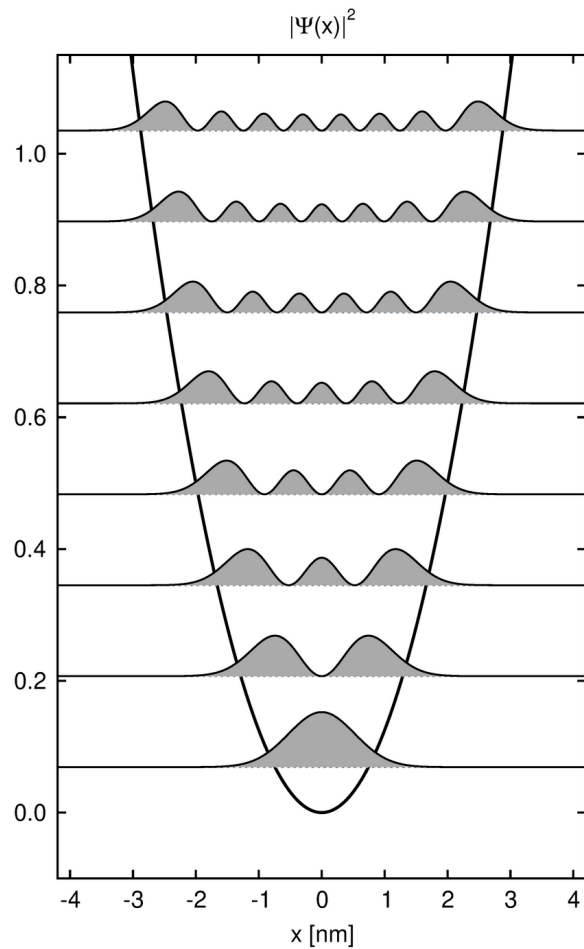
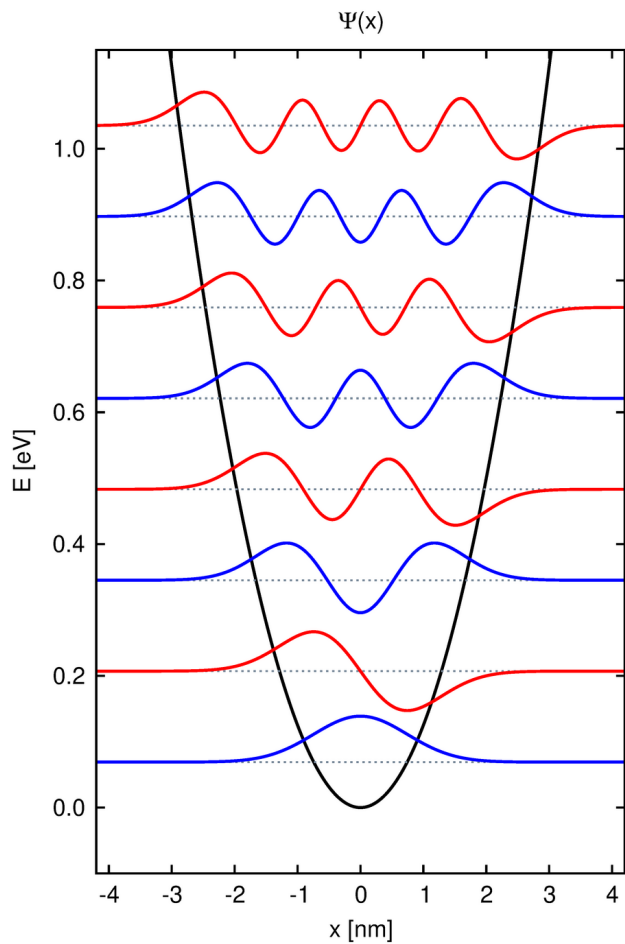


