Problems

2.14. BBGKY for binary mixtures. Consider a binary mixture described by the Hamiltonian (2.53).

$$\begin{aligned} H = &\sum_{a=1}^{N_A}\left(\frac{p_{A,a}^2}{2m_A}+V^A(\vec r_{A,a})\right)+\sum_{b=1}^{N_B}\left(\frac{p_{B,b}^2}{2m_B}+V^B(\vec r_{B,b})\right) \\ &+\sum_{a<b}^{N_A}\phi^{AA}(\vec r_{A,a}-\vec r_{A,b})+\sum_{a<b}^{N_B}\phi^{BB}(\vec r_{B,a}-\vec r_{B,b})+\sum_{a=1}^{N_A}\sum_{b=1}^{N_B}\phi^{AB}(\vec r_{A,a}-\vec r_{B,b})\end{aligned} \tag{2.53}$$

Derive the BBGKY equations for the reduced distributions $F^{(n_A,n_B)}$ and write in detail the equations for the cases $F^{(1,0)}$ and $F^{(0,1)}$.

- We start with collecting the needed abbreviations and definitions:
  - Phase space
  $$\Gamma_N = (\vec r_1,\vec p_1,\vec r_2,\vec p_2,\dots,\vec r_N,\vec p_N) = (1,2,\dots,N) \qquad \text{, where } k=\vec r_k,\vec p_k \tag{1}$$
  - symmetrized distribution
  $$\widehat F(\Gamma,t)=\frac{1}{N!}\sum_P F(P\Gamma,t) \tag{2.15}$$
  where P signifies the $N!$ permutations of positions and momenta of the particles.
  - reduced distribution
  $$F^{(n)}(1,2,\dots,n;t)=\frac{N!}{(N-n)!}\int \widehat F(1,2,\dots,N;t)d(n+1)\dots dN \tag{2.17}$$
  with the normalization
  $$\int F^{(n)}(1,2,\dots,n;t)d1\dots dn=\frac{N!}{(N-n)!} \tag{2.18}$$
  - Liouville equation
  $$\frac{\partial F}{\partial t}=-\{H,F\} \tag{2.11}$$
- to obtain the equations for the hierarchy, we
  1. symmetrize the Liouville equation, eq. (2.11), over the N particles
  2. multiply by the prefactor $\frac{N!}{(N-n)!}$ and
  3. integrate over the remainder of the phase space $\int d(n+1)\dots dN$
- general assumption for the N particle Hamiltonian:
  $$H_N=\sum_{a=1}^N h_0(a)+\sum_{a<b}^N\phi(a,b) \tag{2}$$
  - H_N has only separable one-particle and two-particle terms
  - the one-particle Hamiltonian h_0 is separable into kinetic and potential parts
  $$h_0=K_0(\vec p_a)+V_0(\vec r_a)\ , \tag{3}$$
  with the kinetic part depending only on momenta and the potential part depending only on positions.
- for mixtures we have also the extended definitions
  $$\widehat F(1_A\dots N_A;1_B\dots N_B;t)=\frac{1}{N_A!}\frac{1}{N_B!}\sum_{P_A}\sum_{P_B}F(P_A\Gamma_A;P_B\Gamma_B;t) \tag{4}$$
  and
  $$\begin{aligned}&F^{(n_A,n_B)}(1_A,\dots,n_A;1_B,\dots,n_B;t)\\ &=\frac{N_A!}{(N_A-n_A)!}\frac{N_B!}{(N_B-n_B)!}\int\widehat F(1_A\dots N_A;1_B\dots N_B;t)d(n_A+1)\dots dN_Ad(n_B+1)\dots dN_B\end{aligned} \tag{5}$$

Applying now the points 1., 2., and 3. to the Liouville equation for the density function of a mixture gives:

1. symmetrizing

$$\frac{\partial \widehat{F}^{(N_A,N_B)}}{\partial t} = \frac{1}{N_A!}\frac{1}{N_B!}\sum_{P_A}\sum_{P_B} P_A P_B \left[-\{H, F^{(N_A,N_B)}\}\right] \tag{6}$$

