11.1.2: Doing the Path Integral - the Free Particle

The density matrix for the free particle

$$H = \frac{P^2}{2m}$$

will be calculated by doing the discrete path integral explicitly and taking the limit $P \rightarrow \infty$ at the end.

The density matrix expression is

$$\rho(x, x'; \beta) = \lim_{P \rightarrow \infty} \left(\frac{mP}{2\pi\beta\hbar^2}\right)^{P/2} \int dx_2 \cdots dx_P exp \left[-\frac{mP}{2\beta\hbar^2} \sum_{i=1}^{P} (x_{i+1} - x_i)^2\right] |_{x_1 = x, x_{P+1} = x'}$$

Let us make a change of variables to

$$\begin{aligned} u_1 &= x_1 \\ u_k &= x_k - \tilde{x}_k \\ \tilde{x}_k &= \frac{(k-1)x_{k+1} + x_1}{k} \end{aligned} \tag{11.1.2.1}$$

The inverse of this transformation can be worked out explicitly, giving

$$x_1 = u_1$$

$$x_k = \sum_{l=1}^{P+1} \frac{k-1}{l-1} u_l + \frac{P-k+1}{P} u_1$$

The Jacobian of the transformation is simply

$$J = \det \begin{pmatrix} 1 & -1/2 & 0 & 0 & \cdots & \\ 0 & 1 & -2/3 & 0 & \cdots & \\ 0 & 0 & 1 & -3/4 & \cdots & \\ 0 & 0 & 0 & 1 & \cdots & \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdots \end{pmatrix} = 1$$

Let us see what the effect of this transformation is for the case $P = 3$. For $P = 3$, one must evaluate

$$(x_1 - x_2)^2 + (x_2 - x_3)^2 + (x_3 - x_4)^2 = (x - x_2)^2 + (x_2 - x_3)^2 + (x_3 - x')^2$$

According to the inverse formula,

$$x_1 = u_1 \tag{11.1.2.2}$$

$$x_2 = u_2 + \frac{1}{2}u_3 + \frac{1}{3}x' + \frac{2}{3}x \tag{11.1.2.3}$$

$$x_3 = u_3 + \frac{2}{3}x' + \frac{1}{3}x \tag{11.1.2.4}$$

Thus, the sum of squares becomes

$$(x - x_2)^2 + (x_2 - x_3)^2 + (x_3 - x')^2 = (2u_2^2 + \frac{3}{2}u_3^2 + \frac{1}{3}(x - x')^2 = \frac{2}{2-1}u_2^2 + \frac{3}{3-1}u_3^2 + \frac{1}{3}(x - x')^2 \tag{11.1.2.5}$$

From this simple example, the general formula can be deduced:

$$\sum_{i=1}^{P} (x_{i+1} - x_i)^2 = \sum_{k=2}^{P} \frac{k}{k-1} u_k^2 + \frac{1}{P}(x - x')^2$$

Thus, substituting this transformation into the integral gives

$$\rho(x,x';\beta) = \left(\frac{m}{2\pi\beta\hbar^2}\right)^{1/2} \prod_{k=2}^{P} \left(\frac{m_k P}{2\pi\beta\hbar^2}\right)^{1/2} \int du_2 \cdots du_P exp\left[-\sum_{k=2}^{P} \frac{m_k P}{2\beta\hbar^2} u_k^2\right] exp\left[-\frac{m}{2\beta\hbar^2}(x-x')^2\right]$$

where

$$m_k = \frac{k}{k-1} m$$

and the overall prefactor has been written as

$$\left(\frac{mP}{2\pi\beta\hbar^2}\right)^{P/2} = \left(\frac{m}{2\pi\beta\hbar^2}\right)^{1/2} \prod_{k=2}^{P} \left(\frac{m_k P}{2\pi\beta\hbar^2}\right)^{1/2}$$

Now each of the integrals over the u variables can be integrated over independently, yielding the final result

$$\rho(x,x';\beta) = \left(\frac{m}{2\pi\beta\hbar^2}\right)^{1/2} \exp\left[-\frac{m}{2\beta\hbar^2}(x-x')^2\right]$$

In order to make connection with classical statistical mechanics, we note that the prefactor is just $\frac{1}{\lambda}$, where λ

$$\lambda = \left(\frac{2\pi\beta\hbar^2}{m}\right)^{1/2} = \left(\frac{\beta h^2}{2\pi m}\right)^{1/2}$$

is the kinetic prefactor that showed up also in the classical free particle case. In terms of λ, the free particle density matrix can be written as

$$\rho(x,x';\beta) = \frac{1}{\lambda} e^{-\pi(x-x')^2/\lambda^2}$$

Thus, we see that λ represents the spatial width of a free particle at finite temperature, and is called the "**thermal de Broglie wavelength**."