Vlnové funkce vlastních stavů HO



Řešení HO v souřadnicové reprezentaci

$$\Psi_n(\xi) \sim H_n(\xi) e^{-\alpha \xi^2} = \sum_{j=0}^n a_j \xi^j e^{-\alpha \xi^2} \quad \Psi'' = (\xi^2 - \varepsilon) \Psi$$

$$\Psi''(\xi) = \sum_{j=0}^n a_j [4\alpha^2 \xi^{j+2} - 2\alpha(2j+1) \xi^j + j(j-1) \xi^{j-2}] e^{-\alpha \xi^2}$$

$$(\xi^2 - \varepsilon) \Psi = \sum_{j=0}^n a_j (\xi^{j+2} - \varepsilon \xi^j) e^{-\alpha \xi^2}$$

}	a_n	a_{n-1}	a_{n-2}	a_{n-3}	a_{n-4}	a_{n-5}	a_1	a_0				
			a_n	a_{n-1}	a_{n-2}	a_{n-3}	a_3	a_2	a_1	a_0		
					a_n	a_{n-1}	a_5	a_4	a_3	a_2		
}	a_n	a_{n-1}	a_{n-2}	a_{n-3}	a_{n-4}	a_{n-5}	a_1	a_0				
			a_n	a_{n-1}	a_{n-2}	a_{n-3}	a_3	a_2	a_1	a_0		
	ξ^{n+2}	ξ^{n+1}	ξ^n	ξ^{n-1}	ξ^{n-2}	ξ^{n-3}	\dots	ξ^3	ξ^2	ξ^1	ξ^0	

Vlnové funkce vlastních stavů HO

$$\Psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2^n n!}} H_n\left(\sqrt{\frac{m\omega}{\hbar}} x\right) e^{-\frac{m\omega}{2\hbar} x^2}$$

$$E_n = \hbar\omega \left(n + \frac{1}{2}\right)$$

Rodriguesova formule pro H_n

$$H_n(\xi) = (-1)^n e^{\xi^2} \frac{d^n}{d\xi^n} e^{-\xi^2}$$

$$H_5(\xi) = 32\xi^5 - 160\xi^3 + 120\xi$$

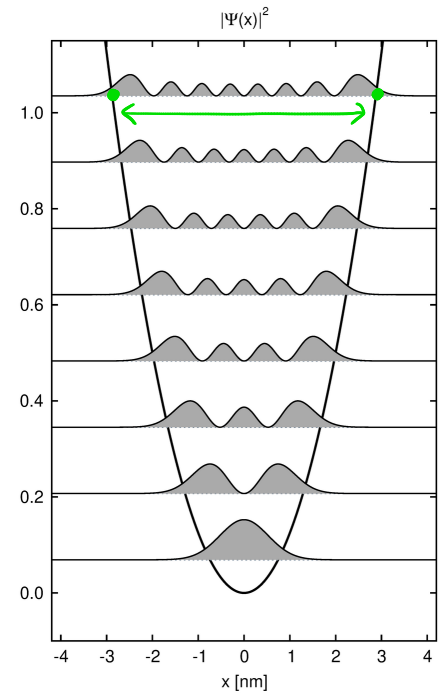
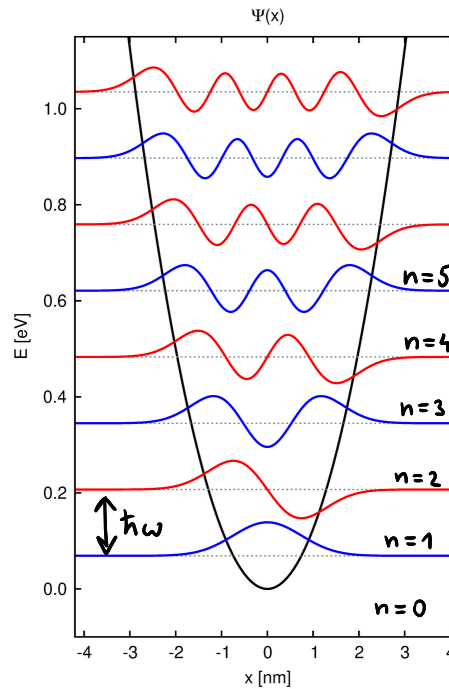
$$H_4(\xi) = 16\xi^4 - 48\xi^2 + 12$$

