Effect of the Width of Gaussian Wave Packets on the Stability of the Nuclei

Supriya Goyal

Department of Physics, GSSDGS Khalsa College, Patiala, Punjab-147001, India
ashuphysics@gmail.com

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Abstract

The role of the range of interaction on the stability of the nuclei propagating with and without momentum dependent interactions is analyzed within the framework of Quantum Molecular Dynamics (QMD) model. A detailed study is carried out by taking different equations of state (i.e., static soft and hard and the momentum dependent soft and hard) for the selected nuclei from $^{12}$C to $^{197}$Au. Comparison is done by using the standard and the double width of the Gaussian wave packets. We find that the effect of the double width of the Gaussian wave packets on the stability of the initial stage nuclei cannot be neglected. The nuclei having double width do not emit free nucleons for a long period of time. Also, the ground state properties of all the nuclei are described well. In the low mass region, the obtained nuclei are less bound but stable. Heavy mass nuclei have proper binding energy and are stable.

Keywords: Quantum Molecular Dynamics Model, Stability of nucleus, Gaussian Width

1. Introduction

Heavy-ion collisions at intermediate energies lead to final states containing many complex fragments. As the beam energy is raised from a few tens to several hundreds of MeV/nucleon, the multiplicity of final fragments increases steadily. The study of nuclear collisions at intermediate energies is primarily motivated by the unique possibilities for probing the physical properties of hot and dense nuclear matter. It is well known that the non-equilibrium effects play an important role in a realistic treatment of heavy-ion collisions [1-4]. The most pronounced effect is from the momentum dependence of the nuclear interaction which leads to an additional repulsion between the nucleons when boosted as in heavy-ion collisions [5]. This repulsive interaction vanishes for relative momentum zero and increases logarithmically with the incident energy. Since the fate of the reaction depends not only on the density, but also on the momentum space [1-5], therefore, momentum dependent potentials have been implemented into the early molecular dynamics as well as into the time dependent meson field approach [6]. All these models predict a significant influence of non-local interactions on the collective flow, particle production, rapidity distribution, anisotropy ratio, density and temperature etc [1, 2, 4, 6-9]. The effect of MDI on the stability of the nuclei has been discussed in detail in Ref. [10]. During the evolution of a single cold nucleus, it has been found that the inclusion of MDI increases the emission of free nucleons and light charged particles (2≤A≤4), but no heavier fragments are emitted artificially.

One of the common problems of the simulation of a heavy-ion reaction is the proper description of the ground state nuclei. The problem is more severe, once the momentum dependent interactions are included. The nucleus build up in the initial stage should be stable in its ground state as well as on a time scale comparable with the time span needed for the nucleus-nucleus collision. A lot of improvements have been done on molecular dynamic models to improve the stability of the ground state nuclei, and to reproduce the correct binding energies and the root-mean-square radii for all types of nuclei.

Mancusi et al. [11] gave an improved version of the JAERI quantum molecular dynamics model (JQMD) to get the consistent results which were not reproduced by the original JQMD [12] model because of the unfaithfully reproduced quantum mechanical ground state of nuclei in a semi classical framework. The improved version included a covariant treatment of two-body interactions and scattering and also an improved ground state initialization algorithm.

The sensitivity of neutron production to the semi classical molecular initial ground state configuration effects is shown in Ref. [13]. Implementation of a proper semi classical ground state initialization is done for the description of all the neutron spectra in proton-induced reactions at intermediate energies.
Paula et al. [14] has investigated the stability of $^{197}$Au nucleus by using a simulation based on molecular dynamics and chromatic restructured aggregation. The initial distribution is also obtained by searching the minimum energy state with the functional cooling method [15-18]. This method has been successful in reproducing the experimental data up to about 80 MeV. Stability of the nucleus is also taken care in the models used to study relativistic energy heavy-ion reactions [19].

