3.4. The Spectrum of the O(N) Symmetric Rigid Rotator

The group $O(N)$ is the group of all $N \times N$ orthogonal matrices. Since each such matrix also represents a rotation in an N-D space, a rigid rotator in an N-D space belongs to $O(N)$.

The relevant (dimensionless) hamiltonian is

$$H = \frac{1}{2} \mathbf{L}^2 \tag{3.35}$$

where $\mathbf{L}$ is the N-D angular momentum. The components of $\mathbf{L}$ also serve as the N generators of the Lie algebra associated with the Lie group $O(N)$.

Eq(3.35) describes the motion of a particle on an $(N-1)$-D unit sphere S^{N-1}. If the sphere is parametrized in terms of coordinates q^i, eq(3.35) becomes

$$H = \frac{1}{2} g^{ij}(\mathbf{q})\, p_i\, p_j \tag{3.36}$$

where g_{ij} is the metric tensor.

For example, let $\mathbf{r}$ be a unit vector in R^N. Then there exists $\mathbf{q} \in R^{N-1}$ such that

$$\mathbf{r} = \left(\mathbf{q},\ \sqrt{1-\mathbf{q}^2} \right) \qquad \text{i.e.,} \qquad r_i = \begin{cases} q_i & \text{for } i = 1, \ldots, N-1 \\ \sqrt{1-\mathbf{q}^2} & \text{for } i = N \end{cases}$$

where

$$\mathbf{q}^2 = \sum_{i=1}^{N-1} q_i^2 = \delta_{ij}\, d\, q^i\, d\, q^j$$

Proof: Since the metric tensor for R^N is δ_{ij}, we have

$$\mathbf{r}^2 = \mathbf{q}^2 + \left(\sqrt{1-\mathbf{q}^2} \right)^2 = 1 \qquad (\ \mathbf{r} \text{ is indeed a unit vector } \forall\ \mathbf{q} \text{ so that } \mathbf{r} \in S^{N-1}\ )$$

Treating $\mathbf{r}$ as an N-D vector in R^N, the line element is given by

$$d\, r^2 \equiv (d\, \mathbf{r})^2 = \delta_{ij}\, d\, q^i\, d\, q^j + \left(d \sqrt{1-\mathbf{q}^2} \right)^2$$

Using

$$d \sqrt{1-\mathbf{q}^2} = -\frac{\mathbf{q} \cdot d\, \mathbf{q}}{\sqrt{1-\mathbf{q}^2}} = -\frac{\delta_{ij}\, q^i\, d\, q^j}{\sqrt{1-\mathbf{q}^2}}$$

$$\left(d \sqrt{1-\mathbf{q}^2} \right)^2 = \left(1-\mathbf{q}^2\right)^{-1} \delta_{ik}\, q^k\, d\, q^i\, \delta_{jm}\, q^m\, d\, q^j$$

we have

$$d\, r^2 = \left[\delta_{ij} + \left(1-\mathbf{q}^2\right)^{-1} \delta_{ik}\, \delta_{jm}\, q^k\, q^m \right] d\, q^i\, d\, q^j$$

Treating $\mathbf{r}$ as a $(N-1)$-D vector in the curved space S^{N-1} & parametrized by $\mathbf{q}$, we have, by definition,

$$d\, r^2 = g_{ij}\, d\, q^i\, d\, q^j$$

Equating the two expressions for $d\, r^2$, we obtain the metric tensor

$$g_{ij} = \delta_{ij} + \left(1-\mathbf{q}^2\right)^{-1} \delta_{ik}\, \delta_{jm}\, q^k\, q^m \tag{3.37a}$$

$$= \delta_{ij} + \left(1-\mathbf{q}^2\right)^{-1} q_i\, q_j \qquad (\ q_i = \delta_{ik}\, q^k\ )$$

Note that numerically, $q_i = q^i$.

