A new truncation scheme for BBGKY hierarchy: conservation of energy and time reversibility

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Abstract. We propose a new truncation scheme for Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy. We approximate the three particle distribution function $f_3(1,2,3,t)$ in terms of $f_2(1,2,t)$, $f_1(3,t)$ and two point correlation functions \{g_2(1,3,t), g_2(2,3,t)\}. Further $f_2$ is expressed in terms of $f_1(1,t)$ and $g_2(1,2,t)$ to close the hierarchy, resulting a set of coupled kinetic equations for $f_1$ and $g_2$. In this paper we show that, for velocity independent correlations, the kinetic equation for $f_1$ reduces to the model proposed by Martys [Martys N S 1999 IJMPC 10 1367-1382]. In the steady state limit, the kinetic equation for $g_2$ reduces to Born-Green-Yvon (BGY) hierarchy for homogeneous density. We also prove that the present scheme respects the energy conservation and under specific circumstances, time symmetry i.e., \( \frac{dH(t)}{dt} = 0 \) where $H(t)$ refers to the Boltzmann’s H-function.

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1. Introduction

Consider a system of \( N \) interacting gas molecules present in a volume \( V \) under the influence of an external potential \( U(\vec{r}) \). From Liouville’s theorem one can say that, the \( s \)-particle phase space distribution function \( f_s(1, 2, \cdots, s, t) \), \( (1 \leq s \leq N - 1) \) of such a system is related to the \( (s + 1) \)-particle distribution function through BBGKY hierarchy \([1, 2]\) of equations,

\[
\frac{\partial f_s}{\partial t} + \sum_{i=1}^{s} \vec{v}_i \cdot \vec{\nabla}_{\vec{r}_i} f_s = - \sum_{i=1}^{s} \sum_{j=1}^{s} \frac{\partial f_s}{\partial \vec{p}_i} \cdot \frac{\partial}{\partial \vec{r}_i} \left( \frac{1}{2} \sum_{j=1 \atop j \neq i}^{s} \phi_{ij} \right) = \sum_{i=1}^{s} \int \frac{\partial f_{s+1}}{\partial \vec{p}_i} \cdot \frac{\partial \phi_{i,s+1}}{\partial \vec{r}_i} \, d\omega_{s+1} \ .
\]

In the above, \( \phi_{ij} = \phi(|\vec{r}_i - \vec{r}_j|) \) is the pair interaction potential between \( i^{th} \) and \( j^{th} \) particles, \( \vec{F}_i = -\vec{\nabla} U(\vec{r}_i) \) and

\[
f_s(1, 2, \cdots, s, t) = \frac{N!}{(N-s)!} \int \prod_{r=s+1}^{N} d\omega_r \, \rho(1, 2, \cdots, N, t) \quad (2)
\]

where \( \rho(1, 2, \cdots, N, t) \) is phase space density of the total system. One need to approximate the higher order distribution functions \( f_{s+1}, \ (1 \leq s \leq N - 1) \) to obtain a closed set of equations for \( f_s \). Solution of these kinetic equations holds importance in understanding the transport processes in dense gaseous systems. There were recent investigations in this direction e.g., \([3, 4]\), where hierarchy is truncated at \( f_2 \) to derive a model kinetic equation for \( f_1 \). In this context, we propose a new closure scheme for the hierarchy at the level of three particle distribution function \( f_3(1, 2, 3, t) \). The scheme and respective calculation is discussed in the following section.

2. New scheme of closure for hierarchy

From \([1]\), we get for \( s = 1 \) and \( s = 2 \) as

\[
\frac{\partial f_1(1)}{\partial t} + \vec{v}_1 \cdot \vec{\nabla}_{\vec{r}_1} f_1(1) = \int \frac{\partial \phi_{12}}{\partial \vec{r}_1} \cdot \frac{\partial f_2(1, 2)}{\partial \vec{v}_1} \, d^3r_2 \, d^3v_2 \quad (3)
\]

