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On the Origin of the Fluctuation and Dissipation in Wave Packet Dynamics

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1. Introduction

- ⋆ History of Microscopic Transport Models
- ⋆ Sources of Fluct. and Dissp.

2. Why Can Energy Expectation Value of W.P. Fluctuate ?

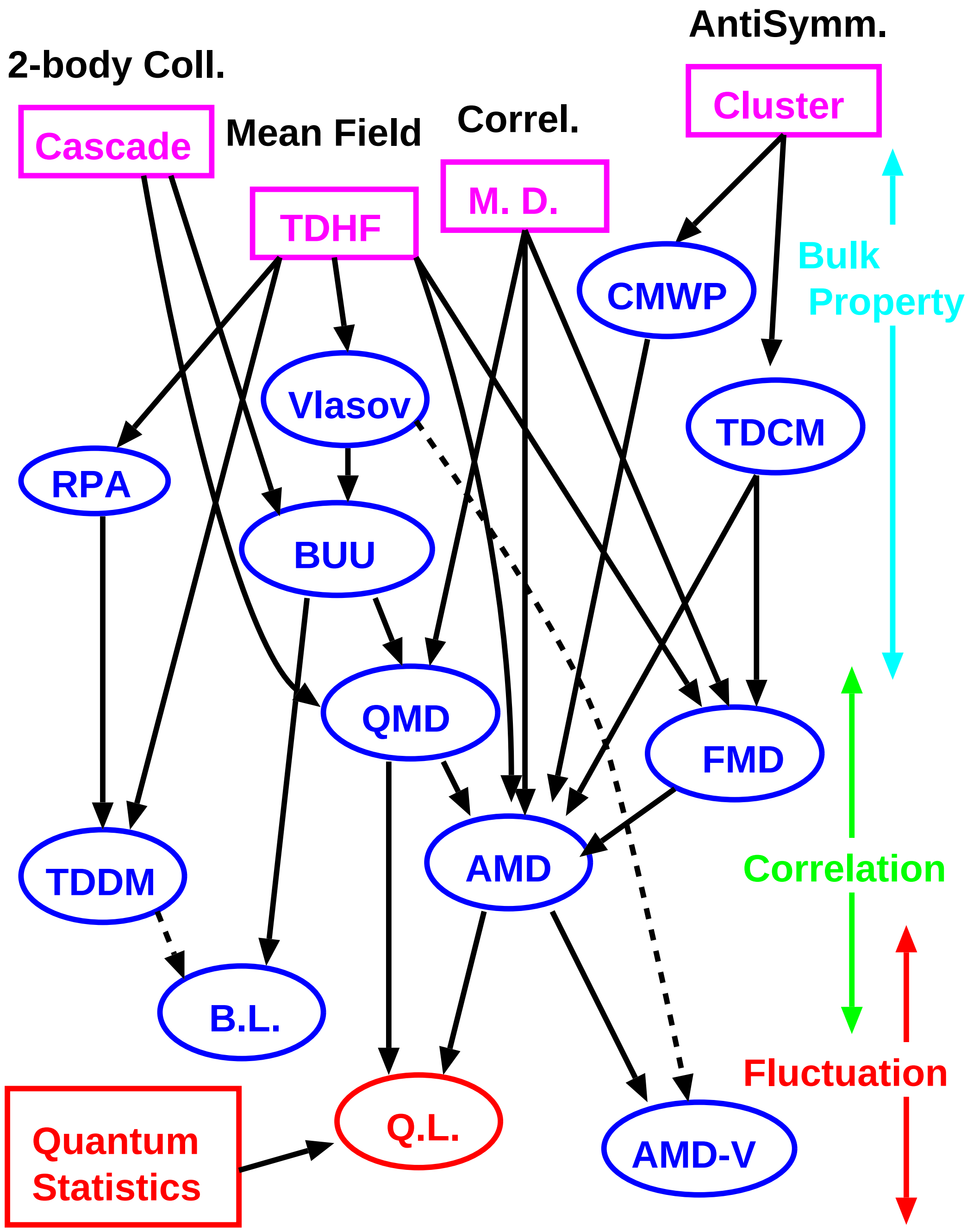
- ⋆ Time-Dependent Density Matrix theory
- ⋆ Wave Packets in Microcanonical Ensemble

3. Nuclear and Atomic Fragment Formation

- ⋆ Thermal Fragmentation
  — Similarities and Difference
  of Nuclear and Atomic Cluster Formation
- ⋆ IMF formation from Au+Au Collision
  (MSU/ALADIN data and FOPI data)

4. Summary

History of Microscopic Transport Models



Sources of Fluctuation & Dissipation

- ⋆ Initial State Correlation/Orientation
  (M.D., FMD, AMD, ...)
  - ∘ Fragment Correlation in Proj./Targ.
    (c.f. Feldmeier, Takemoto)
- ⋆ Two-Body Collision
  (Cascade, QMD, AMD, B.L., ...)
- ⋆ Mean Field/Shape Instability
  (M.D., BUU, B.L., AMD-V, ...)
  - ∘ Exponential Growth in Spinodal Region
    (c.f. Bauer, Chomaz, Toshi. Maruyama)
  - ∘ Neck, Ring, Bubble Formation
- ⋆ Created Two-body Correlation (TDDM)
  - ∘ Ladder and Ring type Diagram (c.f. Tohyama)
- ⋆ Channel Branching due to Wave Packet Diffusion
  (AMD-V)
  - ∘ Short-time Vlasov-type Evolution
    + Branching to a AMD state (c.f. Ono)
- ⋆ Inherent Energy Fluctuation of Wave Packets (Q.L.)

Problem:

- ⋆ Which can make copious fragments ?
- ⋆ Which can kill and enhance collective motion ?

