S6.B. Reduced Density Matrices and the Wigner Distribution

The quantum 1- and 2- body operators in an N-body system take the respective forms

$$\hat{O}_{(1)}^{N} = \sum_{i=1}^{N} \hat{O}(\hat{\boldsymbol{X}}_i) = \sum_{i=1}^{N} \hat{O}(\hat{\boldsymbol{q}}_i , \hat{\boldsymbol{p}}_i) \tag{6.77}$$

$$\hat{O}_{(2)}^{N} = \sum_{i<j}^{N(N-1)/2} \hat{O}\left(\hat{\boldsymbol{X}}_i,\ \hat{\boldsymbol{X}}_j\right) = \sum_{i<j}^{N(N-1)/2} \hat{O}(\hat{\boldsymbol{q}}_i , \hat{\boldsymbol{q}}_j , \hat{\boldsymbol{p}}_i, \hat{\boldsymbol{p}}_j) \tag{6.78}$$

where operator $\hat{\boldsymbol{X}}_i$ of the i^{th} particle acts only on states for the i^{th} particle.

In the position basis or x-representation,

$$\begin{aligned}
\langle O_{(1)}(t) \rangle &= \mathrm{Tr}\left[\hat{O}_{(1)}^{N} \hat{\rho}(t) \right] \\
&= \sum_{i=1}^{N} \int d\boldsymbol{x}_1 \ldots \int d\boldsymbol{x}_N \int d\boldsymbol{y}_1 \ldots \int d\boldsymbol{y}_N \\
&\qquad * \left\langle \boldsymbol{x}_1,\ \ldots,\ \boldsymbol{x}_N \,\middle|\, \hat{O}(\hat{\boldsymbol{X}}_i) \,\middle|\, \boldsymbol{y}_1,\ \ldots,\ \boldsymbol{x}_N \right\rangle \\
&\qquad * \left\langle \boldsymbol{y}_1,\ \ldots,\ \boldsymbol{x}_N \,\middle|\, \hat{\rho}\left(\hat{\boldsymbol{X}}^N, t\right) \,\middle|\, \boldsymbol{x}_1,\ \ldots,\ \boldsymbol{x}_N \right\rangle \\
&\equiv \sum_{i=1}^{N} \int d\boldsymbol{x}^N \int d\boldsymbol{y}^N \left\langle \boldsymbol{x}^N \,\middle|\, \hat{O}(\hat{\boldsymbol{X}}_i) \,\middle|\, \boldsymbol{y}^N \right\rangle \left\langle \boldsymbol{y}^N \,\middle|\, \hat{\rho}\left(\hat{\boldsymbol{X}}^N, t\right) \,\middle|\, \boldsymbol{x}^N \right\rangle \\
&= \sum_{i=1}^{N} \int d\boldsymbol{x}^N \int d\boldsymbol{y}^N \prod_{j\neq i} \delta(\boldsymbol{x}_j - \boldsymbol{y}_j) \left\langle \boldsymbol{x}_i \,\middle|\, \hat{O}(\hat{\boldsymbol{X}}_i) \,\middle|\, \boldsymbol{y}_i \right\rangle \left\langle \boldsymbol{y}^N \,\middle|\, \hat{\rho}\left(\hat{\boldsymbol{X}}^N, t\right) \,\middle|\, \boldsymbol{x}^N \right\rangle \\
&= \sum_{i=1}^{N} \int d\boldsymbol{x}^N \int d\boldsymbol{y}_i \left\langle \boldsymbol{x}_i \,\middle|\, \hat{O}(\hat{\boldsymbol{X}}_i) \,\middle|\, \boldsymbol{y}_i \right\rangle \left\langle \boldsymbol{x}^N_{\boldsymbol{x}_i\to\boldsymbol{y}_i} \,\middle|\, \hat{\rho}\left(\hat{\boldsymbol{X}}^N, t\right) \,\middle|\, \boldsymbol{x}^N \right\rangle \\
&= \frac{1}{N}\sum_{i=1}^{N} \int d\boldsymbol{x}_i \int d\boldsymbol{y}_i \left\langle \boldsymbol{x}_i \,\middle|\, \hat{O}(\hat{\boldsymbol{X}}_i) \,\middle|\, \boldsymbol{y}_i \right\rangle \left\langle \boldsymbol{y}_i \,\middle|\, \hat{\rho}_{(1)}\left(\hat{\boldsymbol{X}}_i, t\right) \,\middle|\, \boldsymbol{x}_i \right\rangle
\end{aligned} \tag{6.79a}$$

where

$$\left| \boldsymbol{x}^N \right\rangle = \left| \boldsymbol{x}_1,\ \ldots,\ \boldsymbol{x}_N \right\rangle \qquad \int d\boldsymbol{x}^N = \int d\boldsymbol{x}_1 \ldots \int d\boldsymbol{x}_N$$

$\boldsymbol{x}^N_{\boldsymbol{x}_i\to\boldsymbol{y}_i}$ is $\boldsymbol{x}^N$ with $\boldsymbol{x}_i$ replaced by $\boldsymbol{y}_i$.

The 1-body reduced density operator is defined as

$$\hat{\rho}_{(1)}\left(\hat{\boldsymbol{X}}_i, t\right) \equiv N \int d\boldsymbol{x}^N_{\backslash i} \left\langle \boldsymbol{x}^N_{\backslash i} \,\middle|\, \hat{\rho}\left(\hat{\boldsymbol{X}}^N, t\right) \,\middle|\, \boldsymbol{x}^N_{\backslash i} \right\rangle \tag{6.80a}$$

where $\boldsymbol{x}^N_{\backslash i}$ is $\boldsymbol{x}^N$ with $\boldsymbol{x}_i$ taken out.

The corresponding 1-body reduced density matrix has elements

$$\left\langle \boldsymbol{y}_i \,\middle|\, \hat{\rho}_{(1)}\left(\hat{\boldsymbol{X}}_i, t\right) \,\middle|\, \boldsymbol{x}_i \right\rangle = N \int d\boldsymbol{z}^N_{\backslash i} \left\langle \boldsymbol{z}^N_{\boldsymbol{z}_i\to\boldsymbol{y}_i} \,\middle|\, \hat{\rho}\left(\hat{\boldsymbol{X}}^N, t\right) \,\middle|\, \boldsymbol{z}^N_{\boldsymbol{z}_i\to\boldsymbol{x}_i} \right\rangle \tag{6.80}$$

Note the absence of $\int d\boldsymbol{p}^N_{\backslash i}$, as compared to the definition for the classical case, (6.63) in §S6.A.

This is of course due to the fact that either $\{ \mid \boldsymbol{x} \rangle \}$ or $\{ \mid \boldsymbol{p} \rangle \}$ alone is already a complete basis for the Hilbert space. Thus, the phase space is an over-specified basis for quantum systems, as emphasized by the uncertainty principle. The quantum case is discussed in detail in App.B.

Since the integrals give the same results for all i, (6.79a) gives

$$\langle O_{(1)}(t) \rangle = \int d\boldsymbol{x} \int d\boldsymbol{y} \left\langle \boldsymbol{x} \,\middle|\, \hat{O}(\hat{\boldsymbol{X}}) \,\middle|\, \boldsymbol{y} \right\rangle \left\langle \boldsymbol{y} \,\middle|\, \hat{\rho}_{(1)}\left(\hat{\boldsymbol{X}}, t\right) \,\middle|\, \boldsymbol{x} \right\rangle \tag{6.79}$$

$$= \int d\boldsymbol{x} \left\langle \boldsymbol{x} \,\middle|\, \hat{O}(\hat{\boldsymbol{X}})\, \hat{\rho}_{(1)}\left(\hat{\boldsymbol{X}}, t\right) \,\middle|\, \boldsymbol{x} \right\rangle$$

$$= \text{Tr}\left[\hat{O}\, \hat{\rho}_{(1)}(t) \right]$$

Similarly, for the 2-body operator,

$$\langle O_{(2)}(t) \rangle = \text{Tr}\left[\hat{O}_{(2)}^{N}\, \hat{\rho}(t) \right]$$

$$\equiv \sum_{i<j}^{N(N-1)/2} \int d\boldsymbol{x}^N \int d\boldsymbol{y}^N \left\langle \boldsymbol{x}^N \,\middle|\, \hat{O}\left(\hat{\boldsymbol{X}}_i, \hat{\boldsymbol{X}}_j\right) \,\middle|\, \boldsymbol{y}^N \right\rangle \left\langle \boldsymbol{y}^N \,\middle|\, \hat{\rho}\left(\hat{\boldsymbol{X}}^N, t\right) \,\middle|\, \boldsymbol{x}^N \right\rangle$$

$$= \sum_{i<j}^{N(N-1)/2} \int d\boldsymbol{x}^N \int d\boldsymbol{y}^N \prod_{k\neq i,j} \delta(\boldsymbol{x}_k - \boldsymbol{y}_k) \left\langle \boldsymbol{x}_i, \boldsymbol{x}_j \,\middle|\, \hat{O}\left(\hat{\boldsymbol{X}}_i, \hat{\boldsymbol{X}}_j\right) \,\middle|\, \boldsymbol{y}_i, \boldsymbol{y}_j \right\rangle$$

$$* \left\langle \boldsymbol{y}^N \,\middle|\, \hat{\rho}\left(\hat{\boldsymbol{X}}^N, t\right) \,\middle|\, \boldsymbol{x}^N \right\rangle$$

$$= \sum_{i<j}^{N(N-1)/2} \int d\boldsymbol{x}^N \int d\boldsymbol{y}_i \int d\boldsymbol{y}_j \left\langle \boldsymbol{x}_i, \boldsymbol{x}_j \,\middle|\, \hat{O}\left(\hat{\boldsymbol{X}}_i, \hat{\boldsymbol{X}}_j\right) \,\middle|\, \boldsymbol{y}_i, \boldsymbol{y}_j \right\rangle$$

$$* \left\langle \boldsymbol{x}^N_{\boldsymbol{x}_i\to\boldsymbol{y}_i,\, \boldsymbol{x}_j\to\boldsymbol{y}_j} \,\middle|\, \hat{\rho}\left(\hat{\boldsymbol{X}}^N, t\right) \,\middle|\, \boldsymbol{x}^N \right\rangle$$

$$= \frac{2}{N(N-1)} \sum_{i<j}^{N(N-1)/2} \int d\boldsymbol{x}_i \int d\boldsymbol{x}_j \int d\boldsymbol{y}_i \int d\boldsymbol{y}_j \tag{6.81a}$$

$$* \left\langle \boldsymbol{x}_i, \boldsymbol{x}_j \,\middle|\, \hat{O}\left(\hat{\boldsymbol{X}}_i, \hat{\boldsymbol{X}}_j\right) \,\middle|\, \boldsymbol{y}_i, \boldsymbol{y}_j \right\rangle \left\langle \boldsymbol{y}_i, \boldsymbol{y}_j \,\middle|\, \hat{\rho}_2\left(\hat{\boldsymbol{X}}_i, \hat{\boldsymbol{X}}_j, t\right) \,\middle|\, \boldsymbol{x}_i, \boldsymbol{x}_j \right\rangle$$

where

$$\hat{\rho}_{(2)}\left(\hat{\boldsymbol{X}}_i, \hat{\boldsymbol{X}}_j, t\right) \equiv \frac{1}{2} N(N-1) \int d\boldsymbol{x}^N_{\setminus(i,j)} \left\langle \boldsymbol{x}^N_{\setminus(i,j)} \,\middle|\, \hat{\rho}\left(\hat{\boldsymbol{X}}^N, t\right) \,\middle|\, \boldsymbol{x}^N_{\setminus(i,j)} \right\rangle \tag{6.82a}$$

$$\left\langle \boldsymbol{y}_i, \boldsymbol{y}_j \,\middle|\, \hat{\rho}_2\left(\hat{\boldsymbol{X}}_i, \hat{\boldsymbol{X}}_j, t\right) \,\middle|\, \boldsymbol{x}_i, \boldsymbol{x}_j \right\rangle$$

$$= \frac{1}{2} N(N-1) \int d\boldsymbol{z}^N_{\setminus(i,j)} \left\langle \boldsymbol{z}^N_{\boldsymbol{z}_i\to\boldsymbol{y}_i,\, \boldsymbol{z}_j\to\boldsymbol{y}_j} \,\middle|\, \hat{\rho}\left(\hat{\boldsymbol{X}}^N, t\right) \,\middle|\, \boldsymbol{z}^N_{\boldsymbol{z}_i\to\boldsymbol{x}_i,\, \boldsymbol{z}_j\to\boldsymbol{x}_j} \right\rangle \tag{6.82}$$