and

\[
\frac{\partial f_2(1, 2)}{\partial t} + \vec{v}_1 \cdot \vec{\nabla}_{r_1} f_2 + \vec{v}_2 \cdot \vec{\nabla}_{r_2} f_2 + \frac{\vec{F}_{12}}{m} \cdot (\vec{\nabla}_{v_1} - \vec{\nabla}_{v_2}) f_2 = \int \left[ \frac{\partial \phi_{13}}{\partial \vec{r}_1} \cdot \frac{\partial f_3(1, 2, 3)}{\partial \vec{v}_1} + \frac{\partial \phi_{23}}{\partial \vec{r}_2} \cdot \frac{\partial f_3(1, 2, 3)}{\partial \vec{v}_2} \right] \, d^3r_3 \, d^3v_3 \quad (4)
\]

respectively, in absence of external forces (\( \vec{F} = 0 \)). The above set of equations is not closed as \( f_3 \) is not known. We approximate \( f_3 \) in terms of its lower order distribution functions,

\[
f_3(1, 2, 3) = f_2(1, 2) \ f_1(1, 3) \ g_2(1, 3) \ g_2(2, 3) \quad (5)
\]

and

\[
f_2(1, 2) = f_1(1) \ f_1(2) \ g_2(1, 2) \ . \quad (6)
\]
From (3) and (2), we get
\[
\frac{\partial f_1(1)}{\partial t} + \vec{v}_1 \cdot \vec{\nabla}_r f_1(1) = \int \frac{\partial \phi_{12}}{\partial \vec{r}_1} \cdot \frac{\partial}{\partial v_1} [f_1(1) f_2(2, 1, 2)] d^3 r_2 d^3 v_2 ,
\]
\[
= \frac{\partial f_1(1)}{\partial v_1} \cdot \int \frac{\partial \phi_{12}}{\partial \vec{r}_1} f_1(2) g_2(1, 2) d^3 r_2 d^3 v_2 +
+ f_1(1) \int \frac{\partial \phi_{12}}{\partial \vec{r}_1} \cdot \frac{\partial g_2(1, 2)}{\partial v_1} f_1(2) d^3 r_2 d^3 v_2 .
\] (7)

The above equation can be rewritten as,
\[
\left[ \frac{\partial}{\partial t} + \vec{v}_1 \cdot \vec{\nabla}_r + \bar{a}^{(1)}_{int}(1) \cdot \frac{\partial}{\partial v_1} \right] \ln(f_1(1)) = (\vec{\nabla}_r^+ \cdot \vec{\nabla}_{v_1^+}) \Phi^{(1)}_{eff}(1^+, 2) ,
\] (8)

where
\[
\bar{a}^{(1)}_{int}(1) = - \int \frac{\partial \phi_{12}}{\partial \vec{r}_1} f_1(2) g_2(1, 2) d^3 r_2 d^3 v_2 \]
(9)
and
\[
\Phi^{(1)}_{eff}(1^+, 2) = \int \phi_{1^+} g_2(1^+, 2) f_1(2) d^3 r_2 d^3 v_2 .
\] (10)

From (4) and (5), we write,
\[
\frac{\partial f_2(1, 2)}{\partial t} + \vec{v}_1 \cdot \vec{\nabla}_r f_2(1, 2) + \vec{v}_2 \cdot \vec{\nabla}_r f_2(1, 2) + \frac{\vec{F}_{12}}{m} \cdot (\vec{\nabla}_{v_1} - \vec{\nabla}_{v_2}) f_2(1, 2) =
\]
\[
= \int [C_1 + C_2] d^5(3)
\] (11)

