Quantum Fluctuation Effects on Nuclear and Atomic Fragmentations

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Abstract. We investigate the nuclear fragmentation and atomic cluster formation by means of the recently proposed Quantal Langevin treatment. The mass distribution of the noble gas clusters is calculated to be affected significantly near the critical temperature by quantum fluctuations, and this effect is in the opposite direction to that in nuclear fragmentation processes. This tendency can be understood through the effective classical temperature for the observables.

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. For example, various intrinsic excited states of clusters are necessarily mixed in a classical wave packet description, while only one eigen state from these states is realized in the asymptotic region of actual fragmentation processes. When this projection to a single eigen state is taken into account, the intrinsic cluster motion is expected to have more fluctuations — fluctuations of the realized intrinsic excitation energies around the average excitation energies of wave packets — than those expected in a classical treatment.

We have shown that this quantal energy fluctuations significantly affect the statistical properties of nuclei, and that effect can be included in dynamical treatments by means of a Quantal Langevin force [1]. For the atomic cluster formation, it is generally believed that this kind of quantal effects would be negligible. However, the level separation of small clusters is not negligibly small compared with the critical temperature. For example, in the case of argon atoms interacting via the Lennard-Jones potential,

$V_{ij} = 4\epsilon((\sigma/r_{ij})^{12} - (\sigma/r_{ij})^6)$, the effective level spacing D is around 0.2ϵ, while the critical temperature is around 0.5ϵ.

In this work, we compare the quantum fluctuation effects on the nuclear fragmentation [1] and atomic cluster formation [2] processes. The calculated results show that the quantum fluctuation also affects the statistical properties of noble gas clusters, especially at around the critical temperatures.

QUANTAL LANGEVIN MODEL

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, $T = 1/\beta$.

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 [1], this inherent energy dispersion modifies the statistical weight for a given wave packet $|Z\rangle$ relative to the naive form expected in an usual MD treatment [3],

$$\mathcal{W}_\beta(\boldsymbol{Z}) \;\equiv\; \langle \boldsymbol{Z}|\exp(-\beta\hat{H})|\boldsymbol{Z}\rangle \;\simeq \exp\left(-\frac{\mathcal{H}}{D}(1-e^{-\beta D})\right) \;\neq\; \exp(-\beta\mathcal{H}) \;, \quad (1)$$

where $\mathcal{H} = \langle Z|\hat{H}|Z\rangle$ and $D = \sigma_{E}^2/\mathcal{H}$ is the effective level spacing. The relaxation towards this approximate quantal equilibrium can be described by the Fokker-Planck equation for the distribution of wave-packet parameters, or its equivalent Langevin equation,

$$\dot{\boldsymbol{p}} = \boldsymbol{f} - \alpha\beta\boldsymbol{M}\cdot(\boldsymbol{v}-\boldsymbol{u}) \;-\beta\boldsymbol{M}\cdot\boldsymbol{u} \;+\boldsymbol{g}\cdot\boldsymbol{\xi} \;, \quad (2)$$

$$\alpha = \frac{1-\exp(-\beta D)}{\beta D} < 1 \;, \quad \boldsymbol{v} = \frac{\partial\mathcal{H}}{\partial\boldsymbol{p}} \;, \quad \boldsymbol{f} = -\frac{\partial\mathcal{H}}{\partial\boldsymbol{r}} \;, \quad \boldsymbol{M} = \boldsymbol{g}\cdot\boldsymbol{g} \;, \quad (3)$$

and its canonical conjugate equation for $\boldsymbol{r}$. 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 this Quantal Langevin equation (2), the normal Einstein relation ($\alpha = 1$) is modified: Since α is smaller than unity, the resulting Fokker-Planck equation gives smaller friction, thus in effect relatively larger fluctuations will arise.

In addition to modifying the statistical weight, the energy fluctuation also causes a intrinsic distortion within each wave packet. The necessity of this distortion can be already seen in the definition of the mean value of an operator $\hat{O}$,

$$\prec \hat{O} \succ_\beta \;\equiv \frac{1}{\mathcal{Z}_\beta}\mathrm{Tr}\left(\hat{O}\, e^{-\beta\hat{H}}\right) = \frac{1}{\mathcal{Z}_\beta}\int d\Gamma_z\; \mathcal{O}_\beta(\boldsymbol{Z})\; \mathcal{W}_\beta(\boldsymbol{Z}) \;, \quad (4)$$

$$\mathcal{O}_\beta(\boldsymbol{Z}) \equiv \langle Z|\exp(-\beta\hat{H}/2)\hat{O}\exp(-\beta\hat{H}/2)|Z\rangle \;/\; \mathcal{W}_\beta(\boldsymbol{Z}) \;. \quad (5)$$

