Лекция 14

Кинетика квантовых систем (часть 2)

Уравнение Линблада для наблюдаемых

$$\langle F_A \rangle_{\rho_A} = \mathbf{Tr}\left(\hat{\rho}_A^{(S)}(t)\ \hat{F}_A^{(S)}\right) = \mathbf{Tr}\left(\hat{\rho}_{A\,0}\ \hat{F}_A^{(H)}(t)\right).$$

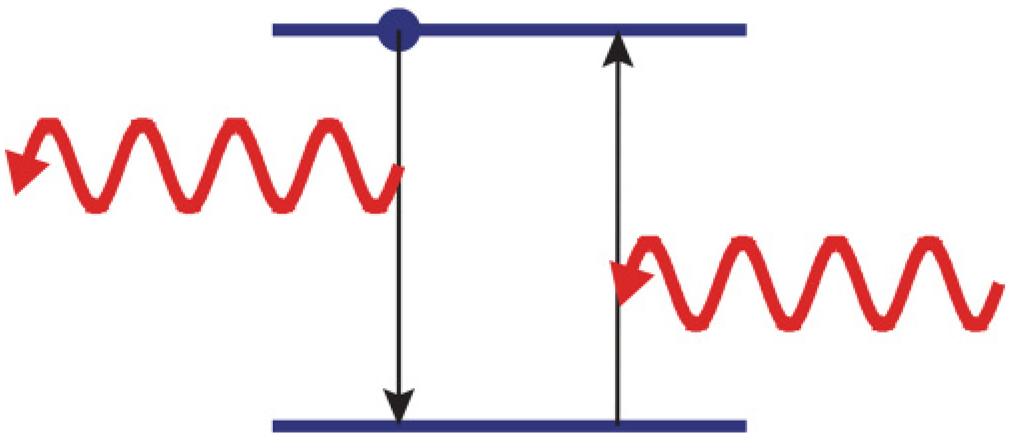
$$\hat{F}_A^H(t) = \hat{M}_k^+(t)\hat{F}_A\hat{M}_k(t),$$

$$\hat{\rho}_A^{(S)}(t) = \hat{M}_k(t)\hat{\rho}_A^{(S)}\hat{M}_k^+(t).$$

$$\frac{d}{dt}\hat{\rho}_A^S = \frac{1}{i\hbar}\left[\hat{H},\hat{\rho}_A^S\right] + L_k\hat{\rho}L_k^+ - \frac{1}{2}\left\{L_k^+L_k,\hat{\rho}\right\},$$

$$\frac{d}{dt}\hat{F}_A^H(t) = \frac{\partial}{\partial t}\hat{F}_A^H(t) - \frac{1}{i\hbar}\left[\hat{H},\hat{F}_A^H(t)\right] + L_k^+\hat{F}_A^H(t)L_k - \frac{1}{2}\left\{L_kL_k^+,\hat{F}_A^H(t)\right\}.$$

Пример: двухуровневая система



$$\frac{d}{dt}\hat{\rho} = \frac{1}{i\hbar}\left[\hat{H},\hat{\rho}\right] + L_k\hat{\rho}L_k^+ - \frac{1}{2}\left\{L_k^+L_k,\hat{\rho}\right\} = \frac{1}{i\hbar}\left[\varepsilon_0\hat{\sigma}^+\hat{\sigma}^-,\hat{\rho}\right] + \gamma\left(\hat{\sigma}^-\hat{\rho}\hat{\sigma}^+ - \frac{1}{2}\left\{\hat{\sigma}^+\hat{\sigma}^-,\hat{\rho}\right\}\right),$$

$$\hat{\sigma}^+ = \left|1\right\rangle\left\langle 0\right|, \hat{\sigma}^- = \left|0\right\rangle\left\langle 1\right|, \hat{\sigma}^+\hat{\sigma}^- = \left|1\right\rangle\left\langle 1\right|, \ldots$$

Преобразование во «вращающуюся» систему координат…

$$\hat{\rho} \to e^{-i\hat{H}t/\hbar}\hat{\rho}e^{i\hat{H}t/\hbar},$$

$$\frac{d}{dt}\hat{\rho} = \gamma\left(\hat{\sigma}^-(t)\hat{\rho}\hat{\sigma}^+(t) - \frac{1}{2}\left\{\hat{\sigma}^+(t)\hat{\sigma}^-(\mathrm{t}), \hat{\rho}\right\}\right),$$

$$\hat{\sigma}^+(t) = e^{i\hat{H}t/\hbar}\left|1\right\rangle\left\langle 0\right|e^{-i\hat{H}t/\hbar},$$

$$\frac{\partial}{\partial t}\hat{\sigma}^+(t) = \frac{i}{\hbar}e^{i\hat{H}t/\hbar}\left[\hat{H}, \hat{\sigma}^+\right]e^{-i\hat{H}t/\hbar} = \frac{i}{\hbar}e^{i\hat{H}t/\hbar}\left[\varepsilon_0\hat{\sigma}^+\hat{\sigma}^-, \hat{\sigma}^+\right]e^{-i\hat{H}t/\hbar} = \frac{i}{\hbar}\varepsilon_0\hat{\sigma}^+(t),$$

$$\hat{\sigma}^+(t) = e^{\frac{i}{\hbar}\varepsilon_0 t}\hat{\sigma}^+, \hat{\sigma}^-(t) = e^{-\frac{i}{\hbar}\varepsilon_0 t}\hat{\sigma}^-.$$