2. multiplying

$$\frac{N_A!}{(N_A-n_A)!}\frac{N_B!}{(N_B-n_B)!}\frac{\partial \widehat{F}^{(N_A,N_B)}}{\partial t} = \frac{1}{(N_A-n_A)!}\frac{1}{(N_B-n_B)!}\sum_{P_A}\sum_{P_B} P_A P_B \left[-\{H, F^{(N_A,N_B)}\}\right] \tag{7}$$

3. integrating

$$\frac{\partial F^{(n_A,n_B)}}{\partial t} = \frac{1}{(N_A-n_A)!}\frac{1}{(N_B-n_B)!}\int_{A_{n+1}^N}\int_{B_{n+1}^N}\sum_{P_A}\sum_{P_B} P_A P_B \left[-\{H, F^{(N_A,N_B)}\}\right] \ , \tag{8}$$

where we introduced the abbreviation

$$\int_{A_{n+1}^N} := \int d(n_A+1)\dots dN_A \ . \tag{9}$$

4. expanding the Hamiltonian

$$\begin{aligned} \frac{\partial F^{(n_A,n_B)}}{\partial t} &= \frac{1}{(N_A-n_A)!}\frac{1}{(N_B-n_B)!}\int_{A_{n+1}^N}\int_{B_{n+1}^N}\sum_{P_A}\sum_{P_B} P_A P_B \qquad (10)\\ &\times \left[-\left\{\left(\sum_{a=1}^{N_A} h_A(a) + \sum_{b=1}^{N_B} h_B(b) + \sum_{a<a'}^{N_A}\phi_{aa'}^{AA} + \sum_{b<b'}^{N_B}\phi_{bb'}^{BB} + \sum_{a=1}^{N_A}\sum_{b=1}^{N_B}\phi_{ab}^{AB}\right), F^{(N_A,N_B)}\right\}\right]\\ &= - \quad \boxed{1} \quad - \quad \boxed{2} \quad - \quad \boxed{3} \quad - \quad \boxed{4} \quad - \quad \boxed{5} \end{aligned}$$

with

$$\boxed{1} = \frac{1}{(N_A-n_A)!}\frac{1}{(N_B-n_B)!}\int_{A_{n+1}^N}\int_{B_{n+1}^N}\sum_{P_A}\sum_{P_B} P_A P_B \left\{\sum_{a=1}^{N_A} h_A(a), F^{(N_A,N_B)}\right\} \tag{11}$$

$$\boxed{2} = \frac{1}{(N_A-n_A)!}\frac{1}{(N_B-n_B)!}\int_{A_{n+1}^N}\int_{B_{n+1}^N}\sum_{P_A}\sum_{P_B} P_A P_B \left\{\sum_{b=1}^{N_B} h_B(b), F^{(N_A,N_B)}\right\} \tag{12}$$

$$\boxed{3} = \frac{1}{(N_A-n_A)!}\frac{1}{(N_B-n_B)!}\int_{A_{n+1}^N}\int_{B_{n+1}^N}\sum_{P_A}\sum_{P_B} P_A P_B \left\{\sum_{a<a'}^{N_A} \phi_{aa'}^{AA}, F^{(N_A,N_B)}\right\} \tag{13}$$

$$\boxed{4} = \frac{1}{(N_A-n_A)!}\frac{1}{(N_B-n_B)!}\int_{A_{n+1}^N}\int_{B_{n+1}^N}\sum_{P_A}\sum_{P_B} P_A P_B \left\{\sum_{b<b'}^{N_B} \phi_{bb'}^{BB}, F^{(N_A,N_B)}\right\} \tag{14}$$

$$\boxed{5} = \frac{1}{(N_A-n_A)!}\frac{1}{(N_B-n_B)!}\int_{A_{n+1}^N}\int_{B_{n+1}^N}\sum_{P_A}\sum_{P_B} P_A P_B \left\{\sum_{a=1}^{N_A}\sum_{b=1}^{N_B} \phi_{ab}^{AB}, F^{(N_A,N_B)}\right\} \tag{15}$$

Discussing the terms:

- Since $\boxed{1}$ and $\boxed{2}$ have the same structure, like $\boxed{3}$ and $\boxed{4}$, too, we can discuss them together.

