4.2: The Quantum Mechanical Trace

Thus far our understanding of ergodicity is rooted in the dynamics of classical mechanics. A Hamiltonian flow which is ergodic is one in which time averages can be replaced by phase space averages using the microcanonical ensemble. What happens, though, if our system is quantum mechanical, as all systems ultimately are?

The Density Matrix

First, let us consider that our system S will in general be in contact with a world W. We call the union of S and W the universe, $U = W \cup S$. Let $\left| N \right\rangle$ denote a quantum mechanical state of W, and let $\left| n \right\rangle$ denote a quantum mechanical state of S. Then the most general wavefunction we can write is of the form

$$\left| \Psi \right\rangle = \sum_{N,n} \Psi_{N,n} \left| N \right\rangle \otimes \left| n \right\rangle . \tag{4.2.1}$$

Now let us compute the expectation value of some operator $\hat{\mathcal{A}}$ which acts as the identity within W, meaning $\left\langle N \right| \hat{\mathcal{A}} \left| N' \right\rangle = \hat{A}\, \delta_{NN'}$, where $\hat{A}$ is the 'reduced' operator which acts within S alone. We then have

$$\begin{aligned} \left\langle \Psi \right| \hat{\mathcal{A}} \left| \Psi \right\rangle &= \sum_{N,N'} \sum_{n,n'} \Psi^*_{N,n} \, \Psi_{N',n'} \, \delta_{NN'} \left\langle n \right| \hat{A} \left| n' \right\rangle \\ &= \mathsf{Tr} \big(\hat{\varrho} \, \hat{A} \big) , \end{aligned}$$

where

$$\hat{\varrho} = \sum_{N} \sum_{n,n'} \Psi^*_{N,n} \, \Psi_{N,n'} \left| n' \right\rangle \left\langle n \right| \tag{4.2.2}$$

is the *density matrix*. The time-dependence of $\hat{\varrho}$ is easily found:

$$\begin{aligned} \hat{\varrho}(t) &= \sum_{N} \sum_{n,n'} \Psi^*_{N,n} \, \Psi_{N,n'} \left| n'(t) \right\rangle \left\langle n(t) \right| \\ &= e^{-i\hat{H}t/\hbar} \, \hat{\varrho} \, e^{+i\hat{H}t/\hbar} , \end{aligned}$$

where $\hat{H}$ is the Hamiltonian for the system S. Thus, we find

$$i\hbar \, \frac{\partial \hat{\varrho}}{\partial t} = \big[\hat{H}, \hat{\varrho} \big] . \tag{4.2.3}$$

Note that the density matrix evolves according to a slightly different equation than an operator in the Heisenberg picture, for which

$$\hat{A}(t) = e^{+iHt/\hbar} \, A \, e^{-i\hat{H}t/\hbar} \qquad \Longrightarrow \qquad i\hbar \, \frac{\partial \hat{A}}{\partial t} = \big[\hat{A}, \hat{H} \big] = -\big[\hat{H}, \hat{A} \big] . \tag{4.2.4}$$

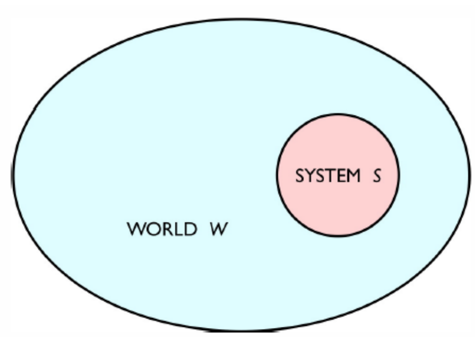

Figure 4.2.1: A system S in contact with a 'world' W. The union of the two, universe $U = W \cup S$, is said to be the 'universe'.

For Hamiltonian systems, we found that the phase space distribution $\varrho(q, p, t)$ evolved according to the Liouville equation,

$$i \, \frac{\partial \varrho}{\partial t} = L \, \varrho , \tag{4.2.5}$$

where the Liouvillian L is the differential operator

$$L=-i\sum_{j=1}^{Nd}\left\{\frac{\partial \hat{H}}{\partial p_j}\frac{\partial}{\partial q_j}-\frac{\partial \hat{H}}{\partial q_j}\frac{\partial}{\partial p_j}\right\}. \tag{4.2.6}$$

