1.18. Density of States and Tracelog

Let $| E_n \rangle$ be the eigenstates of $\hat{H}$, (1.536) becomes

$$Z(T) = \mathrm{Tr}\, e^{-\hat{H}/k_B T} \tag{1.577}$$

$$= \sum_n \left\langle E_n \middle| e^{-\hat{H}/k_B T} \middle| E_n \right\rangle$$

$$= \sum_n e^{-E_n / k_B T} \tag{1.578}$$

$$= \int d E\, \rho(E)\, e^{-E / k_B T} \tag{1.579}$$

where

$$\rho(E) = \sum_n \delta(E - E_n) \tag{1.580}$$

is just another expression of the density of states defined in (1.558).

With the help of the density of states operator

$$\hat{\rho}(E) \equiv \delta\left(E - \hat{H}\right) \tag{1.581a}$$

(1.580) can also be written as

$$\rho(E) = \mathrm{Tr}\, \hat{\rho}(E) \tag{1.581}$$

Setting

$$\beta = \frac{1}{k_B T} = -\frac{i}{\hbar} t$$

the Fourier transform of $Z(T)$ is

$$\tilde{Z}(E) = \int_{-\infty}^{\infty} d t\, e^{i E t / \hbar} Z(t)$$

$$= -i \hbar \int_{-i\infty}^{i\infty} d \beta\, e^{-\beta E} Z(\beta)$$

$$= -i \hbar \int_{-i\infty}^{i\infty} d \beta\, e^{-\beta E}\, \mathrm{Tr}\, e^{-\beta \hat{H}} \tag{1.582}$$

$$= -i \hbar \sum_n \int_{-i\infty}^{i\infty} d \beta\, e^{-\beta (E - E_n)}$$

$$= \sum_n \int_{-\infty}^{\infty} d t\, e^{i (E - E_n) t / \hbar}$$

$$= 2 \pi \sum_n \delta(E - E_n)$$

$$= 2 \pi \rho(E) \tag{1.582}$$

The number of states up to energy E is [c.f. (1.551)]

$$\mathcal{N}(E) = \int_{E'' \le E_0}^{E} d E'\, \rho(E') \tag{1.583}$$

where E_0 is the ground state energy.

Using (1.580), we have

$$\mathcal{N}(E) = \sum_{n=0}^{\infty} \int_{-\infty}^{E} d E'\, \delta(E' - E_n)$$

Now,

$$\int_{-\infty}^{E} dE'\,\delta(E'-E_n) = \begin{cases} 1 & \text{if } E > E_n \\ 0 & \text{if } E < E_n \end{cases}$$
$$= \theta(E - E_n)$$

The case $E = E_n$ requires special attention:

$$\int_{-\infty}^{E_n} dE'\,\delta(E'-E_n) = \int_{-\infty}^{E_n} dE' \int_{-\infty}^{\infty} \frac{dt}{2\pi\hbar} e^{i(E'-E_n)t/\hbar}$$
$$= \frac{1}{2\pi i} \mathcal{P} \int_{-\infty}^{\infty} \frac{dt}{t}$$
$$= \frac{1}{2}$$

where $\mathcal{P}$ denotes the principal value and we've used

$$\mathcal{P} \int_{-\infty}^{\infty} \frac{dt}{t} = \int_C \frac{dz}{z} \qquad C = \text{small counterclockwise semi – circle around origin}$$
$$= i \int_0^{\pi} d\phi \qquad z = r e^{i\phi}$$
$$= i\pi$$

Hence

$$\mathcal{N}(E) = \sum_n \theta(E - E_n) \tag{1.584}$$

with

$$\lim_{E \to E_n} \theta(E - E_n) = \frac{1}{2} \tag{1.584a}$$

Thus,

$$\mathcal{N}(E_m) = \sum_{n=0}^{\infty} \theta(E_m - E_n)$$
$$= \sum_{n=0}^{m-1} 1 + \lim_{E_n \to E_m} \theta(E_m - E_n)$$
$$= m + \frac{1}{2} \tag{1.585}$$

This formula will serve to determine the energies of bound states from approximations to $\omega(E)$ in §4.7.

Consider the trace of the logarithm (or tracelog) of the operator $\hat{H} - E\,\hat{1}$,

$$\operatorname{Tr}\ln\left(\hat{H} - E\right) = \sum_n \ln(E_n - E) \tag{1.586}$$
$$= \int_{-\infty}^{\infty} dE'\,\rho(E')\ln(E' - E) \tag{1.587}$$
$$= \operatorname{Tr} \int_{-\infty}^{\infty} dE'\,\delta\!\left(E' - \hat{H}\right)\ln(E' - E) \tag{1.587a}$$

where (1.581) was used.

