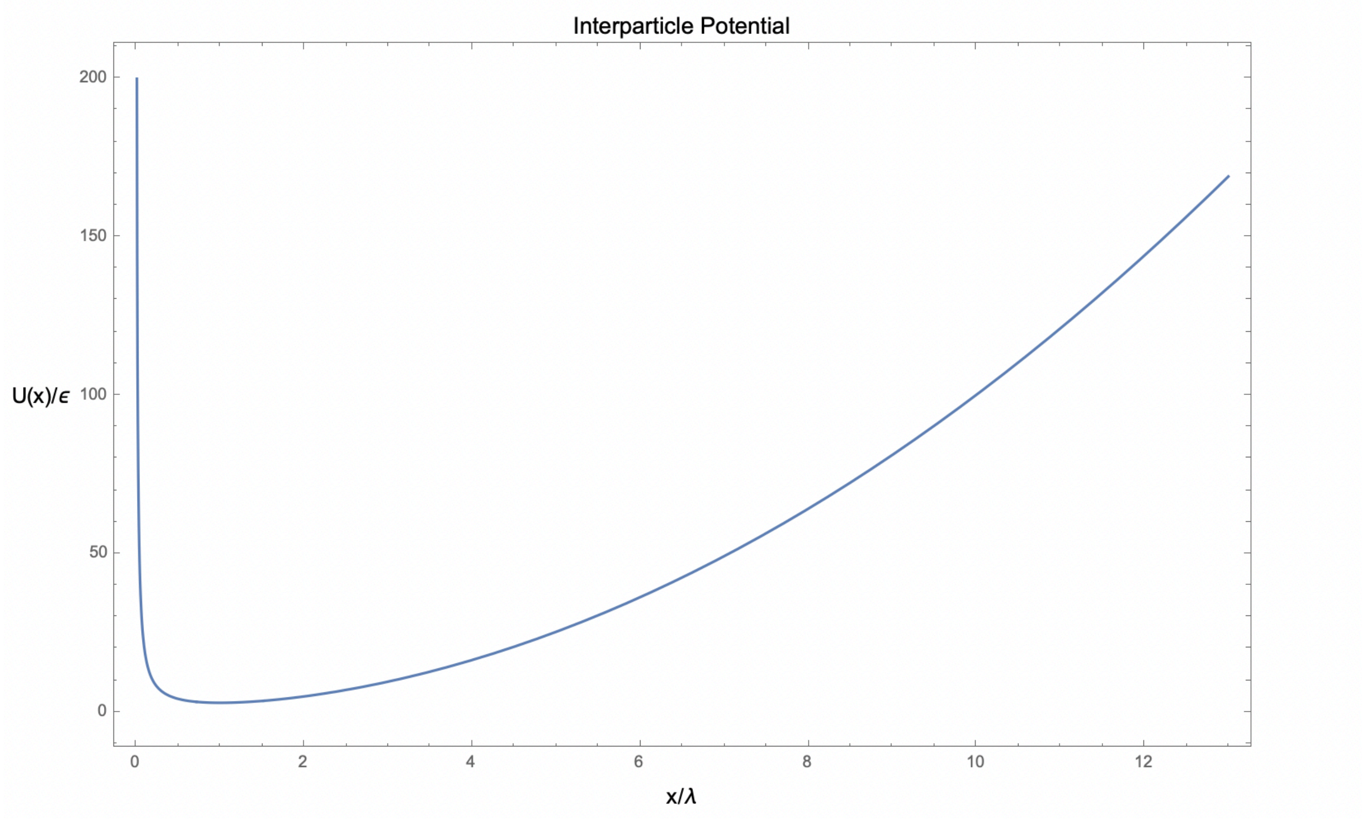
We consider a simple model which exhibits thermal expansion.

Source: Undergrad Stat Mech course

It is known that atoms and molecules tend to attract one another at long distances due to dipole-dipole interactions, and to strongly repel one another at short distances due to Coulomb interactions. A toy model that qualitatively captures these features is the potential energy

$$U(x) = \varepsilon\left(2\frac{\lambda}{x} + \left(\frac{x}{\lambda}\right)^2\right), \quad x > 0$$



