The Ehrenfest Theorems

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1 Classical Preliminaries

A classical system with n degrees of freedom is described by n second order ordinary differential equations on the configuration space (n independent coordinates) in the Lagrangian representation

$$\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{q}_j} - \frac{\partial \mathcal{L}}{\partial q_j} = 0 \tag{1}$$

and $2n$ first order ordinary differential equations on the phase space (n independent coordinates and the conjugate momentum of each coordinate) in the Hamiltonian representation

$$\frac{dq_j}{dt} = +\frac{\partial \mathcal{H}}{\partial p_j} \qquad\qquad \frac{dp_j}{dt} = -\frac{\partial \mathcal{H}}{\partial q_j} \tag{2}$$

The first set of equations is called the Euler-Lagrange equations and the second set is called the Hamiltonian equations of motion.

Functions describing particles depend on time implicitly through the time dependence of the particle's coordinates and momenta; they may also depend explicitly on time: $f = f(q(t), p(t), t)$. The time derivative of such functions has the form

$$\begin{aligned}
\frac{df}{dt} &= \frac{\partial f}{\partial t} + \frac{\partial f}{\partial q_i}\frac{dq_i}{dt} + \frac{\partial f}{\partial p_i}\frac{dp_i}{dt} \\
&= \frac{\partial f}{\partial t} + \frac{\partial f}{\partial q_i}\frac{\partial \mathcal{H}}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial \mathcal{H}}{\partial q_i} \\
&= \frac{\partial f}{\partial t} + \{f, \mathcal{H}\}
\end{aligned} \tag{3}$$

The partial derivative provides information about the *explicit* time dependence of the function. The *implicit* time dependence, depending on the motion of the particle, is provided by the *Poisson bracket*:

$$\{f, g\} \equiv \sum_j \frac{\partial f}{\partial q_j}\frac{\partial g}{\partial p_j} - \frac{\partial f}{\partial p_j}\frac{\partial g}{\partial q_j} \tag{4}$$

2 Classical - Quantum Correspondence

An elegant formulation of Quantum Theory is given in terms of a relation between the Poisson bracket of Classical Mechanics and the commutator (Lie) bracket of Quantum Mechanics:

$$\begin{array}{ccc} \text{Classical Mechanics} & & \text{QuantumMechanics} \\ & & \\ \{f, g\} & \leftrightarrow & \dfrac{[\hat{f}, \hat{g}]}{i\hbar} \end{array} \tag{5}$$

The hat $\hat{}$ on the right hand side indicates that the correspondents are operators.

To see how this works, we observe directly from Equ.(4) that $\{q_j, p_k\} = \delta_{jk}$. From this and the Classical $\rightarrow$ Quantum mapping Equ.(5) we observe that $[\hat{q}_j, \hat{p}_k] = i\hbar\delta_{jk}$. Thiss relation can be satisfied in one of two obvious ways, one emphasizing the coordinates (the usual), the other emphasizing their conjugate momenta:

$$\begin{array}{ccc} \text{Representation} & \hat{q}_j & \hat{p}_k \\ \hline \text{Coordinate} & q_j & \dfrac{\hbar}{i}\dfrac{\partial}{\partial q_k} \\ \text{Momentum} & -\dfrac{\hbar}{i}\dfrac{\partial}{\partial p_j} & p_k \end{array} \tag{6}$$

A final piece of the puzzle that we need is the time-dependent Schrödinger equation. For a free particle with wavefunction $\psi(x) = e^{ikx}$ the momentum is $\hbar k$ by looking at the eigenvalue of the momentum operator $\hat{p} = (\hbar/i)\partial/\partial x$. If we would like to represent the time-dependence of a free particle moving to the right with a momentum $\hbar k$ in the form $e^{ikx-\omega t}$ we must choose the time-dependent form of the Schrödinger equation to be

$$\mathcal{H}\psi(x,t) = +i\hbar\frac{\partial\psi(x,t)}{\partial t}$$

3 Ehrenfest Theorems

The "Ehrenfest Theorem" comprises a whole class of results, all of which assume the same form:

$$\begin{array}{ccc} \text{Classical Mechanics} & \rightarrow & \text{Quantum Mechanics} \\ & & \\ \dfrac{d}{dt}A = B & \rightarrow & \dfrac{d}{dt}\langle\hat{A}\rangle = \langle\hat{B}\rangle \end{array} \tag{7}$$

To show this, we write down the time derivative of an expectation value as follows:

$$\frac{d}{dt}\langle \hat{A} \rangle = \frac{d}{dt}\int \psi^*(x,t)\hat{A}\psi(x,t)dV =$$

$$\int \psi^*(x,t)\frac{\partial \hat{A}}{\partial t}\psi(x,t)dV + \int \frac{\partial \psi^*(x,t)}{\partial t}\hat{A}\psi(x,t)dV + \int \psi^*(x,t)\hat{A}\frac{\partial \psi(x,t)}{\partial t}dV \quad (8)$$

In the expression above we can replace $\frac{\partial \psi(x,t)}{\partial t}$ by $\mathcal{H}/i\hbar$ and we can replace $\frac{\partial \psi^*(x,t)}{\partial t}$ by $-\mathcal{H}/i\hbar$. The result is

$$\frac{d}{dt}\langle \hat{A} \rangle = \langle \frac{\partial \hat{A}}{\partial t} \rangle + \langle \frac{[\hat{A}, \mathcal{H}]}{i\hbar} \rangle \tag{9}$$

Equation (9) for Quantum systems is identical to Equ. (3) for Classical systems through the Quantum-Classical correspondence of Equ. (5). This is "Ehrenfest's Theorem."

