Two-phase separated and disperse flow : towards a two-scale diffuse interface model with geometrical variables

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Industrial and scientific interests

$\longrightarrow$ **Study of complex two-phase flows**

[Le Chenadec, 2012]

Industrial applications :

- Liquid fuel injection : consumption, pollutants, ... ,
- Aerospace, propulsion,
- Leakage scenario in water systems of nuclear power plants.

Scientific challenge of the atomization process :

- Multiscale problem,
- Critical droplet size distribution for industrial process,
- Difficulty with DNS : no convergence with mesh refinement [Ling, Fuster & al, 2017], highly dependent on the interface dynamics.

Towards a unified reduced-order model for atomization

Separated phase

Eulerian approach with :

Averaged equations [Ishii, 1984] [Drew, 1988],
Postulated equations [Truesdell, 1969] [Baer & Nunziato, 1986].

Disperse phase

Kinetic based approach [Massot & al, 2010]
or
Lagrangian tracking of the droplets [Zamansky & al, 2014].

The models for separated phase do not degenerate well into the ones adapted to disperse phase.
The models for disperse phase require an initially postulated droplet distribution.

$\longrightarrow$ **How do we unify the two approaches ?**

- Coupling between the two numerical strategies [Le Touze, 2015] [Cordesse & al, 2018],
- First steps towards a unified reduced-order models with sub-scale phenomena [Devassy & al, 2015] : transport of surface area density Σ.

Our goal : A model for the mixed and separated phase using geometric variables Σ, H, G for a sub-scale model which degenerates into a disperse model.

Introduction to Stationary Action Principle

The SAP derives **consistent momentum and energy equations** from a Lagrangian.

$$\mathcal{L} = U - T, \qquad \delta\mathcal{A} = \int_T \int_\Omega \mathcal{L}(y, y', t) dxdt = 0. \tag{1}$$

Example : Euler equations

$$\mathcal{L}(u,\rho) = \frac{1}{2}\rho u^2 - \rho e(\rho).$$
$$\delta\mathcal{A} = \delta\mathcal{A}_u + \delta\mathcal{A}_\rho = 0.$$

$$\partial_t \rho + \nabla \cdot (\rho u) = 0.$$

$$\Rightarrow \begin{cases} \partial_t(\rho u) + \nabla \cdot (\rho u \otimes u) + \nabla(p(\rho)) = 0, \\ \partial_t(E) + \nabla \cdot ((E+p)u) = 0, \end{cases} \tag{2}$$

with $E = \rho u^2 + \rho e(\rho)$.

Barotropic case : the energy holds as the mathematical entropy [Cordesse, 2020].

Derivation of a two-phase model using SAP

Recovering the transport of volumic fraction

Still assuming mass conservation

One-velocity model with α-**dependency**	$\mathcal{L}(u,\rho,\alpha) = \frac{1}{2}\rho u^2 - \rho e(\rho,\alpha).$	No equation on α and $p_1 = p_2$.
With a **sub-scale kinetic** energy	$\mathcal{L}(u,\rho,\alpha,D_t\alpha) = \frac{1}{2}\rho u^2 + \frac{1}{2}\nu(\alpha)(D_t\alpha)^2 - \rho e(\rho,\alpha).$	Additional **“sub-scale” momentum** equation, **System** ruling the dynamics of α and $D_t\alpha$.

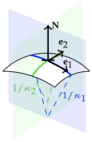
This last sub-scale kinetic energy can be interpreted using the Rayleigh-Plesset's model of a pulsating bubble [Drui, 2017].

$\longrightarrow$ **Let's look for other sub-scale energies depending on α, Σ, H, G.** [Cordesse & al, 2020][Di Battista, 2021]

Introduction and motivation to geometric variables

From a local description of a surface ...

