MOLECULAR DYNAMICS WITH QUANTUM FLUCTUATIONS AND ITS APPLICATION TO HEAVY ION COLLISIONS

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The effects of quantum fluctuations are studied by using the recently developed Quantal Langevin model. It is shown that we can understand various thermal and dynamical aspects of nuclear matter, such as the caloric curve, fragment mass distribution in a thermal environment, and abundant IMF productions in Au+Au collisions in a consistent and microscopic way by taking account of the inherent energy fluctuations within the wave packet wave functions.

1 Introduction

Molecular dynamics presents a powerful tool for elucidating the features of mesoscopic systems in various fields, including nuclear physics. Largely owing to the advances of computational power, it becomes possible to simulate the dynamical evolution of large systems from a microscopic point of view. In most of these approaches, the time-evolution of (possibly anti-symmetrized) product wave packets are simulated by applying the time-dependent variational principle, and two-body collisions are usually included. The latter generate fluctuations around the mean trajectory and help to form fragments.

When we address the problem of quantum fluctuation, the applicability of these approaches becomes doubtful. Since the two-body collision term is added in a classical way and the time-dependent variational principle only concerns the expectation value of the Hamiltonian, the operator nature or the fluctuation of the Hamiltonian is ignored. This problem might be essential to the statistical properties of nuclei. The statistical weight is known to be expanded in $\beta = 1/T$, like $\langle \exp(-\beta\mathcal{H})\rangle = \exp(-\beta\langle\hat{H}\rangle + \beta^2\sigma_E^2/2 + \cdots)$, where $\sigma_E^2 = \langle\hat{H}^2\rangle - \mathcal{H}^2$ is the energy dispersion within a given state. For moving wave packets, although this energy dispersion is not necessarily small, it is assumed to play no role in molecular dynamics. This possible defect in statistics may be serious in describing fragmentation, if nuclear multifragmentation is caused by the the instability of nuclear matter [1−3].

In this report, we present the way to take approximate account of this energy dispersion in statistics and dynamics following the recently developed

Quantal Langevin model [4]. The energy dispersion modifies the statistical weight in a statistical context, while it appears as a Langevin-type stochastic term in dynamics. We would like to emphasize that both of the statistics and dynamics are improved based on the same idea that the wave packets are not energy eigen states and they involves inherent energy fluctuations.

2 From Quantumn Statistics to Dynamics with Fluctuations

Since one of the largest aim of heavy-ion physics is to explore various phases of nuclear matter and to study the associated phase transition between them, it is necessary to investigate heavy-ion dynamics in the relation with the statistical properties of nuclear system. The statistical equilibrium properties of a wave packet dynamics is determined by the probability distribution to find wave packets after long time evolution. For example, this probability becomes $\delta(E-\langle\hat{H}\rangle)$ in classical molecular dynamics, and $\exp(-\beta\langle\hat{H}\rangle)$ when a (classical-)Langevin force which satisfies the Einstein relation is added.

On the other hand, the quantum statistical mechanics tells us this probability distribution at equilibrium, $\mathcal{W}=\langle\exp(-\beta\hat{H})\rangle$ and $\mathcal{W}=\langle\delta(E-\hat{H})\rangle$ for canonical and microcanonical ensemble, respectively. Once this probability distribution is given, we can construct a model which dynamically produces the desired equilibrium distribution $\mathcal{W}$ at equilibrium. For example, we can adopt a Fokker-Planck type equation or its equivalent *Quantal Langevin* equation,

$$\frac{Dq_i}{Dt} = \sum_j \left(-M_{ij}\frac{\partial \log \mathcal{W}}{\partial q_j} + g_{ij}\zeta_j \right) , \quad \boldsymbol{M} = \boldsymbol{g}\cdot\boldsymbol{g} \qquad (1)$$

where $\{q_i\}$ are canonical variable parameters satisfying $d\Gamma=\prod_i dq_i$, $\boldsymbol{M}$ represents the mobility tensor, and ζ is the white noise.