$$\Downarrow$$

$$\frac{d}{dt}\hat{\rho} = \gamma\left(\hat{\sigma}^-\hat{\rho}\hat{\sigma}^+ - \frac{1}{2}\left\{\hat{\sigma}^+\hat{\sigma}^-, \hat{\rho}\right\}\right).$$

$$\frac{d}{dt}\hat{\rho} = \gamma\left(\hat{\sigma}^{-}\hat{\rho}\hat{\sigma}^{+} - \frac{1}{2}\left\{\hat{\sigma}^{+}\hat{\sigma}^{-}, \hat{\rho}\right\}\right).$$

$$\rho(t) = a(t)\left|0\right\rangle\left\langle 0\right| + b(t)\left|0\right\rangle\left\langle 1\right| + b^*(t)\left|1\right\rangle\left\langle 0\right| + c(t)\left|1\right\rangle\left\langle 1\right|, \tag{12}$$

with $\left|0\right\rangle$ being the ground state, $\left|1\right\rangle$ being the excited state and $a(t) + c(t) = 1 \quad \forall t$. $\sigma_- = \left|0\right\rangle\left\langle 1\right|$ and $\sigma_+ = \left|1\right\rangle\left\langle 0\right|$. We have assumed that there is no free Hamiltonian for the system ($h_0^S + h_{LS}^S = 0$) for simplicity.

We can explicitly solve this master equation by evaluating the right hand side for a general $\rho(t) = \begin{pmatrix} a(t) & b(t) \\ b^*(t) & c(t) \end{pmatrix}$:

$$\begin{aligned} \begin{pmatrix} \dot{a}(t) & \dot{b}(t) \\ \dot{b}^*(t) & \dot{c}(t) \end{pmatrix} &= \gamma\left(\begin{pmatrix} c(t) & 0 \\ 0 & 0 \end{pmatrix} - \frac{1}{2}\begin{pmatrix} 0 & 0 \\ b^*(t) & c(t) \end{pmatrix} - \frac{1}{2}\begin{pmatrix} 0 & b(t) \\ 0 & c(t) \end{pmatrix}\right) \\ &= \begin{pmatrix} \gamma c(t) & -\frac{\gamma}{2}b(t) \\ -\frac{\gamma}{2}b^*(t) & -c(t) \end{pmatrix} \end{aligned} \tag{13}$$

This matrix equation defines two scalar differential equations:

$$\begin{aligned} \dot{c}(t) &= -\gamma c(t) \\ \dot{b}(t) &= -\frac{\gamma}{2}b(t) \end{aligned}$$

$$\frac{d}{dt}\hat{\rho} = \gamma\left(\hat{\sigma}^{-}\hat{\rho}\hat{\sigma}^{+} - \frac{1}{2}\left\{\hat{\sigma}^{+}\hat{\sigma}^{-}, \hat{\rho}\right\}\right).$$

$$\dot{c}(t) = -\gamma c(t)$$
$$\dot{b}(t) = -\frac{\gamma}{2} b(t)$$

Solving these and using $a(t) + c(t) = 1$, gives us the density matrix at any time t:

$$\rho(t) = \begin{pmatrix} 1 - e^{-\gamma t}c(0) & e^{-\frac{\gamma}{2}t}b(0) \\ e^{-\frac{\gamma}{2}t}b^*(0) & e^{-\gamma t}c(0) \end{pmatrix}$$

Exercise: If we begin in the excited state ($\rho(0) = |1\rangle\langle 1|$) what is the state at long times? If we begin in an equal superposition of the excited and ground states ($\rho(0) = |+\rangle\langle +|$), what is the state at long times?

Найдем операторы Крауса

$$\boxed{\hat{\rho}(t) = \sum \hat{M}_k(t)\hat{\rho}(t=0)\hat{M}_k^+(t).}$$

В нашей задаче, k=0,1.

$$\hat{\rho}(t) = \begin{pmatrix} a(t) & b(t) \\ b^*(t) & c(t) \end{pmatrix} = \begin{pmatrix} 1 - e^{-\gamma t}c(0) & e^{-\gamma t/2}b(0) \\ e^{-\gamma t/2}b^*(0) & e^{-\gamma t}c(0) \end{pmatrix} =$$

$$= \hat{M}_0(t)\hat{\rho}(t=0)\hat{M}_0^+(t) + \hat{M}_1(t)\hat{\rho}(t=0)\hat{M}_1^+(t).$$

$$\hat{M}_0 = \hat{1} + \left(\hat{L}_0 - \frac{i\hat{H}_A}{\hbar}\right)\Delta t;$$
$$\hat{M}_{k'} = \hat{L}_{k'}\sqrt{\Delta t} \quad \textbf{при} \quad k' \neq 0$$

$$\hat{L}_0 = -\frac{1}{2}\sum_{k'\neq 0}\hat{L}^{\dagger}_{k'}\hat{L}_{k'}$$

$$\hat{L}_1^- = \hat{\sigma}^-\sqrt{\gamma},$$
$$\hat{L}_0 = -\frac{1}{2}\hat{L}_1^+\hat{L}_1^- = -\frac{1}{2}\gamma\hat{\sigma}^+\hat{\sigma}^-.$$

