INNOCOM 97, Nov. 14, 1997

Molecular Dynamics with Quantum Fluctuations and Its Application to Heavy-Ion Collisions

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1. Introduction

2. Statistical Properties of Wave Packet System

- ⋆ **Energy Dispersion and Harmonic Approx.**
- ⋆ **Caloric Curve of Nuclear Matter**

3. Fragmentation at Fixed Temperature

- ⋆ **Quantum Langevin Model at Fixed β**
- ⋆ **Nuclear and Atomic Fragment Formation**

4. Application to Heavy-Ion Collisions

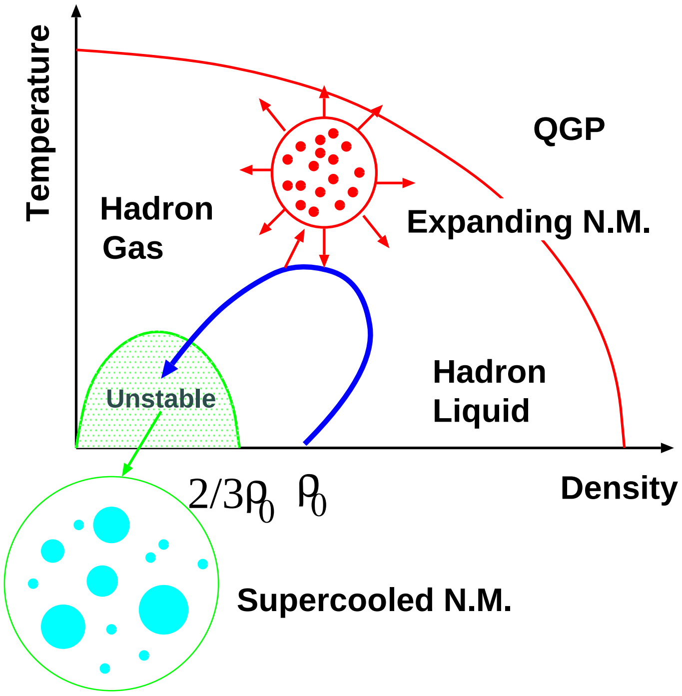
- ⋆ **Quantum Langevin Model at Fixed E**
- ⋆ **IMF formation from Au+Au Collision (MSU/ALADIN data and FOPI data)**

5. Summary and Outlook

A.O. and J. Randrup, PRL 75('95), 596
A.O. and J. Randrup, AOP 253('97), 279
A.O. and J. Randrup, PL B394('97), 260
A.O. and J. Randrup, PRA 55('97), 3315R
A.O. et al., NN97 Proc, NPA ('97), in press
Y.Hirata, Y.Nara, A.O., T.Harada, and J.Randrup, in preparation

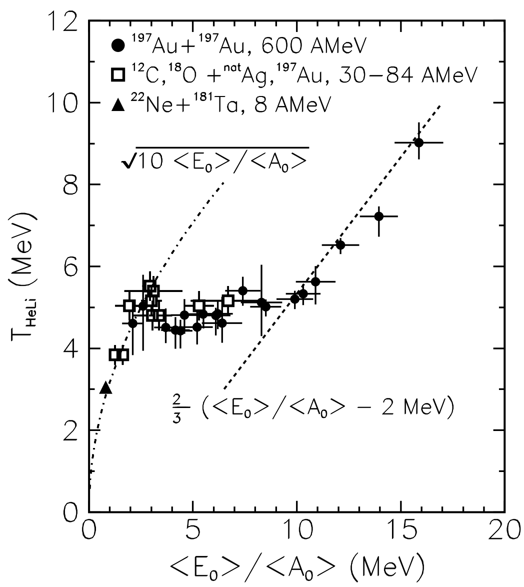
Nuclear Liquid-Gas Phase Transition

- Phase Diagram



- Caloric Curve

J.Pochadzalla et al., PRL75('95),1040.



(Low-T: $E^*/A = aT^2$
$\rightarrow$ High-T: $E^* = 1.5T + c$)

Problem:

If L.G.P.T. is responsible
for Multifragmentation,
Statistical Property is Essential.

$\rightarrow$ Can we understand it
in Microscopic Transport Models ?

