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Entropy and the Kac Master Equation

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Probabilistic model for N colliding particles (Kac 1956)

(i) For a collision randomly and uniformly pick a pair (i, j) of particles.

(ii) Randomly pick a 'scattering angle' with uniform probability.

(iii) Update the velocities by a rotation, i.e.,

$$(v_i, v_j) \to (v_i^*(\theta), v_j^*(\theta)) := (\sin(\theta)v_i + \cos(\theta)v_j, \cos(\theta)v_i - \sin(\theta)v_j)$$

(iv) Assume that the collision times are exponentially distributed, i.e, the probabiltity that the first collision time is larger than t is given by e^{-t}.

$$\mathbf{v} = (v_1, v_2, \cdots, v_N)$$

Energy is conserved.

$$\mathbf{v}^2 = \sum_{i=1}^{N} v_i^2 = N$$

Momentum is not conserved.

Looking for an evolution on probability distributions

$$F(\mathbf{v}) \in L^1(\mathbb{S}^{N-1}(\sqrt{N}), \mu^N)\ ,\ \mathbf{v} = (v_1, v_2, \ldots, v_N)$$

This setup models a spatially homogenous gas.

Given an initial distribution $F_0(\mathbf{v})$

$$F(\mathbf{v},t) = e^{-Nt(I-Q)}F_0 = \sum_{k=0}^{\infty} \frac{e^{-Nt}(Nt)^k}{k!} Q^k F_0$$

satisfies the linear Kac master equation

$$\frac{\mathrm{d}}{\mathrm{d}t}F(\mathbf{v},t) = -N(I-Q)F(\mathbf{v},t) \ , \ F(\mathbf{v},0) = F_0(\mathbf{v})$$

$$R_{i,j}\Phi := \frac{1}{2\pi}\int_0^{2\pi} \Phi(v_1,\cdots,v_i^*(\theta),\cdots,v_j^*(\theta),\cdots,v_N)\mathrm{d}\theta$$

$$Q = \begin{pmatrix} N \\ 2 \end{pmatrix}^{-1} \sum_{i<j} R_{i,j}$$

$$N(Q - I) = \frac{2}{N-1}\sum_{i<j}(R_{i,j} - I)$$

The collision rate of particular particle colliding with any other within a time interval dt is $2dt$.

The (negative) Entropy

$$S(F) = \int_{\mathbb{S}^{N-1}} F \log F d\mu^N$$

Cercignani's conjecture, formulated orginally for the Boltzmann equation

$$S(F(t)) \le e^{-ct} S(F_0)\ ,\ \ c > 0\ .$$

Entropy production, McKean, Carlen-Carvalho

$$\Gamma_N = \inf_F - \frac{\frac{d}{dt} S(F(t))}{S(F)}\bigg|_{t=0} = \inf_F \frac{\int_{\mathbb{S}^{N-1}} N(I-Q) F \log F d\mu^N}{S(F)}$$

$$\frac{dS}{dt}(F(t)) \le -\Gamma_N S(F(t))$$

C. Villani, 2003

$$\Gamma_N \geq \frac{2}{N-1}$$

Amit Einav, 2012

$$\Gamma_N \approx \frac{1}{N} \, .$$

The indications are that exponential decay of the entropy does not hold for general initial conditions.

Problem: Is there an initial condition F_0 such that

$$S(F(t)) \geq c(1 - \frac{t}{N}) S(F_0) \ ?$$

What are physically reasonable situations where one can expect exponential decay in entropy at a rate independent of N?

A good candidate is a 'small system' coupled to a large system in thermal equilibrium.

Joint work with Federico Bonetto

Warm up: System interacting with a thermostat

$$\frac{\partial f}{\partial t} = -\lambda M(I-Q)f - \mu \sum_{j=1}^{M} (I-R_j)f =: \mathcal{L}_T f \ . \tag{1}$$

$$R_j f := \frac{1}{2\pi}\int dw \frac{1}{2\pi}\int_0^{2\pi} d\theta \sqrt{\frac{\beta}{2\pi}} e^{-\frac{\beta}{2} w_j^{*2}(\theta)} f(\mathbf{v}_j(\theta, w))$$

$$\mathbf{v}_j(\theta, w) = (v_1, ..., v_j \cos(\theta) + w \sin(\theta), ..., v_M) \ , \ w_j^*(\theta) = -v_j \sin(\theta) + w \cos(\theta)$$

.