Quantum Stat. Mech. of Wave Packets

Energy Fluctuation of Wave Packets

$$\sigma_E^2 = \langle \hat{H}^2 \rangle - \langle \hat{H} \rangle^2 \neq 0$$

modifies Statisitcal Weight !

- **Partition Function in Wave Packet Basis**

$$|\mathbf{Z}\rangle : \textbf{Wave Packet}, \quad \mathbf{1} = \int d\Gamma\, |\mathbf{Z}\rangle\langle\mathbf{Z}|$$

$$\mathcal{Z}_\beta \equiv \mathrm{Tr}\left(\exp(-\beta \hat{H})\right) = \int d\Gamma\ \mathcal{W}_\beta(\mathbf{Z})$$

$$\mathcal{W}_\beta(\mathbf{Z}) \equiv \langle \mathbf{Z}| \exp(-\beta \hat{H}) |\mathbf{Z}\rangle \neq \exp(-\beta \langle \hat{H} \rangle)$$

- **Thermal Average**

$$\prec \hat{O} \succ_\beta \equiv \frac{1}{\mathcal{Z}_\beta} \mathrm{Tr}\left(\hat{O} \exp(-\beta \hat{H})\right) = \frac{1}{\mathcal{Z}_\beta} \int d\Gamma\, \mathcal{W}_\beta(\mathbf{Z})\ \mathcal{O}_\beta(\mathbf{Z})$$

$$\mathcal{O}_\beta(\mathbf{Z}) \equiv \frac{\langle \mathbf{Z}_{\beta/2}|\hat{O}|\mathbf{Z}_{\beta/2}\rangle}{\langle \mathbf{Z}_{\beta/2}|\mathbf{Z}_{\beta/2}\rangle} \neq \langle \hat{O} \rangle$$

$$|\mathbf{Z}_{\beta/2}\rangle \equiv \exp(-\beta \hat{H}/2)|\mathbf{Z}\rangle \neq |\mathbf{Z}\rangle$$

$\cdots$ **Intrinsic Distortion of W.P.**

- **Harmonic Approximation**

$$\mathcal{W}_\beta(\mathbf{Z}) \approx \exp\left[-\frac{\mathcal{H}}{D}\left(1 - e^{-\beta D}\right)\right] = \exp(-\beta\mathcal{H} + \beta^2\sigma_E^2/2 + \cdots)$$

$\cdots$ **Improved β Expansion**

$$D(\mathbf{Z}) \equiv \sigma_E^2/\mathcal{H}$$

$$\mathcal{H}_\beta(\mathbf{Z}) \equiv -\frac{\partial \log \mathcal{W}_\beta(\mathbf{Z})}{\partial\beta} = \frac{\langle \mathbf{Z}_{\beta/2}|\hat{H}|\mathbf{Z}_{\beta/2}\rangle}{\langle \mathbf{Z}_{\beta/2}|\mathbf{Z}_{\beta/2}\rangle} \approx \mathcal{H}(\mathbf{Z})\ e^{-\beta D}$$

$\cdots$ **Distortion reduces E^* !**

Soluble Example

- **One Particle in a Harmonic Oscillator**

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2 \hat{r}^2}{2}$$

$$\mathcal{H} = \hbar\omega \bar{Z} Z = \frac{p^2}{2m} + \frac{m\omega^2 r^2}{2} \qquad \left(Z = \sqrt{\nu} r + \frac{i\,p}{2\hbar\sqrt{\nu}} \right)$$

$$D(\mathbf{Z}) \equiv \langle \mathbf{Z} | \hat{H}^2 - \mathcal{H}^2 | \mathbf{Z} \rangle / \mathcal{H} = \hbar\omega$$

$$\mathcal{W}_\beta(\mathbf{Z}) \equiv \langle \mathbf{Z} | \exp(-\beta \hat{H}) | \mathbf{Z} \rangle = \exp(-\alpha \beta \mathcal{H}) \qquad \left(\alpha = \frac{1 - e^{-\beta\hbar\omega}}{\beta\hbar\omega} < 1 \right)$$

$$\prec \hat{H} \succ_\beta^U \equiv \frac{1}{\mathcal{Z}_\beta} \int d\Gamma \, \mathcal{W}_\beta(\mathbf{Z}) \; \mathcal{H}(\mathbf{Z}) = \frac{T}{\alpha} > T$$

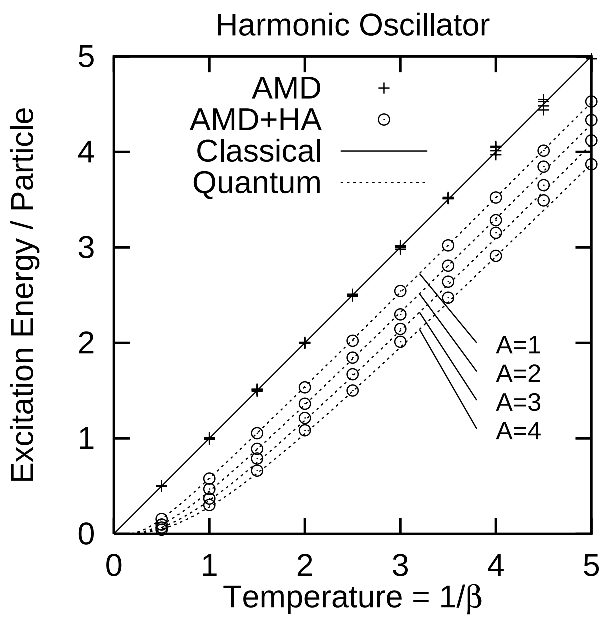
$\cdots$ **w.o Distortion = Wrong !**

$$\prec \hat{H} \succ_\beta = \frac{1}{\mathcal{Z}_\beta} \int d\Gamma \, \mathcal{W}_\beta(\mathbf{Z}) \; \mathcal{H}_\beta(\mathbf{Z}) = \frac{\hbar\omega}{e^{\beta\hbar\omega} - 1} \qquad \cdots \textbf{Exact}$$

$\cdots$ **Larger Fluctuations + Intrinsic Distortion = Exact**

- **Fermions in a Harmonic Oscillator**

(A.O. and J.Randrup, NPA 565('93),474.)