We see that at zero temperature, a particle will be found where

$$U'(x) = 0 = -2\varepsilon\lambda/x^2 + 2x\varepsilon/\lambda^2 \iff$$

$$2\varepsilon\lambda^3 = 2\varepsilon x^3 \iff x = \lambda.$$

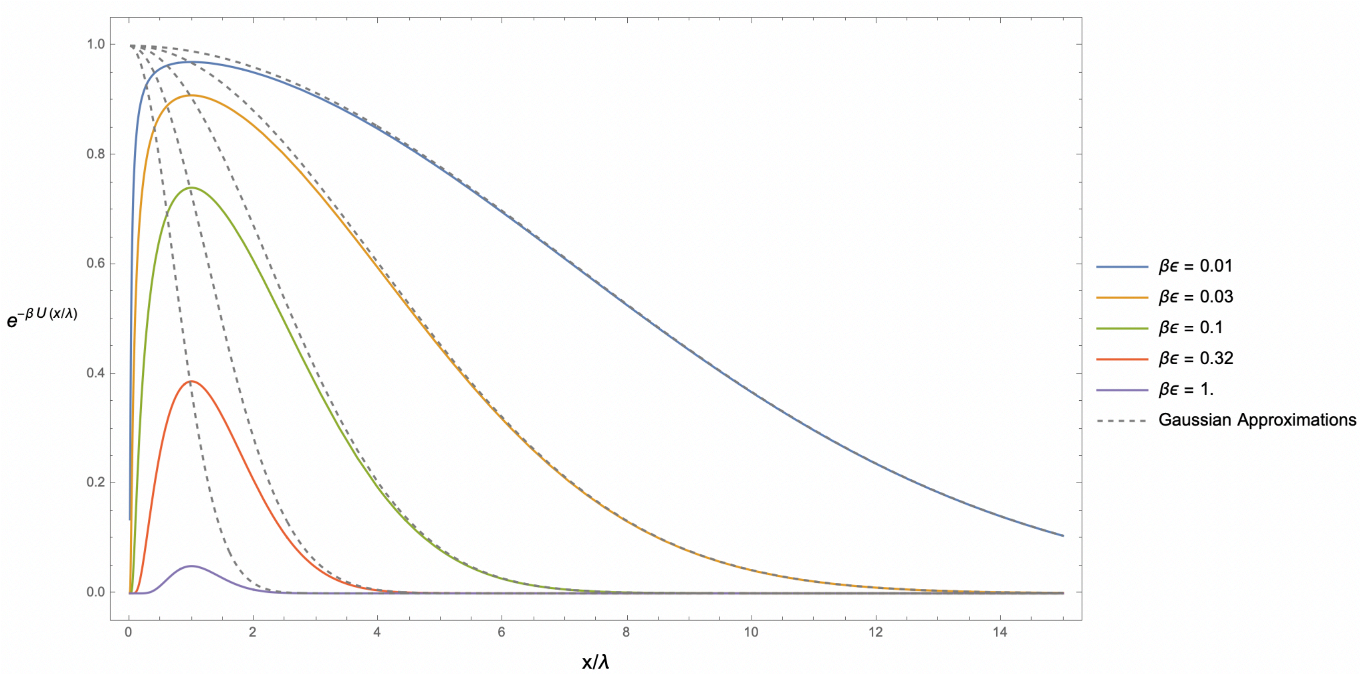
We now compute its average position at finite temperature.

$$\langle x \rangle = \frac{1}{Z}\int_0^\infty x e^{-\beta U(x)}\,dx =$$

$$\int_0^\infty x\, e^{-\beta\varepsilon(2\lambda/x + (x/\lambda)^2)}\,dx \Big/ \int_0^\infty e^{-\beta\varepsilon(2\lambda/x + (x/\lambda)^2)}\,dx$$

We are interested in the high-temperature limit $\beta\varepsilon \ll 1$, which means that for most values of x,

$$e^{-\beta\varepsilon(2\lambda/x + (x/\lambda))^2} \approx e^{-\beta\varepsilon(x/\lambda)^2}$$



Clearly this approximation improves as $\beta\varepsilon \to 0$. It thus follows that

$$\langle x \rangle \approx \lambda^2 \int_0^\infty \left(\frac{x}{\lambda}\right) e^{-\beta\varepsilon (x/\lambda)^2} d(x/\lambda) \Big/ \lambda \int_0^\infty e^{-\beta\varepsilon (x/\lambda)^2} d(x/\lambda)$$

$$= \lambda \int_0^\infty \alpha e^{-\beta\varepsilon\alpha^2} d\alpha \Big/ \int_0^\infty e^{-\beta\varepsilon\alpha^2} d\alpha =$$

$$\lambda \cdot \frac{1}{2\beta\varepsilon} \frac{2\sqrt{\beta\varepsilon}}{\sqrt{\pi}} = \frac{\lambda}{\sqrt{\pi\beta\varepsilon}} = \lambda \sqrt{\frac{T}{\pi\varepsilon k_B}} \implies$$

$$\boxed{\left\langle \frac{x}{\lambda} \right\rangle = \sqrt{\frac{T}{\pi\varepsilon k_B}} \equiv \sqrt{\frac{T}{\pi T_0}}}$$

where we have defined $T_0 = \varepsilon k_B$ to be the natural energy scale of the model. Thus, this model clearly exhibits thermal expansion, as the particle's average position increases with the temperature.