7.7 Virial Theorem

In quantum mechanics the virial theorem is a particular case of a general property of stationary states. Since we focus on energy eigenstates, we are considering time-independent Hamiltonians. We will write the stationary states as follows:

$$\Psi(\mathbf{x}, t) = e^{-iEt/\hbar}\, \psi(\mathbf{x}). \tag{7.7.1}$$

Consider now the main equation (5.2.5) governing the time dependence of the expectation value of a time-independent operator $\hat{Q}$:

$$i\hbar \frac{d}{dt}\langle \hat{Q} \rangle = \left\langle [\hat{Q}, \hat{H}] \right\rangle. \tag{7.7.2}$$

If the expectation value is taken on a stationary state Ψ, then both sides of the equation vanish. The left-hand side vanishes because, as we showed in section 6.1, the expectation value of any time-independent operator on a stationary state is time independent. Therefore, the time derivative kills $\langle \hat{Q} \rangle$. The vanishing of the right-hand side is also simple to see:

$$\left\langle [\hat{Q}, \hat{H}] \right\rangle = \langle \Psi, [\hat{Q}, \hat{H}]\Psi \rangle = \langle e^{-iEt/\hbar}\psi, [\hat{Q}, \hat{H}]e^{-iEt/\hbar}\psi \rangle. \tag{7.7.3}$$

Since the operators $\hat{Q}$ and $\hat{H}$ do not involve time derivatives, the time-dependent phases can go out of the inner product and cancel each other:

$$\left\langle [\hat{Q}, \hat{H}] \right\rangle = \langle \psi, [\hat{Q}, \hat{H}]\psi \rangle. \tag{7.7.4}$$

Finally, expanding out the commutator using the Hermiticity of $\hat{H}$ and the relation $\hat{H}\psi = E\psi$, we have

$$\left\langle [\hat{Q}, \hat{H}] \right\rangle = \langle \psi, \hat{Q}\hat{H}\psi \rangle - \langle \hat{H}\psi, \hat{Q}\psi \rangle = E\langle \psi, \hat{Q}\psi \rangle - E\langle \psi, \hat{Q}\psi \rangle = 0. \tag{7.7.5}$$

We have thus confirmed the following:

Lemma. *For any time-independent* $\hat{Q}$, *a time-independent Hamiltonian* $\hat{H}$, and an energy eigenstate $\Psi = \exp(-iEt/\hbar)\psi$, we have $\langle [\hat{Q}, \hat{H}] \rangle_\Psi = \langle [\hat{Q}, \hat{H}] \rangle_\psi = 0$

You may have noticed that requiring $\hat{Q}$ to be time independent is not really needed for the above lemma; all that is required is that $\hat{Q}$ contain no time derivatives. Still, all familiar applications use time-independent $\hat{Q}$ operators.

This lemma is useful because, using suitably chosen $\hat{Q}$ operators, we can often learn important facts about the expectation values of operators on energy eigenstates. The vanishing of $\langle [\hat{Q}, \hat{H}] \rangle_\psi$ has interesting consequences. The most familiar application deals with the Hamiltonian for a point particle moving in a potential. If the problem is one-dimensional, the Hamiltonian is the sum of the kinetic plus potential energies:

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}). \tag{7.7.6}$$

We then choose $\hat{Q} = \hat{x}\hat{p}$ and compute

$$[\hat{x}\hat{p}, \hat{H}] = \left[\hat{x}\hat{p}, \frac{\hat{p}^2}{2m}\right] + [\hat{x}\hat{p}, V(x)]. \tag{7.7.7}$$

The first commutator is computed using the derivation property ((5.2.8), second equation), as well as (5.2.15):

$$\left[\hat{x}\hat{p}, \frac{\hat{p}^2}{2m}\right] = \frac{1}{2m}[\hat{x}, \hat{p}^2]\,\hat{p} = \frac{1}{2m}2i\hbar\hat{p}\,\hat{p} = 2i\hbar\,\frac{\hat{p}^2}{2m}. \tag{7.7.8}$$