Even with AntiSymm.,

$E^* = T = 1/\beta$

without σ_E^2 **Effects**

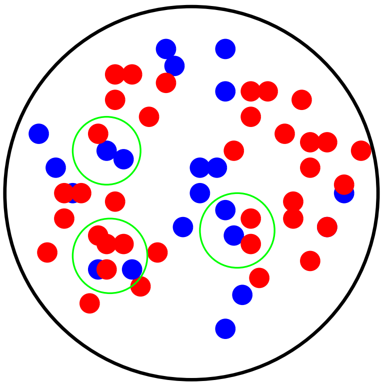
$\Downarrow$

Improved by H.A.

incl. A**-dep.**

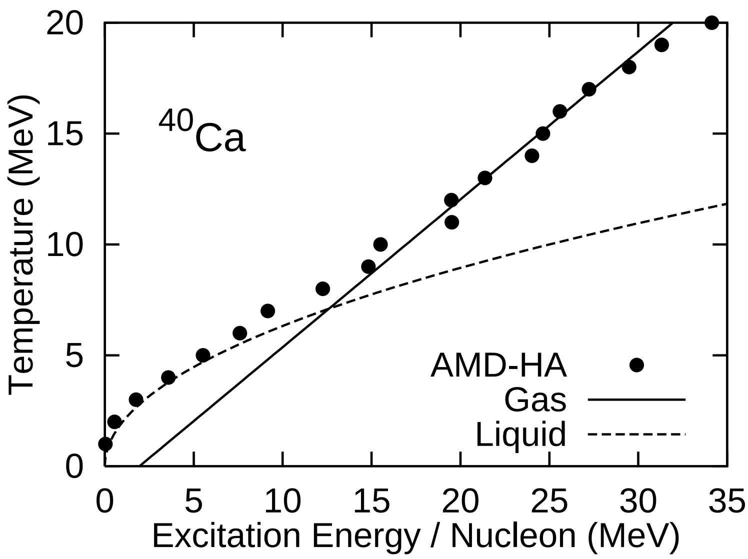
Statistical Properties of Nuclei

(A.O. and J.Randrup, PRL 75('95),596;AOP 253('97),279;
A.O. et al., Proc. NN97, NPA, in press.)



- ⋆ Equilibrium in a Sphere $R = r_0 A^{1/3}$ ($r_0 = 2.0$ fm)
- ⋆ AMD w.f. and $\mathcal{H}$ (Volkov)
- ⋆ Harmonic Approx.
- ⋆ Metropolis Sampling

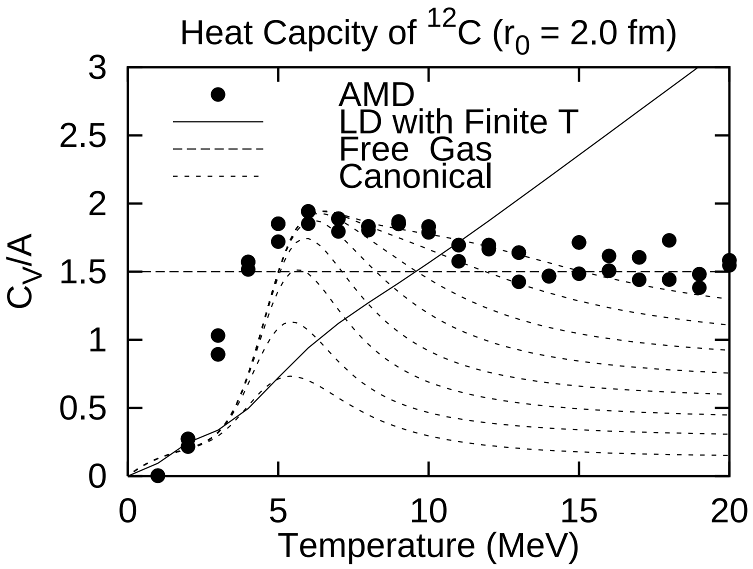
• Caloric Curve



G: $T = \frac{2}{3}(E/A - 2)$ MeV

L: $T = 2\sqrt{E/A}$ MeV

• Heat Capacity



Multifragmentation ?
Canonical
→ upto 9-body

Quantal Langevin Equation at Fixed T

- **Equilibrium Distribution**

$$\phi_{\rm eq}(\mathbf{Z}) \equiv \exp(-\mathcal{F}(\mathbf{Z})) = \langle \mathbf{Z}| e^{-\beta \hat{H}} |\mathbf{Z}\rangle$$
$$\approx \exp(-\alpha\beta\mathcal{H}) \quad \textbf{(Harmonic Approx.)}$$

- **Fokker-Planck Equation:** $\phi_{\rm eq}$ **= Static Solution**

$$\frac{D\phi(\mathbf{Z};t)}{Dt} = \frac{\partial}{\partial \mathbf{q}} \cdot \left(\mathbf{M} \cdot \frac{\partial \mathcal{F}}{\partial \mathbf{q}} + \mathbf{M} \cdot \frac{\partial}{\partial \mathbf{q}} \right) \phi \ , \quad \{\mathbf{q}\} = \{\mathbf{r}, \mathbf{p}\}$$

$$\mathbf{M} = \mathbf{g} \cdot \mathbf{g} : \quad \textbf{Mobility Tensor}$$

- **Equivalent Langevin Equation at Fixed** E

$$\dot{\mathbf{p}} = \mathbf{f} - \alpha\beta\mathbf{M}^p \cdot (\mathbf{v} - \mathbf{u}) - \beta\mathbf{M}^p \cdot \mathbf{u} + \mathbf{g}^p \cdot \zeta^p \ ,$$
$$\dot{\mathbf{r}} = \mathbf{v} + \alpha\beta\mathbf{M}^r \cdot \mathbf{f} \qquad\qquad + \mathbf{g}^r \cdot \zeta^r \ ,$$

