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# 伏見汎関数による 非平衡状態でのエントロピー生成の記述

- Introduction
- Entropy production in Quantum Mechanics
- Entropy production in Quantum Field Theory
- Summary

“Towards a Theory of Entropy Production in the Little and Big Bang”

T. Kunihiro, B. Muller, A. Ohnishi, A. Schafer

Eprint:0809.4831

# Various Entropies

- エントロピーとは何か？10文字以内で答えよ。  
「乱雑さを表す示量変数」(10文字)  
(学部1年生によく出した試験問題)

- von Neumann entropy

$$S_{vN} = -\text{Tr}[\hat{\rho} \log \hat{\rho}] = -\sum_n w_n \log w_n$$

- Wehrl entropy (Discrete level  $\rightarrow$  phase space)

$$S_{Wehrl} = -\int d\Gamma f \log f$$

- Kolmogorov-Sinai entropy = Entropy growth rate in classical non-linear dynamics

$$S_{KS} = \sum_n \lambda_n \theta(\lambda_n)$$

$\lambda_n$  = Lyapunov exponent

$$\delta X_i = \delta X_i(t=0) \exp(\lambda_i t)$$

# Entropy production in Quantum Mechanics

- Pure state  $\rightarrow$  Entropy = 0

$$i \hbar \frac{\partial \psi}{\partial t} = H \psi \rightarrow \rho_{nm} = 1 (n = m = \text{occupied}), 0 (\text{other})$$

$\rightarrow$  We need “something else” than Schrodinger equation !

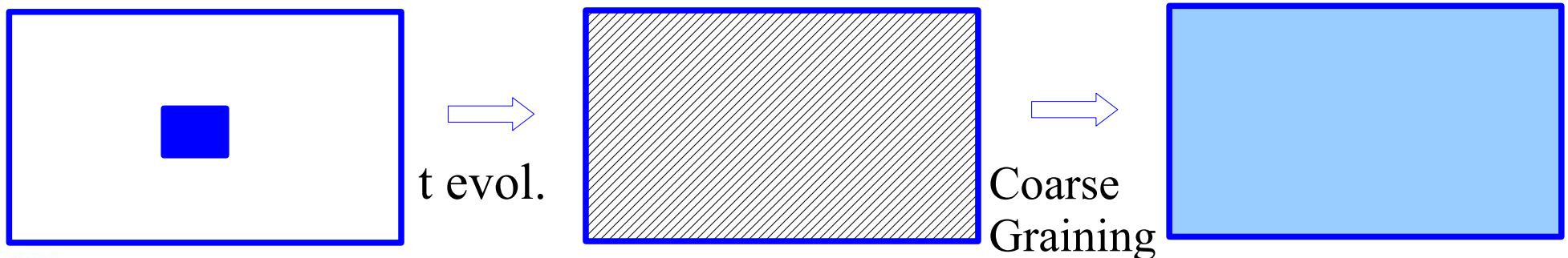
- Two kind of information loss

- Interaction with unobserved environment

$$S = -\text{Tr} [\rho_S \log \rho_S], \quad \rho_S = \text{Tr}_E \rho$$

- Loss of practically obtainable information due to increasing complexity of phase space distribution

$\rightarrow$  Some kind of “Coarse Graining” is necessary



# Coarse Graining

- N-body → Projection to product wave functions

$$S = \int d\Gamma \left[ -f \log f + \sigma (1 + \sigma f) \log (1 + \sigma f) \right]$$

( $\sigma = \pm 1$  for bosons/fermions)

- Advanced treatment with spectral function  
T. Kita, JPSJ75('06)114005, Yu. B. Ivanov, J. Knoll, D.N. Voskresensky, NPA672(00)313, A. Nishiyama, arXiv:0810.5003.  
→ “single particle energy” is necessary in advanced treatment.

- Smearing of phase space distribution function

- Wigner function is not always positive.  
→ Husimi function

*We study the entropy production  
in quantum mechanics and field theory  
with Husimi function / functional*

