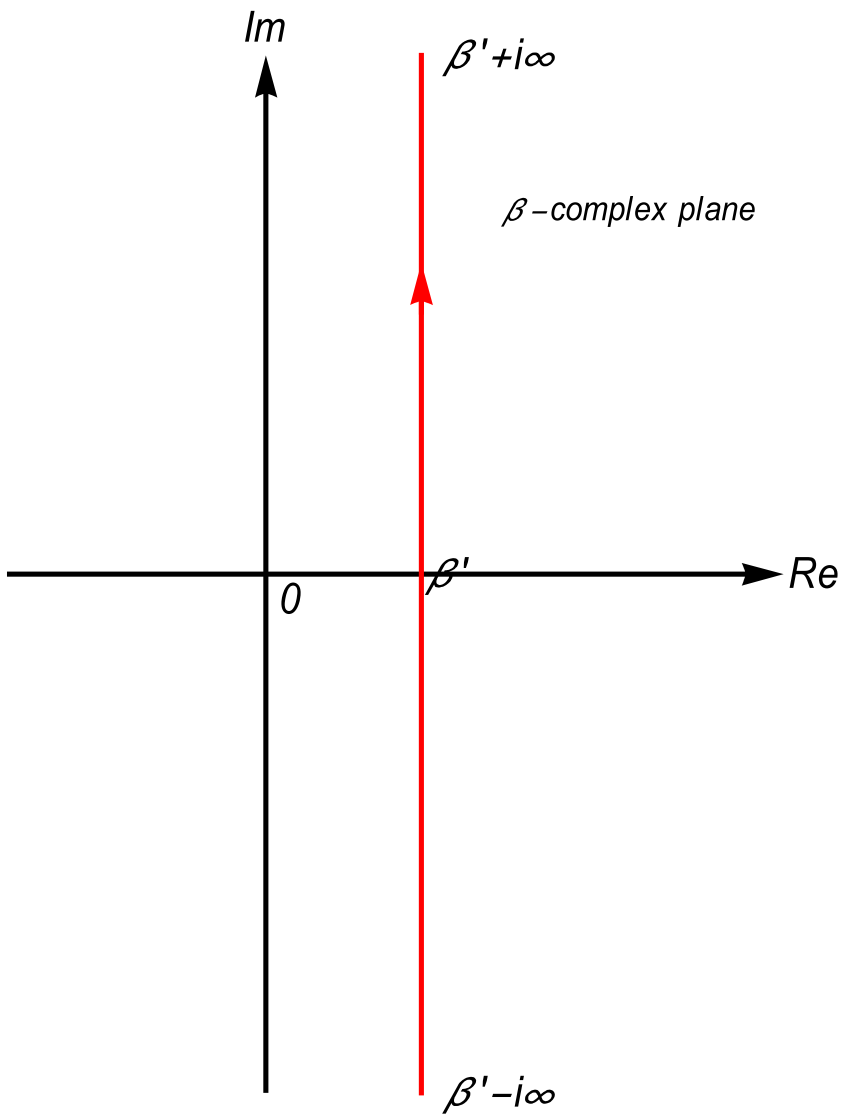
The inverse Laplace transform of the partition function is the number of energy levels per unit energy interval (density of states)

$$Z(\beta) = \sum_s e^{-\beta E_s}$$

The inverse Laplace transform $\Omega(\varepsilon)$ is, by definition,

$$\Omega(E) = \frac{1}{2\pi i}\int_{\beta'-i\infty}^{\beta'+i\infty} d\beta\, e^{\beta E} Z(\beta)$$

(Bromwich-Wagner integral)



Then we have

$$\Omega(E) = \frac{1}{2\pi i}\int_{\beta'-i\infty}^{\beta''+i\infty} d\beta\, e^{\beta E} Z(\beta)$$

$$= \sum_s \frac{1}{2\pi i}\int_{\beta'-i\infty}^{\beta''+i\infty} d\beta\, e^{\beta(E-E_s)}$$

For $\beta = \beta' + iy$ with $y = -\infty$ to ∞,

$$d\beta = i dy, \qquad (\beta' = 0)$$

$$\Omega(E)=\sum_s \frac{1}{2\pi}\int_{-\infty}^{\infty} dy\, e^{i(E-E_s)y}=\sum_s \delta(E-E_s)$$

in terms of the Dirac delta function. Thus $\Omega(E)$ is the density of states.

2. Entropy

One writes the integrand in the form

$$e^{-\beta E}\Omega(E)=\exp[\ln\Omega(E)-\beta E]$$

The exponent of the above expression is expanded in the neighborhood of E^* (let E^* be the value of E which maximizes the integrand)

$$\ln\Omega(E)-\beta E=\ln D(E^*)-\beta E^*+\frac{1}{1!}\left(E-E^*\right)\frac{\partial}{\partial E^*}[\ln\Omega(E^*)-\beta E^*]$$
$$+\frac{1}{2!}\left(E-E^*\right)^2\frac{\partial^2}{\partial E^{*2}}[\ln\Omega(E^*)-\beta E^*]$$

Noting that

$$\frac{\partial}{\partial E^*}\ln\Omega(E^*)=\beta\,,\qquad \frac{\partial^2}{\partial E^{*2}}\ln\Omega(E^*)<0\,,$$

we get

$$\ln\Omega(E)-\beta E=\ln\Omega(E^*)-\beta E^*+\frac{1}{2}\left(E-E^*\right)^2\frac{\partial^2}{\partial E^{*2}}\ln\Omega(E^*)\ .$$

where the linear term becomes zero.

$$\Omega(E)e^{-\beta E}=\Omega(E^*)e^{-\beta E^*}\exp[-\frac{1}{2\sigma_{E^*}^{\ 2}}\left(E-E^*\right)^2]$$

(Gaussian distribution ; mean E^* and standard deviation σ_{E^*})

Here we define

$$\frac{1}{\sigma_{E^*}{}^2} = -\frac{\partial^2}{\partial E^{*2}} \ln \Omega(E^*)$$