$\boxed{1}$ In $\boxed{1}$ (or $\boxed{2}$) we have only the single particle Hamiltonian and we sum over all particles. Therefore the permutations just rearrange the appearance of terms in the sum, but do not change the sum. So we get

$$\sum_{P_A}\sum_{P_B} P_A P_B \left\{\sum_{a=1}^{N_A} h_A(a), F^{(N_A,N_B)}\right\} = \sum_{a=1}^{N_A}\left\{h_A(a), \sum_{P_A}\sum_{P_B} P_A P_B F^{(N_A,N_B)}\right\}$$
$$= \sum_{a=1}^{N_A}\left\{h_A(a), N_A! N_B! \widehat{F}^{(N_A,N_B)}\right\} \tag{16}$$

- For the integration we have to split the remaining sum into the two ranges $1\dots n_A$ and $(n_A+1)\dots N_A$:

$$\boxed{1} = \frac{N_A!}{(N_A-n_A)!}\frac{N_B!}{(N_B-n_B)!}\int_{A^N_{n+1}}\int_{B^N_{n+1}}\left(\sum_{a=1}^{n_A} + \sum_{a=n_A+1}^{N_A}\right)\left\{h_A(a), \widehat{F}^{(N_A,N_B)}\right\}$$
$$= \sum_{a=1}^{n_A}\left\{h_A(a), F^{(n_A,n_B)}\right\} + \frac{N_A!}{(N_A-n_A)!}\frac{N_B!}{(N_B-n_B)!}\sum_{a=n_A+1}^{N_A}\int_{A^N_{n+1}}\int_{B^N_{n+1}}$$
$$\times\left(\frac{\partial h_A(a)}{\partial \vec{p}_a}\frac{\partial \widehat{F}^{(N_A,N_B)}}{\partial \vec{r}_a} - \frac{\partial \widehat{F}^{(N_A,N_B)}}{\partial \vec{p}_a}\frac{\partial h_A(a)}{\partial \vec{r}_a}\right) \tag{17}$$

But the second term can be rewritten

$$\frac{\partial h_A(a)}{\partial \vec{p}_a}\frac{\partial \widehat{F}^{(N_A,N_B)}}{\partial \vec{r}_a} - \frac{\partial \widehat{F}^{(N_A,N_B)}}{\partial \vec{p}_a}\frac{\partial h_A(a)}{\partial \vec{r}_a} = \frac{\partial}{\partial \vec{p}_a}\left(h_A(a)\frac{\partial \widehat{F}^{(N_A,N_B)}}{\partial \vec{r}_a}\right) - \frac{\partial}{\partial \vec{r}_a}\left(h_A(a)\frac{\partial \widehat{F}^{(N_A,N_B)}}{\partial \vec{p}_a}\right) \tag{18}$$

and since it is integrated over, vanishes.
So we get simply:

$$\boxed{1} = \sum_{a=1}^{n_A}\left\{h_A(a), F^{(n_A,n_B)}\right\} \tag{19}$$
$$\boxed{2} = \sum_{b=1}^{n_B}\left\{h_B(b), F^{(n_A,n_B)}\right\} \tag{20}$$

$\boxed{3}$ In $\boxed{3}$ (or $\boxed{4}$) we still have only the single particle Hamiltonian and we sum over all particles. Therefore the permutations just rearrange the appearance of terms in the sum, but do not change the sum, even when we sum over pairs of positions. So we get

$$\sum_{P_A}\sum_{P_B} P_A P_B \left\{\sum_{a<a'}^{N_A} \phi^{AA}_{aa'}, F^{(N_A,N_B)}\right\} = \sum_{a<a'}^{N_A}\left\{\phi^{AA}_{aa'}, \sum_{P_A}\sum_{P_B} P_A P_B F^{(N_A,N_B)}\right\}$$
$$= \sum_{a<a'}^{N_A}\left\{\phi^{AA}_{aa'}, N_A! N_B! \widehat{F}^{(N_A,N_B)}\right\} \tag{21}$$

