# 11.1.3: Dominant Paths in the Propagator and Density Matrix

Let us first consider the real time quantum propagator. The quantity appearing in the exponential is an integral of

$$\frac{1}{2}m\dot{x}^2 - U(x) \equiv L(x,\dot{x})$$

which is known as the Lagrangian in classical mechanics. We can ask, which paths will contribute most to the integral

$$\int_0^t ds\left[\frac{m}{2}\dot{x}^2(s) - U(x(s))\right] = \int_0^t ds L(x(s),\dot{x}(s)) = S[x]$$

known as the *action integral*. Since we are integrating over a complex exponential $\exp(\frac{iS}{\hbar})$, which is oscillatory, those paths away from which small deviations cause no change in $S$ (at least to first order) will give rise to the dominant contribution. Other paths that cause $\exp(\frac{iS}{\hbar})$ to oscillate rapidly as we change from one path to another will give rise to phase decoherence and will ultimately cancel when integrated over. Thus, we consider two paths $x(s)$ and a nearby one constructed from it $x(s)+\delta x(s)$ and demand that the change in $S$ between these paths be 0

$$S[x+\delta x] - S[x] = 0$$

Note that, since $x(0) = x$ and $x(t) = x'$, $\delta x(0) = \delta x(t) = 0$, since *all* paths must begin at $x$ and end at $x'$. The change in $S$ is

$$\delta S = S[x+\delta x] - S[x] = \int_0^t ds L(x+\delta x, \dot{x}+\delta\dot{x}) - \int_0^t ds L(x,\dot{x})$$

Expanding the first term to first order in $\delta x$, we obtain

$$\delta S = \int_0^t ds\left[L(x,\dot{x}) + \frac{\partial L}{\partial \dot{x}}\delta\dot{x} + \frac{\partial L}{\partial x}\delta x\right] - \int_0^t L(x,\dot{x}) = \int_0^t ds\left[\frac{\partial L}{\partial \dot{x}}\delta\dot{x} + \frac{\partial L}{\partial x}\delta x\right]$$

The term proportional to $\delta\dot{x}$ can be handled by an integration by parts:

$$\int_0^t ds\frac{\partial L}{\partial \dot{x}}\delta\dot{x} = \int_0^t \frac{\partial L}{\partial \dot{x}}\frac{d}{dt}\delta x = \frac{\partial L}{\partial \dot{x}}\partial x|_0^t - \int_0^t ds\frac{d}{dt}\frac{\partial L}{\partial \dot{x}}\delta x$$

because $\delta x$ vanishes at 0 and $t$, the surface term is 0, leaving us with

$$\delta S = \int_0^t ds\left[-\frac{d}{dt}\frac{\partial L}{\partial \dot{x}} + \frac{\partial L}{\partial x}\right]\delta x = 0$$

Since the variation itself is arbitrary, the only way the integral can vanish, in general, is if the term in brackets vanishes:

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{x}} - \frac{\partial L}{\partial x} = 0$$

This is known as the **Euler-Lagrange equation** in classical mechanics. For the case that $L = m\dot{x}/2 - U(x)$, they give

$$\frac{d}{dt}(m\dot{x}) + \frac{\partial U}{\partial x} = 0$$

$$m\ddot{x} = -\frac{\partial U}{\partial x}$$

which is just Newton's equation of motion, subject to the conditions that $x(0)$, $x(t) = x'$. Thus, the classical path and those near it contribute the most to the path integral.

The classical path condition was derived by requiring that $\delta S = 0$ to first order. This is known as an action *stationarity* principle. However, it turns out that there is also a **principle of least action,** which states that the classical path minimizes the action as well. This is an important consideration when deriving the dominant paths for the density matrix, which takes the form

$$\rho(x,x';\beta) = \int_{x(0)=x}^{x(\beta\hbar=x'} \mathcal{D}x(\cdot) exp\left[-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau\left(\frac{m}{2}\dot{x}(\tau) + U(x(\tau))\right)\right]$$

The action appearing in this expression is

$$S_E[x] = \int_0^{\beta\hbar} d\tau \left[\frac{m}{2}\dot{x}^2 + U(x(\tau))\right] = \int_0^{\beta\hbar} d\tau H(x, \dot{x})$$

which is known as the **Euclidean action** and is just the integral over a path of the total energy or *Euclidean Lagrangian* $H(x, \dot{x})$. Here, we see that a minimum action principle is needed, since the smallest values of $S_E$ will contribute most to the integral. Again, we require that to first order $S_E[x + \delta x] - S_E[x] = 0$. Applying the same logic as before, we obtain the condition

$$\frac{d}{d\tau}\frac{\partial H}{\partial \dot{x}} - \frac{\partial H}{\partial x} = 0$$

$$m\ddot{x} = \frac{\partial}{\partial x}U(x)$$

which is just Newton's equation of motion on the inverted potential surface $-U(x)$, subject to the conditions $x(0) = x$, $x(\beta\hbar) = x'$. For the partition function $Q(\beta)$, the same equation of motion must be solved, but subject to the conditions that $x(0) = x(\beta\hbar)$, i.e., periodic paths.