Title : COSCOM_C - Cooperative Scattering & Optomechanics code (classical model)

Date : 2022-01-11

The code *coscom_c.jl* is a Julia code which simulates cooperative scattering from a classical/thermal gas of atoms, including optomechanical effects. The code solves what are essentially the Bloch equations for each atom in the limit of weak excitation, together with Newton's equations of motion for the atomic position and velocity/momentum.

1. Equations

The coherence of atom j can be described using eq. (4) of [Bachelard, Piovella etc.](#) :

$$\frac{d\beta_j}{dt} = \left(i\Delta - \frac{\Gamma}{2}\right)\beta_j - i\frac{\Omega(\mathbf{r})}{2} - \frac{\Gamma}{2}\sum_{m\neq j} G_{jm}\beta_m$$

where

$$G_{jm} = \frac{\exp(ik|\mathbf{r}_j - \mathbf{r}_m|)}{ik|\mathbf{r}_j - \mathbf{r}_m|}$$

and the force on atom j can be described by

$$\mathbf{F}_j = -\hbar\left(\beta_j \nabla\Omega^* + c.c.\right) + i\frac{\hbar\Gamma}{2}\left(\sum_{m\neq j}\nabla G_{jm}\beta_m\beta_j^* - c.c.\right)$$

where ∇ is understood as differentiating with respect to $\mathbf{r}_j$. As

$$\nabla G_{jm} = \left(\frac{1}{q_{jm}} + \frac{i}{q_{jm}^2}\right)e^{iq_{jm}}k\hat{\mathbf{r}}_{jm}$$

where $q_{jm} = k|\mathbf{r}_j - \mathbf{r}_m|$ and $\hat{\mathbf{r}}_{jm}$ is a unit vector pointing in the direction of $\mathbf{r}_{jm}$. Consequently

$$\mathbf{F}_j = -\hbar(\beta_j\nabla\Omega^* + cc) - \hbar k\Gamma\sum_{m\neq j}\beta_j^*\beta_m\left(\frac{\sin q_{jm}}{q_{jm}} + \frac{\cos q_{jm}}{q_{jm}^2}\right)\hat{\mathbf{r}}_{\mathbf{jm}}.$$

Using the dimensionless variables :

$$X = kx \ , \ Y = ky \ , \ Z = kz \ , \ \mathbf{R} = k\mathbf{r}$$

$$\tau = \Gamma t$$

$$\bar{\Delta} = \frac{\Delta}{\Gamma} \ , \ \bar{\Omega} = \frac{\Omega}{\Gamma}$$

then the above can be written as

$$\frac{d^2\mathbf{R}_j}{d\tau^2} = -\frac{\hbar k^2}{m\Gamma}(\beta_j \bar{\nabla}\bar{\Omega}^* + c.c.) - \frac{\hbar k^2}{m\Gamma}\sum_{m\neq j}\beta_j^*\beta_m\left(\frac{\sin q_{jm}}{q_{jm}} + \frac{\cos q_{jm}}{q_{jm}^2}\right)\hat{\mathbf{r}}_{\mathbf{jm}}$$

and

$$\frac{d\beta_j}{d\tau} = \left(i\bar{\Delta} - \frac{1}{2}\right)\beta_j - i\frac{\bar{\Omega}(\mathbf{r})}{2} - \frac{1}{2}\sum_{m\neq j} G_{jm}\beta_m.$$

As

$$\hat{\mathbf{r}}_{\mathbf{jm}} = \frac{\mathbf{r}_j - \mathbf{r}_m}{|\mathbf{r}_j - \mathbf{r}_m|} = \frac{\mathbf{R}_j - \mathbf{R}_m}{q_{jm}} = \frac{X_j - X_m}{q_{jm}}\hat{\mathbf{i}} + \frac{Y_j - Y_m}{q_{jm}}\hat{\mathbf{j}} + \frac{Z_j - Z_m}{q_{jm}}\hat{\mathbf{k}}$$

then the components can be expressed as

$$\frac{d^2\mathbf{X}_j}{d\tau^2} = -2\bar{\omega}_r(\beta_j\frac{\partial\bar{\Omega}^*}{\partial X} + c.c.) - 2\bar{\omega}_r\sum_{m\neq j}\beta_j^*\beta_m\left(\frac{\sin q_{jm}}{q_{jm}} + \frac{\cos q_{jm}}{q_{jm}^2}\right)\left(\frac{X_j - X_m}{q_{jm}}\right)$$