The partition function $Z(\beta)$ can be written as

$$\begin{aligned} Z_C(\beta) &= \int_0^\infty dE\, e^{-\beta\varepsilon} \Omega(E) \\ &= \Omega(E^*) e^{-\beta E^*} \int_{-\infty}^{\infty} dE \exp[-\frac{1}{2\sigma_{E^*}{}^2}\left(E - E^*\right)^2] \end{aligned}$$

or

$$Z_C(\beta) = \sqrt{2\pi}\sigma_{E^*}\Omega(E^*)\, e^{-\beta E^*}$$

The logarithm of $Z(\beta)$ can be written in the form

$$\ln Z(\beta) = \ln[\sqrt{2\pi}\sigma_{E^*}\Omega(E^*)] - \beta E^*$$

The Helmholtz free energy is

$$\begin{aligned} F &= U - ST \\ &= -k_B T \ln Z(\beta) \\ &= -k_B T \ln[\sqrt{2\pi}\sigma_{E^*}\Omega(E^*)] + E^* \\ &= U - k_B T \ln[\sqrt{2\pi}\sigma_{E^*}\Omega(E^*)] \end{aligned}$$

where $U = E$. Thus the entropy S is given by

$$S = k_B \ln[\sqrt{2\pi}\sigma_{E^*}\Omega(E^*)]$$

((**Note**))

$$\ln \Omega(E) - \beta E = \ln \Omega(E^*) - \beta E^* - \frac{1}{2\sigma_{E^*}{}^2}\left(E - E^*\right)^2$$

or

$$\Omega(E) = \Omega(E^*)e^{\beta(E-E^*)} \exp[-\frac{1}{2\sigma_{E^*}{}^2}\left(E - E^*\right)^2 \ ]$$

or

$$\frac{\Omega(E^*)e^{-\beta E^*}}{\Omega(E^*)e^{-\beta E^*}} = \exp[-\frac{1}{2\sigma_{E^*}{}^2}\left(E - E^*\right)^2 \ ]$$

which is a Gaussian distribution function with average energy E^* and fluctuation σ_{E^*}

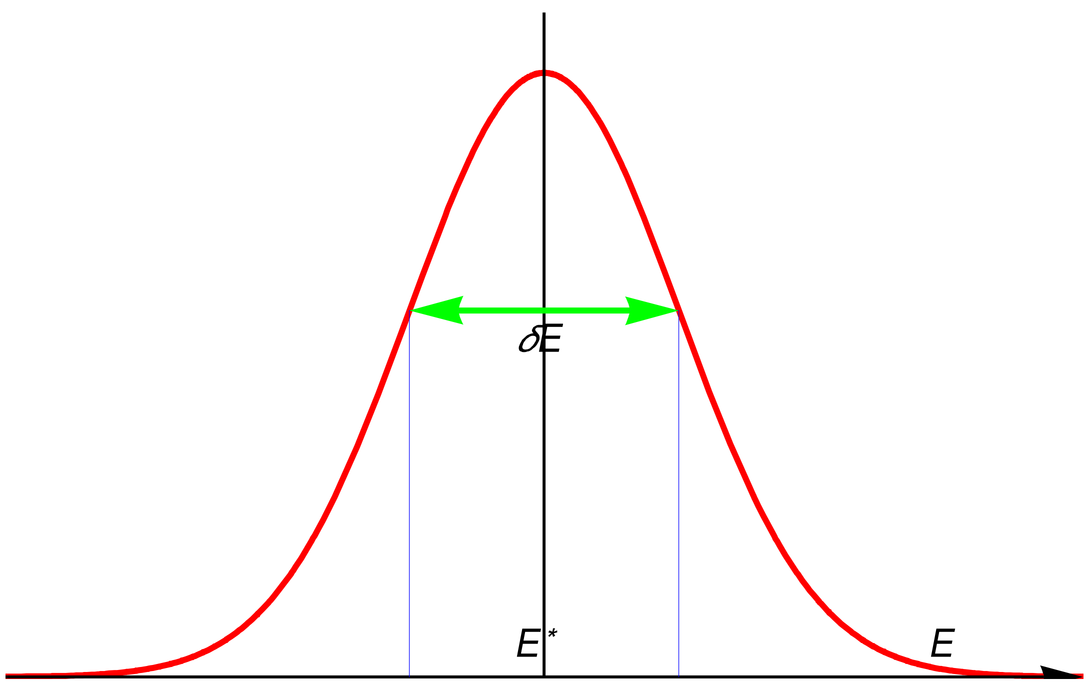


Fig. $\dfrac{\Omega(E^*)e^{-\beta E^*}}{\Omega(E^*)e^{-\beta E^*}}$ vs E. Gaussian distribution function with mean E^* and standard deviation δE

3. Convolution (Faltung) of the density of states

We consider the two kinds of partition functions,

$$Z_1(\beta) = \int_0^\infty d\varepsilon_1 e^{-\beta\varepsilon_1}\Omega_1(\varepsilon_1)\,,$$

$$Z_2(\beta) = \int_0^\infty d\varepsilon_2 e^{-\beta\varepsilon_2} \Omega_2(\varepsilon_2)$$

We calculate the product of these partition functions

$$Z_1(\beta)Z_1(\beta) = \int_0^\infty d\varepsilon_1 e^{-\beta\varepsilon_1} \Omega_1(\varepsilon_1) \int_0^\infty d\varepsilon_2 e^{-\beta\varepsilon_2} \Omega_2(\varepsilon_2)$$

$$= \int_0^\infty d\varepsilon_1 \int_0^\infty d\varepsilon_2 e^{-\beta(\varepsilon_1+\varepsilon_2)} \Omega_1(\varepsilon_1)\Omega_2(\varepsilon_2)$$

We introduce new variables;

$$\varepsilon_1 + \varepsilon_2 = \varepsilon, \qquad \varepsilon_1 = \varepsilon'$$

$$0 \le \varepsilon < \infty, \qquad 0 \le \varepsilon' \le \varepsilon$$

$$Z_1(\beta)Z_2(\beta) = \int_0^\infty d\varepsilon e^{-\beta\varepsilon} \int_0^\varepsilon d\varepsilon' \Omega_1(\varepsilon')\Omega_2(\varepsilon - \varepsilon') = \int_0^\infty d\varepsilon e^{-\beta\varepsilon} \Omega_1 * \Omega_2$$

Thus $Z_1(\beta)Z_2(\beta)$ is the Laplace transform of the convolution of the density of states

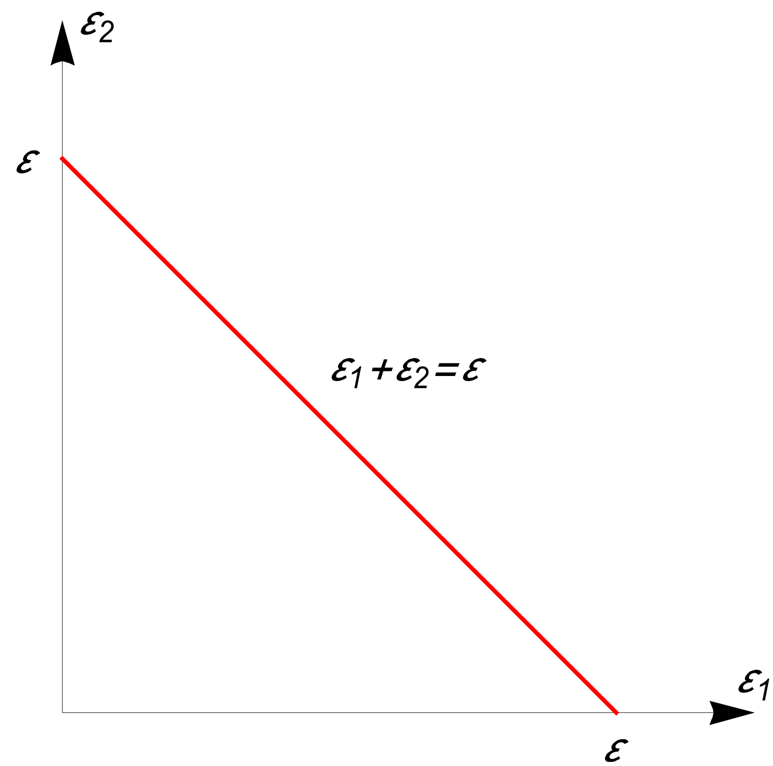
$$\Omega_1 * \Omega_2 = \int_0^\varepsilon d\varepsilon' \Omega_1(\varepsilon')\Omega_2(\varepsilon - \varepsilon').$$