$$H_3(\xi) = 8\xi^3 - 12\xi$$

$$H_2(\xi) = 4\xi^2 - 2$$

$$H_1(\xi) = 2\xi$$

$$H_0(\xi) = 1$$



Bestiář vlnových funkcí

1.2 Hermitovy polynomy

- prvních několik Hermitových polynomů

$$\begin{aligned}
 H_0(x) &= 1 & H_4(x) &= 16x^4 - 48x^2 + 12 \\
 H_1(x) &= 2x & H_5(x) &= 32x^5 - 160x^3 + 120x \\
 H_2(x) &= 4x^2 - 2 & H_6(x) &= 64x^6 - 480x^4 + 720x^2 - 120 \\
 H_3(x) &= 8x^3 - 12x & H_7(x) &= 128x^7 - 1344x^5 + 3360x^3 - 1680x
 \end{aligned}$$

- rekurenční relace

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x) \quad H'_n(x) = 2nH_{n-1}(x) \quad (7)$$

- Rodriguesova formule

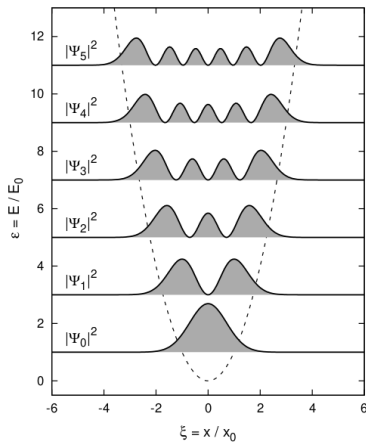
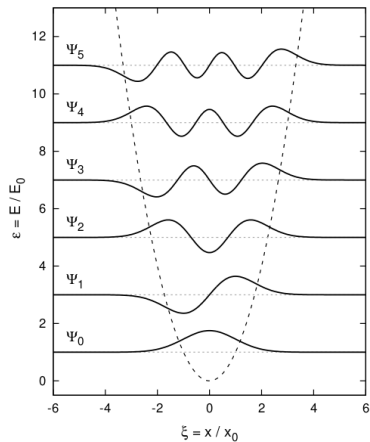
$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2} \quad (8)$$

- ortogonalita Hermitových polynomů

$$\int_{-\infty}^{\infty} H_n(x) H_m(x) e^{-x^2} dx = 2^n n! \sqrt{\pi} \delta_{nm} \quad (9)$$

- Hermitovy polynomy lze získat Taylorovým rozvojem tzv. vytvářející funkce

$$e^{2xt-t^2} = \sum_{n=0}^{\infty} H_n(x) \frac{t^n}{n!} \quad (10)$$



Bestiář (z [latinského](#) *bestiarium* od *bestia* - dravé zvíře, dravec) je kniha nebo její část, obsahující popisy skutečných i mytických zvířat a jiných bytostí.