Попробуем угадать ответ:

$$\hat{M}_0(t) = \sqrt{1-p(t)}\hat{\sigma}^+\hat{\sigma}^- = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{1-p(t)} \end{pmatrix} \approx \hat{1} - \frac{1}{2}p(t)\hat{\sigma}^+\hat{\sigma}^-,$$
$$\hat{M}_1(t) = \hat{\sigma}^-\sqrt{p(t)}.$$

$$\hat{M}_0(t) = \sqrt{1-p(t)}\hat{\sigma}^+\hat{\sigma}^- = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{1-p(t)} \end{pmatrix} \approx \hat{1} - \frac{1}{2}p(t)\hat{\sigma}^+\hat{\sigma}^-,$$

$$\hat{M}_1(t) = \hat{\sigma}^-\sqrt{p(t)}.$$

$$\hat{\rho}(t) = \begin{pmatrix} a(t) & b(t) \\ b^*(t) & c(t) \end{pmatrix} = \begin{pmatrix} 1-e^{-\gamma t}c(0) & e^{-\gamma t/2}b(0) \\ e^{-\gamma t/2}b^*(0) & e^{-\gamma t}c(0) \end{pmatrix} =$$

$$= \hat{M}_0(t)\hat{\rho}(t=0)\hat{M}_0^+(t) + \hat{M}_1(t)\hat{\rho}(t=0)\hat{M}_1^+(t) =$$

$$= \begin{pmatrix} a(0)+p(t)c(0) & \sqrt{p(t)}b(0) \\ \sqrt{p(t)}b^*(0) & p(t)c(0) \end{pmatrix},$$

$$p(t) = e^{-\gamma t}.$$

H-теорема для уравнений Линблада

(согласно S. Abe, Phys. Rev. E 94, 022106 (2016)
и (или) Journal of Physics: Conf. Series 1035 (2018) 012001

$$\boxed{\mathrm{S}_\alpha(\hat{\rho}) = \frac{1}{1-\alpha}\ln\left(\mathrm{tr}\,\hat{\rho}^\alpha\right).} \Rightarrow \boxed{\mathrm{S}_{\alpha\to1}(\hat{\rho}) = -\mathrm{tr}\,\hat{\rho}\ln\left(\hat{\rho}\right).}$$

$$\hat{\rho} = \sum_i p_i \left|u_i\right\rangle\left\langle u_i\right|.$$

$$\Downarrow$$

$$\boxed{\mathrm{S}_\alpha(\hat{\rho}) = \frac{1}{1-\alpha}\ln\left(\sum_i p_i^\alpha\right).}$$

$$\frac{d}{dt}\hat{\rho} = \frac{1}{i\hbar}\left[\hat{H},\hat{\rho}\right] + L_k\hat{\rho}L_k^+ - \frac{1}{2}\left\{L_k^+L_k,\hat{\rho}\right\}.$$

$$\boxed{\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{S}_\alpha(\hat{\rho}) = \frac{\alpha}{(1-\alpha)\,\mathrm{tr}\,\hat{\rho}^\alpha}\,\mathrm{tr}\left(\hat{\rho}^{\alpha-1}\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}\right) = \\
&= \frac{\alpha}{(1-\alpha)\,\mathrm{tr}\,\hat{\rho}^\alpha}\,\mathrm{tr}\left(\hat{\rho}^{\alpha-1}\left\{\frac{1}{i\hbar}\left[\hat{H},\hat{\rho}\right] + L_k\hat{\rho}L_k^+ - \frac{1}{2}\left\{L_k^+L_k,\hat{\rho}\right\}\right\}\right) = \\
&= \frac{\alpha}{(1-\alpha)\,\mathrm{tr}\,\hat{\rho}^\alpha}\,\mathrm{tr}\left(\hat{\rho}^{\alpha-1}\left\{L_k\hat{\rho}L_k^+ - \frac{1}{2}\left\{L_k^+L_k,\hat{\rho}\right\}_+\right\}\right).
\end{aligned}}$$

$$\boxed{\begin{gathered}\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{S}_\alpha(\hat\rho)=\sum_k\Gamma_k,\\ \Gamma_k=\frac{\alpha}{(1-\alpha)\,\mathrm{tr}\,\hat\rho^\alpha}\mathrm{tr}\left(\hat\rho^{\alpha-1}\left\{\hat L_k\hat\rho\hat L_k^+-\frac{1}{2}\left\{\hat L_k^+\hat L_k,\hat\rho\right\}_+\right\}\right).\end{gathered}}$$

- Ниже будет доказано, что

$$\boxed{\begin{gathered}\Gamma_k>\left\langle\left[\hat L_k^+,\hat L_k\right]_-\right\rangle_\alpha,\\ \langle\ldots\rangle_\alpha=\frac{\mathrm{tr}\left(\hat\rho^\alpha\ldots\right)}{\mathrm{tr}\,\hat\rho^\alpha}.\end{gathered}}$$

$$\hat{\rho} = \sum_i p_i \left| u_i \right\rangle \left\langle u_i \right|.$$

$$\Gamma_k = \frac{\alpha}{(1-\alpha)\,\mathrm{tr}\,\hat{\rho}^\alpha} \mathrm{tr}\left(\hat{\rho}^{\alpha-1} \left\{ \hat{L}_k \hat{\rho} \hat{L}_k^+ - \frac{1}{2} \left\{ \hat{L}_k^+ \hat{L}_k, \hat{\rho} \right\}_+ \right\} \right) =$$

$$= \frac{\alpha}{(1-\alpha)\,\mathrm{tr}\,\hat{\rho}^\alpha} \left(\sum_{i,j} p_i^{\alpha-1} p_j \left| \left\langle u_i \right| \hat{L}_k \left| u_j \right\rangle \right|^2 - \sum_i p_i^\alpha \left\langle u_i \right| \hat{L}_k^+ \hat{L}_k \left| u_i \right\rangle \right) =$$

$$= \frac{\alpha}{(1-\alpha)\,\mathrm{tr}\,\hat{\rho}^\alpha} \left(\sum_{i,j} p_i^{\alpha-1} p_j \left| \left\langle u_i \right| \hat{L}_k \left| u_j \right\rangle \right|^2 - \sum_{ij} p_j^\alpha \left| \left\langle u_i \right| \hat{L}_k \left| u_j \right\rangle \right|^2 \right) =$$

$$\frac{\alpha}{(1-\alpha)\,\mathrm{tr}\,\hat{\rho}^\alpha} \left(\sum_{i,j} \left| \left\langle u_i \right| \hat{L}_k \left| u_j \right\rangle \right|^2 \left[p_i^{\alpha-1} - p_j^{\alpha-1} \right] p_j \right).$$