The inverse metric tensor is

$$g^{ij} = \delta^{ij} - q^i q^j \tag{3.37}$$

which is easily verified as follows.

$$g^{ik} g_{kj} = \left(\delta^{ik} - q^i q^k\right) \left[\delta_{kj} + \left(1 - \boldsymbol{q}^2\right)^{-1} q_k q_j\right]$$

Using

$$\delta^{ik} \delta_{kj} = \delta^i_j \qquad\qquad q_k q^k = \boldsymbol{q}^2$$

we have

$$g^{ik} g_{kj} = \delta^i_j + \left(1 - \boldsymbol{q}^2\right)^{-1} q^i q_j - q^i q_j - \left(1 - \boldsymbol{q}^2\right)^{-1} \boldsymbol{q}^2 q^i q_j$$
$$= \delta^i_j$$

Adapting eq(3.23-5) to the present case, we have

$$\langle \boldsymbol{q}'' \mid e^{-\beta H} \mid \boldsymbol{q}' \rangle = \int \left[\sqrt{g[\boldsymbol{q}(t)]}\; d\boldsymbol{q}(t)\right] \exp\left[-\frac{1}{2}\int_0^\beta dt\, g_{ij}[\boldsymbol{q}(t)]\, \dot{q}^i \dot{q}^j\right] \tag{3.38}$$

where g is the determinant of the matrix $\boldsymbol{g}$ representing the metric tensor g_{ij}, and

$$\left[\sqrt{g[\boldsymbol{q}(t)]}\; d\,q(t)\right] = \lim_{\substack{n\to\infty \\ \varepsilon\to 0}} \left(2\pi\hbar\varepsilon\right)^{-nN/2} \prod_{k=1}^{n} \sqrt{\det \boldsymbol{g}(\boldsymbol{q}_k)}$$

In terms of $\boldsymbol{r} \in R^N$, we have $g_{ij} = \delta_{ij}$. Using $\delta(1 - \boldsymbol{r}^2(t))$ to constraint $\boldsymbol{r} \in S^{N-1}$, we have

$$\langle \boldsymbol{r}'' \mid e^{-\beta H} \mid \boldsymbol{r}' \rangle = \int_{\boldsymbol{r}(0)=\boldsymbol{r}'}^{\boldsymbol{r}(\beta)=\boldsymbol{r}''} \left[d\,\boldsymbol{r}(t)\, \delta\left(1 - \boldsymbol{r}^2(t)\right)\right] \exp\left(-\frac{1}{2}\int_0^\beta dt\, \dot{\boldsymbol{r}}^2\right) \tag{3.39}$$

Note that unlike the $O(2)$ case, S^{N-1} for $N > 2$ are simply-connected, which means all loops on it can be contracted to a point. All paths that differ only in the number of extra loops are thus topologically equivalent.

High Temperature Expansion

The classical solution to eq(3.35) is

$$\boldsymbol{L} = \dot{\theta}\, \hat{\boldsymbol{L}} = \text{const}$$

where θ is the rotation angle measured in the plane perpendicular to the rotational axis $\hat{\boldsymbol{L}}$.

The classical path from $\boldsymbol{r}'$ to $\boldsymbol{r}''$ in time β is therefore given by

$$\boldsymbol{r}_c(t) = R(t)\, \boldsymbol{r}'$$

where

$$R(t) = \begin{pmatrix} \cos\left(\theta \frac{t}{\beta}\right) & -\sin\left(\theta \frac{t}{\beta}\right) \\ \sin\left(\theta \frac{t}{\beta}\right) & \cos\left(\theta \frac{t}{\beta}\right) \end{pmatrix} \tag{3.40a}$$

is a rotation in the plane $(\boldsymbol{r}', \boldsymbol{r}'')$ defined by $\boldsymbol{r}'$ & $\boldsymbol{r}''$ and θ is the angle between $\boldsymbol{r}'$ & $\boldsymbol{r}''$ given by

$$\cos\theta = \boldsymbol{r}' \cdot \boldsymbol{r}'' \qquad \text{with} \qquad 0 \le \theta \le \pi$$

Caution: Our $R(t)$ is the inverse of that used in Zinn-Justin's text.

$$\boldsymbol{r}_c(0) = \boldsymbol{r}' = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \& \qquad \boldsymbol{r}_c(\beta) = \boldsymbol{r}'' = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix}$$

In the classical path approximation, we set

$$\boldsymbol{r}(t) = R(t)\, \boldsymbol{\rho}(t)$$

$$\rightarrow \qquad \boldsymbol{r}^2 = \boldsymbol{r}^T \boldsymbol{r} = \boldsymbol{\rho}^T R^T R\, \boldsymbol{\rho} = \boldsymbol{\rho}^T \boldsymbol{\rho} = \boldsymbol{\rho}^2 \qquad (\, T = \text{transpose}\,)$$