We have studied the statistical equilibrium properties by applying the *harmonic approximation* to the statistical weight [4],

$$\mathcal{W} \approx \exp\left(-\alpha\beta\mathcal{H}\right) , \quad \alpha = \frac{1-\exp(-\beta D)}{\beta D} < 1 , \quad D = \frac{\sigma_E^2}{\mathcal{H}} . \qquad (2)$$

In the left panel of Fig. 1, we show the nuclear caloric curve calculted by using the above statistical weight directly. In the right panel, on the other hand, we show the fragment mass distribution at given temperatures calculated by applying the Quantal Langevin equation (1) derived from the statistical weight (2). It is clear that both of the caloric curve and thermal fragmentation are improved by taking account of quantum fluctuations. For example, in the caloric curve, the transition from quantal behavior $T \propto \sqrt{E}$ to the classical behavior

$T = 2E/3A +$ constant is clearly seen as the excitation grows. In thermal fragmentations, in the Quantal Langevin treatment, more fragments are formed than in the classical case, and the results of the fragment grandcanonical model are well reproduced.

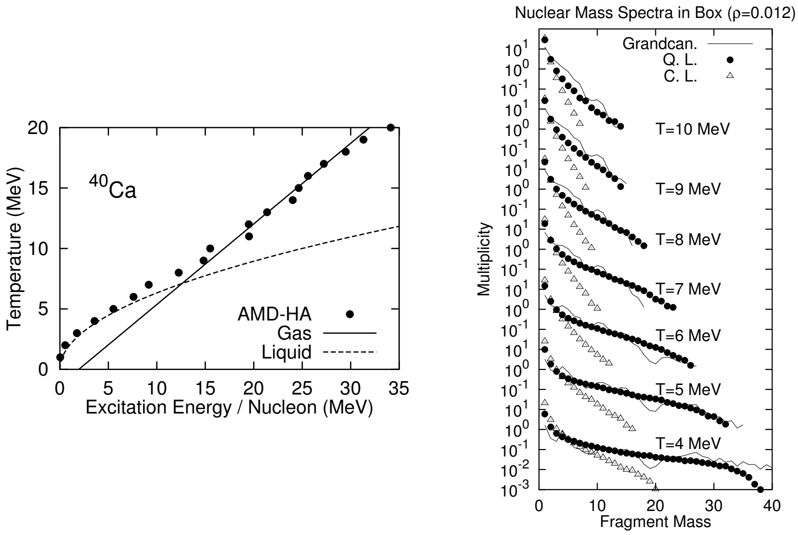

Figure 1: Statistical properties of nuclei. Left: Caloric curve of ^{40}Ca [4]. The mean excitation energy per nucleon E^*/A for a canonical ensemble of 40 nucleons (20 protons and 20 neutrons) confined in a sphere with a radius 2.0 $A^{1/3}$ fm as a function of the temperature T. Circles show the calculated results with the harmonic approximation based on the AMD model. Solid and dashed lines show the temperature in gas and liquid phase. Right: Nuclear fragment mass distribution at given temperagures in a box with the periodic boundary condition [5]. Solid circles and open triangles show the results of the QMD simulation with the quantal and classical Langevin force, respectively. In the figure, the grandcanonical fragment population is also shown (solid line).

3 Multifragment Formation from Heavy-Ion Collision

In the situations with a specified energy, where a microcanonical ensemble will appear if the evolution time is long enough, it is also possible to apply the Quantal Langevin model by assuming a corresponding statistical weight for each wave packet,

$$\mathcal{W} = \langle \delta(E - \hat{H}) \rangle \ \propto \ \frac{(\mathcal{H}/D)^{E/D}}{\Gamma(E/D+1)} \exp(-\mathcal{H}/D) \ . \tag{3}$$

The last relation assumes that the spectral function is given by a continuous Poisson distribution. With this statistical weight and the resultant Quantal Langevin equation, we have studied the intermediate-mass fragment (IMF) formation in ^{197}Au+^{197}Au collision [2] and have shown that the fragments with low excitation are enhanced by incorporating the quantal fluctuation [5].

