2.4. Partition Function. Correlation Functions

Assume H to be t-independent with discrete spectrum.

The Quantum Partition Function

$$\mathcal{Z}(\beta) = \operatorname{tr} e^{-\beta H}$$

For t-independent H, solution to eq(2.5) is

$$U(t, t') = e^{-(t-t')H/\hbar}$$

so that

$$U(\hbar\beta, 0) = e^{-\beta H}$$

$$\therefore \qquad \mathcal{Z}(\beta) = \operatorname{tr} U(\hbar\beta, 0)$$

$$= \int d\boldsymbol{q} \, \langle \boldsymbol{q} \mid U(\hbar\beta, 0) \mid \boldsymbol{q} \rangle$$

$$= \lim_{\substack{n\to\infty \\ \varepsilon\to 0}} \left(\frac{m}{2\pi\hbar\varepsilon} \right)^{nd/2} \int \prod_{k=1}^{n} d^d q_k \exp\left(-\frac{1}{\hbar} S[\boldsymbol{q}, \varepsilon] \right)$$

$$= \int [d\boldsymbol{q}(t)] \exp\left(-\frac{S(\boldsymbol{q})}{\hbar} \right) \quad \text{with} \quad \boldsymbol{q}(0) = \boldsymbol{q}(\hbar\beta) \tag{2.31}$$

Note that the trace operation means that there're now n, instead of $n-1$, integrals as in eq(2.19).

With $\tau = \frac{t}{\hbar}$, eq(2.18) becomes

$$\frac{S(\boldsymbol{q})}{\hbar} = \int_0^\beta d\tau \left\{ \frac{1}{2\hbar^2} m \dot{\boldsymbol{q}}^2(\tau) + V[\boldsymbol{q}(\tau)] \right\} \tag{2.32}$$

$$= -\int_0^\beta d\tau \, L$$

The Harmonic Oscillator

For the harmonic oscillator, eq(2.28) gives

$$\langle q'' \mid U_0(\hbar\beta, 0) \mid q' \rangle = \exp\left(-\frac{1}{\hbar} S_0[q_c] \right) \mathcal{N}(\omega; \hbar\beta)$$

where, from eq(2.27),

$$S_0[q_c] = \frac{m\omega}{2\sinh\omega\hbar\beta} \left\{ -2q'q'' + \left[(q'')^2 + (q')^2 \right] \cosh\omega\hbar\beta \right\}$$

The periodic boundary condition in eq(2.31) requires $q' = q'' = q_0$ so that

$$S_0[q_c] = \frac{m\omega}{\sinh\omega\hbar\beta} q_0^2 (-1 + \cosh\omega\hbar\beta)$$

$$= \frac{2m\omega}{\sinh\omega\hbar\beta} q_0^2 \sinh^2 \frac{\omega\hbar\beta}{2}$$

$$= \frac{m\omega}{\cosh\frac{\omega\hbar\beta}{2}} q_0^2 \sinh\frac{\omega\hbar\beta}{2}$$

$$= m\omega q_0^2 \tanh\frac{\omega\hbar\beta}{2}$$

Hence,

$$\begin{aligned}\mathcal{Z}_0(\beta) &= \operatorname{tr} U_0(\hbar\beta, 0)\\ &= \int dq \,\langle q \mid U_0(\hbar\beta, 0) \mid q\rangle\\ &= \mathcal{N}(\omega;\hbar\beta)\int_{-\infty}^{\infty} dq_0 \exp\left(-\frac{1}{\hbar} m\,\omega\, q_0^2 \tanh\frac{\omega\hbar\beta}{2}\right)\\ &= \mathcal{N}(\omega;\hbar\beta)\sqrt{\frac{\pi\hbar}{m\,\omega\tanh\frac{\omega\hbar\beta}{2}}}\end{aligned} \tag{2.33}$$

The Large β Limit

Since H is t-independent, $\mathcal{Z}(\beta)$ will not be affected if eq(2.32) is written as

$$\frac{S(\boldsymbol{q})}{\hbar} = \int_{-\beta/2}^{\beta/2} d\tau \left\{\frac{1}{2\hbar^2} m\,\dot{\boldsymbol{q}}^2(\tau) + V[\boldsymbol{q}(\tau)]\right\} \tag{2.32a}$$

with the boundary condition $\boldsymbol{q}(\beta/2) = \boldsymbol{q}(-\beta/2)$.