Operators act on probability distributions in $L^1(\mathbb{R}^M)$. Energy no longer conserved.

$$K(f) := \frac{1}{2}\sum_{i=1}^{M}\int_{\mathbb{R}^M} v_i^2 f(v_1,\ldots,v_M)dv_1\cdots dv_M \ ,$$

$$\frac{dK}{dt} = -\frac{\mu}{2}\left(K - \frac{M}{2\beta}\right) \ .$$

Unique equilibrium state: Gaussian with temperature β^{-1}

$$G_\beta(\mathbf{v}) = \left(\sqrt{\frac{\beta}{2\pi}}\right)^M e^{-\frac{\beta\sum_{i=1}^M v_i^2}{2}}$$

Relative entropy

$$S(f|G_\beta) = \int_{\mathbb{R}^M} f \log \frac{f}{G_\beta} d\mathbf{v}$$

Theorem (Bonetto-L-Vaidyanathan)

Let $f(t)$ be the solution of the master equation (1) with initial condition f_0. Then

$$S(f(t)|G_\beta) \le e^{-\mu t/2} S(f_0|G_\beta) \ .$$

The rate $\mu/2$ is best possible, **(Vaidyanathan)**

System interacting with a finite reservoir

$$\partial_t F = \mathcal{L}F := \mathcal{L}_S F + \mathcal{L}_R F + \mathcal{L}_I F \ , \quad F(\mathbf{v}, \mathbf{w}, t)$$

$$\mathcal{L}_S = \frac{\lambda_S}{M-1} \sum_{i<j=1}^{M} (R_{i,j} - I) \ , \ \mathcal{L}_R = \frac{\lambda_R}{N-1} \sum_{M+1 \le i<j}^{M+N} (R_{i,j} - I)$$

$$\mathcal{L}_I = \frac{\mu}{N} \sum_{i=1}^{M} \sum_{j=M+1}^{M+N} (R_{i,j}^I - I)$$

Initital conditions

The reservoir R should be initially in equilibrium,

while no assumption should be made about the system S

$$F_0(\mathbf{v}, \mathbf{w}) = f_0(\mathbf{v}) G_{N,\beta}(\mathbf{w})$$

where $G_{N,\beta}$ is a Gaussian of temperature β^{-1}

Note that through the interaction term, correlations will be building up over time. In particular the reservoir will be out of equilibrium after a finite time.

Equilibrium State for finite reservoir system

$$\int_{SO(N+M)} F_0(R^{-1}(\mathbf{v},\mathbf{w}))dR \neq G_{M+N,\beta}(\mathbf{v},\mathbf{w})$$

Equilibrium State for the thermostated system

$$G_{M,\beta}(\mathbf{v}) = \left(\sqrt{\frac{\beta}{2\pi}}\right)^M e^{-\frac{\beta\sum_{i=1}^M v_i^2}{2}}$$

How do the thermostated model and the finite reservoir model compare?
The Gabetta-Toscani-Wennberg metric

$$d_2(F,G) = \sup_{|\vec{\xi}|\neq 0} \frac{|\widehat{F}(\vec{\xi}) - \widehat{G}(\vec{\xi})|}{|\vec{\xi}|^2}$$

$$d_2(f^{\otimes N}, g^{\otimes N}) = d_2(f,g)\ !$$

$F(v,w,t)$ solution of the finite reservoir system.

$f(v,t)$ solution of the thermostated system.

Initial conditions:

$$F(v,w,0) = f_0(v) G_{N,\beta}(w)\ ,\ \ f(v,0) = f_0(v)\ .$$

Theorem (Bonetto, L, Tossounian, Vaidyanathan (2017))

Under reasonable assumptions of f

$$d_2(F(\cdot,t), f(\cdot,t)G_{N,\beta}(\cdot)) \leq$$
$$K_1\frac{M}{N}(1-e^{-\frac{\mu t}{4}})\sqrt{d_2(f(\cdot,0),G_{M,\beta}(\cdot))+K_2\sqrt{d_2(f(\cdot,0),G_{M,\beta}(\cdot))}}$$

Rate of decay of entropy for the system interacting with finite reservoir?