The jacobian of the transformation is

$$J = \det R = 1$$

so that eq(3.39) becomes

$$\left\langle \boldsymbol{r}'' \,\middle|\, e^{-\beta H} \,\middle|\, \boldsymbol{r}' \right\rangle = \int_{\boldsymbol{\rho}(0) = \boldsymbol{\rho}(\beta) = \boldsymbol{r}'} \left[d\,\boldsymbol{\rho}(t)\, \delta\big(1 - \boldsymbol{\rho}^2(t)\big)\right] \exp[-S(\boldsymbol{\rho})] \tag{3.40}$$

where

$$S(\boldsymbol{\rho}) = \frac{1}{2} \int_0^\beta dt \left\{ \frac{d}{dt} [R(t)\, \boldsymbol{\rho}(t)] \right\}^2$$

Since $R(t)$ has no effect on any vector that is perpendicular to $(\boldsymbol{r}', \boldsymbol{r}'')$, it acts like the identity in the subspace orthogonal to $(\boldsymbol{r}', \boldsymbol{r}'')$. We therefore decompose $\boldsymbol{\rho}$ as

$$\boldsymbol{\rho} = \boldsymbol{\rho}_T + u\, \hat{\boldsymbol{u}} + v\, \hat{\boldsymbol{v}}$$

(3.40b)

where $\boldsymbol{\rho}_T$ is the component orthogonal to $(\boldsymbol{r}', \boldsymbol{r}'')$, while $\hat{\boldsymbol{u}}$ & $\hat{\boldsymbol{v}}$ are any pair of orthogonal unit vectors that span $(\boldsymbol{r}', \boldsymbol{r}'')$. The natural choice is

$$\hat{\boldsymbol{u}} = \boldsymbol{r}' = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \& \qquad \hat{\boldsymbol{v}} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Consideration of the B.C. gives

$$\boldsymbol{r}(0) = \boldsymbol{r}' \qquad \& \qquad R(0) = \boldsymbol{I}$$

$$\to \quad \boldsymbol{\rho}(0) = \boldsymbol{r}' = \hat{\boldsymbol{u}} \qquad \text{so that } \boldsymbol{\rho}_T(0) = 0\,, \quad u(0) = 1 \quad \& \quad v(0) = 0 \tag{3.42a}$$

$$\boldsymbol{r}(\beta) = \boldsymbol{r}'' \in (\boldsymbol{r}', \boldsymbol{r}'') \quad \to \quad \boldsymbol{\rho}_T(\beta) = 0\,, \quad u(\beta) = \cos\theta \quad \& \quad v(\beta) = \sin\theta$$

Taking the square of eq(3.40b) gives the constraint

$$\boldsymbol{\rho}^2 = \boldsymbol{\rho}_T^2 + u^2 + v^2 = 1 \tag{3.42}$$

Operating with R on eq(3.40b) gives

$$\begin{aligned} R\,\boldsymbol{\rho} &= \boldsymbol{\rho}_T + u\, R\, \hat{\boldsymbol{u}} + v\, R\, \hat{\boldsymbol{v}} \\ &= \boldsymbol{\rho}_T + u \begin{pmatrix} \cos\left(\theta \frac{t}{\beta}\right) \\ \sin\left(\theta \frac{t}{\beta}\right) \end{pmatrix} + v \begin{pmatrix} -\sin\left(\theta \frac{t}{\beta}\right) \\ \cos\left(\theta \frac{t}{\beta}\right) \end{pmatrix} \\ &= \boldsymbol{\rho}_T + \left[u \cos\left(\theta \frac{t}{\beta}\right) - v \sin\left(\theta \frac{t}{\beta}\right) \right] \hat{\boldsymbol{u}} + \left[u \sin\left(\theta \frac{t}{\beta}\right) + v \cos\left(\theta \frac{t}{\beta}\right) \right] \hat{\boldsymbol{v}} \end{aligned}$$

$$\begin{aligned} \therefore \quad \frac{d}{dt}[R(t)\, \boldsymbol{\rho}(t)] = \dot{\boldsymbol{\rho}}_T &+ \left[\dot{u} \cos\left(\theta \frac{t}{\beta}\right) - \dot{v} \sin\left(\theta \frac{t}{\beta}\right) - \frac{\theta}{\beta} u \sin\left(\theta \frac{t}{\beta}\right) - \frac{\theta}{\beta} v \cos\left(\theta \frac{t}{\beta}\right) \right] \hat{\boldsymbol{u}} \\ &+ \left[\dot{u} \sin\left(\theta \frac{t}{\beta}\right) + \dot{v} \cos\left(\theta \frac{t}{\beta}\right) + \frac{\theta}{\beta} u \cos\left(\theta \frac{t}{\beta}\right) - \frac{\theta}{\beta} v \sin\left(\theta \frac{t}{\beta}\right) \right] \hat{\boldsymbol{v}} \end{aligned}$$