Local main curvatures κ_1, κ_2 give :



$$dS = |e_1 \times e_2|^{\frac{1}{2}},$$
$$H = \frac{1}{2}(\kappa_1 + \kappa_2), \qquad (3)$$
$$G = \kappa_1 \kappa_2.$$

... to a statistical one. [Pope, 1988]

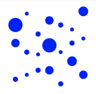
With a Surface Density Function (SDF) $F(x, t, \xi = (H, G, v_I))$:

$$\Sigma = \int F(x,t,\xi)d\xi,$$
$$\Sigma \langle H \rangle = \int HF(x,t,\xi)d\xi, \qquad (4)$$
$$\Sigma \langle G \rangle = \int GF(x,t,\xi)d\xi.$$

With F^d the Discrete SDF (DSDF) [Essadki, 2018],

Number Density Function (NDF) $\overset{DSDF}{\leftrightarrow}$ Averaged geometric variables

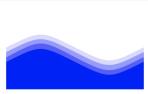
Disperse phase



NDF $n(x,t,\xi) = \frac{G}{4\pi} F^d(x,t,\xi)$

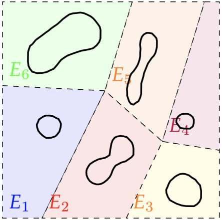
via the Gauss-Bonnet theorem.

Separated phase



SDF represents a non-localized interface.

Introduction and motivation to geometric variables



... to a statistical one. [Pope, 1988]

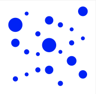
With a Surface Density Function (SDF) $F(x, t, \xi = (H, G, v_I))$:

$$\Sigma = \int F(x, t, \xi) d\xi,$$
$$\Sigma \langle H \rangle = \int HF(x, t, \xi) d\xi, \qquad (5)$$
$$\Sigma \langle G \rangle = \int GF(x, t, \xi) d\xi.$$

With F^d the Discrete SDF (DSDF) [Essadki, 2018],

$$\text{Number Density Function (NDF)} \overset{DSDF}{\leftrightarrow} \text{Averaged geometric variables}$$

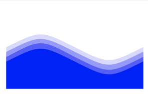
Disperse phase



NDF $n(x, t, \tilde{\xi}) = \frac{G}{4\pi} F^d(x, t, \tilde{\xi})$

via the Gauss-Bonnet theorem.

Separated phase



SDF represents a non-localized interface.

Link with moments of a spherical droplets distribution

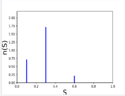
[Essadki, 2018] New phase space $\tilde{\xi} = (\tilde{H}, \tilde{S}, V, \tilde{v}_I)$ through $\tilde{G} = \frac{4\pi}{\tilde{S}}$.

$$
\begin{aligned}
\frac{1}{4\pi}\Sigma\langle G\rangle &= \frac{1}{4\pi}\int \tilde{G}F^d(x,t,\tilde{\xi})d\tilde{\xi} &&= \int n(x,t,\tilde{\xi})d\tilde{\xi} &&= m_0\\
\frac{1}{\sqrt{4\pi}}\Sigma\langle H\rangle &= \frac{1}{\sqrt{4\pi}}\int \frac{1}{\sqrt{\tilde{G}}}\tilde{G}F^d(x,t,\tilde{\xi})d\tilde{\xi} &&= \int \sqrt{\tilde{S}}n(x,t,\tilde{\xi})d\tilde{\xi} &&= m_{1/2}\\
\Sigma &= \int \frac{1}{\tilde{G}}\tilde{G}F^d(x,t,\tilde{\xi})d\tilde{\xi} &&= \int \tilde{S}n(x,t,\tilde{\xi})d\tilde{\xi} &&= m_1\\
6\sqrt{\pi}\alpha &= && 6\sqrt{\pi}\int \frac{4}{3}\pi\left(\frac{\tilde{S}}{4\pi}\right)^{3/2}n(x,t,\tilde{\xi})d\tilde{\xi} &&= m_{3/2}
\end{aligned}
$$

For spherical droplets : $n(x,t,\tilde{\xi}) = \tilde{n}(x,t,\tilde{S},\tilde{v}_I)\delta(\tilde{H}-\tilde{H}_{\tilde{S}}(\tilde{S}))\delta(V-V_{\tilde{S}}(\tilde{S}))$.

