The H atoms in ZrH_2 can be modeled as a one-dimensional harmonic oscillator. Here the force is linear and restorative

$$F(x) = -Cx \tag{1}$$

where C is the force constant and the potential is given by

$$V(x) = -\frac{\mathrm{d}}{\mathrm{d}x}F(x) = \frac{1}{2}m\omega^2 x^2 \tag{2}$$

where

$$C = m\omega^2 \ . \tag{3}$$

The energy of an excitation is

$$E = \hbar\,\omega \ . \tag{4}$$

Q: What is the force constant for the H atom?

The time-independent Schrödinger equation for a particle with the potential given in Equation 2 is

$$-\frac{\hbar^2}{2\,m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\,\psi(x) + \frac{1}{2}m\omega^2\psi(x) = E\psi(x) \ . \tag{5}$$

The allowed values of the energy can be shown to be

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \qquad n = 0, 1, 2, \ldots \tag{6}$$

For $n = 0$ the wavefunction is given by

$$\psi_0(x) = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} e^{-m\omega x^2/(2\hbar)} \ . \tag{7}$$

For a particle in state n, the average value of x^2 may be determined from the wavefunction.

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 |\psi_n(x)|^2 \mathrm{d}x \tag{8}$$

Q: What is the average thermal displacement, $\sqrt{\langle x^2 \rangle}$, of a hydrogen atom in ZrH_2 for $n = 0$? How does this compare to the value of the Debye-Waller factor determined from the exponential fit to the Q-dependence of the elastic line?

Hint:

$$\int_{-\infty}^{\infty} x^{2p} e^{-cx^2} \mathrm{d}x = \frac{1 \cdot 3 \cdot 5 \cdots (2p-1)}{(2c)^p}\sqrt{\frac{\pi}{c}} \tag{9}$$

Useful constants and unit conversions:

$\hbar = \frac{h}{2\pi} = 1.054572\times10^{-34}$ J·s $= 6.582119\times10^{-16}$ eV·s

$\hbar c = 3.1615\times10^{-26}$ J·m $= 197.33$ eV· nm

$m_{\text{neutron}} = 1.6749\times10^{-27}$ kg $= 939.57$ MeV$/c^2$

$c = 2.99792458\times10^{-8}$ m/s^2

1 eV $= 1.6022\times10^{-19}$ J