- For the integration we have to split the remaining double sum into three ranges for a and a':

$$\sum_{a<a'}^{N_A} = \sum_{a=1}^{N_A-1}\sum_{a'=a+1}^{N_A} = \sum_{a=1}^{n_A-1}\sum_{a'=a+1}^{n_A} + \sum_{a=1}^{n_A}\sum_{a'=n_A+1}^{N_A} + \sum_{a=n_A+1}^{N_A-1}\sum_{a'=a+1}^{N_A} \tag{22}$$

The first sum is independent of the integrals:

$$\boxed{3_1} = \frac{N_A!}{(N_A-n_A)!}\frac{N_B!}{(N_B-n_B)!}\int_{A^N_{n+1}}\int_{B^N_{n+1}}\sum_{a=1}^{n_A-1}\sum_{a'=a+1}^{n_A}\left\{\phi^{AA}_{aa'}, \widehat{F}^{(N_A,N_B)}\right\} = \sum_{a<a'}^{n_A}\left\{\phi^{AA}_{aa'}, F^{(n_A,n_B)}\right\} \tag{23}$$

In the second sum we can rename the summation index a' and give it always the name $\tilde{a}$. Then the second term has $(N_A - n_A)$ identical integrals over $\tilde{a}$:

$$\boxed{3_2} = \frac{N_A!}{(N_A-n_A)!}\frac{N_B!}{(N_B-n_B)!}\int_{A^N_{n+1}}\int_{B^N_{n+1}}\sum_{a=1}^{n_A}\sum_{a'=n_A+1}^{N_A}\left\{\phi^{AA}_{aa'},\widehat{F}^{(N_A,N_B)}\right\}$$
$$= \frac{N_A!}{(N_A-n_A)!}\frac{N_B!}{(N_B-n_B)!}\sum_{a=1}^{n_A}\int d\tilde{a}\int_{A^N_{n+2}}\int_{B^N_{n+1}}\left\{\phi^{AA}_{a\tilde{a}},\widehat{F}^{(N_A,N_B)}\right\}\sum_{a'=n_A+1}^{N_A}$$
$$= \sum_{a=1}^{n_A}\int d\tilde{a}\left\{\phi^{AA}_{a\tilde{a}},\frac{N_A!}{(N_A-n_A-1)!}\frac{N_B!}{(N_B-n_B)!}\int_{A^N_{n+2}}\int_{B^N_{n+1}}\widehat{F}^{(N_A,N_B)}\right\}$$
$$= \sum_{a=1}^{n_A}\int d\tilde{a}\left\{\phi^{AA}_{a\tilde{a}},F^{(n_A+1,n_B)}\right\} \tag{24}$$

The last sum can be treated in a similar way as eq. (17) and (18), since we integrate over all the summation indices:

$$\frac{\partial\phi^{AA}_{aa'}}{\partial\vec{p}_j}\frac{\partial\widehat{F}^{(N_A,N_B)}}{\partial\vec{r}_j} - \frac{\partial\widehat{F}^{(N_A,N_B)}}{\partial\vec{p}_j}\frac{\partial\phi^{AA}_{aa'}}{\partial\vec{r}_j} = \frac{\partial}{\partial\vec{p}_j}\left(\phi^{AA}_{aa'}\frac{\partial\widehat{F}^{(N_A,N_B)}}{\partial\vec{r}_j}\right) - \frac{\partial}{\partial\vec{r}_j}\left(\phi^{AA}_{aa'}\frac{\partial\widehat{F}^{(N_A,N_B)}}{\partial\vec{p}_j}\right) \tag{25}$$

and since it is integrated over, vanishes.
So we get simply:

$$\boxed{3} = \sum_{a<a'}^{n_A}\left\{\phi^{AA}_{aa'},F^{(n_A,n_B)}\right\} + \sum_{a=1}^{n_A}\int d\tilde{a}\left\{\phi^{AA}_{a\tilde{a}},F^{(n_A+1,n_B)}\right\} \tag{26}$$

$$\boxed{4} = \sum_{b<b'}^{n_B}\left\{\phi^{BB}_{bb'},F^{(n_A,n_B)}\right\} + \sum_{b=1}^{n_B}\int d\tilde{b}\left\{\phi^{BB}_{b\tilde{b}},F^{(n_A,n_B+1)}\right\} \tag{27}$$

where $\tilde{a}$ and $\tilde{b}$ are the names for the additional variables the appear in $F^{(n+1)}$ compared to $F^{(n)}$.