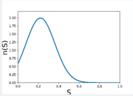
The distribution closure can be :

A quadrature of moments



$$n(S) = \sum_i n_i\delta(S-S_i).$$

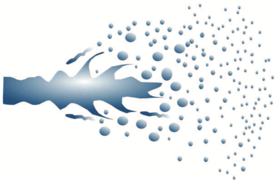
A maximization of entropy



$$n(S_0) = \arg\min(E[n]),$$
$$E[n] = \int n(S)\ln(n(S))dS.$$

Introduction and methodology

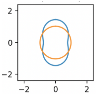
$\longrightarrow$ Goal : Find the right variables to describe a polydisperse distribution of oscillating variables.



The linear model of Rayleigh (1883)

Incompressibility	$\Delta\phi = 0,$
Momentum	$\partial_t \phi + \frac{1}{2}\left\|\nabla\phi\right\|^2 = \frac{1}{\rho}\nabla p,$
Laplace's pressure law	$p = -\sigma H,$
Kinematic closure	$\partial_t R = \partial_r \phi - \frac{1}{R^2}\nabla_S \phi \cdot \nabla_S R.$

$\longrightarrow$ R is harmonic along each spherical mode.



Perturbation along mode Y_2^0 in the same spirit as the TAB model [O'Rourke & Amsden, 1987].

$\longrightarrow$ Similar to [Drui, 2017] and the sub-scale "micro-inertia" of bubble pulsations :

Step 1

Find the right variables through E_k and E_p.

Step 2

Choose $\xi = (S_0, \ldots)$ to link with the NDF.

Step 3

Distribution closure and energies for SAP.

Identification of the variables for the first order dynamic

Formalism of [Plümacher, 2020] on the unit sphere $\mathbb{S}^2$.

Potential energy

$$E_p = \sigma(S - S_0). \qquad (6)$$

Kinetic energy

$$E_k = \frac{1}{2}\rho \int_V \nabla\phi \cdot \nabla\phi dV. \qquad (7)$$

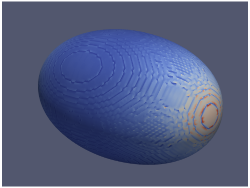
At order 2 :

$$E_p = \frac{1}{2}\sigma f(2) x_2^2 = \frac{1}{2}\rho R_0^3 \omega_2^2 x_2^2,$$
$$E_k = \frac{1}{2}\rho R_0^3 \dot{x}_2^2, \qquad (8)$$

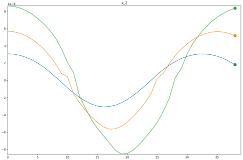
with $\boxed{x_2 = \frac{\langle Y_2^0, R^{(1)} \rangle}{\sqrt{2}}}$, and $R = R_0 + R^{(1)} + R^{(2)} + \ldots$

Then, $\ddot{x}_2 + \omega_2^2 x_2 = 0,$

$$\text{with} \quad \omega_l^2 = \frac{\sigma}{\rho R_0^3} f(l) = \frac{\sigma}{\rho R_0^3} l(l+2)(l-1). \qquad (9)$$



[CORIA - ARCHER]



$x_2(t)$

Identification of the variables for the first order dynamic

Link with geometric variables

Differential geometry

First variations of average geometric quantities [Deserno, 2015]:

$$\delta V = \int_{\mathbb{S}^2} \left[R_0^2 \left(R^{(1)} + R^{(2)} + R^{(3)} \right) + R_0 \left((R^{(1)})^2 + 2R^{(1)}R^{(2)} \right) + \frac{1}{3} R^{(3)} \right] dS,$$

$$\delta S = \int_{\mathbb{S}^2} \left[2R_0 \left(R^{(1)} + R^{(2)} + R^{(3)} \right) + \left((R^{(1)})^2 + 2R^{(1)}R^{(2)} \right) - \frac{1}{2} \left(R^{(1)} \Delta_{\mathbb{S}^2} R^{(1)} + R^{(2)} \Delta_{\mathbb{S}^2} R^{(1)} + R^{(1)} \Delta_{\mathbb{S}^2} R^{(2)} \right) \right] dS. \quad (10)$$