Accordingly, any distribution $\varrho(\Lambda_1,\ldots,\Lambda_k)$ which is a function of constants of the motion $\Lambda_a(q,p)$ is a stationary solution to the Liouville equation: $\partial_t\,\varrho(\Lambda_1,\ldots,\Lambda_k)=0$. Similarly, any quantum mechanical density matrix which commutes with the Hamiltonian is a stationary solution to Equation 4.2.3. The corresponding microcanonical distribution is

$$\hat{\varrho}_E=\delta\big(E-\hat{H}\big)\,. \tag{4.2.7}$$

Averaging the DOS

If our quantum mechanical system is placed in a finite volume, the energy levels will be discrete, rather than continuous, and the density of states (DOS) will be of the form

$$D(E)=\mathsf{Tr}\;\delta\big(E-\hat{H}\big)=\sum_l\delta(E-E_l)\,, \tag{4.2.8}$$

where $\{E_l\}$ are the eigenvalues of the Hamiltonian $\hat{H}$. In the thermodynamic limit, $V\to\infty$, and the discrete spectrum of kinetic energies remains discrete for all finite V but must approach the continuum result. To recover the continuum result, we average the DOS over a window of width ΔE:

$$\overline{D(E)}=\frac{1}{\Delta E}\int\limits_E^{E+\Delta E}\!dE'\;D(E')\,. \tag{4.2.9}$$

If we take the limit $\Delta E\to 0$ but with $\Delta E\gg\delta E$, where δE is the spacing between successive quantized levels, we recover a smooth function, as shown in Figure 4.2.2. We will in general drop the bar and refer to this function as $D(E)$. Note that $\delta E\sim 1/D(E)=e^{-N\phi(\varepsilon,v)}$ is (typically) *exponentially* small in the size of the system, hence if we took $\Delta E\propto V^{-1}$ which vanishes in the thermodynamic limit, there are still exponentially many energy levels within an interval of width ΔE.

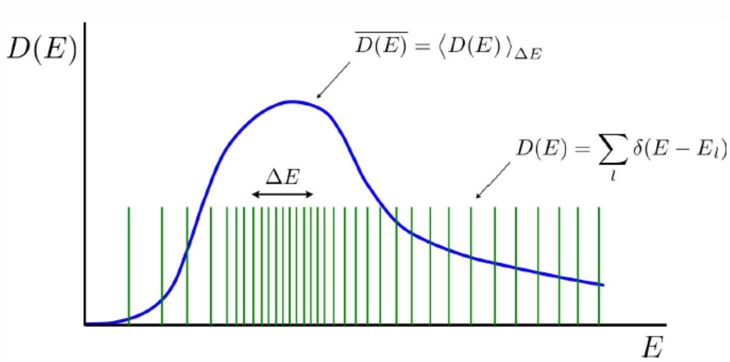

Figure 4.2.2: Averaging the quantum mechanical discrete density of states yields a continuous curve.

Coherent States

The quantum-classical correspondence is elucidated with the use of *coherent states*. Recall that the one-dimensional harmonic oscillator Hamiltonian may be written

$$\begin{aligned}\hat{H}_0&=\frac{p^2}{2m}+\frac{1}{2}m\,\omega_0^2\,q^2\\&=\hbar\omega_0\,\big(a^\dagger a+\tfrac{1}{2}\big)\,,\end{aligned}$$

where a and $a^\dagger$ are *ladder operators* satisfying $\big[a,a^\dagger\big]=1$, which can be taken to be

$$a=\ell\,\frac{\partial}{\partial q}+\frac{q}{2\ell}\qquad,\qquad a^\dagger=-\ell\,\frac{\partial}{\partial q}+\frac{q}{2\ell}\,, \tag{4.2.10}$$

with $\ell=\sqrt{\hbar/2m\omega_0}$. Note that

$$q=\ell\left(a+a^{\dagger}\right) \qquad , \qquad p=\frac{\hbar}{2i\ell}\left(a-a^{\dagger}\right) . \tag{4.2.11}$$

The ground state satisfies $a\,\psi_0(q)=0$, which yields

$$\psi_0(q)=(2\pi\ell^2)^{-1/4}\,e^{-q^2/4\ell^2} . \tag{4.2.12}$$

The normalized *coherent state* $\mid z\,\rangle$ is defined as

$$\mid z\,\rangle=e^{-\frac{1}{2}|z|^2}\,e^{za^{\dagger}}\mid 0\,\rangle=e^{-\frac{1}{2}|z|^2}\sum_{n=0}^{\infty}\frac{z^n}{\sqrt{n!}}\mid n\,\rangle . \tag{4.2.13}$$

The overlap of coherent states is given by

$$\langle\, z_1\mid z_2\,\rangle=e^{-\frac{1}{2}|z_1|^2}\,e^{-\frac{1}{2}|z_2|^2}\,e^{\bar{z}_1 z_2} , \tag{4.2.14}$$

hence different coherent states are not orthogonal. Despite this nonorthogonality, the coherent states allow a simple resolution of the identity,

$$1=\int\frac{d^2z}{2\pi i}\mid z\,\rangle\langle\, z\mid \quad ; \quad \frac{d^2z}{2\pi i}\equiv\frac{d\,Re z\,d\,Im z}{\pi} \tag{4.2.15}$$

which is straightforward to establish.

