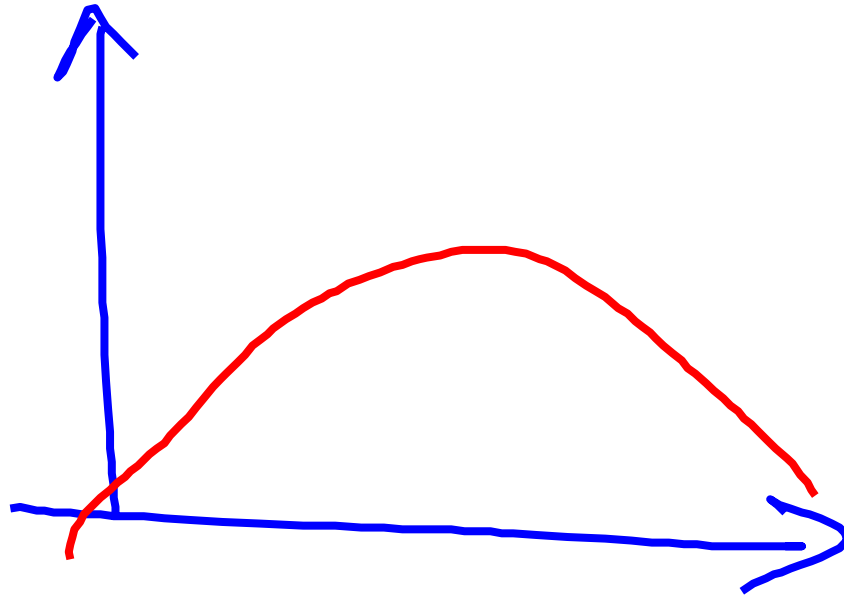


3.320: Lecture 13 (Mar 17 2005)

MOLECULAR DYNAMICS (PLAY IT AGAIN SAM)

A Particle Is a Particle Is a Particle

$$m \frac{d^2 \vec{r}}{dt^2} = F(\vec{r}) \quad \xrightarrow{\quad} \quad \begin{matrix} \vec{r}(t) \\ \vec{v}(t) \end{matrix}$$



N coupled equations

$$m_i \frac{d^2 \vec{r}_i}{dt^2} = \vec{F}_i(\vec{r}_1, \dots, \vec{r}_N)$$

- The force depends on positions only (not velocities)
- The total energy of the system is conserved (microcanonical evolution)

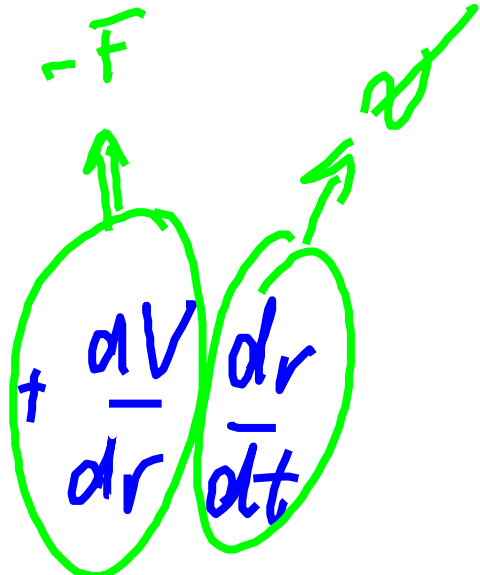
Conservation of the total energy

$$\frac{d}{dt} \left(\frac{1}{2} m v^2 + V(r) \right)$$

$\Downarrow$

$$\frac{1}{2} m 2 v a + \frac{dV}{dt} \Rightarrow m \cancel{v} a + \frac{dV}{dr} \frac{dr}{dt}$$

$ma - F$



以上内容仅为本文档的试下载部分，为可阅读页数的一半内容。如要下载或阅读全文，请访问：<https://d.book118.com/198141134026006104>