Penning Trap Lagrangian

Adam C. Keith

June 2, 2015

Lagrangian in the lab frame:

$$
\begin{aligned}
L &= \sum_{i=1}^{N}\left[\frac{1}{2}m_i\left(\dot{x}_i^2+\dot{y}_i^2+\dot{z}_i^2\right)-\frac{1}{2}m_i\omega_z^2\left(z_i^2-\frac{x_i^2+y_i^2}{2}\right)-\frac{1}{2}m_i\omega_z^2 GV_w\left[\left(x_i^2-y_i^2\right)\cos 2\omega t-2x_iy_isin2\omega t\right]-\right.\\
&\quad\left.\frac{eB}{2}\left(\dot{x}_iy_i-\dot{y}_ix_i\right)-\frac{ke^2}{2}\sum_{j\neq i}^{N}\frac{1}{r_{ij}}\right] \qquad (1)
\end{aligned}
$$

with $\frac{\omega_z}{2\pi}$ the axial trapping frequency, $\frac{\omega_z}{2\pi}$ the crystal rotation frequency, G a geometrical factor relating trap electrodes, and V_w relating to the strength of the rotating wall potential. Moving to a frame rotating at ω we have the new Lagrangian:

$$
\begin{aligned}
L &= \sum_{i=1}^{N}\left[\frac{1}{2}m_i\left(\dot{x}_i^2+\dot{y}_i^2+\dot{z}_i^2\right)+\frac{1}{2}m_i\left(2\omega-\frac{eB}{m_i}\right)\left(\dot{x}_iy_i-\dot{y}_ix_i\right)-\frac{1}{2}m_i\omega_z^2z_i^2+\right.\\
&\quad\left.\frac{1}{2}m_i\left(\omega^2+\frac{\omega_z^2}{2}-\frac{eB\omega}{m_i}\right)\left(x_i^2+y_i^2\right)-\frac{1}{2}m_i\omega_z^2GV_w\left(x_i^2-y_i^2\right)-\frac{ke^2}{2}\sum_{j\neq i}^{N}\frac{1}{r_{ij}}\right] \qquad (2)
\end{aligned}
$$

with all coordinates in rotating frame. Let's write the characteristic length and time scales as $l_0^3=\frac{ke^2}{\frac{1}{2}m_{Be}\omega_z^2}$ and $t_0=\frac{1}{\omega_z}$ where m_{Be} is the Beryllium ion mass. We also write the cyclotron frequency $\frac{eB}{m_{Be}}=\omega_c\omega_z$ and the rotation frequency as $\omega=\omega_r\omega_z$. With these definitions and substitutions we divide the Lagrangian by $\frac{ke^2}{l_0}$:

$$
\begin{aligned}
L &= \sum_{i=1}^{N}\left[m_i\left(\dot{x}_i^2+\dot{y}_i^2+\dot{z}_i^2\right)+m_i\left(2\omega_r-\frac{\omega_c}{m_i}\right)\left(\dot{x}_iy_i-\dot{y}_ix_i\right)-m_iz_i^2+m_i\left(\omega_r^2+\frac{1}{2}-\frac{\omega_c\omega_r}{m_i}\right)\left(x_i^2+y_i^2\right)-\right.\\
&\quad\left.GV_wm_i\left(x_i^2-y_i^2\right)-\frac{1}{2}\sum_{j\neq i}^{N}\frac{1}{r_{ij}}\right] \qquad (3)
\end{aligned}
$$

with all coordinates in dimensionless form and m_i overloaded as fraction of Beryllium ion mass.

Now we expand the Lagrangian about the equilibrium positions in all variables. We assume at equilibrium all velocities are zero and force a planar structure so that all $z_i=0$. This causes the expanded Lagrangian to separate in to a Lagrangian for the axial direction and one in the plane. For the axial direction,

$$\frac{\partial L}{\partial \dot{z}_\alpha} = -2m_\alpha z_\alpha + \sum_{j\neq\alpha}^{N} \frac{z_\alpha - z_j}{r_{\alpha j}^3} \tag{4}$$

$$\frac{\partial L}{\partial z_\alpha} = 2m_\alpha \dot{z}_\alpha \tag{5}$$

which both vanish at equilibrium as do the partials involving x and z or y and z (or $\dot{z}$). The only partials that don't vanish at equilibrium are