Under incompressibility ($\delta V = 0$), order 2 devlopment and mode 2 perturbation, we obtain :

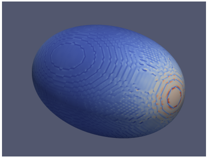
$$x_2^2 = \frac{S - S_0}{2}, \begin{cases} x_2 > 0 \text{ if prolate,} \\ x_2 < 0 \text{ if oblate.} \end{cases} \quad (11)$$

$$\boxed{E_p = \frac{1}{2} 4\sigma \left(\sqrt{S - S_0} \right)^2, \qquad E_k = \frac{1}{2} \frac{\rho R_0^3}{2} \left(\partial_t \left(\sqrt{S - S_0} \right) \right)^2.} \quad (12)$$

x_2 is the right quantity which drives the motion studied in [Cordesse & al, 2020].

DNS validation of the first order model and non-linearity

Measure of geometric variables ($\langle G \rangle$ below) on a droplet DNS using Mercur(v)e[1] [Di Battista, 2021]

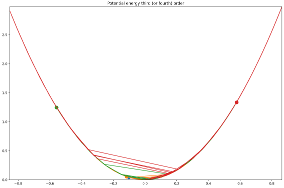


[CORIA - ARCHER]

DNS post-processing of geometric quantities combined with differential geometry tools enable to precisely study non-linear behaviour.

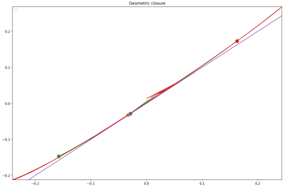
Second order potential energy

$$E_p = \frac{1}{2} 8 x_2^2$$



Geometric closure

$$\tilde{S} - \tilde{S}_0 = f\left(R_0\left(\tilde{S}\tilde{H} - \tilde{S}_0\tilde{H}_0\right)\right)$$



[1] gitlab.com/rubendibattista/mercurve

New distribution variable for droplets oscillations

Extension of M. Essadki's NDF by defining :

$$\tilde{\xi} = \left(\tilde{H}, \tilde{S}_0, \tilde{\psi}, \tilde{v}_l\right), \qquad \text{with} \qquad \tilde{\psi} = \sqrt{\frac{\tilde{S} - \tilde{S}_0}{\tilde{S}_0}}. \qquad (13)$$

For oscillating droplets : $\boxed{n(x, t, \tilde{\xi}) = \bar{n}(x, t, \tilde{S}_0, \tilde{\psi}, \tilde{v}_l)\delta(\tilde{H} - \tilde{H}_{\tilde{S}_0,\tilde{\psi}}(\tilde{S}_0, \tilde{\psi})).}$

Link geometric variables to moments of n :

$$\begin{aligned}
\frac{1}{4\pi}\Sigma\langle G\rangle &= m_{0,0}, \\
\frac{1}{\sqrt{4\pi}}\Sigma\langle H\rangle &= m_{1/2,0} + m_{1/2,2}, \\
\Sigma &= m_1 + m_{1,2}, \\
6\sqrt{\pi}\alpha &= m_{3/2,0}.
\end{aligned}$$

Differential geometry

At order 2,
$\tilde{S} - \tilde{S}_0 = R_0\left(\tilde{S}\tilde{H} - \tilde{S}_0\tilde{H}_0\right)$,
and $\hat{H}(\tilde{S}_0, \tilde{\psi})$ is then explicit.

$\longrightarrow$ Two new moments are available : $m_{1/2,2}$ and $m_{1,2}$.
$\longrightarrow$ When we reach sphericity, $m_{1/2,2}$ and $m_{1,2}$ go to zero and **the model degenerates towards a model of polydisperse spherical droplets**.