Harmonická aproximace

$$m_H = 1.674 \cdot 10^{-27} \text{ kg}$$

$$m_{Cl} = 58.9 \cdot 10^{-27} \text{ kg}$$

$$m = \frac{m_H m_{Cl}}{m_H + m_{Cl}} \approx m_H$$

Morseův potenciál

$$V(r) = D(e^{-2\alpha \xi} - 2e^{-\alpha \xi})$$

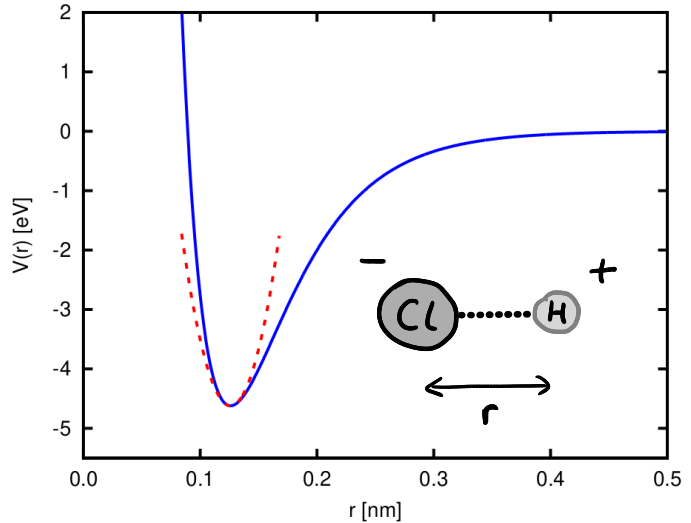
$$\xi = \frac{r-r_0}{r_0}, \quad r_0 = 0.126 \text{ nm}, \quad D = 4.62 \text{ eV}, \quad \alpha = 2.38$$

Taylorův rozvoj v okolí minima

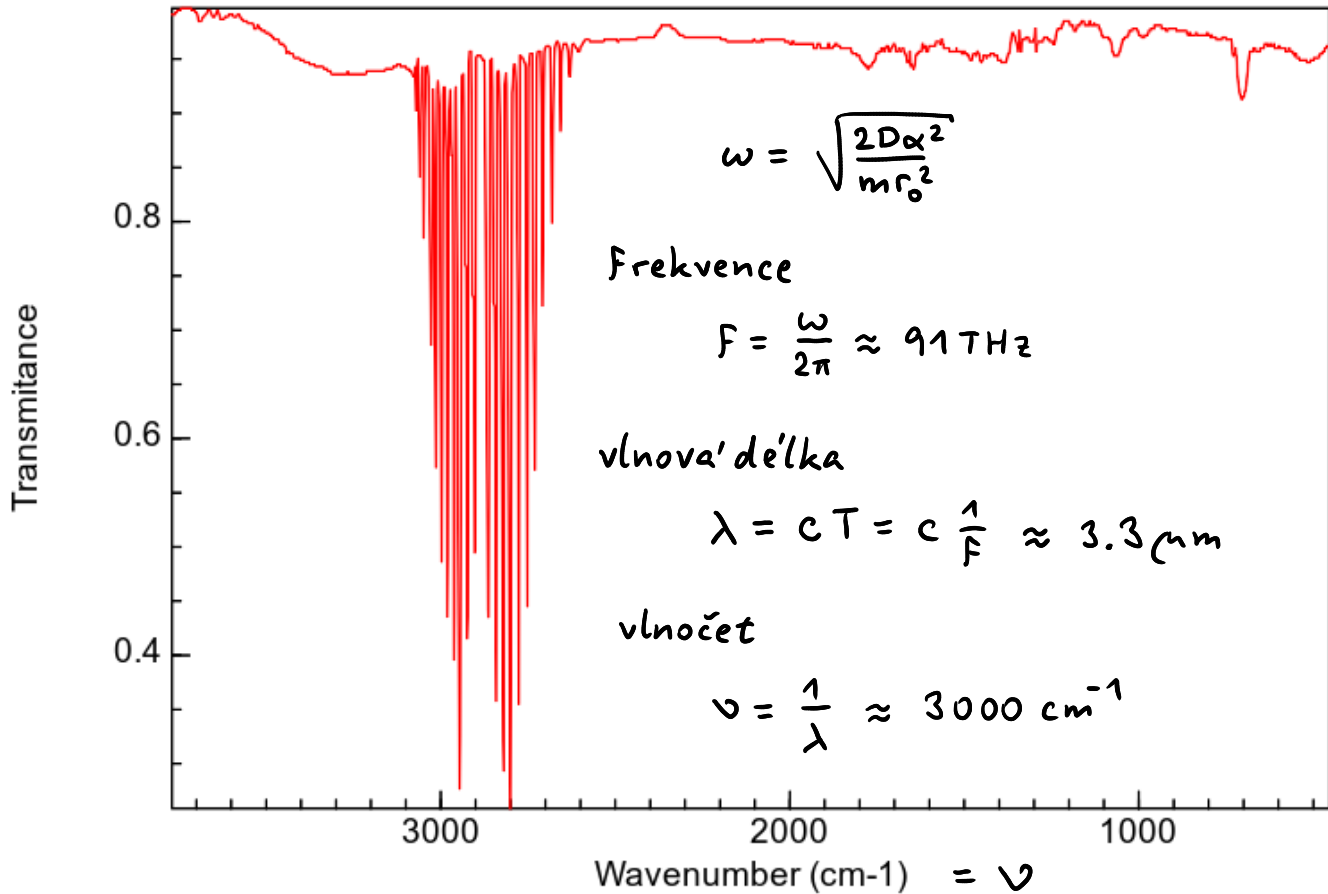
$$V(r) \approx V(r_0) + \frac{dV}{dr} \Big|_{r_0} (r-r_0) + \frac{1}{2} \frac{d^2V}{dr^2} \Big|_{r_0} (r-r_0)^2$$