- In the Poisson bracket we have to sum over all possible pairs of coordinates and momenta. But if the pair does not appear in the potential ϕ, the result of the individual term of the Poisson bracket vanishes:

$$\left\{\phi^{AA}_{aa'},F\right\} = \sum_j^{N_A,N_B}\left[\frac{\partial\phi^{AA}_{aa'}}{\partial\vec{p}_j}\frac{\partial F}{\partial\vec{r}_j} - \frac{\partial F}{\partial\vec{p}_j}\frac{\partial\phi^{AA}_{aa'}}{\partial\vec{r}_j}\right] = -\frac{\partial F}{\partial\vec{p}_a}\frac{\partial\phi^{AA}_{aa'}}{\partial\vec{r}_a} - \frac{\partial F}{\partial\vec{p}_{a'}}\frac{\partial\phi^{AA}_{aa'}}{\partial\vec{r}_{a'}} \tag{28}$$

  – and with the same argument as in eq. (17) and (18), since we integrate for $\boxed{3}$ and $\boxed{4}$ over over $\tilde{a}$ and $\tilde{b}$, these indices will again not appear in the derivatives, giving the simpler result

$$\boxed{3} = \sum_{a<a'}^{n_A}\left\{\phi^{AA}_{aa'},F^{(n_A,n_B)}\right\} - \sum_{a=1}^{n_A}\int d\tilde{a}\frac{\partial\phi^{AA}_{a\tilde{a}}}{\partial\vec{r}_a}\frac{\partial}{\partial\vec{p}_a}F^{(n_A+1,n_B)} \tag{29}$$

$$\boxed{4} = \sum_{b<b'}^{n_B}\left\{\phi^{BB}_{bb'},F^{(n_A,n_B)}\right\} - \sum_{b=1}^{n_B}\int d\tilde{b}\frac{\partial\phi^{BB}_{b\tilde{b}}}{\partial\vec{r}_b}\frac{\partial}{\partial\vec{p}_b}F^{(n_A+1,n_B)} \tag{30}$$

$\boxed{5}$ In $\boxed{5}$ we still have now the real mixed particle Hamiltonian and we sum over all particles of both species. Therefore the permutations again just rearrange the appearance of the terms in the sum, but do not change the sum. So we get

$$\sum_{P_A}\sum_{P_B}P_AP_B\left\{\sum_{a=1}^{N_A}\sum_{b=1}^{N_B}\phi^{AB}_{ab},F^{(N_A,N_B)}\right\} = \sum_{a=1}^{N_A}\sum_{b=1}^{N_B}\left\{\phi^{AB}_{ab},\sum_{P_A}\sum_{P_B}P_AP_BF^{(N_A,N_B)}\right\}$$
$$= \sum_{a=1}^{N_A}\sum_{b=1}^{N_B}\left\{\phi^{AB}_{ab},N_A!N_B!\widehat{F}^{(N_A,N_B)}\right\} \tag{31}$$

- For the integration we have to split the double sum now into four ranges for a and b:

$$\sum_{a=1}^{N_A}\sum_{b=1}^{N_B} = \sum_{a=1}^{n_A}\sum_{b=1}^{n_B} + \sum_{a=n_A+1}^{N_A}\sum_{b=1}^{n_B} + \sum_{a=1}^{n_A}\sum_{b=n_B+1}^{N_B} + \sum_{a=n_A+1}^{N_A}\sum_{b=n_B+1}^{N_B} \tag{32}$$