In the sum of the square of the coefficients of $\hat{\boldsymbol{u}}$ & $\hat{\boldsymbol{v}}$, the cross-terms $\dot{u}\,\dot{v}$, $\dot{u}\,u$ & $\dot{v}\,v$ cancel out so that

$$\to \quad \frac{d}{dt}[R(t)\, \boldsymbol{\rho}(t)]^2 = \dot{\boldsymbol{\rho}}_T^2 + \dot{u}^2 + \dot{v}^2 + \left(\frac{\theta}{\beta}\right)^2 (u^2 + v^2) + 2\, \frac{\theta}{\beta} (-\dot{u}\, v + u\, \dot{v})$$

$$\therefore \quad S(\boldsymbol{\rho}) = \frac{1}{2} \int_0^\beta dt \left\{ \dot{\boldsymbol{\rho}}_T^2 + \dot{u}^2 + \dot{v}^2 + \left(\frac{\theta}{\beta}\right)^2 (u^2 + v^2) + 2\, \frac{\theta}{\beta} (-\dot{u}\, v + u\, \dot{v}) \right\} \tag{3.41}$$

Since the classical path means setting $\boldsymbol{\rho} = \boldsymbol{r}'$, it corresponds to the case $\boldsymbol{\rho}_T = 0$, $u = 1$ & $v = 0$.

Eq(3.42) indicates that fluctuations about the classical path involve small $\boldsymbol{\rho}_T$ & v.

We therefore eliminate u using

$$u = \sqrt{1 - \boldsymbol{\rho}_T^2 - v^2}$$

& expand $S(\boldsymbol{\rho})$ in powers of $\boldsymbol{\rho}_T$ & v.

Using

$$\dot{u} = -\frac{\boldsymbol{\rho}_T \cdot \dot{\boldsymbol{\rho}}_T + v\,\dot{v}}{\sqrt{1 - \boldsymbol{\rho}_T^2 - v^2}}$$

we have

$$S(\boldsymbol{\rho}) = \frac{1}{2}\int_0^\beta d\,t \left\{ \dot{\boldsymbol{\rho}}_T^2 + \frac{\left(\boldsymbol{\rho}_T \cdot \dot{\boldsymbol{\rho}}_T + v\,\dot{v}\right)^2}{1 - \boldsymbol{\rho}_T^2 - v^2} + \dot{v}^2 + \left(\frac{\theta}{\beta}\right)^2 \left(1 - \boldsymbol{\rho}_T^2\right) \right.$$

$$\left. + 2\,\frac{\theta}{\beta} \left(\frac{\boldsymbol{\rho}_T \cdot \dot{\boldsymbol{\rho}}_T + v\,\dot{v}}{\sqrt{1 - \boldsymbol{\rho}_T^2 - v^2}}\, v + \sqrt{1 - \boldsymbol{\rho}_T^2 - v^2}\;\dot{v} \right) \right\}$$

Keeping only the leading order term, we have

$$S_0(\boldsymbol{\rho}) = \frac{1}{2}\int_0^\beta d\,t \left(\frac{\theta}{\beta}\right)^2 = \frac{\theta^2}{2\,\beta}$$

Whereas the classical path approximation is valid only in the high temperature ($\beta \to \infty$) limit, we also require S_0 to be the dominant term in S. Hence, S_0 must be of order 1 so that $\theta = O\left(\sqrt{\beta}\right)$.

The next order terms give rise to Gaussian integrals in the path integral,

$$S_1 = \frac{1}{2}\int_0^\beta d\,t \left\{ \dot{\boldsymbol{\rho}}_T^2 - \left(\frac{\theta}{\beta}\right)^2 \boldsymbol{\rho}_T^2 + \dot{v}^2 + 2\,\frac{\theta}{\beta}\,\dot{v} \right\} \qquad (3.41a)$$

$$= S_T + S_v$$

where

$$S_T = \frac{1}{2}\int_0^\beta d\,t \left\{ \dot{\boldsymbol{\rho}}_T^2 - \left(\frac{\theta}{\beta}\right)^2 \boldsymbol{\rho}_T^2 \right\}$$

$$S_v = \frac{1}{2}\int_0^\beta d\,t \left(\dot{v}^2 + 2\,\frac{\theta}{\beta}\,\dot{v} \right)$$

