S6.C. Microscopic Balance Equations

The fundamental commutation relations for an N particle system are

$$
\begin{aligned}
&[\hat{\boldsymbol{q}}_i, \hat{\boldsymbol{q}}_j] = 0 \qquad [\hat{\boldsymbol{p}}_i, \hat{\boldsymbol{p}}_j] = 0 \qquad i, j = 1, \ldots, N \\
&[\hat{q}_{i\alpha}, \hat{q}_{j\beta}] = 0 \qquad [\hat{p}_{i\alpha}, \hat{p}_{j\beta}] = 0 \quad \alpha, \beta = x, y, z \\
&[\hat{\boldsymbol{q}}_i, \hat{\boldsymbol{p}}_j] = i\hbar\,\delta_{ij}\,\hat{I} \\
&[\hat{q}_{i\alpha}, \hat{p}_{j\beta}] = i\hbar\,\delta_{ij}\,\delta_{\alpha\beta}
\end{aligned} \tag{6.97}
$$

Using

$$
\begin{aligned}
[A, BC] &= ABC - BCA \\
&= ABC - BAC + BAC - BCA \\
&= [A, B]\,C + B\,[A, C]
\end{aligned}
$$

we have

$$
\begin{aligned}
[\hat{p}_{i\alpha}, \hat{q}_{j\beta}^2] &= [\hat{p}_{i\alpha}, \hat{q}_{j\beta}]\,\hat{q}_{j\beta} + \hat{q}_{j\beta}\,[\hat{p}_{i\alpha}, \hat{q}_{j\beta}] \\
&= -2\,i\hbar\,\delta_{\alpha\beta}\,\hat{q}_{i\beta} \\
[\hat{p}_{i\alpha}, \hat{q}_{j\beta}^3] &= [\hat{p}_{i\alpha}, \hat{q}_{j\beta}^2]\,\hat{q}_{j\beta} + \hat{q}_{j\beta}^2\,[\hat{p}_{i\alpha}, \hat{q}_{j\beta}] \\
&= -3\,i\hbar\,\delta_{\alpha\beta}\,\hat{q}_{i\beta}^2 \\
&\vdots \\
[\hat{p}_{i\alpha}, \hat{q}_{j\beta}^n] &= -n\,i\hbar\,\delta_{\alpha\beta}\,\hat{q}_{i\beta}^{n-1}
\end{aligned}
$$

$$
\begin{aligned}
[\hat{p}_{i\alpha}, F(\hat{\boldsymbol{q}}^N)] &= \sum_{n=0}^{\infty} \frac{1}{n!} \left.\frac{\partial^n F(\hat{\boldsymbol{q}}^N)}{\partial \hat{q}_{i\alpha}^n}\right|_{\hat{q}_{i\alpha}=0} [\hat{p}_{i\alpha}, \hat{q}_{i\alpha}^n] \\
&= \sum_{n=0}^{\infty} \frac{1}{n!} \left.\frac{\partial^n F(\hat{\boldsymbol{q}}^N)}{\partial \hat{q}_{i\alpha}^n}\right|_{\hat{q}_{i\alpha}=0} \left(-n\,i\hbar\,\hat{q}_{i\alpha}^{n-1}\right) \\
&= -i\hbar \sum_{n=1}^{\infty} \frac{1}{(n-1)!} \left.\frac{\partial^n F(\hat{\boldsymbol{q}}^N)}{\partial \hat{q}_{i\alpha}^n}\right|_{\hat{q}_{i\alpha}=0} \hat{q}_{i\alpha}^{n-1} \\
&= -i\hbar\,\frac{\partial F(\hat{\boldsymbol{q}}^N)}{\partial \hat{q}_{i\alpha}}
\end{aligned} \tag{6.98a}
$$

or

$$
[\hat{\boldsymbol{p}}_i, F(\hat{\boldsymbol{q}}^N)] = -i\hbar\,\frac{\partial F(\hat{\boldsymbol{q}}^N)}{\partial \hat{\boldsymbol{q}}_i} \qquad = -i\hbar\,\nabla_{\hat{\boldsymbol{q}}_i} F(\hat{\boldsymbol{q}}^N) \tag{6.98}
$$

Note: using the Taylor expansion, it is easy to show that

$$
\frac{\partial F(\hat{\boldsymbol{q}}^N)}{\partial \hat{\boldsymbol{q}}_i} = \left.\frac{\partial F(\boldsymbol{q}^N)}{\partial \boldsymbol{q}_i}\right|_{\boldsymbol{q}_i \to \hat{\boldsymbol{q}}_i}
$$

Similarly,

$$
\begin{aligned}
[\hat{q}_{i\alpha}, G(\hat{\boldsymbol{p}}^N)] &= \sum_{n=0}^{\infty} \frac{1}{n!} \left.\frac{\partial^n G(\hat{\boldsymbol{p}}^N)}{\partial \hat{p}_{i\alpha}^n}\right|_{q_{i\alpha}=0} [\hat{q}_{i\alpha}, \hat{p}_{i\alpha}^n] \\
&= i\hbar\,\frac{\partial G(\hat{\boldsymbol{p}}^N)}{\partial \hat{p}_{i\alpha}}
\end{aligned} \tag{6.99a}
$$

$$
[\hat{\boldsymbol{q}}_i, G(\hat{\boldsymbol{p}}^N)] = i\hbar\,\frac{\partial G(\hat{\boldsymbol{p}}^N)}{\partial \hat{\boldsymbol{p}}_i} = i\hbar\,\nabla_{\hat{\boldsymbol{p}}_i} G(\hat{\boldsymbol{p}}^N) \tag{6.99}
$$

Consider the Hamiltonian

$$\hat{H}^N = \sum_{i=1}^{N} \frac{\hat{\boldsymbol{p}}_i^2}{2m} + \sum_{i<j}^{N(N-1)/2} \hat{V}\left(\left| \hat{\boldsymbol{q}}_i - \hat{\boldsymbol{q}}_j \right| \right) \qquad (6.100)$$

$$= \sum_{i=1}^{N} \frac{\hat{p}_{i\alpha}\hat{p}_{i\alpha}}{2m} + \frac{1}{2} \sum_{i,j=1\ (i\neq j)}^{N} \hat{V}_{ij} \qquad (6.100a)$$

where

$$\alpha = x, y, z$$

$$\hat{V}_{ij} \equiv \hat{V}\left(\left| \hat{\boldsymbol{q}}_i - \hat{\boldsymbol{q}}_j \right| \right) = \hat{V}(\hat{r}_{ij}) \qquad \hat{r}_{ij} = \left| \hat{\boldsymbol{q}}_i - \hat{\boldsymbol{q}}_j \right|$$

and the Einstein’s convention of implicit summation over repeated indices will be assumed for the Cartesian components.