The second commutator gives us

$$[\hat{x}\hat{p}, V(\hat{x})] = \hat{x}[\hat{p}, V(\hat{x})] = \frac{\hbar}{i}\,\hat{x}\frac{dV}{d\hat{x}}, \tag{7.7.9}$$

using the result (5.2.14) for the commutator of $\hat{p}$ with an arbitrary function of $\hat{x}$. Having computed the two contributions to $[\hat{x}\hat{p}, \hat{H}]$, the vanishing expectation value on a stationary state gives

$$\Big\langle [\hat{x}\hat{p}, \hat{H}] \Big\rangle = 2i\hbar\Big\langle \frac{\hat{p}^2}{2m}\Big\rangle - i\hbar\Big\langle \hat{x}\frac{dV}{d\hat{x}}\Big\rangle = 0. \tag{7.7.10}$$

We have therefore shown that

$$\boxed{\Big\langle \frac{\hat{p}^2}{2m}\Big\rangle = \frac{1}{2}\Big\langle \hat{x}\frac{dV}{d\hat{x}}\Big\rangle.} \tag{7.7.11}$$

This is the **virial theorem** for one-dimensional potentials: it relates the expectation value of the kinetic energy, the left-hand side, to the expectation value of a simple function of the potential, both evaluated on the same arbitrary energy eigenstate. Note that for a quadratic potential $V(\hat{x}) = \gamma\hat{x}^2$, with γ a constant,

$$\tfrac{1}{2}\hat{x}\frac{d}{d\hat{x}}V(\hat{x}) = \tfrac{1}{2}\hat{x}\,2\gamma\hat{x} = \gamma\hat{x}^2 = V(\hat{x}), \tag{7.7.12}$$

which means that for a quadratic potential the expectation values of the kinetic and the potential energies are the same!

The three-dimensional version of the virial theorem gives a useful equality when we consider a particle moving in a central potential, meaning that $V(\mathbf{x})$ is in fact a function $V(r)$ of the length r of the position vector $\mathbf{x}$. The Hamiltonian is then

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + V(r). \tag{7.7.13}$$

This time we consider the commutator of $\hat{H}$ with $\hat{\mathbf{x}} \cdot \hat{\mathbf{p}}$, the analog of the one-dimensional $\hat{x}\hat{p}$:

$$\hat{\mathbf{x}} \cdot \hat{\mathbf{p}} = \sum_{k=1}^{3} \hat{x}_k \hat{p}_k = \hat{x}_1 \hat{p}_1 + \hat{x}_2 \hat{p}_2 + \hat{x}_3 \hat{p}_3. \tag{7.7.14}$$

We thus have

$$[\hat{\mathbf{x}} \cdot \hat{\mathbf{p}}, \hat{H}] = \Big[\hat{\mathbf{x}} \cdot \hat{\mathbf{p}}, \frac{\hat{\mathbf{p}}^2}{2m} + V(r)\Big] = \frac{1}{2m}[\hat{\mathbf{x}} \cdot \hat{\mathbf{p}}, \hat{\mathbf{p}}^2] + \sum_{k=1}^{3} \hat{x}_k [\hat{p}_k, V(r)], \tag{7.7.15}$$

where we noted that $\hat{x}_k$ commutes with $V(r)$ because all $\hat{x}$ operators commute with each other, and ultimately, r is a function of the $\hat{x}_k$'s. Let us look at the first commutator:

$$\begin{aligned}[\hat{\mathbf{x}} \cdot \hat{\mathbf{p}}, \hat{\mathbf{p}}^2] &= [\hat{x}_1 \hat{p}_1 + \hat{x}_2 \hat{p}_2 + \hat{x}_3 \hat{p}_3\,,\ \hat{p}_1^2 + \hat{p}_2^2 + \hat{p}_3^2] \\ &= [\hat{x}_1 \hat{p}_1\,, \hat{p}_1 \hat{p}_1] + [\hat{x}_2 \hat{p}_2\,, \hat{p}_2 \hat{p}_2] + [\hat{x}_3 \hat{p}_3\,, \hat{p}_3 \hat{p}_3],\end{aligned} \tag{7.7.16}$$

because the only nontrivial commutators happen between $\hat{x}$'s and $\hat{p}$'s with the same index. The above commutators are of the same form as in the one-dimensional case. You can quickly check that

$$[\hat{\mathbf{x}} \cdot \hat{\mathbf{p}}\,, \hat{\mathbf{p}}^2] = 2i\hbar\, \hat{\mathbf{p}}^2. \tag{7.7.17}$$