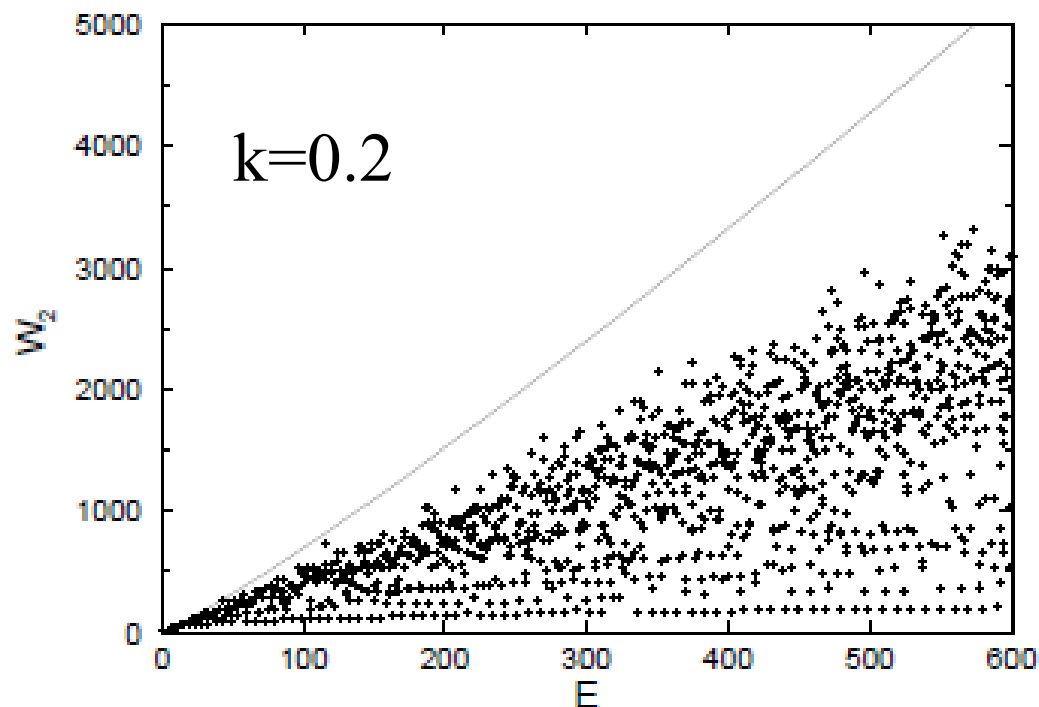
# Complexity Degree: Second Moment

- Small average Husimi function would be a measure of chaoticity  
Sugita, Aiba, J. Phys. A 36 (2001), 9081.

$$H = \frac{1}{2}(p_x^2 + p_y^2) + \frac{1}{2}(x^4 + y^4) - kx^2y^2,$$

$$W_2(\rho_H) = \frac{1}{M_2(\rho_H)},$$

$$M_2(\rho_H) = \int \frac{dpdq}{(2\pi\hbar)^k} \rho_H(\mathbf{p}, \mathbf{q})^2.$$



# TDHF and Vlasov Equation

- Time-Dependent Mean Field Theory (e.g., TDHF)  $i\hbar \frac{\partial \phi_i}{\partial t} = h \phi_i$

- Density Matrix

$$\rho(r, r') = \sum_i^{\text{Occ}} \phi_i(r) \phi_i^*(r') \rightarrow \rho_W = f \text{ (phase space density)}$$

- TDHF for Density Matrix

$$i\hbar \frac{\partial \rho}{\partial t} = [h, \rho] \rightarrow \frac{\partial f}{\partial t} = \{h_W, f\}_{P.B.} + O(\hbar^2)$$

- Wigner Transformation and Wigner-Kirkwood Expansion  
(Ref.: Ring-Schuck)

$$O_W(r, p) \equiv \int d^3s \exp(-i p \cdot s / \hbar) \langle r + s/2 | O | r - s/2 \rangle$$

$$(AB)_W = A_W \exp(i\hbar \Lambda) B_W \quad \Lambda \equiv \nabla'_r \cdot \nabla_p - \nabla'_p \cdot \nabla_r \quad (\nabla' \text{ acts on the left})$$

$$[A, B]_W = 2i A_W \sin(\hbar \Lambda / 2) B_W = i\hbar \{A_W, B_W\}_{P.B.} + O(\hbar^3)$$

# Test Particle Method

- Vlasov Equation

$$\frac{\partial f}{\partial t} - \{h_W, f\}_{P.B.} = \frac{\partial f}{\partial t} + v \cdot \nabla_r f - \nabla U \cdot \nabla_p f = 0$$

- Classical Hamiltonian

$$h_W(r, p) = \frac{p^2}{2m} + U(r, p)$$

- Test Particle Method (C. Y. Wong, 1982)

$$f(r, p) = \frac{1}{N_0} \sum_i^{AN_0} \delta(r - r_i) \delta(p - p_i) \quad \rightarrow \quad \frac{dr_i}{dt} = \nabla_p h_w, \quad \frac{dp_i}{dt} = -\nabla_r h_w,$$