where
\[
C_1 = \frac{\partial \phi_{13}}{\partial \vec{r}_1} \cdot \frac{\partial}{\partial v_1} [f_2(1, 2) f_1(3) g_2(1, 3) g_2(2, 3)] ,
\]
\[
C_2 = \frac{\partial \phi_{23}}{\partial \vec{r}_2} \cdot \frac{\partial}{\partial v_2} [f_2(1, 2) f_1(3) g_2(1, 3) g_2(2, 3)] ,
\]
and \(d^5(3) = d^3 r_3 d^3 v_3\) respectively. The above equation can be further simplified as,
\[
[S']_{12} \ln(g_2(1, 2)) = - a^{eff}_{int}(1^+ 2) \cdot \vec{\nabla}_{v_1} \ln(f_1(1)) -
- a^{eff}_{int}(12^+) \cdot \vec{\nabla}_{v_2} \ln(f_1(2)) +
+ (\vec{\nabla}_r^+ \cdot \vec{\nabla}_{v_1^+}) \left[ \Psi^{(2)}(1^+ 2) - \Phi^{(1)}_{eff}(1^+ 2) \right] +
+ (\vec{\nabla}_r^+ \cdot \vec{\nabla}_{v_2^+}) \left[ \Psi^{(2)}(12^+) - \Phi^{(1)}_{eff}(12^+) \right] .
\] (12)

Here,
\[
[S']_{12} = \frac{\partial}{\partial t} + \vec{v}_1 \cdot \vec{\nabla}_r + \vec{v}_2 \cdot \vec{\nabla}_r + a^{(2)}_{int}(1^+ 2) \cdot \vec{\nabla}_{v_1} + a^{(2)}_{int}(12^+) \cdot \vec{\nabla}_{v_2} ,
\] (13)
\[
\Psi^{(2)}(1^+ 2) = \int \phi(1^+ 3) g_2(1^+ 3) f_1(3) g_2(2, 3) d^3(3) ,
\] (14)
\[
\Psi^{(2)}(12^+) = \int \phi(2^+ 3) g_2(2^+ 3) f_1(3) g_2(1, 3) d^3(3) ,
\] (15)
BBGKY hierarchy - new truncation scheme

\[ a_{\text{eff}}^{(1+2)} = a_{\text{int}}^{(2)}(1+2) - a_{\text{int}}^{(1)}(1), \]
\[ a_{\text{eff}}^{(12^+)} = a_{\text{int}}^{(2)}(12^+) - a_{\text{int}}^{(1)}(2). \]

where

\[ a_{\text{int}}^{(1+2)} = - \int \frac{\partial \phi_{13}}{\partial \vec{r}_1} f_1(3) \, g_2(1, 3) \, g_2(2, 3) \, d^3(3), \]
\[ a_{\text{int}}^{(12^+)} = - \int \frac{\partial \phi_{23}}{\partial \vec{r}_2} f_1(3) \, g_2(1, 3) \, g_2(2, 3) \, d^3(3). \]

Equations (16) and (17) together form a closed set of equations. A numerical solution of these coupled integro-differential equations can be obtained for a given initial condition on \( f_1 \) and \( g_2 \). Unlike the earlier models [4, 5, 6], velocity and time dependence of \( g_2 \) is retained in the present model. Hence it yields more reliable results of time evolution of \( f_1 \). In the following subsection, we present the total energy conservation succeeded by a discussion on time behavior of Boltzmann’s H-function for the present truncation scheme.

2.1. Conservation of total energy

The time rate of change of local kinetic energy (\( K_{\text{loc}}(\vec{r}) \)) can be calculated as,
\[
\frac{d}{dt} \left( K_{\text{loc}}(\vec{r}_1, t) \right) = \int d^3 v_1 \left( \frac{1}{2} m v_1^2 \right) \, d^3(2) \left\{ \frac{1}{m} \int \left[ \frac{\partial \phi_{13}}{\partial \vec{r}_1} \cdot \frac{\partial f_3}{\partial \vec{v}_1} + \frac{\partial \phi_{23}}{\partial \vec{r}_2} \cdot \frac{\partial f_3}{\partial \vec{v}_2} \right] d^3(3) \right\}. \tag{21}
\]

Upon integrating by parts with respect to \( \vec{v}_1 \) and \( \vec{v}_2 \), assuming \( f_3 \) vanishes at infinite velocities, the above equation results in
\[
\frac{d}{dt} \left( K_{\text{loc}}(\vec{r}_1, t) \right) = - \int d^3 \vec{v}_1 \, d^3(2) \, d^3(3) \left[ \vec{v}_1 \cdot \vec{\nabla}_{r_1} \phi_{13} \right] f_3(1, 2, 3, t). \tag{22}
\]

