量子力学 第9回レポート [redacted] (ほそく)

$\boxed{Z: 分配関数}$

$$P(E_m) = \frac{1}{Z} \exp\left(-\frac{E_n}{k_BT}\right)$$

エネルギーは k_BT に比例する.

分配関数

$$Z = \underbrace{\sum_{n=0}^{\infty} \exp\left(-\frac{(n+\frac{1}{2})\hbar\omega}{k_BT}\right)}_{\exp\left(-\frac{n\hbar\omega}{k_BT}\right)\exp\left(-\frac{\hbar\omega}{2k_BT}\right)}$$

$$= \exp\left(-\frac{\hbar\omega}{2k_BT}\right) \underbrace{\sum_{n=0}^{\infty} \exp\left(-\frac{n\hbar\omega}{k_BT}\right)}_{\frac{1}{1-\exp\left(-\frac{\hbar\omega}{k_BT}\right)}}$$

$$\boxed{Z = \frac{\exp\left(-\frac{\hbar\omega}{2k_BT}\right)}{1-\exp\left(-\frac{\hbar\omega}{k_BT}\right)}}$$

分配関数

$$\nu = \frac{1}{2\pi}\sqrt{\frac{k}{\mu}}$$

$|m\rangle$ をとる確率

$$P(E_m) = \frac{1}{Z} \exp\left(-\frac{E_n}{kT}\right)$$

$$= e^{\hbar\omega/2kT}\left(1 - e^{-\hbar\omega/kT}\right) \cdot e^{-\frac{E_m}{kT}}$$

$h\nu$

基底状態

$$\boxed{P(E_0) = 1 - e^{-\hbar\omega/kT}}$$

前提条件

h

$$\boxed{\hbar = \frac{h}{2\pi}[}$$

rad/s rad

$$[h\nu[1/s] = E]$$

〈2原子分子の並進と振動〉

$$\hat{H}\Psi(x_G, x) = E\Psi(x_G, x)$$

$$\left[-\frac{\hbar^2}{2M}\cdot\frac{d^2}{dx_G^2} - \frac{\hbar^2}{2\mu}\frac{d^2}{dx^2} + V(x - x_0)\right]\Psi(x_G, x) = E\Psi(x_G, x)$$

$$\left[-\frac{\hbar^2}{2M}\cdot\frac{d^2}{dx_G^2} - \frac{\hbar^2}{2\mu}\cdot\frac{d^2}{dx^2} + V(x - x_0)\right]\phi(x_G)\varphi(x) = E\phi(x_G)\varphi(x)$$

$$-\frac{\hbar^2}{2M}\cdot\frac{d^2}{dx_G^2}\cdot\underline{\phi(x_G)}\,\varphi(x) - \frac{\hbar^2}{2\mu}\cdot\frac{d^2}{dx^2}\cdot\phi(x_G)\cdot\varphi(x) + V(x - x_0)\cdot\phi(x_G)\varphi(x)$$

$$= E\underline{\phi(x_G)}\,\varphi(x)$$

両辺を $\phi(x_G)\ \varphi(x)$ でわると

$$-\frac{\hbar^2}{2M}\frac{1}{\phi(x_G)}\frac{d^2}{dx_G^2}\phi(x_G) - \frac{\hbar^2}{2\mu}\cdot\frac{1}{\varphi(x)}\frac{d^2}{dx^2}\varphi(x) + V(x - x_0) = E$$

〈2原子分子の並進と振動〉

前提
(S.E = シュレディンガーの式)