Eq(3.40) thus becomes

$$\left\langle \boldsymbol{r}'' \,\middle|\, e^{-\beta H} \,\middle|\, \boldsymbol{r}' \right\rangle \approx e^{-\theta^2/2\beta}\, \mathcal{I}_T\, \mathcal{I}_v$$

where

$$\mathcal{I}_T = \int [\,d\,\boldsymbol{\rho}_T(t)\,]\, e^{-S_T}$$

$$\mathcal{I}_v = \int [\,d\,v(t)\,]\, e^{-S_v}$$

Since $\boldsymbol{\rho} \in R^N$, eq(3.40b) indicates $\boldsymbol{\rho}_T \in R^{N-2}$ & $v \in R$.

From eq(3.42a), we have

$$\boldsymbol{\rho}_T(0) = \boldsymbol{\rho}_T(\beta) = 0$$

so that $\boldsymbol{\rho}_T$ is a periodic function that can be expanded as a Fourier series (with $\beta \to \infty$)

$$\boldsymbol{\rho}_T(t) = C \sum_{n=1}^{\beta} \tilde{\boldsymbol{\rho}}_n \sin\frac{n\,\pi\,t}{\beta} \qquad (C = \text{const})$$

To determine C, we try to match the $q(t)$ equation just above eq(2.57) as follows

$$\boldsymbol{\rho}_T(t) = \frac{C}{2i}\sum_{n=1}^{\beta} \tilde{\boldsymbol{\rho}}_n \left(e^{i n\pi t/\beta} - e^{-i n\pi t/\beta}\right)$$

$$= \frac{C}{2i}\sum_{n=-\beta}^{\beta} \tilde{\boldsymbol{\rho}}_n\, e^{i n\pi t/\beta} \qquad\qquad (\ \tilde{\boldsymbol{\rho}}_{-n} = -\tilde{\boldsymbol{\rho}}_n\ )$$

$$= \frac{1}{\sqrt{2\beta}}\sum_{n=-2\beta/2}^{2\beta/2} \tilde{\boldsymbol{\rho}}_n\, e^{2 i n\pi t/2\beta}$$

$$\rightarrow \qquad C = i\sqrt{\frac{2}{\beta}}$$

$$\therefore \qquad \boldsymbol{\rho}_T(t) = i\sqrt{\frac{2}{\beta}}\sum_{n=1}^{\beta\to\infty} \tilde{\boldsymbol{\rho}}_n \sin\frac{n\pi t}{\beta}$$

Setting

$$\boldsymbol{\rho}_n = i\,\tilde{\boldsymbol{\rho}}_n$$

we have

$$\tilde{\boldsymbol{\rho}}_n\cdot\tilde{\boldsymbol{\rho}}_{-n} = \boldsymbol{\rho}_n^2$$

$$\boldsymbol{\rho}_T(t) = \sqrt{\frac{2}{\beta}}\sum_{n=1}^{\beta\to\infty} \boldsymbol{\rho}_n \sin\frac{n\pi t}{\beta}$$

(3.41b)

For each component of $\boldsymbol{\rho}_T$, the jacobian of the transformation is

$$J(\beta) = \left(\frac{2}{\beta}\right)^{\beta/2} \det \boldsymbol{A} \qquad \text{with} \qquad A_{jk} = \sin\frac{jk\pi}{\beta}$$

$$\rightarrow \qquad \boldsymbol{\rho}_T^2(t) = \frac{2}{\beta}\sum_{m,n=1}^{\beta} \boldsymbol{\rho}_n\cdot\boldsymbol{\rho}_m \sin\frac{n\pi t}{\beta}\sin\frac{m\pi t}{\beta}$$

$$\dot{\boldsymbol{\rho}}_T(t) = \sqrt{\frac{2}{\beta}}\sum_{n=1}^{\beta} \frac{n\pi}{\beta}\boldsymbol{\rho}_n \cos\frac{n\pi t}{\beta}$$

$$\dot{\boldsymbol{\rho}}_T^2(t) = \frac{2}{\beta}\left(\frac{\pi}{\beta}\right)^2\sum_{m,n=1}^{\beta} n\,m\,\boldsymbol{\rho}_n\cdot\boldsymbol{\rho}_m \cos\frac{n\pi t}{\beta}\cos\frac{m\pi t}{\beta}$$

$$\therefore \qquad \dot{\boldsymbol{\rho}}_T^2 - \left(\frac{\theta}{\beta}\right)^2\boldsymbol{\rho}_T^2 = \frac{2}{\beta}\left(\frac{\pi}{\beta}\right)^2\sum_{m,n=1}^{\beta} \boldsymbol{\rho}_n\cdot\boldsymbol{\rho}_m\left[n\,m\cos\frac{n\pi t}{\beta}\cos\frac{m\pi t}{\beta} - \left(\frac{\theta}{\pi}\right)^2\sin\frac{n\pi t}{\beta}\sin\frac{m\pi t}{\beta}\right]$$