Distribution closure and averaged energies

Mono-disperse closure

$$n(S_0,\psi) = n_1\delta(S_0-(S_0)_1)\delta(\psi-\psi_1), \quad (14)$$

3 moments needed :
$m_{0,0}$, $m_{3/2,0}$, $m_{1,2}$.

Poly-disperse closure

$$\begin{aligned} n(S_0,\psi) =& n_1\delta(S_0-(S_0)_1)\delta(\psi-\psi_1) \\ &+ n_2\delta(S_0-(S_0)_2)\delta(\psi-\psi_2), \end{aligned} \quad (15)$$

6 moments needed :
$m_{0,0}$, $m_{1/2,0}$, $m_{1,0}$, $m_{3/2,0}$, $m_{1/2,2}$, $m_{1,2}$.

For the mono-disperse closure,

$$n = m_{0,0}, \quad (S_0)_1 = \left(\frac{m_{3/2,0}}{m_{0,0}}\right)^{2/3}, \quad \psi_1 = \frac{(m_{1,2}^{1/2})}{(m_{0,0})^{1/6}(m_{3/2,0})^{1/3}}. \quad (16)$$

Assuming equi-probable phase within our droplets collection, the potential and kinetic energies read :

$$\boxed{E_{p,coll} = \frac{1}{2}2\sigma\left(\Sigma-\Sigma_0\right), \qquad E_{k,coll} = \frac{3\pi^{3/2}}{8}\rho\frac{\alpha}{\Sigma\langle G\rangle}\left(\partial_t\sqrt{\Sigma-\Sigma_0}\right)^2}. \quad (17)$$

$\longrightarrow$ Subscale energies for the derivation of a reduced-order model with SAP.

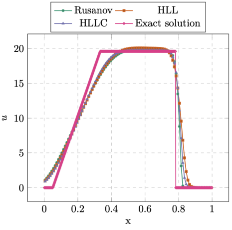
A Finite-Volume solver : Josiepy

Josiepy[2] is a Finite-Volume solver created by R. Di Battista which solves :

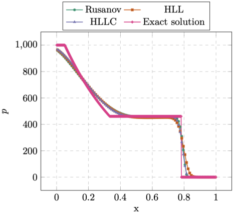
$$\partial_t \mathrm{q} + \nabla \cdot \left(\underline{F}(\mathrm{q}) + \underline{\underline{\underline{D}}}(\mathrm{q}) \cdot \nabla \mathrm{q} \right) + \underline{\underline{B}}(\mathrm{q}) \cdot \nabla \mathrm{q} = \mathrm{s}(\mathrm{q}). \tag{18}$$

Good to know about Josiepy

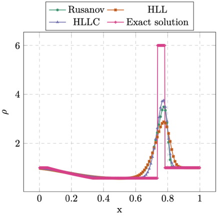
- An open-source solver using Python and the Numpy library,
- Hands-on implementation : a new model requires only to add F, D and B for the state q under scrutiny,
- Classical space schemes (Rusanov, HLL, HLLC, Upwind) and time schemes (Runge-Kutta) are available.



(a) Velocity profile



(b) Pressure profile



(c) Density profile

[2] gitlab.com/rubendibattista/josiepy

Application to a two-phase model with interfacial density

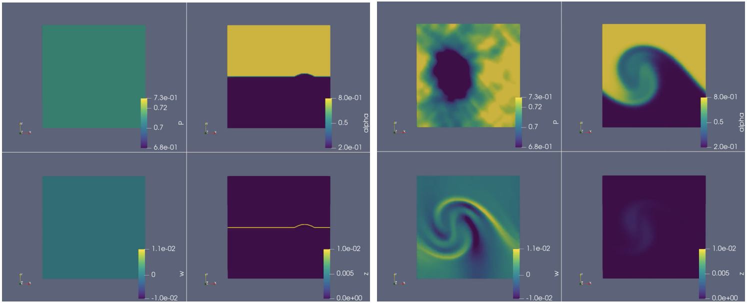
For our targeted model, we would have at most :

$$q = (\alpha\rho_k, \alpha\rho u_k, \alpha\rho e_k, \alpha, \Sigma, \Sigma \langle G \rangle, \Sigma \langle H \rangle, m_{1/2,2}, m_{1,2}), \qquad k = 1, 2. \tag{19}$$