$$\uparrow \\ v_{\text{minimu}} = 0$$

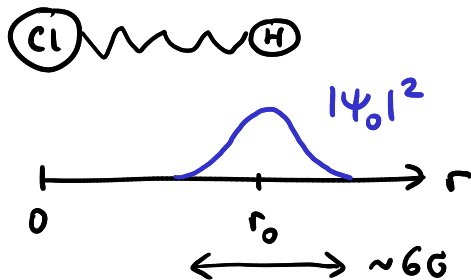
$$\underbrace{\hspace{10em}}_{k = m\omega^2 = \frac{2D\alpha^2}{r_0^2}} \rightarrow \omega = \sqrt{\frac{2D\alpha^2}{m r_0^2}}$$



HYDROGEN CHLORIDE INFRARED SPECTRUM



Nulbodové oscilace

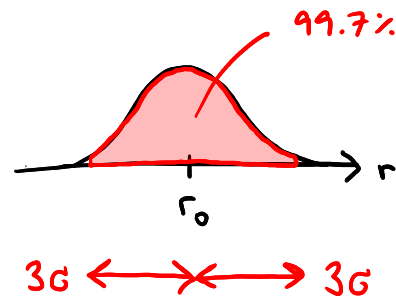
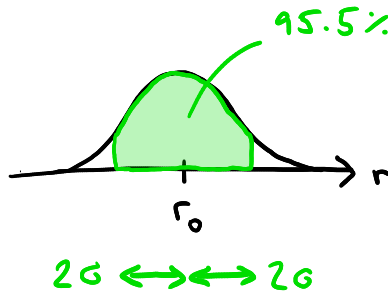
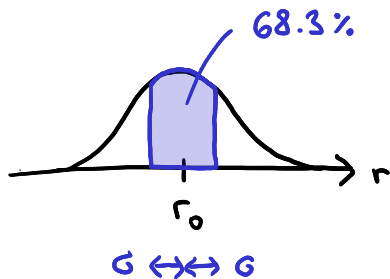


$$\psi_0(r-r_0) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}(r-r_0)^2}$$

$$|\psi_0|^2 \sim e^{-\frac{m\omega}{\hbar}(r-r_0)^2} = e^{-\frac{(r-r_0)^2}{2\sigma^2}}$$

$$\sigma = \sqrt{\frac{\hbar}{2m\omega}} \approx 0.0075 \text{ nm} \approx 6\% r_0$$

s $P = 68\%$ padne vzdálenost H a Cl do intervalu $(r_0 - \sigma, r_0 + \sigma)$



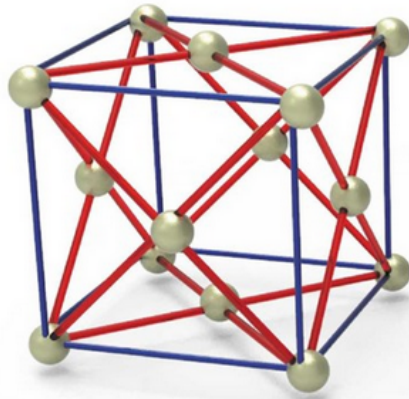
Nulbodové oscilace v krystalech

Lindemannovo kritérium

- krystal roztaje, pokud $\Delta r = \sqrt{\langle (r - r_0)^2 \rangle}$ překročí 10-15% r_0 , kde r_0 je vzdálenost sousedních atomů