In the Heisenberg picture [see (6.57)], we have

$$\frac{\partial \hat{q}_{i\alpha}}{\partial t} = \frac{1}{i\hbar}\left[\hat{q}_{i\alpha}, \hat{H}^N \right]$$

$$= \frac{1}{i\hbar}\frac{1}{2m}\sum_{j=1}^{N}\left[\hat{q}_{i\alpha},\ \hat{p}_{j\beta}\hat{p}_{j\beta}\right]$$

$$= \frac{1}{i\hbar}\frac{1}{2m}\sum_{j=1}^{N} i\hbar \frac{\partial\, \hat{p}_{j\beta}\hat{p}_{j\beta}}{\partial \hat{p}_{i\alpha}}$$

$$= \frac{1}{2m}\sum_{j=1}^{N} 2\,\delta_{ij}\,\delta_{\alpha\beta}\,\hat{p}_{j\beta}$$

$$= \frac{\hat{p}_{i\alpha}}{m} \qquad (6.101a)$$

$$\rightarrow \qquad \frac{\partial \hat{\boldsymbol{q}}_i}{\partial t} = \frac{\hat{\boldsymbol{p}}_i}{m} \qquad (6.101)$$

Similarly,

$$\frac{\partial \hat{p}_{i\alpha}}{\partial t} = \frac{1}{i\hbar}\left[\hat{p}_{i\alpha}, \hat{H}^N \right]$$

$$= \frac{1}{2i\hbar}\sum_{j,k=1\ (j\neq k)}^{N}\left[\hat{p}_{i\alpha},\ \hat{V}_{jk}\right]$$

$$= -\frac{1}{2}\sum_{j,k=1\ (j\neq k)}^{N}\left(\delta_{ij}\frac{\partial \hat{V}_{ik}}{\partial \hat{q}_{i\alpha}} + \delta_{ik}\frac{\partial \hat{V}_{ji}}{\partial \hat{q}_{i\alpha}} \right)$$

$$= -\frac{1}{2}\left(\sum_{k=1\ (k\neq i)}^{N}\frac{\partial \hat{V}_{ik}}{\partial \hat{q}_{i\alpha}} + \sum_{j=1\ (j\neq i)}^{N}\frac{\partial \hat{V}_{ji}}{\partial \hat{q}_{i\alpha}} \right)$$

$$= -\sum_{j=1\,(\neq i)}^{N}\frac{\partial \hat{V}_{ij}}{\partial \hat{q}_{i\alpha}}$$

$$= \sum_{j=1\,(\neq i)}^{N}\hat{F}_{ij\alpha} \qquad (6.102a)$$

where

$$\hat{F}_{ij\alpha} \equiv -\frac{\partial \hat{V}_{ij}}{\partial \hat{q}_{i\alpha}} = -\frac{\partial \hat{r}_{ij}}{\partial \hat{q}_{i\alpha}}\hat{V}'_{ij} \qquad \hat{V}'_{ij} \equiv \frac{d\hat{V}_{ij}}{d\hat{r}_{ij}}$$

Using

$$\hat{r}_{ij} = \sqrt{\left(\hat{q}_{i\alpha}-\hat{q}_{j\alpha}\right)\left(\hat{q}_{i\alpha}-\hat{q}_{j\alpha}\right)} = \hat{r}_{ji} \qquad V_{ij} = V_{ji}$$

we have

$$\frac{\partial \hat{r}_{ij}}{\partial \hat{q}_{i\alpha}} = \frac{\hat{q}_{i\alpha} - \hat{q}_{j\alpha}}{\hat{r}_{ij}} = -\frac{\hat{q}_{j\alpha} - \hat{q}_{i\alpha}}{\hat{r}_{ji}} = -\frac{\partial \hat{r}_{ij}}{\partial \hat{q}_{j\alpha}}$$

so that

$$\hat{F}_{ij\alpha} = -\frac{\hat{q}_{i\alpha} - \hat{q}_{j\alpha}}{\hat{r}_{ij}} \hat{V}'_{ij} \qquad (6.102b)$$

$$\hat{F}_{ji\alpha} \equiv \frac{\partial \hat{V}_{ji}}{\partial \hat{q}_{j\alpha}} = \frac{\partial \hat{r}_{ji}}{\partial \hat{q}_{j\alpha}} \hat{V}'_{ji} = \frac{\partial \hat{r}_{ij}}{\partial \hat{q}_{j\alpha}} \hat{V}'_{ij} = -\hat{F}_{ij\alpha} \qquad (6.102c)$$

(6.102a) can be written as

$$\frac{\partial \hat{\boldsymbol{p}}_i}{\partial t} = -\sum_{j=1\,(\neq i)}^{N} \frac{\partial \hat{V}_{ij}}{\partial \hat{\boldsymbol{q}}_i} = \sum_{j=1\,(\neq i)}^{N} \hat{\boldsymbol{F}}_{ij} \qquad (6.102)$$

From the classical expressions for the particle density at point $\boldsymbol{R}$,

$$n(\boldsymbol{q}^N; \boldsymbol{R}) = \sum_{i=1}^{N} \delta(\boldsymbol{q}_i - \boldsymbol{R}) = \sum_{i=1}^{N} \prod_{\alpha} \delta(q_{i\alpha} - R_\alpha)$$

we obtain the quantized version as

$$\hat{n}\left(\hat{\boldsymbol{q}}^N; \boldsymbol{R}\right) = \sum_{i=1}^{N} \delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}) = \sum_{i=1}^{N} \prod_{\alpha} \delta(\hat{q}_{i\alpha} - R_\alpha) \qquad (6.104)$$