(1)

Если $0 < \alpha < 1$ и $0 < \lambda < 1$

$$[\lambda p_i + (1-\lambda)p_j]^\alpha > \lambda p_i^\alpha + (1-\lambda)p_j^\alpha$$

$$y^\alpha - 1 \leqslant \alpha(y-1)$$

$$\Downarrow$$

(2)

$$p_i^\alpha\left[\lambda + (1-\lambda)\frac{p_j}{p_i}\right]^\alpha \leqslant p_i^\alpha\left\{\alpha\left[\lambda + (1-\lambda)\frac{p_j}{p_i} - 1\right] + 1\right\}$$

(3)

(1)-(2) $\Rightarrow$ $$p_i^\alpha\left\{\alpha\left[\lambda + (1-\lambda)\frac{p_j}{p_i} - 1\right] + 1\right\} > \lambda p_i^\alpha + (1-\lambda)p_j^\alpha$$

$$p_i^\alpha \left\{ \alpha \left[\lambda + (1-\lambda)\frac{p_j}{p_i} - 1 \right] + 1 \right\} > \lambda p_i^\alpha + (1-\lambda) p_j^\alpha$$

Замечаем, что $1-\lambda$ сокращается!!!

$$\alpha p_i^{\alpha-1} p_j > (\alpha-1) p_i^\alpha + p_j^\alpha$$

$$\Gamma_k = \frac{1}{(1-\alpha)\,\mathrm{tr}\,\hat{\rho}^\alpha}\left(\sum_{i,j}\left|\langle u_i|\hat{L}_k|u_j\rangle\right|^2\left[\alpha p_i^{\alpha-1}p_j - \alpha p_j^{\alpha-1}p_j\right]\right) >$$

$$\frac{1}{(1-\alpha)\,\mathrm{tr}\,\hat{\rho}^\alpha}\left(\sum_{i,j}\left|\langle u_i|\hat{L}_k|u_j\rangle\right|^2\left[(\alpha-1)p_i^\alpha + p_j^\alpha - \alpha p_j^{\alpha-1}p_j\right]\right) =$$

$$= \frac{1}{(1-\alpha)\,\mathrm{tr}\,\hat{\rho}^\alpha}\left(\sum_{i,j}\left|\langle u_i|\hat{L}_k|u_j\rangle\right|^2\left[(\alpha-1)p_i^\alpha - (\alpha-1)p_j^\alpha\right]\right) =$$

$$= \frac{1}{\mathrm{tr}\,\hat{\rho}^\alpha}\left(\sum_{i,j}\left|\langle u_i|\hat{L}_k|u_j\rangle\right|^2\left[p_j^\alpha - p_i^\alpha\right]\right).$$

$$\sum_{i,j}\left|\langle u_i|\hat{L}_k|u_j\rangle\right|^2\left[p_j^\alpha - p_i^\alpha\right] = \sum_{i,j}\langle u_i|\hat{L}_k|u_j\rangle\langle u_j|\hat{L}_k^+|u_i\rangle\left[p_j^\alpha - p_i^\alpha\right] =$$

$$= \sum_j p_j^\alpha\langle u_j|\hat{L}_k^+\hat{L}_k|u_j\rangle - \sum_i p_i^\alpha\langle u_i|\hat{L}_k\hat{L}_k^+|u_i\rangle = \sum_j p_j^\alpha\left\langle u_j\left|\left[\hat{L}_k^+,\hat{L}_k\right]_-\right|u_j\right\rangle = \left\langle\left[\hat{L}_k^+,\hat{L}_k\right]_-\right\rangle_\alpha \operatorname{tr}\hat{\rho}^\alpha .$$

$$\Gamma_k = \frac{1}{(1-\alpha)\operatorname{tr}\hat{\rho}^\alpha}\left(\sum_{i,j}\left|\langle u_i|\hat{L}_k|u_j\rangle\right|^2\left[\alpha p_i^{\alpha-1}p_j - \alpha p_j^{\alpha-1}p_j\right]\right) >$$

$$= \frac{1}{\operatorname{tr}\hat{\rho}^\alpha}\left(\sum_{i,j}\left|\langle u_i|\hat{L}_k|u_j\rangle\right|^2\left[p_j^\alpha - p_i^\alpha\right]\right) = \left\langle\left[\hat{L}_k^+,\hat{L}_k\right]_-\right\rangle_\alpha .$$

Подводим итоги

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{S}_\alpha(\hat{\rho}) = \sum_k \Gamma_k,$$

$$\Gamma_k = \frac{\alpha}{(1-\alpha)\,\mathrm{tr}\,\hat{\rho}^\alpha}\mathrm{tr}\left(\hat{\rho}^{\alpha-1}\left\{\hat{L}_k\hat{\rho}\hat{L}_k^+ - \frac{1}{2}\left\{\hat{L}_k^+\hat{L}_k,\hat{\rho}\right\}_+\right\}\right) > \left\langle\left[\hat{L}_k^+,\hat{L}_k\right]_-\right\rangle_\alpha .$$