$$\frac{\partial L}{\partial \dot{z}_\beta}\frac{\partial L}{\partial \dot{z}_\alpha} = 2m_\alpha \delta_{\alpha\beta} \tag{6}$$

$$\frac{\partial L}{\partial z_\beta}\frac{\partial L}{\partial z_\alpha} = \delta_{\alpha\beta}\left[-2m_\alpha + \sum_{j\neq\alpha}^{N} \frac{r_{\alpha j}^2 - 3\left(z_\alpha - z_j\right)^2}{r_{\alpha j}^5}\right] - \left(1-\delta_{\alpha\beta}\right)\frac{r_{\alpha\beta}^2 - 3\left(z_\alpha - z_\beta\right)^2}{r_{\alpha\beta}^5} \tag{7}$$

Thus, the expanded Lagrangian in the axial direction is

$$L = \frac{1}{2}\sum_{i=1}^{N} 2m_i \dot{z}_i^2 + \frac{1}{2}\sum_{i,j}^{N} z_i z_j \left(\delta_{ij}\left[-2m_i + \sum_{k\neq i}^{N}\frac{1}{\bar{r}_{ik}^3}\right] - \left(1-\delta_{ij}\right)\frac{1}{\bar{r}_{ij}^3}\right) \tag{8}$$

where z_i is overloaded to be the distance away from equilibrium position and $\bar{r}_{ji}$ is the equilibrium distance between ions.

We now Taylor expand the Lagrangian in x_i, y_i, $\dot{x}_i$, and $\dot{y}_i$. I'll write out all the derivatives explicitly:

$$\frac{\partial L}{\partial x_\alpha} = -m_\alpha\left[2\omega_r - \omega_c\right]\dot{y}_\alpha + 2m_\alpha\left(\omega_r^2 + \frac{1}{2} - \frac{\omega_r\omega_c}{m_\alpha} - GV_w\right)x_\alpha + \sum_{j\neq\alpha}^{N}\frac{x_\alpha - x_j}{r_{\alpha j}^3} \tag{9}$$

$$\frac{\partial L}{\partial y_\alpha} = m_\alpha\left[2\omega_r - \omega_c\right]\dot{x}_\alpha + 2m_\alpha\left(\omega_r^2 + \frac{1}{2} - \frac{\omega_r\omega_c}{m_\alpha} + GV_w\right)y_\alpha + \sum_{j\neq\alpha}^{N}\frac{y_\alpha - y_j}{r_{\alpha j}^3} \tag{10}$$

The above derivatives vanish at equilibrium, by definition. The following two derivatives DO NOT vanish...

$$\frac{\partial L}{\partial \dot{x}_\alpha} = 2m_\alpha \dot{x}_\alpha + m_\alpha\left[2\omega_r - \omega_c\right]y_\alpha \tag{11}$$

$$\frac{\partial L}{\partial \dot{y}_\alpha} = 2m_\alpha \dot{y}_\alpha - m_\alpha\left[2\omega_r - \omega_c\right]x_\alpha \tag{12}$$

$$\begin{aligned}\frac{\partial}{\partial x_\beta}\frac{\partial}{\partial x_\alpha}L \quad &= \quad \delta_{\alpha\beta}\left[2m_\alpha\left(\omega_r^2 + \frac{1}{2} - \frac{\omega_r\omega_c}{m_\alpha} - GV_w\right) + \sum_{j\neq\alpha}^{N}\frac{r_{\alpha j}^2 - 3\left(x_\alpha - x_j\right)^2}{r_{\alpha j}^5}\right] + \\ &\quad - \left(1-\delta_{\alpha\beta}\right)\frac{r_{\alpha\beta}^2 - 3\left(x_\alpha - x_\beta\right)^2}{r_{\alpha\beta}^5}\end{aligned} \tag{13}$$