The first sum is independent of the integrals:

$$\boxed{5_1} = \frac{N_A!}{(N_A-n_A)!}\frac{N_B!}{(N_B-n_B)!}\int_{A^N_{n+1}}\int_{B^N_{n+1}}\sum_{a=1}^{n_A}\sum_{b=1}^{n_B}\left\{\phi^{AB}_{ab},\widehat{F}^{(N_A,N_B)}\right\} = \sum_{a=1}^{n_A}\sum_{b=1}^{n_B}\left\{\phi^{AB}_{ab},F^{(n_A,n_B)}\right\} \tag{33}$$

In the second sum we can rename one summation index a and give it always the name $\tilde{a}$. Then the second term has (N_A-n_A) identical integrals over $\tilde{a}$:

$$\begin{aligned}\boxed{5_2} &= \frac{N_A!}{(N_A-n_A)!}\frac{N_B!}{(N_B-n_B)!}\int_{A^N_{n+1}}\int_{B^N_{n+1}}\sum_{a=n_A+1}^{N_A}\sum_{b=1}^{n_B}\left\{\phi^{AB}_{ab},\widehat{F}^{(N_A,N_B)}\right\}\\ &= \frac{N_A!}{(N_A-n_A)!}\frac{N_B!}{(N_B-n_B)!}\sum_{b=1}^{n_B}\int d\tilde{a}\int_{A^N_{n+2}}\int_{B^N_{n+1}}\left\{\phi^{AB}_{\tilde{a}b},\widehat{F}^{(N_A,N_B)}\right\}\sum_{a=n_A+1}^{N_A}\\ &= \sum_{b=1}^{n_B}\int d\tilde{a}\left\{\phi^{AB}_{\tilde{a}b},\frac{N_A!}{(N_A-n_A-1)!}\frac{N_B!}{(N_B-n_B)!}\int_{A^N_{n+2}}\int_{B^N_{n+1}}\widehat{F}^{(N_A,N_B)}\right\}\\ &= \sum_{b=1}^{n_B}\int d\tilde{a}\left\{\phi^{AB}_{\tilde{a}b},F^{(n_A+1,n_B)}\right\}\end{aligned} \tag{34}$$

With the same logic for the Poisson bracket as eq. (28) we get

$$\boxed{5_2} = -\sum_{b=1}^{n_B}\int d\tilde{a}\frac{\partial\phi^{AB}_{\tilde{a}b}}{\partial\vec{r}_b}\frac{\partial}{\partial\vec{p}_b}F^{(n_A+1,n_B)} \tag{35}$$

In a similar way we get the third term by exchanging a and b:

$$\begin{aligned}\boxed{5_3} &= \frac{N_A!}{(N_A-n_A)!}\frac{N_B!}{(N_B-n_B)!}\int_{A^N_{n+1}}\int_{B^N_{n+1}}\sum_{a=1}^{n_A}\sum_{b=n_B+1}^{N_B}\left\{\phi^{AB}_{ab},\widehat{F}^{(N_A,N_B)}\right\}\\ &= -\sum_{a=1}^{n_A}\int d\tilde{b}\frac{\partial\phi^{AB}_{a\tilde{b}}}{\partial\vec{r}_a}\frac{\partial}{\partial\vec{p}_a}F^{(n_A,n_B+1)}\end{aligned} \tag{36}$$

In the last sum we have to rename both of the summation indices and like in the previous equations we will call them $\tilde{a}$ and $\tilde{b}$:

$$\begin{aligned}\boxed{5_4} &= \frac{N_A!}{(N_A-n_A)!}\frac{N_B!}{(N_B-n_B)!}\int_{A^N_{n+1}}\int_{B^N_{n+1}}\sum_{a=n_A+1}^{N_A}\sum_{b=n_B+1}^{N_B}\left\{\phi^{AB}_{ab},\widehat{F}^{(N_A,N_B)}\right\}\\ &= \frac{N_A!}{(N_A-n_A)!}\frac{N_B!}{(N_B-n_B)!}\int d\tilde{a}\int d\tilde{b}\int_{A^N_{n+2}}\int_{B^N_{n+2}}\left\{\phi^{AB}_{\tilde{a}\tilde{b}},\widehat{F}^{(N_A,N_B)}\right\}\sum_{a=n_A+1}^{N_A}\sum_{b=n_B+1}^{N_B}\\ &= \int d\tilde{a}\int d\tilde{b}\left\{\phi^{AB}_{\tilde{a}\tilde{b}},F^{(n_A+1,n_B+1)}\right\}\end{aligned} \tag{37}$$