Kelvin-Helmotz instability on a model with interfacial area density [Lhuillier, 2004]

$$\partial_t \Sigma + \nabla \cdot (\Sigma u) = \frac{2}{3}\Sigma \nabla \cdot u + s_\Sigma(x, t, \Sigma). \tag{20}$$

The initial interfacial imperfection within a velocity shear triggers the instability.
(Test-case from [Di Battista, 2021])



From top-left to bottom-right : Pressure, volumic fraction α, $\omega = \frac{D_t\alpha}{\rho Y \Sigma^2}$, $z = \frac{\Sigma^{2/3}}{\rho^{1/2}}$.

Conclusion and perspectives

Conclusion

- Identification of a new variable to describe droplets oscillations with two new corresponding moments $m_{1/2,2}$ and $m_{1,2}$,
- Derivation of kinetic and potential energies for SAP with both mono-disperse and poly-disperse quadratures,
- An efficient environment to study non-linearity with DNS post-processing of geometric variables with Mercur(v)e, differential geometry and computational algebra.

Perspectives

- Derivation of a new set of equations with SAP using the new variable x_2,
  [A. Loison, R. Di Battista, S. Kokh, M. Massot, T. Pichard. *Diffuse interface model for two-phase two-scale flow using stationary action principle, geometrical variables and a finite-volume method*. In preparation]
- Add non-linear dynamics / geometrical closures to the model,
- Development and implementation of specific schemes for Josiepy to stay in the moments space for the kinetic approach (work in collaboration with K. Ait-Ameur),
- Application to model with evaporation (work in collaboration with W. Haegeman, ONERA)
- Investigate exchange terms between large and sub-scale using DNS.
  [A. Loison, S. Kokh, M. Massot, T. Pichard. *Sub-scale modeling for eulerian two-phase flows : analysis of a perturbed droplet using differential geometry*. In preparation]

Non-linear dynamics of the droplet

The next order of the dynamics gives us :

$$E_k = \frac{1}{2}\rho R_0^3 \dot{x}_l{}^2, \qquad \text{and} \qquad E_p = \sigma\left(\frac{f(l)}{2}x_l^2 - \frac{g(l)}{3R_0}x_l^3\right), \tag{21}$$

with $x_l = \epsilon \frac{1}{\sqrt{l^*}} \left\langle Y_{l^*}^{m^*}, R^{(1)} + \epsilon R^{(2)} + \epsilon \frac{l^*+3}{8} \frac{(R^{(1)})^2}{R_0} \right\rangle.$

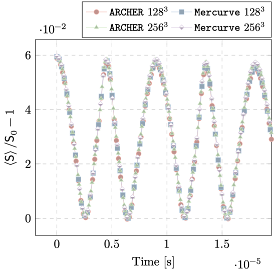
Third order variations of both S and SH give us that :

$$x_l = \sqrt[3]{\frac{3R_0}{h(l^*) - g(l^*)}\left(R_0(S\langle H\rangle - (S\langle H\rangle)_0) - (S - S_0)\right)}. \tag{22}$$

And the dynamic is given by :

$$\ddot{x}_2 + \omega^2 x_2 - \frac{g(2)}{f(2)}\frac{x_2^2}{R_0} = 0. \tag{23}$$

DNS with post-processing to get x_l confirms the same behaviour as the one of the ODE.