From the above, we can write,
\[
\frac{d}{dt} (K_{\text{tot}}(t)) = - \int d^3(1) d^3(3) \left[ \vec{v}_1 \cdot \vec{\nabla}_{r_1} \phi_{13} \right] f_2(1, 3, t), \tag{23}
\]
where
\[
K_{\text{tot}}(t) = \int K_{\text{loc}}(\vec{r}, t) \, d^3 r. \tag{24}
\]

Assuming only two-body interactions, the time rate of change of total potential energy can be written as,
\[
\frac{d}{dt} (\Phi_{\text{tot}}(t)) = \frac{1}{2} \int \phi_{12} \, \frac{\partial f_2}{\partial t} \, d^3(1) \, d^3(2), \tag{25}
\]
where
\[
\Phi_{\text{tot}}(t) = \frac{1}{2} \int \phi_{12} \, f_2(1, 2, t) \, d^3(1) \, d^3(2). \tag{26}
\]
is the total potential energy of the system at any instant of time $t$. From (4) and (25), we write
\[
\frac{d}{dt} (\Phi_{\text{tot}}(t)) = \frac{1}{2} \int \phi_{12} \left\{ -[\Theta] f_2 + \int \left( \frac{\partial \phi_{13}}{\partial \bar{r}_1} \frac{\partial \phi_2}{\partial \bar{v}_1} + \frac{\partial \phi_{23}}{\partial \bar{r}_2} \cdot \frac{\partial \phi_3}{\partial \bar{v}_2} \right) d^3(3) \right\} d^3(1) d^3(2) .
\] (27)

where
\[
\Theta = \bar{v}_1 \cdot \bar{\nabla}r_1 + \bar{v}_2 \cdot \bar{\nabla}r_2 + \frac{\bar{F}_{12}}{m} \cdot (\bar{\nabla}v_1 - \bar{\nabla}v_2) .
\] (28)

Upon integrating by parts with respect to $\bar{v}_1$, $\bar{v}_2$, $\bar{r}_1$ and $\bar{r}_2$, assuming the distribution function vanishes at $v = \pm \infty$ and $r = \pm \infty$, we obtain
\[
\frac{d}{dt} (\Phi_{\text{tot}}(t)) = \int d^3(1) d^3(2) (\bar{v}_1 \cdot \bar{\nabla}r_1 \phi_{12}) f_2(1, 2, t) .
\] (29)

Hence, from (23) and (29), we notice that
\[
\frac{d}{dt} (K_{\text{tot}}(t)) = -\frac{d}{dt} (\Phi_{\text{tot}}(t)) ,
\] (30)

and hence the total energy is conserved.

2.2. H-function and time reversibility

We have the Boltzmann’s H-function defined as,
\[
H(t) = \int d^3(1) f_1(1, t) \ln f_1(1, t) .
\] (31)

From (3), the time rate of change of $H(t)$ can be written as,
\[
\frac{dH(t)}{dt} = -\int d^3(1) d^3(2) \left( \bar{\nabla}_r \phi_{12} \cdot \bar{\nabla}_v \ln f_1(1, t) \right) f_2(1, 2, t)
\] (32)
\[
= -\int d^3(1) d^3(2) \left( \bar{\nabla}_r \phi_{12} \cdot \bar{\nabla}_v f_1(1, t) \right) f_1(2, t) g_2(1, 2, t) .
\] (33)

(using (6)) (34)

Now, assuming the density is homogeneous, we can write
\[
g_2(1, 2, t) = g_2(r_{12}, v_{12}, t) ,
\] (35)

where $r_{12} = |\bar{r}_2 - \bar{r}_1|$ and $v_{12} = |\bar{v}_2 - \bar{v}_1|$ respectively. Hence from (33) and (35),
\[
\frac{dH(t)}{dt} = \int d^3r_1 \hat{r}_1 \cdot \int d^3v_1 \hat{v}_1 \frac{\partial f_1(1, t)}{\partial v_1} \left[ I_{12} \right]
\] (36)

where
\[
\left[ I_{12} \right] = \int d^3r_{12} d^3v_{12} f_1(2, t) g_2(r_{12}, v_{12}, t) \frac{\partial \phi_{12}}{\partial r_{12}} .
\] (37)

