VIRIAL THEOREM

Yubo "Paul" Yang

April 6, 2018

Classical and Non-relativistic Statement

Virial theorem originates from non-relativistic Classical thermodynamics and states

$$\frac{d}{dt}\left(\sum_{i=1}^{N}\boldsymbol{r}_i\cdot\boldsymbol{p}_i\right) =2T-nV \tag{1}$$

$$T =\sum_{i=1}^{N}\frac{p_i^2}{2m_i} \tag{2}$$

$$V =\frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}U(|\boldsymbol{r}_1-\boldsymbol{r}_2|) \tag{3}$$

for N particles interacting via isotropic pair potential $U(|\boldsymbol{r}_1-\boldsymbol{r}_2|)\propto|\boldsymbol{r}_1-\boldsymbol{r}_2|^n$. $\boldsymbol{r}$ is the position of particle i. $\boldsymbol{p}_i$ is its momentum. T is the total kinetic energy of all N particles. V is the total potential energy. $\boldsymbol{r}_i,\boldsymbol{p}_i,T,V$ are all functions of time t.

Define the term in parentheses to be $G\equiv\sum\limits_{i=1}^{N}\boldsymbol{r}_i\cdot\boldsymbol{p}_i$, then the time average of eq. (1) is

$$\frac{1}{t_f-t_i}\left(G(t_f)-G(t_i)\right)=2\langle T\rangle-n\langle V\rangle. \tag{4}$$

If $G(t)$ is bounded, then $G(t_f)-G(t_i)$ is finite. Therefore, in the limit of infinite time average, $\frac{1}{t_f-t_i}$ drives the LHS to zero. If the system is ergodic, i.e. time average = ensemble average, then the thermal averages of kinetic and potential energies are related as

$$\langle T\rangle=\frac{n}{2}\langle V\rangle. \tag{5}$$

The Virial theorem is widely used in astrophysics, where stars interact via gravitational attraction $U(r)\propto r^{-2}$, i.e. $n=2$. In this case, eq. (5) reduces to

$$\langle T\rangle=\langle V\rangle. \tag{6}$$

Unfortunately, eq. (6) is often mis-quoted as *the Virial theorem*.

Derivation

To derive the Classical non-relativistic version of Virial theorem eq. 1, one may use product rule on the LHS of eq. (1) and plug in physics. Necessary physics: momentum is related to the time evolution of position $\boldsymbol{p}_i = m\frac{d}{dt}\boldsymbol{r}_i$, whereas force is related to the time evolution of momentum $\boldsymbol{f}_i = \frac{d}{dt}\boldsymbol{p}_i$. Finally, force can be related to the spatial variation of potential $\boldsymbol{f}_i = -\frac{d}{d\boldsymbol{r}_i}V$ or $\boldsymbol{f}_i = -\nabla_{\boldsymbol{r}_i}V$ if you hate vector being in the denominator.

The kinetic piece is straight-forward

$$\boxed{\sum_{i=1}^{N} \frac{d\boldsymbol{r}_i}{dt} \cdot \boldsymbol{p}_i = 2T.} \tag{7}$$

The potential piece is a bit tricky

$$\sum_{k=1}^{N} \boldsymbol{r} \cdot \frac{d\boldsymbol{p}_k}{dt} = \sum_{k=1}^{N} \boldsymbol{r}_k \cdot \boldsymbol{f}_k. \tag{8}$$

First, define $\boldsymbol{f}_{kj}$ to be the force that particle j exerts on particle k, so that

$$\boldsymbol{f}_k = \sum_{j=1, j\neq k}^{N} \boldsymbol{f}_{kj}. \tag{9}$$

Next, split the sum in two pieces and use Newton's 3^{rd} law ($\boldsymbol{f}_{jk} = -\boldsymbol{f}_{kj}$)

$$\begin{aligned} \sum_{k=1}^{N} \sum_{j=1, j\neq k}^{N} \boldsymbol{r}_k \cdot \boldsymbol{f}_{kj} &= \left(\sum_{j<k} \boldsymbol{r}_k \cdot \boldsymbol{f}_{kj} \right) + \left(\sum_{j>k} \boldsymbol{r}_k \cdot \boldsymbol{f}_{kj} \right) \\ &= \sum_{j<k} \left(\boldsymbol{r}_k \cdot \boldsymbol{f}_{kj} - \boldsymbol{r}_j \cdot \boldsymbol{f}_{kj} \right) \\ &= \sum_{j<k} \boldsymbol{r}_{kj} \cdot \boldsymbol{f}_{kj}. \end{aligned} \tag{10}$$

Finally, obtain force from spherical pair potential $U(r) \propto r^n \Rightarrow U'(r) = nU(r)/r$

$$\boldsymbol{f}_{kj} = -\frac{dU(r_{kj})}{d\boldsymbol{r}_{kj}} = -U'(r_{kj})\hat{\boldsymbol{r}}_{jk} = -nU(r_{kj})\hat{\boldsymbol{r}}_{kj}. \tag{11}$$

Therefore, the potential piece

$$\begin{aligned} \boxed{\sum_{k=1}^{N} \boldsymbol{r} \cdot \frac{d\boldsymbol{p}_k}{dt}} =& \sum_{k=1}^{N} \sum_{j<k} \boldsymbol{r}_{kj} \cdot \boldsymbol{f}_{kj} \\ =& -n \sum_{k=1}^{N} \sum_{j<k} U(r_{kj}) \\ =& \boxed{-nV}. \end{aligned} \tag{12}$$