Microscopic Transport Models
to Nuclear Multi-Fragmentation

- **(Semi-)Classical M.D.-type Models**

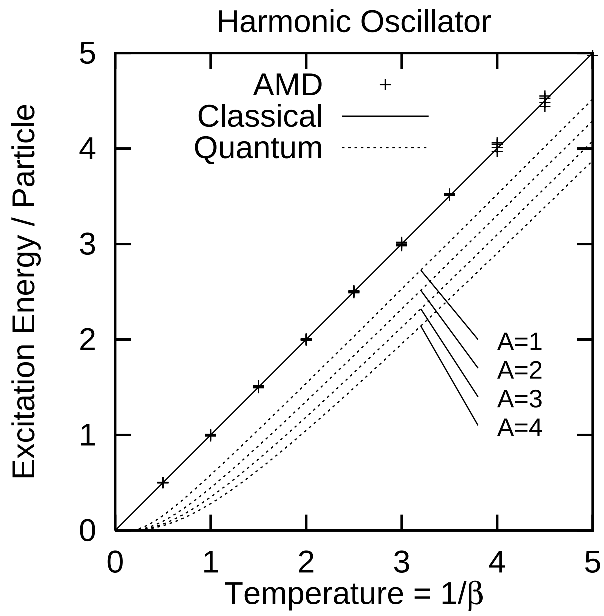
A.O. and J.Randrup, NPA 565('93),474.
c.f. Schnack-Feldmeier, NPA 601('96), 181.
Ono-Horiuchi, PRC 53('96), 2341.

⋆ **Equation of Motion**

$$\dot{\mathbf{r}} = \frac{\partial \mathcal{H}}{\partial \mathbf{p}}$$
$$\dot{\mathbf{p}} = -\frac{\partial \mathcal{H}}{\partial \mathbf{r}}$$

⋆ **Partition Function**

$$\mathcal{Z} = \int d\Gamma \exp(-\beta \mathcal{H})$$



→ $E^* \propto T \equiv 1/\beta$ **even at low** T

→ **Too Small** T (≃ **Strength of Flucts.) at a given** E

- **Transport Models with Fluctuations**

1. Boltzmann-Langevin Approach
2. AMD-V (Ono-Horiuchi)
3. Quantum Langevin Model (Ohnishi-Randrup)

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**

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

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

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

- **Thermal Average**

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

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

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

$\cdots$ **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 !**

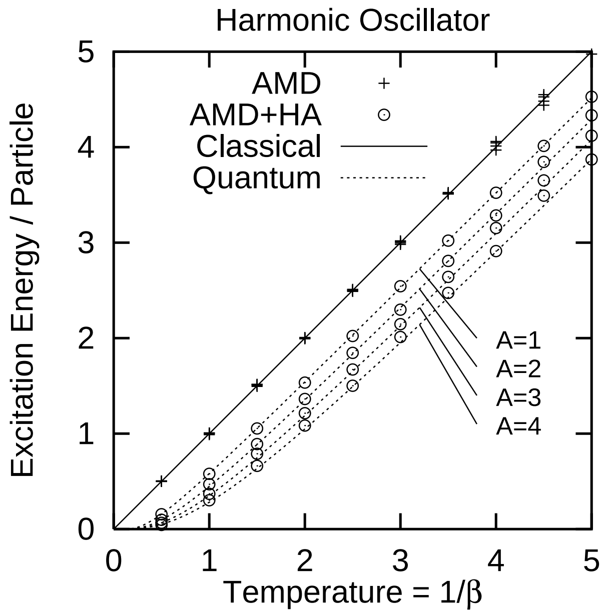
$$\prec \hat{H} \succ_\beta = \frac{1}{\mathcal{Z}_\beta}\int d\Gamma\, \mathcal{W}_\beta(\mathbf{Z})\;\mathcal{H}_\beta(\mathbf{Z}) = \frac{\hbar\omega}{e^{\beta\hbar\omega}-1}$$

$\cdots$ **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**

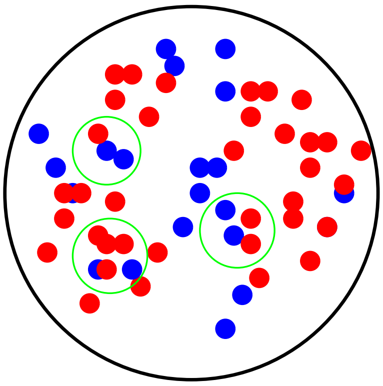
$\Downarrow$

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.)