Thus, when basis wave functions are not the energy eigen states, the mean value of $\hat{O}$ is not a weighted average of $\langle \boldsymbol{Z}|\hat{O}|\boldsymbol{Z}\rangle$, but a weighted average of the quantum expectation values under the distorted state, $\mathcal{O}_\beta(\boldsymbol{Z})$. The intrinsic distortion is calculated by replacing the time t by the imaginary time $i\tau$ in the equation of motion. The resulting distorted parameter is then given by solving the following cooling equation until $\tau = \hbar\beta/2$.

$$\frac{d\boldsymbol{p}_n}{d\tau} = -\frac{2\Delta p^2}{\hbar}\left(\boldsymbol{v}_n - \boldsymbol{u}_n\right) . \tag{6}$$

APPLICATION TO FRAGMENT FORMATION

Now, we apply the above Quantal Langevin model to the fragment formation processes of nucleons and atoms. 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 a molecular dynamics. In the atomic case, the dynamics of 100 argon atoms in a box interacting via Lennard-Jones potential is simulated. It is interesting to note that the quantum fluctuation lowers the critical temperature by about 20 % in the atomic cluster formation. This modification comes from the agitation of the cluster intrinsic motion by the quantum fluctuation. On the other hand, the quantal fluctuation effect on the nuclear fragmentation is opposite to that on atomic cluster formation. Namely, the inclusion of the quantum Langevin force produces a steeper slope in the atomic cluster mass distribution at high temperatures, and vice versa in nuclear cases.

This difference of quantum effects can be intuitively understood by considering the effective classical temperature of the Quantal Langevin model [2]. By applying the Einstein relation, the effective temperature for the wave packet parameters is calculated to be $T_{\rm eff} = D/(1-\exp(-D/T)) > T$. This effective temperature is suitable for the description of atomic cluster formation; since the separation of atoms ($\sim \sigma$) is much larger than the wave packet width, the intrinsic distortion effects can be ignored. In the case of nuclear fragmentation, however, the width of the wave packet is comparable to the nucleon separation, then the intrinsic distortion can modify the fragment configuration. In the mechanically stable region, the distorted momentum is given by solving the cooling equation (6), $\boldsymbol{p}'_n(t) \equiv \boldsymbol{p}_n(t, \tau = \hbar/2T) = e^{-D/2T}\,\boldsymbol{p}_n(t)$. The effective temperature for this distorted parameter is given by $T'_{\rm eff} = D/(\exp(D/T)-1) < T$, and this applies to nuclear fragmentations.

Although the intrinsic distortion does not largely affect the atomic cluster formation, it modifies the excitation energy of each cluster. This mismatch may be related to the necessity to distinguish intrinsic and external temperature in the description of cluster formation [4].

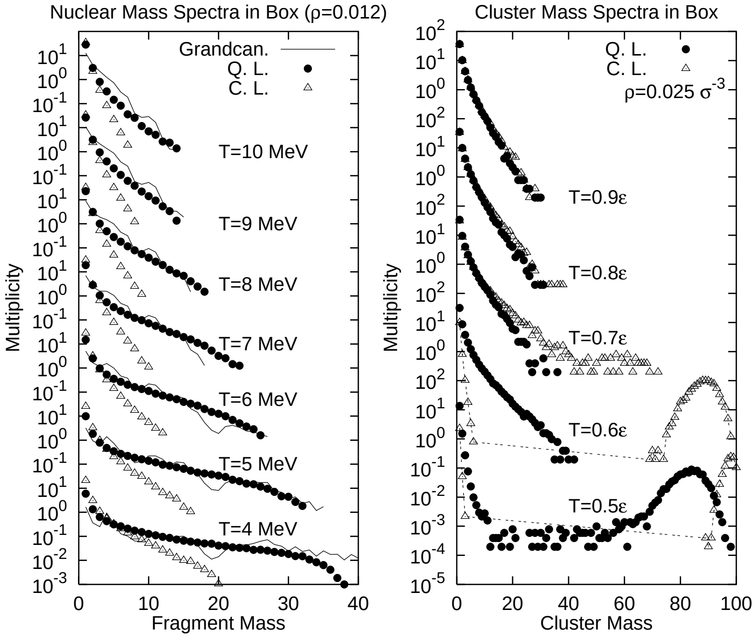

FIGURE 1. Nuclear (left) and cluster (right) mass distribution at given temperatures in a box. Solid circles and open triangles show the results of the simulation with the quantal and classical Langevin force, respectively. In the nuclear case, the grandcanonical fragment population is also shown (solid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

SUMMARY

The quantum fluctuation are shown to affect fragmentation processes in various ways. The combined effects of the modified Einstein relation and the intrinsic distortion of wave packets provides different effects depending on the system and observables. In atomic cluster formation processes, it will be interesting to see the difference between the intrinsic temperature of clusters and the external (or inter-cluster) temperature, since the quantum fluctuation will cause a gap between them.

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