

Равенство Яржинского (Jarzynski), 1997

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$$\vec{z} = (\vec{q}, \vec{p})$$

$$H(\vec{z}, \lambda_t) = H_0(\vec{z}) - \lambda_t Q(\vec{z})$$

$$\rho_0(\vec{z}_0) = e^{-\beta H_0(\vec{z}_0)} / Z_0, \quad Z_0 = \int d\vec{z}_0 e^{-\beta H_0(\vec{z}_0)}$$

Работа: $W[\vec{z}_0, \lambda] = H(\vec{z}_\tau, \lambda_\tau) - H(\vec{z}_0, \lambda_0)$

$$\dot{q}_t = \frac{\partial H(\vec{z}_t, \lambda_t)}{\partial p}$$

$$W[\vec{z}_0, \lambda] = \int_0^\tau dt \dot{\lambda}_t \frac{\partial H(\vec{z}_t, \lambda_t)}{\partial \lambda_t} = - \int_0^\tau dt \dot{\lambda}_t Q_t$$

$$\dot{p}_t = - \frac{\partial H(\vec{z}_t, \lambda_t)}{\partial q}$$

Теорема

$$\langle e^{-\beta W} \rangle_\lambda = e^{-\beta \Delta F}$$

$$\Delta F = -\beta^{-1} \ln \frac{Z(\lambda_\tau)}{Z(\lambda_0)}$$

$$Z(\lambda_\tau) = \int d\vec{z} e^{-\beta H(\vec{z}, \lambda_\tau)}$$

$$\langle e^{-\beta W} \rangle_\lambda = \int e^{-\beta W[\vec{z}_0, \lambda]} \rho(\vec{z}_0) d\vec{z}_0 \geq e^{-\beta \int W \rho(\vec{z}) d\vec{z}}$$

Следствие

$$\langle W \rangle \geq \Delta F$$

$$\leftarrow e^{-\beta \langle W \rangle} \leq e^{-\beta \Delta F}$$

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