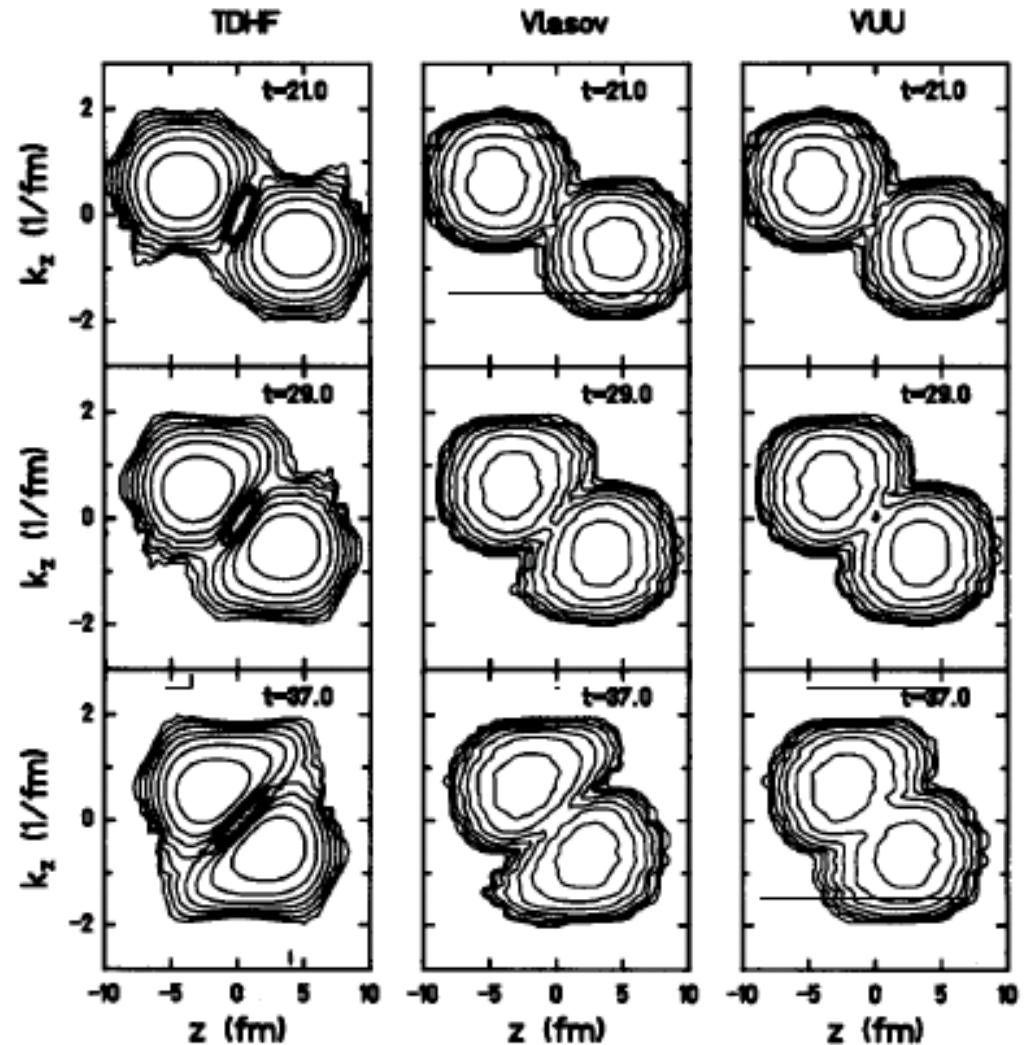
*Mean Field Evolution can be simulated*

*by Classical Test Particles*

*→ Opened a possibility to Simulate High Energy HIC  
including Two-Body Collisions in Cascade*

# Comparison of TDHF, Vlasov and BUU(VUU)

- Ca+Ca, 40 A MeV  
(Cassing-Metag-Mosel-Niita, Phys. Rep. 188 (1990) 363).





# Wigner Function

- Example: Inverted Harmonic Oscillator

$$\hat{H} = \frac{1}{2}\hat{p}^2 - \frac{1}{2}\lambda^2\hat{x}^2$$

- Equation of Motion

$$\frac{\partial W}{\partial t} = \frac{2}{\hbar} H \sin(\hbar \Lambda / 2) W = \{H, W\}_{P.B.}$$

$$(AB)_W = A_W \exp(i \hbar \Lambda) B_W \quad \Lambda \equiv \nabla'_r \cdot \nabla_p - \nabla'_p \cdot \nabla_r \quad (\nabla' \text{ acts on the left})$$

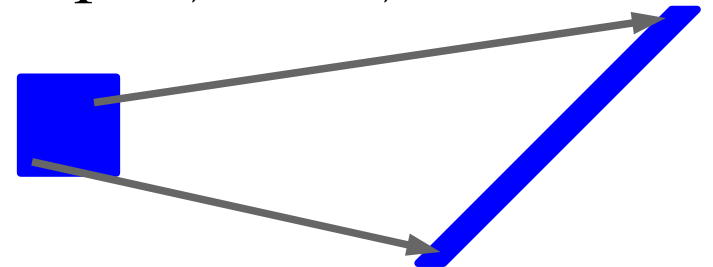
H contains only  $p^2$  and  $x^2 \rightarrow$  No  $O(\hbar^3)$  terms

$\rightarrow$  Classical EOM gives exact results

$$\frac{dx}{dt} = p, \quad \frac{dp}{dt} = \lambda^2 x \rightarrow \begin{pmatrix} x \\ p/\lambda \end{pmatrix} = \begin{pmatrix} \cosh \lambda t & \sinh \lambda t \\ \sinh \lambda t & \cosh \lambda t \end{pmatrix} \begin{pmatrix} x_0 \\ p_0/\lambda \end{pmatrix}$$