For $\mathcal{L}_T$ we have the decay

$$S(f(t)|G_\beta) \leq e^{-\mu t/2} S(f_0|G_\beta) \ .$$

Choose $\beta = 2\pi$ from now on

Define

$$f(\mathbf{v}, t) := \int_{\mathbb{R}^N} e^{\mathcal{L}t} F_0(\mathbf{v}, \mathbf{w}) d\mathbf{w}$$

$$F_0(\mathbf{v}, \mathbf{w}) = f_0(\mathbf{v}) e^{-\pi|\mathbf{w}|^2}$$

$$S(f) := S(f|e^{-\pi|\mathbf{v}|^2}) = \int_{\mathbb{R}^M} f(\mathbf{v}) \log\left(\frac{f(\mathbf{v})}{e^{-\pi|\mathbf{v}|^2}}\right) d\mathbf{v} < \infty$$

Cannot expect that $S(f(t))$ tends to zero.

The Gaussian is not the equilibrium state

$$\int_{SO(N+M)} F(R^{-1}(\mathbf{v},\mathbf{w}))dR \neq G_{M,\beta}(\mathbf{v})G_{N,\beta}(\mathbf{w})$$

$$\int_{\mathbb{R}^N}\int_{SO(N+M)} F(R^{-1}(\mathbf{v},\mathbf{w}))dRd\mathbf{w} \neq G_{M,\beta}(\mathbf{v})$$

Replace the uniform measure $\frac{d\theta}{2\pi}$ by $\rho(\theta)d\theta$

and assume that

$$\int_0^{2\pi} \rho(\theta)\sin\theta\cos\theta d\theta = 0$$

,

We do not assume local reversibility!

Theorem (Bonetto-Geisinger-L-Ried)

Assume that the entropy of f_0 relative to the thermal state is finite

$$S(f_0) = \int_{\mathbb{R}^M} f_0(\mathbf{v}) \log\left(\frac{f_0(\mathbf{v})}{e^{-\pi|\mathbf{v}|^2}}\right) d\mathbf{v} < \infty$$

Then for $N \geq M$

$$S(f(t)) \leq \left[\frac{M}{N+M} + \frac{N}{N+M} e^{-\mu(\rho)\frac{N+M}{N}t}\right] S(f_0)$$

where

$$\mu(\rho) = \mu \int_0^{2\pi} \rho(\theta) \sin(\theta)^2 d\theta$$

Some ideas for a proof

$$f_0(\mathbf{v}) = h_0(\mathbf{v})e^{-\pi|\mathbf{v}|^2}$$

$$e^{\mathcal{L}t}F_0(\mathbf{v},\mathbf{w}) = e^{-\pi(|\mathbf{v}|^2+|\mathbf{w}|^2)}e^{\mathcal{L}t}h_0(\mathbf{v},\mathbf{w})$$

$$F_0(\mathbf{v},\mathbf{w}) = h_0(\mathbf{v})e^{-\pi(|\mathbf{v}|^2+|\mathbf{w}|^2)}$$

$$f(\mathbf{v},t) = h(\mathbf{v},t)e^{-\pi|\mathbf{v}|^2}\ , \ \text{where } h(\mathbf{v},t) = \int_{\mathbb{R}^N} e^{\mathcal{L}t}h_0(\mathbf{v},\mathbf{w})e^{-\pi|\mathbf{w}|^2}d\mathbf{w}$$

$$S(f(t)) = \int h(\mathbf{v},t)\log h(\mathbf{v},t)e^{-\pi\mathbf{v}^2}dv$$

$$S(f_0) = \int h_0\log h_0 e^{-\pi\mathbf{v}^2}dv$$

$$\Lambda = \lambda_S \frac{M}{2} + \lambda_R \frac{N}{2} + \mu M$$

$$\frac{\lambda_S}{\Lambda(M-1)} \, , \; \frac{\lambda_R}{\Lambda(N-1)} \, , \; \frac{\mu}{\Lambda N} \, ,$$