Using

$$\int_0^\beta dt\cos\frac{n\pi t}{\beta}\cos\frac{m\pi t}{\beta} = \frac{\beta}{2}\delta_{nm} \qquad \& \qquad \int_0^\beta dt\sin\frac{n\pi t}{\beta}\sin\frac{m\pi t}{\beta} = \frac{\beta}{2}\delta_{nm}$$

we have

$$\frac{1}{2}\int_0^\beta dt\left\{\dot{\boldsymbol{\rho}}_T^2 - \left(\frac{\theta}{\beta}\right)^2\boldsymbol{\rho}_T^2\right\} = \frac{1}{2}\left(\frac{\pi}{\beta}\right)^2\sum_{n=1}^{\beta}\boldsymbol{\rho}_n^2\left[n^2 - \left(\frac{\theta}{\pi}\right)^2\right] \qquad (3.41c)$$

Thus, each of the $N-2$ components of $\boldsymbol{\rho}_n$ gives the same contribution to $\mathcal{I}_T$, namely,

$$\int_{-\infty}^{\infty} d\rho \exp\left\{-\frac{1}{2}\left(\frac{\pi}{\beta}\right)^2 \rho^2 \left[n^2 - \left(\frac{\theta}{\pi}\right)^2\right]\right\} = \sqrt{\frac{2\beta^2}{\pi\left[n^2 - \left(\frac{\theta}{\pi}\right)^2\right]}}$$

$$= \sqrt{\frac{2\beta^2}{\pi}} \frac{1}{n\sqrt{1-\left(\frac{\theta}{n\pi}\right)^2}}$$

$$\therefore \qquad \mathcal{I}_T = \left\{J(\beta)\left(\frac{2\beta^2}{\pi}\right)^{\beta/2} \frac{1}{\beta\,!} \prod_{n=1}^{\beta}\left[1-\left(\frac{\theta}{n\pi}\right)^2\right]^{-1/2}\right\}^{N-2}$$

As $\beta \to \infty$, Sterling's formula gives

$$\frac{\beta^\beta}{\beta!} \approx \frac{e^\beta}{\sqrt{2\pi\beta}}$$

Using

$$\prod_{n=1}^{\beta}\left[1-\left(\frac{\theta}{n\pi}\right)^2\right] = \frac{\sin\theta}{\theta} \qquad \text{[see G-R, eq(1.431.1)]}$$

we have

$$\mathcal{I}_T = \left\{J(\beta)\frac{e^\beta}{\sqrt{2\pi\beta}}\sqrt{\frac{\theta}{\sin\theta}}\right\}^{N-2}$$

For $\mathcal{I}_v$, we start by writing

$$S_v = \frac{1}{2}\int_0^\beta dt\left[\left(\dot{v}+\frac{\theta}{\beta}\right)^2 - \left(\frac{\theta}{\beta}\right)^2\right]$$

$$= -\frac{\theta^2}{2\beta} + \frac{1}{2}\int_0^\beta dt\,\dot{w}^2 \qquad \left(\dot{w} = \dot{v} + \frac{\theta}{\beta}\right)$$

Using eq(3.42a), we have

$$w = v + \frac{\theta}{\beta}t$$

$$w(0) = v(0) = 0$$

$$w(\beta) = v(\beta) + \theta = \sin\theta + \theta$$

By eq(2.10), we have

$$\mathcal{I}_v = e^{\theta^2/2\beta}\frac{e^{-(\sin\theta+\theta)^2/2\beta}}{\sqrt{2\pi\beta}}$$

$$\therefore \qquad \left\langle \boldsymbol{r}'' \,\middle|\, e^{-\beta H} \,\middle|\, \boldsymbol{r}' \right\rangle \approx \frac{1}{\sqrt{2\pi\beta}}\exp\left[-\frac{(\sin\theta+\theta)^2}{2\beta}\right]\left\{J(\beta)\frac{e^\beta}{\sqrt{2\pi\beta}}\sqrt{\frac{\theta}{\sin\theta}}\right\}^{N-2}$$

$$= K(\beta)\exp\left[-\frac{(\sin\theta+\theta)^2}{2\beta}\right]\left(\frac{\theta}{\sin\theta}\right)^{(N-2)/2} \qquad (3.43a)$$

where

$$K(\beta) = \frac{1}{\sqrt{2\pi\beta}} \left(J(\beta) \frac{e^{\beta}}{\sqrt{2\pi\beta}} \right)^{N-2} = \left(J(\beta)\, e^{\beta} \right)^{N-2} (2\pi\beta)^{-(N-1)/\beta}$$