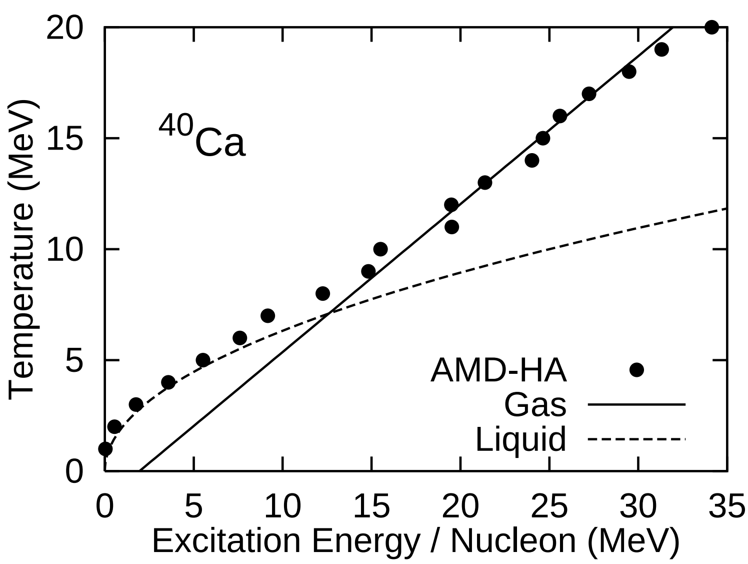
⋆ Equilibrium in a Sphere $R = r_0 A^{1/3}$ ($r_0 = 2.0$ fm)

⋆ AMD w.f. and $\mathcal{H}$ (Volkov)

⋆ Harmonic Approx.

⋆ Metropolis Sampling

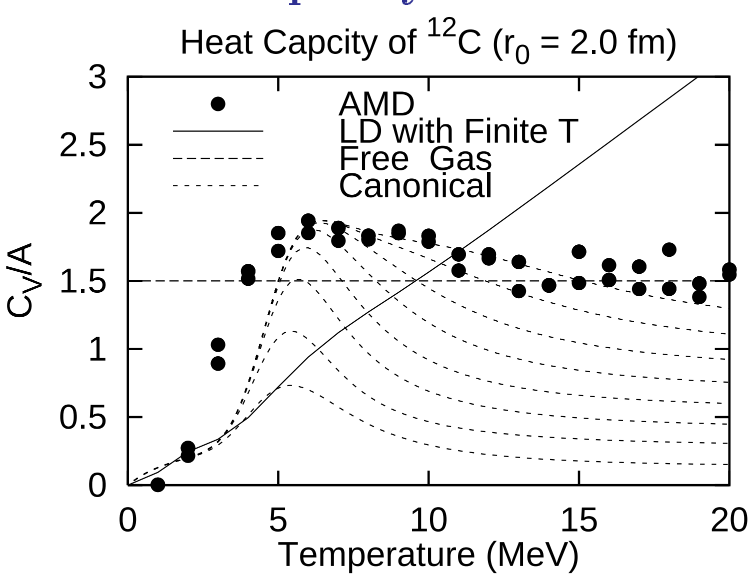
- **Caloric Curve**



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**

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

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

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

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

- **Equivalent Langevin Equation at Fixed** E

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

Drift **Diffusion**

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

(Smaller Friction = Larger Fluctuation)

$\star$ $\mathbf{u}$ **: 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** $\cdots\exp(-\beta\hat{H}/2)|\mathbf{Z}\rangle$

