Quantum Fluctuation Effects on Nuclear Fragment and Atomic Cluster Formation

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We investigate the nuclear fragmentation and atomic cluster formation by means of the recently proposed quantal Langevin treatment. It is shown that the effect of the quantal fluctuation is in the opposite direction in nuclear fragment and atomic cluster size distribution. This tendency is understood through the effective classical temperature for the observables.

1 Introduction

Molecular dynamics presents a powerful tool for elucidating both statistical and dynamical properties of mesoscopic systems. While quantitative insight can be obtained in many cases, the foundation and interpretation of such approaches can be problematic when quantum systems are addressed, since the energy fluctuations are necessarily present in wave packet wave functions whose effects are neglected in molecular dynamics.

We have shown this quantal energy fluctuations significantly affect the statistical properties of nuclei [1, 2], and that effect can be included in dynamical treatments by means of a quantal Langevin force. This quantal Langevin force distributes the ensemble according to the probabilities $\langle \exp(-\beta \hat{H}) \rangle$ and $\langle \delta(E - \hat{H}) \rangle$ in the canonical and microcanonical cases, respectively, within the harmonic approximation [2], while the probabilities are $\exp(-\beta \langle \hat{H} \rangle)$ and $\delta(E - \langle \hat{H} \rangle)$ with the normal treatment.

In this short report, we apply this quantal Langevin model to the nuclear fragmentation and the atomic cluster formation of noble gases. These two processes have been extensively studied by using molecular dynamics, although the role of quantum effects is different. While atomic nuclei are highly quantal objects, atomic clusters are believed to be described by classical dynamics.

2 Quantal Langevin Model

2.1 Quantal Langevin Equation

We first give a condensed description of the recently introduced quantal Langevin model for the situation when the system can be regarded as being in thermal equilibrium at a given temperature.

The treatment seeks to take account of the energy fluctuations present in a system being described in terms of many-body wave packets. As we have already discussed in detail in Ref. [2], this inherent energy dispersion modifies the statistical weight relative to the naive the classical form,

$$\mathcal{W}_\beta(\boldsymbol{Z}) \;\equiv\; \langle \boldsymbol{Z} | \exp(-\beta \hat{H}) | \boldsymbol{Z} \rangle \;\neq\; \exp(-\beta \mathcal{H}) \;. \tag{1}$$

Here $\mathcal{H} = \langle \boldsymbol{Z} | \hat{H} | \boldsymbol{Z} \rangle$ is the expectation value of the Hamiltonian in the given wave-packet state $|\boldsymbol{Z}\rangle$ and thus the last quantity represent the usual classical statistical weight. The complex parameter

set $\boldsymbol{Z} = \{\boldsymbol{z}_1, \boldsymbol{z}_2, \ldots \boldsymbol{z}_A\}$ is related to the phase space coordinates, $\boldsymbol{z}_n = \boldsymbol{r}_n/2\Delta r + i\boldsymbol{p}_n/2\Delta p$, where Δr and Δp are widths of wave packet. By invoking the harmonic approximation, it is possible to obtain a good description of the statistical weight by means of a simple "free energy",

$$\mathcal{F}_\beta(\boldsymbol{Z}) \equiv -\log \mathcal{W}_\beta(\boldsymbol{Z}) = \frac{\mathcal{H}}{D}\left(1 - \exp(-\beta D)\right) \ , \tag{2}$$

where $D = \sigma_E^2/E^*$ is the effective level spacing. (The energy of the wave packet relative to its ground state is denoted by E^* and σ_E^2 is the associated variance.)