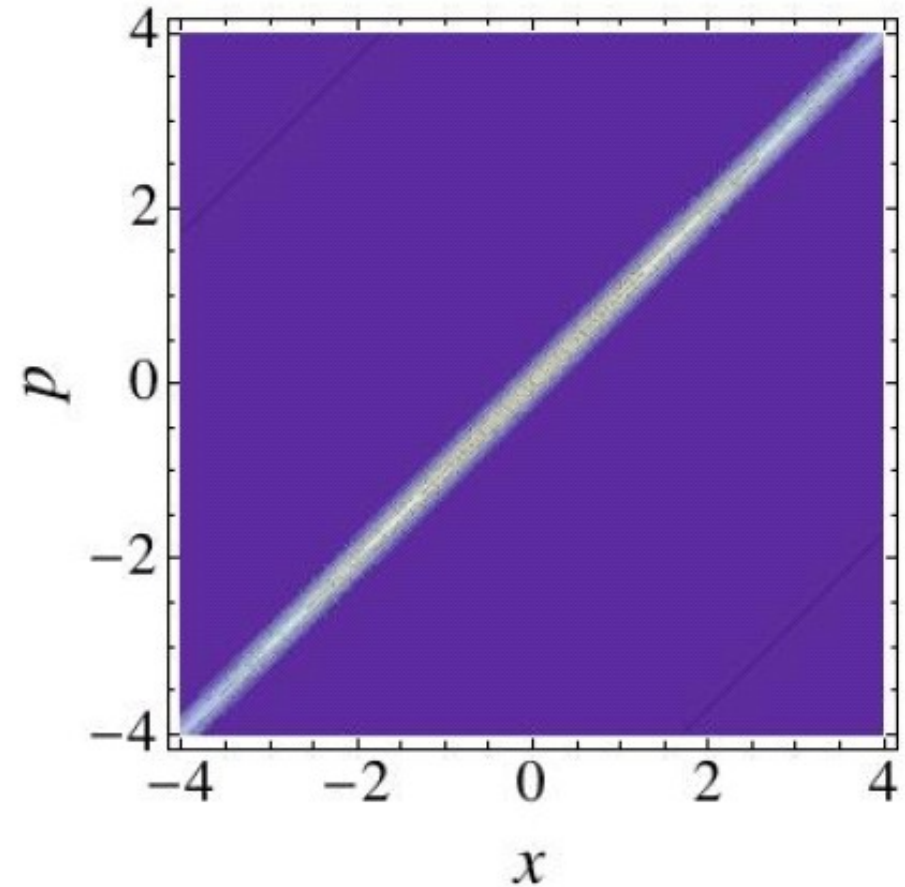
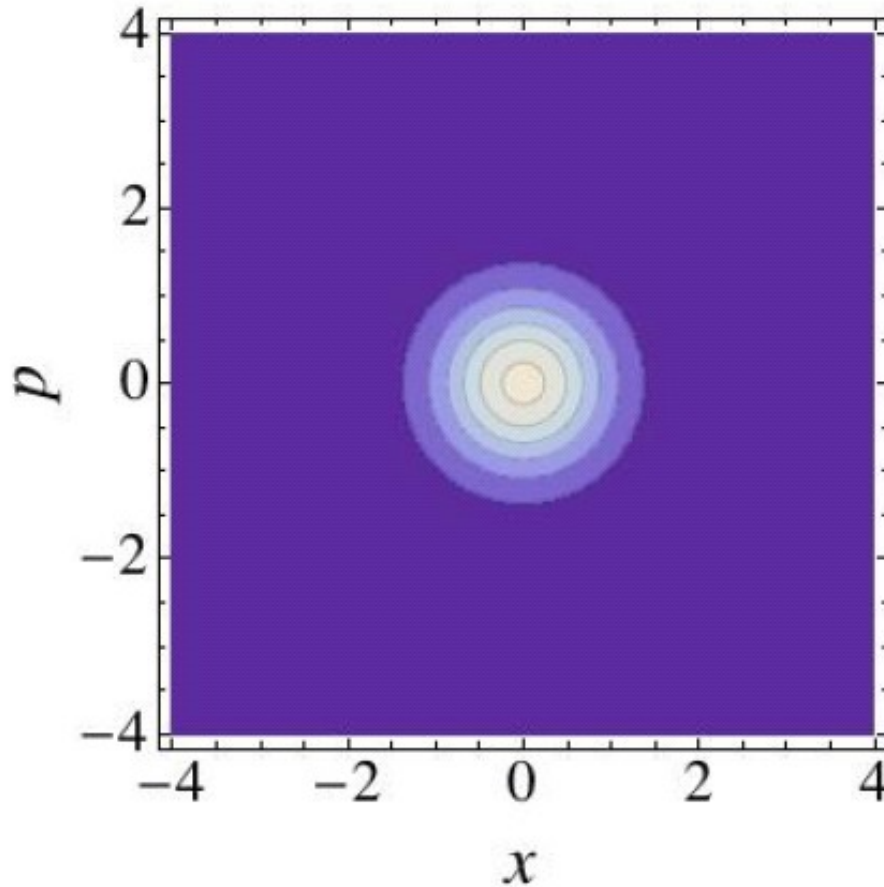
- Solution : Wigner function is constant along the classical path

$$W(x, p; t) = W(x_0(x, p, t), p_0(x, p, t); t=0)$$



# Evolution of the Wigner Function

- Liouville theorem → conservation of the phase space volume
  - Exponential growth in  $(x+p/\lambda)$ , Exponential narrowing in  $(x-p/\lambda)$



$$\hat{\mathcal{H}} = \frac{1}{2}\hat{p}^2 - \frac{1}{2}\lambda^2\hat{x}^2 \quad \lambda=1, \lambda t=0, 2$$

# Wigner-Wehrl Entropy Growth Rate

## ■ Wigner-Wehrl entropy

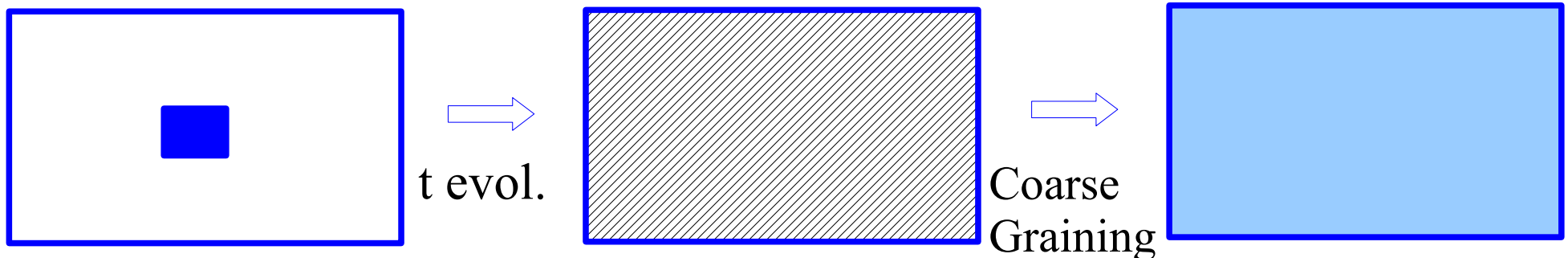
$$S_W(t) = \int d\Gamma W(x, p; t) \log W(x, p; t)$$