A cooling procedure via Pauli potential is also reported in the literature [13, 17, 18, 20-22]. The introduction of a repulsive Pauli potential forbids the nucleons of the same spin and isospin to come close in the phase space. A self-consistent minimization of the energy of the nucleus results in a reasonable ground state due to the Pauli potential mimicking the fermionic properties of the nucleons. In case of low-energy reactions such as fusion, fission, and deep inelastic collision process the microscopic simulations by using the molecular dynamics have not been studied except for a few works [16] because several extra nucleons are emitted during the collision processes in the calculations. This is due to the insufficient stability of initial ground state nuclei. Therefore, Maruyama et al. [21] have proposed a solution of this problem by including the so called Pauli potential into effective interaction. They treated the width of each wave packet as a dynamical variable. Models that adopt such repulsive interactions reproduce the binding energies of nuclear ground states but gives spurious repulsions in the collision process.

In the present work, we aim to investigate the stability of nuclei propagating with and without momentum dependent interactions in the framework of QMD model. The typical time for a heavy-ion reaction is around 200 fm/c. For this time non-interacting nuclei have to be stable, otherwise, one cannot be sure that the results really reveal the physics or are just numerical artifacts. Since in QMD model each nucleon is represented by a Gaussian wave packet with a certain width $L$, which is a free parameter in the model. The very small values of $L$ are excluded because then the nuclei would become unstable after initialization. Thus, the value of $L$ presents the limit for a semi classical theory. As noted in Ref. [7, 24], the value of $L$ determines the interaction range of the nucleons and influences the density distribution of finite systems. This value affects the ground state properties of finite nuclei and infinite nuclear matter below saturation densities while it does not change those of infinite nuclear matter above saturation densities [18]. The width of the Gaussian has strong influence on the variables such as collective flow, multifragmentation, pion and kaon production in heavy-ion collisions at intermediate energy [7, 25]. In Ref. [7], the Gaussian width was taken as $L = 1.08 \text{ fm}^2$ for the reaction of $^{40}\text{Ca} + ^{90}\text{Zr}$ and $L = 2.16 \text{ fm}^2$ for the reaction of $^{197}\text{Au} + ^{197}\text{Au}$. A system-size dependent width along with other constraints has also been used by Wang et al. [26] to study the fusion reactions and also to reproduce the data of fusion cross-section for $^{40}\text{Ca} + ^{90,92}\text{Zr}$ at energies near the barrier. The role of the width of Gaussian wave packets in multifragmentation has been analyzed in detail by Singh and Puri [27]. They find that the effect of different widths depends on the physical conditions and excitation energy of the system. Some attempts with limited success have also been made by using the realistic time dependent width of the Gaussian [28].

From above discussion, it seems to us that it is worthwhile to make a further study of the influence of the Gaussian widths on the stability of the individual nuclei propagating with and without momentum dependent interactions. From the review of the literature we find that different models which are used to study heavy-ion collisions at intermediate and high energies, takes different forms of the potentials to get realistic results [7, 12, 21, 29]. In the low energy region also, several sets of parameters are present for the phenomenological forces. All these parameters reproduce the ground state properties of nuclei with similar accuracy [30]. Due to the importance of the nuclear interactions in the fate of the reaction, further development in the form of the nuclear potential are still going on. It means that a clear and well defined nuclear potential is still not present in the literature. In our present study, we have given a new method to obtain the stable nuclei with QMD model by varying the width of the Gaussian wave packets, which was ignored in the earlier studies. By increasing the range of the interaction the system is not getting over-bound which will be shown later.

For the present study, constant values of $L = 1.08 \text{ fm}^2$ and $L = 2.16 \text{ fm}^2$ are used. These values are referred hereafter as $L^\text{norm}$ and $L^\text{broad}$ respectively. To check the stability of the initialized nuclei, we let the single nuclei to evolve for at least 200 fm/c and then the ground state properties including the root-mean-square radii, the binding energy, and the density distribution are checked. If the bulk properties and their time evolution are good enough and there is no spurious nucleon emission for a long time, only then we can say that we have got the stable nuclei. The details of the QMD model which is used to follow the reaction dynamics can be found in Ref. [31].