But applying the logic of eq. (28) we see, that this term vanishes.
So we get:

$$\begin{aligned}\boxed{5} &= \sum_{a=1}^{n_A}\sum_{b=1}^{n_B}\left\{\phi^{AB}_{ab},F^{(n_A,n_B)}\right\} + \sum_{b=1}^{n_B}\int d\tilde{a}\left\{\phi^{AB}_{\tilde{a}b},F^{(n_A+1,n_B)}\right\} + \sum_{a=1}^{n_A}\int d\tilde{b}\left\{\phi^{AB}_{a\tilde{b}},F^{(n_A,n_B+1)}\right\}\\ &+ \int d\tilde{a}\int d\tilde{b}\left\{\phi^{AB}_{\tilde{a}\tilde{b}},F^{(n_A+1,n_B+1)}\right\}\\ &= \sum_{a=1}^{n_A}\sum_{b=1}^{n_B}\left\{\phi^{AB}_{ab},F^{(n_A,n_B)}\right\} - \sum_{b=1}^{n_B}\int d\tilde{a}\frac{\partial\phi^{AB}_{\tilde{a}b}}{\partial\vec{r}_b}\frac{\partial}{\partial\vec{p}_b}F^{(n_A+1,n_B)} - \sum_{a=1}^{n_A}\int d\tilde{b}\frac{\partial\phi^{AB}_{a\tilde{b}}}{\partial\vec{r}_a}\frac{\partial}{\partial\vec{p}_a}F^{(n_A,n_B+1)}\end{aligned} \tag{38}$$

Writing the n particle Hamiltonian as

$$H_n = \sum_{a=1}^{n_A} h_A(a) + \sum_{b=1}^{n_B} h_B(b) + \sum_{a<a'}^{n_A} \phi^{AA}_{aa'} + \sum_{b<b'}^{n_B} \phi^{BB}_{bb'} + \sum_{a=1}^{n_A}\sum_{b=1}^{n_B} \phi^{AB}_{ab} \tag{39}$$

we can write the hierarchy as

$$\begin{aligned}
\frac{\partial}{\partial t} F^{(n_A,n_B)} = & -\left\{H_n, F^{(n_A,n_B)}\right\} + \int d\tilde{a} \sum_{a=1}^{n_A} \frac{\partial \phi^{AA}_{a\tilde{a}}}{\partial \vec{r}_a}\frac{\partial}{\partial \vec{p}_a} F^{(n_A+1,n_B)} + \int d\tilde{b} \sum_{b=1}^{n_B} \frac{\partial \phi^{BB}_{b\tilde{b}}}{\partial \vec{r}_b}\frac{\partial}{\partial \vec{p}_b} F^{(n_A,n_B+1)} \\
& + \int d\tilde{a} \sum_{b=1}^{n_B} \frac{\partial \phi^{AB}_{\tilde{a}b}}{\partial \vec{r}_b}\frac{\partial}{\partial \vec{p}_b} F^{(n_A+1,n_B)} + \int d\tilde{b} \sum_{a=1}^{n_A} \frac{\partial \phi^{AB}_{a\tilde{b}}}{\partial \vec{r}_a}\frac{\partial}{\partial \vec{p}_a} F^{(n_A,n_B+1)} \\
= & -\left\{H_n, F^{(n_A,n_B)}\right\} + \int d\tilde{a} \left[\sum_{a=1}^{n_A} \frac{\partial \phi^{AA}_{a\tilde{a}}}{\partial \vec{r}_a}\frac{\partial}{\partial \vec{p}_a} + \sum_{b=1}^{n_B} \frac{\partial \phi^{AB}_{\tilde{a}b}}{\partial \vec{r}_b}\frac{\partial}{\partial \vec{p}_b}\right] F^{(n_A+1,n_B)} \\
& + \int d\tilde{b} \left[\sum_{b=1}^{n_B} \frac{\partial \phi^{BB}_{b\tilde{b}}}{\partial \vec{r}_b}\frac{\partial}{\partial \vec{p}_b} + \sum_{a=1}^{n_A} \frac{\partial \phi^{AB}_{a\tilde{b}}}{\partial \vec{r}_a}\frac{\partial}{\partial \vec{p}_a}\right] F^{(n_A,n_B+1)}
\end{aligned} \tag{40}$$