Drift **Diffusion**

⋆ **Modified Einstein Relation:** $\alpha = \dfrac{1 - e^{-\beta D}}{\beta D} < 1$

(Smaller Friction = Larger Fluctuation)

⋆ $\mathbf{u}$ **: Local Collective Velocity ≈ Classical**

⋆ $\prec \zeta_i(t)\zeta_j(t') \succ = 2\delta(t - t')$ **: White Noise**

- **Intrinsic Distortion of Wave Packets** $\cdots \exp(-\beta\hat{H}/2)|\mathbf{Z}\rangle$

Imaginary Time Evolution = Cooling upto $\tau = \beta\hbar/2$

$$\frac{d\mathbf{p}}{d\tau} = -\frac{2\Delta p^2}{\hbar}(\mathbf{v} - \mathbf{u}) \ , \quad \frac{d\mathbf{r}}{d\tau} = \frac{2\Delta r^2}{\hbar}\mathbf{f}$$

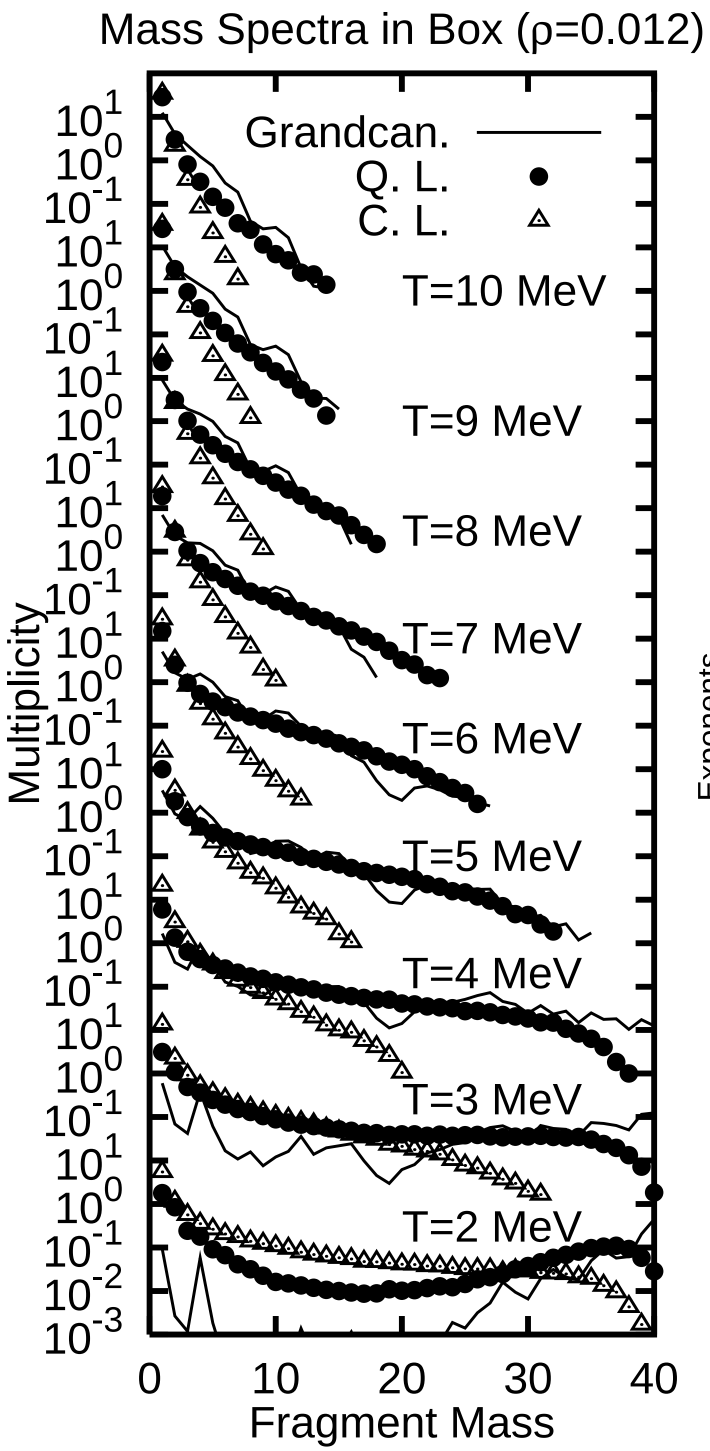
Thermal Fragmentation of Nuclei

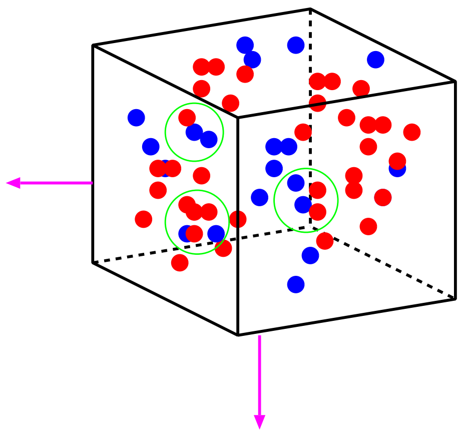
(A.O. and J. Randrup, PL B394('97), 260)

⋆ Equilibrium in a Box with Periodic B.C.