- Constant  $W$  along the classical path
- Liouville theorem :  $J(x(t), p(t) / x(t=0), p(t=0)) = 1$

$$\begin{aligned} S_W(t) &= \int d\Gamma W(x, p; t) \log W(x, p; t) \\ &= \int d\Gamma_0 W(x_0, p_0; t=0) \log W(x_0, p_0, t=0) = \text{const.} \end{aligned}$$

→ # of “touched” phase space cell increases,  
but no Entropy Production

→ Coarse Graining is necessary to evaluate the entropy  
coming from the complexity in the phase space



# Husimi Function

## ■ Husimi Function

- Coarse grained Wigner function by the Gaussian satisfying uncertainty principle

$$H_{\Delta}(p, x; t) \equiv \int \frac{dp' dx'}{\pi \hbar} \exp \left( -\frac{1}{\hbar \Delta} (p - p')^2 - \frac{\Delta}{\hbar} (x - x')^2 \right) W(p', x'; t)$$

- Expectation value of the density matrix with a coherent state  
→ Semi-Positive definite ( $H_{\Delta} \geq 0$ )

$$H_{\Delta}(p, x; t) = \langle z | \hat{\rho} | z \rangle$$

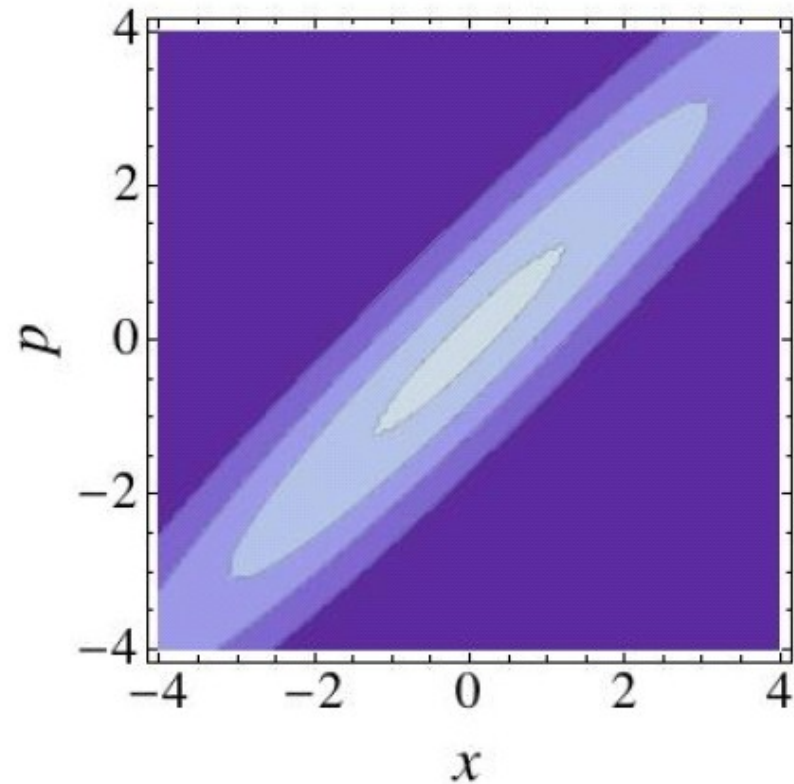
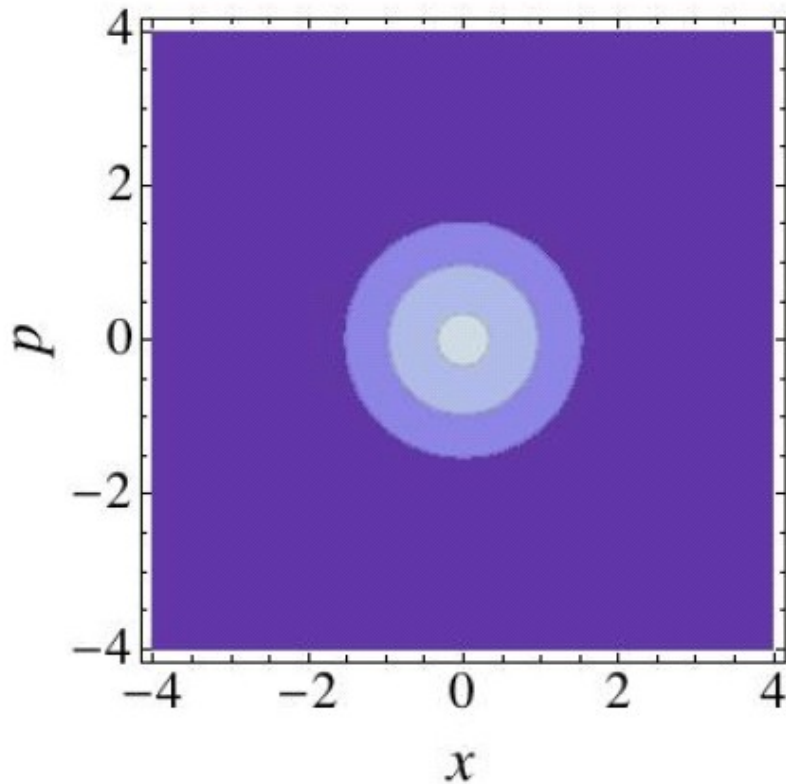
$$|z\rangle = e^{-\bar{z}z/2} \exp(z a^+) |0_{\Delta}\rangle, \quad z = \sqrt{\nu} x + \frac{i}{2\hbar\sqrt{\nu}} p, \quad \nu = \Delta/2\hbar$$

## ■ Husimi-Wehrl Entropy

$$S_{H,\Delta}(t) = - \int \frac{dp dx}{2\pi\hbar} H_{\Delta}(p, x; t) \ln H_{\Delta}(p, x; t)$$