Since the integrals give the same results for all pairs of (i, j), (6.81a) gives

$$\langle O_{(2)}(t) \rangle = \int d\boldsymbol{x}_1 \int d\boldsymbol{x}_2 \int d\boldsymbol{y}_1 \int d\boldsymbol{y}_2 \left\langle \boldsymbol{x}_1, \boldsymbol{x}_2 \,\middle|\, \hat{O}\left(\hat{\boldsymbol{X}}_1, \hat{\boldsymbol{X}}_2\right) \,\middle|\, \boldsymbol{y}_1, \boldsymbol{y}_2 \right\rangle \tag{6.81}$$

$$* \left\langle \boldsymbol{y}_1, \boldsymbol{y}_2 \,\middle|\, \hat{\rho}_2\left(\hat{\boldsymbol{X}}_1, \hat{\boldsymbol{X}}_2, t\right) \,\middle|\, \boldsymbol{x}_1, \boldsymbol{x}_2 \right\rangle$$

$$= \int d\boldsymbol{x}_1 \int d\boldsymbol{x}_2 \left\langle \boldsymbol{x}_1, \boldsymbol{x}_2 \,\middle|\, \hat{O}\left(\hat{\boldsymbol{X}}_1, \hat{\boldsymbol{X}}_2\right) \hat{\rho}_2\left(\hat{\boldsymbol{X}}_1, \hat{\boldsymbol{X}}_2, t\right) \,\middle|\, \boldsymbol{x}_1, \boldsymbol{x}_2 \right\rangle$$

$$= \text{Tr}\left[\hat{O}\, \hat{\rho}_{(2)}(t) \right] \tag{6.81b}$$

Note that we choose (6.81-2) to differ from Reichl's by a factor of $\frac{1}{2}$ in order to obtain (6.81b).

The 1- and 2- particle reduced Wigner function are defined as

$$f_1(\boldsymbol{k}, \boldsymbol{R}, t) \equiv \int d\boldsymbol{r}\, e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \left\langle \boldsymbol{R} - \frac{1}{2}\boldsymbol{r} \,\middle|\, \hat{\rho}_{(1)}(t) \,\middle|\, \boldsymbol{R} + \frac{1}{2}\boldsymbol{r} \right\rangle \tag{6.83}$$

$$= \int d\boldsymbol{r}\, e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} \left\langle \boldsymbol{R} + \frac{1}{2}\boldsymbol{r} \,\middle|\, \hat{\rho}_{(1)}(t) \,\middle|\, \boldsymbol{R} - \frac{1}{2}\boldsymbol{r} \right\rangle \qquad [\,\boldsymbol{r} \to -\boldsymbol{r}\,]$$

$$f_2(\boldsymbol{k}_1, \boldsymbol{k}_2, \boldsymbol{R}_1, \boldsymbol{R}_2, t) \equiv \int d\boldsymbol{r}_1 \int d\boldsymbol{r}_2\, e^{i\boldsymbol{k}_1\cdot\boldsymbol{r}_1} e^{i\boldsymbol{k}_2\cdot\boldsymbol{r}_2} * \left\langle \boldsymbol{R}_1 - \frac{1}{2}\boldsymbol{r}_1,\ \boldsymbol{R}_2 - \frac{1}{2}\boldsymbol{r}_2 \,\middle|\, \hat{\rho}_{(2)}(t) \,\middle|\, \boldsymbol{R}_1 + \frac{1}{2}\boldsymbol{r}_1,\ \boldsymbol{R}_2 + \frac{1}{2}\boldsymbol{r}_2 \right\rangle \qquad (6.84)$$

Note that the matrix elements in (6.83-4) are the complex conjugate of those used by Reichl. The reason for our choice is to obtain (6.86).

$f_1(\boldsymbol{k}, \boldsymbol{R}, t)$ is the closest quantum analog to the classical distribution function $f(\boldsymbol{p}, \boldsymbol{q}, t)$. In particular, (6.83) gives

$$\begin{aligned}\int \frac{d\boldsymbol{k}}{(2\pi)^3} f_1(\boldsymbol{k}, \boldsymbol{R}, t) &= \int d\boldsymbol{r}\, \delta(\boldsymbol{r}) \left\langle \boldsymbol{R} - \frac{1}{2}\boldsymbol{r} \,\middle|\, \hat{\rho}_{(1)}(t) \,\middle|\, \boldsymbol{R} + \frac{1}{2}\boldsymbol{r} \right\rangle \\ &= \langle \boldsymbol{R} \,|\, \hat{\rho}_{(1)}(t) \,|\, \boldsymbol{R} \rangle \\ &= n(\boldsymbol{R}, t) \qquad (6.85) \\ &= \text{average number of particle at point } \boldsymbol{R} \text{ and time } t.\end{aligned}$$

Using

$$\boldsymbol{x} = \boldsymbol{R} + \frac{1}{2}\boldsymbol{r} \qquad \boldsymbol{y} = \boldsymbol{R} - \frac{1}{2}\boldsymbol{r}$$

$$J = \det \begin{vmatrix} \frac{\partial x_\alpha}{\partial r_\beta} & \frac{\partial x_\alpha}{\partial R_\beta} \\ \frac{\partial y_\alpha}{\partial r_\beta} & \frac{\partial y_\alpha}{\partial R_\beta} \end{vmatrix} \qquad [\ \alpha \ \& \ \beta \text{ are Cartesian component indices.}\ ]$$

$$= \det \begin{vmatrix} \frac{1}{2}\delta_{\alpha\beta} & \delta_{\alpha\beta} \\ -\frac{1}{2}\delta_{\alpha\beta} & \delta_{\alpha\beta} \end{vmatrix} = \det \begin{vmatrix} \frac{1}{2}\hat{I} & \hat{I} \\ -\frac{1}{2}\hat{I} & \hat{I} \end{vmatrix}$$

$$= \det \begin{vmatrix} \hat{I} & 0 \\ -\frac{1}{2}\hat{I} & \hat{I} \end{vmatrix} \qquad [\ \text{Gaussian elimination used.}\ ]$$

$$= 1 \qquad [\ \text{Determinant is lower triangular with diagonal elements all equal to 1.}\ ]$$

we have

$$d\boldsymbol{x}\, d\boldsymbol{y} = |\, J \,|\ d\boldsymbol{r}\, d\boldsymbol{R} = d\boldsymbol{r}\, d\boldsymbol{R}$$

Let $\boldsymbol{x}$ & $\boldsymbol{y}$ be the positions of 2 identical particles, then $\boldsymbol{R} = \frac{1}{2}(\boldsymbol{x} + \boldsymbol{y})$ gives the center of mass position and $\boldsymbol{r} = \boldsymbol{x} - \boldsymbol{y}$ the relative coordinates.

Let the momentum eigenstate in the x-representation be

$$\langle \boldsymbol{x} \,|\, \boldsymbol{k} \rangle = e^{i\boldsymbol{k}\cdot\boldsymbol{x}} \qquad (6.85a)$$

(6.83) then gives

$$f_1(\boldsymbol{k}, \boldsymbol{R}, t) = \int d\boldsymbol{r}\, e^{i\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{y})} \langle \boldsymbol{y} \,|\, \hat{\rho}_{(1)}(t) \,|\, \boldsymbol{x} \rangle \qquad (6.85b)$$

$$\begin{aligned}\int d\boldsymbol{R}\, f_1(\boldsymbol{k}, \boldsymbol{R}, t) &= \int d\boldsymbol{x} \int d\boldsymbol{y}\, e^{i\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{y})} \langle \boldsymbol{y} \,|\, \hat{\rho}_{(1)}(t) \,|\, \boldsymbol{x} \rangle \\ &= \int d\boldsymbol{x} \int d\boldsymbol{y}\, \langle \boldsymbol{k} \,|\, \boldsymbol{y} \rangle \langle \boldsymbol{y} \,|\, \hat{\rho}_{(1)}(t) \,|\, \boldsymbol{x} \rangle \langle \boldsymbol{x} \,|\, \boldsymbol{k} \rangle \\ &= \langle \boldsymbol{k} \,|\, \hat{\rho}_{(1)}(t) \,|\, \boldsymbol{k} \rangle \qquad (6.86) \\ &= n(\boldsymbol{k}, t) \\ &= \text{average number of particle with momentum } \hbar\boldsymbol{k} \text{ and time } t.\end{aligned}$$

Note that with the normalization choice (6.85a), we have

$$\int \frac{d\boldsymbol{k}}{(2\pi)^3} e^{i\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{y})} = \delta(\boldsymbol{x} - \boldsymbol{y}) = \langle \boldsymbol{x} \,|\, \boldsymbol{y} \rangle$$

$$= \int \frac{d\boldsymbol{k}}{(2\pi)^3} \langle \boldsymbol{x} \mid \boldsymbol{k} \rangle \langle \boldsymbol{k} \mid \boldsymbol{y} \rangle$$

so that the completeness relation of $\{ \mid \boldsymbol{k} \rangle \}$ is given by

$$\int \frac{d\boldsymbol{k}}{(2\pi)^3} \mid \boldsymbol{k} \rangle \langle \boldsymbol{k} \mid = \hat{I}$$

as opposed to

$$\int d\boldsymbol{x} \mid \boldsymbol{x} \rangle \langle \boldsymbol{x} \mid = \hat{I}$$

See App.B for another choice of normalization for $\langle \boldsymbol{x} \mid \boldsymbol{k} \rangle$.