$S - S_0$ from [Di Battista, 2021]

Polydisperse closure

Let's use the 6 moments $m_{0,0}$, $m_{1/2,0}$, $m_{1,0}$, $m_{3/2,0}$, $m_{1/2,2}$, $m_{1,2}$, for the quadrature closure :

$$n(S_0,\xi) = n_1\delta(S_0-(S_0)_1)\delta(\xi-\xi_1) + n_2\delta(S_0-(S_0)_2)\delta(\xi-\xi_2). \tag{24}$$

With $\Delta = (m_{0,0}m_{3/2,0} - m_{1,0}m_{1/2,0})^2 - 4(m_{0,0}m_{1,0} - m_{1/2,0}^2)(m_{1/2,0}m_{3/2,0} - m_{1,0}^2)$, we obtain :

$$\begin{aligned} n_1 &= \frac{1}{2}\left(m_{0,0} + \frac{m_{0,0}(m_{1,0}m_{1/2,0} - m_{0,0}m_{3/2,0}) + 2m_{1/2,0}(m_{0,0}m_{1,0} - m_{1/2,0}^2)}{\sqrt{\Delta}}\right), \\ n_2 &= \frac{1}{2}\left(m_{0,0} - \frac{m_{0,0}(m_{1,0}m_{1/2,0} - m_{0,0}m_{3/2,0}) + 2m_{1/2,0}(m_{0,0}m_{1,0} - m_{1/2,0}^2)}{\sqrt{\Delta}}\right), \end{aligned} \tag{25}$$

$$\begin{aligned} (S_0)_1 &= \frac{(m_{0,0}m_{3/2,0} - m_{1,0}m_{1/2,0})\sqrt{\Delta} + (m_{0,0}m_{3/2,0} - m_{1,0}m_{1/2,0})^2 + 2m_{0,0}m_{1,0}^3 - 2m_{1,0}m_{1/2,0}m_{3/2,0}m_{0,0} + 2m_{1/2,0}^3m_{3/}}{2\left(m_{1/2,0}^2 - m_{0,0}m_{1,0}\right)^2} \\ (S_0)_2 &= \frac{(m_{0,0}m_{3/2,0} - m_{1,0}m_{1/2,0})\sqrt{\Delta} + (m_{0,0}m_{3/2,0} - m_{1,0}m_{1/2,0})^2 + 2m_{0,0}m_{1,0}^3 - 2m_{1,0}m_{1/2,0}m_{3/2,0}m_{0,0} + 2m_{1/2,0}^3m_{3/}}{2\left(m_{1/2,0}^2 - m_{0,0}m_{1,0}\right)^2} \end{aligned} \tag{26}$$

And two other expressions using the 6 moments for ξ_1 and ξ_2.

Oscillating model with Hamiltonian mechanics

Given kinetic and potential energies :

$$E_p = \frac{1}{2} 2\sigma \left(\Sigma - \Sigma_0\right), \qquad E_k = \frac{3\pi^{3/2}}{8} \rho \frac{\alpha}{\Sigma \langle G \rangle} \left(\partial_t \sqrt{\Sigma - \Sigma_0}\right)^2. \tag{27}$$

We assumed $\partial_t \alpha = \partial_t(\Sigma \langle G \rangle) = 0$ and we note :

$$m = \frac{3\pi^{3/2}}{4} \rho \frac{\alpha}{\Sigma \langle G \rangle}, \qquad p = m \left(\partial_t \sqrt{\Sigma - \Sigma_0}\right), \qquad q = \sqrt{\Sigma - \Sigma_0}. \tag{28}$$

The hamiltonian : $H = \frac{p^2}{2m} + E_p$, then $\begin{cases} \dot{q} = \partial_p H, \\ \dot{p} = -\partial_q H, \end{cases}$

$$\begin{aligned} \dot{q} &= \frac{p}{m}, \\ \dot{p} &= -2\sigma q, \end{aligned} \tag{29}$$

$$\ddot{q} + \frac{2\sigma}{m} q = 0. \tag{30}$$

We recover the harmonic oscillator.