# Evolution of the Husimi Function

- Coherent state broadening of phase space
  - Minimum width in  $(x-p/\lambda) \rightarrow$  phase space dist. func. is smeared !



$$\hat{\mathcal{H}} = \frac{1}{2}\hat{p}^2 - \frac{1}{2}\lambda^2\hat{x}^2 \quad \lambda=1, \lambda t=0, 2$$

# Husimi-Wehrl Entropy Growth Rate

## ■ Example

- Initial Cond.= g.s. of HO with freq.  $\omega$
- Hamiltonian = Inverted HO with freq.  $\lambda$

$$\hat{\mathcal{H}} = \frac{1}{2}\hat{p}^2 - \frac{1}{2}\lambda^2\hat{x}^2$$

$$S_{H,\Delta}(t) = \ln \frac{\sqrt{A(t)}}{2} + 1 = \frac{1}{2} \ln \frac{A(t)}{4} + 1$$

$$A(t) = 2(\sigma\rho \cosh 2\lambda t + 1 + \delta\delta')$$

$$\begin{aligned} \frac{dS_{H,\Delta}}{dt} &= \int \frac{dp dx}{2\pi\hbar} \frac{\partial H_{\Delta}}{\partial t} \ln H_{\Delta} + \frac{\partial}{\partial t} \int \frac{dp dx}{2\pi\hbar} H_{\Delta} = \int \frac{dp dx}{2\pi\hbar} \frac{\partial H_{\Delta}}{\partial t} \ln H_{\Delta} \\ &= \frac{\lambda \sigma\rho \sinh 2\lambda t}{\sigma\rho \cosh 2\lambda t + 1 + \delta\delta'} \xrightarrow{t \rightarrow \infty} \lambda \end{aligned}$$

*Kolmogorov-Sinai entropy appears  
in quantum mechanical problem  
with Husimi coarse graining !*

# Wigner Functional

- Canonical variables

(x, p) : Classical and Quantum Mechanics

( $\Phi, \Pi$ ): Field Theory

→ Wigner *Functional*

- Coordinate representation

$$W[\Pi(x), \Phi(x); t] = \int \mathcal{D}\varphi(x) e^{-i \int dx \Pi(x)\varphi(x)} \\ \times \langle \Phi(x) + \frac{1}{2}\varphi(x) | \hat{\rho}(t) | \Phi(x) - \frac{1}{2}\varphi(x) \rangle$$

- Momentum representation

$$W[\Phi(p), \Pi(p); t] = \int \mathcal{D}\varphi(p) \exp \left[ -i \int_0^\infty dp (\Pi^*(p)\varphi(p) + \Pi(p)\varphi^*(p)) \right] \\ \times \langle \Phi(p) + \frac{1}{2}\varphi(p) | \hat{\rho}(t) | \Phi(p) - \frac{1}{2}\varphi(p) \rangle$$

# Equation of Motion of Wigner Functional

- Hamiltonian in the momentum representation

$$\hat{H}_0 = \int_0^\infty \frac{dp}{2\pi} \left( \hat{\Pi}^\dagger(p) \hat{\Pi}(p) + (p^2 + m^2) \hat{\Phi}^\dagger(p) \hat{\Phi}(p) \right)$$

$$\hat{H} = \hat{H}_0 + V[\Phi]$$

$$\frac{\partial W[\Phi, \Pi; t]}{\partial t} = \{H, W\}_{PB} + O(\hbar^2)$$

- As far as the power of  $\Phi$  and  $\Pi$  is less than or equal to 2, classical EOM gives correct time evolution.  
→ Similar treatment to the quantum mechanics

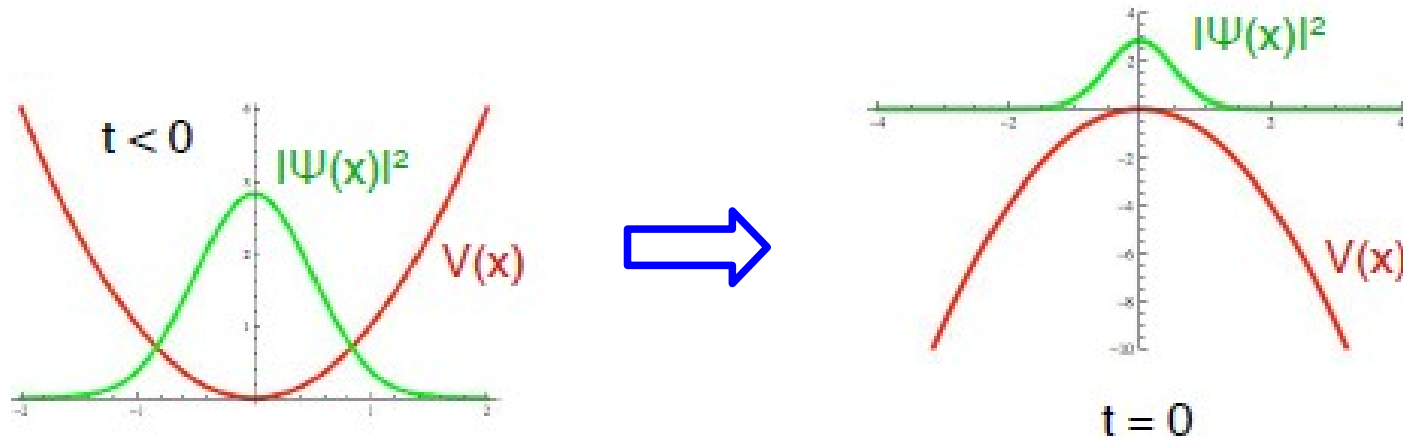


# Roll-Over Transition

- Spontaneous symmetry breaking of the vacuum  
→ Simple example: roll-over transition

$$\hat{H}(t) = \frac{p^2}{2} + \frac{m(t)^2}{2}x^2$$

$$\text{with } m^2(t) = m^2 \theta(-t) - \mu^2 \theta(t)$$



# Wigner Functional during Roll-Over

- Wigner functional is constant along classical path

$$W[\Pi, \Phi; t] = C \exp \left[ - \int \frac{dp}{2\pi} \left( \frac{|\Pi_p^0|^2}{E_p} + E_p |\Phi_p^0|^2 \right) \right]$$