The Wigner functions can be used to take phase space averages the same way as the classical distribution functions. For example, the average current is given by

$$\langle \boldsymbol{j}(t) \rangle = \mathrm{Tr}\left[\hat{\boldsymbol{v}}\, \rho(t) \right] = \mathrm{Tr}\left[\frac{\hat{\boldsymbol{p}}}{m} \rho(t) \right]$$

$$= \int d\boldsymbol{x} \int d\boldsymbol{y} \left\langle \boldsymbol{x} \,\middle|\, \frac{\hat{\boldsymbol{p}}}{m} \,\middle|\, \boldsymbol{y} \right\rangle \left\langle \boldsymbol{y} \mid \hat{\rho}_{(1)}(t) \mid \boldsymbol{x} \right\rangle \qquad \text{[(6.79) used.]}$$

$$= \int \frac{d\boldsymbol{k}}{(2\pi)^3} \int d\boldsymbol{x} \int d\boldsymbol{y} \left\langle \boldsymbol{x} \,\middle|\, \frac{\hat{\boldsymbol{p}}}{m} \,\middle|\, \boldsymbol{k} \right\rangle \langle \boldsymbol{k} \mid \boldsymbol{y} \rangle \left\langle \boldsymbol{y} \mid \hat{\rho}_{(1)}(t) \mid \boldsymbol{x} \right\rangle$$

$$= \int \frac{d\boldsymbol{k}}{(2\pi)^3} \int d\boldsymbol{x} \int d\boldsymbol{y}\, \frac{\hbar \boldsymbol{k}}{m} e^{i\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{y})} \left\langle \boldsymbol{y} \mid \hat{\rho}_{(1)}(t) \mid \boldsymbol{x} \right\rangle$$

$$= \int \frac{d\boldsymbol{k}}{(2\pi)^3} \frac{\hbar \boldsymbol{k}}{m} \int d\boldsymbol{R} \int d\boldsymbol{r}\; e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \left\langle \boldsymbol{R} - \frac{1}{2}\boldsymbol{r} \,\middle|\, \hat{\rho}_{(1)}(t) \,\middle|\, \boldsymbol{R} + \frac{1}{2}\boldsymbol{r} \right\rangle$$

$$= \int \frac{d\boldsymbol{k}}{(2\pi)^3} \frac{\hbar \boldsymbol{k}}{m} \int d\boldsymbol{R}\, f_1(\boldsymbol{k}, \boldsymbol{R}, t) \qquad (6.87a)$$

$$= \int d\boldsymbol{R} \,\langle \boldsymbol{j}(\boldsymbol{R}, t) \rangle$$

where

$$\langle \boldsymbol{j}(\boldsymbol{R}, t) \rangle = \int \frac{d\boldsymbol{k}}{(2\pi)^3} \frac{\hbar \boldsymbol{k}}{m} f_1(\boldsymbol{k}, \boldsymbol{R}, t) \qquad (6.87)$$

is the average current density at position $\boldsymbol{R}$ and time t.

Caution: the Wigner functions are not positive semi-definite and hence cannot be interpreted as probability densities.

We now derive the equation of motion for $f_1(\boldsymbol{k}, \boldsymbol{R}, t)$ given a Hamiltonian

$$\hat{H} = \sum_{i=1}^{N} \frac{\hat{\boldsymbol{p}}_i^2}{2m} + \sum_{i<j}^{N(N-1)/2} V(\hat{\boldsymbol{q}}_i - \hat{\boldsymbol{q}}_j) \qquad (6.88)$$

$$= \sum_{i=1}^{N} \hat{K}_i + \sum_{i<j}^{N(N-1)/2} \hat{V}_{ij}$$

$$= \hat{\mathcal{K}} + \hat{\mathcal{V}}$$

Combining (6.80a) with the Liouville equation

$$i\hbar \frac{\partial}{\partial t} \hat{\rho}(t) = \left[\hat{H},\ \hat{\rho}(t) \right] \qquad (6.53)$$

we have

$$i\hbar \frac{\partial}{\partial t} \hat{\rho}_{(1)}\left(\hat{\boldsymbol{X}}_i,\ t\right) = N \int d\boldsymbol{x}_{\setminus i}^{N} \left\langle \boldsymbol{x}_{\setminus i}^{N} \,\middle|\, \left[\hat{H},\ \hat{\rho}\left(\hat{\boldsymbol{X}}^{N}, t\right) \right] \,\middle|\, \boldsymbol{x}_{\setminus i}^{N} \right\rangle \qquad (6.88a)$$

Consider 1st the term with the kinetic energy $\hat{K}_i$,

$$
\begin{aligned}
& N \int d\boldsymbol{x}_{\setminus i}^N \left\langle \boldsymbol{x}_{\setminus i}^N \left| \left[\hat{K}_i,\ \hat{\rho}(t) \right] \right| \boldsymbol{x}_{\setminus i}^N \right\rangle \\
&= N \int d\boldsymbol{x}_{\setminus i}^N \int d\boldsymbol{z}_{\setminus i}^N \left\{ \left\langle \boldsymbol{x}_{\setminus i}^N \mid \hat{K}_i \mid \boldsymbol{z}_{\setminus i}^N \right\rangle \left\langle \boldsymbol{z}_{\setminus i}^N \mid \hat{\rho}(t) \mid \boldsymbol{x}_{\setminus i}^N \right\rangle \right. \\
&\qquad \left. - \left\langle \boldsymbol{x}_{\setminus i}^N \mid \hat{\rho}(t) \mid \boldsymbol{z}_{\setminus i}^N \right\rangle \left\langle \boldsymbol{z}_{\setminus i}^N \mid \hat{K}_i \mid \boldsymbol{x}_{\setminus i}^N \right\rangle \right\} \\
&= N \int d\boldsymbol{x}_{\setminus i}^N \int d\boldsymbol{z}_{\setminus i}^N \left\{ \left\langle \boldsymbol{x}_{\setminus i}^N \mid \boldsymbol{z}_{\setminus i}^N \right\rangle \hat{K}_i \left\langle \boldsymbol{z}_{\setminus i}^N \mid \hat{\rho}(t) \mid \boldsymbol{x}_{\setminus i}^N \right\rangle \right. \\
&\qquad \left. - \left\langle \boldsymbol{x}_{\setminus i}^N \mid \hat{\rho}(t) \mid \boldsymbol{z}_{\setminus i}^N \right\rangle \hat{K}_i \left\langle \boldsymbol{z}_{\setminus i}^N \mid \boldsymbol{x}_{\setminus i}^N \right\rangle \right\} \\
&= N \int d\boldsymbol{x}_{\setminus i}^N \int d\boldsymbol{z}_{\setminus i}^N \left\{ \hat{K}_i \left\langle \boldsymbol{z}_{\setminus i}^N \mid \hat{\rho}(t) \mid \boldsymbol{x}_{\setminus i}^N \right\rangle - \left\langle \boldsymbol{x}_{\setminus i}^N \mid \hat{\rho}(t) \mid \boldsymbol{z}_{\setminus i}^N \right\rangle \hat{K}_i \right\} \prod_{j \neq i} \delta(\boldsymbol{z}_j - \boldsymbol{x}_j) \\
&= N \int d\boldsymbol{x}_{\setminus i}^N \left\{ \hat{K}_i \left\langle \boldsymbol{x}_{\setminus i}^N \mid \hat{\rho}(t) \mid \boldsymbol{x}_{\setminus i}^N \right\rangle - \left\langle \boldsymbol{x}_{\setminus i}^N \mid \hat{\rho}(t) \mid \boldsymbol{x}_{\setminus i}^N \right\rangle \hat{K}_i \right\} \\
&= \hat{K}_i \hat{\rho}_{(1)} \left(\hat{\boldsymbol{X}}_i, t \right) - \hat{\rho}_{(1)} \left(\hat{\boldsymbol{X}}_i, t \right) \hat{K}_i \\
&= \left[\hat{K}_i,\ \hat{\rho}_{(1)} \left(\hat{\boldsymbol{X}}_i, t \right) \right]
\end{aligned}
$$

For $j \neq i$,

$$
\begin{aligned}
& N \int d\boldsymbol{x}_{\setminus i}^N \left\langle \boldsymbol{x}_{\setminus i}^N \left| \left[\hat{K}_j,\ \hat{\rho}(t) \right] \right| \boldsymbol{x}_{\setminus i}^N \right\rangle \\
&= N \int d\boldsymbol{x}_{\setminus i}^N \int d\boldsymbol{z}_{\setminus i}^N \left\{ \left\langle \boldsymbol{x}_{\setminus i}^N \mid \hat{K}_j \mid \boldsymbol{z}_{\setminus i}^N \right\rangle \left\langle \boldsymbol{z}_{\setminus i}^N \mid \hat{\rho}(t) \mid \boldsymbol{x}_{\setminus i}^N \right\rangle \right. \\
&\qquad \left. - \left\langle \boldsymbol{x}_{\setminus i}^N \mid \hat{\rho}(t) \mid \boldsymbol{z}_{\setminus i}^N \right\rangle \left\langle \boldsymbol{z}_{\setminus i}^N \mid \hat{K}_j \mid \boldsymbol{x}_{\setminus i}^N \right\rangle \right\} \\
&= N \int d\boldsymbol{x}_{\setminus i}^N \int d\boldsymbol{z}_{\setminus i}^N \left\{ \left\langle \boldsymbol{x}_{\setminus i}^N \mid \hat{K}_j \mid \boldsymbol{z}_{\setminus i}^N \right\rangle \left\langle \boldsymbol{z}_{\setminus i}^N \mid \hat{\rho}(t) \mid \boldsymbol{x}_{\setminus i}^N \right\rangle \right. \qquad [\ \boldsymbol{z} \leftrightarrow \boldsymbol{x} \text{ in } 2^{\text{nd}} \text{ term }] \\
&\qquad \left. - \left\langle \boldsymbol{z}_{\setminus i}^N \mid \hat{\rho}(t) \mid \boldsymbol{x}_{\setminus i}^N \right\rangle \left\langle \boldsymbol{x}_{\setminus i}^N \mid \hat{K}_j \mid \boldsymbol{z}_{\setminus i}^N \right\rangle \right\} \\
&= 0
\end{aligned}
$$

Therefore, the kinetic energy term in (6.88a) gives

$$
N \int d\boldsymbol{x}_{\setminus i}^N \left\langle \boldsymbol{x}_{\setminus i}^N \left| \left[\hat{\mathcal{K}},\ \hat{\rho}(t) \right] \right| \boldsymbol{x}_{\setminus i}^N \right\rangle = \left[\hat{K}_i,\ \hat{\rho}_{(1)} \left(\hat{\boldsymbol{X}}_i, t \right) \right] \qquad \forall\ i \qquad (6.88b)
$$