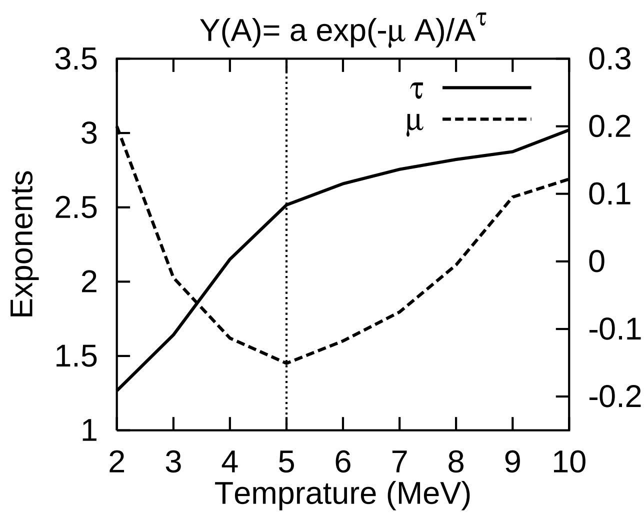
⋆ Time-Average by using QMD (Gogny) +Q.L.

- **Mass Dist. at Fixed T**





- **Critical Properties**



$$Y(A) \propto e^{-\mu A}/A^{\tau}$$

$$\tau \simeq 2.5$$

Quantal Langevin Equation at Fixed E

- **Equilibrium Distribution $\cdots$ Q. Microcan.**

$$\phi_{\rm eq}(\mathbf{Z}) \equiv \exp(-\mathcal{F}(\mathbf{Z})) = \langle \mathbf{Z} | \delta(E - \hat{H}) | \mathbf{Z} \rangle \neq \delta(E - \mathcal{H})$$

- **Fokker-Planck Equation: $\phi_{\rm eq}$ = Static Solution**

$$\frac{D\phi(\mathbf{Z};t)}{Dt} = \frac{\partial}{\partial \mathbf{q}} \cdot \left(\mathbf{M} \cdot \frac{\partial \mathcal{F}}{\partial \mathbf{q}} + \mathbf{M} \cdot \frac{\partial}{\partial \mathbf{q}} \right) \phi \ , \quad \{\mathbf{q}\} = \{\mathbf{r}, \mathbf{p}\}$$

$$\mathbf{M} = \mathbf{g} \cdot \mathbf{g} : \quad \text{Mobility Tensor}$$

- **Equivalent Langevin Equation at Fixed E**

$$\begin{aligned} \dot{\mathbf{p}} &= \mathbf{f} - \beta_{\mathcal{H}} \mathbf{M}^p \cdot (\mathbf{v} - \mathbf{u}) + \mathbf{g}^p \cdot \zeta^p \ , \\ \dot{\mathbf{r}} &= \mathbf{v} + \beta_{\mathcal{H}} \mathbf{M}^r \cdot \mathbf{f} \qquad\qquad + \mathbf{g}^r \cdot \zeta^r \ , \end{aligned}$$

Drift **Diffusion**

$\star$ **Effective Inverse Temperature:**

$$\beta_{\mathcal{H}} \equiv \frac{\partial \mathcal{F}}{\partial \mathcal{H}} \approx \frac{\mathcal{H} - E}{\sigma_E^2} \qquad (\text{Harm. Approx. to } \langle \mathbf{Z} | \delta(E - \hat{H}) | \mathbf{Z} \rangle)$$

$\cdots$ **Drift Term Acts as a Energy Recovering Force**

$\star$ $\mathbf{u}$ **: Local Collective Velocity $\approx$ Classical**

$\star$ $\prec \zeta_i(t) \zeta_j(t') \succ = 2\delta(t - t')$ **: White Noise**

- **Intrinsic Distortion of Wave Packets** $\cdots \sqrt{\delta(E - \hat{H})} | \mathbf{Z} \rangle$

Canonical-type Distortion is used.

$$\frac{d\mathbf{p}}{d\tau} = -\frac{2\Delta p^2}{\hbar} (\mathbf{v} - \mathbf{u}) \ , \quad \frac{d\mathbf{r}}{d\tau} = \frac{2\Delta r^2}{\hbar} \mathbf{f}$$

until $\mathcal{H} = E$ before making an observation

Soluble Example

• **Distinguishable Particles in a Harmonic Oscillator**
(A.O. and J.Randrup, AOP 253('97),279.)

⋆ **Number of States = Phase Volume**

$$\Omega(E) = \frac{(E+N-1)!}{E!\,(N-1)!} = \frac{\Gamma(E+N)}{\Gamma(E+1)\Gamma(N)}$$

$$\frac{1}{T} \equiv \frac{\partial}{\partial E}\log(\Omega(E))$$

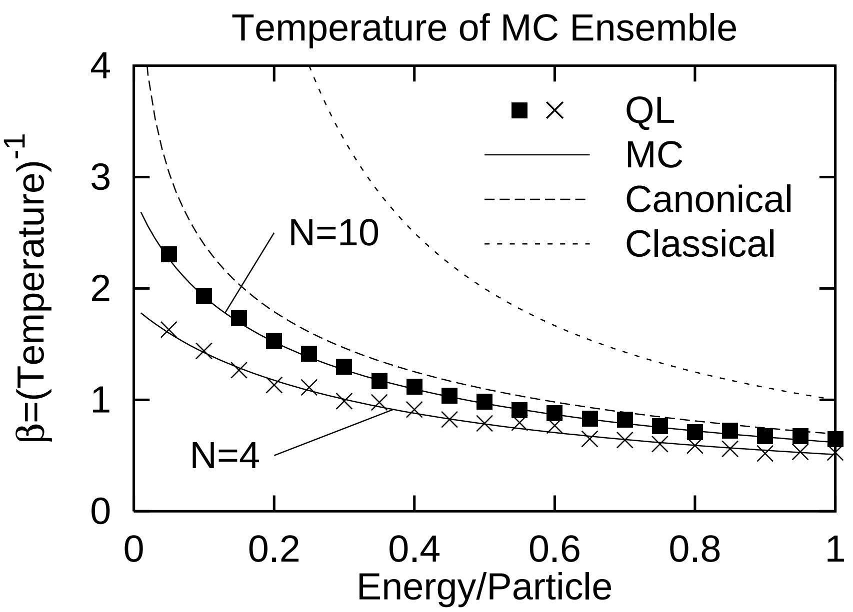
⋆ **Harm. Approx. to** $\langle \mathbf{Z}|\delta(E-\hat{H})|\mathbf{Z}\rangle$