- Unstable modes

$$\Phi_p^0 = \Phi_p(t) \cosh \lambda_p t - \frac{\Pi_p(t)}{\lambda_p} \sinh \lambda_p t$$

$$\Pi_p^0 = \Pi_p(t) \cosh \lambda_p t - \lambda_p \Phi_p(t) \sinh \lambda_p t$$

- Stable modes

$$\Phi_p^0 = \Phi_p(t) \cos \omega_p t - \frac{\Pi_p(t)}{\omega_p} \sin \omega_p t$$

$$\Pi_p^0 = \Pi_p(t) \cos \omega_p t + \omega_p \Phi_p(t) \sin \omega_p t$$

# Husimi-Wehrl Entropy

- Husimi-Wehrl entropy

$$S_{H,\Delta}(t) = \int \frac{D\Pi D\Phi}{2\pi} H_{\Delta} \ln H_{\Delta}$$

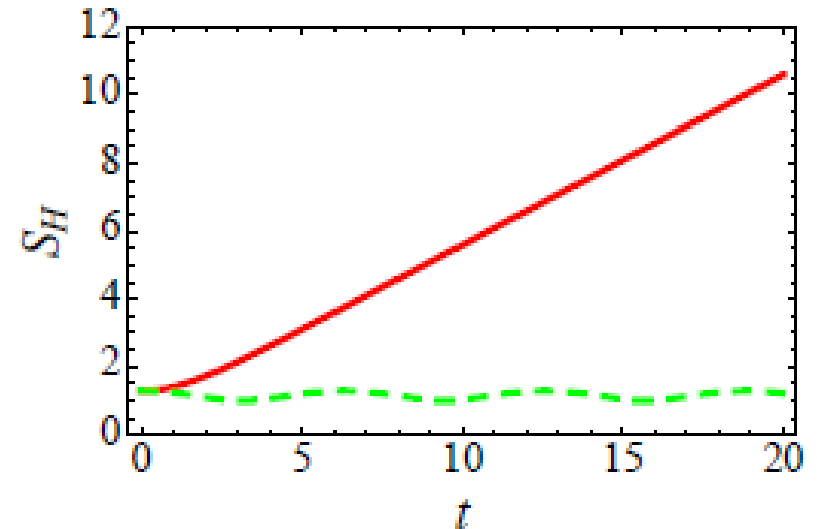
$$= V \int_{|p|<\mu} \frac{dp}{2\pi} \left[ \frac{1}{2} \ln \frac{A_p(t)}{4} + 1 \right] + V \int_{|p|>\mu} \frac{dp}{2\pi} \left[ \frac{1}{2} \ln \frac{\bar{A}_p(t)}{4} + 1 \right]$$

$$\frac{dS_{H,\Delta}}{dt} = V \int_{|p|<\mu} \frac{dp}{2\pi} \frac{\sigma_p(\Delta^2 + \lambda_p^2) \sinh 2\lambda_p t}{A_p(t)\Delta} + V \int_{|p|>\mu} \frac{dp}{2\pi} \frac{\bar{\delta}_p(\omega_p^2 - \Delta^2) \sin 2\omega_p t}{\bar{A}_p(t)\Delta}$$

$$\xrightarrow{t \rightarrow \infty} V \int_{-\mu}^{\mu} \frac{dp}{2\pi} \lambda_p = \frac{V \mu^2}{8}$$

$$A_p(t) = \frac{\Delta^2 + \lambda_p^2}{\lambda_p \Delta} \cosh 2\lambda_p t + 2 + \delta_p \frac{\Delta^2 - \lambda_p^2}{\lambda_p \Delta},$$

$$\bar{A}_p(t) = \frac{\Delta^2 + \omega_p^2}{\omega_p \Delta} + 2 + \delta_p \frac{\Delta^2 - \omega_p^2}{\omega_p \Delta} \cos 2\omega_p t$$



# Summary

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- Early stage entropy production and/or thermalization is one of the largest remaining problem in RHIC physics.
- Entropy production of isolated quantum system requires some kind of coarse graining.
- Here we have discussed the entropy production in quantum mechanical and field theoretical problems by using the Wigner function/functional, and its coarse graining, Husimi function/functional.
- With Husimi function(al), the entropy growth rate is found to be described by the Kolmogorov-Sinai (KS) entropy, which is the sum of the positive Lyapunov exponent, in the case of inverted HO potential and Roll-over transitions.