4 Simple Applications

The following results are immediate:

$$\begin{aligned}
\frac{d}{dt}\langle \mathbf{x} \rangle &= \langle \frac{\mathbf{p}}{m} \rangle \\
\frac{d}{dt}\langle \mathbf{p} \rangle &= \langle -\frac{\partial V}{\partial \mathbf{x}} \rangle = \langle \mathbf{F} \rangle \\
\frac{d}{dt}\langle \mathbf{L} \rangle &= \langle \mathbf{r} \times \mathbf{F} \rangle
\end{aligned} \tag{10}$$

The Hamiltonian equations of motion are obtained as follows. Set $\hat{A} = \hat{q}_j$. In this case

$$\frac{d}{dt}\langle q_j \rangle = \frac{1}{i\hbar}\langle [q_j, \mathcal{H}] \rangle = \frac{1}{i\hbar}\langle i\hbar \frac{\partial}{\partial p_j}\mathcal{H} \rangle = \langle \frac{\partial \mathcal{H}}{\partial p_j} \rangle \tag{11}$$

The replacement of the commutator $[q_j, \mathcal{H}]$ by the derivative $i\hbar\frac{\partial}{\partial p_j}\mathcal{H}$ is a direct application of Equ. (6). In a similar way we find Ehrenfest's limit for the other of Hamilton's equations. The symmetry is

$$\frac{dq_j}{dt} = +\frac{\partial \mathcal{H}}{\partial p_j} \quad \rightarrow \quad \frac{d\langle q_j \rangle}{dt} = +\langle \frac{\partial \mathcal{H}}{\partial p_j} \rangle \tag{12}$$

$$\tag{13}$$

$$\frac{dp_k}{dt} = -\frac{\partial \mathcal{H}}{\partial q_k} \quad \rightarrow \quad \frac{d\langle p_k \rangle}{dt} = -\langle \frac{\partial \mathcal{H}}{\partial q_k} \rangle \tag{14}$$

$$\tag{15}$$

If there is any uncertainty about taking the partial derivative of the operator $\mathcal{H}$ with respect to a coordinate or a momentum, the commutator (over $\pm i\hbar$) can be taken instead.

5 Virial Theorem

The Virial of Clausius is defined by

$$G = \sum_j p_j q_j = \mathbf{p} \cdot \mathbf{q} \tag{16}$$

The Virial has the dimensions of Action ($dA = \sum pdq$). Its time derivative has expressions in terms of useful physical quantities (kinetic energy, force)

$$\frac{dG}{dt} = \sum_j \frac{dq_j}{dt} p_j + q_j \frac{dp_j}{dt} = \frac{\mathbf{p}}{m} \cdot \mathbf{p} + \mathbf{r} \cdot \mathbf{F} = 2T - \mathbf{r} \cdot \nabla V \tag{17}$$

and in terms of Euler-like operators on the Hamiltonian

$$\frac{dG}{dt} = \sum_j p_j \frac{dq_j}{dt} + q_j \frac{dp_j}{dt} = \sum_j \left(p_j \frac{\partial}{\partial p_j} - q_j \frac{\partial}{\partial q_j} \right) \mathcal{H} \tag{18}$$

The Virial Theorem is different from classical expressions given in previous sections in that it is a statistical statement. It is an expression of long time averages:

$$\overline{G} = \lim_{\tau \to \infty} \frac{1}{\tau} \int_0^\tau \frac{dG}{dt} \, dt = \lim_{\tau \to \infty} \frac{1}{\tau} \int_0^\tau \left(2T - \sum_j q_j \frac{\partial}{\partial q_j} V \right) \, dt = \overline{2T} - \overline{q \cdot \nabla V} \tag{19}$$

If the motion is periodic or, more generally it is bounded, $G(q(\tau), p(\tau)) - G(q(0), p(0))$ is bounded so the limit above vanishes. If the potential is a homogeneous function of the coordinates, so that $V(q) = \alpha |q|^n$, then by Euler's theorem and the boundedness of the motion we find

$$\overline{2T} - n\overline{V} = 0 \tag{20}$$

This is the standard equipartition of energy theorem for systems in thermodynamic equilibrium. For Coulomb potentials ($n = -1$) this result tells us that the mean value of the potential energy is twice the mean value of the kinetic energy, and of opposite sign.

The Quantum Mechanical statement of this theorem is also different from expressions given previously, in that it must involve two averaging operations. Spatial averages are denoted by $\langle \ \rangle$ and temporal averages are denoted by $\overline{}$. The Virial is defined as a symmetrized generalization of the classical expression:

$$\hat{G} = \sum_j \frac{1}{2}[\hat{p}_j, \hat{q}_j]_+ = \sum_j \frac{1}{2}(\hat{p}_j\hat{q}_j + \hat{q}_j\hat{p}_j) \tag{21}$$

The time derivative is given by the usual expression

$$\frac{d}{dt}\langle\hat{G}\rangle = \langle[\hat{G}, \mathcal{H}]\rangle \tag{22}$$

The commutators are easily computed. They give $2T$ and $\mathbf{r} \cdot \mathbf{F}$ as before. Integrating the time derivative, we find for bound states

$$\overline{\langle 2T - \mathbf{q} \cdot \nabla V \rangle} = 0 \tag{23}$$

The result for a homogeneous potential of degree n is

$$\overline{\langle 2T \rangle} = n\overline{\langle V \rangle} \tag{24}$$

We observe that spatial expectation values are time-dependent in general, but expectation values in an eigenstate are time independent. In an eigenstate the statement above is true at all times, not only on average, so we find for a bound eigenstate in a homogeneous potential

$$\langle 2T \rangle = n\langle V \rangle \tag{25}$$