The relaxation towards this approximate quantal equilibrium can be described by the following Fokker-Planck equation for the distribution $\phi(\boldsymbol{Z})$ of wave-packet parameters,

$$\frac{D\phi}{Dt} \ = \ \left[-\sum_i \frac{\partial}{\partial q_i} V_i + \ \sum_{ij} \frac{\partial}{\partial q_i} M_{ij} \frac{\partial}{\partial q_j}\right] \phi \ , \quad V_i \ = \ -\sum_j M_{ij} \frac{\partial \mathcal{F}_\beta}{\partial q_j} \ , \tag{3}$$

where q_i represents either $\boldsymbol{r}_n$ or $\boldsymbol{p}_n$. It is easy to check that the statistical equilibrium distribution, $\phi_{\rm eq} = \exp(-\mathcal{F}_\beta)$, is a stationary solution to the above Fokker-Planck equation. Moreover, when the classical statistical weight is employed (*i.e.* when $\mathcal{F}_\beta^C = \beta\mathcal{H}$), the drift and the diffusion coefficients of the Fokker-Planck equation satisfy the usual Einstein relation, corresponding to $\alpha = 1$ in (4). On the other hand, when the quantal statistical weight obtained with the harmonic approximation is used, eq. (2), the relation is modified. For example, if the effective level spacing D does not depend strongly on the wave-packet parameters, the drift coefficient reduced by the factor α,

$$V_i = -\alpha\beta \sum_j M_{ij} \frac{\partial \mathcal{H}}{\partial q_j} \ , \quad \alpha = \frac{1 - \exp(-\beta D)}{\beta D} \ . \tag{4}$$

Since α is smaller than unity, the resulting Fokker-Planck equation gives smaller friction, thus in effect relatively larger fluctuations will arise.

It is convenient to solve the Fokker-Planck transport equation by means of a Langevin method. Within the framework of QMD the Langevin equation becomes

$$\dot{\boldsymbol{p}} \ = \ \boldsymbol{f} - \alpha\beta \boldsymbol{M}^p \cdot (\boldsymbol{v} - \boldsymbol{u}) \ - \beta \boldsymbol{M}^p \cdot \boldsymbol{u} \ + \boldsymbol{g}^p \cdot \boldsymbol{\xi}^p \ , \tag{5}$$

$$\dot{\boldsymbol{r}} \ = \ \boldsymbol{v} + \alpha\beta \boldsymbol{M}^r \cdot \boldsymbol{f} + \boldsymbol{g}^r \cdot \boldsymbol{\xi}^r \ , \tag{6}$$

$$\boldsymbol{v} = \frac{\partial \mathcal{H}}{\partial \boldsymbol{p}} \ , \quad \boldsymbol{f} = -\frac{\partial \mathcal{H}}{\partial \boldsymbol{r}} \ , \quad \boldsymbol{M}^p = \boldsymbol{g}^p \cdot \boldsymbol{g}^p \ , \quad \boldsymbol{M}^r = \boldsymbol{g}^r \cdot \boldsymbol{g}^r \ . \tag{7}$$

Here $\boldsymbol{r}$ and $\boldsymbol{p}$ are the phase-space centroid parameters for the wave packet, ξ is used to denote random numbers drawn from a normal distribution with a variance equal to two, and $\boldsymbol{u}$ is a local collective velocity. In these equations, we have omitted the diffusion-induced drift term and that part of the mobility tensor that connects $\boldsymbol{r}$ and $\boldsymbol{p}$.

2.2 Thermal Distortion and Observation

In addition to modifying the statistical weight, the energy fluctuation also modifies the meaning of wave packet ensemble, since it causes a thermal distortion of the spectral strength distribution of the energy eigencomponents within each wave packet. The distortion operator $\exp(-\beta\hat{H}/2)$ reduces the expectation value of the Hamiltonian in the particular state $|\boldsymbol{Z}\rangle$. The thermal distortion is calculated by replacing the time t by the imaginary time $i\tau$ in the equation of motion. The resulting "evolution" is then described by a cooling equation,

$$\frac{d\boldsymbol{p}_n}{d\tau} = -\frac{2\Delta p^2}{\hbar}\left(\boldsymbol{v}_n - \boldsymbol{u}_n\right) \ , \quad \frac{d\boldsymbol{r}_n}{d\tau} = \frac{2\Delta r^2}{\hbar} \boldsymbol{f}_n \ , \tag{8}$$

with which the state should be propagated until $\tau = \hbar\beta/2$. Here, $\boldsymbol{v}$ is again replaced by $\boldsymbol{v} - \boldsymbol{u}$ in order to leave the collective (or cluster) motion unaffected.