The equation of motion for $\hat{n}$ is

$$\begin{aligned}
\frac{\partial \hat{n}\left(\hat{\boldsymbol{q}}^N; \boldsymbol{R}\right)}{\partial t} &= \frac{1}{i\hbar}\left[\hat{n}\left(\hat{\boldsymbol{q}}^N; \boldsymbol{R}\right), \hat{H}^N\right] \\
&= \frac{1}{i\hbar}\left[\sum_{i=1}^{N} \delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}), \sum_{j=1}^{N} \frac{\hat{\boldsymbol{p}}_j^2}{2m}\right] \\
&= \frac{1}{i\hbar}\sum_{i=1}^{N}\left[\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}), \frac{\hat{p}_{i\alpha}\hat{p}_{i\alpha}}{2m}\right] \\
&= \frac{1}{i\hbar}\sum_{i=1}^{N}\left(\left[\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}), \hat{p}_{i\alpha}\right]\frac{\hat{p}_{i\alpha}}{2m} + \frac{\hat{p}_{i\alpha}}{2m}\left[\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}), \hat{p}_{i\alpha}\right]\right) \\
&= \sum_{i=1}^{N}\left(\frac{\partial \delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})}{\partial \hat{q}_{i\alpha}}\frac{\hat{p}_{i\alpha}}{2m} + \frac{\hat{p}_{i\alpha}}{2m}\frac{\partial \delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})}{\partial \hat{q}_{i\alpha}}\right) \\
&= -\sum_{i=1}^{N}\left(\frac{\partial \delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})}{\partial R_\alpha}\frac{\hat{p}_{i\alpha}}{2m} + \frac{\hat{p}_{i\alpha}}{2m}\frac{\partial \delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})}{\partial R_\alpha}\right) \\
&= -\frac{\partial}{\partial R_\alpha}\sum_{i=1}^{N}\left(\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})\frac{\hat{p}_{i\alpha}}{2m} + \frac{\hat{p}_{i\alpha}}{2m}\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})\right) \\
&= -\frac{\partial}{\partial R_\alpha}\hat{J}^n_\alpha\left(\hat{\boldsymbol{q}}^N, \hat{\boldsymbol{p}}^N; \boldsymbol{R}\right) \qquad (6.103a)
\end{aligned}$$

where

$$\hat{J}^n_\alpha\left(\hat{\boldsymbol{q}}^N, \hat{\boldsymbol{p}}^N; \boldsymbol{R}\right) = \frac{1}{2m}\sum_{i=1}^{N}\left(\hat{p}_{i\alpha}\,\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}) + \delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})\,\hat{p}_{i\alpha}\right) \qquad (6.105a)$$

is the α^{th} component of the current density operator at $\boldsymbol{R}$.

(6.103a) can be written in vector form as

$$\frac{\partial \hat{n}\left(\hat{\boldsymbol{q}}^N; \boldsymbol{R}\right)}{\partial t} = -\frac{\partial}{\partial \boldsymbol{R}} \cdot \sum_{i=1}^{N}\left(\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})\frac{\hat{\boldsymbol{p}}_i}{2m} + \frac{\hat{\boldsymbol{p}}_i}{2m}\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})\right)$$

$$= -\frac{\partial}{\partial \boldsymbol{R}} \cdot \hat{\boldsymbol{J}}^n \left(\hat{\boldsymbol{q}}^N, \hat{\boldsymbol{p}}^N; \boldsymbol{R}\right)$$
$$= -\nabla_{\boldsymbol{R}} \cdot \hat{\boldsymbol{J}}^n \left(\hat{\boldsymbol{q}}^N, \hat{\boldsymbol{p}}^N; \boldsymbol{R}\right) \qquad (6.103)$$

where

$$\hat{\boldsymbol{J}}^n \left(\hat{\boldsymbol{q}}^N, \hat{\boldsymbol{p}}^N; \boldsymbol{R}\right) = \frac{1}{2\,m} \sum_{i=1}^{N} \left(\hat{\boldsymbol{p}}_i \, \delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}) + \delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}) \, \hat{\boldsymbol{p}}_i \right) \qquad (6.105)$$

is the current density operator at $\boldsymbol{R}$.

(6.103) is the balance equation for the particle number density n.

Note that (6.105) can be obtained from the classical version

$$\boldsymbol{J}^n(\boldsymbol{q}^N, \boldsymbol{p}^N; \boldsymbol{R}) = \sum_{i=1}^{N} \frac{\boldsymbol{p}_i}{m} \delta(\boldsymbol{q}_i - \boldsymbol{R})$$

by applying the quantization rule that all products of $\hat{\boldsymbol{q}}$ & $\hat{\boldsymbol{p}}$ must be symmetrized to keep the resultant operator Hermitian.

The momentum density operator at $\boldsymbol{R}$ is defined as

$$\hat{\boldsymbol{J}}^p \left(\hat{\boldsymbol{q}}^N, \hat{\boldsymbol{p}}^N; \boldsymbol{R}\right) = \frac{1}{2} \sum_{i=1}^{N} \left(\hat{\boldsymbol{p}}_i \, \delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}) + \delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}) \, \hat{\boldsymbol{p}}_i \right) \qquad (6.106a)$$
$$= m \, \hat{\boldsymbol{J}}^n \left(\hat{\boldsymbol{q}}^N, \hat{\boldsymbol{p}}^N; \boldsymbol{R}\right)$$

with Cartesian components

$$\hat{J}^p_\alpha \left(\hat{\boldsymbol{q}}^N, \hat{\boldsymbol{p}}^N; \boldsymbol{R}\right) = \frac{1}{2} \sum_{i=1}^{N} \left(\hat{p}_{i\alpha} \, \delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}) + \delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}) \, \hat{p}_{i\alpha} \right) \qquad (6.106b)$$

Similar to the case of $\hat{n}$, the balance equation for $\hat{\boldsymbol{J}}^p$ is related to the equation of motion as

$$\frac{\partial \hat{J}^p_\alpha}{\partial t} = \frac{1}{i\hbar} \left[\hat{J}^p_\alpha, \hat{H}^N \right] = -\frac{\partial}{\partial R_\beta} \hat{\mathbb{J}}^p_{\beta\alpha} \qquad (6.106c)$$

or

$$\frac{\partial \hat{\boldsymbol{J}}^p}{\partial t} = \frac{1}{i\hbar} \left[\hat{\boldsymbol{J}}^p, \hat{H}^N \right] = -\nabla_{\boldsymbol{R}} \cdot \hat{\mathbb{J}}^p \qquad (6.106)$$

where the momentum current density tensor $\hat{\mathbb{J}}^p$ is to be determined as follows.