### 2. Results and Discussion

For the present analysis, the selected nuclei i.e. $^{12}\text{C}$, $^{40}\text{Ca}$, $^{93}\text{Nb}$, and $^{197}\text{Au}$ are simulated with different equations of state (i.e., Soft, Hard, SMD, and HMD). Since the study is on single nucleus, therefore, the different values of impact parameter, energy, and cross-section have no meaning.
Since it has been shown in the work by Vermani et al. [10] that the number of nucleons emitted by the $^{197}$Au and $^{58}$Ni nuclei at the final time of 200 fm/c are 5 and 3, respectively for Soft EOS. However, when analysis was done with SMD, their numbers increased to 19 and 7 for $^{197}$Au and $^{58}$Ni nuclei, respectively. It was found in Ref. [10] that out of the 19 units emitted by the $^{197}$Au, 15 are in terms of free nucleons. It means that the main contribution of the emitted units goes to free nucleons. Therefore, in the present study, we have treated all the emitted units at the final time step as free nucleons. It is worth mentioning that in Ref. [10] the standard value of the Gaussian wave packet width i.e. $L = 1.08$ fm$^2$ was taken for whole analysis. The impact of doubling the width of Gaussian wave packets on the stability of the nuclei initialized with Soft, Hard, SMD, and HMD equations of state will be discussed in the detail in the present study.

In Fig. 1, we see that $A_{\text{max}}$ decreases and multiplicity of free nucleons increases with time. The effect is much more pronounced for SMD EOS as compared to Soft EOS. From Fig. 1, we also see that the multiplicity of the free nucleons reduces nearly to zero with $L_{\text{broad}}$ for both Soft and SMD equations of state. The similar trend has been seen for the nuclei propagating with Hard and HMD EOS (not shown here).

In Fig. 2, we see that many nucleons in case of $L_{\text{stand}}$ leave the surface and thus are not bounded by the potentials generated by all its fellow nucleons. Thus they get emitted out. Approximately $2(4)$, $4(15)$, and $4(31)$ nucleon gets unbound at 200 fm/c for $^{40}$Ca, $^{93}$Nb, and $^{197}$Au nuclei with Soft (SMD) EOS, respectively. But when we increase the interaction range, we find that the nucleons which come close to the surface are pulled back by the other nucleons. Thus all the nucleons remain confined in a sphere. The number of nucleons thus emitted with $L_{\text{broad}}$ are $0(2)$, $0(2)$, and $0(0)$ for $^{40}$Ca, $^{93}$Nb, and $^{197}$Au nuclei with Soft (SMD) EOS, respectively. As a next step we check the ground state properties of initialized nuclei like binding energy, root-mean-square radii, and density distribution.

In Fig. 3, we see clearly that all the nuclei having $L_{\text{broad}}$ have a constant value of radii close to the experimental values and with very small fluctuations over the entire time span. For the SMD case, the deviation of the radii for all the nuclei having $L_{\text{stand}}$ width from the experimental values is large as compared to Soft EOS. But when we increased the width of the Gaussian wave packets, the root-mean-square radii for all the nuclei matches well with their true values for both Soft and SMD equations of state.
Figure 2: Trajectories of the free nucleons emitted with \( L_{\text{stand}} \) in the field of other bound nucleons is displayed for a time span of 200 fm/c. The trajectories are shown for the \(^{40}\text{Ca} \), \(^{93}\text{Nb} \), and \(^{197}\text{Au} \) nuclei. Column 1 and 2 from left are for Soft EOS with \( L_{\text{stand}} \) and \( L_{\text{broad}} \), respectively, whereas column 3 and 4 are for SMD with \( L_{\text{stand}} \) and \( L_{\text{broad}} \), respectively. Only single event is generated to obtain the number of emitted nucleons. To visualize the size of the system, we show also a sphere of radius \( r = 1.3 \times A^{1/3} \), where \( A \) is the mass of the nuclei. The solid circles represent the position of the nucleons at initial time.