or

$$Z_1(\beta)Z_1(\beta) = \int_0^\infty d\varepsilon e^{-\beta\varepsilon} \int_0^\varepsilon d\varepsilon' \Omega_1(\varepsilon')\Omega_2(\varepsilon - \varepsilon')$$

$$= \int_0^\infty d\varepsilon e^{-\beta\varepsilon} \int_0^\varepsilon d\varepsilon' \Omega_1(\varepsilon - \varepsilon')\Omega_2(\varepsilon')$$

$$= \int_0^\infty d\varepsilon e^{-\beta\varepsilon} \Omega_1 * \Omega_2$$



((**Note**))

$$\Omega_{12}(E)=\Omega_1*\Omega_2=\int_0^E dE'\Omega_1(E')\Omega_2(E-E') \qquad \text{(convolution)}$$

$$\begin{aligned}
Z_{1+2}(\beta)&=\int_0^\infty e^{-\beta E}\Omega_{12}(E)dE\\
&=\int_0^\infty dE e^{-\beta E}\int_0^E dE_1\Omega_1(E_1)\Omega_2(E-E_1)\\
&=\int_0^\infty dE_1\int_{E_1}^\infty dE e^{-\beta E}\Omega_1(E_1)\Omega_2(E-E_1)
\end{aligned}$$

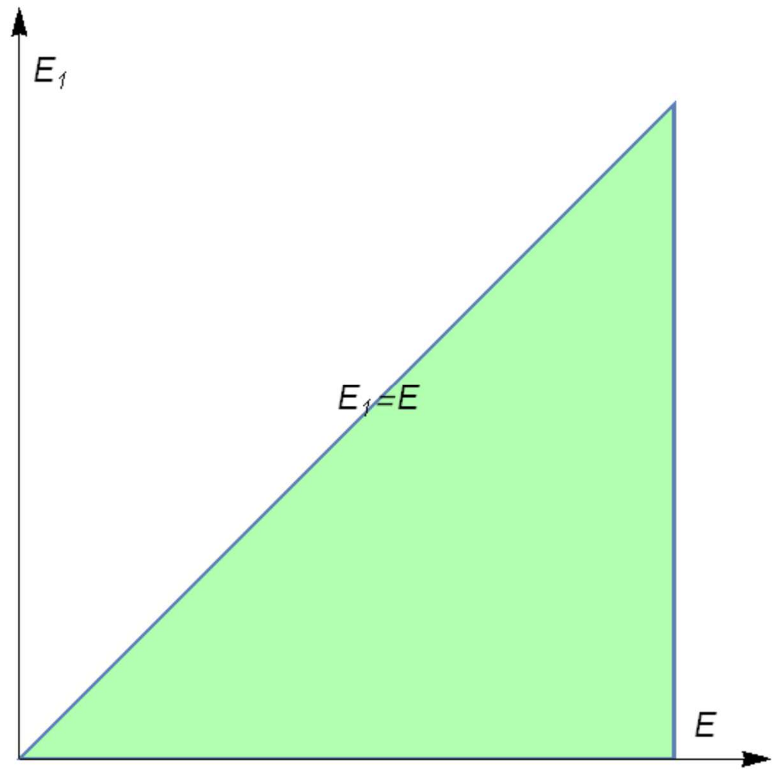


Fig. Region of integration. (a) $0 < E_1 < E$ for the integration over E_1. (b) $E_1 < E < \infty$

Here we put $E = E_1 + E_2$

$$Z_{1+2}(\beta) = \int_0^\infty e^{-\beta\varepsilon_1}\Omega_1(E_1)dE_1 \int_0^\infty dE_2 e^{-\beta E_2}\Omega_2(E_2) = Z_1(\beta)Z_2(\beta)$$

4. The method of steepest decent (saddle point method)

In calculating $\Omega(E)$, one writes the integrand in the form

$$e^{\beta E}Z(\beta) = \exp[\ln Z(\beta) + \beta E]$$

and chooses as integration path a straight line (from $\beta^* - i\infty$ to $\beta^* + i\infty$ in the β-complex plane, with β^* determined by

$$\frac{\partial}{\partial\beta^*}\ln Z(\beta^*) = - E$$

The exponent of the above expression is expanded in the neighborhood of β^*,

$$\ln Z(\beta) + \beta E = \ln Z(\beta^*) + \beta^* E + \left(\beta - \beta^*\right)[\frac{\partial}{\partial \beta^*} \ln Z(\beta^*) + E]$$