При $\alpha \to 1$, получаем стандартную энтропию

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{S}(\hat{\rho}) = -\sum_k \mathrm{tr}\left(\ln(\hat{\rho})\left\{\hat{L}_k\hat{\rho}\hat{L}_k^+ - \frac{1}{2}\left\{\hat{L}_k^+\hat{L}_k,\hat{\rho}\right\}_+\right\}\right) > \sum_k\left\langle\left[\hat{L}_k^+,\hat{L}_k\right]_-\right\rangle.$$

Примеры, иллюстрирующие H-теорему.

$$\frac{d}{dt}\hat{\rho} = \gamma\left(\hat{\sigma}^{-}\hat{\rho}\hat{\sigma}^{+} - \frac{1}{2}\left\{\hat{\sigma}^{+}\hat{\sigma}^{-},\hat{\rho}\right\}\right),$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{S}(\hat{\rho}) > \left\langle\left[\hat{L}_1^{+},\hat{L}_1\right]_{-}\right\rangle = \gamma\left\langle\left[\hat{\sigma}^{+},\hat{\sigma}^{-}\right]_{-}\right\rangle =$$

$$= \gamma\left\langle\left[|1\rangle\langle 0|,|0\rangle\langle 1|\right]_{-}\right\rangle = \gamma\left\langle|1\rangle\langle 1| - |0\rangle\langle 0|\right\rangle = \gamma\left(P_1 - P_0\right) = \gamma\left(2e^{-\gamma t}c(0) - 1\right).$$

$$\hat{\rho}(t) = \begin{pmatrix} a(t) & b(t) \\ b^*(t) & c(t) \end{pmatrix} = \begin{pmatrix} 1 - e^{-\gamma t}c(0) & e^{-\gamma t/2}b(0) \\ e^{-\gamma t/2}b^*(0) & e^{-\gamma t}c(0) \end{pmatrix} =$$