Since the first integral in (36) is the vector sum of all possible directions, we get
\[
\frac{dH(t)}{dt} = 0 .
\] (38)

Since we have a closed equation for $f_2(1, 2)$, let us define the $H$-function as,
\[
H_2(t) = \int d^3(1) d^3(2) f_2(1, 2, t) \ln f_2(1, 2, t) .
\] (39)
From (4), we can write

$$\frac{dH_2(t)}{dt} = \int d^3(1) \, d^3(2) \, d^3(3) \left[ \nabla_{r_1} \phi_{13} \cdot \nabla_{v_1} f_3 + \nabla_{r_2} \phi_{23} \cdot \nabla_{v_2} f_3 \right] \ln f_2(1, 2) \cdot (40)$$

Upon integrating by parts with respect to $\vec{v}_1$ and $\vec{v}_2$, the above equation becomes

$$\frac{dH_2}{dt} = -\int d^3(1) \, d^3(2) \, d^3(3) \left[ \nabla_{r_1} \phi_{13} \cdot \nabla_{v_1} \ln f_2(1, 2) + \nabla_{r_2} \phi_{23} \cdot \nabla_{v_2} \ln f_2(1, 2) \right] f_3 \cdot (41)$$

From (5) and (6), we get

$$\frac{dH_2}{dt} = -\int d^3(1) \, d^3(2) \, d^3(3) \left[ \nabla_{r_1} \phi_{13} \cdot \nabla_{v_1} \ln f_1(1) + \nabla_{r_2} \phi_{23} \cdot \nabla_{v_2} \ln f_1(2) \right] f_3 \cdot (42)$$

By integrating out the 3rd particle that is not necessary, the above equation reduces to

$$\frac{dH_2}{dt} = -2\int d^3(1) \, d^3(3) \left[ \nabla_{r_1} \phi_{13} \cdot \nabla_{v_1} \ln f_1(1) \right] f_2(1, 3) \cdot (43)$$

Note that the above integral is same as in (32). Hence, from the same argument as before, one can conclude for a homogeneous medium that

$$\frac{dH_2(t)}{dt} = 0 \cdot (44)$$

In the following section we present the case when the two point correlations are independent of velocity and time.

### 2.3. Velocity and time independent correlations

Let us assume that $g_2$ is independent of momentum and time. Then, (8) reduces to

$$\left[ \frac{\partial}{\partial t} + \vec{v}_1 \cdot \nabla_{r_1} + \vec{a}_{int}^{(1)}(1) \cdot \frac{\partial}{\partial \vec{v}_1} \right] \ln(f_1) = 0 \cdot (45)$$

since there is no velocity and time dependence in $g_2$. Hence (45) can be written as,

$$\left[ \frac{\partial}{\partial t} + \vec{v}_1 \cdot \nabla_{r_1} \right] f_1(1) = -\vec{a}_{int}^{(1)}(1) \cdot \frac{\partial}{\partial \vec{v}_1} f_1(1) \cdot (46)$$

where,

$$\vec{a}_{int}^{(1)} = -\int \frac{\partial \phi_{12}}{\partial r_1} f_1(2) g_2(1, 2) \, d^3(2)$$

$$= -\int \frac{\partial \phi_{12}}{\partial r_1} f_1(\vec{r}_2, \vec{v}_2, t) \, g_2(\vec{r}_1, \vec{r}_2) \, d^3(2)$$

$$\vec{a}_{int}^{(1)}(\vec{r}_1, t) = -\int \rho(\vec{r}_2, t) g_2(\vec{r}_1, \vec{r}_2) \, \frac{\partial \phi_{12}}{\partial \vec{r}_1} \, d^3 r_2$$

$$= \vec{a}_{int}^{(m)}(\vec{r}_1, t)$$

In the above, mass density $\rho(\vec{r}, t)$ is defined as,

$$\rho(\vec{r}, t) = \int f_1(\vec{r}, \vec{v}, t) \, d^3 v \cdot (48)$$
and $\tilde{a}^{(m)}_{\text{int}}(\vec{r}_1, t)$ refers to the mean-field force term in the Martys’ kinetic equation, see [4, 5] for more details. Hence if we drop the momentum and time dependence in $g_2$, the first of the coupled equations, (8) reduces to the Martys kinetic equation,

$$\frac{\partial f_1}{\partial t} + \vec{v}_1 \cdot \frac{\partial f_1}{\partial \vec{r}_1} + \tilde{a}_{\text{ext}} \cdot \frac{\partial f_1}{\partial \vec{v}_1} = \Omega_1,$$