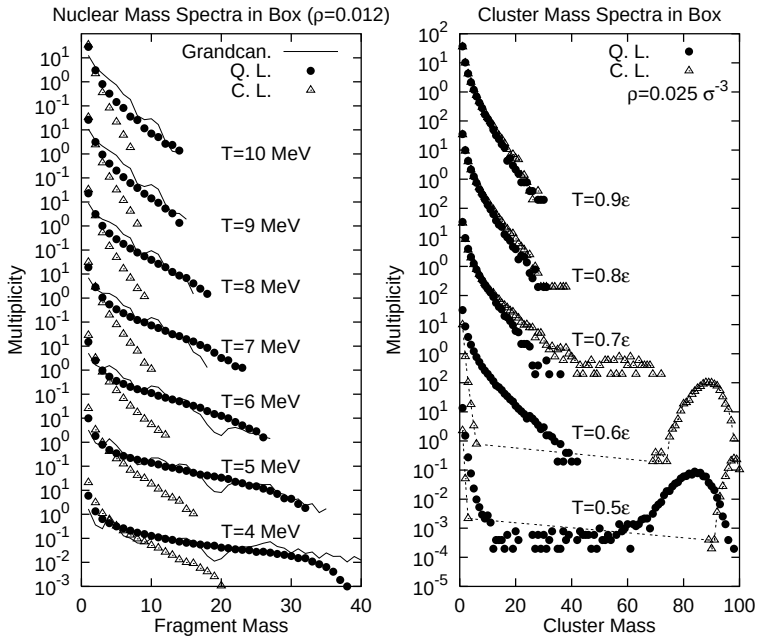

Figure 1: Nuclear (left) and cluster (right) mass distribution at given temperatures in a box. Solid circles and open triangles show the results of the simulation with the quantal and classical Langevin force. In nuclear case, fragment grandcanonical calculation is also shown (solid line).

3 Application to Fragment Formation Processes

In this section, we show the calculated results of nuclear fragmentation [3] and atomic cluster formation [4] processes by means of Langevin models with and without quantal fluctuations. In a Langevin model without quantal fluctuations, the classical Einstein relation is kept ($\alpha = 1$), and the thermal distortion does not exist.

In Fig. 1, we show the nuclear fragment and atomic cluster mass distributions at given temperatures. In the nuclear case, we put 40 nucleons in a box with periodic boundary condition, and quantal or classical (normal) Langevin force is included in the Quantum Molecular Dynamics (QMD) model. In the atomic case, the dynamics of 100 argon atoms in a box interacting via Lennard-Jones potential is simulated.

It is clear that the quantal fluctuation effect on the atomic cluster mass distribution is opposite to that on nuclear fragmentation. Namely, the inclusion of the quantum Langevin force tends to produce more heavy fragments in the nuclear case, and vice versa in atomic cases.

These features are intuitively understood by considering the corresponding effective classical temperature. The effective temperature can be estimated by means of the Einstein relation as the square of the diffusion coefficient divided by the drift coefficient. In the case of atomic clusters, the distances of atoms are much larger than the wave packet width, then the thermal distortion does not modify the cluster configuration. Then the corresponding effective temperature can be obtained from Eq. (5),

$$T_{\rm eff} = \frac{\nu T}{\alpha \nu} = \frac{T}{\alpha} = D/(1 - {\rm e}^{-D/T}) > T \ . \tag{9}$$

This expectation is indeed borne out, as shown in Fig. 2 where we compare the cluster mass distribution obtained with the quantal model at $T = 0.5\epsilon$ to the result of the classical treatment carried out at the corresponding effective temperature $T_{\rm eff} = 0.62\epsilon$. The quantitative similarity between the two distributions is remarkable and supports the above discussion.