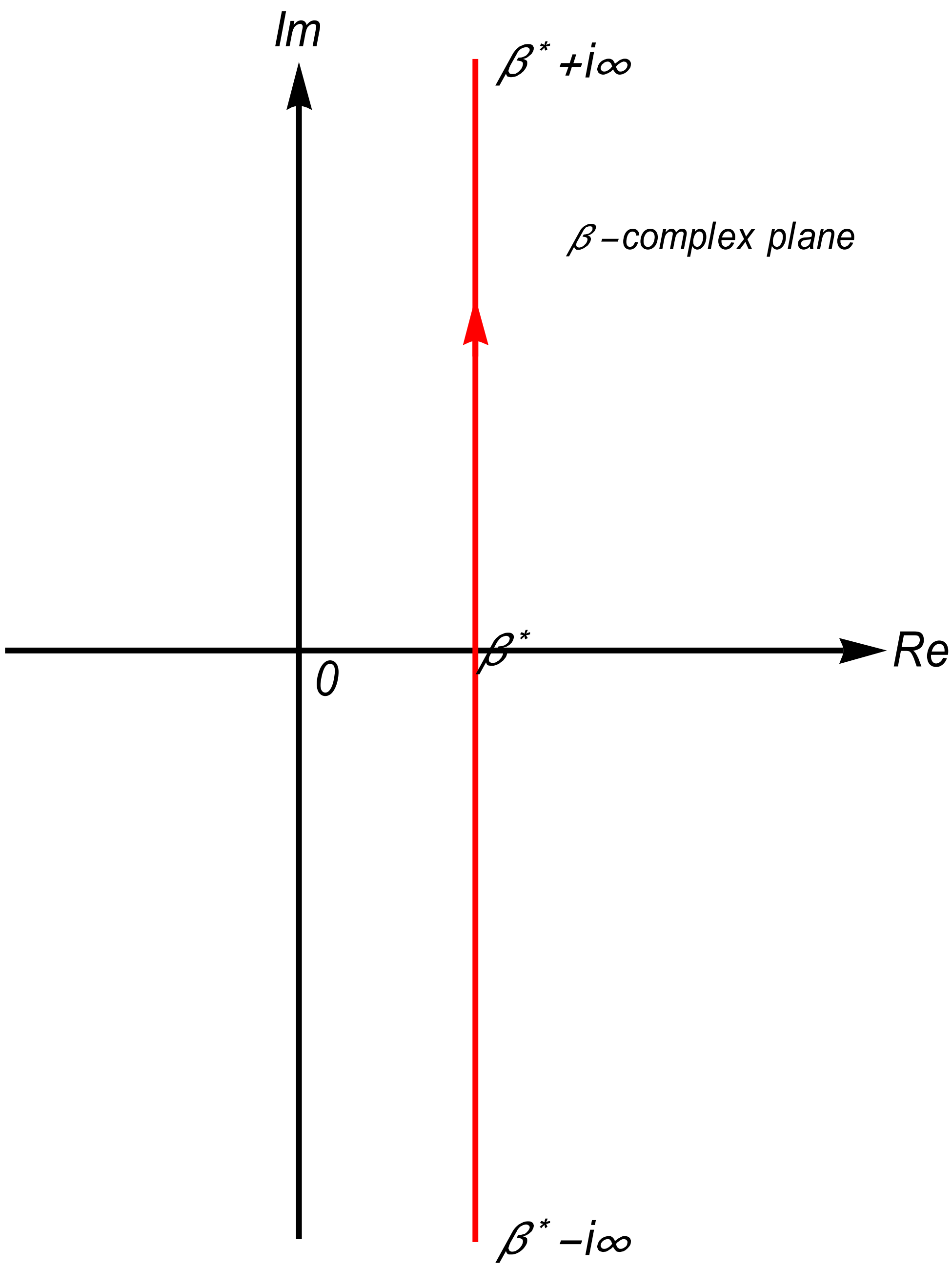
$$+ \frac{1}{2}\left(\beta - \beta^*\right)^2 [\frac{\partial^2}{\partial \beta^{*2}} \ln Z(\beta^*)] + ...$$

$$= \ln Z(\beta^*) + \beta^* E + \frac{1}{2}\left(\beta - \beta^*\right)^2 [\frac{\partial^2}{\partial \beta^{*2}} \ln Z(\beta^*)] + ...$$

Then the integral is approximated as

$$\Omega(E) = \frac{1}{2\pi i} \int_{\beta^* - i\infty}^{\beta^* + i\infty} d\beta \, e^{\beta E} Z(\beta)$$

$$= \frac{1}{2\pi i} \int_{\beta^* - i\infty}^{\beta^* + i\infty} d\beta \exp[\ln Z(\beta^*) + \beta^* E] \exp[\frac{1}{2}\left(\beta - \beta^*\right)^2 [\frac{\partial^2}{\partial \beta^{*2}} \ln Z(\beta^*)]$$



For $\beta = \beta^* + i\beta''$, $\quad d\beta = i d\beta''$

$$\Omega(E) = \frac{1}{2\pi i}\int_{\beta^*-i\infty}^{\beta^*+i\infty} d\beta \exp[\ln Z(\beta^*) + \beta^* E]\exp[\frac{1}{2}(\beta-\beta^*)^2[\frac{\partial^2}{\partial\beta^{*2}}\ln Z(\beta^*)]$$

$$= \frac{1}{2\pi}\exp[\ln Z(\beta^*) + \beta^* E]\int_{-\infty}^{\infty} d\beta'' \exp[-\frac{1}{2}\beta''^2 \frac{\partial^2 \ln Z(\beta^*)}{\partial\beta^{*2}}]$$

$$= \frac{1}{\sqrt{2\pi\frac{\partial^2 \ln Z(\beta^*)}{\partial\beta^{*2}}}}\exp[\ln Z(\beta^*) + \beta^* E]$$

Therefore, the logarithm of this expression gives

$$\ln\Omega(E) = \ln Z(\beta^*) + \beta^* E - \frac{1}{2}\ln[2\pi\frac{\partial^2 \ln Z(\beta^*)}{\partial\beta^{*2}}].$$

The second term may be neglected in comparison with the first term. Thus one gets

$$\ln\Omega(E) = \ln Z(\beta^*) + \beta^* E$$

where

$$\frac{\partial}{\partial\beta^*}\ln Z(\beta^*) = -E.$$

6. Canonical ensemble

$$Z_C(N,\beta,V)$$

$$Z_G(\mu,\beta,V) = \sum_{N=0}\sum_{i\{N\}}\exp[\beta(\mu N - E_i(N)]$$
$$= \sum_{N=0}\exp(\beta\mu N)Z_C(N,\beta,V)$$

$$Z_C(N,\beta,V) = \sum_{i\{N\}}\exp[-\beta E_i(N)] \qquad \text{(quantum mechanics)}$$

$$Z_C(N,\beta,V) = \int d^N\Gamma \exp[-\beta H(N)] \qquad \text{(classical mechanics)}$$

7. Ground canonical ensemble

$$Z_G(\beta,\mu) = \sqrt{2\pi}\sigma_{E^*}\sqrt{2\pi}\sigma_{N^*}\Omega(N^*,E^*,V)\,e^{-\beta E^*}e^{\beta\mu N^*}$$
$$= 2\pi\sigma_{E^*}\sigma_{N^*}\Omega(N^*,E^*,V)\,e^{-\beta E^*}e^{\beta\mu N^*}$$

$$\frac{1}{\sigma_{E^*}{}^2} = -\frac{\partial^2}{\partial E^{*2}}\ln\Omega(N^*,E^*,V), \qquad \frac{1}{\sigma_{N^*}{}^2} = -\frac{\partial^2}{\partial N^{*2}}\ln\Omega(N^*,E^*,V)$$

$$\frac{\partial}{\partial E^*}\ln\Omega(N^*,E^*,V) = \beta, \qquad \frac{\partial}{\partial N^*}\ln\Omega(N^*,E^*,V) = -\mu\beta$$

$$\ln Z_G(\beta,\mu) = \ln(2\pi\sigma_{E^*}\sigma_{N^*}) + \ln\Omega(N^*,E^*,V) - \beta E^* + \beta\mu N^*$$

$$\frac{\Omega(N)e^{\mu\beta N}}{\Omega(N^*)e^{\mu\beta N^*}} = \exp[-\frac{1}{2\sigma_{N^*}{}^2}\left(N-N^*\right)^2\ ]$$