case $F^{(1,0)}$

$$\begin{aligned}
\left[\frac{\partial}{\partial t} + \{H_n,\cdot\}\right] F^{(1,0)}[\vec{r}_a,\vec{p}_a;t] = & \int d\tilde{a} \left[\sum_{a=1}^{1} \frac{\partial \phi^{AA}_{a\tilde{a}}}{\partial \vec{r}_a}\frac{\partial}{\partial \vec{p}_a} + \sum_{b=1}^{0} \frac{\partial \phi^{AB}_{\tilde{a}b}}{\partial \vec{r}_b}\frac{\partial}{\partial \vec{p}_b}\right] F^{(2,0)} \\
& + \int d\tilde{b} \left[\sum_{b=1}^{0} \frac{\partial \phi^{BB}_{b\tilde{b}}}{\partial \vec{r}_b}\frac{\partial}{\partial \vec{p}_b} + \sum_{a=1}^{1} \frac{\partial \phi^{AB}_{a\tilde{b}}}{\partial \vec{r}_a}\frac{\partial}{\partial \vec{p}_a}\right] F^{(1,1)} \\
= & \int d\tilde{a} \frac{\partial \phi^{AA}_{a\tilde{a}}}{\partial \vec{r}_a}\frac{\partial}{\partial \vec{p}_a} F^{(2,0)}[\vec{r}_a,\vec{p}_a,\vec{r}_{\tilde{a}},\vec{p}_{\tilde{a}};t] \\
& + \int d\tilde{b} \frac{\partial \phi^{AB}_{a\tilde{b}}}{\partial \vec{r}_a}\frac{\partial}{\partial \vec{p}_a} F^{(1,1)}[\vec{r}_a,\vec{p}_a;\vec{r}_{\tilde{b}},\vec{p}_{\tilde{b}};t]
\end{aligned} \tag{41}$$

case $F^{(0,1)}$

$$\begin{aligned}
\left[\frac{\partial}{\partial t} + \{H_n,\cdot\}\right] F^{(0,1)}[\vec{r}_b,\vec{p}_b;t] = & \int d\tilde{a} \left[\sum_{a=1}^{0} \frac{\partial \phi^{AA}_{a\tilde{a}}}{\partial \vec{r}_a}\frac{\partial}{\partial \vec{p}_a} + \sum_{b=1}^{1} \frac{\partial \phi^{AB}_{\tilde{a}b}}{\partial \vec{r}_b}\frac{\partial}{\partial \vec{p}_b}\right] F^{(1,1)} \\
& + \int d\tilde{b} \left[\sum_{b=1}^{1} \frac{\partial \phi^{BB}_{b\tilde{b}}}{\partial \vec{r}_b}\frac{\partial}{\partial \vec{p}_b} + \sum_{a=1}^{0} \frac{\partial \phi^{AB}_{a\tilde{b}}}{\partial \vec{r}_a}\frac{\partial}{\partial \vec{p}_a}\right] F^{(0,2)} \\
= & \int d\tilde{a} \frac{\partial \phi^{AB}_{\tilde{a}b}}{\partial \vec{r}_b}\frac{\partial}{\partial \vec{p}_b} F^{(1,1)}[\vec{r}_{\tilde{a}},\vec{p}_{\tilde{a}};\vec{r}_b,\vec{p}_b;t] \\
& + \int d\tilde{b} \frac{\partial \phi^{BB}_{b\tilde{b}}}{\partial \vec{r}_b}\frac{\partial}{\partial \vec{p}_b} F^{(0,2)}[\vec{r}_b,\vec{p}_b,\vec{r}_{\tilde{b}},\vec{p}_{\tilde{b}};t]
\end{aligned} \tag{42}$$