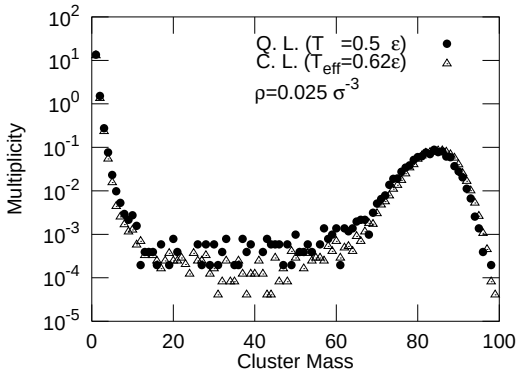

Figure 2: The cluster mass distribution obtained with either the quantal Langevin model at $T = 0.5\epsilon$ (solid circles) or the classical Langevin model at the corresponding effective temperature $T_{\rm eff} = 0.62\epsilon$ (open triangles), at the density $\rho = 0.025\ \sigma^{-3}$.

On the other hand, the thermal distortion strongly modify the nucleon configuration in nuclear fragmentation, and the above discussion does not hold. In order to illustrate this feature, we consider here the evolution of the distorted momentum (*i.e.* the solution to Eq. (8)) which is given by

$$\boldsymbol{p}'_i(t) \equiv \boldsymbol{p}_i(t, \tau = \frac{\hbar}{2T}) = \mathrm{e}^{-D/2T}\, \boldsymbol{p}_i(t)\ . \tag{10}$$

Thus, in the rest frame of the nuclear fragment, the distorted momenta of the constituent nucleons are governed by a modified Langevin equation,

$$\dot{\boldsymbol{p}'} = \mathrm{e}^{-D/2T}\boldsymbol{f} - \alpha\nu \boldsymbol{M}^2 \cdot \boldsymbol{p}' + \mathrm{e}^{-D/2T}\sqrt{\nu T}\boldsymbol{M}\cdot\boldsymbol{\zeta}\ . \tag{11}$$

We can again invoke the Einstein relation and extract an effective temperature for the intrinsic cluster motion,

$$T'_{\rm eff} = \frac{\mathrm{e}^{-D/T}\nu T}{\alpha\nu} = D/(\mathrm{e}^{D/T} - 1) < T\ . \tag{12}$$

It has been shown that calculations with classical molecular dynamics at this equivalent temperature $T'_{\rm eff}$ yields results that are very similar to the exact quantal results for the real temperature T, for non-interacting particles in a harmonic potential [2, 5, 6, 7].

In nuclear fragmentation, the normal Langevin model at this effective temperature $T'_{\rm eff}$ gives a similar fragment mass distribution to the quantal Langevin model at T, except the region around the critical temperature. At around the critical temperature, the system is mechanically unstable, and a small fluctuation induces a large difference after the thermal distortion. At higher and lower temperatures than the critical one, the system is mechanically stable, and the above discussion approximately holds.

4 Summary

In the present report, we have applied a recently developed quantal Langevin model to systems of nucleons and argon atoms in thermal equilibrium. The basic features of the quantal Langevin model can be summarized as *larger fluctuations*($\alpha \leq 1$) and the *thermal distortion*. The combination of these two points appears as different effects in nuclear fragmentation and atomic cluster formation. In the atomic case, the distortion effects are small and the effective classical temperature becomes higher than the actual temperature. Namely, quantum fluctuations gives a steeper slope in the size

distribution. In the nuclear case, however, the distortion strongly modifies nucleon configurations, then the quantum fluctuation enhances fragment yield.

As it was pointed out at this meeting, the quantal fluctuation effect shown in this work seems to be too large in the atomic case, since the distance between atoms is much larger than the width of the wave packet and the classical dynamics is believed to be valid. However, a small width in r-space leads to a large width in p-space. Therefore, the associated energy fluctuation can be non-negligible. In our estimate, the "level spacing" is $D \approx 0.2265\ \epsilon$, where ϵ is the depth of the Lennard-Jones potential. Compared with the critical (classical) temperature at low densities ($\approx 0.6\epsilon$), this value is far from negligible. This may be related to the treatment of cluster intrinsic degrees of freedom in Ref. [8]. Ikeshoji et al. treat the cluster-intrinsic degrees of freedom in a different way from the cluster-translational motion. Therefore, we expect that there is still room for taking account for the quantal fluctuation in atomic dynamics.

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