To begin,

$$\left[\hat{p}_{i\alpha} \, \delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}), \; \hat{H}^N \right]$$
$$= \left[\hat{p}_{i\alpha} \, \delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}), \; \sum_{j=1}^{N} \frac{\hat{p}_{j\beta} \hat{p}_{j\beta}}{2\,m} + \frac{1}{2} \sum_{j,k=1\,(j\neq k)}^{N} \hat{V}_{jk} \right]$$
$$= \hat{p}_{i\alpha} \left[\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}), \; \sum_{j=1}^{N} \frac{\hat{p}_{j\beta} \hat{p}_{j\beta}}{2\,m} \right] + \left[\hat{p}_{i\alpha}, \; \frac{1}{2} \sum_{j,k=1\,(j\neq k)}^{N} \hat{V}_{jk} \right] \delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})$$

The commutators were already evaluated to obtain (6.102-3), giving

$$\frac{1}{i\hbar} \left[\hat{p}_{i\alpha} \, \delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}), \; \hat{H}^N \right]$$
$$= -\frac{\hat{p}_{i\alpha}}{2\,m} \frac{\partial}{\partial R_\beta} \left[\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}) \, \hat{p}_{i\beta} + \hat{p}_{i\beta} \, \delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}) \right] + \sum_{j=1\,(\neq i)}^{N} \hat{F}_{ij\alpha} \, \delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})$$

Similarly,

$$\frac{1}{i\hbar} \left[\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}) \, \hat{p}_{i\alpha}, \; \hat{H}^N \right]$$

$$= \frac{1}{i\hbar}\left[\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})\,\hat{p}_{i\alpha},\ \sum_{j=1}^{N}\frac{\hat{p}_{j\beta}\hat{p}_{j\beta}}{2m} + \frac{1}{2}\sum_{j,k=1\,(j\neq k)}^{N}\hat{V}_{jk}\right]$$

$$= \frac{1}{i\hbar}\,\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})\left[\hat{p}_{i\alpha},\ \frac{1}{2}\sum_{j,k=1\,(j\neq k)}^{N}\hat{V}_{jk}\right] + \left[\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}),\ \sum_{j=1}^{N}\frac{\hat{p}_{j\beta}\hat{p}_{j\beta}}{2m}\right]\hat{p}_{i\alpha}$$

$$= \delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})\sum_{j=1\,(\neq i)}^{N}\hat{F}_{ij\alpha} - \frac{1}{2m}\frac{\partial}{\partial R_\beta}\left[\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})\,\hat{p}_{i\beta} + \hat{p}_{i\beta}\,\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})\right]\hat{p}_{i\alpha}$$

Hence,

$$\frac{1}{i\hbar}\left[\hat{J}^{p}_{\alpha},\ \hat{H}^{N}\right] = -\frac{1}{4m}\frac{\partial}{\partial R_\beta}\sum_{i=1}^{N}\Big[\hat{p}_{i\alpha}\,\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})\,\hat{p}_{i\beta} + \hat{p}_{i\alpha}\hat{p}_{i\beta}\,\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}) + \delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})\,\hat{p}_{i\beta}\hat{p}_{i\alpha} + \hat{p}_{i\beta}\,\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})\,\hat{p}_{i\alpha}\Big] + \sum_{i,j=1\,(i\neq j)}^{N}\hat{F}_{ij\alpha}\,\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}) \tag{6.107a}$$

As will be shown momentarily,

$$\sum_{i,j=1\,(i\neq j)}^{N}\hat{F}_{ij\alpha}\,\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}) = \frac{\partial}{\partial R_\beta}(\mathcal{S}_1 + \mathcal{S}_2 + \mathcal{S}_3) \tag{6.107b}$$

where

$$\mathcal{S}_1 = \frac{1}{4}\sum_{i,j=1\,(i\neq j)}^{N}(\hat{q}_{i\alpha} - \hat{q}_{j\alpha})\,\hat{F}_{ij\beta}\,\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})$$

$$\mathcal{S}_2 = \frac{1}{4}\sum_{i,j=1\,(i\neq j)}^{N}(\hat{q}_{i\beta} - \hat{q}_{j\beta})\,\hat{F}_{ij\alpha}\,\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}) = \mathcal{S}_1\,(\alpha \leftrightarrow \beta)$$

$$\mathcal{S}_3 = -\frac{1}{2}\sum_{i,j=1\,(i\neq j)}^{N}\delta_{\alpha\beta}(\hat{q}_{i\gamma} - \hat{q}_{j\gamma})\,\hat{F}_{ij\gamma}\,\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})$$

Note that the tensor $\mathcal{S} = \mathcal{S}_1 + \mathcal{S}_2 + \mathcal{S}_3$ is symmetric and traceless, i.e.,

$$\mathcal{S}_{\alpha\beta} = \mathcal{S}_{\beta\alpha} \qquad \mathrm{Tr}\,\mathcal{S} = \mathcal{S}_{\alpha\alpha} = 0$$

(6.106) & (6.107a) then give

$$\mathbb{J}^{p}_{\alpha\beta} = \frac{1}{4m}\sum_{i=1}^{N}\Big[\hat{p}_{i\alpha}\,\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})\,\hat{p}_{i\beta} + \hat{p}_{i\alpha}\hat{p}_{i\beta}\,\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}) + \delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})\,\hat{p}_{i\beta}\hat{p}_{i\alpha} + \hat{p}_{i\beta}\,\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})\,\hat{p}_{i\alpha}\Big] - \frac{1}{4}\sum_{i,j=1\,(i\neq j)}^{N}\Big[(\hat{q}_{i\alpha} - \hat{q}_{j\alpha})\,\hat{F}_{ij\beta} + (\hat{q}_{i\beta} - \hat{q}_{j\beta})\,\hat{F}_{ij\alpha} - 2\,\delta_{\alpha\beta}(\hat{q}_{i\gamma} - \hat{q}_{j\gamma})\,\hat{F}_{ij\gamma}\Big]\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}) \tag{6.107}$$