For the potential energy $\hat{V}_{ij}$ term, we have, with $j \neq i$ understood,

$$
\begin{aligned}
& N \int d\boldsymbol{x}_{\setminus i}^N \left\langle \boldsymbol{x}_{\setminus i}^N \left| \left[\hat{V}_{ij},\ \hat{\rho}(t) \right] \right| \boldsymbol{x}_{\setminus i}^N \right\rangle \\
&= N \int d\boldsymbol{x}_{\setminus i}^N \int d\boldsymbol{z}_{\setminus i}^N \left\{ \left\langle \boldsymbol{x}_{\setminus i}^N \mid \hat{V}_{ij} \mid \boldsymbol{z}_{\setminus i}^N \right\rangle \left\langle \boldsymbol{z}_{\setminus i}^N \mid \hat{\rho}(t) \mid \boldsymbol{x}_{\setminus i}^N \right\rangle \right. \\
&\qquad \left. - \left\langle \boldsymbol{x}_{\setminus i}^N \mid \hat{\rho}(t) \mid \boldsymbol{z}_{\setminus i}^N \right\rangle \left\langle \boldsymbol{z}_{\setminus i}^N \mid \hat{V}_{ij} \mid \boldsymbol{x}_{\setminus i}^N \right\rangle \right\} \\
&= N \int d\boldsymbol{x}_{\setminus i}^N \int d\boldsymbol{z}_{\setminus i}^N \left\{ \hat{V} \left(\hat{\boldsymbol{q}}_i - \boldsymbol{z}_j \right) \left\langle \boldsymbol{z}_{\setminus i}^N \mid \hat{\rho}(t) \mid \boldsymbol{x}_{\setminus i}^N \right\rangle \right. \\
&\qquad \left. - \left\langle \boldsymbol{x}_{\setminus i}^N \mid \hat{\rho}(t) \mid \boldsymbol{z}_{\setminus i}^N \right\rangle \hat{V} \left(\hat{\boldsymbol{q}}_i - \boldsymbol{x}_j \right) \right\} \prod_{k \neq i} \delta(\boldsymbol{z}_k - \boldsymbol{x}_k) \\
&= N \int d\boldsymbol{x}_{\setminus i}^N \left\{ \hat{V} \left(\hat{\boldsymbol{q}}_i - \boldsymbol{x}_j \right) \left\langle \boldsymbol{x}_{\setminus i}^N \mid \hat{\rho}(t) \mid \boldsymbol{x}_{\setminus i}^N \right\rangle - \left\langle \boldsymbol{x}_{\setminus i}^N \mid \hat{\rho}(t) \mid \boldsymbol{x}_{\setminus i}^N \right\rangle \hat{V} \left(\hat{\boldsymbol{q}}_i - \boldsymbol{x}_j \right) \right\} \\
&= \frac{2}{N-1} \int d\boldsymbol{x}_j \left\{ \hat{V} \left(\hat{\boldsymbol{q}}_i - \boldsymbol{x}_j \right) \left\langle \boldsymbol{x}_j \left| \hat{\rho}_{(2)} \left(\hat{\boldsymbol{X}}_i, \hat{\boldsymbol{X}}_j, t \right) \right| \boldsymbol{x}_j \right\rangle \right. \\
&\qquad \left. - \left\langle \boldsymbol{x}_j \left| \hat{\rho}_{(2)} \left(\hat{\boldsymbol{X}}_i, \hat{\boldsymbol{X}}_j, t \right) \right| \boldsymbol{x}_j \right\rangle \hat{V} \left(\hat{\boldsymbol{q}}_i - \boldsymbol{x}_j \right) \right\} \\
&= \frac{2}{N-1} \int d\boldsymbol{x}_j \left\langle \boldsymbol{x}_j \left| \left[\hat{V} \left(\hat{\boldsymbol{q}}_i - \hat{\boldsymbol{q}}_j \right),\ \hat{\rho}_{(2)} \left(\hat{\boldsymbol{X}}_i, \hat{\boldsymbol{X}}_j, t \right) \right] \right| \boldsymbol{x}_j \right\rangle
\end{aligned}
$$

For the potential energy $\hat{V}_{jk}$ term with $j, k \neq i$,

$$N \int d\boldsymbol{x}_{\backslash i}^{N} \left\langle \boldsymbol{x}_{\backslash i}^{N} \,\middle|\, \left[\hat{V}_{jk},\ \hat{\rho}(t)\right] \,\middle|\, \boldsymbol{x}_{\backslash i}^{N} \right\rangle$$

$$= N \int d\boldsymbol{x}_{\backslash i}^{N} \int d\boldsymbol{z}_{\backslash i}^{N} \left\{ \left\langle \boldsymbol{x}_{\backslash i}^{N} \,\middle|\, \hat{V}_{jk} \,\middle|\, \boldsymbol{z}_{\backslash i}^{N} \right\rangle \left\langle \boldsymbol{z}_{\backslash i}^{N} \,\middle|\, \hat{\rho}(t) \,\middle|\, \boldsymbol{x}_{\backslash i}^{N} \right\rangle - \left\langle \boldsymbol{x}_{\backslash i}^{N} \,\middle|\, \hat{\rho}(t) \,\middle|\, \boldsymbol{z}_{\backslash i}^{N} \right\rangle \left\langle \boldsymbol{z}_{\backslash i}^{N} \,\middle|\, \hat{V}_{jk} \,\middle|\, \boldsymbol{x}_{\backslash i}^{N} \right\rangle \right\}$$

$$= N \int d\boldsymbol{x}_{\backslash i}^{N} \int d\boldsymbol{z}_{\backslash i}^{N} \left\{ V(\boldsymbol{x}_j - \boldsymbol{x}_k) \left\langle \boldsymbol{z}_{\backslash i}^{N} \,\middle|\, \hat{\rho}(t) \,\middle|\, \boldsymbol{x}_{\backslash i}^{N} \right\rangle - \left\langle \boldsymbol{x}_{\backslash i}^{N} \,\middle|\, \hat{\rho}(t) \,\middle|\, \boldsymbol{z}_{\backslash i}^{N} \right\rangle V(\boldsymbol{x}_j - \boldsymbol{x}_k) \right\} \prod_{m \neq i} \delta(\boldsymbol{z}_m - \boldsymbol{x}_m)$$

$$= N \int d\boldsymbol{x}_{\backslash i}^{N} \left\{ V(\boldsymbol{x}_j - \boldsymbol{x}_k) \left\langle \boldsymbol{x}_{\backslash i}^{N} \,\middle|\, \hat{\rho}(t) \,\middle|\, \boldsymbol{x}_{\backslash i}^{N} \right\rangle - \left\langle \boldsymbol{x}_{\backslash i}^{N} \,\middle|\, \hat{\rho}(t) \,\middle|\, \boldsymbol{x}_{\backslash i}^{N} \right\rangle V(\boldsymbol{x}_j - \boldsymbol{x}_k) \right\}$$

$$= 0$$

Therefore, the potential energy term in (6.88a) gives

$$N \int d\boldsymbol{x}_{\backslash i}^{N} \left\langle \boldsymbol{x}_{\backslash i}^{N} \,\middle|\, \left[\hat{\mathcal{V}},\ \hat{\rho}(t)\right] \,\middle|\, \boldsymbol{x}_{\backslash i}^{N} \right\rangle = \frac{1}{2} N \sum_{j,\,k\,(j \neq k)} \int d\,x_{\backslash i}^{N} \left\langle \boldsymbol{x}_{\backslash i}^{N} \,\middle|\, \left[\hat{V}_{jk},\ \hat{\rho}(t)\right] \,\middle|\, \boldsymbol{x}_{\backslash i}^{N} \right\rangle$$

$$= \frac{1}{N-1} \sum_{j\,(\neq i)} \int d\boldsymbol{x}_j \left\langle \boldsymbol{x}_j \,\middle|\, \left[\hat{V}(\hat{\boldsymbol{q}}_i - \boldsymbol{x}_j),\ \hat{\rho}_{(2)}\!\left(\hat{\boldsymbol{X}}_i, \hat{\boldsymbol{X}}_j, t\right)\right] \,\middle|\, \boldsymbol{x}_j \right\rangle \tag{6.88c}$$

(6.88a) thus becomes

$$i\hbar \frac{\partial}{\partial t} \hat{\rho}_{(1)}\!\left(\hat{\boldsymbol{X}}_i,\ t\right) = \left[\hat{K}_i,\ \hat{\rho}_{(1)}\!\left(\hat{\boldsymbol{X}}_i, t\right)\right] + \frac{1}{N-1} \sum_{j\,(\neq i)} \int d\boldsymbol{x}_j \left\langle \boldsymbol{x}_j \,\middle|\, \left[\hat{V}(\hat{\boldsymbol{q}}_i - \boldsymbol{x}_j),\ \hat{\rho}_{(2)}\!\left(\hat{\boldsymbol{X}}_i, \hat{\boldsymbol{X}}_j, t\right)\right] \,\middle|\, \boldsymbol{x}_j \right\rangle$$

Since every term in the sum gives the same value, we can write this as

$$i\hbar \frac{\partial}{\partial t} \hat{\rho}_{(1)}\!\left(\hat{\boldsymbol{X}}_1,\ t\right) = \left[\hat{K}_1,\ \hat{\rho}_{(1)}\!\left(\hat{\boldsymbol{X}}_1, t\right)\right] + \int d\boldsymbol{x}_2 \left\langle \boldsymbol{x}_2 \,\middle|\, \left[\hat{V}(\hat{\boldsymbol{q}}_1 - \boldsymbol{x}_2),\ \hat{\rho}_{(2)}\!\left(\hat{\boldsymbol{X}}_1, \hat{\boldsymbol{X}}_2, t\right)\right] \,\middle|\, \boldsymbol{x}_2 \right\rangle \tag{6.89a}$$

Using

$$\left\langle \boldsymbol{x}_1 \,\middle|\, \hat{K}_1 \hat{\rho}_{(1)}\!\left(\hat{\boldsymbol{X}}_1, t\right) \,\middle|\, \boldsymbol{y}_1 \right\rangle = -\frac{\hbar^2}{2m} \int d\boldsymbol{z}_1\, \nabla_{\boldsymbol{x}_1}^2 \langle \boldsymbol{x}_1 \mid \boldsymbol{z}_1 \rangle \left\langle \boldsymbol{z}_1 \,\middle|\, \hat{\rho}_{(1)}\!\left(\hat{\boldsymbol{X}}_1, t\right) \,\middle|\, \boldsymbol{y}_1 \right\rangle$$

$$= -\frac{\hbar^2}{2m} \int d\boldsymbol{z}_1\, \delta(\boldsymbol{x}_1 - \boldsymbol{z}_1)\, \nabla_{\boldsymbol{x}_1}^2 \left\langle \boldsymbol{z}_1 \,\middle|\, \hat{\rho}_{(1)}\!\left(\hat{\boldsymbol{X}}_1, t\right) \,\middle|\, \boldsymbol{y}_1 \right\rangle$$

$$= -\frac{\hbar^2}{2m} \nabla_{\boldsymbol{x}_1}^2 \left\langle \boldsymbol{x}_1 \,\middle|\, \hat{\rho}_{(1)}\!\left(\hat{\boldsymbol{X}}_1, t\right) \,\middle|\, \boldsymbol{y}_1 \right\rangle$$

$$\left\langle \boldsymbol{x}_1 \,\middle|\, \hat{\rho}_{(1)}\!\left(\hat{\boldsymbol{X}}_1, t\right) \hat{K}_1 \,\middle|\, \boldsymbol{y}_1 \right\rangle = -\frac{\hbar^2}{2m} \int d\boldsymbol{z}_1 \left\langle \boldsymbol{x}_1 \,\middle|\, \hat{\rho}_{(1)}\!\left(\hat{\boldsymbol{X}}_1, t\right) \,\middle|\, \boldsymbol{z}_1 \right\rangle \nabla_{\boldsymbol{z}_1}^2 \langle \boldsymbol{z}_1 \mid \boldsymbol{y}_1 \rangle$$