$$\frac{d^2\mathbf{Y}_j}{d\tau^2} = -2\bar{\omega}_r(\beta_j\frac{\partial\bar{\Omega}^*}{\partial Y} + c.c.) - 2\bar{\omega}_r\sum_{m\neq j}\beta_j^*\beta_m\left(\frac{\sin q_{jm}}{q_{jm}} + \frac{\cos q_{jm}}{q_{jm}^2}\right)\left(\frac{Y_j - Y_m}{q_{jm}}\right)$$

$$\frac{d^2\mathbf{Z}_j}{d\tau^2} = -2\bar{\omega}_r(\beta_j\frac{\partial\bar{\Omega}^*}{\partial Z} + c.c.) - 2\bar{\omega}_r\sum_{m\neq j}\beta_j^*\beta_m\left(\frac{\sin q_{jm}}{q_{jm}} + \frac{\cos q_{jm}}{q_{jm}^2}\right)\left(\frac{Z_j - Z_m}{q_{jm}}\right)$$

where $\bar{\omega}_r = \frac{\hbar k^2}{2m\Gamma}$ is a dimensionless recoil frequency. Defining the dimensionless momentum

$$\mathbf{P} = \frac{m\mathbf{v}}{\hbar k}$$

then the above can be written as a series of 1st order ODEs :

$$\frac{dX}{d\tau} = 2\bar{\omega}_r P_x \quad , \quad \frac{dY}{d\tau} = 2\bar{\omega}_r P_y \quad , \quad \frac{dZ}{d\tau} = 2\bar{\omega}_r P_z,$$

$$\frac{dP_{xj}}{d\tau} = -(\beta_j\frac{\partial\bar{\Omega}^*}{\partial X} + c.c.) - \sum_{m\neq j}\beta_j^*\beta_m\left(\frac{\sin q_{jm}}{q_{jm}} + \frac{\cos q_{jm}}{q_{jm}^2}\right)\left(\frac{X_j - X_m}{q_{jm}}\right)$$

$$\frac{d\mathbf{P}_{\mathbf{y}j}}{d\tau} = -(\beta_j\frac{\partial\bar{\Omega}^*}{\partial Y} + c.c.) - \sum_{m\neq j}\beta_j^*\beta_m\left(\frac{\sin q_{jm}}{q_{jm}} + \frac{\cos q_{jm}}{q_{jm}^2}\right)\left(\frac{Y_j - Y_m}{q_{jm}}\right)$$

$$\frac{d\mathbf{P}_{\mathbf{z}j}}{d\tau} = -(\beta_j\frac{\partial\bar{\Omega}^*}{\partial Z} + c.c.) - \sum_{m\neq j}\beta_j^*\beta_m\left(\frac{\sin q_{jm}}{q_{jm}} + \frac{\cos q_{jm}}{q_{jm}^2}\right)\left(\frac{Z_j - Z_m}{q_{jm}}\right).$$

2. Implementation

- If N is the number of atoms then set up a state vector, sv, consisting of $7N$ elements where e.g.

$$sv[1:N] = X$$

$$sv[N+1:2N] = Y$$

$$sv[2N+1:3N] = Z$$

$$sv[3N+1:4N] = P_x$$

$$sv[4N+1:5N] = P_y$$

$$sv[5N+1:6N] = P_z$$

$$sv[6N+1:7N] = \beta$$

- Initialise sv
- Integrate sv using e.g. RK4 method

3. Cutoff

Equations for the derivatives of $P_{x,y,z}$ and β require evaluation of q_{jm} which is evaluated as

$$q_{jm} = \sqrt{(X_j - X_m)^2 + (Y_j - Y_m)^2 + (Z_j - Z_m)^2}$$

As $q_{jm} \to 0$, it is necessary to introduce a cutoff, ϵ , so that the derivatives do not become singular. This can be done using the method of Plummer e.g. amending the calculation of q_{jm} to

$$q_{jm} = \sqrt{(X_j - X_m)^2 + (Y_j - Y_m)^2 + (Z_j - Z_m)^2 + \epsilon^2}.$$

4. Input parameters

- $\bar{\omega}_r$: Dimensionless recoil frequency ($= \frac{\omega_r}{\Gamma}$)
- $\bar{\Delta}$: Dimensionless detuning ($= \frac{\Delta}{\Gamma}$)
- $\bar{\Omega}$: Dimensionless Rabi frequency ($= \frac{\Omega}{\Gamma}$)
- ϵ : Dimensionless cutoff distance ($= k \times d_{min}$) where d_{min} is the cutoff distance. If $d_{min} = \lambda$, then $\epsilon = 2\pi$.

5. Output files

- positions.dat : Contains t, X, Y
- momenta.dat : Contains t, P_x, P_y