In tensor (dyadic) form

$$\mathbb{J}^p = \frac{1}{4m}\sum_{i=1}^{N}\{\hat{\boldsymbol{p}}_i\,\delta(\hat{\boldsymbol{q}}_i-\boldsymbol{R})\,\hat{\boldsymbol{p}}_i+\hat{\boldsymbol{p}}_i\,\hat{\boldsymbol{p}}_i\,\delta(\hat{\boldsymbol{q}}_i-\boldsymbol{R}) \qquad (6.107c)$$

$$+\left[\hat{\boldsymbol{p}}_i\,\delta(\hat{\boldsymbol{q}}_i-\boldsymbol{R})\,\hat{\boldsymbol{p}}_i+\hat{\boldsymbol{p}}_i\,\hat{\boldsymbol{p}}_i\,\delta(\hat{\boldsymbol{q}}_i-\boldsymbol{R})\right]^+\}$$

$$-\frac{1}{4}\sum_{i,j=1\,(i\neq j)}^{N}\left\{(\hat{\boldsymbol{q}}_i-\hat{\boldsymbol{q}}_j)\,\hat{\boldsymbol{F}}_{ij}+\hat{\boldsymbol{F}}_{ij}(\hat{\boldsymbol{q}}_i-\hat{\boldsymbol{q}}_j)\right.$$

$$\left.-2\left[(\hat{\boldsymbol{q}}_i-\hat{\boldsymbol{q}}_j)\cdot\hat{\boldsymbol{F}}_{ij}\right]\boldsymbol{I}\right\}\delta(\hat{\boldsymbol{q}}_i-\boldsymbol{R})$$

Note that the tensor $\mathbb{J}^p$ is symmetric as well as Hermitian, i.e.,

$$\mathbb{J}^{p+}=\mathbb{J}^p=\mathbb{J}^{pT} \qquad \text{or} \qquad \mathbb{J}^{p+}_{\alpha\beta}=\mathbb{J}^p_{\beta\alpha}=\mathbb{J}^p_{\alpha\beta}$$

To prove (6.107b), consider the 1st term on the R.H.S.,

$$\frac{\partial}{\partial R_\beta}S_1=\frac{1}{4}\frac{\partial}{\partial R_\beta}\sum_{i,j=1\,(i\neq j)}^{N}(\hat{q}_{i\alpha}-\hat{q}_{j\alpha})\,\hat{F}_{ij\beta}\,\delta(\hat{\boldsymbol{q}}_i-\boldsymbol{R})$$

$$=\frac{1}{4}\sum_{i,j=1\,(i\neq j)}^{N}(\hat{q}_{i\alpha}-\hat{q}_{j\alpha})\,\hat{F}_{ij\beta}\,\frac{\partial}{\partial R_\beta}\delta(\hat{\boldsymbol{q}}_i-\boldsymbol{R})$$

$$=-\frac{1}{4}\sum_{i,j=1\,(i\neq j)}^{N}(\hat{q}_{i\alpha}-\hat{q}_{j\alpha})\,\hat{F}_{ij\beta}\,\frac{\partial}{\partial \hat{q}_{i\beta}}\delta(\hat{\boldsymbol{q}}_i-\boldsymbol{R})$$

$$=\frac{1}{4}\sum_{i,j=1\,(i\neq j)}^{N}\frac{\partial\,(\hat{q}_{i\alpha}-\hat{q}_{j\alpha})\,\hat{F}_{ij\beta}}{\partial \hat{q}_{i\beta}}\,\delta(\hat{\boldsymbol{q}}_i-\boldsymbol{R}) \qquad [\,f\,\delta'(x)=-f'\,\delta(x)\,]$$

$$=\frac{1}{4}\sum_{i,j=1\,(i\neq j)}^{N}\left[\delta_{\alpha\beta}\,\hat{F}_{ij\beta}+(\hat{q}_{i\alpha}-\hat{q}_{j\alpha})\,\frac{\partial \hat{F}_{ij\beta}}{\partial \hat{q}_{i\beta}}\right]\delta(\hat{\boldsymbol{q}}_i-\boldsymbol{R})$$

$$=\frac{1}{4}\sum_{i,j=1\,(i\neq j)}^{N}\left[\hat{F}_{ij\alpha}+(\hat{q}_{i\alpha}-\hat{q}_{j\alpha})\,\frac{\partial \hat{F}_{ij\beta}}{\partial \hat{q}_{i\beta}}\right]\delta(\hat{\boldsymbol{q}}_i-\boldsymbol{R})$$

From (6.102b), we have

$$\frac{\partial \hat{F}_{ij\alpha}}{\partial \hat{q}_{i\beta}}=-\frac{\partial^2\,\hat{r}_{ij}}{\partial \hat{q}_{i\beta}\,\partial \hat{q}_{i\alpha}}\,\hat{V}'_{ij}-\frac{\partial\,\hat{r}_{ij}}{\partial \hat{q}_{i\alpha}}\,\frac{\partial\,\hat{r}_{ij}}{\partial \hat{q}_{i\beta}}\,\hat{V}''_{ij}$$

$$=-\left[\delta_{\alpha\beta}\,\frac{1}{\hat{r}_{ij}}-\frac{(\hat{q}_{i\alpha}-\hat{q}_{j\alpha})(\hat{q}_{i\beta}-\hat{q}_{j\beta})}{\hat{r}_{ij}^3}\right]\hat{V}'_{ij}-\frac{(\hat{q}_{i\alpha}-\hat{q}_{j\alpha})(\hat{q}_{i\beta}-\hat{q}_{j\beta})}{\hat{r}_{ij}^2}\,\hat{V}''_{ij}$$

$$=\frac{\partial \hat{F}_{ij\beta}}{\partial \hat{q}_{i\alpha}} \qquad [\text{ Symmetric in } \alpha \,\&\, \beta.\ ]$$

$$\rightarrow \qquad \frac{\partial \hat{F}_{ij\beta}}{\partial \hat{q}_{i\beta}}=-\left[\frac{3}{\hat{r}_{ij}}-\frac{(\hat{q}_{i\beta}-\hat{q}_{j\beta})(\hat{q}_{i\beta}-\hat{q}_{j\beta})}{\hat{r}_{ij}^3}\right]\hat{V}'_{ij}-\frac{(\hat{q}_{i\beta}-\hat{q}_{j\beta})(\hat{q}_{i\beta}-\hat{q}_{j\beta})}{\hat{r}_{ij}^2}\,\hat{V}''_{ij}$$

$$=-\frac{2}{\hat{r}_{ij}}\,\hat{V}'_{ij}-\hat{V}''_{ij}$$

Hence,

$$\frac{\partial\,(\hat{q}_{i\alpha}-\hat{q}_{j\alpha})\,\hat{F}_{ij\beta}}{\partial \hat{q}_{i\beta}}=\delta_{\alpha\beta}\,\hat{F}_{ij\beta}+(\hat{q}_{i\alpha}-\hat{q}_{j\alpha})\,\frac{\partial \hat{F}_{ij\beta}}{\partial \hat{q}_{i\beta}}$$