$$\rho_E(\mathbf{Z}) \equiv \langle \mathbf{Z}|\delta(E-\hat{H})|\mathbf{Z}\rangle \approx \; e^{-\mathcal{H}} \frac{\mathcal{H}^E}{\Gamma(E+1)}$$

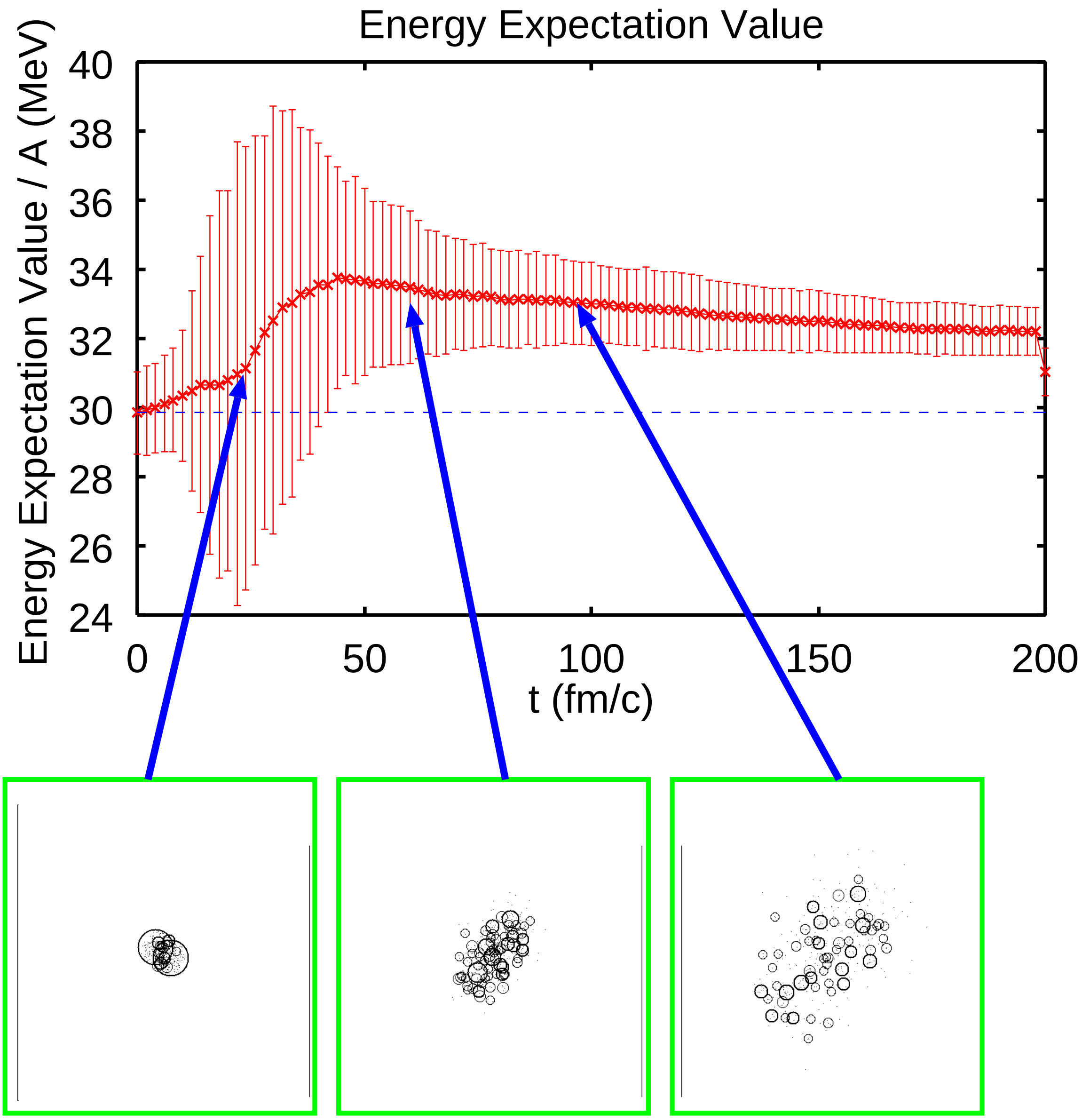
⋆ **Quantal Langevin Model**

$$\frac{1}{T} \equiv \frac{1}{\Omega(E)} \int d\Gamma \rho_E(\mathbf{Z}) \;\beta_E(\mathbf{Z}) \approx \prec \beta_E(\mathbf{Z}) \succ_{TimeAverage}$$

$$\beta_E(\mathbf{Z}) \equiv \frac{\partial \log(\rho_E(\mathbf{Z}))}{\partial E} \qquad > \beta_{\mathcal{H}}$$