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

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

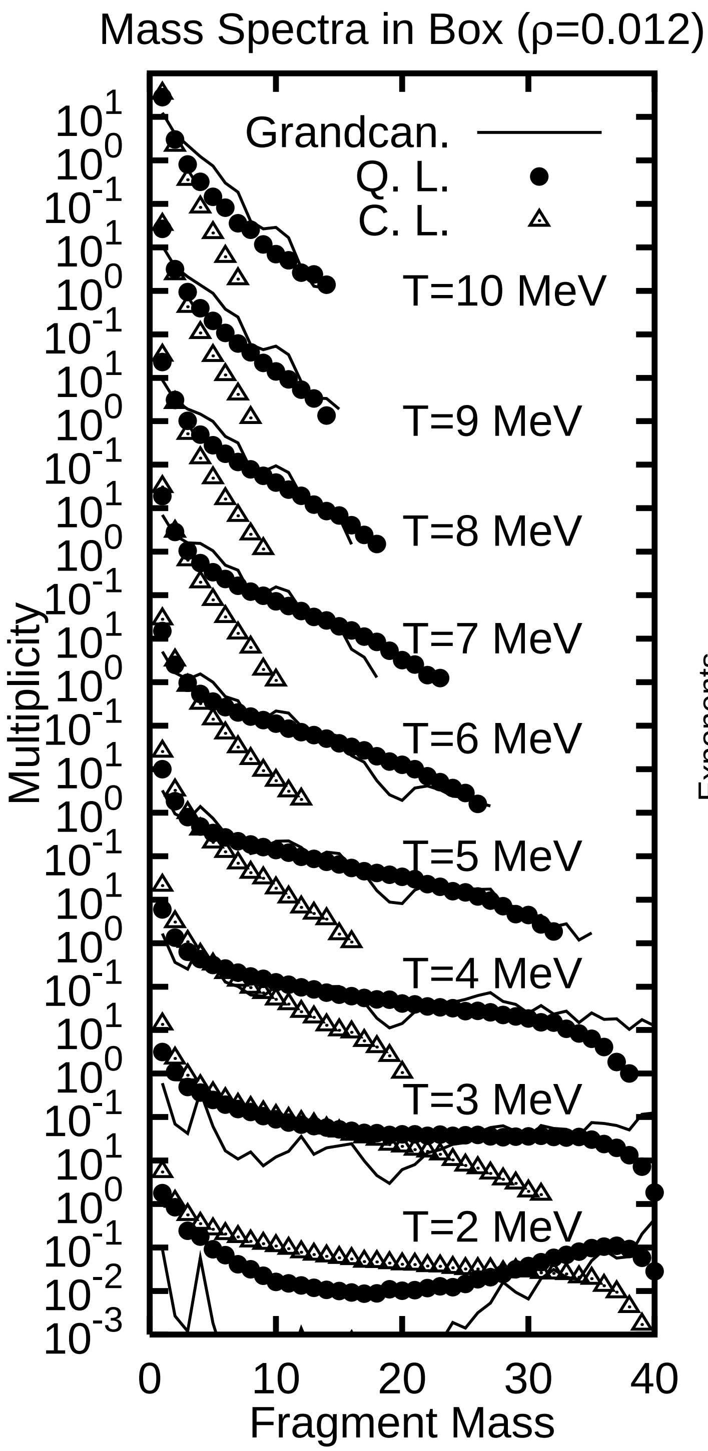
Thermal Fragmentation of Nuclei

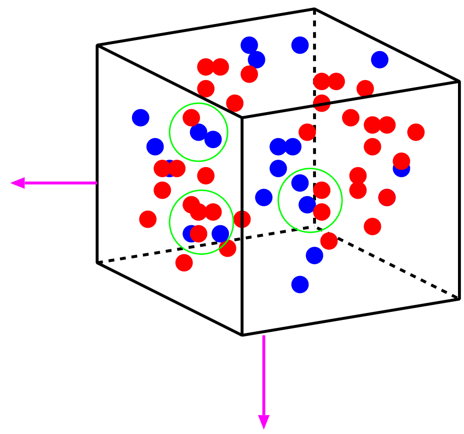
(A.O. and J. Randrup, PL B394('97), 260)

⋆ Equilibrium in a Box with Periodic B.C.

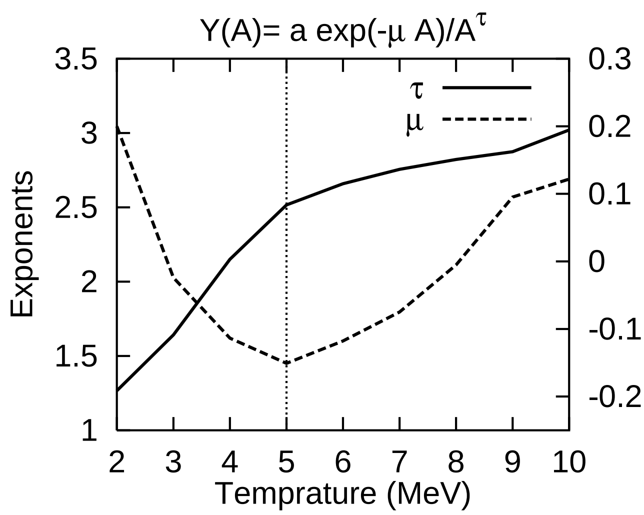
⋆ Time-Average by using QMD (Gogny) +Q.L.

