Single particle with coordinate q and momentum p moving in a one-dimensional periodic potential[1] of the form:

$$U(q,L) = \frac{m\omega^2 L^2}{4\pi^2}\left[1 - \cos\left(\frac{2\pi q}{L}\right)\right].$$

The partition function in the NPT ensemble is:

$$\mathcal{Z}_{NPT} = \int_0^\infty \mathrm{d}L e^{-\beta PL} \mathcal{Z}_{NVT}.$$

where

$$\mathcal{Z}_{NVT} = \frac{1}{h}\sqrt{2\pi m\beta} \int_0^L \mathrm{d}q e^{-\beta U(q,L)}$$

and

$$\mathcal{Z}_{NPT} = \int_0^\infty \mathrm{d}L e^{-\beta PL} \frac{1}{h}\sqrt{2\pi m\beta} L e^{-\frac{\beta m\omega^2 L^2}{4\pi^2}} I_0\left(\frac{\beta m\omega^2 L^2}{4\pi^2}\right).$$

The length and position distribution functions are:

$$\begin{aligned}
\rho(L) &= \frac{1}{\mathcal{Z}_{NPT}} e^{-\beta PL} \frac{1}{h}\sqrt{2\pi m\beta} L e^{-\frac{\beta m\omega^2 L^2}{4\pi^2}} I_0\left(\frac{\beta m\omega^2 L^2}{4\pi^2}\right) \\
\rho(q) &= \frac{1}{\mathcal{Z}_{NPT}} \frac{1}{h}\sqrt{2\pi m\beta} \int_q^\infty \mathrm{d}L e^{-\beta PL} e^{-\beta U(q,L)} \qquad (1)
\end{aligned}$$

where I_0 is the Bessel functions of the first kind, the length and position distribution functions need to be calculated numerically, for which we study the following physical situation in particular $T = 1$, $P = 1$, $m = 1$, $\omega = 1$, $k_B = 1$ and $h = 1$.

References

[1] Mark E. Tuckerman. *Statistical Mechanics: Theory and Molecular Simulation*. Oxford University Press, first edition, 2010.