

$$\int_{-\infty}^{\infty} dt \left\{ \frac{1}{2m} \left[-\frac{i\hbar}{\alpha} \frac{\delta}{\delta \chi(t)} - m \frac{d\chi(t)}{dt} \right]^2 - \frac{m}{2} \left[\frac{d\chi(t)}{dt} \right]^2 \right\} \Phi[\chi] = 0$$

離散化

$$\sum_{k=-\infty}^{\infty} \varepsilon \left\{ \frac{1}{2m} \left(-\frac{i\hbar}{\alpha} \frac{1}{\varepsilon} \frac{\partial}{\partial \chi(k\varepsilon)} - m \frac{\chi(k\varepsilon+\varepsilon) - \chi(k\varepsilon)}{\varepsilon} \right)^2 - \frac{m}{2} \left[\frac{\chi(k\varepsilon+\varepsilon) - \chi(k\varepsilon)}{\varepsilon} \right]^2 \right\} \Phi(\dots, \chi(\varepsilon), \chi(2\varepsilon), \dots) = 0$$

ハミルトニアン

$$H(p; x) = Q \phi(x) + [1/(2M)] \sum_k [p^k - QA^k(x)]^2$$

$$x^k \equiv \chi(k\varepsilon)$$

$$M = m\varepsilon\alpha^2, Q = m;$$

$$A^k(x) = \alpha(x^{k+1} - x^k),$$

$$\phi(x) = -[1/(2\varepsilon)] \sum_k (x^{k+1} - x^k)^2$$

正準方程式

$$\frac{dx^j}{d\tau} = \frac{\partial H}{\partial p^j}$$

$$\frac{dx^j}{d\tau} = \frac{1}{M} [p^j - QA^j(x)]$$

$$t = j\varepsilon$$

$$\frac{dp^j}{d\tau} = -\frac{\partial H}{\partial x^j}$$

$$\frac{dp^j}{d\tau} = -Q \partial_j \phi(x) + \frac{Q}{M} \sum_k [p^k - QA^k(x)] \partial_j A^k(x)$$

$$\frac{d^2 x^j}{d\tau^2} = \frac{1}{\varepsilon\alpha} \left[\frac{dx^{j-1}}{d\tau} - \frac{dx^{j+1}}{d\tau} \right] + \frac{2}{\varepsilon^2\alpha^2} \left[x^j - \frac{1}{2}(x^{j-1} + x^{j+1}) \right]$$