In the large β limit, eq(2.32) becomes

$$\frac{S(\boldsymbol{q})}{\hbar} = \int_0^{\infty} d\tau \left\{\frac{1}{2\hbar^2} m\,\dot{\boldsymbol{q}}^2(\tau) + V[\boldsymbol{q}(\tau)]\right\} \qquad \text{with} \qquad q(0) = q(\infty)$$

while eq(2.32a) becomes

$$\frac{S(\boldsymbol{q})}{\hbar} = \int_{-\infty}^{\infty} d\tau \left\{\frac{1}{2\hbar^2} m\,\dot{\boldsymbol{q}}^2(\tau) + V[\boldsymbol{q}(\tau)]\right\} \qquad \text{with} \qquad q(-\infty) = q(\infty)$$

The explicitly time translation invariant version from eq(2.23a) is clearly preferable.

Classical and Quantum Statistical Physics

Consider the discrete time path integral

$$\mathcal{Z}(n,\varepsilon) = \int \prod_{k=1}^{n} dq_k\, e^{-S[\boldsymbol{q};\varepsilon]} \tag{2.34}$$

with

$$\begin{aligned}S[\boldsymbol{q};\varepsilon] &= \frac{1}{\hbar}\sum_{k=1}^{n}\left[m\frac{(q_k - q_{k-1})^2}{2\varepsilon} + \varepsilon V(q_k)\right]\\ &= \frac{\varepsilon}{\hbar}\sum_{k=1}^{n}\left[\frac{1}{2} m\left(\frac{q_k - q_{k-1}}{\varepsilon}\right)^2 + V(q_k)\right]\end{aligned} \tag{2.34a}$$

& the periodic boundary condition

$$q_0 = q_n$$

If we define a hamiltonian

$$H = \sum_{k=1}^{n}\left[\frac{1}{2} m\,\dot{q}_k^2 + V(q_k)\right] \qquad \text{with} \qquad \dot{q}_k = \frac{q_k - q_{k-1}}{\varepsilon}$$

then

$$\mathcal{Z}(n,\varepsilon) = \int \prod_{k=1}^{n} dq_k\, e^{-\varepsilon H/\hbar}$$

can be taken as the classical partition function of a 1-D lattice at inverse temperature $\beta\hbar = \varepsilon$.
Note that ε here is necessarily a real time so that the momentum of the particle at site k is $p_k = m\,\dot{q}_k$.
The approximation becomes exact in the thermodynamic limit ($n \to \infty$) & high temperatures ($\varepsilon \to 0$).

Let

$$S(q\,,\,q') = \frac{1}{\hbar}\left[\,m\,\frac{(q-q')^2}{2\,\varepsilon} + \frac{1}{2}\,\varepsilon\,V(q) + \frac{1}{2}\,\varepsilon\,V(q')\,\right] \qquad (2.35)$$

$$= \frac{\varepsilon}{\hbar}\left\{\,\frac{1}{2}\,m\left(\frac{q-q'}{\varepsilon}\right)^2 + \frac{1}{2}[\,V(q) + V(q')\,]\right\}$$

$$\rightarrow \qquad S[\boldsymbol{q}\,;\,\varepsilon] = \sum_{k=1}^{n} S\,(q_{k-1}\,,\,q_k)$$

$$e^{-S[\boldsymbol{q}\,;\varepsilon]} = \prod_{k=1}^{n} e^{-S(q_{k-1},\,q_k)}$$

$$\mathcal{Z}(n,\,\varepsilon) = \prod_{k=1}^{n}\int d\,q_k\,e^{-S(q_{k-1},\,q_k)}$$

Let

$$\mathcal{T}(q,\,q') = e^{-S(q\,,\,q')}$$

We define the transfer matrix $\boldsymbol{T}$ by as an operator with matrix elements $\mathcal{T}(q,\,q')$, i.e.,

$$\langle\,q'\mid \boldsymbol{T}\mid q\,\rangle = \mathcal{T}\,(q,\,q') = e^{-S(q\,,\,q')} \qquad (2.36)$$

$$\mathcal{Z}(n,\,\varepsilon) = \int d\,q_1 \ldots \int d\,q_n\,\langle\,q_n\mid \boldsymbol{T}\mid q_{n-1}\,\rangle \ldots \langle\,q_2\mid \boldsymbol{T}\mid q_1\,\rangle\langle\,q_1\mid \boldsymbol{T}\mid q_n\,\rangle$$

$$\equiv \prod_{k=1}^{n}\int d\,q_k\,\langle\,q_k\mid \boldsymbol{T}\mid q_{k-1}\,\rangle \quad \text{with} \qquad q_0 = q_n$$

$$= \int d\,q_n\left\langle\,q_n\mid \boldsymbol{T}^n\mid q_n\,\right\rangle$$

$$= \mathrm{tr}\boldsymbol{T}^n \qquad (2.36a)$$

For $\varepsilon \to 0$, $\boldsymbol{T}$ can be taken as the 1-particle quantum operator