Difference between eq(3.43a) & eq(3.43) in Zinn-Justin's text is due to the fact that the latter treated

1. $\mathcal{I}_\nu$ as independent of θ.
2. $J(\beta) = 1$.

Spectral Extraction

$$\langle \mathbf{r}'' \mid e^{-\beta H} \mid \mathbf{r}' \rangle = \sum_l \langle \mathbf{r}'' \mid e^{-\beta H} \mid l \rangle \langle l \mid \mathbf{r}' \rangle \qquad \text{where} \qquad H \mid l \rangle = E_l \mid l \rangle$$
$$= \sum_l e^{-\beta E_l} \langle \mathbf{r}'' \mid l \rangle \langle l \mid \mathbf{r}' \rangle$$
$$= \sum_l e^{-\beta E_l}\, \psi_l(\mathbf{r}'')\, \psi_l^*(\mathbf{r}')$$

Assuming $\{\psi_l\}$ are orthonormal, we have

$$\int d\mathbf{r}''\, \psi_k^*(\mathbf{r}) \langle \mathbf{r}'' \mid e^{-\beta H} \mid \mathbf{r}' \rangle = \int d\mathbf{r}'' \sum_l e^{-\beta E_l}\, \psi_k^*(\mathbf{r}'')\, \psi_l(\mathbf{r}'')\, \psi_l^*(\mathbf{r}')$$
$$= e^{-\beta E_k}\, \psi_k^*(\mathbf{r}')$$

$$\to \qquad e^{-\beta E_l} = \int d\mathbf{r}'' \frac{\psi_l^*(\mathbf{r}'')}{\psi_l^*(\mathbf{r}')} \langle \mathbf{r}'' \mid e^{-\beta H} \mid \mathbf{r}' \rangle \qquad (3.43b)$$

where $\qquad H\,\psi_l(\mathbf{r}) = E_l\, \psi_l(\mathbf{r})$

n-Sphere

Ref: All properties of the n-sphere used here are derived in the file n-sphere.pdf.

For an $(N-1)$-D sphere S^{N-1} embedded in N-D space, the spherical coordinates are given by

$$\boldsymbol{\theta} = \{\theta_1, \ .., \ \theta_{N-1}\} = \{\theta_1, \ .., \ \theta_{N-2}, \phi\}$$

where $\qquad \theta_1, \ ..., \ \theta_{N-2} \in [0, \pi] \qquad$ but $\qquad \phi \in [0, 2\pi]$

As given by eq(16c) in n-sphere.pdf, the spherical Laplacian $\nabla^2_{S^{N-1}}$ satisfies

$$\nabla^2_{S^{N-1}} Y(\boldsymbol{\theta}) = -l\,(l + N - 2)\, Y(\boldsymbol{\theta})$$

In the spectral extraction eq(3.43a), $\langle \mathbf{r}'' \mid e^{-\beta H} \mid \mathbf{r}' \rangle$ is a function of the angular separation θ only.
Using the results of n-sphere.pdf, we therefore set $\theta = \theta_1$ & [see eq(16b) of n-sphere.pdf],

$$Y(\boldsymbol{\theta}) = Y_{1\,l}(\cos\theta_1) = C_l^{(N-2)/2}(\cos\theta_1) \qquad (3.44a)$$

where $C_l^{\alpha}(x)$ are the Gegenbauer (or ultraspherical) polynomials.