$$= -\frac{\hbar^2}{2m} \int d\boldsymbol{z}_1\, \delta(\boldsymbol{z}_1 - \boldsymbol{y}_1)\, \nabla_{\boldsymbol{z}_1}^2 \left\langle \boldsymbol{x}_1 \,\middle|\, \hat{\rho}_{(1)}\!\left(\hat{\boldsymbol{X}}_1, t\right) \,\middle|\, \boldsymbol{z}_1 \right\rangle$$

$$= -\frac{\hbar^2}{2m} \nabla_{\boldsymbol{y}_1}^2 \left\langle \boldsymbol{x}_1 \,\middle|\, \hat{\rho}_{(1)}\!\left(\hat{\boldsymbol{X}}_1, t\right) \,\middle|\, \boldsymbol{y}_1 \right\rangle$$

we have

$$\left\langle \boldsymbol{x}_1 \,\middle|\, \left[\hat{K}_1,\ \hat{\rho}_{(1)}(t)\right] \,\middle|\, \boldsymbol{y}_1 \right\rangle = -\frac{\hbar^2}{2m} \left(\nabla_{\boldsymbol{x}_1}^2 - \nabla_{\boldsymbol{y}_1}^2\right) \langle \boldsymbol{x}_1 \mid \hat{\rho}_{(1)}(t) \mid \boldsymbol{y}_1 \rangle$$

$$= -\frac{\hbar^2}{2m}(\nabla_{x_1}+\nabla_{y_1})\cdot(\nabla_{x_1}-\nabla_{y_1})\langle \boldsymbol{x}_1 \mid \hat{\rho}_{(1)}(t) \mid \boldsymbol{y}_1 \rangle$$

Similarly,

$$\left\langle \boldsymbol{x}_1 \,\middle|\, \int d\boldsymbol{x}_2 \left\langle \boldsymbol{x}_2 \,\middle|\, \hat{V}(\hat{\boldsymbol{q}}_1 - \boldsymbol{x}_2)\,\hat{\rho}_{(2)}\left(\hat{\boldsymbol{X}}_1, \hat{\boldsymbol{X}}_2, t\right) \,\middle|\, \boldsymbol{x}_2 \right\rangle \,\middle|\, \boldsymbol{y}_1 \right\rangle$$

$$= \int d\boldsymbol{x}_2\; V(\boldsymbol{x}_1 - \boldsymbol{x}_2)\left\langle \boldsymbol{x}_1, \boldsymbol{x}_2 \,\middle|\, \hat{\rho}_{(2)}\left(\hat{\boldsymbol{X}}_1, \hat{\boldsymbol{X}}_2, t\right) \,\middle|\, \boldsymbol{y}_1, \boldsymbol{x}_2 \right\rangle$$

$$\left\langle \boldsymbol{x}_1 \,\middle|\, \int d\boldsymbol{x}_2 \left\langle \boldsymbol{x}_2 \,\middle|\, \hat{\rho}_{(2)}\left(\hat{\boldsymbol{X}}_1, \hat{\boldsymbol{X}}_2, t\right)\hat{V}(\hat{\boldsymbol{q}}_1 - \boldsymbol{x}_2) \,\middle|\, \boldsymbol{x}_2 \right\rangle \,\middle|\, \boldsymbol{y}_1 \right\rangle$$

$$= \int d\boldsymbol{x}_2\; V(\boldsymbol{y}_1 - \boldsymbol{x}_2)\left\langle \boldsymbol{x}_1, \boldsymbol{x}_2 \,\middle|\, \hat{\rho}_{(2)}\left(\hat{\boldsymbol{X}}_1, \hat{\boldsymbol{X}}_2, t\right) \,\middle|\, \boldsymbol{y}_1, \boldsymbol{x}_2 \right\rangle$$

$$\to \quad \int d\boldsymbol{x}_2 \left\langle \boldsymbol{x}_2 \,\middle|\, \left[\hat{V}(\hat{\boldsymbol{q}}_1 - \boldsymbol{x}_2), \hat{\rho}_{(2)}\left(\hat{\boldsymbol{X}}_1, \hat{\boldsymbol{X}}_2, t\right)\right] \,\middle|\, \boldsymbol{x}_2 \right\rangle$$

$$= \int d\boldsymbol{x}_2 \left(V(\boldsymbol{x}_1 - \boldsymbol{x}_2) - V(\boldsymbol{y}_1 - \boldsymbol{x}_2)\right)\left\langle \boldsymbol{x}_1, \boldsymbol{x}_2 \,\middle|\, \hat{\rho}_{(2)}\left(\hat{\boldsymbol{X}}_1, \hat{\boldsymbol{X}}_2, t\right) \,\middle|\, \boldsymbol{y}_1, \boldsymbol{x}_2 \right\rangle$$

(6.89a) thus gives

$$i\hbar\frac{\partial}{\partial t}\langle \boldsymbol{x}_1 \mid \hat{\rho}_{(1)}(t) \mid \boldsymbol{y}_1 \rangle = -\frac{\hbar^2}{2m}(\nabla_{x_1}+\nabla_{y_1})\cdot(\nabla_{x_1}-\nabla_{y_1})\langle \boldsymbol{x}_1 \mid \hat{\rho}_{(1)}(t) \mid \boldsymbol{y}_1 \rangle \qquad (6.89)$$
$$+\int d\boldsymbol{x}_2\,\left[V(\boldsymbol{x}_1 - \boldsymbol{x}_2) - V(\boldsymbol{y}_1 - \boldsymbol{x}_2)\right]\langle \boldsymbol{x}_1, \boldsymbol{x}_2 \mid \hat{\rho}_{(2)}(t) \mid \boldsymbol{y}_1, \boldsymbol{x}_2 \rangle$$

Note that the RHS of (6.89) is the negative of that of Reichl’s.

Setting

$$\boldsymbol{R} = \frac{1}{2}(\boldsymbol{x}_1 + \boldsymbol{y}_1) \qquad \boldsymbol{r} = \boldsymbol{x}_1 - \boldsymbol{y}_1$$

$$\to \quad \boldsymbol{x}_1 = \boldsymbol{R} + \frac{1}{2}\boldsymbol{r} \qquad \boldsymbol{y}_1 = \boldsymbol{R} - \frac{1}{2}\boldsymbol{r}$$

(6.89) becomes

$$i\hbar\frac{\partial}{\partial t}\left\langle \boldsymbol{R} + \frac{1}{2}\boldsymbol{r} \,\middle|\, \hat{\rho}_{(1)}(t) \,\middle|\, \boldsymbol{R} - \frac{1}{2}\boldsymbol{r} \right\rangle = -\frac{\hbar^2}{m}\nabla_{\boldsymbol{R}}\cdot\nabla_{\boldsymbol{r}}\left\langle \boldsymbol{R} + \frac{1}{2}\boldsymbol{r} \,\middle|\, \hat{\rho}_{(1)}(t) \,\middle|\, \boldsymbol{R} - \frac{1}{2}\boldsymbol{r} \right\rangle$$
$$+\int d\boldsymbol{x}_2\left[V\left(\boldsymbol{R} + \frac{1}{2}\boldsymbol{r} - \boldsymbol{x}_2\right) - V\left(\boldsymbol{R} - \frac{1}{2}\boldsymbol{r} - \boldsymbol{x}_2\right)\right]\left\langle \boldsymbol{R} + \frac{1}{2}\boldsymbol{r}, \boldsymbol{x}_2 \,\middle|\, \hat{\rho}_{(2)}(t) \,\middle|\, \boldsymbol{R} - \frac{1}{2}\boldsymbol{r}, \boldsymbol{x}_2 \right\rangle$$
$$(6.89a)$$

If we $\int d\boldsymbol{r}\, e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}$ the whole equation, the 1-particle terms become [see (6.83)]

$$\int d\boldsymbol{r}\, e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}\, i\hbar\frac{\partial}{\partial t}\left\langle \boldsymbol{R} + \frac{1}{2}\boldsymbol{r} \,\middle|\, \hat{\rho}_{(1)}(t) \,\middle|\, \boldsymbol{R} - \frac{1}{2}\boldsymbol{r} \right\rangle = i\hbar\frac{\partial}{\partial t}f_1(\boldsymbol{k}, \boldsymbol{R}, t) \qquad (a)$$

and

$$-\int d\boldsymbol{r}\, e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}\frac{\hbar^2}{m}\nabla_{\boldsymbol{R}}\cdot\nabla_{\boldsymbol{r}}\left\langle \boldsymbol{R} + \frac{1}{2}\boldsymbol{r} \,\middle|\, \hat{\rho}_{(1)}(t) \,\middle|\, \boldsymbol{R} - \frac{1}{2}\boldsymbol{r} \right\rangle$$
$$= \frac{\hbar^2}{m}\nabla_{\boldsymbol{R}}\cdot\int d\boldsymbol{r}\left(\nabla_{\boldsymbol{r}} e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}\right)\left\langle \boldsymbol{R} + \frac{1}{2}\boldsymbol{r} \,\middle|\, \hat{\rho}_{(1)}(t) \,\middle|\, \boldsymbol{R} - \frac{1}{2}\boldsymbol{r} \right\rangle$$
$$= -i\frac{\hbar^2}{m}\boldsymbol{k}\cdot\nabla_{\boldsymbol{R}}\int d\boldsymbol{r}\, e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}\left\langle \boldsymbol{R} + \frac{1}{2}\boldsymbol{r} \,\middle|\, \hat{\rho}_{(1)}(t) \,\middle|\, \boldsymbol{R} - \frac{1}{2}\boldsymbol{r} \right\rangle$$
$$= -i\frac{\hbar^2}{m}\boldsymbol{k}\cdot\nabla_{\boldsymbol{R}} f_1(\boldsymbol{k}, \boldsymbol{R}, t) \qquad (b)$$

The 2-particle term requires more work. To begin, the inverse of (6.84) gives

$$\left\langle \boldsymbol{R}_1 + \frac{1}{2}\boldsymbol{r}_1\,,\ \boldsymbol{R}_2 + \frac{1}{2}\boldsymbol{r}_2 \,\middle|\, \hat{\rho}_{(2)}(t) \,\middle|\, \boldsymbol{R}_1 - \frac{1}{2}\boldsymbol{r}_1\,,\ \boldsymbol{R}_2 - \frac{1}{2}\boldsymbol{r}_2 \right\rangle$$
$$= \int \frac{d\boldsymbol{k}_1}{(2\pi)^3} \int \frac{d\boldsymbol{k}_2}{(2\pi)^3} e^{i\boldsymbol{k}_1\cdot\boldsymbol{r}_1} e^{i\boldsymbol{k}_2\cdot\boldsymbol{r}_2} f_2(\boldsymbol{k}_1, \boldsymbol{k}_2, \boldsymbol{R}_1, \boldsymbol{R}_2, t)$$
$$= \left\langle \boldsymbol{x}_1\,,\ \boldsymbol{x}_2 \,\middle|\, \hat{\rho}_{(2)}(t) \,\middle|\, \boldsymbol{y}_1\,,\ \boldsymbol{y}_2 \right\rangle$$