$$=\hat{F}_{ij\alpha}+(\hat{q}_{i\alpha}-\hat{q}_{j\alpha})\,\frac{\partial \hat{F}_{ij\beta}}{\partial \hat{q}_{i\beta}}$$

$$= \hat{F}_{ij\alpha} - (\hat{q}_{i\alpha} - \hat{q}_{j\alpha})\left(\frac{2}{\hat{r}_{ij}}\hat{V}'_{ij} + \hat{V}''_{ij}\right)$$

so that

$$\frac{\partial}{\partial R_\beta}\mathcal{S}_1 = \frac{1}{4}\sum_{i,j=1\,(i\neq j)}^{N}\left[\hat{F}_{ij\alpha} - (\hat{q}_{i\alpha} - \hat{q}_{j\alpha})\left(\frac{2}{\hat{r}_{ij}}\hat{V}'_{ij} + \hat{V}''_{ij}\right)\right]\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})$$

Similarly, the 2nd term on the R.H.S. of (6.107b) gives

$$\frac{\partial}{\partial R_\beta}\mathcal{S}_2 = \frac{1}{4}\frac{\partial}{\partial R_\beta}\sum_{i,j=1\,(i\neq j)}^{N}(\hat{q}_{i\beta} - \hat{q}_{j\beta})\hat{F}_{ij\alpha}\,\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})$$

$$= \frac{1}{4}\sum_{i,j=1\,(i\neq j)}^{N}(\hat{q}_{i\beta} - \hat{q}_{j\beta})\hat{F}_{ij\alpha}\frac{\partial}{\partial R_\beta}\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})$$

$$= -\frac{1}{4}\sum_{i,j=1\,(i\neq j)}^{N}(\hat{q}_{i\beta} - \hat{q}_{j\beta})\hat{F}_{ij\alpha}\frac{\partial}{\partial \hat{q}_{i\beta}}\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})$$

$$= \frac{1}{4}\sum_{i,j=1\,(i\neq j)}^{N}\frac{\partial\,(\hat{q}_{i\beta} - \hat{q}_{j\beta})\hat{F}_{ij\alpha}}{\partial \hat{q}_{i\beta}}\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})$$

Using

$$\frac{\partial\,(\hat{q}_{i\beta} - \hat{q}_{j\beta})\hat{F}_{ij\alpha}}{\partial \hat{q}_{i\beta}} = 3\hat{F}_{ij\alpha} + (\hat{q}_{i\beta} - \hat{q}_{j\beta})\frac{\partial \hat{F}_{ij\alpha}}{\partial \hat{q}_{i\beta}}$$

$$= 3\hat{F}_{ij\alpha} - \left[\frac{\hat{q}_{i\alpha} - \hat{q}_{j\alpha}}{\hat{r}_{ij}} - \frac{(\hat{q}_{i\alpha} - \hat{q}_{j\alpha})\hat{r}_{ij}^2}{\hat{r}_{ij}^3}\right]\hat{V}'_{ij} - \frac{(\hat{q}_{i\alpha} - \hat{q}_{j\alpha})\hat{r}_{ij}^2}{\hat{r}_{ij}^2}\hat{V}''_{ij}$$

$$= 3\hat{F}_{ij\alpha} - (\hat{q}_{i\alpha} - \hat{q}_{j\alpha})\hat{V}''_{ij}$$

we have

$$\frac{\partial}{\partial R_\beta}\mathcal{S}_2 = \frac{1}{4}\frac{\partial}{\partial R_\beta}\sum_{i,j=1\,(i\neq j)}^{N}\left[3\hat{F}_{ij\alpha} - (\hat{q}_{i\alpha} - \hat{q}_{j\alpha})\hat{V}''_{ij}\right]\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})$$

Thus,

$$\frac{\partial}{\partial R_\beta}(\mathcal{S}_1 + \mathcal{S}_2) = \sum_{i,j=1\,(i\neq j)}^{N}\left[\hat{F}_{ij\alpha} - \frac{1}{2}(\hat{q}_{i\alpha} - \hat{q}_{j\alpha})\left(\frac{1}{\hat{r}_{ij}}\hat{V}'_{ij} + \hat{V}''_{ij}\right)\right]\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}) \qquad \text{(a)}$$

Now,

$$\sum_{i,j=1\,(i\neq j)}^{N}(\hat{q}_{i\alpha} - \hat{q}_{j\alpha})\left(\frac{1}{\hat{r}_{ij}}\hat{V}'_{ij} + \hat{V}''_{ij}\right)\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})$$

$$= \sum_{i,j=1\,(i\neq j)}^{N}\left(\frac{\hat{q}_{i\alpha} - \hat{q}_{j\alpha}}{\hat{r}_{ij}}\right)\left(\hat{r}_{ij}\hat{V}'_{ij}\right)'\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})$$

$$= \sum_{i,j=1\,(i\neq j)}^{N}\frac{\partial \hat{r}_{ij}}{\partial \hat{q}_{i\alpha}}\frac{d\,\hat{r}_{ij}\hat{V}'_{ij}}{d\,\hat{r}_{ij}}\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})$$

$$= \sum_{i,j=1\,(i\neq j)}^{N}\frac{\partial\,\hat{r}_{ij}\hat{V}'_{ij}}{\partial \hat{q}_{i\alpha}}\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})$$

$$= -\sum_{i,j=1\,(i\neq j)}^{N}\hat{r}_{ij}\hat{V}'_{ij}\frac{\partial}{\partial \hat{q}_{i\alpha}}\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})$$

$$= \sum_{i,j=1\,(i\neq j)}^{N} \hat{r}_{ij}\,\hat{V}'_{ij}\,\frac{\partial}{\partial R_\alpha}\,\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})$$

$$= \frac{\partial}{\partial R_\alpha}\sum_{i,j=1\,(i\neq j)}^{N} \hat{r}_{ij}\,\hat{V}'_{ij}\,\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})$$

$$= -\frac{\partial}{\partial R_\alpha}\sum_{i,j=1\,(i\neq j)}^{N} (\hat{q}_{i\beta} - \hat{q}_{j\beta})\,\hat{F}_{ij\beta}\,\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})$$

$$= -\frac{\partial}{\partial R_\beta}\sum_{i,j=1\,(i\neq j)}^{N} \delta_{\alpha\beta}\,(\hat{q}_{i\gamma} - \hat{q}_{j\gamma})\,\hat{F}_{ij\gamma}\,\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})$$

$$= 2\,\frac{\partial}{\partial R_\beta}\,S_3 \qquad \text{(b)}$$

where we have used the result from (6.102b) that

$$(\hat{q}_{i\alpha} - \hat{q}_{j\alpha})\,\hat{F}_{ij\alpha} = -\frac{(\hat{q}_{i\alpha} - \hat{q}_{j\alpha})(\hat{q}_{i\alpha} - \hat{q}_{j\alpha})}{\hat{r}_{ij}}\,\hat{V}'_{ij} = -\hat{r}_{ij}\,\hat{V}'_{ij}$$

Putting (b) back in (a) turns it into (6.107b) and the proof is complete.