To gain some physical intuition about the coherent states, define

$$z\equiv\frac{Q}{2\ell}+\frac{i\ell P}{\hbar} \tag{4.2.16}$$

and write $\mid z\,\rangle\equiv\mid Q,P\,\rangle$. One finds (*exercise!*)

$$\psi_{Q,P}(q)=\langle\, q\mid z\,\rangle=(2\pi\ell^2)^{-1/4}\,e^{-iPQ/2\hbar}\,e^{iPq/\hbar}\,e^{-(q-Q)^2/4\ell^2} , \tag{4.2.17}$$

hence the coherent state $\psi_{Q,P}(q)$ is a wavepacket Gaussianly localized about $q=Q$, but oscillating with average momentum P.

For example, we can compute

$$\begin{aligned}\big\langle\, Q,P\,\big|\,q\,\big|\,Q,P\,\big\rangle &=\big\langle\, z\,\big|\,\ell\,(a+a^{\dagger})\,\big|\,z\,\big\rangle=2\ell\;Re\,z=Q\\ \big\langle\, Q,P\,\big|\,p\,\big|\,Q,P\,\big\rangle &=\big\langle\, z\,\big|\,\frac{\hbar}{2i\ell}\,(a-a^{\dagger})\,\big|\,z\,\big\rangle=\frac{\hbar}{\ell}\;Im\,z=P\end{aligned}$$

as well as

$$\begin{aligned}\big\langle\, Q,P\,\big|\,q^2\,\big|\,Q,P\,\big\rangle &=\big\langle\, z\,\big|\,\ell^2\,(a+a^{\dagger})^2\,\big|\,z\,\big\rangle=Q^2+\ell^2\\ \big\langle\, Q,P\,\big|\,p^2\,\big|\,Q,P\,\big\rangle &=-\big\langle\, z\,\big|\,\frac{\hbar^2}{4\ell^2}(a-a^{\dagger})^2\,\big|\,z\,\big\rangle=P^2+\frac{\hbar^2}{4\ell^2} .\end{aligned}$$

Thus, the root mean square fluctuations in the coherent state $\mid Q,P\,\rangle$ are

$$\Delta q=\ell=\sqrt{\frac{\hbar}{2m\omega_0}} \qquad , \qquad \Delta p=\frac{\hbar}{2\ell}=\sqrt{\frac{m\hbar\omega_0}{2}}, \tag{4.2.18}$$

and $\Delta q\cdot\Delta p=\frac{1}{2}\,\hbar$. Thus we learn that the coherent state $\psi_{Q,P}(q)$ is localized in phase space, in both position and momentum. If we have a general operator $\hat{A}(q,p)$, we can then write

$$\big\langle\, Q,P\,\big|\,\hat{A}(q,p)\,\big|\,Q,P\,\big\rangle=A(Q,P)+\mathcal{O}(\hbar) , \tag{4.2.19}$$

where $A(Q,P)$ is formed from $\hat{A}(q,p)$ by replacing $q\to Q$ and $p\to P$.

Since

$$\frac{d^2z}{2\pi i} \equiv \frac{d\,Re z\,d\,Im z}{\pi} = \frac{dQ\,dP}{2\pi\hbar}\;, \tag{4.2.20}$$

we can write the trace using coherent states as

$$\mathsf{Tr}\,\hat{A} = \frac{1}{2\pi\hbar}\int\limits_{-\infty}^{\infty}\!dQ\int\limits_{-\infty}^{\infty}\!dP\,\big\langle\,Q,P\,\big|\,\hat{A}\,\big|\,Q,P\,\big\rangle\;. \tag{4.2.21}$$

We now can understand the origin of the factor $2\pi\hbar$ in the denominator of each (q_i, p_i) integral over classical phase space in Equation ???.

Note that ω_0 is arbitrary in our discussion. By increasing ω_0, the states become more localized in q and more plane wave like in p. However, so long as ω_0 is finite, the width of the coherent state in each direction is proportional to $\hbar^{1/2}$, and thus vanishes in the classical limit.