Setting $\boldsymbol{r}_2 = 0$, we have $\boldsymbol{x}_2 = \boldsymbol{R}_2$ and

$$\left\langle \boldsymbol{x}_1\,,\ \boldsymbol{x}_2 \,\middle|\, \hat{\rho}_{(2)}(t) \,\middle|\, \boldsymbol{y}_1\,,\ \boldsymbol{x}_2 \right\rangle = \left\langle \boldsymbol{R}_1 + \frac{1}{2}\boldsymbol{r}_1\,,\ \boldsymbol{x}_2 \,\middle|\, \hat{\rho}_{(2)}(t) \,\middle|\, \boldsymbol{R}_1 - \frac{1}{2}\boldsymbol{r}_1\,,\ \boldsymbol{x}_2 \right\rangle$$
$$= \int \frac{d\boldsymbol{k}_1}{(2\pi)^3} \int \frac{d\boldsymbol{k}_2}{(2\pi)^3} e^{i\boldsymbol{k}_1\cdot\boldsymbol{r}_1} f_2(\boldsymbol{k}_1, \boldsymbol{k}_2, \boldsymbol{R}_1, \boldsymbol{x}_2, t)$$

Removing all subscript 1 gives

$$\left\langle \boldsymbol{x}\,,\ \boldsymbol{x}_2 \,\middle|\, \hat{\rho}_{(2)}(t) \,\middle|\, \boldsymbol{y}\,,\ \boldsymbol{x}_2 \right\rangle = \left\langle \boldsymbol{R} + \frac{1}{2}\boldsymbol{r}\,,\ \boldsymbol{x}_2 \,\middle|\, \hat{\rho}_{(2)}(t) \,\middle|\, \boldsymbol{R} - \frac{1}{2}\boldsymbol{r}\,,\ \boldsymbol{x}_2 \right\rangle$$
$$= \int \frac{d\boldsymbol{k}'}{(2\pi)^3} \int \frac{d\boldsymbol{k}_2}{(2\pi)^3} e^{i\boldsymbol{k}'\cdot\boldsymbol{r}} f_2(\boldsymbol{k}', \boldsymbol{k}_2, \boldsymbol{R}_1, \boldsymbol{x}_2, t)$$

$$\rightarrow \qquad V(\boldsymbol{x} - \boldsymbol{x}_2) \left\langle \boldsymbol{x}\,,\ \boldsymbol{x}_2 \,\middle|\, \hat{\rho}_{(2)}(t) \,\middle|\, \boldsymbol{y}\,,\ \boldsymbol{x}_2 \right\rangle$$
$$= \int \frac{d\boldsymbol{k}'}{(2\pi)^3} \int \frac{d\boldsymbol{k}_2}{(2\pi)^3} V\left(\boldsymbol{R} + \frac{1}{2}\boldsymbol{r} - \boldsymbol{x}_2\right) e^{i\boldsymbol{k}'\cdot\boldsymbol{r}} f_2(\boldsymbol{k}', \boldsymbol{k}_2, \boldsymbol{R}_1, \boldsymbol{x}_2, t)$$
$$= \int \frac{d\boldsymbol{k}'}{(2\pi)^3} \int \frac{d\boldsymbol{k}_2}{(2\pi)^3} V\left(\boldsymbol{R} + \frac{1}{2i}\frac{\partial}{\partial \boldsymbol{k}'} - \boldsymbol{x}_2\right) e^{i\boldsymbol{k}'\cdot\boldsymbol{r}} f_2(\boldsymbol{k}', \boldsymbol{k}_2, \boldsymbol{R}_1, \boldsymbol{x}_2, t)$$

$$V(\boldsymbol{y} - \boldsymbol{x}_2) \left\langle \boldsymbol{x}\,,\ \boldsymbol{x}_2 \,\middle|\, \hat{\rho}_{(2)}(t) \,\middle|\, \boldsymbol{y}\,,\ \boldsymbol{x}_2 \right\rangle$$
$$= \int \frac{d\boldsymbol{k}'}{(2\pi)^3} \int \frac{d\boldsymbol{k}_2}{(2\pi)^3} V\left(\boldsymbol{R} - \frac{1}{2}\boldsymbol{r} - \boldsymbol{x}_2\right) e^{i\boldsymbol{k}'\cdot\boldsymbol{r}} f_2(\boldsymbol{k}', \boldsymbol{k}_2, \boldsymbol{R}_1, \boldsymbol{x}_2, t)$$
$$= \int \frac{d\boldsymbol{k}'}{(2\pi)^3} \int \frac{d\boldsymbol{k}_2}{(2\pi)^3} V\left(\boldsymbol{R} - \frac{1}{2i}\frac{\partial}{\partial \boldsymbol{k}'} - \boldsymbol{x}_2\right) e^{i\boldsymbol{k}'\cdot\boldsymbol{r}} f_2(\boldsymbol{k}', \boldsymbol{k}_2, \boldsymbol{R}_1, \boldsymbol{x}_2, t)$$

Hence, the 2-particle term becomes

$$\int d\boldsymbol{r}\, e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} \int d\boldsymbol{x}_2 \left[V(\boldsymbol{x} - \boldsymbol{x}_2) - V(\boldsymbol{y} - \boldsymbol{x}_2) \right] \left\langle \boldsymbol{x}, \boldsymbol{x}_2 \,\middle|\, \hat{\rho}_{(2)}(t) \,\middle|\, \boldsymbol{y}, \boldsymbol{x}_2 \right\rangle$$
$$= \int d\boldsymbol{r}\, e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} \int \frac{d\boldsymbol{k}'}{(2\pi)^3} \int \frac{d\boldsymbol{k}_2}{(2\pi)^3} \int d\boldsymbol{x}_2$$
$$* \left[V\left(\boldsymbol{R} + \frac{1}{2i}\frac{\partial}{\partial \boldsymbol{k}'} - \boldsymbol{x}_2\right) - V\left(\boldsymbol{R} - \frac{1}{2i}\frac{\partial}{\partial \boldsymbol{k}'} - \boldsymbol{x}_2\right) \right] e^{i\boldsymbol{k}'\cdot\boldsymbol{r}} f_2(\boldsymbol{k}', \boldsymbol{k}_2, \boldsymbol{R}, \boldsymbol{x}_2, t)$$
$$= \int d\boldsymbol{k}' \int \frac{d\boldsymbol{k}_2}{(2\pi)^3} \int d\boldsymbol{x}_2 \left[V\left(\boldsymbol{R} + \frac{1}{2i}\frac{\partial}{\partial \boldsymbol{k}'} - \boldsymbol{x}_2\right) - V\left(\boldsymbol{R} - \frac{1}{2i}\frac{\partial}{\partial \boldsymbol{k}'} - \boldsymbol{x}_2\right) \right]$$
$$* \delta(\boldsymbol{k} - \boldsymbol{k}')\, f_2(\boldsymbol{k}', \boldsymbol{k}_2, \boldsymbol{R}, \boldsymbol{x}_2, t)$$
$$= \int \frac{d\boldsymbol{k}_2}{(2\pi)^3} \int d\boldsymbol{x}_2 \left[V\left(\boldsymbol{R} + \frac{1}{2i}\frac{\partial}{\partial \boldsymbol{k}} - \boldsymbol{x}_2\right) - V\left(\boldsymbol{R} - \frac{1}{2i}\frac{\partial}{\partial \boldsymbol{k}} - \boldsymbol{x}_2\right) \right] f_2(\boldsymbol{k}, \boldsymbol{k}_2, \boldsymbol{R}, \boldsymbol{x}_2, t) \qquad \text{(c)}$$

Putting (a-c) into (6.89a) gives

$$\frac{\partial}{\partial t} f_1(\boldsymbol{k}, \boldsymbol{R}, t) = -\frac{\hbar}{m} \boldsymbol{k}\cdot\nabla_{\boldsymbol{R}} f_1(\boldsymbol{k}, \boldsymbol{R}, t) + \frac{1}{i\hbar} \int \frac{d\boldsymbol{k}_2}{(2\pi)^3} \int d\boldsymbol{x}_2 \qquad (6.91)$$
$$* \left[V\left(\boldsymbol{R} + \frac{1}{2i}\frac{\partial}{\partial \boldsymbol{k}} - \boldsymbol{x}_2\right) - V\left(\boldsymbol{R} - \frac{1}{2i}\frac{\partial}{\partial \boldsymbol{k}} - \boldsymbol{x}_2\right) \right] f_2(\boldsymbol{k}, \boldsymbol{k}_2, \boldsymbol{R}, \boldsymbol{x}_2, t)$$

With $\boldsymbol{p} = \hbar \boldsymbol{k}$, this becomes

$$\frac{\partial}{\partial t} f_1(\boldsymbol{p}, \boldsymbol{R}, t) + \frac{1}{m} \boldsymbol{p} \cdot \nabla_{\boldsymbol{R}} f_1(\boldsymbol{p}, \boldsymbol{R}, t) = \frac{1}{i\hbar} \int \frac{d\boldsymbol{p}_2}{(2\pi\hbar)^3} \int d\boldsymbol{x}_2 \qquad (6.92a)$$

$$* \left[V\left(\boldsymbol{R} + \frac{\hbar}{2i} \frac{\partial}{\partial \boldsymbol{p}} - \boldsymbol{x}_2\right) - V\left(\boldsymbol{R} - \frac{\hbar}{2i} \frac{\partial}{\partial \boldsymbol{p}} - \boldsymbol{x}_2\right) \right] f_2(\boldsymbol{p}, \boldsymbol{p}_2, \boldsymbol{R}, \boldsymbol{x}_2, t)$$

Setting

$$f_n{}'(\boldsymbol{p}_1, \ldots, \boldsymbol{p}_n, \boldsymbol{R}_1, \ldots, \boldsymbol{R}_n, t) = \frac{1}{\hbar^{3n}} f_n(\boldsymbol{p}_1, \ldots, \boldsymbol{p}_n, \boldsymbol{R}_1, \ldots, \boldsymbol{R}_n, t) \qquad (6.93)$$

(6.92a) becomes

$$\frac{\partial}{\partial t} f_1{}'(\boldsymbol{p}, \boldsymbol{R}, t) + \frac{1}{m} \boldsymbol{p} \cdot \nabla_{\boldsymbol{R}} f_1{}'(\boldsymbol{p}, \boldsymbol{R}, t) = \frac{1}{i\hbar} \int \frac{d\boldsymbol{p}_2}{(2\pi)^3} \int d\boldsymbol{x}_2 \qquad (6.92)$$

$$* \left[V\left(\boldsymbol{R} + \frac{\hbar}{2i} \frac{\partial}{\partial \boldsymbol{p}} - \boldsymbol{x}_2\right) - V\left(\boldsymbol{R} - \frac{\hbar}{2i} \frac{\partial}{\partial \boldsymbol{p}} - \boldsymbol{x}_2\right) \right] f_2{}'(\boldsymbol{p}, \boldsymbol{p}_2, \boldsymbol{R}, \boldsymbol{x}_2, t)$$

The potential term can now be expanded in powers of $\hbar$, with $\hbar \to 0$ giving the classical kinetic equation.