Energy

The energy density operator at $\boldsymbol{R}$ is defined as

$$\hat{h}\left(\hat{\boldsymbol{q}}^N, \hat{\boldsymbol{p}}^N; \boldsymbol{R}\right) = \frac{1}{2}\sum_{i=1}^{N}\left(\hat{H}_i\,\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}) + \delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})\,\hat{H}_i\right) \qquad (6.110)$$

where

$$\hat{H}_i = \frac{\hat{p}_{i\alpha}\,\hat{p}_{i\alpha}}{2\,m} + \frac{1}{2}\sum_{j=1\,(j\neq i)}^{N} \hat{V}_{ij} \qquad (6.111)$$

$$\hat{H}^N = \sum_{i=1}^{N} \hat{H}_i$$

The balance equation for $\hat{h}$ is related to the equation of motion as

$$\frac{\partial\,\hat{h}}{\partial\,t} = \frac{1}{i\,\hbar}\left[\hat{h}, \hat{H}^N\right] = -\frac{\partial}{\partial R_\alpha}\,\hat{\mathbb{J}}^h_\alpha \qquad (6.111a)$$

where the energy current density $\hat{\mathbb{J}}^h$ is to be determined as follows.

To begin,

$$\left[\hat{h}, \hat{H}^N\right] = \left[\frac{1}{2}\sum_{i=1}^{N}\left(\hat{H}_i\,\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}) + \delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})\,\hat{H}_i\right), \sum_{j=1}^{N}\hat{H}_j\right]$$

$$= \frac{1}{2}\sum_{i,j=1}^{N}\left\{\hat{H}_i\left[\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}), \hat{H}_j\right] + \left[\hat{H}_i\,, \hat{H}_j\right]\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})\right. \qquad (6.111b)$$

$$\left. + \delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})\left[\hat{H}_i\,, \hat{H}_j\right] + \left[\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}), \hat{H}_j\right]\hat{H}_i\right\}$$

Now, in the derivation of (6.103a), we have already shown that

$$\frac{1}{i\,\hbar}\left[\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}), \hat{H}_j\right] = -\delta_{ij}\,\frac{\partial}{\partial R_\alpha}\left(\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})\,\frac{\hat{p}_{i\alpha}}{2\,m} + \frac{\hat{p}_{i\alpha}}{2\,m}\,\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})\right)$$

Using

$$\frac{1}{i\,\hbar}\left[\hat{p}_{i\alpha}\,, \sum_{k=1\,(k\neq j)}^{N} \hat{V}_{jk}\right] = -\sum_{k=1\,(k\neq j)}^{N} \frac{\partial\,\hat{V}_{jk}}{\partial\,\hat{q}_{i\alpha}}$$

$$= \sum_{k=1\ (k\neq j)}^{N} \left(\delta_{ij} \hat{F}_{ik\alpha} + \delta_{ik} \hat{F}_{ij\alpha} \right)$$

we have

$$\frac{1}{i\hbar}\left[\hat{H}_i\ ,\ \hat{H}_j\right] = \frac{1}{i\hbar}\left[\frac{\hat{p}_{i\alpha}\hat{p}_{i\alpha}}{2m}\ ,\ \frac{1}{2}\sum_{k=1\ (k\neq j)}^{N}\hat{V}_{jk}\right] + \frac{1}{i\hbar}\left[\frac{1}{2}\sum_{k=1\ (k\neq i)}^{N}\hat{V}_{ik}\ ,\ \frac{\hat{p}_{j\alpha}\hat{p}_{j\alpha}}{2m}\right]$$

$$= \frac{1}{4m}\sum_{k=1\ (k\neq j)}^{N}\left\{\hat{p}_{i\alpha}\left(\delta_{ij}\hat{F}_{ik\alpha} + \delta_{ik}\hat{F}_{ij\alpha}\right) + \left(\delta_{ij}\hat{F}_{ik\alpha} + \delta_{ik}\hat{F}_{ij\alpha}\right)\hat{p}_{i\alpha}\right\}$$

$$-\frac{1}{4m}\sum_{k=1\ (k\neq i)}^{N}\left\{\hat{p}_{j\alpha}\left(\delta_{ij}\hat{F}_{jk\alpha} + \delta_{jk}\hat{F}_{ji\alpha}\right) + \left(\delta_{ij}\hat{F}_{jk\alpha} + \delta_{jk}\hat{F}_{ji\alpha}\right)\hat{p}_{j\alpha}\right\}$$

Keeping in mind that the sums over i & j are unrestricted, while that over k is constrained with $k \neq i$ or j, we have

$$\frac{1}{i\hbar}\sum_{i,j=1}^{N}\left[\hat{H}_i\ ,\ \hat{H}_j\right]\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})$$

$$= \frac{1}{4m}\left\{\sum_{i,k=1\ (k\neq i)}^{N}\hat{p}_{i\alpha}\hat{F}_{ik\alpha}\,\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}) + \sum_{j,k=1\ (k\neq j)}^{N}\hat{p}_{k\alpha}\hat{F}_{kj\alpha}\,\delta(\hat{\boldsymbol{q}}_k - \boldsymbol{R})\right.$$

$$+ \sum_{i,k=1\ (k\neq i)}^{N}\hat{F}_{ik\alpha}\hat{p}_{i\alpha}\,\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}) + \sum_{j,k=1\ (k\neq j)}^{N}\hat{F}_{kj\alpha}\hat{p}_{k\alpha}\,\delta(\hat{\boldsymbol{q}}_k - \boldsymbol{R})$$