$$\mathcal{L} = \Lambda Q - \Lambda I$$

$$Q = \sum_{1 \leq i < j \leq M+N} \lambda_{i,j} R_{i,j}$$

$$\sum_{1 \leq i < j \leq M+N} \lambda_{i,j} = 1$$

Power series expansion for the time evolution

$$(e^{\mathcal{L}t}h_0)(\mathbf{v},\mathbf{w}) =$$

$$e^{-\Lambda t}\sum_{k=0}^{\infty}\frac{\Lambda^k t^k}{k!}Q^k h_0(\mathbf{v},\mathbf{w})$$

$$Q^k h_0(\mathbf{v},\mathbf{w}) = \sum_{\underline{\alpha}}\lambda_{\underline{\alpha}}\int \rho_{\underline{\theta}}d\underline{\theta}\; h_0([\Pi_{j=1}^k r_{\alpha_j}(\theta_j)]^{-1}(\mathbf{v},\mathbf{w}))$$

$$\sum_{\underline{\alpha}}\lambda_{\underline{\alpha}}\int \rho_{\underline{\theta}}d\underline{\theta} = \sum_{\alpha_1,\ldots,\alpha_k}\lambda_{\alpha_1}\cdots\lambda_{\alpha_k}\int \rho(\theta_1)d\theta_1\cdots\rho(\theta_k)d\theta_k$$

$$\mathcal{N}_{k,\underline{\alpha},\underline{\theta}}\, h_0(\mathbf{v}) := \int_{\mathbb{R}^N} h_0([\Pi_{j=1}^k r_{\alpha_j}(\theta_j)]^{-1}(\mathbf{v},\mathbf{w}))e^{-\pi|\mathbf{w}|^2}d\mathbf{w}$$

Convexity

$$S(f(t)) \leq e^{-\Lambda t} \sum_{k=0}^{\infty} \frac{\Lambda^k t^k}{k!} \sum_{\underline{\alpha}} \lambda_{\underline{\alpha}} \int \rho_{\underline{\theta}} d\underline{\theta} \;\; S(\mathcal{N}_{k,\underline{\alpha},\underline{\theta}}\, h_0)$$

$$S(\mathcal{N}_{k,\underline{\alpha},\underline{\theta}}\, h_0) = \int_{\mathbb{R}^M} \mathcal{N}_{k,\underline{\alpha},\underline{\theta}}\, h_0(\mathbf{v}) \log \left[\mathcal{N}_{k,\underline{\alpha},\underline{\theta}}\, h_0(\mathbf{v}) \right] e^{-\pi|\mathbf{v}|^2} d\mathbf{v}$$

$$[\Pi_{j=1}^{k} r_{\alpha_j}(\theta_j)]^{-1} = \begin{bmatrix} A_k(\underline{\alpha},\underline{\theta}) & B_k(\underline{\alpha},\underline{\theta}) \\ C_k(\underline{\alpha},\underline{\theta}) & D_k(\underline{\alpha},\underline{\theta}) \end{bmatrix}$$

$$\mathcal{N}_{k,\underline{\alpha},\underline{\theta}} h_0(\mathbf{v}) = \int_{\mathbb{R}^N} h_0(A_k(\underline{\alpha},\underline{\theta})\mathbf{v} + B_k(\underline{\alpha},\underline{\theta})\mathbf{w}) e^{-\pi|\mathbf{w}|^2} d\mathbf{w}$$

$$= \int_{\mathbb{R}^M} h_0(A_k(\underline{\alpha},\underline{\theta})\mathbf{v} + \left(I_M - A_k(\underline{\alpha},\underline{\theta})A_k(\underline{\alpha},\underline{\theta})^T\right)^{1/2} \mathbf{w}) e^{-\pi|\mathbf{w}|^2} d\mathbf{w}$$

$$A_k(\underline{\alpha},\underline{\theta}) = U_k(\underline{\alpha},\underline{\theta})\Gamma_k(\underline{\alpha},\underline{\theta})V_k(\underline{\alpha},\underline{\theta})^T \ , \ \ \Gamma_k(\underline{\alpha},\underline{\theta}) = [\gamma_1, \cdots, \gamma_M] \ , \ 0 \leq \gamma_j \leq 1$$

$$= \int_{\mathbb{R}^M} h_{0,U_k(\underline{\alpha},\underline{\theta})}(\Gamma_k(\underline{\alpha},\underline{\theta})V_k(\underline{\alpha},\underline{\theta})^T\mathbf{v} + \left(I_M - \Gamma_k(\underline{\alpha},\underline{\theta})^2\right)^{1/2} \mathbf{w}) e^{-\pi|\mathbf{w}|^2} d\mathbf{w}$$