(6.87a) can be easily generalized to the case of a 1-particle operator that depends only on $\hat{\boldsymbol{p}}$:

$$\langle O(t) \rangle = \text{Tr}\left[\hat{O}(\hat{\boldsymbol{p}})\, \rho_{(1)}(t)\right]$$

$$= \int \frac{d\boldsymbol{p}}{(2\pi)^3} \int d\boldsymbol{R}\; O(\boldsymbol{p})\, f_1{}'(\boldsymbol{p}, \boldsymbol{R}, t) \qquad (6.94a)$$

which takes the form of a classical phase space average. [Note however that f_1 is not a probability distribution since it can take negative values (see Exercise 6.7).]

Similarly, for a 1-particle operator that depends only on $\hat{\boldsymbol{q}}$:

$$\langle O(t) \rangle = \text{Tr}\left[\hat{O}(\hat{\boldsymbol{q}})\, \rho_{(1)}(t)\right]$$

$$= \int d\boldsymbol{x} \int d\boldsymbol{y} \left\langle \boldsymbol{x} \,\middle|\, \hat{O}(\hat{\boldsymbol{q}}) \,\middle|\, \boldsymbol{y} \right\rangle \left\langle \boldsymbol{y} \,\middle|\, \hat{\rho}_{(1)}(t) \,\middle|\, \boldsymbol{x} \right\rangle$$

$$= \int d\boldsymbol{x} \int d\boldsymbol{y}\; O(\boldsymbol{y})\, \delta(\boldsymbol{x} - \boldsymbol{y}) \left\langle \boldsymbol{y} \,\middle|\, \hat{\rho}_{(1)}(t) \,\middle|\, \boldsymbol{x} \right\rangle$$

$$= \int d\boldsymbol{x}\; O(\boldsymbol{x}) \left\langle \boldsymbol{x} \,\middle|\, \hat{\rho}_{(1)}(t) \,\middle|\, \boldsymbol{x} \right\rangle \qquad (6.94b)$$

Inverting (6.85b), we have

$$\left\langle \boldsymbol{y} \,\middle|\, \hat{\rho}_{(1)}(t) \,\middle|\, \boldsymbol{x} \right\rangle = \int \frac{d\boldsymbol{k}}{(2\pi)^3} e^{-i\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{y})} f_1(\boldsymbol{k}, \boldsymbol{R}, t)$$

$$\to \qquad \left\langle \boldsymbol{x} \,\middle|\, \hat{\rho}_{(1)}(t) \,\middle|\, \boldsymbol{x} \right\rangle = \int \frac{d\boldsymbol{k}}{(2\pi)^3} f_1(\boldsymbol{k}, \boldsymbol{x}, t)$$

(6.94b) thus becomes

$$\langle O(t) \rangle = \int \frac{d\boldsymbol{k}}{(2\pi)^3} \int d\boldsymbol{x}\; O(\boldsymbol{x})\, f_1(\boldsymbol{k}, \boldsymbol{x}, t)$$

$$= \int \frac{d\boldsymbol{p}}{(2\pi)^3} \int d\boldsymbol{x}\; O(\boldsymbol{x})\, f_1{}'(\boldsymbol{p}, \boldsymbol{x}, t) \qquad (6.94c)$$

which has the form of (6.94a).

On the other hand, the quantized form $\hat{O}(\hat{\boldsymbol{q}}, \hat{\boldsymbol{p}})$ of a classical 1-particle phase function $O(\boldsymbol{q}, \boldsymbol{p})$ is not unique. Thus, the integral

$$\int \frac{d\mathbf{p}}{(2\pi)^3} \int d\mathbf{x}\ O(\mathbf{x}, \mathbf{p})\, f_1{}'(\mathbf{p}, \mathbf{x}, t)$$

may not agree with the average given by

$$\langle O(t) \rangle = \mathrm{Tr}\left[\hat{O}, \hat{\rho}_{(1)}(t)\right]$$

for some quantized form $\hat{O}(\hat{\boldsymbol{q}}, \hat{\boldsymbol{p}})$.

For a classical phase space function $O(\boldsymbol{q}, \boldsymbol{p})$ with Fourier transform

$$O(\boldsymbol{q}, \boldsymbol{p}) = \int \frac{d\boldsymbol{\eta}}{(2\pi)^3} \int d\boldsymbol{\sigma}\, e^{i(\boldsymbol{\eta}\cdot\boldsymbol{q} - \boldsymbol{\sigma}\cdot\boldsymbol{p})}\, \tilde{O}(\boldsymbol{\eta}, \boldsymbol{\sigma}) \tag{6.94}$$

The Weyl correspondence gives the quantum version of the operator as

$$\hat{O}(\hat{\boldsymbol{q}}, \hat{\boldsymbol{p}}) = \int \frac{d\boldsymbol{\eta}}{(2\pi)^3} \int d\boldsymbol{\sigma}\, e^{i(\boldsymbol{\eta}\cdot\hat{\boldsymbol{q}} - \boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}})}\, \tilde{O}(\boldsymbol{\eta}, \boldsymbol{\sigma}) \tag{6.95a}$$

so that

$$\left\langle \boldsymbol{x} \,\middle|\, \hat{O}(\hat{\boldsymbol{q}}, \hat{\boldsymbol{p}}) \,\middle|\, \boldsymbol{y} \right\rangle = \int \frac{d\boldsymbol{\eta}}{(2\pi)^3} \int d\boldsymbol{\sigma} \left\langle \boldsymbol{x} \,\middle|\, e^{i(\boldsymbol{\eta}\cdot\hat{\boldsymbol{q}} - \boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}})} \,\middle|\, \boldsymbol{y} \right\rangle \tilde{O}(\boldsymbol{\eta}, \boldsymbol{\sigma}) \tag{6.95}$$

Consider the Zassenhaus formula

$$e^{t(\hat{X}+\hat{Y})} = e^{t\hat{X}} \prod_{n=1}^{\infty} e^{t^n C_n} \tag{d}$$

where

$$C_1 = \hat{Y} \qquad C_2 = -\frac{1}{2!}\left[\hat{X}, \hat{Y}\right] \qquad C_3 = \frac{1}{3!}\left(2\left[\hat{Y}, \left[\hat{X}, \hat{Y}\right]\right] + \left[\hat{X}, \left[\hat{X}, \hat{Y}\right]\right]\right)$$

If $\left[\hat{X}, \hat{Y}\right]$ is central, i.e., $\left[\hat{X}, \hat{Y}\right]$ commutes with both $\hat{X}$ and $\hat{Y}$, (d) reduces to

$$e^{t(\hat{X}+\hat{Y})} = e^{t\hat{X}}\, e^{t\hat{Y}} \exp\left(-\frac{1}{2!} t^2 \left[\hat{X}, \hat{Y}\right]\right) \tag{e}$$

Setting

$$\hat{X} = \boldsymbol{\eta}\cdot\hat{\boldsymbol{q}} \qquad \hat{Y} = -\boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}} \qquad t = i$$

we have

$$\left[\hat{X}, \hat{Y}\right] = \left[\eta_i \hat{q}_i, -\sigma_j \hat{p}_j\right] = -\eta_i \sigma_j\, i\hbar\, \delta_{ij} = -i\hbar\, \eta_i \sigma_i = -i\hbar\, \boldsymbol{\eta}\cdot\boldsymbol{\sigma}$$

$$\left[\hat{Y}, \left[\hat{X}, \hat{Y}\right]\right] = \left[\hat{X}, \left[\hat{X}, \hat{Y}\right]\right] = 0$$

$$e^{i(\boldsymbol{\eta}\cdot\hat{\boldsymbol{q}} - \boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}})} = e^{i\boldsymbol{\eta}\cdot\hat{\boldsymbol{q}}}\, e^{-i\boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}}}\, e^{-i\hbar\boldsymbol{\eta}\cdot\boldsymbol{\sigma}/2}$$

so that

$$\begin{aligned}
\left\langle \boldsymbol{x} \,\middle|\, e^{i(\boldsymbol{\eta}\cdot\hat{\boldsymbol{q}} - \boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}})} \,\middle|\, \boldsymbol{y} \right\rangle &= e^{-i\hbar\boldsymbol{\eta}\cdot\boldsymbol{\sigma}/2} \left\langle \boldsymbol{x} \,\middle|\, e^{i\boldsymbol{\eta}\cdot\hat{\boldsymbol{q}}}\, e^{-i\boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}}} \,\middle|\, \boldsymbol{y} \right\rangle \\
&= e^{-i\hbar\boldsymbol{\eta}\cdot\boldsymbol{\sigma}/2}\, e^{i\boldsymbol{\eta}\cdot\boldsymbol{x}} \left\langle \boldsymbol{x} \,\middle|\, e^{-i\boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}}} \,\middle|\, \boldsymbol{y} \right\rangle \\
&= e^{-i\hbar\boldsymbol{\eta}\cdot\boldsymbol{\sigma}/2}\, e^{i\boldsymbol{\eta}\cdot\boldsymbol{x}} \int \frac{d\boldsymbol{k}}{(2\pi)^3} \left\langle \boldsymbol{x} \,\middle|\, e^{-i\boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}}} \,\middle|\, \boldsymbol{k} \right\rangle \left\langle \boldsymbol{k} \,\middle|\, \boldsymbol{y} \right\rangle \\
&= e^{-i\hbar\boldsymbol{\eta}\cdot\boldsymbol{\sigma}/2}\, e^{i\boldsymbol{\eta}\cdot\boldsymbol{x}} \int \frac{d\boldsymbol{k}}{(2\pi)^3}\, e^{-i\hbar\boldsymbol{\sigma}\cdot\boldsymbol{k}}\, e^{i\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{y})} \\
&= e^{-i\hbar\boldsymbol{\eta}\cdot\boldsymbol{\sigma}/2}\, e^{i\boldsymbol{\eta}\cdot\boldsymbol{x}}\, \delta(\boldsymbol{x} - \boldsymbol{y} - \hbar\boldsymbol{\sigma})
\end{aligned}$$

(6.95) thus becomes

$$\left\langle \boldsymbol{x} \,\middle|\, \hat{O}(\hat{\boldsymbol{q}}, \hat{\boldsymbol{p}}) \,\middle|\, \boldsymbol{y} \right\rangle = \int \frac{d\boldsymbol{\eta}}{(2\pi)^3} \int d\boldsymbol{\sigma}\, e^{-i\hbar\boldsymbol{\eta}\cdot\boldsymbol{\sigma}/2}\, e^{i\boldsymbol{\eta}\cdot\boldsymbol{x}}\, \delta(\boldsymbol{x} - \boldsymbol{y} - \hbar\boldsymbol{\sigma})\, \tilde{O}(\boldsymbol{\eta}, \boldsymbol{\sigma})$$

$$= \int \frac{d\boldsymbol{\eta}}{(2\pi)^3} \, e^{-i\boldsymbol{\eta}\cdot(\boldsymbol{x}-\boldsymbol{y})/2} e^{i\boldsymbol{\eta}\cdot\boldsymbol{x}} \, \tilde{O}(\boldsymbol{\eta}, \boldsymbol{x}-\boldsymbol{y})$$
$$= \int \frac{d\boldsymbol{\eta}}{(2\pi)^3} \, e^{i\boldsymbol{\eta}\cdot(\boldsymbol{x}+\boldsymbol{y})/2} \, \tilde{O}(\boldsymbol{\eta}, \boldsymbol{x}-\boldsymbol{y})$$
$$= \int \frac{d\boldsymbol{\eta}}{(2\pi)^3} \, e^{i\boldsymbol{\eta}\cdot\boldsymbol{R}} \, \tilde{O}(\boldsymbol{\eta}, \boldsymbol{r})$$