Since

$$\operatorname{Tr}\hat{H}^{-\nu} = \sum_{n=0}^{\infty} \frac{1}{E_n^{\nu}} \tag{1.589a}$$

bears certain resemblance with the Riemann zeta function

$$\zeta(\nu) = \sum_{n=1}^{\infty} \frac{1}{n^{\nu}}$$

we define the operator zeta function associated with $\hat{H}$ as

$$\hat{\zeta}_{\hat{H}}(\nu) = \hat{H}^{-\nu} \tag{1.588}$$

so that its trace is the generalized zeta function

$$\zeta_{\hat{H}}(\nu) = \mathrm{Tr}\,\hat{\zeta}_{\hat{H}}(\nu) = \sum_{n=0}^{\infty} \frac{1}{E_n^{\nu}} \tag{1.589}$$

Now,

$$\frac{\partial}{\partial \nu} \ln \hat{H}^{-\nu} = \frac{\partial}{\partial \nu}\left(-\nu \ln \hat{H}\right) = -\ln \hat{H}$$

is valid for all ν.

Setting $\nu = 0$, we have

$$\mathrm{Tr} \ln \hat{H} = -\mathrm{Tr} \frac{\partial}{\partial \nu} \ln \hat{H}^{-\nu} \bigg|_{\nu=0} \tag{1.589a}$$

Using the Taylor expansion of $f(\hat{H})$, one can easily prove that

$$\mathrm{Tr}\, f(\hat{H}) = \sum_n f(E_n)$$

(1.598a) thus becomes

$$\begin{aligned}\mathrm{Tr} \ln \hat{H} &= -\sum_n \frac{\partial}{\partial \nu} \ln E_n^{-\nu} \bigg|_{\nu=0} \\ &= -\sum_n \frac{1}{E_n^{-\nu}} \frac{\partial}{\partial \nu} E_n^{-\nu} \bigg|_{\nu=0} \\ &= -\frac{\partial}{\partial \nu} \sum_n E_n{}^{-\nu} \bigg|_{\nu=0} \\ &= -\frac{\partial}{\partial \nu} \zeta_{\hat{H}}(\nu) \bigg|_{\nu=0} \end{aligned} \tag{1.590}$$

Now,

$$\begin{aligned}\frac{\partial}{\partial E} \mathrm{Tr} \ln\left(\hat{H} - E\right) = \mathrm{Tr} \frac{\partial}{\partial E} \ln\left(\hat{H} - E\right) \\ = \mathrm{Tr} \frac{1}{E - \hat{H}} = \sum_n \frac{1}{E - E_n} \\ = \frac{1}{i\hbar} \mathrm{Tr}\, \hat{R}(E) = \frac{1}{i\hbar} \sum_n R_n(E)\end{aligned} \tag{1.591}$$

where the resolvent $\hat{R}$ was defined in (1.315).

To avoid the singularities at $E = E_n$, we switch to

$$\frac{\partial}{\partial E} \mathrm{Tr} \ln\left(\hat{H} - E - i\eta\right) = \sum_n \frac{1}{E - E_n + i\eta} \tag{1.591a}$$

Using

$$\frac{1}{x \pm i\delta} = \mathcal{P} \frac{1}{x} \mp i\pi\, \delta(x) \tag{1.325}$$

we have

$$-\frac{1}{\pi} \operatorname{Im} \frac{\partial}{\partial E} \operatorname{Tr} \ln\left(\hat{H} - E - i\,\eta\right) = \sum_n \delta(E - E_n) = \rho(E) \qquad (1.326)$$

Assuming the spectrum of $\hat{H}$ is bounded below, i.e., E_0 is finite, then

$$\lim_{E \to -\infty} \operatorname{Tr} \ln\left(\hat{H} - E - i\,\eta\right) = 0$$

Integrating (1.326) over E then gives

$$\begin{aligned} -\frac{1}{\pi} \operatorname{Im} \int_{-\infty}^{E} d\,E' \frac{\partial}{\partial E'} \operatorname{Tr} \ln\left(\hat{H} - E' - i\,\eta\right) \\ = -\frac{1}{\pi} \operatorname{Im} \operatorname{Tr} \ln\left(\hat{H} - E - i\,\eta\right) \\ = \sum_n \int_{-\infty}^{E} d\,E'\, \delta(E' - E_n) = \sum_n \theta(E - E_n) \\ = \int_{-\infty}^{E} d\,E'\, \rho(E') = \mathcal{N}(E) \qquad (1.593) \end{aligned}$$