- **Mass Dist. at Fixed T**





- **Critical Properties**



$$Y(A) \propto e^{-\mu A}/A^{\tau}(A \leq 15)$$
$$\tau \simeq 2.5$$

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**

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

Drift Diffusion

$\star$ Effective Inverse Temperature:

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

$\cdots$ 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.)

$\star$ **Number of States = Phase Volume**

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

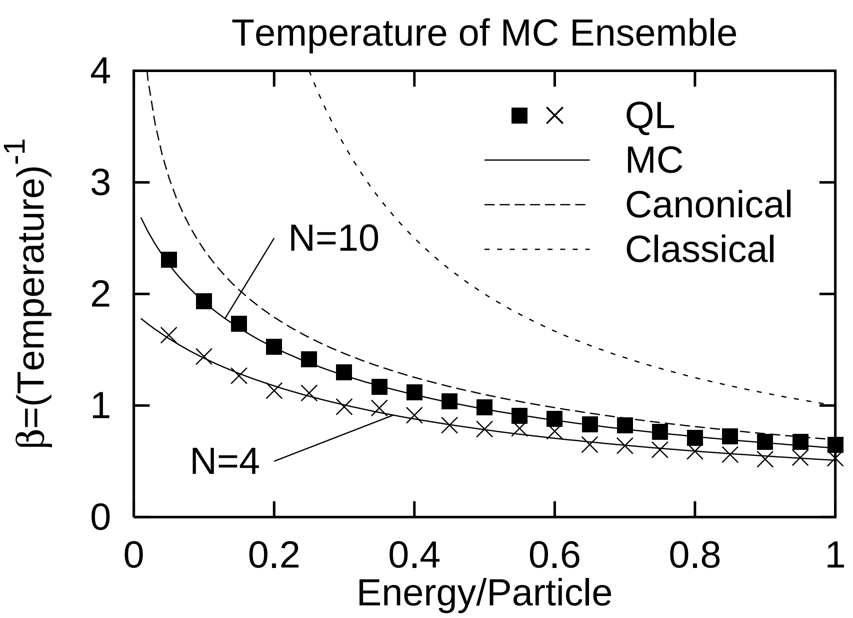
$\star$ **Harm. Approx. to** $\langle \mathbf{Z}|\delta(E-\hat{H})|\mathbf{Z}\rangle$