In Fig 2, we compare the calculated results shown in our previous work [5] and the recently published data by FOPI group [3]. Including the quantum fluctuation effects (QL) cleary improves the description of fragment formation. However, it still underestimates light fragment yields. This may be because the two nucleon collision term, which is included in a classical way, somewhat spoils the quantal nature generated by the Quantal Langevin force. In order to avoid this defect partly, we have included scattering of 0s-clusters at low nucleon densities (QLb). Namely, when a well defined 0s-cluster $(d, t, {}^3\mathrm{He}, \alpha)$ collides with other nucleons or 0s-clusters at nuclear surface, they are made to scatter elastically with the probability of a half even at high colliding energies of these clusters (shadow scattering). This cluster-cluster scattering enhances light charged fragment yields. In addition, IMF mulitplicities are increased, probably because these light charged particles can coalesce to make IMF. The largest remaining problem now lies in the formation of very light ($A = 3$) fragments, which may not be made through the instability of matter, but will be made by cluster-cluster rearrangement in nuclei or coalescence of d-N.

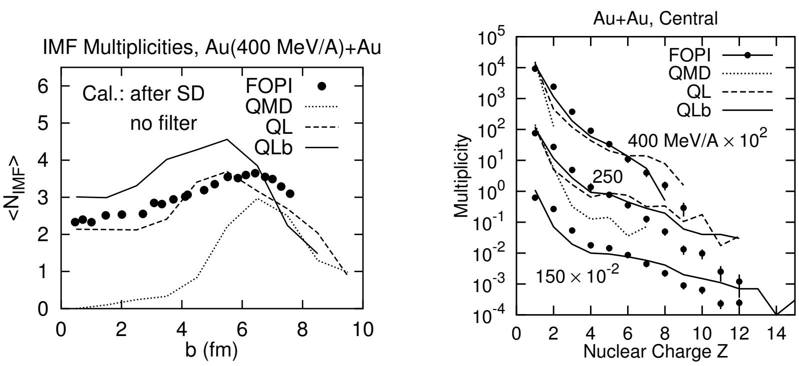

Figure 2: Fragment formation in Au+Au collisions. Left: Dotted, dashed, and solid lines show the calculated IMF ($3 \leq Z \leq 15$) multiplicities by using QMD, QMD with Quantal Langevin force (QL), and QL with cluster-cluster scattering (QLb), respectively. Statistical decay is included in the calculation, and no filter is included. Data [3] are shown by filled circles. Right: Fragment charge distribution from central Au+Au collisions. Dotted, dashed, and solid lines show the calculated results with QMD, QL, and QLb, respectively. Data [3] including detector efficiency correction are shown by filled circles.

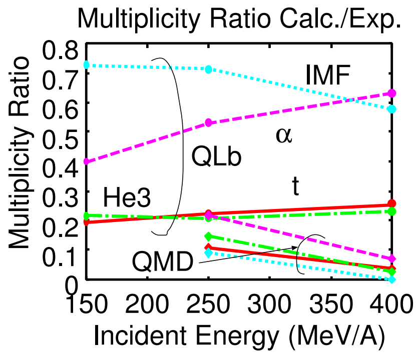

Figure 3: Multiplicity ratio of the calculated results to the experimental data [3].

4 Summary and Outlook

We have studied the effects of quantum fluctuations induded by the energy dispersion of wave packets in statistics and dynamics. Although it has been discussed that anti-symmetrized wave packet dynamics has quantal statistical properties in non-evaporative processes by adjusting the temprature parameter without including the quantum fluctuations discussed here [6,7], it becomes necessary to include other types of fluctuations for evaporative processes [6]. In this work, on the other hand, it has been emphasized that the energy dispersion in a wave packet improves the statistical properties of the system, and the same energy dispersion also improves the description of fragment formation.

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