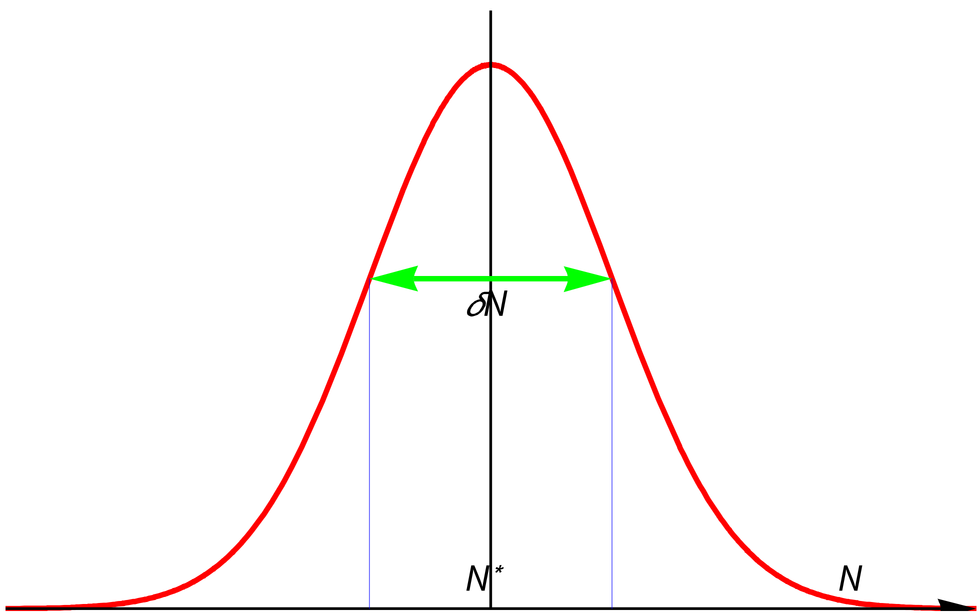


Fig. $\frac{\Omega(N)e^{\mu\beta N}}{\Omega(N^*)e^{\mu\beta N^*}}$ vs *N*. Gaussian distribution function with mean N^* and standard deviation δN.

8. Application-I: Simple harmonics

Multiplicity of simple harmonics (*N* oscillator systems)

$$\Omega_N(E) = \frac{1}{2\pi i}\int_{\beta^*-i\infty}^{\beta^*+i\infty} d\beta\ e^{\beta E} Z_N(\beta)$$

where

$$Z_N = Z_1^{\ N} = e^{-\frac{N\hbar\omega\beta}{2}}(1-e^{-\hbar\omega\beta})^{-N}$$

with

$$Z_1 = \sum_{n=0}^{\infty} e^{-\hbar\omega\beta(n+\frac{1}{2})} = \frac{e^{-\frac{\hbar\omega\beta}{2}}}{1-e^{-\hbar\omega\beta}}$$

Thus we get

$$\begin{aligned}\Omega_N(E) &= \frac{1}{2\pi i}\int_{\beta^*-i\infty}^{\beta^*+i\infty} d\beta\ e^{\beta(E-\frac{\hbar\omega}{2})}(1-e^{-\hbar\omega\beta})^{-N} \\ &= \frac{1}{2\pi i} e^{-\frac{\beta\hbar\omega}{2}} \int_{\beta^*-i\infty}^{\beta^*+i\infty} d\beta\ e^{\beta E}(1-e^{-\hbar\omega\beta})^{-N}\end{aligned}$$

$$\begin{aligned}\Omega_N(E) &= \frac{1}{2\pi i}\int_{\beta^*-i\infty}^{\beta^*+i\infty} e^{\beta E} d\beta e^{-\frac{\beta\hbar\omega}{2}}\ (1-e^{-\hbar\omega\beta})^{-N} \\ &= \frac{1}{2\pi i}\int_{\beta^*-i\infty}^{\beta^*+i\infty} e^{\beta E} d\beta\ \sum_{M=0}^{\infty}\binom{-N}{M}(-1)^M e^{-(M+\frac{1}{2})\hbar\omega\beta} \\ &= \frac{1}{2\pi i}\int_{\beta^*-i\infty}^{\beta^*+i\infty} e^{\beta E} d\beta\ \sum_{M=0}^{\infty}\frac{(N+M-1)!}{(N-1)!M!} e^{-(M+\frac{1}{2})\hbar\omega\beta}\end{aligned}$$

where

$$\binom{-N}{M}(-1)^M = \frac{(N+M-1)!}{(N-1)!M!}$$

This formula can be proved by using the Mathematica. Thus we get

$$\Omega_N(E) = \sum_{M=0}^{\infty} \frac{(N+M-1)!}{(N-1)!M!} \frac{1}{2\pi i} \int_{\beta^*-i\infty}^{\beta^*+i\infty} e^{\beta[E-(M+\frac{1}{2}N)\hbar\omega]} d\beta$$
$$= \sum_{M=0}^{\infty} \frac{(N+M-1)!}{(N-1)!M!} \delta[E-(M+\frac{1}{2})\hbar\omega]$$

where

$$\frac{1}{2\pi i} \int_{\beta^*-i\infty}^{\beta^*+i\infty} e^{a\beta} d\beta \ = \delta(a)$$

So the number of arrangement for $E = (M + \frac{1}{2})\hbar\omega$ is

$$\frac{(N+M-1)!}{(N-1)!M!}$$

9. Application-II: ideal gas

Using expressions for the partition function of classical ideal gases, evaluate the density of states $\Omega(E)$ by the inverse Laplace transform. For simplicity, the gas molecules are assumed to be of one kind. Ignore the internal degrees of freedom.