$$\boldsymbol{T} = e^{-\varepsilon\,h/\hbar}$$

where, since ε is a real time,

$$h = \frac{1}{2}\,m\,(\hat{\dot{q}})^2 + V(\hat{q}) = \frac{1}{2\,m}\,\hat{p}^2 + V(\hat{q}) \qquad (2.36b)$$

is the 1-particle hamiltonian so that

$$S(q\,,\,q') \approx \frac{\varepsilon}{\hbar}\,\langle\,q'\mid h\mid q\,\rangle$$

$$\rightarrow \qquad \mathcal{T}(q,\,q') \approx \left\langle\,q'\,\middle|\,e^{-\varepsilon\,h/\hbar}\,\middle|\,q\,\right\rangle$$

In the thermodynamic limit ($n \to \infty$)

$$\mathcal{Z}(n,\,\varepsilon) \approx \mathrm{tr}\,e^{-n\,\varepsilon\,h/\hbar}$$

$$= \sum_k g_k\,e^{-n\,\varepsilon\,e_k/\hbar} \qquad (g_k = \text{degeneracy of the } k^{\text{th}} \text{ excited state})$$

$$\approx e^{-n\,\varepsilon\,e_0/\hbar}$$

where e_0 is the 1-particle ground state energy & we've assumed $g_0 = 1$.

The free energy is given by

$$\mathcal{W}_n = -\frac{\hbar}{\varepsilon}\ln\mathcal{Z}(n,\,\varepsilon)$$

$$= n\,e_0$$

On the other hand, taking $S[\boldsymbol{q};\,\varepsilon]$ as an approximation to the 1-particle action $S(\boldsymbol{q})$ in eq(2.31), we see that

$$\mathcal{Z}(\beta) = \lim_{\substack{n\to\infty \\ \varepsilon\to 0}} \left(\frac{m}{2\pi\hbar\varepsilon}\right)^{n/2} \mathcal{Z}(n,\varepsilon)\Bigg|_{\varepsilon=\beta\hbar}$$

$$\mathcal{W} = -\frac{1}{\beta}\ln\mathcal{Z}(\beta)$$

$$= -\frac{\hbar}{\varepsilon}\left\{\frac{n}{2}\ln\frac{m}{2\pi\hbar\varepsilon} + \ln\mathcal{Z}(n,\varepsilon)\right\}$$

$$= n\,e_0 - \frac{n\hbar}{2\varepsilon}\ln\frac{m}{2\pi\hbar\varepsilon}$$

$$\rightarrow \qquad \frac{\mathcal{W}}{n} = e_0 - \frac{\hbar}{2\varepsilon}\ln\frac{m}{2\pi\hbar\varepsilon}$$

Thus, the 0-D (1-particle) quantum statistics is related to the 1-D classical statistics.
More generally, the d-D (1-particle) quantum statistics is related to the $(d+1)$-D classical statistics.

Keeping ε small but finite, we see that

$$\lim_{\beta\to\infty}\left[\mathcal{Z}(\beta) = \operatorname{tr} e^{-\beta H}\right] \qquad \text{(low temperature limit)}$$

corresponds to

$$\lim_{n\to\infty}\left[\mathcal{Z}(n,\varepsilon) \approx \operatorname{tr} e^{-n\varepsilon h/\hbar}\right] \qquad \text{(thermodynamic limit)}$$

Correlation Functions

In classical statistics, an m-point correlation function is given by

$$\langle q_{i_1} q_{i_2} \ldots q_{i_m}\rangle = \frac{1}{\mathcal{Z}(n,\varepsilon)}\int\left(\prod_{k=1}^{n} d\,q_k\right) q_{i_1} q_{i_2}\ldots q_{i_m}\, e^{-S[\boldsymbol{q};\,\varepsilon]} \qquad (2.37)$$

Assuming

$$0 < i_1 \le i_2 \ldots \le i_m < n \qquad (2.37a)$$

we can write

$$S[\boldsymbol{q};\varepsilon] = \sum_{j=1}^{m+1} S\left(q_{i_{j-1}},\, q_{i_j}\right) \qquad \text{with} \qquad i_0 = 0 \qquad i_{m+1} = n$$

Using eq(2.36), we can integrate all q_k's except q_0, q_{i_1}, q_{i_2}, ..., & q_{i_m} to get

$$\langle q_{i_1} q_{i_2}\ldots q_{i_m}\rangle = \frac{1}{\mathcal{Z}(n,\varepsilon)}\int d\,q_0 \int d\,q_{i_1} \ldots \int d\,q_{i_m}\, \langle q_0 | \boldsymbol{T}^{n-i_m} | q_{i_m}\rangle q_{i_m}$$
$$\times \langle q_{i_m} | \boldsymbol{T}^{i_m - i_{m-1}} | q_{i_{m-1}}\rangle q_{i_{m-1}} \ldots q_{i_2} \langle q_{i_2} | \boldsymbol{T}^{i_2-i_1} | q_{i_1}\rangle q_{i_1} \langle q_{i_1} | \boldsymbol{T}^{i_1} | q_0\rangle$$

One can check that the power of $\boldsymbol{T}$ is n, as required by eq(2.36a).