From (6.79), we have

$$\langle O \rangle = \int d\boldsymbol{x} \int d\boldsymbol{y} \left\langle \boldsymbol{x} \mid \hat{O} \mid \boldsymbol{y} \right\rangle \left\langle \boldsymbol{y} \mid \hat{\rho}_{(1)} \mid \boldsymbol{x} \right\rangle$$
$$= \int d\boldsymbol{x} \int d\boldsymbol{y} \int \frac{d\boldsymbol{\eta}}{(2\pi)^3} \, e^{i\boldsymbol{\eta}\cdot\boldsymbol{R}} \, \tilde{O}(\boldsymbol{\eta}, \boldsymbol{r}) \left\langle \boldsymbol{y} \mid \hat{\rho}_{(1)} \mid \boldsymbol{x} \right\rangle$$
$$= \int d\boldsymbol{R} \int d\boldsymbol{r} \int \frac{d\boldsymbol{\eta}}{(2\pi)^3} \, e^{i\boldsymbol{\eta}\cdot\boldsymbol{R}} \, \tilde{O}(\boldsymbol{\eta}, \boldsymbol{r}) \left\langle \boldsymbol{y} \mid \hat{\rho}_{(1)} \mid \boldsymbol{x} \right\rangle$$
$$= \int d\boldsymbol{r} \int \frac{d\boldsymbol{\eta}}{(2\pi)^3} \, \tilde{O}(\boldsymbol{\eta}, \boldsymbol{r}) \, \tilde{f}_1(\boldsymbol{\eta}, \boldsymbol{r}, t)$$
$$= \int d\boldsymbol{r} \int \frac{d\boldsymbol{p}}{(2\pi)^3} \, \tilde{O}(\boldsymbol{p}, \boldsymbol{r}) \, \tilde{f}_1{}'(\boldsymbol{p}, \boldsymbol{r}, t) \qquad (6.96)$$

where

$$\tilde{f}_1(\boldsymbol{k}, \boldsymbol{r}, t) = \int d\boldsymbol{R} \; e^{i\boldsymbol{k}\cdot\boldsymbol{R}} \left\langle \boldsymbol{y} \mid \hat{\rho}_{(1)} \mid \boldsymbol{x} \right\rangle$$
$$= \int d\boldsymbol{R} \; e^{i\boldsymbol{k}\cdot\boldsymbol{R}} \left\langle \boldsymbol{R} - \frac{1}{2}\boldsymbol{r} \,\middle|\, \hat{\rho}_{(1)} \,\middle|\, \boldsymbol{R} + \frac{1}{2}\boldsymbol{r} \right\rangle$$

Exercise 6.7

Compute the Wigner function for a system with a density operator

$$\hat{\rho} = \hbar\sqrt{a\,b}\,\left(e^{-a\hat{x}^2} e^{-b\hat{p}^2} + e^{-b\hat{p}^2} e^{-a\hat{x}^2}\right)$$

Answer

The matrix elements of $\hat{\rho}$ are

$$\langle x \mid \hat{\rho} \mid y \rangle = \hbar\sqrt{a\,b}\,\left\langle x \,\middle|\, \left(e^{-a\hat{x}^2} e^{-b\hat{p}^2} + e^{-b\hat{p}^2} e^{-a\hat{x}^2}\right) \,\middle|\, y \right\rangle$$
$$= \hbar\sqrt{a\,b}\,\left\langle x \,\middle|\, e^{-a x^2} e^{-b\hat{p}^2} + e^{-b\hat{p}^2} e^{-a y^2} \right) \,\middle|\, y \right\rangle$$
$$= \hbar\sqrt{a\,b}\,\left(e^{-a x^2} + e^{-a y^2}\right) \left\langle x \,\middle|\, e^{-b\hat{p}^2} \,\middle|\, y \right\rangle$$

Using

$$\left\langle x \,\middle|\, e^{-b\hat{p}^2} \,\middle|\, y \right\rangle = \int \frac{d\,p}{2\pi\hbar} \left\langle x \,\middle|\, e^{-b\hat{p}^2} \,\middle|\, p \right\rangle \langle p \mid y \rangle$$
$$= \int \frac{d\,p}{2\pi\hbar} \, e^{-b p^2} \langle x \mid p \rangle \langle p \mid y \rangle$$
$$= \int \frac{d\,p}{2\pi\hbar} \, e^{-b p^2} \, e^{i p (x-y)/\hbar}$$
$$= \frac{1}{2\hbar\sqrt{b\,\pi}} \exp\left(-\frac{(x-y)^2}{4\,b\,\hbar^2}\right)$$

[See §Code below.]

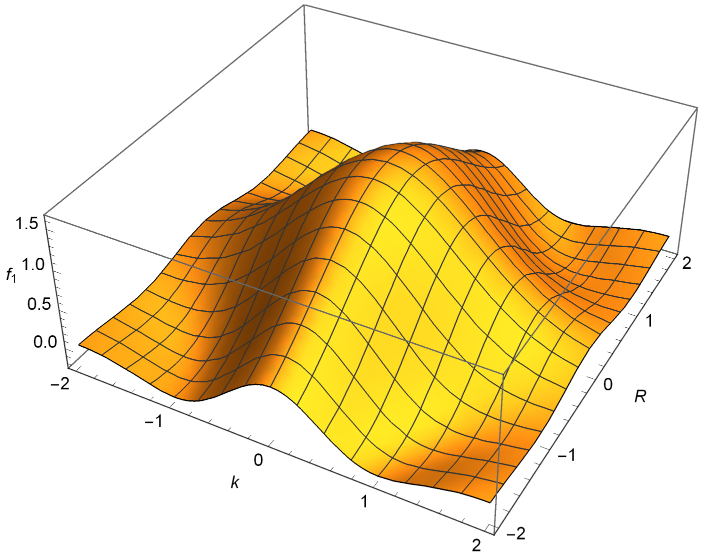
we have

$$\langle x \mid \hat{\rho} \mid y \rangle = \frac{1}{2}\sqrt{\frac{a}{\pi}}\left(e^{-a x^2} + e^{-a y^2}\right)\exp\left(-\frac{(x-y)^2}{4 b \hbar^2}\right) \tag{1}$$

From (6.83), we have

$$\begin{aligned} f_1(k, R) &= \int_{-\infty}^{\infty} d r\, e^{i k r} \left\langle R - \frac{1}{2} r \,\middle|\, \hat{\rho} \,\middle|\, R + \frac{1}{2} r \right\rangle \\ &= \int_{-\infty}^{\infty} d r\, e^{i k r} \langle y \mid \hat{\rho} \mid x \rangle \\ &= \frac{1}{2}\sqrt{\frac{a}{\pi}} \int_{-\infty}^{\infty} d r\, e^{i k r} \left(e^{-a\left(R+\frac{1}{2} r\right)^2} + e^{-a\left(R-\frac{1}{2} r\right)^2} \right) \exp\left(-\frac{r^2}{4 b \hbar^2}\right) \\ &= \sqrt{\frac{a b \hbar^2}{1 + a b \hbar^2}}\, e^{-\frac{a R^2 + 2 b k^2 \hbar^2}{1 + a b \hbar^2}} \left(e^{\frac{b k (k - 2 i a R) \hbar^2}{1 + a b \hbar^2}} + e^{\frac{b k (k + 2 i a R) \hbar^2}{1 + a b \hbar^2}} \right) \\ &= \sqrt{\frac{a b \hbar^2}{1 + a b \hbar^2}}\, e^{-\frac{a R^2 + b k^2 \hbar^2}{1 + a b \hbar^2}} \left(e^{-\frac{2 i a b k R \hbar^2}{1 + a b \hbar^2}} + e^{\frac{2 i a b k R \hbar^2}{1 + a b \hbar^2}} \right) \\ &= \sqrt{\frac{4 a b \hbar^2}{1 + a b \hbar^2}}\, e^{-\frac{a R^2 + b k^2 \hbar^2}{1 + a b \hbar^2}} \cos\left(\frac{2 a b k R \hbar^2}{1 + a b \hbar^2}\right) \end{aligned} \tag{2}$$

Plot of f_1 for $a = 1$, $b = 2$, $\hbar = 1$. [See §Code below.]



Code

Assuming$\left[b > 0 \,\&\&\, \hbar > 0 \,\&\&\, x > 0 \,\&\&\, y > 0,\ \int_{-\infty}^{\infty} \frac{1}{2 \pi \hbar} e^{-b p^2} e^{i p (x-y)/\hbar} d p \right]$

$$\frac{e^{-\frac{(x-y)^2}{4 b \hbar^2}}}{2 \sqrt{b} \sqrt{\pi}\, \hbar}$$

$$A = \text{Assuming}\Big[a > 0 \,\&\&\, b > 0 \,\&\&\, \hbar > 0 \,\&\&\, R > 0 \,\&\&\, k > 0,\; \int_{-\infty}^{\infty} e^{i k r}\left(e^{-a\left(R+\frac{1}{2}r\right)^2} + e^{-a\left(R-\frac{1}{2}r\right)^2}\right)\text{Exp}\left[-\frac{r^2}{4 b \hbar^2}\right] dr\Big]$$

$$2\, e^{-\frac{a R^2 + 2 b k^2 \hbar^2}{1 + a b \hbar^2}}\left(e^{\frac{b k (k - 2 i a R)\hbar^2}{1 + a b \hbar^2}} + e^{\frac{b k (k + 2 i a R)\hbar^2}{1 + a b \hbar^2}}\right)\sqrt{\pi}\,\hbar\sqrt{\frac{b}{1 + a b \hbar^2}}$$

$$f[k\_, R\_] := \sqrt{\frac{4 a b \hbar^2}{1 + a b \hbar^2}}\; e^{-\frac{a R^2 + b k^2 \hbar^2}{1 + a b \hbar^2}}\,\text{Cos}\left[\frac{2 a b k R \hbar^2}{1 + a b \hbar^2}\right] \;/.\; \{a \to 1, b \to 2, \hbar \to 1\}$$

```
f[k, R]
```

$$2\sqrt{\frac{2}{3}}\; e^{\frac{1}{3}\left(-2 k^2 - R^2\right)}\,\text{Cos}\left[\frac{4 k R}{3}\right]$$

```
Plot3D[f[k, R], {k, -2, 2}, {R, -2, 2},
    AxesLabel → {"k", "R", "f1"}]
```