- **Example of Energy Fluctuation**

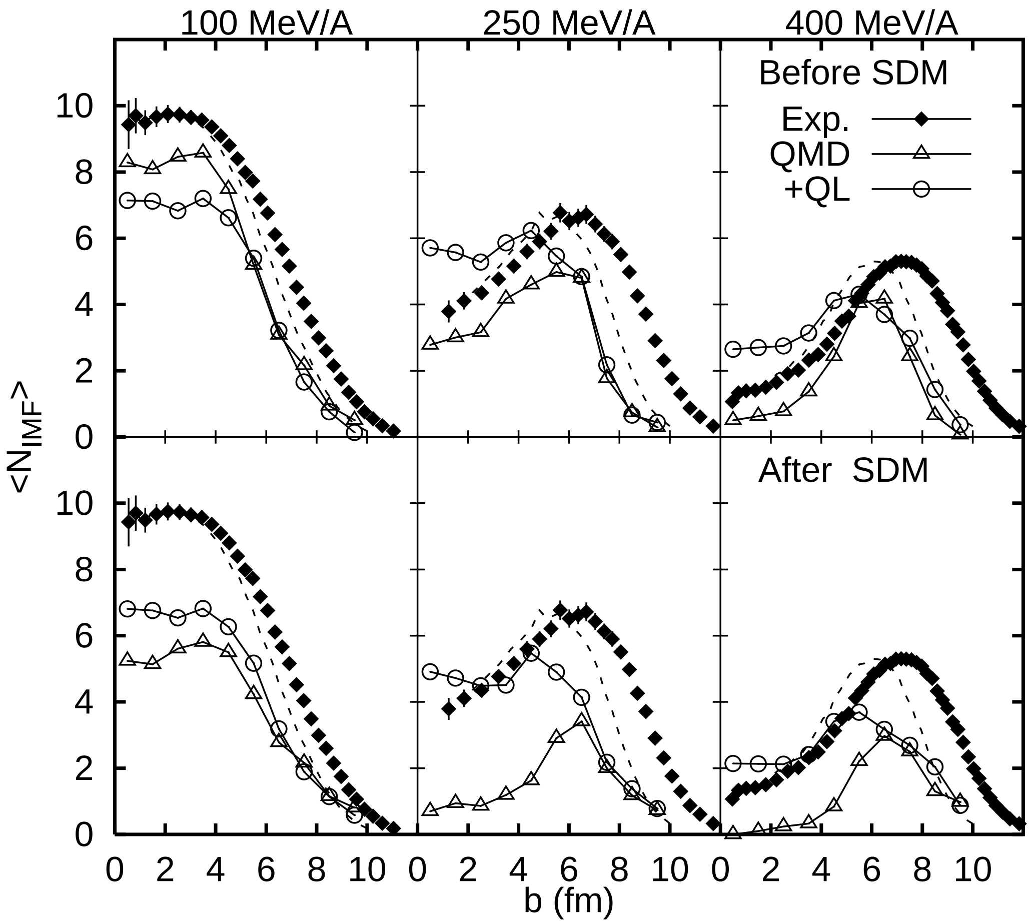


Multifragmentation from Au+Au

• **MSU/ALADIN Data —**

E_{inc} and b-dependence of IMF Multiplicities

M.B.Tsang et al., PRL 71 ('93), 1502.
A.O. and J. Randrup, PL B394('97), 260.
c.f. Iwamoto et al. PTP 98('97),87.
Barz et al. PLB 359('96),261.



⋆ **Exp.:** b_{imp} **sort = PM,** $3 \leq Z_{imf} \leq 30$

⋆ **Calc.: QMD, Gogny+Pauli, No Det. Eff. is incl.**

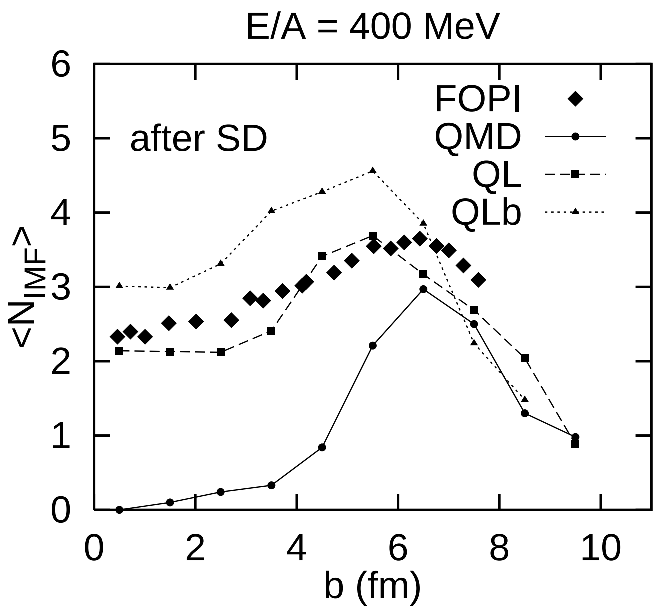
→ **Dynamically Produced Fragments are cool enough to Survive Statistical Decay in QMD-QL !**