The partition function for the ideal free gas is given by

$$Z_N(\beta) = \frac{1}{N!} Z_1(\beta)^N = \frac{V^N}{N!}\left(\frac{m}{2\pi\hbar^2\beta}\right)^{3N/2}$$

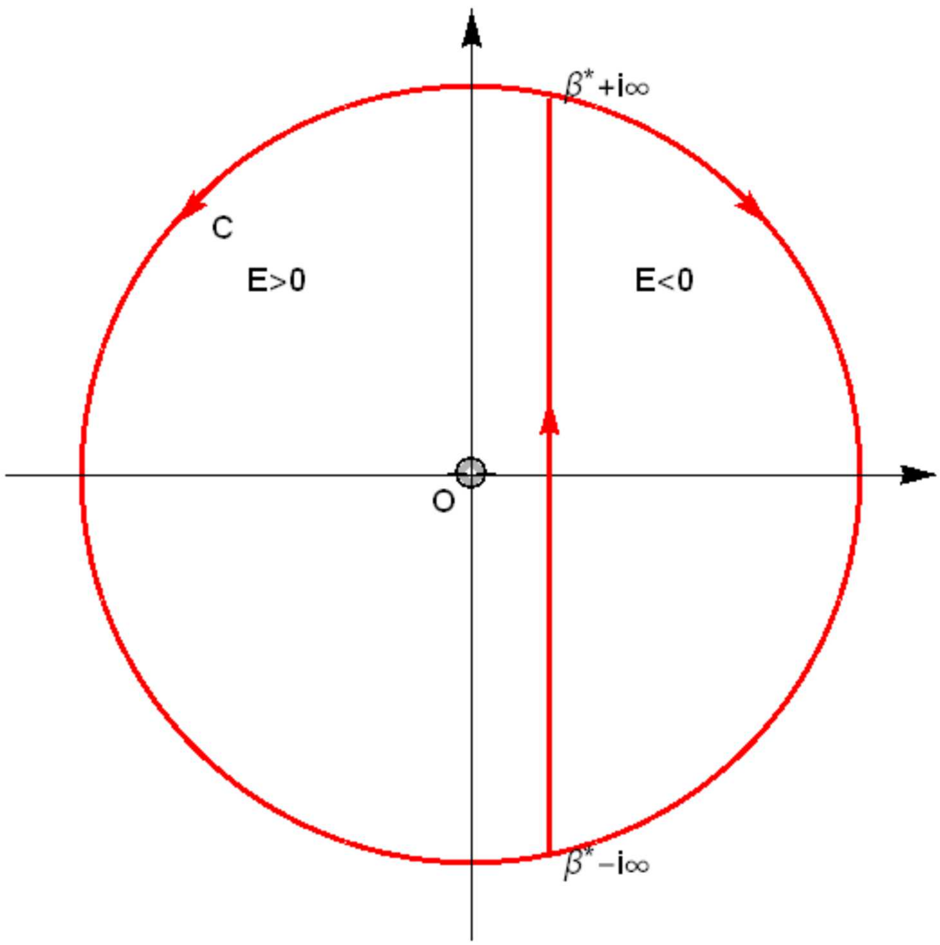
We now evaluate the density of states

$$\Omega(E) = \frac{1}{2\pi i} \int_{\beta^*-i\infty}^{\beta^*+i\infty} d\beta \ \mathrm{e}^{\beta E} Z_N(\beta)$$
$$= \frac{V^N}{N!}\left(\frac{m}{2\pi\hbar^2}\right)^{3N/2} \frac{1}{2\pi i} \int_{\beta^*-i\infty}^{\beta^*+i\infty} d\beta \ \mathrm{e}^{\beta E} \frac{1}{\beta^{3N/2}} \qquad \text{(Bromwich-Wagner)}$$

where $\beta^* > 0$. Using the Jordan lemma, the integral can be rewritten as

$$I = \frac{1}{2\pi i}\int_{\beta^*-i\infty}^{\beta^*+i\infty} d\beta \; \mathrm{e}^{\beta E}\,\frac{1}{\beta^{3N/2}}$$
$$= \frac{1}{2\pi i}\int_C d\beta \; \mathrm{e}^{\beta E}\,\frac{1}{\beta^{3N/2}}$$

where the contour C is in the left-half plane of the complex plane (E>0).



The case of even *N*

The function $g(\beta) = \frac{1}{\beta^{3N/2}}$ has a pole of rank $3N/2$ (integer) at the origin, which are inside the contour C. Using the Cauchy's theorem

$$\frac{1}{2\pi i}\int_C \frac{f(z)dz}{(z-a)^{n+1}} = \frac{1}{n!} f^{(n)}(a)$$

we have

$$I = \frac{E^{(3N/2)-1}}{\Gamma(3N/2)}$$

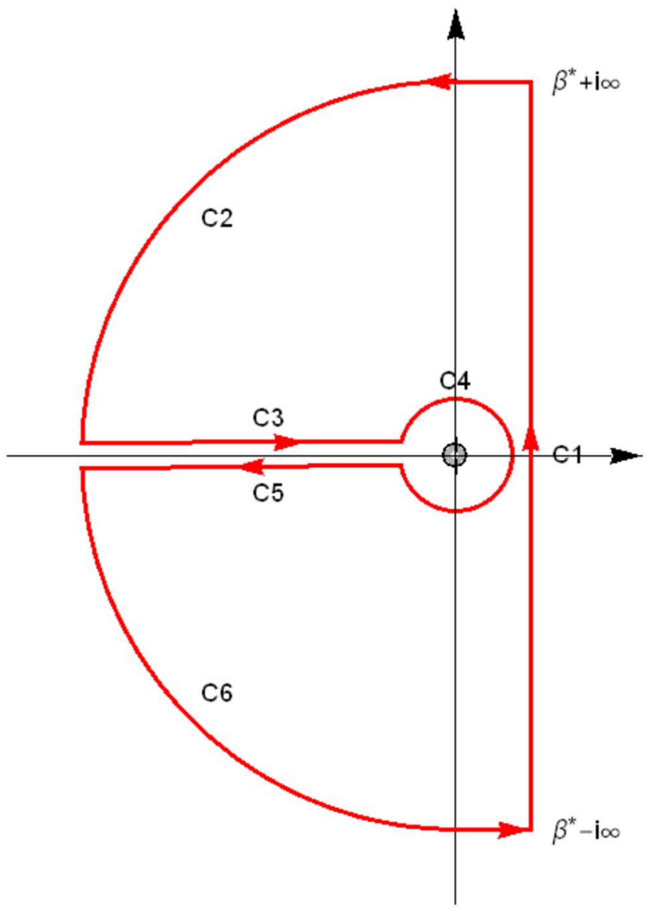
The case of odd *N*

When $N = 2n+1$ (n; integer)

$$g(\beta) = \frac{1}{\beta^{3N/2}} = \frac{1}{\beta^{3n+1+\frac{1}{2}}} = \frac{1}{\beta^{3n+1}} \frac{1}{\sqrt{s}}$$

Because of the factor $\sqrt{s}$, the function $g(\beta)$ is discontinuous on the negative real axis. In this case, the contour C should be changed as the path $C_1 \to C_2 \to C_3 \to C_4 \to C_5 \to C_6$. Inside the path there is no pole. According to the Cauchy's theorem,

$$0 = \int_{\beta^*-i\infty}^{\beta^*+i\infty} d\beta\ \mathrm{e}^{\beta E} \frac{1}{\beta^{3N/2}} + \int_{C_2} d\beta\ \mathrm{e}^{\beta E} \frac{1}{\beta^{3N/2}} + \int_{C_3} d\beta\ \mathrm{e}^{\beta E} \frac{1}{\beta^{3N/2}}$$
$$+ \int_{C_4} d\beta\ \mathrm{e}^{\beta E} \frac{1}{\beta^{3N/2}} + \int_{C_5} d\beta\ \mathrm{e}^{\beta E} \frac{1}{\beta^{3N/2}} + \int_{C_6} d\beta\ \mathrm{e}^{\beta E} \frac{1}{\beta^{3N/2}}$$