$C_n^{\alpha}(x)$ are orthogonal polynomials with normalization [see G-R, eq(7.313.1)]

$$\int_{-1}^{1} d\,x \left(1 - x^2\right)^{(2\nu-1)/2} C_m^{\nu}(x)\, C_n^{\nu}(x) = \delta_{m\,n} \frac{\pi\, 2^{1-2\nu}\, \Gamma(2\nu + n)}{n!\,(n+\nu)\,[\Gamma(\nu)]^2}$$
$$= \int_0^{\pi} d\,\theta \sin^{2\nu}\theta\, C_m^{\nu}(\cos\theta)\, C_n^{\nu}(\cos\theta)$$

Another important relation is [see G-R, eq(7.311.1)] that for $m \neq 0$,

$$\int_{-1}^{1} d\,x\left(1-x^2\right)^{(2\,v-1)/2}\ C_m^v(x) = \begin{cases} 0 & \text{for} \quad m \neq 0 \\ \dfrac{\sqrt{\pi}\ \Gamma[(2\,m+1)/2\,]}{v\,!} & \text{for} \quad m = 0 \end{cases} \tag{3.44b}$$

$$= \int_0^{\pi} d\,\theta \sin^{2\,v}\theta\ C_m^v(\cos\theta)$$

Using eq(3.44a) on eq(3.43b), we have

$$e^{-\beta\,E_l} \propto \int_0^{\pi} d\,\theta\ \sin^{N-2}\theta\, C_l^{(N-2)/2}(\cos\theta)\left(\frac{\theta}{\sin\theta}\right)^{(N-2)/2} \exp\left[-\frac{(\sin\theta+\theta)^2}{2\,\beta}\right]$$

$$= \int_0^{\pi} d\,\theta\ C_l^{(N-2)/2}(\cos\theta)\,(\theta\sin\theta)^{(N-2)/2}\exp\left[-\frac{(\sin\theta+\theta)^2}{2\,\beta}\right] \tag{3.45a}$$

where we've set $k_1 = l$ since $k_j = 0\ \forall\ j > 1$.

For $\beta \to 0$, the exponential vanishes except for $\theta \to 0$. Eq(3.45a) can therefore be approximated by

$$e^{-\beta\,E_l} \propto \int_{-\infty}^{\infty} d\,\theta\ C_l^{(N-2)/2}(\cos\theta)\ \theta^{N-2}\exp\left(-\frac{2\,\theta^2}{\beta}\right) \tag{3.45b}$$

Using the *Mathematica* code

```
GegenbauerC[(n - 2) / 2, ℓ, Cos[θ]] + O[θ]^4
```

we get

$$C_l^{(N-2)/2}(\cos\theta) = A\left\{1 - \frac{(N-2)\,(4\,l+N-2)}{4\,(2\,l+1)}\ \theta^2 + O\left(\theta^4\right)\right\} \tag{3.45c}$$

where

$$A = C_l^{(N-2)/2}(1) = \frac{2^{1-2\,l}\sqrt{\pi}\ \Gamma\left(2\,l+\frac{1}{2}\,(N-2)\right)}{(l-1)!\ \Gamma\left(\frac{N}{2}\right)\Gamma\left(l+\frac{1}{2}\right)}$$

Note that the coefficient of θ^2 in eq(3.45c) differs considerably from that given by Zinn-Justin. However, eq(3.45c) is the correct expression because it gives better numerical results.

Putting eq(3.45c) into eq(3.45b), we get

$$e^{-\beta\,E_l} \propto A\int_{-\infty}^{\infty} d\,\theta\left\{1 - \frac{(N-2)\,(4\,l+N-2)}{4\,(2\,l+1)}\ \theta^2 + \dots\right\}\theta^{N-2}\exp\left(-\frac{2\,\theta^2}{\beta}\right)$$

$$= B\left(1 - \frac{(N-1)\,(N-2)\,(4\,l+N-2)}{16\,(2\,l+1)}\,\beta + O\left(\beta^2\right)\right)$$

where

$$B = 16\left[1+(-)^N\right]2^{-(N+9)/2}\ \beta^{-(N-1)/2}\ \Gamma[(N-1)/2]\,A$$

Writing

$$e^{-\beta\,E_l} = e^{-\beta\,E_0}\left(1 - \frac{(N-1)\,(N-2)\,(4\,l+N-2)}{16\,(2\,l+1)}\,\beta + O\left(\beta^2\right)\right)$$

$$\approx e^{-\beta\,E_0}\exp\left(-\frac{(N-1)\,(N-2)\,(4\,l+N-2)}{16\,(2\,l+1)}\,\beta\right)$$

we have

$$E_l = E_0 + \frac{(N-1)\,(N-2)\,(4\,l+N-2)}{16\,(2\,l+1)}$$

which differs considerably from the correct result [see eq(16c) of n-sphere.pdf]

$$E_l = E_0 + \frac{1}{2} l (l + N - 2) \tag{3.46}$$