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

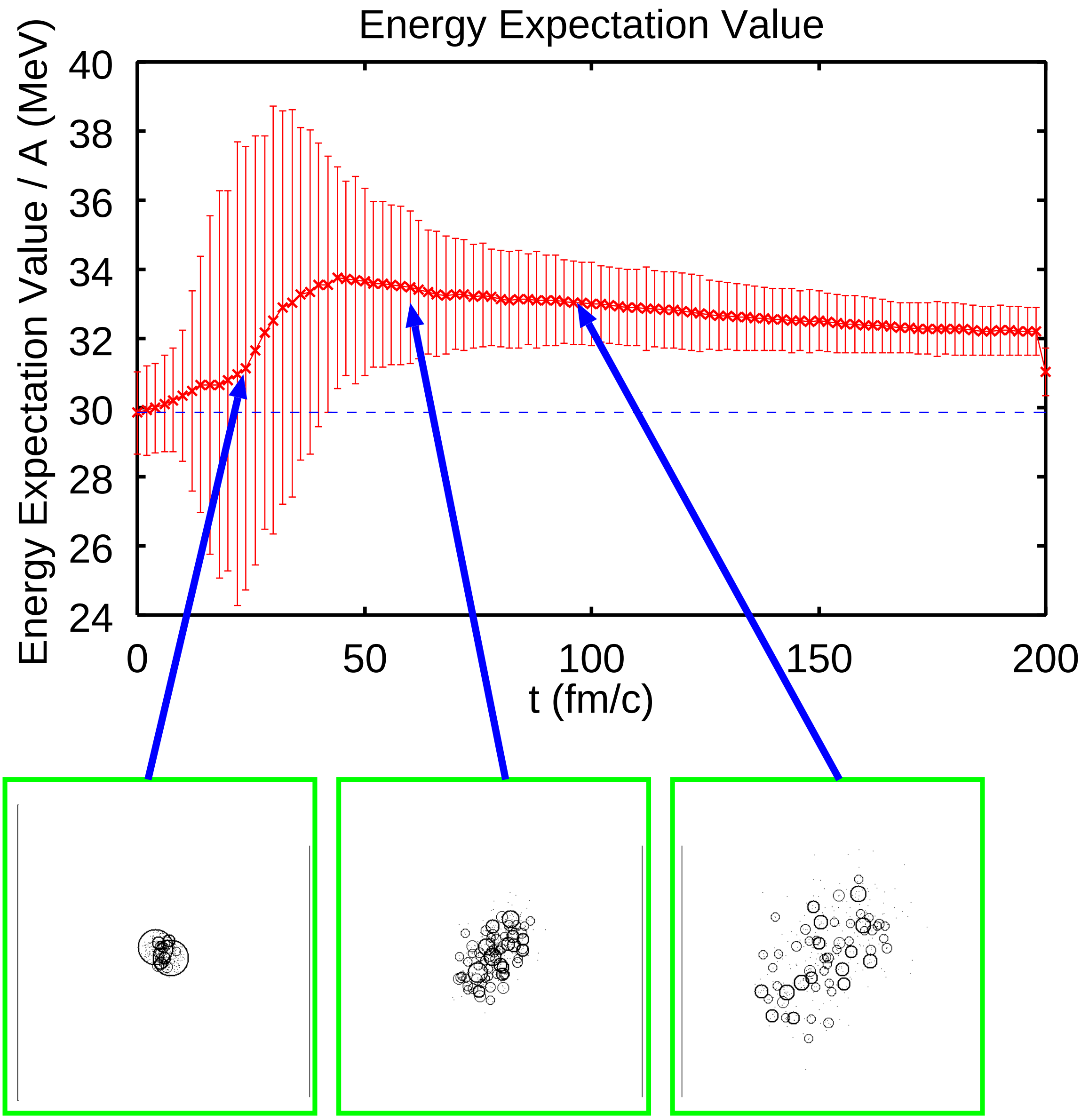
$\star$ **Quantal Langevin Model**

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

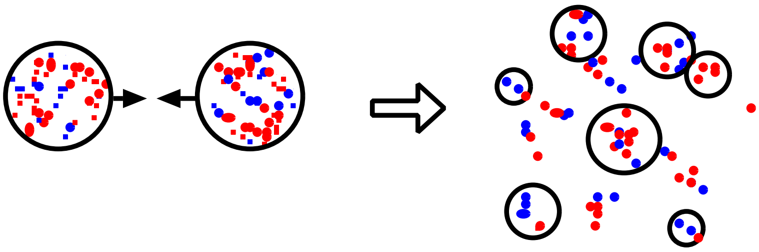
$$\beta_E(\mathbf{Z}) \equiv \frac{\partial\log(\rho_E(\mathbf{Z}))}{\partial E} \qquad > \beta_{\mathcal{H}}$$