$$- \sum_{i,k=1\ (k\neq i)}^{N}\hat{p}_{i\alpha}\hat{F}_{ik\alpha}\,\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}) - \sum_{i,k=1\ (k\neq i)}^{N}\hat{p}_{k\alpha}\hat{F}_{ki\alpha}\,\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})$$

$$\left. - \sum_{i,k=1\ (k\neq i)}^{N}\hat{F}_{ik\alpha}\hat{p}_{i\alpha}\,\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}) - \sum_{i,k=1\ (k\neq i)}^{N}\hat{F}_{ki\alpha}\hat{p}_{k\alpha}\,\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})\right\}$$

$$= \frac{1}{4m}\left\{\sum_{j,k=1\ (k\neq j)}^{N}\left(\hat{p}_{k\alpha}\hat{F}_{kj\alpha} + \hat{F}_{kj\alpha}\hat{p}_{k\alpha}\right)\delta(\hat{\boldsymbol{q}}_k - \boldsymbol{R})\right.$$

$$\left. - \sum_{i,k=1\ (k\neq i)}^{N}\left(\hat{p}_{k\alpha}\hat{F}_{ki\alpha} + \hat{F}_{ki\alpha}\hat{p}_{k\alpha}\right)\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})\right\}$$

$$= \frac{1}{4m}\left\{\sum_{i,k=1\ (k\neq i)}^{N}\left(\hat{p}_{i\alpha}\hat{F}_{ik\alpha} + \hat{F}_{ik\alpha}\hat{p}_{i\alpha}\right)\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})\right.$$

$$\left. - \sum_{i,k=1\ (k\neq i)}^{N}\left(\hat{p}_{k\alpha}\hat{F}_{ki\alpha} + \hat{F}_{ki\alpha}\hat{p}_{k\alpha}\right)\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})\right\}$$

$$= \frac{1}{4m}\sum_{i,k=1\ (k\neq i)}^{N}\left[\left(\hat{p}_{i\alpha} + \hat{p}_{k\alpha}\right)\hat{F}_{ik\alpha} + \hat{F}_{ik\alpha}\left(\hat{p}_{i\alpha} + \hat{p}_{k\alpha}\right)\right]\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})$$

$$= \frac{1}{2m}\sum_{i,k=1\ (k\neq i)}^{N}\left(\hat{p}_{i\alpha} + \hat{p}_{k\alpha}\right)\hat{F}_{ik\alpha}\,\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}) \qquad \left[\ \frac{\partial\hat{F}_{ik\alpha}}{\partial\hat{q}_{i\alpha}} = -\frac{\partial\hat{F}_{ik\alpha}}{\partial\hat{q}_{k\alpha}}\ \right]$$

$$= \frac{1}{2m}\sum_{i,j=1\ (j\neq i)}^{N}\left(\hat{p}_{i\alpha} + \hat{p}_{j\alpha}\right)\hat{F}_{ij\alpha}\,\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})$$

Similarly,

$$\frac{1}{i\hbar}\sum_{i,j=1}^{N}\delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})\left[\hat{H}_i\ ,\ \hat{H}_j\right]$$

$$= \frac{1}{2m} \sum_{i,j=1\ (j\neq i)}^{N} \delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}) (\hat{p}_{i\alpha} + \hat{p}_{j\alpha}) \hat{F}_{ij\alpha}$$

$$= \frac{1}{2m} \sum_{i,j=1\ (j\neq i)}^{N} \delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}) \hat{F}_{ij\alpha} (\hat{p}_{i\alpha} + \hat{p}_{j\alpha})$$

(6.111b) thus becomes

$$\frac{\partial \hat{h}}{\partial t} = \frac{1}{i\hbar} \left[\hat{h}, \hat{H}^N \right]$$

$$= -\frac{1}{4m} \frac{\partial}{\partial R_\alpha} \sum_{i=1}^{N} \Big\{ \hat{H}_i \delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}) \hat{p}_{i\alpha} + \hat{H}_i \hat{p}_{i\alpha} \delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})$$

$$+ \delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}) \hat{p}_{i\alpha} \hat{H}_i + \hat{p}_{i\alpha} \delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}) \hat{H}_i \Big\}$$

$$+ \frac{1}{4m} \sum_{i,j=1\ (j\neq i)}^{N} \Big\{ (\hat{p}_{i\alpha} + \hat{p}_{j\alpha}) F_{ij\alpha} \delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})$$

$$+ \delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}) F_{ij\alpha} (\hat{p}_{i\alpha} + \hat{p}_{j\alpha}) \Big] \Big\}$$

Using (6.107b), we have

$$\frac{\partial \hat{h}}{\partial t} = -\frac{\partial}{\partial R_\alpha} \mathbb{J}_\alpha^h = -\nabla_{\boldsymbol{R}} \cdot \mathbb{J}^h \qquad (6.109)$$

where

$$\mathbb{J}_\alpha^h = \frac{1}{4m} \sum_{i=1}^{N} \Big\{ \hat{H}_i \delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}) \hat{p}_{i\alpha} + \hat{H}_i \hat{p}_{i\alpha} \delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}) \qquad (6.112)$$

$$+ \delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}) \hat{p}_{i\alpha} \hat{H}_i + \hat{p}_{i\alpha} \delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}) \hat{H}_i \Big\}$$

$$- \frac{1}{4m} \sum_{i,j=1\ (j\neq i)}^{N} \Big\{ (\hat{p}_{i\beta} + \hat{p}_{j\beta}) \Big[(\hat{q}_{i\alpha} - \hat{q}_{j\alpha}) \hat{F}_{ij\beta} + (\hat{q}_{i\beta} - \hat{q}_{j\beta}) \hat{F}_{ij\alpha}$$

$$- 2\delta_{\alpha\beta} (\hat{q}_{i\gamma} - \hat{q}_{j\gamma}) \hat{F}_{ij\gamma} \Big] \delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R})$$

$$+ \delta(\hat{\boldsymbol{q}}_i - \boldsymbol{R}) \Big[(\hat{q}_{i\alpha} - \hat{q}_{j\alpha}) \hat{F}_{ij\beta} + (\hat{q}_{i\beta} - \hat{q}_{j\beta}) \hat{F}_{ij\alpha}$$

$$- 2\delta_{\alpha\beta} (\hat{q}_{i\gamma} - \hat{q}_{j\gamma}) \hat{F}_{ij\gamma} \Big] (\hat{p}_{i\beta} + \hat{p}_{j\beta}) \Big\}$$