$$h_{0,U_k(\underline{\alpha},\underline{\theta})}(\mathbf{v}) = h_0(U_k(\underline{\alpha},\underline{\theta})\mathbf{v})$$

$$\mathcal{N}_{k,\underline{\alpha},\underline{\theta}}\, h_0(\mathbf{v}) =$$

$$\int_{\mathbb{R}^M} h_{0,U_k(\underline{\alpha},\underline{\theta})}(\Gamma_k(\underline{\alpha},\underline{\theta})\mathbf{v} + \left(I_M - \Gamma_k(\underline{\alpha},\underline{\theta})^2\right)^{1/2}\mathbf{w})e^{-\pi|\mathbf{w}|^2}d\mathbf{w} =$$

$$\int_{\mathbb{R}^M} h_{0,U_k}(\gamma_1 v_1 + (1-\gamma_1^2)^{1/2} w_1, \ldots, \gamma_M v_M + (1-\gamma_M^2)^{1/2} w_M) e^{-\pi \sum_{j=1}^M w_j^2} dw_1 \cdots dw_M$$

Ornstein-Uhlenbeck type operator

$$\mathcal{N}_a h(v) = \int_{\mathbb{R}} h(av + \sqrt{1-a^2}w)e^{-\pi w^2}dw\ ,\ 0 \le a \le 1$$

Hypercontractivity in entropic form

Theorem

Assume that $h : \mathbb{R} \to \mathbb{R}_+$ has finite entropy, i.e.,

$$S(h) = \int_{\mathbb{R}} h(v) \log h(v) e^{-\pi v^2} dv < \infty$$

then

$$S(\mathcal{N}_a h) \leq a^2 S(h) + (1 - a^2) \|h\|_1 \log \|h\|_1$$

A computation

$$S(\mathcal{N}_{a,b}h) = S(\mathcal{N}_a\mathcal{N}_b h) \leq a^2 S(\mathcal{N}_b h) + (1-a^2)S(\mathcal{N}_b h^1)$$

$$\leq a^2b^2S(h)+a^2(1-b^2)S(h^2)+(1-a^2)b^2S(h^1)+(1-a^2)(1-b^2)\|h\|_1\log\|h\|_1$$

$$h^1(v_2) = \int_{\mathbb{R}} dv_1 e^{-\pi v_1^2} h(v_1,v_2)\ ,\ \ h^2(v_2) = \int_{\mathbb{R}} dv_2 e^{-\pi v_2^2} h(v_1,v_2)$$

$$\|h\|_1 = \int_{\mathbb{R}^2} dv_1 dv_2 e^{-\pi[v_1^2+v_2^2]} h(v_1,v_2)$$

Theorem

Let $\int_{\mathbb{R}^M} h_0(\mathbf{v})e^{-\pi|\mathbf{v}|^2}d\mathbf{v} = 1$ and assume that $S(h_0) < \infty$. Then

$$S(\mathcal{N}_{k,\underline{\alpha},\underline{\theta}}\, h_0) \leq$$
$$\sum_{\sigma\subset\{1,\ldots,M\}} \Pi_{i\in\sigma^{\rm c}}\gamma_i^2\Pi_{j\in\sigma}(1-\gamma_j^2) \int_{\mathbb{R}^M} h_0(\mathbf{v}) \log h^{\sigma}_{0,U_k}(P_{\sigma^c}U_k^T\mathbf{v})e^{-\pi|\mathbf{v}|^2}d\mathbf{v}$$

where

$$h_{U_k}(\mathbf{v}) = h(U_k(\underline{\alpha},\underline{\theta})\mathbf{v})$$

and the σ marginal $h^{\sigma}_{U_k}$ is given by

$$h^{\sigma}_{U_k}(\mathbf{u}) = \int_{\mathbb{R}^\sigma} h(U_k(\mathbf{u}',\mathbf{u}))e^{-\pi|\mathbf{u}'|^2}d\mathbf{u}'$$