The second commutator in (7.7.15) involves the commutator $[\hat{p}_k, V(r)]$. Recall that in one dimension we showed that $[\hat{p}, V(\hat{x})] = \frac{\hbar}{i}\frac{dV}{dx}$. Since, as an operator in position space, $\hat{p}_k = \frac{\hbar}{i}\frac{\partial}{\partial x_k}$ (see (3.3.26)), this time we have $[\hat{p}_k, V(\mathbf{x})] = \frac{\hbar}{i}\frac{\partial V}{\partial x_k}$. Therefore,

$$\sum_{k=1}^{3} \hat{x}_k [\hat{p}_k, V(r)] = \sum_{k=1}^{3} \hat{x}_k \frac{\hbar}{i} \frac{\partial V(r)}{\partial x_k} = -i\hbar \sum_{k=1}^{3} \hat{x}_k \frac{\partial V(r)}{\partial r} \frac{\partial r}{\partial \hat{x}_k}. \tag{7.7.18}$$

Using $r^2 = \hat{x}_1^2 + \hat{x}_2^2 + \hat{x}_3^2$, we can evaluate the partial derivative of r with respect to any coordinate:

$$\frac{\partial r}{\partial \hat{x}_k} = \frac{1}{2r}\frac{\partial r^2}{\partial \hat{x}_k} = \frac{1}{2r}(2\hat{x}_k) = \frac{\hat{x}_k}{r}. \tag{7.7.19}$$

Therefore, the commutator gives

$$\sum_{k=1}^{3} \hat{x}_k [\hat{p}_k,\, V(r)] = -i\hbar \sum_{k=1}^{3} \frac{\hat{x}_k \hat{x}_k}{r} \frac{\partial V(r)}{\partial r} = -i\hbar\, r \frac{\partial V(r)}{\partial r}. \tag{7.7.20}$$

All in all, we have found that

$$[\, \hat{\mathbf{x}} \cdot \hat{\mathbf{p}}\, , \hat{H}] = 2i\hbar \frac{\hat{\mathbf{p}}^2}{2m} - i\hbar\, r \frac{\partial V(r)}{\partial r}. \tag{7.7.21}$$

The vanishing expectation value of the commutator on any energy eigenstate now gives the relation

$$\boxed{\left\langle \frac{\hat{\mathbf{p}}^2}{2m} \right\rangle = \frac{1}{2} \left\langle r \frac{\partial V}{\partial r} \right\rangle.} \tag{7.7.22}$$

This is the three-dimensional version of the virial theorem in quantum mechanics.

The first formulation of the virial theorem, due to Rudolf Clausius (1870), was in the context of classical mechanics. The analog of expectation value in quantum mechanics is time average. Similarly, the analog of a stationary state is a system exhibiting periodic motion or, if not periodic, at least motion in which positions and momenta are bounded in time. For a quantity $\mathcal{O}$ built from position and momenta, the classical average $\langle \cdots \rangle_{\text{cl}}$ over a time period τ is defined by

$$\langle \mathcal{O} \rangle_{\text{cl}} \equiv \frac{1}{\tau} \int_0^{\tau} \mathcal{O}(t) dt. \tag{7.7.23}$$

For a periodic system with period T, the average over T of the time derivative of $\mathcal{O}$ vanishes:

$$\left\langle \frac{d\mathcal{O}}{dt} \right\rangle_{\text{cl}} = \frac{1}{T} \int_0^{T} \frac{d\mathcal{O}}{dt}(t) dt = \mathcal{O}(T) - \mathcal{O}(0) = 0, \tag{7.7.24}$$

by the periodicity condition. This is the classical analog of the vanishing of the time derivative of the expectation value of a quantum operator $\hat{Q}$. As you will verify in problem 7.13, the classical form of the virial theorem follows by choosing $\mathcal{O} = \sum_\alpha \mathbf{r}_\alpha \cdot \mathbf{p}_\alpha$, where the sum of the products of position and momenta is over all the particles of the system. The resulting form of the classical virial theorem is completely analogous to (7.7.22).

The virial theorem was applied by Fritz Zwicky in 1933 to the Coma cluster of galaxies, a cluster containing over one thousand galaxies and located about 32 million light-years away from us. Estimates of average kinetic energies obtained by Doppler shift measurements, together with the virial theorem, led to an estimate for the total mass of the cluster. From an analysis of luminosity, it became clear that the matter in stars and in hot interstellar gas cannot account, by a large factor, for the total mass of the cluster. This led Zwicky to postulate the existence of *dark matter*. With much better measurements since, it seems that about 9% of the mass of the Coma cluster is in the form of dark matter.