$$= \hat{M}_0(t)\hat{\rho}(t=0)\hat{M}_0^{+}(t) + \hat{M}_1(t)\hat{\rho}(t=0)\hat{M}_1^{+}(t).$$

```
In[•]:= ρ[t_, c_, b_, γ_] := ( 1 - c Exp[-γ t]    b Exp[-γ t / 2] )
                             ( b* Exp[-γ t / 2]    c Exp[-γ t]     )

In[•]:= S[t_, c_, b_, γ_] := -Tr[ρ[t, c, b, γ] MatrixLog[ρ[t, c, b, γ]]] // FullSimplify
                              след              логарифм матрицы              упростить в пол

In[•]:= Plot[S[t, 1, 0, 1], {t, 0, 5}, AxesLabel → {time, Entropy}, PlotLabel → S[t],
        график функции                 обозначения на осях   энтропия   пометка графика
         LabelStyle → Directive[14]]
         стиль отметки  директива
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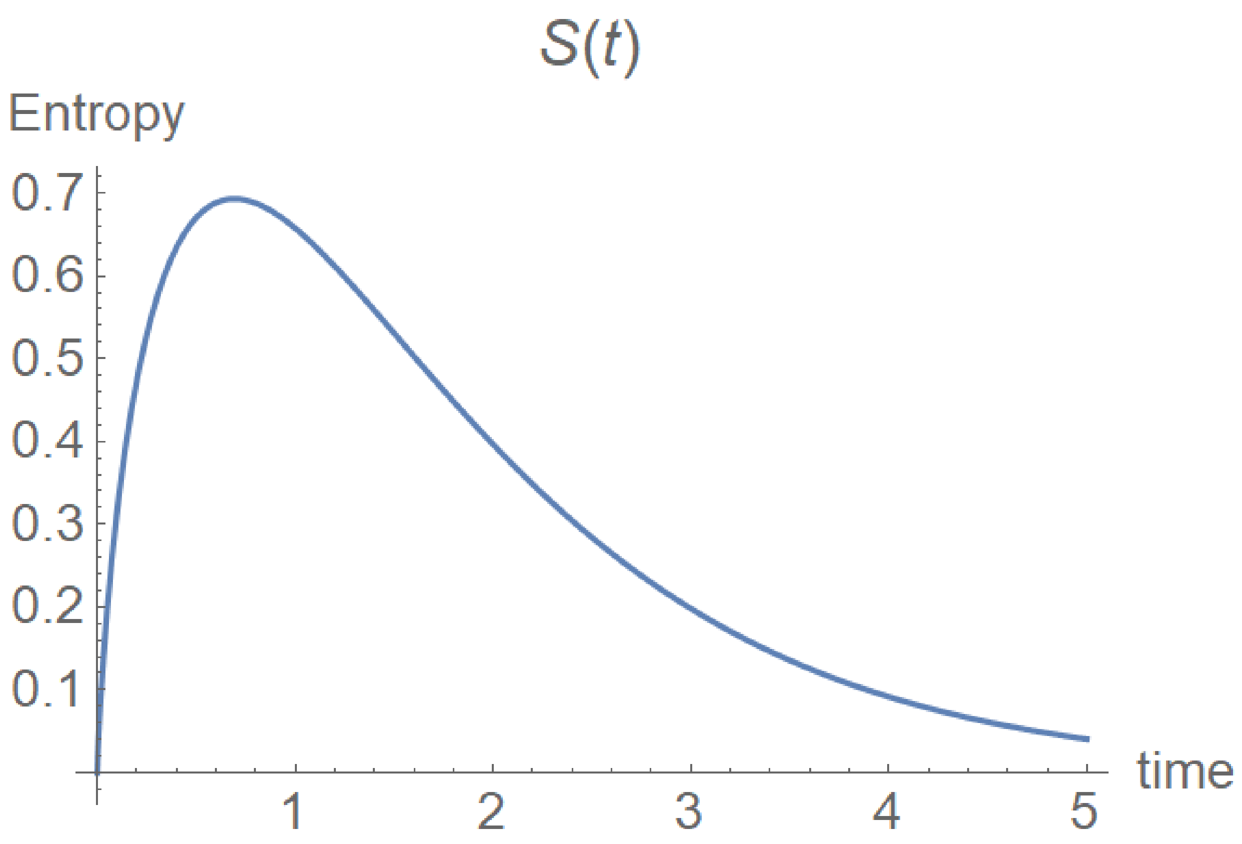
Out[•]=



Уравнения Паули (Master equation)

$$\frac{\partial}{\partial t}\hat{\rho} = \frac{1}{i\hbar}\left[\hat{H}, \hat{\rho}\right] + \mathrm{L}\ \hat{\rho}\,\mathrm{L}^{+} - \frac{1}{2}\left\{\mathrm{L}^{+}\mathrm{L}, \hat{\rho}\right\},$$

$$\hat{\rho}_{ik} = \delta_{ik} P_i,$$

$$\frac{\partial}{\partial t} P_i = L_{ik} P_k L_{ik}^{*} - \frac{1}{2}\left(L_{ki}^{*} L_{ki} P_i + P_i L_{ki}^{*} L_{ki}\right) = W_{ik} P_k - W_{ki} P_i,$$

$$W_{ik} = \left|L_{ik}\right|^2.$$

$$\frac{\partial}{\partial t} P_i = W_{ik} P_k - W_{ki} P_i.$$

Решим уравнение Паули

$$\frac{d}{dt}\hat{\rho} = \gamma\left(\hat{\sigma}^{-}\hat{\rho}\hat{\sigma}^{+} - \frac{1}{2}\left\{\hat{\sigma}^{+}\hat{\sigma}^{-}, \hat{\rho}\right\}\right),$$

$$W_{01} = \left|L_{01}\right|^{2} = \gamma.$$

$$\frac{\partial}{\partial t}P_i = W_{ik}P_k - W_{ki}P_i.$$

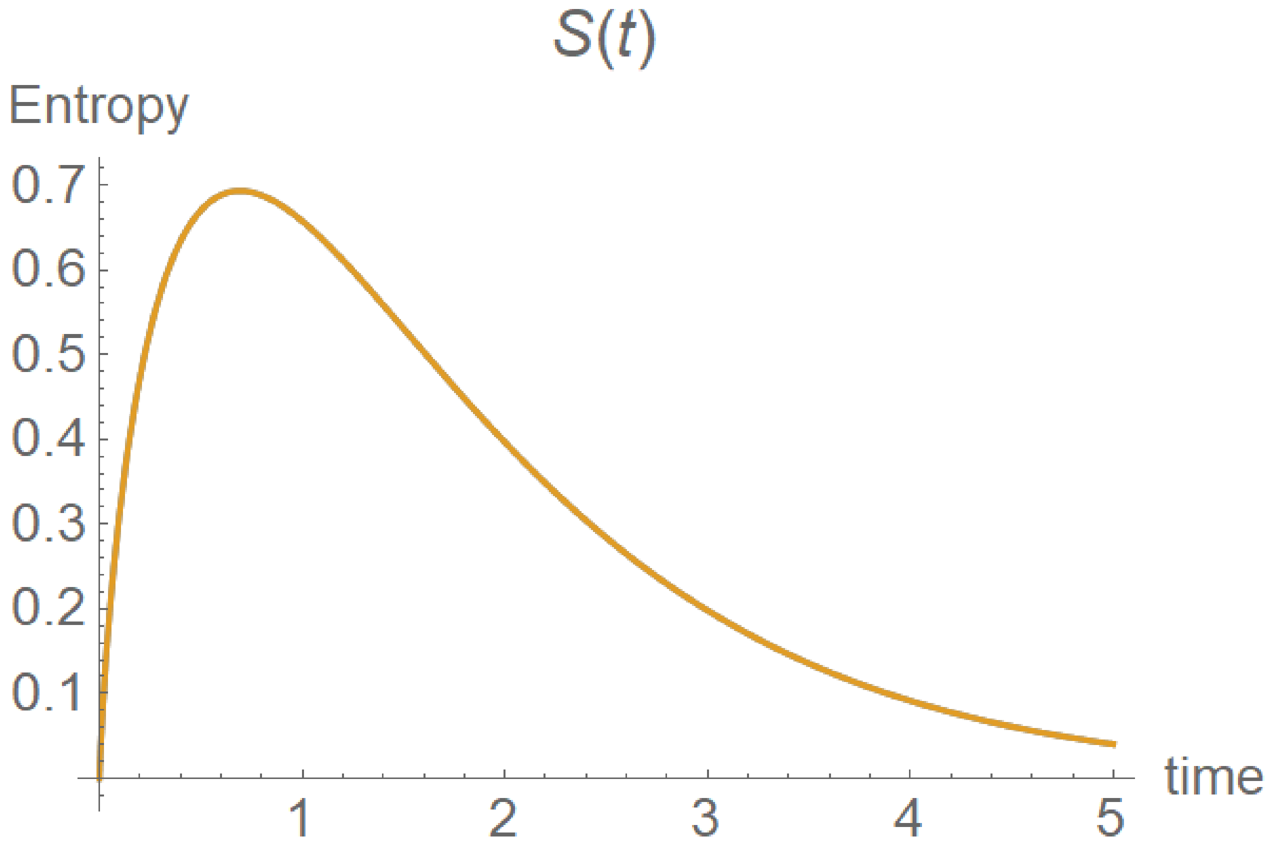
$$\frac{\partial}{\partial t}\begin{pmatrix} P_0 \\ P_1 \end{pmatrix} = \begin{pmatrix} \gamma P_1 \\ -\gamma P_1 \end{pmatrix}.$$

$$\begin{pmatrix} P_0 \\ P_1 \end{pmatrix} = \begin{pmatrix} 1 - P_1(t) \\ P_1(0)e^{-\gamma t} \end{pmatrix}.$$

Найдем энтропию

$$\begin{pmatrix} P_0 \\ P_1 \end{pmatrix} = \begin{pmatrix} 1 - P_1(t) \\ P_1(0) e^{-\gamma t} \end{pmatrix}.$$