According to the Jordan's lemma, we have

$$\int_{C_3} d\beta \ e^{\beta E} \frac{1}{\beta^{3N/2}} = 0 \, , \qquad \int_{C_6} d\beta \ e^{\beta E} \frac{1}{\beta^{3N/2}} = 0$$

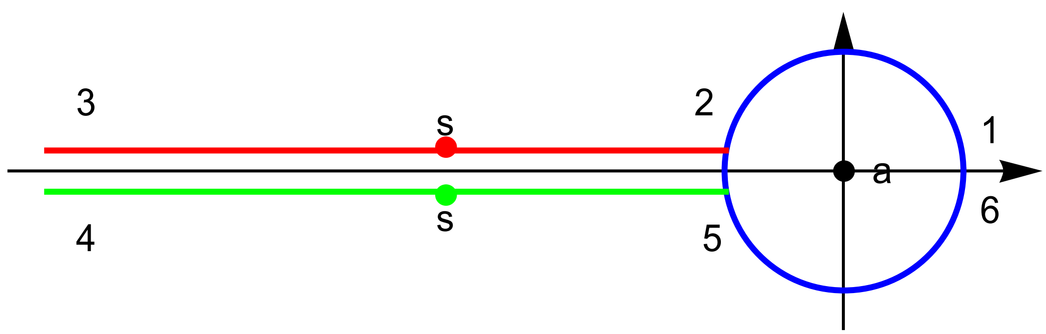
(a) The path integrals along the path C_3 and path C_5

The path $3 \rightarrow 2$: $\beta - 0 = se^{i\pi}$

$$
\begin{aligned}
I_3 &= \int_{C_3} d\beta \ \mathrm{e}^{\beta E} \frac{1}{\beta^{3N/2}} \\
&= e^{-i\frac{3\pi N}{2}} \int_{\infty}^{0} e^{i\pi} ds \frac{e^{-sE}}{s^{3N/2}} \\
&= -e^{-i\frac{3\pi N}{2}} e^{i\pi} \int_{0}^{\infty} ds \frac{e^{-sE}}{s^{3N/2}} \\
&= e^{-i\frac{3\pi N}{2}} \int_{0}^{\infty} ds \frac{e^{-sE}}{s^{3N/2}}
\end{aligned}
$$

The path $5 \rightarrow 4$: $\qquad \beta - 0 = se^{-i\pi}$

$$
\begin{aligned}
I_5 &= \int_{C_5} d\beta \ \mathrm{e}^{\beta E} \frac{1}{\beta^{3N/2}} \\
&= e^{i\frac{3\pi N}{2}} e^{-i\pi} \int_{0}^{\infty} ds \frac{e^{-sE}}{s^{3N/2}} \\
&= -e^{i\frac{3\pi N}{2}} \int_{0}^{\infty} ds \frac{e^{-sE}}{s^{3N/2}}
\end{aligned}
$$



Then we have

$$
I_3 + I_5 = -2i \sin(\frac{3\pi N}{2}) \int_{0}^{\infty} ds \frac{e^{-sE}}{s^{3N/2}}
$$

For $N = 2n + 1$

$$\sin(\frac{3\pi N}{2}) = \sin[\frac{3\pi(2n+1)}{2}]$$

$$= \sin(3\pi n + \frac{3\pi}{2})$$

$$= \sin(n\pi + \frac{3\pi}{2})$$

$$= \sin(\frac{3\pi}{2})\cos(n\pi)$$

$$= (-1)^{n+1}$$

$$= (-1)^{\frac{N+1}{2}}$$

We calculate the integral

$$J = \int_0^\infty ds \frac{e^{-sE}}{s^{3N/2}}$$

When $N = 2n+1$

$$J(E) = \int_0^\infty ds \frac{e^{-sE}}{s^{(3n+1)+1/2}} = \int_0^\infty ds \frac{1}{s^{(3n+1)}} \frac{e^{-sE}}{\sqrt{s}}$$

Thus we get

$$\frac{dJ(E)}{dE} = \int_0^\infty ds \frac{(-s)}{s^{(3n+1)}} \frac{e^{-sE}}{\sqrt{s}} = (-1)\int_0^\infty ds \frac{1}{s^{3n}} \frac{e^{-sE}}{\sqrt{s}}$$

$$\frac{d^2 J(E)}{dE^2} = (-1)^2 \int_0^\infty ds \frac{1}{s^{3n-1}} \frac{e^{-sE}}{\sqrt{s}}$$

Similarly, we have

$$\frac{d^{(3n+1)} J(E)}{dE^{(3n+1)}} = J^{(3n+1)}(E) = (-1)^{3n+1} \int_0^\infty ds \frac{e^{-sE}}{\sqrt{s}} = (-1)^{3n+1} \sqrt{\frac{\pi}{E}}$$

where

$$\int_0^\infty ds \frac{e^{-sE}}{\sqrt{s}} = \sqrt{\frac{\pi}{E}}$$

From the sequential integration of the above relation, we get

$$J(E) = (-1)^{\frac{3N-1}{2}} \pi \frac{1}{\sqrt{\pi}\frac{1}{2}\cdot\frac{3}{2}\cdot\frac{5}{2}.........(\frac{3N}{2}-1)} E^{\frac{3N}{2}-1}$$

$$= \frac{(-1)^{\frac{3N-1}{2}} \pi}{\Gamma(\frac{3N}{2})} E^{\frac{3N}{2}-1}$$

where

$$\Gamma(\frac{3N}{2}) = \sqrt{\pi}\frac{1}{2}\cdot\frac{3}{2}\cdot\frac{5}{2}.........(\frac{3N}{2}-1)$$

Thus we have

$$I_3 + I_5 = -2i(-1)^{\frac{N+1}{2}} \frac{(-1)^{\frac{3N-1}{2}} \pi}{\Gamma(\frac{3N}{2})} E^{\frac{3N}{2}-1}$$

$$= -2i(-1)^{2N} \pi \frac{E^{\frac{3N}{2}-1}}{\Gamma(\frac{3N}{2})}$$

(b) ***C*₄: circle:** $\beta = \varepsilon e^{i\theta}$ (θ changes from π to -π)

$$\int_{C_4} d\beta \ \mathrm{e}^{\beta E} \frac{1}{\beta^{3N/2}}$$

It seems that this integral may diverge. This integral may be included in the path integral on the path C_3 and C_5. In fact, in Kubo's book, this assumption is included in the path integral on the path C_3 and C_5.
[R. Kubo, H. Ichimura, T. Usui, and N. Hashitsume, Statistical Mechanics An Advanced Course with Problems and Solutions (North Holland, 1988)].