# Discussion

- Is the Husimi-Wehrl entropy consistent with the von Neumann entropy in thermal equilibrium ?  
→ Thermal equilibrium with one dim HO potential
- von Neumann entropy

$$S_{vN} \equiv - \sum_{n=0}^{\infty} w_n \ln w_n = \frac{\beta \hbar \omega}{e^{\beta \hbar \omega} - 1} - \ln(1 - e^{-\beta \hbar \omega})$$
$$= -\bar{n} \ln \bar{n} + (\bar{n} + 1) \ln(\bar{n} + 1) .$$

$$\bar{n} = \frac{1}{Z_{\beta}} \sum_{n=0}^{\infty} n w_n = \frac{1}{e^{\beta \hbar \omega} - 1}$$

- Wigner-Wehrl entropy

$$W(z) = B_{\beta} \exp(-B_{\beta} \bar{z} z) \quad B_{\beta} = 2 \tanh(\beta \hbar \omega / 2) = 1/(\bar{n} + 1/2)$$

$$S_W = 1 + \ln \left( \bar{n} + \frac{1}{2} \right)$$

# Discussion

## ■ Husimi-Wehrl entropy

Coherent state

$$|z\rangle = e^{-\bar{z}z/2} \exp(z\hat{a}^\dagger) |0\rangle = e^{-\bar{z}z/2} \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{n!}} |n\rangle$$

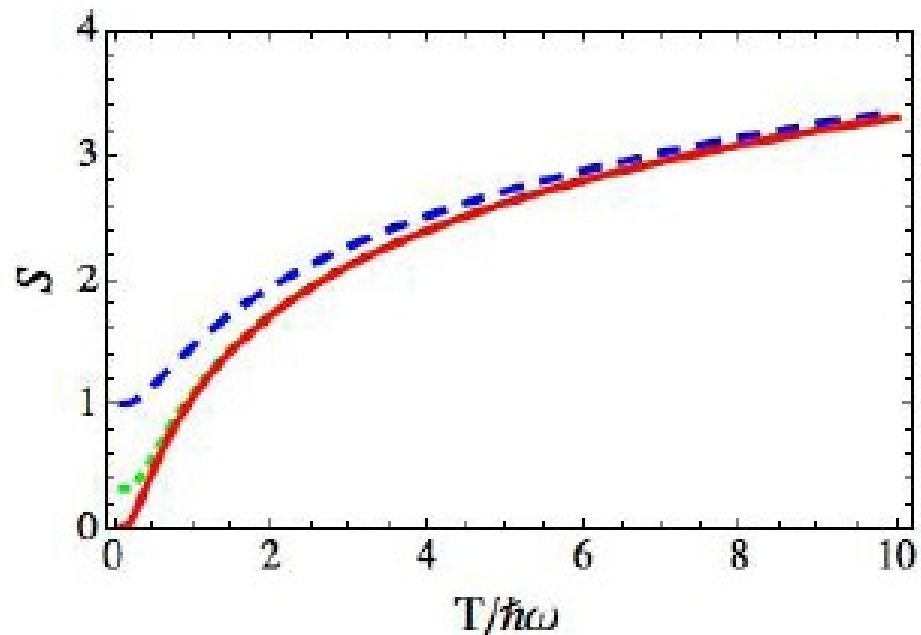
Husimi function

$$\begin{aligned} H(z) &= \langle z | \hat{\rho}_{\text{th}} | z \rangle = \frac{e^{-\bar{z}z}}{\mathcal{Z}_\beta} \sum_{n=0}^{\infty} \frac{(\bar{z}z)^n}{n!} e^{-n\beta\hbar\omega} \\ &= \frac{1}{\mathcal{Z}_\beta} \exp \left[ -\bar{z}z \left( 1 - e^{-\beta\hbar\omega} \right) \right] = A_\beta \exp(-A_\beta \bar{z}z) \\ A_\beta &= 1 - e^{-\beta\hbar\omega} = 1/(\bar{n} + 1) \end{aligned}$$

Husimi-Wehrl entropy

$$S_H = 1 - \ln A_\beta = 1 + \ln(\bar{n} + 1)$$

*With Husimi-Wehrl entropy,  
coarse graining effects  
also appears in equilibrium.*



# Entropy expression in Wave Packet Statistics

## ■ Wave packet statistical mechanics (Ohnishi-Randrup method)

### ● Partition Function

$$\mathcal{Z}_\beta = \int d\Gamma \langle z | e^{-\beta\mathcal{H}} | z \rangle = \int d\Gamma \exp \left[ - \int_0^\beta d\beta' \mathcal{H}_{\beta'}(z) \right] ,$$
$$\mathcal{H}_\beta(z) = -\frac{\partial}{\partial\beta} \ln \langle z | e^{-\beta\mathcal{H}} | z \rangle = \langle z | \mathcal{H} e^{-\beta\mathcal{H}} | z \rangle / \langle z | e^{-\beta\mathcal{H}} | z \rangle$$
$$= \langle z | \mathcal{H} | z \rangle - \beta \sigma_{\mathcal{H}}^2(z) + \mathcal{O}(\beta^2) ,$$

### ● Entropy

$$S = -\frac{\partial F}{\partial T} = \frac{\partial}{\partial T} (T \ln \mathcal{Z}_\beta) = -\beta \frac{\partial}{\partial\beta} \ln \mathcal{Z}_\beta + \ln \mathcal{Z}_\beta$$
$$= \int d\Gamma \frac{\langle z | e^{-\beta\mathcal{H}} | z \rangle}{\mathcal{Z}_\beta} [\beta \mathcal{H}_\beta(z) + \ln \mathcal{Z}_\beta] .$$
$$S_H - S = \int d\Gamma H(z) \left[ \int_0^\beta d\beta' \mathcal{H}_{\beta'}(z) - \beta \mathcal{H}_\beta(z) \right]$$
$$\simeq \int d\Gamma H(z) \left[ \frac{1}{2} \beta^2 \sigma_{\mathcal{H}}^2(z) + \mathcal{O}(\beta^3) \right] .$$

*We have systematic manner how to calculate entropy in equilibrium. Is there any similar method in Non-Eq. cases where single particle description may not be good enough ?*