From (47) we know that $\Omega_1 = \int \frac{\partial \phi(r_{12})}{\partial \vec{r}_1} \cdot \frac{\partial (f_1(1) f_1(2))}{\partial \vec{v}_1} d\vec{r}_2 d\vec{v}_2$.

$$\Omega_1 = \int \frac{\partial \phi(r_{12})}{\partial \vec{v}_1} \cdot \frac{\partial (f_1(1) f_1(2))}{\partial \vec{v}_1} d\vec{r}_2 d\vec{v}_2$$

$$= \frac{\partial f_1(1)}{\partial \vec{v}_1} \cdot \int \frac{\partial \phi(r_{12})}{\partial \vec{r}_1} f_1(2) g_2(\vec{r}_1, \vec{r}_2, t) d\vec{r}_2 d\vec{v}_2$$

$$= - \frac{\partial f_1(1)}{\partial \vec{v}_1} \cdot \tilde{a}_{\text{int}}(\vec{r}_1, t).$$

The second of the set of coupled equations, (12), becomes

$$\left(\vec{v}_1 \cdot \vec{v}_{\vec{r}_1} + \vec{v}_2 \cdot \vec{v}_{\vec{r}_2}\right) \ln(g_2(1, 2)) =$$

$$= \left(\tilde{a}^{(1)}_{\text{int}}(1) - \tilde{a}^{(2)}_{\text{int}}(1+2)\right) \cdot \vec{v}_1 \ln(f_1(1)) +$$

$$+ \left(\tilde{a}^{(1)}_{\text{int}}(2) - \tilde{a}^{(2)}_{\text{int}}(2+2)\right) \cdot \vec{v}_2 \ln(f_1(2)).$$
In the steady state limit, take \( f_1 \) to be a Maxwellian, i.e., \( f_1 \approx A \exp\left(-\frac{\beta}{2}mv^2\right) \). Now, from (50), (54) and (55), one can show that

\[
\vec{\nabla}_{r_1} \ln g_2(\vec{r}_1, \vec{r}_2) = -\beta \phi_{12} - \beta \rho_0 \int g_2(\vec{r}_1, \vec{r}_3) h_2(r_{23}) \frac{\partial \phi_{12}}{\partial \vec{r}_1} d^3r_3,
\]

where we assume the system is homogeneous, \( \rho(\vec{r}_3) \approx \rho_0 \). The above result is a truncated version of the BGY (Born-Green-Yvon) hierarchy, see [7, 8]. Note that the BGY hierarchy relates \( g_2 \) to \( g_3 \) and so on. But the present scheme is equivalent to writing

\[
g_3(1, 2, 3) \approx g_2(1, 2) g_2(2, 3) g_2(3, 1).
\]

From the above, which is called as “Kirkwood superposition approximation,” [9], the BGY hierarchy reduces to (56).

3. Conclusions

In this paper we propose a new closure scheme for BBGKY hierarchy by approximating \( f_3 \) in terms of its lower order distribution functions and two point correlation functions. This resulted in a set of coupled kinetic equations for \( f_1(1, t) \) and \( g_2(1, 2, t) \). Since the momentum and time dependence of \( g_2 \) is retained, it should provide a more reliable estimate of time evolution of \( f_1 \) compared to earlier models [4, 5, 6]. We have also shown that the present model reduces to [4, 6] for velocity independent correlations. Here, we have shown analytically that the current closure scheme respects time symmetry, i.e.,

\[
\frac{dH(t)}{dt} = 0,
\]

for homogeneous density.

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