3.3. The Spectrum of the O(2) Symmetric Rigid Rotator

The (dimensionless) hamiltonian for an $O(2)$ rigid rotator is

$$H = -\frac{1}{2}\frac{\partial^2}{\partial\theta^2} \qquad (3.28)$$

$$H\psi = -\frac{1}{2}\frac{\partial^2\psi}{\partial\theta^2} = E\psi$$

$\rightarrow$ $\psi = c_l e^{il\theta}$

with $E_l = \frac{1}{2} l^2 \qquad (3.29)$

ψ is single-valued, i.e.,

$$\psi(\theta + 2\pi n) = \psi(\theta) \qquad \forall\ n \in \mathbb{Z} \text{ (integers)}$$

$\rightarrow$ $l \in \mathbb{Z}$

i.e., the spectrum is discrete.

Writing

$$H = \frac{1}{2}p^2 = \frac{1}{2}\dot{\theta}^2$$

where

$$p = -i\frac{\partial}{\partial\theta} = \dot{\theta}$$

is the angular momentum, the Lagrangian is

$$L = p\dot{\theta} - H = \frac{1}{2}\dot{\theta}^2 \qquad \text{(real time)}$$

$$= -\frac{1}{2}\left(\frac{d\theta}{dt}\right)^2 \qquad \text{(imaginary time)}$$

The imaginary time action is

$$S(t'', t') = -\int_{t'}^{t''} dt\, L = \frac{1}{2}\int_{t'}^{t''} dt \left(\frac{d\theta}{dt}\right)^2$$

Matrix elements of the evolution operator $e^{-\beta H}$ are

$$\langle \theta'' \mid e^{-\beta H} \mid \theta' \rangle = \int_{\theta(0)=\theta'}^{\theta(\beta)=\theta''} [d\theta(t)]\, e^{-S(\beta,0)}$$

$$= \int_{\theta(0)=\theta'}^{\theta(\beta)=\theta''} [d\theta(t)] \exp\left[-\frac{1}{2}\int_0^\beta dt \left(\frac{d\theta}{dt}\right)^2\right] \qquad (3.30)$$

The Euler-Lagrange eq. is

$$\frac{d^2\theta}{dt^2} = 0 \qquad \rightarrow \qquad \frac{d\theta}{dt} = \text{const} \qquad (3.30a)$$

Since the points $\{\theta + 2\pi n \mid n \in \mathbb{Z}\}$ are all equivalent to the point θ, in going from θ' to θ'', one can taking an infinite number of distinct paths that goes from θ' to $\theta'' + 2\pi n$.

For the classical paths that satisfy eq(3.30a), we have

$$\theta_c(t) = \theta' + t\,\frac{\theta'' - \theta' + 2\pi n}{\beta} \qquad n \in \mathbb{Z} \qquad (3.31)$$

These paths are topologically distinct since they cannot be continuously deformed into each other without leaving the manifold of motion (a circle for our rotator).

As usual, we set

$$\theta(t) = \theta_c(t) + u(t) \qquad (3.32)$$

with

$$u(\beta) = u(0) = 0$$

Hence,

$$\frac{d\theta}{dt} = \frac{\theta'' - \theta' + 2\pi n}{\beta} + \frac{du}{dt}$$

$$\left(\frac{d\theta}{dt}\right)^2 = \left(\frac{\theta'' - \theta' + 2\pi n}{\beta}\right)^2 + 2\left(\frac{\theta'' - \theta' + 2\pi n}{\beta}\right)\frac{du}{dt} + \left(\frac{du}{dt}\right)^2$$

so that

$$S(\beta, 0) = \frac{1}{2\beta}(\theta'' - \theta' + 2\pi n)^2 + \frac{1}{2}\int_0^\beta dt \left(\frac{du}{dt}\right)^2$$

Hence,

$$\langle \theta'' \mid e^{-\beta H} \mid \theta' \rangle = \mathcal{N}(\beta) \sum_{n=-\infty}^{\infty} \exp\left[-\frac{1}{2\beta}(\theta'' - \theta' + 2\pi n)^2\right] \qquad (3.33)$$

where

$$\mathcal{N}(\beta) = \int_{u(\beta)=u(0)=0} [du] \exp\left[-\frac{1}{2}\int_0^\beta dt \left(\frac{du}{dt}\right)^2\right]$$

$$= \frac{1}{\sqrt{2\pi\beta}} \qquad \text{[see eq(2.66b \& 2.68)]}$$

Since $\langle \theta'' \mid e^{-\beta H} \mid \theta' \rangle$ is a periodic function of $\theta'' - \theta'$, it has a Fourier series expansion

$$\langle \theta'' \mid e^{-\beta H} \mid \theta' \rangle = \sum_{l=-\infty}^{\infty} c_l\, e^{i l (\theta'' - \theta')} \qquad (3.34)$$

$$2\pi c_l = \int_0^{2\pi} d(\theta'' - \theta')\, e^{i l (\theta'' - \theta')} \langle \theta'' \mid e^{-\beta H} \mid \theta' \rangle$$

$$= \frac{1}{\sqrt{2\pi\beta}} \sum_{n=-\infty}^{\infty} \int_0^{2\pi} d\theta \exp\left[-\frac{1}{2\beta}(\theta + 2\pi n)^2 + i l \theta\right]$$

$$= \frac{1}{\sqrt{2\pi\beta}} \sum_{n=-\infty}^{\infty} \int_{2\pi n}^{2\pi(n+1)} d\varphi \exp\left(-\frac{1}{2\beta}\varphi^2 + i l \varphi\right) \qquad \varphi = \theta + 2\pi n$$

$$= \frac{1}{\sqrt{2\pi\beta}} \int_{-\infty}^{\infty} d\varphi \exp\left(-\frac{1}{2\beta}\varphi^2 + i l \varphi\right)$$

$$= \exp\left(-\frac{1}{2} l^2 \beta\right)$$

$$= \exp(-E_l \beta)$$