$$S(t) = -P_0(t) \ln P_0(t) - P_1(t) \ln P_1(t).$$



Как же H-теорема???
Все пропало???

Вспомним H-теорему для уравнения Паули

Let $P_i(t)$ be the probability that the system is in a quantum or classical state i at time t. Then write

$$\frac{dP_i}{dt} = \sum_j \left(W_{ij}\, P_j - W_{ji}\, P_i\right) , \tag{2.86}$$

where W_{ij} is the rate at which j makes a transition to i. This is known as the *Master equation*. Note that we can recast the Master equation in the form

$$\frac{dP_i}{dt} = -\sum_j \Gamma_{ij}\, P_j , \tag{2.87}$$

with

$$\Gamma_{ij} = \begin{cases} -W_{ij} & \text{if } i \neq j \\ \sum_k' W_{kj} & \text{if } i = j , \end{cases} \tag{2.88}$$

Lecture Notes on Nonequilibrium Statistical Physics (A Work in Progress)

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Страница 50 про уравнение Паули (Master equation) и H-теорему

2.5.2 Boltzmann's H-theorem

Suppose for the moment that Γ is a symmetric matrix, *i.e.* $\Gamma_{ij} = \Gamma_{ji}$. Then construct the function

$$H(t) = \sum_i P_i(t) \, \ln P_i(t) \, . \tag{2.95}$$

Then

$$\begin{aligned} \frac{dH}{dt} &= \sum_i \frac{dP_i}{dt} \, (1 + \ln P_i) = \sum_i \frac{dP_i}{dt} \, \ln P_i \\ &= -\sum_{i,j} \Gamma_{ij} \, P_j \ln P_i \\ &= \sum_{i,j} \Gamma_{ij} \, P_j \big(\ln P_j - \ln P_i \big) \, , \end{aligned} \tag{2.96}$$

where we have used $\sum_i \Gamma_{ij} = 0$. Now switch $i \leftrightarrow j$ in the above sum and add the terms to get

$$\frac{dH}{dt} = \frac{1}{2} \sum_{i,j} \Gamma_{ij} \big(P_i - P_j \big) \big(\ln P_i - \ln P_j \big) \, . \tag{2.97}$$

$$\frac{dH}{dt} = \frac{1}{2} \sum_{i,j} \Gamma_{ij} \left(P_i - P_j\right) \left(\ln P_i - \ln P_j\right) . \tag{2.97}$$

Note that the $i = j$ term does not contribute to the sum. For $i \neq j$ we have $\Gamma_{ij} = -W_{ij} \leq 0$, and using the result

$$(x - y)\,(\ln x - \ln y) \geq 0 \, , \tag{2.98}$$

we conclude

$$\frac{dH}{dt} \leq 0 \, . \tag{2.99}$$

$$\frac{dP_i}{dt} = -\sum_j \Gamma_{ij}\, P_j\ ,$$

