Molecular Simulation of Materials, Homework 2

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September 18, 2016

1 Problem 1

a) i

$$
\begin{aligned}
\frac{1}{2m_i}\frac{\partial|\mathbf{p}_i|^2}{\partial \mathbf{p}_i} =& \frac{1}{2m_i}\frac{\partial\left[\mathbf{p}_i\cdot\mathbf{p}_i\right]}{\partial \mathbf{p}_i},\\
=& \frac{1}{2m_i}\frac{\partial\left[p_{i1}^2+p_{i2}^2+p_{i3}^2\right]}{\partial p_{ij}},\\
=& \frac{1}{2m_i}\begin{Bmatrix} 2p_{i1}\\ 2p_{i2}\\ 2p_{i3}\end{Bmatrix},\\
=& \frac{2\mathbf{p}_i}{2m_i},\\
=& \frac{\mathbf{p}_i}{m_i}.
\end{aligned}
$$

ii

$$
\begin{aligned}
\frac{\partial r_{ij}}{\partial \mathbf{r}_i} =& \frac{\partial\sqrt{\left(r_{i1}-r_{j1}\right)^2+\left(r_{i2}-r_{j2}\right)^2+\left(r_{i3}-r_{j3}\right)^2}}{\partial \mathbf{r}_i},\\
=& \begin{Bmatrix}
\frac{1}{2}\left[\left(r_{i1}-r_{j1}\right)^2+\left(r_{i2}-r_{j2}\right)^2+\left(r_{i3}-r_{j3}\right)^2\right]^{-1/2}2\left(r_{i1}-r_{j1}\right)\\
\frac{1}{2}\left[\left(r_{i1}-r_{j1}\right)^2+\left(r_{i2}-r_{j2}\right)^2+\left(r_{i3}-r_{j3}\right)^2\right]^{-1/2}2\left(r_{i2}-r_{j2}\right)\\
\frac{1}{2}\left[\left(r_{i1}-r_{j1}\right)^2+\left(r_{i2}-r_{j2}\right)^2+\left(r_{i3}-r_{j3}\right)^2\right]^{-1/2}2\left(r_{i3}-r_{j3}\right)
\end{Bmatrix},\\
=& \frac{1}{2}r_{ij}^{-1}2\mathbf{r}_{ij},\\
=& \frac{\mathbf{r}_{ij}}{r_{ij}}.
\end{aligned}
$$

iii

$$
\begin{aligned}
\mathcal{H} =& \mathcal{K}+\mathcal{U},\\
=& \Sigma_i\frac{|\mathbf{p}_i|^2}{2m_i}+\mathcal{U}.
\end{aligned}
$$

TODO: FINISH THIS PROOF

b)

$$
\begin{aligned}
v_{i,x}(t+\Delta t) &= v_{i,x}(t)+\frac{\partial v_{i,x}}{\partial t}\Big|_t(\Delta t)+\frac{1}{2}\frac{\partial^2 v_{i,x}}{\partial t^2}\Big|_t(\Delta t)^2,\\
&= v_{i,x}(t)+\frac{F_{i,x}(t)}{m_i}(\Delta t)+\frac{1}{2}\frac{\partial^2 v_{i,x}}{\partial t^2}\Big|_t(\Delta t)^2.
\end{aligned}
$$

Recall that $v_{i,x}(t+\Delta t/2)=v_{i,x}(t)+F_{i,x}(t)\Delta t/(2m_i)$.

$$
v_{i,x}(t+\Delta t)=v_{i,x}(t+\Delta t/2)+\frac{F_{i,x}(t)}{2m_i}(\Delta t)+\frac{1}{2}\frac{\partial^2 v_{i,x}}{\partial t^2}\Big|_t(\Delta t)^2. \tag{1}
$$

We can simplify (1) further by considering the Taylor expansion of the force:

$$
\begin{aligned}
F_{i,x}(t+\Delta t) &= F_{i,x}(t)+\frac{\partial F_{i,x}}{\partial t}\Big|_t(\Delta t), && (2)\\
&= F_{i,x}(t)+\frac{\partial}{\partial t}\left[m_i\frac{\partial v_{i,x}}{\partial t}\right]\Big|_t(\Delta t), && (3)\\
&= F_{i,x}(t)+m_i\frac{\partial^2 v_{i,x}}{\partial t^2}\Big|_t(\Delta t). && (4)
\end{aligned}
$$

Dividing both sides of (4) by $2m_i$ and plugging into (1) yields the desired result.