- **Example of Energy Fluctuation**

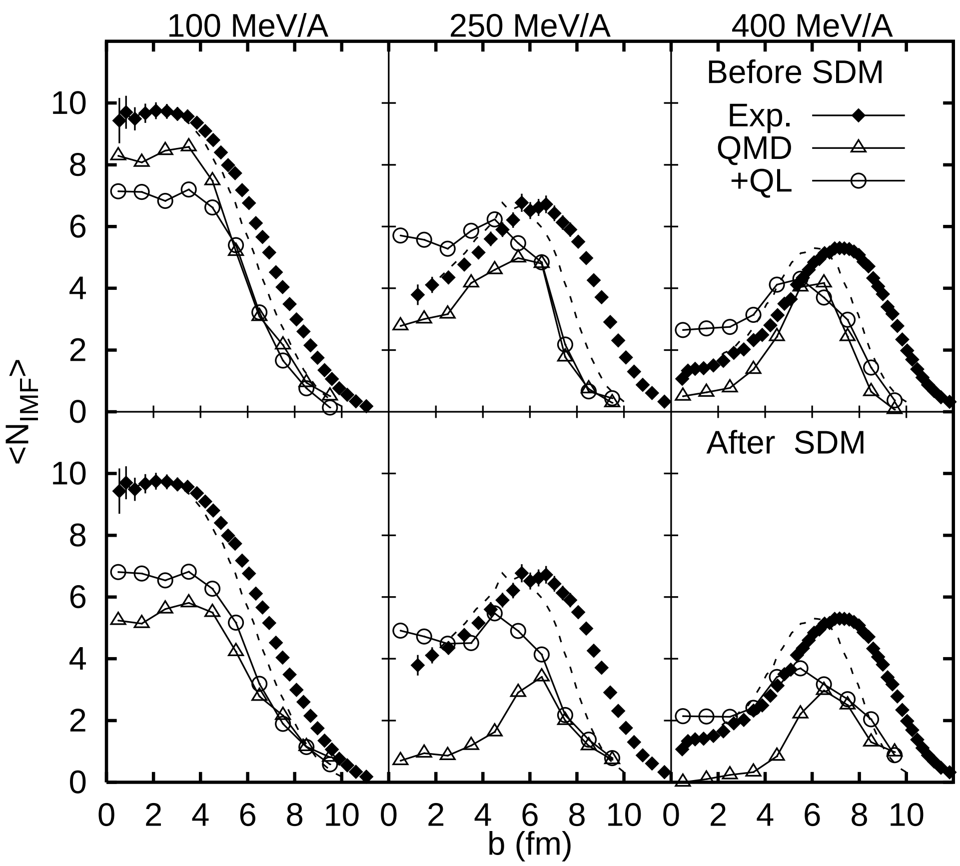


Multifragmentation from Au+Au



- **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.**

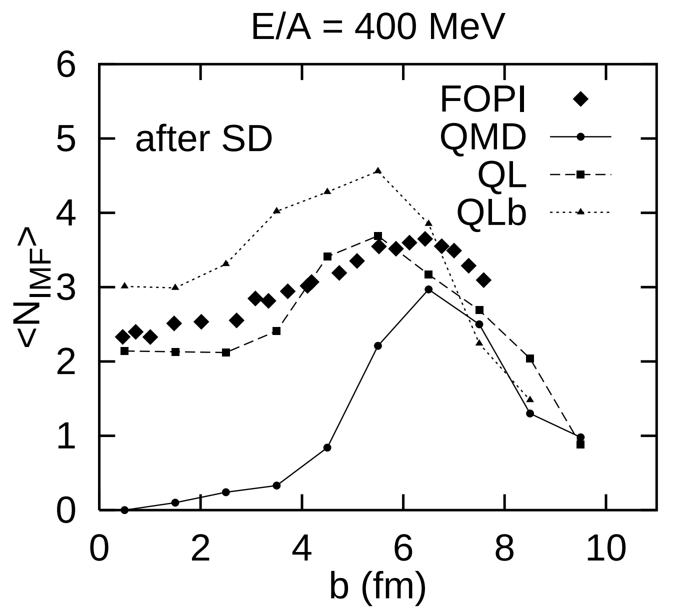
→ Dynamically Produced Fragments are cool enough to Survive Statistical Decay in QMD-QL !

• **FOPI Data —**

IMF Multiplicities and Z Distribution

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

⋆ **IMF Multiplicities**



⋆ **Exp:**

b_{imp} **sort = ERAT**

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

⋆ **Calc.:**

QMD, Gogny+Pauli

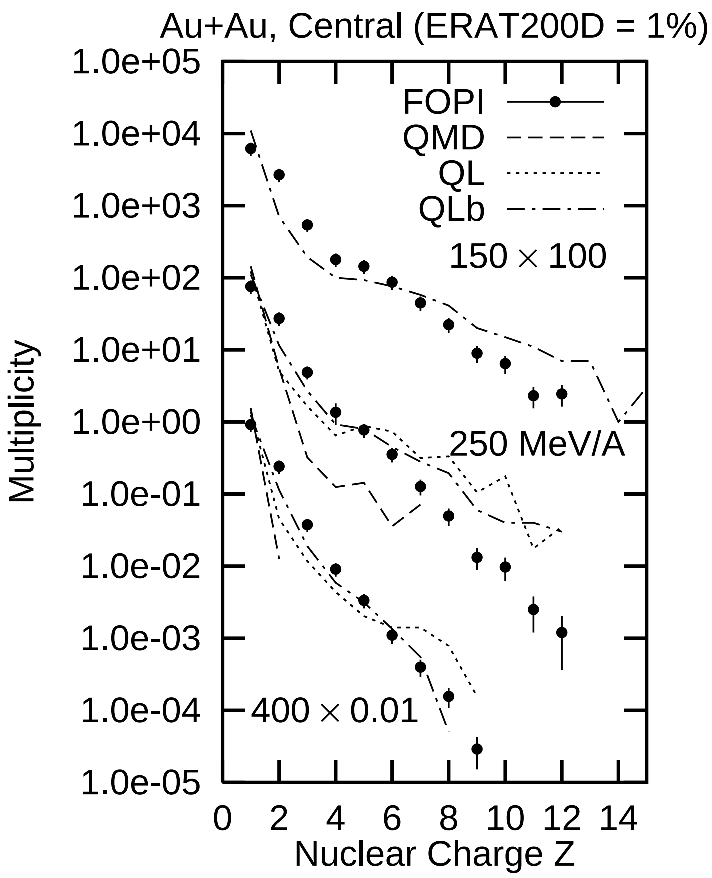
No Det. Eff. is incl.