(c)

$$\frac{1}{2\pi i}\int_{\beta^*-i\infty}^{\beta^*+i\infty} d\beta\, \mathrm{e}^{\beta E}\frac{1}{\beta^{3N/2}} = -\frac{1}{2\pi i}(I_3+I_5)$$

$$= \frac{(-1)}{2\pi i}[-2i(-1)^{2N}\pi\frac{E^{\frac{3N}{2}-1}}{\Gamma(\frac{3N}{2})}]$$

$$= \frac{E^{\frac{3N}{2}-1}}{\Gamma(\frac{3N}{2})}]$$

In conclusion, for any integer (both for even and odd numbers), we have the density of states given by

$$\Omega(E) = \frac{V^N}{N!}\left(\frac{m}{2\pi\hbar^2}\right)^{3N/2}\frac{E^{(3N/2)-1}}{\Gamma(3N/2)}$$

24. Evaluate the state density $\Omega(E)$ for a system composed of N ($N \gg 1$) classical harmonic oscillators having a frequency ω by the inverse transformation (2.6). Determine its asymptotic expression by the saddle-point method. Derive Stirling's formula from it.

Partition function for the simple harmonics:

$$Z_{C1} = \sum_{n=0}^{\infty} e^{-n\beta\hbar\omega} = (1-e^{-\beta\hbar\omega})^{-1}$$

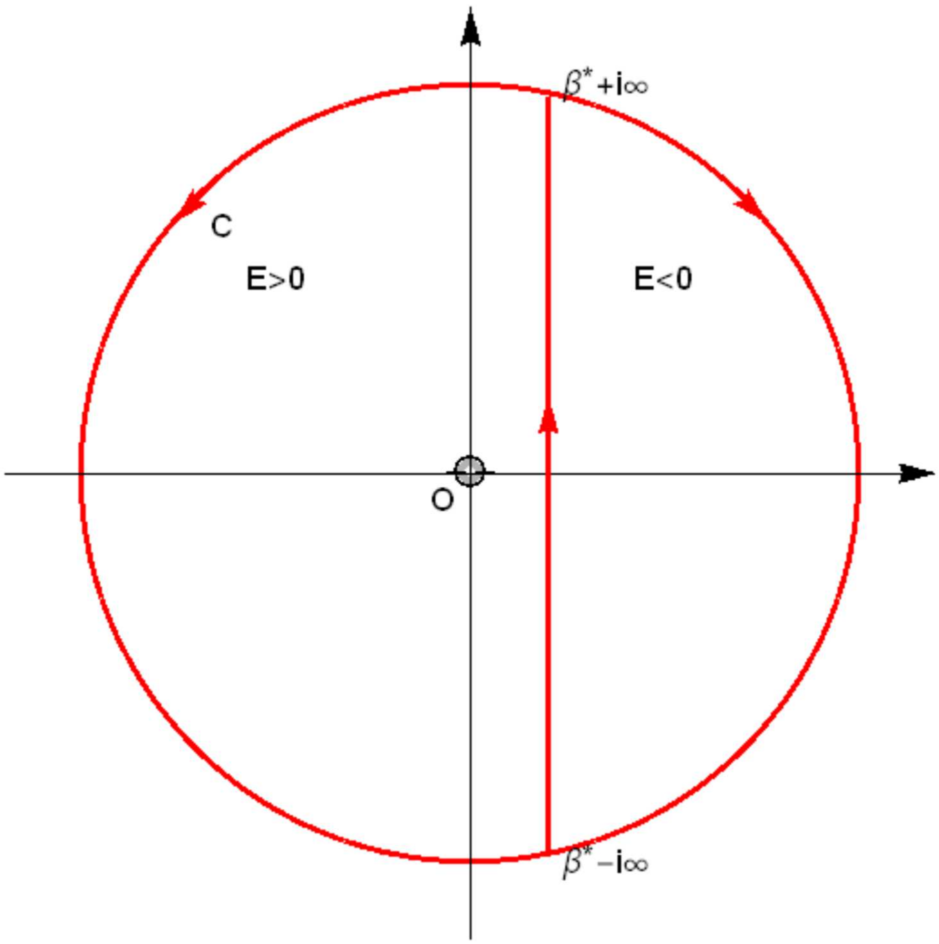
For the system with N-simple harmonics,

$$Z_{CN} = (Z_{C1})^N = (1-e^{-\beta\hbar\omega})^{-N}.$$

The density of states

$$\Omega(E) = \frac{1}{2\pi i}\int_{\beta^*-i\infty}^{\beta^*+i\infty} d\beta\ \mathrm{e}^{\beta E} Z_N(\beta)$$

$$= \frac{1}{2\pi i}\int_{\beta^*-i\infty}^{\beta^*+i\infty} d\beta\ \mathrm{e}^{\beta E} (1-e^{-\beta\hbar\omega})^{-N}$$



According to the Jordan's lemma,

$$\Omega(E,N) = \frac{1}{2\pi i}\int_C d\beta\ \mathrm{e}^{\beta E} (1-e^{-\beta\hbar\omega})^{-N}$$

The integrant has a pole at $\beta = 0$ of the rank *N*. Using the Cauchy's theorem, we get

$$\Omega(E,N) = \text{Residue}[e^{\beta E}(1-e^{-\beta\hbar\omega})^{-N}, \{\beta, 0\}]$$
$$= \frac{1}{\hbar\omega}\frac{(N-1+M)!}{(N-1)!M!}$$

((**Mathematica**))

```
Clear["Global`*"];
f1[N1_] := Exp[β E1] / (1 - Exp[-ħ ω β])^N1 /. E1 → ħ ω M1;
Residue[f1[2], {β, 0}]
```

$$\frac{1+\text{M1}}{\omega\hbar}$$

```
Residue[f1[3], {β, 0}] // Factor
```

$$\frac{(1+\text{M1})(2+\text{M1})}{2\omega\hbar}$$

```
Residue[f1[4], {β, 0}] // Factor
```

$$\frac{(1+\text{M1})(2+\text{M1})(3+\text{M1})}{6\omega\hbar}$$

```
Residue[f1[5], {β, 0}] // Factor
```

$$\frac{(1+\text{M1})(2+\text{M1})(3+\text{M1})(4+\text{M1})}{24\omega\hbar}$$

```
Residue[f1[8], {β, 0}] // Factor
```

$$\frac{(1+\text{M1})(2+\text{M1})(3+\text{M1})(4+\text{M1})(5+\text{M1})(6+\text{M1})(7+\text{M1})}{5040\omega\hbar}$$