Theorem

$$\sum_{\underline{\alpha}} \lambda_{\underline{\alpha}} \int \rho_{\underline{\theta}} d\underline{\theta} \; S(\mathcal{N}_{k,\underline{\alpha},\underline{\theta}} \; h_0)$$

$$\leq \left[\frac{M}{N+M} + \frac{N}{N+M}(1-\mu_\rho \frac{M+N}{\Lambda N})^k\right] S(f_0)$$

$$e^{-\Lambda t} \sum_{k=0}^{\infty} \frac{\Lambda^k t^k}{k!} \left[\frac{M}{N+M} + \frac{N}{N+M}(1-\mu_\rho \frac{M+N}{\Lambda N})^k\right]$$

$$= \frac{M}{N+M} + \frac{N}{N+M} e^{-\mu_\rho \frac{M+N}{N} t}$$

Barthe's version of the Brascamp-Lieb inequalities

For $i = 1, \dots K$, let $H_i \subset \mathbb{R}^M$ be subspaces of dimension d_i and $B_i : \mathbb{R}^M \to H_i$ be linear maps with the property that $B_i B_i^T = I_{H_i}$, the identity map on H_i. Assume further there are non-negative constants $A, c_i, i = 1, \dots, K$ such that

$$\sum_{i=1}^{K} c_i B_i^T B_i = A I_M \ . \tag{2}$$

Then for any non-negative functions $f_i : H_i \to \mathbb{R}$, $i = 1, \dots, K$, and any non-negative function $h \in L^1(\mathbb{R}^M, e^{-\pi|\mathbf{v}|^2} d\mathbf{v})$ with $\|h\|_1 = 1$

$$\sum_{i=1}^{K} c_i \left[\int_{\mathbb{R}^M} h(\mathbf{v}) \log f_i(B_i \mathbf{v}) e^{-\pi|\mathbf{v}|^2} d\mathbf{v} - \log \int_{H_i} f_i(u) e^{-\pi u^2} du \right]$$
$$\leq A \int_{\mathbb{R}^M} h(\mathbf{v}) \log h(\mathbf{v}) e^{-\pi|\mathbf{v}|^2} d\mathbf{v} \tag{3}$$

Carlen – Cordero-Erausquin

$$f_i(u) \Leftrightarrow h_U^{\sigma}(\mathbf{u})$$

$$H_i \Leftrightarrow \mathbb{R}^{\sigma^{\mathrm{c}}}$$

$$P_{\sigma^{\mathrm{c}}} : \mathbb{R}^M \to \mathbb{R}^{\sigma^{\mathrm{c}}}$$

$$B_i \Leftrightarrow P_{\sigma^{\mathrm{c}}} U_k(\underline{\alpha}, \underline{\theta})^T$$

$$B_i B_i^T = I_{H_i} \Leftrightarrow P_{\sigma^{\mathrm{c}}} U_k(\underline{\alpha}, \underline{\theta})^T [P_{\sigma^{\mathrm{c}}} U_k(\underline{\alpha}, \underline{\theta})^T]^T = P_{\sigma^{\mathrm{c}}} P_{\sigma^{\mathrm{c}}}^T = I_{\mathbb{R}^{\sigma^{\mathrm{c}}}}$$

What corresponds to the c_is and to the summation

$$\sum_{i=1}^{K} c_i B_i^T B_i = I_M \ ?$$

Key Computation

$$\sum_{\underline{\alpha}} \lambda_{\underline{\alpha}} \int \rho_{\underline{\theta}} d\underline{\theta}$$

$$\sum_{\sigma \subset \{1,\ldots,M\}} \Pi_{i \in \sigma^{\mathrm{c}}} \gamma_{k,i}(\underline{\alpha}, \underline{\theta})^2 \Pi_{j \in \sigma}(1 - \gamma_{k,j}(\underline{\alpha}, \underline{\theta})^2) U_k(\underline{\alpha}, \underline{\theta}) P_{\sigma^{\mathrm{c}}}^T P_{\sigma^{\mathrm{c}}} U_k(\underline{\alpha}, \underline{\theta})^T$$

$$= A_{k,M} I_M$$

where

$$A_{k,M} = \left[\frac{M}{N+M} + \frac{N}{N+M} (1 - \mu_\rho \frac{M+N}{\Lambda N})^k \right]$$

$$\mu_\rho = \int \rho(\theta) \sin(\theta)^2 d\theta$$

THANK YOU!