$$\Gamma_{ij} = \begin{cases} -W_{ij} & \text{if } i \neq j \\ \sum_k' W_{kj} & \text{if } i = j\ , \end{cases}$$

А если матрица скоростей переходов несимметрична, тогда все иначе!!!

If $\Gamma_{ij} \neq \Gamma_{ji}$, we can still prove a version of the H-theorem. Define a new symmetric matrix

$$\overline{W}_{ij} \equiv W_{ij}\, P_j^{\text{eq}} = W_{ji}\, P_i^{\text{eq}} = \overline{W}_{ji}\ , \tag{2.101}$$

and the generalized H-function,

$$H(t) \equiv \sum_i P_i(t)\, \ln\!\left(\frac{P_i(t)}{P_i^{\text{eq}}}\right) . \tag{2.102}$$

Then

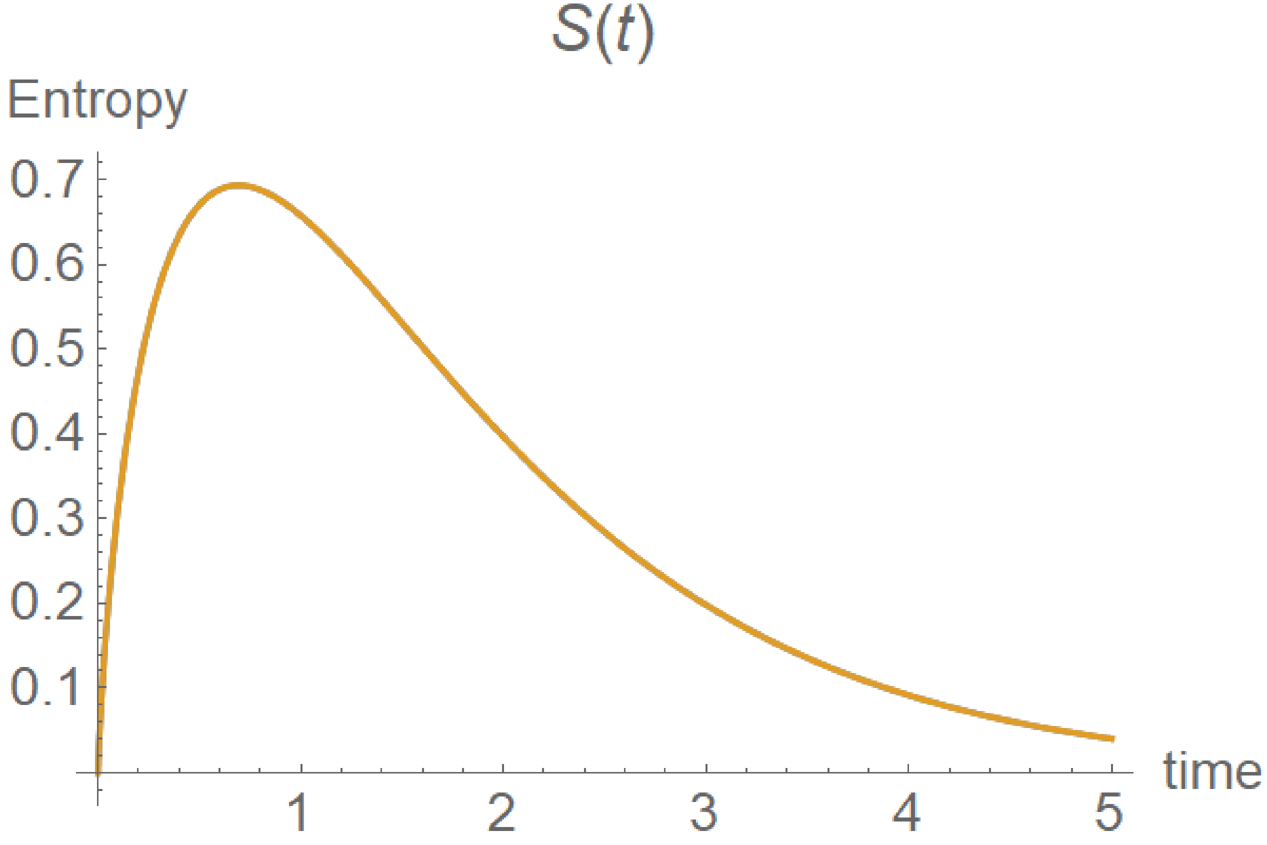
$$\frac{dH}{dt} = -\frac{1}{2} \sum_{i,j} \overline{W}_{ij} \left(\frac{P_i}{P_i^{\text{eq}}} - \frac{P_j}{P_j^{\text{eq}}}\right) \left[\ln\!\left(\frac{P_i}{P_i^{\text{eq}}}\right) - \ln\!\left(\frac{P_j}{P_j^{\text{eq}}}\right) \right] \leq 0\ . \tag{2.103}$$

$$\frac{\partial}{\partial t}\begin{pmatrix} P_0 \\ P_1 \end{pmatrix} = \begin{pmatrix} \gamma P_1 \\ -\gamma P_1 \end{pmatrix}.$$

Найдем энтропию

$$\begin{pmatrix} P_0 \\ P_1 \end{pmatrix} = \begin{pmatrix} 1 - P_1(t) \\ P_1(0)e^{-\gamma t} \end{pmatrix}.$$

$$S(t) = -P_0(t)\ln P_0(t) - P_1(t)\ln P_1(t).$$



В этой задаче равновесное распределение: $P_0 = 1, P_1 = 0$. Не получится ввести H-функцию. На ноль мы делить не можем!

$$H(t) \equiv \sum_i P_i(t)\,\ln\left(\frac{P_i(t)}{P_i^{\mathrm{eq}}}\right)$$

Модифицируем задачу

$$\frac{d}{dt}\hat{\rho} = \gamma_0\left(\hat{\sigma}^-\hat{\rho}\hat{\sigma}^+ - \frac{1}{2}\left\{\hat{\sigma}^+\hat{\sigma}^-, \hat{\rho}\right\}\right) + \gamma_1\left(\hat{\sigma}^+\hat{\rho}\hat{\sigma}^- - \frac{1}{2}\left\{\hat{\sigma}^-\hat{\sigma}^+, \hat{\rho}\right\}\right).$$

Напишем уравнение Паули

$$\frac{\partial}{\partial t}\begin{pmatrix} P_0 \\ P_1 \end{pmatrix} = \begin{pmatrix} \gamma_0 P_1 - \gamma_1 P_0 \\ -\gamma_0 P_1 + \gamma_1 P_0 \end{pmatrix}.$$

$$\gamma_0 P_1^{eq} - \gamma_1 P_0^{eq} = 0$$

$$P_0^{eq} = \frac{\gamma_0}{\gamma_0 + \gamma_1}, P_1^{eq} = \frac{\gamma_1}{\gamma_0 + \gamma_1}.$$