Integrating q_0, which corresponds to taking the trace, gives

$$\langle q_{i_1} q_{i_2}\ldots q_{i_m}\rangle = \frac{1}{\mathcal{Z}(n,\varepsilon)}\int d\,q_{i_1} \ldots \int d\,q_{i_m}\, \langle q_{i_1} | \boldsymbol{T}^{n-i_m+i_1} | q_{i_m}\rangle q_{i_m}$$
$$\times \langle q_{i_m} | \boldsymbol{T}^{i_m - i_{m-1}} | q_{i_{m-1}}\rangle q_{i_{m-1}} \ldots q_{i_2} \langle q_{i_2} | \boldsymbol{T}^{i_2-i_1} | q_{i_1}\rangle q_{i_1}$$

For example,

$$\langle q_4\, q_7\rangle = \frac{1}{\mathcal{Z}(10,\varepsilon)}\int d\,q_4 \int d\,q_7\, \langle q_4 | \boldsymbol{T}^{7} | q_7\rangle q_7 \langle q_7 | \boldsymbol{T}^{3} | q_4\rangle q_4$$

By definition,

$$\hat{q} \mid q\rangle = q \mid q\rangle$$

Hence,

$$\langle q_{i_1} q_{i_2} \ldots q_{i_m}\rangle = \frac{1}{\mathcal{Z}(n,\,\varepsilon)} \int d\,q_{i_1} \ldots \int d\,q_{i_m} \;\langle q_{i_1} \,\Big|\, \boldsymbol{T}^{\,n-i_m+i_1}\,\hat{q} \,\Big|\, q_{i_m}\rangle$$

$$\times \langle q_{i_m} \,\Big|\, \boldsymbol{T}^{\,i_m-i_{m-1}}\,\hat{q} \,\Big|\, q_{i_{m-1}}\rangle \ldots \langle q_{i_2} \,\Big|\, \boldsymbol{T}^{\,i_2-i_1}\,\hat{q} \,\Big|\, q_{i_1}\rangle$$

$$= \frac{1}{\mathcal{Z}(n,\,\varepsilon)}\,\mathrm{tr}\left(\boldsymbol{T}^{\,n-i_m+i_1}\,\hat{q}\;\boldsymbol{T}^{\,i_m-i_{m-1}}\,\hat{q}\;\ldots\;\boldsymbol{T}^{\,i_2-i_1}\,\hat{q}\right)$$

Small ε

Let

$$t_k = \frac{\varepsilon}{\hbar}\,i_k \qquad q_{i_k} = q(t_k) \qquad \beta = n\,\frac{\varepsilon}{\hbar} \tag{2.38a}$$

then with eq(2.36b), we have

$$\langle q_{i_1} q_{i_2} \ldots q_{i_m}\rangle_\beta = \langle q\,(t_1)\,q\,(t_2)\ldots q(t_m)\rangle_\beta$$

$$\equiv Z^{(m)}(t_1,\,t_2,\;\ldots,\,t_m)$$

$$\equiv \frac{1}{\mathcal{Z}(\beta)}\int [d\,\boldsymbol{q}]\;q(t_1)\ldots q(t_m)\,e^{-S(\boldsymbol{q})} \tag{2.39}$$

$$= \frac{1}{\mathcal{Z}(\beta)}\,\mathrm{tr}\left(e^{-(\beta-t_m+t_1)\,h}\,\hat{q}\;e^{-(t_m-t_{m-1})\,h}\,\hat{q}\;\ldots\,e^{-(t_2-t_1)\,h}\,\hat{q}\right) \tag{2.38}$$

Thermodynamic Limit

Since $\beta = n\,\varepsilon$, the thermodynamic limit ($n \to \infty$) in the classical statistics model is the zero temperature limit ($\beta \to \infty$) in the quantum statistics model.