$$\sim \frac{1}{\sqrt{m\omega}} \sim m^{-\frac{1}{4}} \quad \omega \sim \frac{1}{\sqrt{m}}$$

2	He Helium		
9	F Fluorine	10	Ne Neon
17	Cl Chlorine	18	Ar Argon
35	Br Bromine	36	Kr Krypton
53	I Iodine	54	Xe Xenon
85	At Astatine	86	Rn Radon
117	Ts Tenness...	118	Og Oganess...



Ne Ar Kr Xe
Face-centered cubic (fcc)

Lennard-Jonesův potenciál

$$V_{LJ}(r) = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right]$$

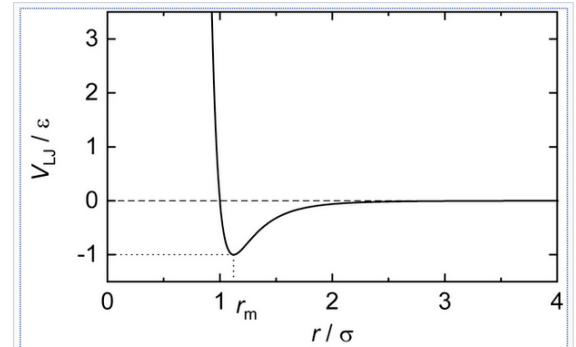
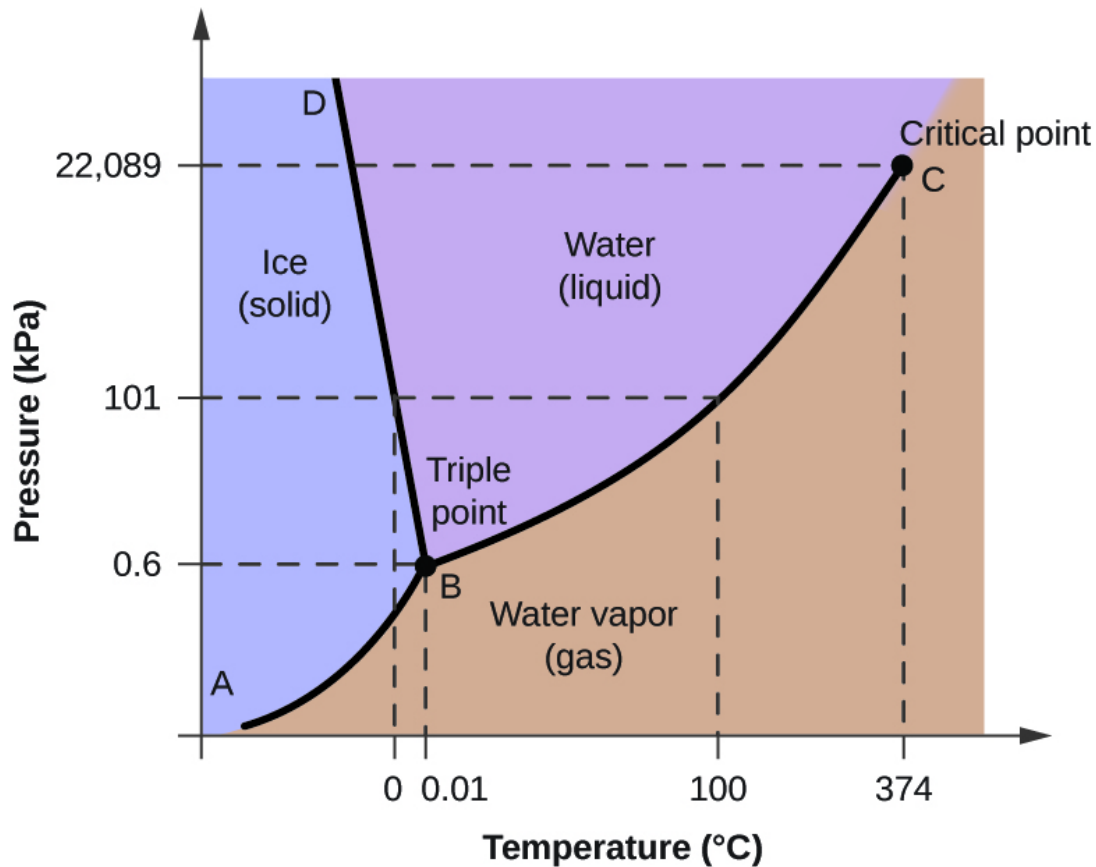
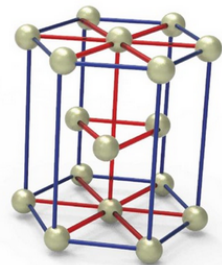
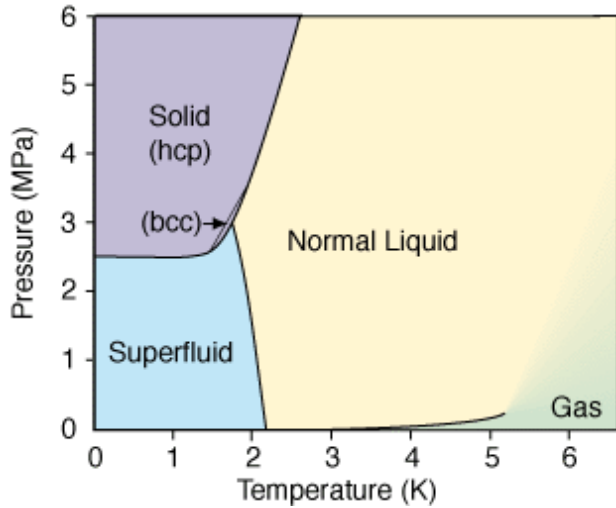