$$\frac{\partial}{\partial y_\beta}\frac{\partial}{\partial y_\alpha}L \;=\; \delta_{\alpha\beta}\left[2m_\alpha\left(\omega_r^2+\frac{1}{2}-\frac{\omega_r\omega_c}{m_\alpha}+GV_w\right)+\sum_{j\neq\alpha}^{N}\frac{r_{\alpha j}^2-3\left(y_\alpha-y_j\right)^2}{r_{\alpha j}^5}\right]+$$
$$-\left(1-\delta_{\alpha\beta}\right)\frac{r_{\alpha\beta}^2-3\left(y_\alpha-y_\beta\right)^2}{r_{\alpha\beta}^5} \tag{14}$$

$$\frac{\partial}{\partial \dot{x}_\beta}\frac{\partial}{\partial \dot{x}_\alpha}L = 2m_\alpha\delta_{\alpha\beta} \tag{15}$$

$$\frac{\partial}{\partial \dot{y}_\beta}\frac{\partial}{\partial \dot{y}_\alpha}L = 2m_\alpha\delta_{\alpha\beta} \tag{16}$$

$$\frac{\partial}{\partial \dot{x}_\beta}\frac{\partial}{\partial x_\alpha}L = 0 \tag{17}$$

$$\frac{\partial}{\partial \dot{y}_\beta}\frac{\partial}{\partial y_\alpha}L = 0 \tag{18}$$

$$\frac{\partial}{\partial \dot{y}_\beta}\frac{\partial}{\partial x_\alpha}L = -m_\alpha\delta_{\alpha\beta}\left[2\omega_r-\omega_c\right] \tag{19}$$

$$\frac{\partial}{\partial \dot{x}_\beta}\frac{\partial}{\partial y_\alpha}L = m_\alpha\delta_{\alpha\beta}\left[2\omega_r-\omega_c\right] \tag{20}$$

$$\frac{\partial}{\partial y_\beta}\frac{\partial}{\partial x_\alpha}L = \delta_{\alpha\beta}\left[-3\sum_{j\neq\alpha}^{N}\frac{\left(y_\alpha-y_j\right)\left(x_\alpha-x_j\right)}{r_{\alpha j}^5}\right]+\left(1-\delta_{\alpha\beta}\right)3\frac{\left(y_\alpha-y_\beta\right)\left(x_\alpha-x_\beta\right)}{r_{\alpha\beta}^5} \tag{21}$$

Thus the expanded Lagrangian is:

$$L=\frac{1}{2}\sum_{i=1}^{N}2m_i\left(\dot{x}_i^2+\dot{y}_i^2\right)+m_i\left(2\omega_r-\omega_c\right)\left(\dot{x}_i(2\bar{y}_i+y_i)-\dot{y}_i(2\bar{x}_i+x_i)\right)+\frac{1}{2}\mathbf{q}^TV\mathbf{q} \tag{22}$$

where x_i, etc is overloaded to be distance away from equilibrium position $\bar{x}_i$ and $\mathbf{q}$ is appropriate vector of positions to make sense with V as matrix of derivatives (Hessian) (just a convenient way to write all the partials compactly). I do not quite understand the factor of two in front of $\bar{x}$ and $\bar{y}$ but doesn't seem to matter. Here are the planar equations of motion.

$$\ddot{z}_i-\frac{1}{2}\sum_{j=1}^{N}\frac{1}{m_i}z_j\left(\delta_{ij}\left[-2m_i+\sum_{k\neq i}^{N}\frac{1}{\bar{r}_{ik}^3}\right]-\left(1-\delta_{ij}\right)\frac{1}{\bar{r}_{ij}^3}\right)=0 \tag{23}$$

$$\ddot{x}_i+\left(2\omega_r-\omega_c\right)\dot{y}_i-\frac{1}{2}\sum_{j=1}^{N}x_j\frac{V_{ij}^{xx}}{m_i}+x_j\frac{V_{ij}^{xy}}{m_i}=0 \tag{24}$$

$$\ddot{y}_i-\left(2\omega_r-\omega_c\right)\dot{x}_i-\frac{1}{2}\sum_{j=1}^{N}y_j\frac{V_{ij}^{yy}}{m_i}+y_j\frac{V_{ij}^{xy}}{m_i}=0 \tag{25}$$

V_{ij}^{xy} is the second order partial with respect to y_j then x_i.

I will add to this how to get both planar and axial normal modes. Hopefully there were no typos or mistakes above!