• **FOPI Data —**

IMF Multiplicities and Z Distribution

W. Reisdorf et al., NP A612 ('97), 493

⋆ **IMF Multiplicities**



⋆ **Exp:**

b_{imp} **sort** $=$ **ERAT**

$3 \le Z_{imf} \le 15$

⋆ **Calc.:**

QMD, Gogny+Pauli

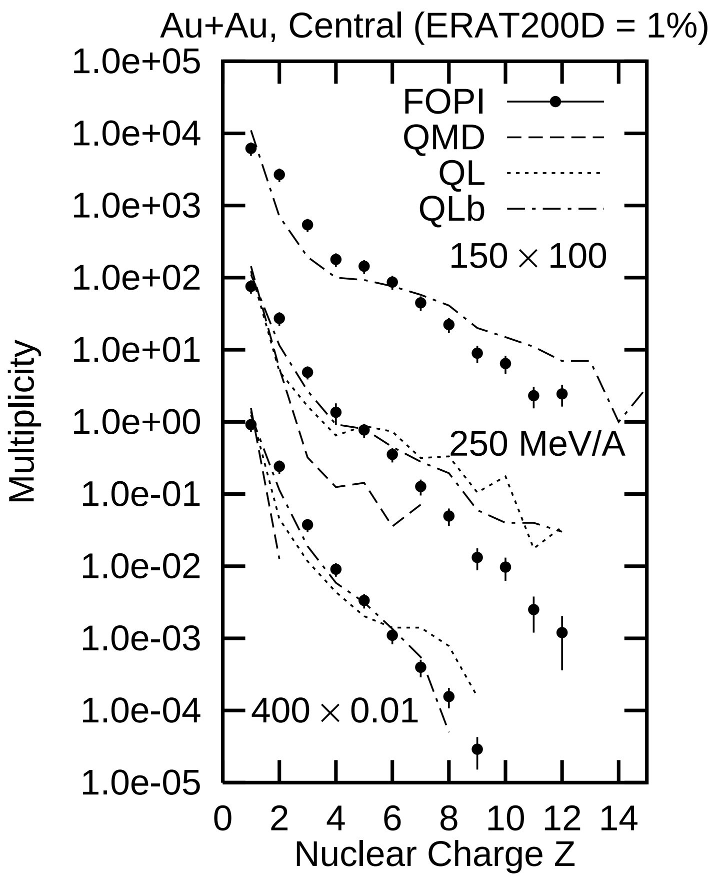
No Det. Eff. is incl.

⋆ **QLb:**

with Cluster coll.

→ **Flatter b dependence with ERAT sort**

⋆ **Charge Distribution**

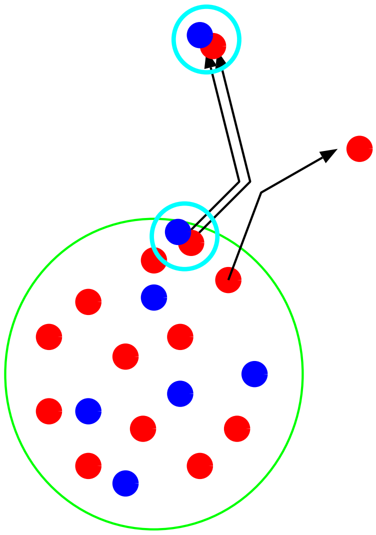


- **Cluster-Cluster Scattering**

Danielewicz and Bertsch, NP A533 ('91), 712: (d, t, h)

Ono et al., PRC 47 ('91), 2652: (Nα)

Y. Nara et al. PL B346 ('95), 217: ($K^{-}\alpha \rightarrow \pi^{4}_{\Lambda}$H)

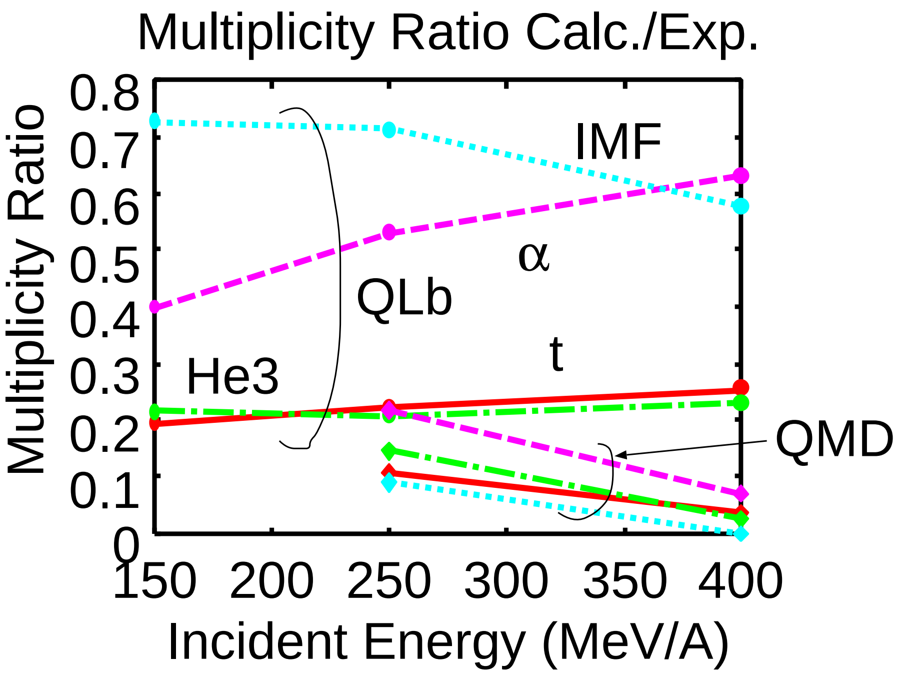


Cluster-Cluster (or N) Scattering

- **Black Disc Ang. Dist. &σ are assumed**
- **Seed of IMFs**
- **Only 0s clusters are considered**

- **Light Charged Particle Multiplicity**

··· **Large underestimate for A=3**



Summary

- Origin of Fluctuation of Wave Packet Energy

1. Wave Packets are not Energy Eigen States.
2.
3. Dynamical Relaxation to Quantum Stat. Equil.
4. Larger Fluctuations (Quantum & Statistical)
   +Intrinsic Distortion (Smaller Excitation Energy)
   Enhancement of Stable Dynamical Fragments

- Achievements

a. Caloric Curve (Liquid → Gas)

b. Thermal Fragmentation (Critical behavior)

c. Dynamical Fragmentation (Au+Au)

- Remaining Problems

⋆ Mobility Tensor M cannot be determined only from stat. requirements.

⋆ Light Charged Particle (LCP) formation ($d, t, {}^3$He$, \alpha$)
Underesitmate by a factor of 4 ∼ 10 for $A = 3$
→ Coalescence ?