Figure 3: Root-mean-square radii of different nuclei as a function of time. The left panel is for Soft EOS and right panel is for SMD. Results obtained with \( L_{\text{stand}} \) are represented with solid lines whereas dashed lines show results with \( L_{\text{broad}} \). The experimental value of root-mean-square radii for all nuclei is shown with dotted shown with dotted line. For each nucleus we display this radius which is average over 100 simulations.
In Fig. 4. we get a quite smooth density distribution with both $L_{\text{stand}}$ and $L_{\text{broad}}$. The central density for SMD is always less than Soft EOS for all the nuclei. The density profile of the ground states of light mass nuclei i.e. for $^{12}$C and $^{40}$Ca has less central density and rather a wide surface shape for the $L_{\text{broad}}$ as compared to $L_{\text{stand}}$. This is because of the few nucleons present at the center of the light nuclei and the smearing out of the nucleus over larger size due to the larger width of the Gaussian wave packets. For the heavy mass nuclei the central density is $\approx 0.15$ nucleon/fm$^3$ for both $L_{\text{stand}}$ and $L_{\text{broad}}$. Same results are obtained for the nuclei propagating with Hard and HMD equations of state.

In Fig. 5, we see from the figure that for the light mass nuclei, the binding energy per nucleon for the $L_{\text{broad}}$ case deviates more from the experimental values for both the Soft and SMD equations of state, whereas for the heavy mass nuclei the binding energy is close to experimental values. One should note that the binding energy is the sum of the density dependent skyrme energy, coulomb energy, and kinetic energy. For the light mass nuclei the nucleon density at the center is less as compared to at the surface. With the increase in the width of the Gaussian, the central density further decreases making the surface more wide as shown in Fig. 4. Due to less central density the skyrme energy which is density dependent, contributes less towards the total binding energy thus decreasing the total binding energy of the light mass nuclei. The kinetic energy which is repulsive in nature decreases with increase in the width but the main contributing factor is of density dependent part of the binding energy. More precisely one can say that the reason for getting the less binding energy for all the nuclei with larger Gaussian width stems from the effect that the nucleus effectively is smeared out over a larger size. Therefore, the central density gets reduced which yields a smaller contribution of the skyrme term and thus a smaller binding energy. It means that the nuclei having $L_{\text{stand}}$ prefer to have more binding energies by emitting the less bound nucleons. But this emission of the nucleons may cause artifacts in the results of heavy-ion collisions. By using $L_{\text{broad}}$ as width we get the less bound but stable nuclei for a long period of time. Similar results are obtained for all the nuclei propagating with Hard and HMD equations of state.

Figure 4: Radial density distribution of the nuclei. We have averaged the local density over the first 100 fm/c for each individual simulation. Then the average over the 200-1000 simulations is taken. The left panel is for Soft EOS and right panel is for SMD. Results obtained with $L_{\text{stand}}$ are represented with solid lines whereas dashed lines show results with $L_{\text{broad}}$. 
The above discussion indicates that for the light mass nuclei propagating with and without momentum dependent interactions the number of free nucleons emitted at final time step reduces nearly to zero by doubling the width of Gaussian. This indicates that one can obtain the stable non-interacting initial nuclei for a long time span but at the cost of decrease in binding energy per nucleon. For the heavy mass nuclei, the double width of the Gaussian wave packets generate properly stable ground states which have correct binding energies, root-mean-square radii, and density distribution.

Summary

Summarizing, we have studied the role of the different widths of the Gaussian wave packets (i.e., $L = 1.08$ fm$^2$ and $L = 2.16$ fm$^2$) on the stability of the ground state nuclei throughout the periodic table for different equations of state namely, Soft, Hard, SMD, and HMD. We find that the double width of the Gaussian wave packet yields stable nuclei which do not emit free nucleons over a long period of time. But these stable nuclei are less bound in case of light mass nuclei. The heavy mass nuclei have proper ground state properties such as binding energy, density distribution, and root-mean-square radii.

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