Assuming a non-degenerate 1-particle ground state, which is always the case in quantum mechanics, we have

$$\mathcal{Z}(\beta) = e^{-\beta\mathcal{W}} \underset{\beta\to\infty}{\longrightarrow} e^{-\beta\,e_0}$$

Using

$$\frac{1}{\mathcal{Z}(\beta)}\langle 0 \,\Big|\, e^{-\beta\,h} = \frac{e^{-\beta\,e_0}}{\mathcal{Z}(\beta)}\langle 0 \mid\, = \langle 0 \mid$$

we have

$$\langle q\,(t_1)\,q\,(t_2)\ldots q(t_m)\rangle_{\beta\to\infty} = \langle 0 \,\Big|\, e^{-(t_1-t_m)\,h}\,\hat{q}\;e^{-(t_m-t_{m-1})\,h}\,\hat{q}\;\ldots\,e^{-(t_2-t_1)\,h}\,\hat{q} \,\Big|\, 0\rangle$$

If h were a constant, the exponential factors would cancel out. Hence, we can write

$$\langle q\,(t_1)\,q\,(t_2)\ldots q(t_m)\rangle_{\beta\to\infty}$$

$$= \langle 0 \,\Big|\, e^{-(t_1-t_m)\,(h-e_0)}\,\hat{q}\;e^{-(t_m-t_{m-1})\,(h-e_0)}\,\hat{q}\;\ldots\,e^{-(t_2-t_1)\,(h-e_0)}\,\hat{q} \,\Big|\, 0\rangle$$

$$= \langle 0 \,\Big|\, \hat{q}\;e^{-(t_m-t_{m-1})\,(h-e_0)}\,\hat{q}\;\ldots\,e^{-(t_2-t_1)\,(h-e_0)}\,\hat{q} \,\Big|\, 0\rangle \tag{2.40}$$

Note that eq(2.37a) dictates

$$0 < t_1 \le t_2 \le \ldots \le t_m < \beta \tag{2.40a}$$

In particular, for $m = 1$, we have

$$\langle q\,(t_1)\rangle_{\beta\to\infty} = \langle 0 \mid \hat{q} \mid 0\rangle$$

which is just a time independent constant & has no dynamical significance.

For $m = 2$, we have

$$\langle q\,(t_1)\,q(t_2)\rangle_{\beta\to\infty} = \langle 0 \,\Big|\, \hat{q}\,e^{-(t_2-t_1)\,(h-e_0)}\,\hat{q} \,\Big|\, 0\rangle$$

$$= \sum_k \langle 0 \mid \hat{q}\, e^{-(t_2-t_1)(h-e_0)} \mid k \rangle \langle k \mid \hat{q} \mid 0 \rangle$$
$$= \sum_k e^{-(t_2-t_1)(e_k-e_0)} \langle 0 \mid \hat{q} \mid k \rangle \langle k \mid \hat{q} \mid 0 \rangle$$
$$= \sum_k e^{-(t_2-t_1)(e_k-e_0)} \left| \langle 0 \mid \hat{q} \mid k \rangle \right|^2$$
$$= \left| \langle 0 \mid \hat{q} \mid 0 \rangle \right|^2 + e^{-(t_2-t_1)(e_1-e_0)} \left| \langle 0 \mid \hat{q} \mid 1 \rangle \right|^2 + \ldots$$

Setting $\langle q(t) \rangle = 0$, we have

$$\langle q(t_1)\, q(t_2) \rangle_{\beta\to\infty} = e^{-(t_2-t_1)(e_1-e_0)} \left| \langle 0 \mid \hat{q} \mid 1 \rangle \right|^2 + \ldots$$

Note that the restriction eq(2.40a) can be implemented by replacing all “time” differences by there absolute values. Hence

$$\langle q(t_1)\, q(t_2) \rangle_{\beta\to\infty} = e^{-|t_2-t_1|(e_1-e_0)} \left| \langle 0 \mid \hat{q} \mid 1 \rangle \right|^2 + \ldots$$

Reverting to the 1-D lattice interpretation via eq(2.38a), we have

$$\langle q_{i_1}\, q_{i_2} \rangle_{\beta\to\infty} \propto e^{-|i_2-i_1|\,\varepsilon(e_1-e_0)/\hbar}$$
$$= e^{-|i_2-i_1|\,a/\xi} \qquad (\, a = \text{lattice constant}\,)$$

so that the correlation length ξ is

$$\xi = \frac{\hbar\, a}{\varepsilon\,(e_1 - e_0)}$$

Thus, ξ diverges in the continuum limit $\varepsilon \to 0$.

Keeping the variables t_1, t_2, …, β fixed when $\varepsilon \to 0$, corresponds to measuring distances on the lattice in correlation length units, that is, in macroscopic units.