Figure 1. Graph of the Lennard-Jones potential V_{LJ} function: Intermolecular potential energy V_{LJ} as a function of the distance of a pair of particles. The potential minimum is at $r = r_{\min} = 2^{1/6}\sigma$.

Fázové diagramy

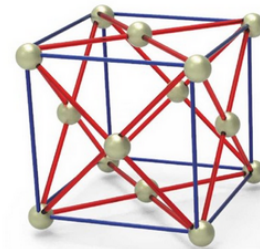
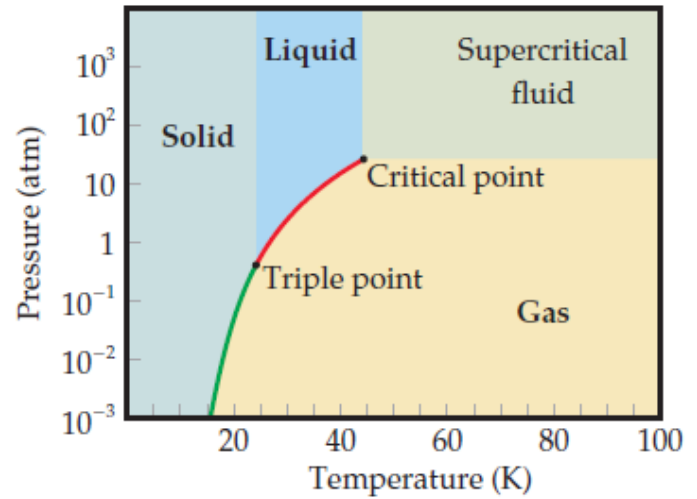


${}^4\text{He}$



He Be Mg
Hexagonal close-packed (hcp)

Ne



Ne Ar Kr Xe
Face-centered cubic (fcc)