⋆ **QLb:**

with Cluster coll.

→ **Flatter b dependence with ERAT sort**

⋆ **Charge Distribution**

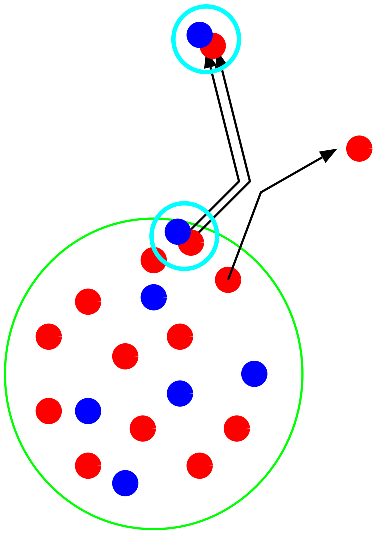


- **Cluster-Cluster Scattering**

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

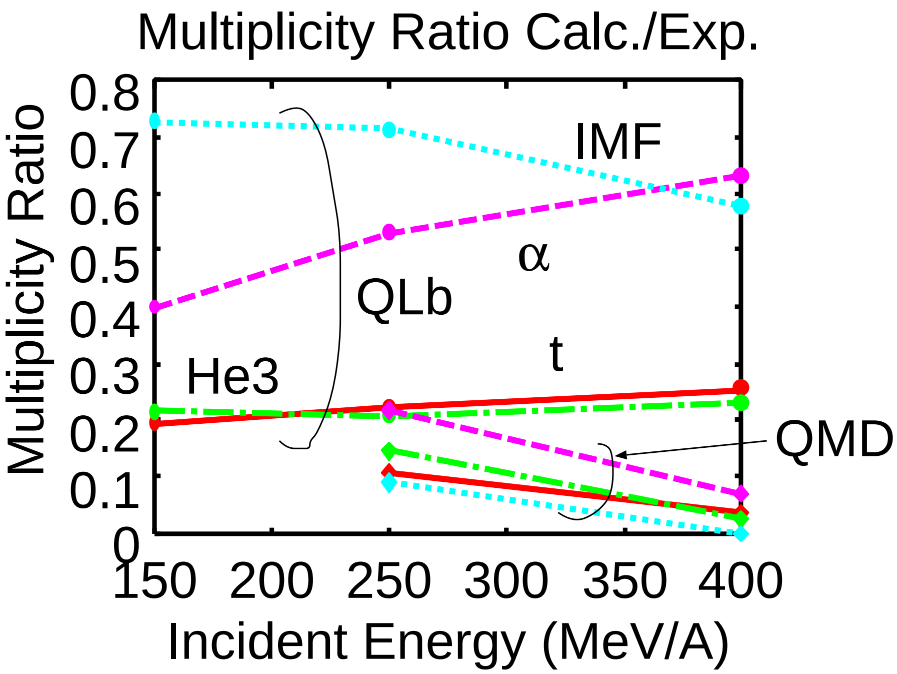
* Black Disc Ang. Dist. &σ are assumed

* Seed of IMFs

* Only 0s clusters are considered

- **Light Charged Particle Multiplicity**

··· **Large underestimate for A=3**



SUMMARY & OUTLOOK

- Quantal Langevin Model

  ⋆ Based on the energy fluctuations of wave packets, which are not energy eigen states.

  ⋆ Dynamical Relaxation to Quantum Stat. Equil.

  ⋆ 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 $4 \sim 10$ for $A = 3$
  → Coalescence ?