Continuum damping effects in nuclear collisions associated with twisted boundary conditions

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The time-dependent Skyrme Hartree-Fock calculations have been performed to study $^{24}$Mg + $^{24}$Mg collisions. The twisted boundary conditions, which can avoid finite box-size effects of the employed 3D coordinate space, have been implemented to compare with the widely used periodic boundary conditions. The prolate deformed $^{24}$Mg has been set to different orientations to study vibrations and rotations of the compound nucleus $^{48}$Cr. Our time evolution results show continuum damping effect persists associated with the twisted averaged boundary conditions after the fusion stage. In particular, the continuum damping width of the rotational amplitudes has been extracted to be around 0.16 MeV. The averaged surface density distributions of the twisted boundary calculations become uniform gas which is different from the structured surface density distributions from calculations with periodic boundary conditions.

Introduction.— The real-time nuclear dynamics such as collective responses, large amplitude collisions and fissions have been studied extensively to probe effective interactions, many-body correlations and transport properties [1][3]. The basic theoretical framework for quantum many-body dynamics is the time-dependent Schrödinger equation with various approximations. In this respect, the microscopic time-dependent Hartree-Fock (TDHF) (or time-dependent density functional theory) was very successful for studies of nuclear dynamics, in particularly the large amplitude dynamics [1][3]. The improved time-dependent-Hartree-Fock-Bogoliubov calculations have also been developed for superfluid systems, relying on tremendous computing capabilities [8][9]. Besides, the quantum molecular dynamics calculations have been widely used for heavy ion collisions at higher energies with two-body dissipations [10]. For small amplitude collective motions, TDHF can match the random phase approximation (RPA), or linear resonance theory [2][11]. For nuclear collisions involving considerable excitation energies, the TDHF without pairing is a reasonable approximation.

TDHF calculations are usually performed in 3D coordinate spaces with periodic boundary conditions [12]. Due to the limits of computational resources, the calculations suffer from a systematic error related to finite box-sizes that were employed. The finite box sizes lead to tiny wave reflections at boundaries or wave interferences between periodic images [13]. Furthermore, the continuum can not be accurately discretized within small coordinate spaces [14]. This is not a serious problem for descriptions of bulk properties but it could be not negligible after long-time evolutions. The important role of continuum in nuclear reactions has also been demonstrated by the widely adopted continuum-discretized coupled-channels calculations [15]. For highly excited compound nuclei produced by fusion reactions, the surface pressures are equilirbized by thermalized continuum gases which allow for particle evaporation [16]. In weakly bound nuclei, the accurate treatment of continuum couplings is important for halo structures and associated dynamics [17][19].

To avoid the dependence of box sizes, the twisted averaged boundary condition (TABC) has been applied to TDHF calculations of giant resonances [20]. The Twisted boundary condition is a generalized periodic boundary condition (PBC) for Bloch waves with non-zero twisted angles. In condensed-matter physics, TABC results by averaging twisted angles can significantly cancel finite box-size effects [21]. Partial TBC has also been found to be useful in Lattice QCD calculations of few body systems [22]. In nuclear physics, the quasiparticle RPA (QRPA) with outgoing boundary conditions has been realized for spherical nuclei [17] but it is extremely difficult for deformed nuclei. It was known that QRPA calculations with not-well discretized continuum can cause false resonance peaks [14][23]. An effective way to smooth resonances of deformed nuclei is to use the absorbing boundary condition (ABC) [13][14]. It has been demonstrated that the TABC and ABC behave similarly in damping effects to smooth the giant resonances [20]. The TDHF calculations can in principle take into account the Landau damping, escaping damping and the damping due to complex configuration couplings [3]. The continuum treatment is essential in all of these damping mechanisms. The ABC calculation has to adjust the imaginary potential to absorb waves exactly at boundaries, and this is tedious. On the other hand, TABC can be easily implemented for complex systems. The TABC is very successful in studying giant resonances but it has not been applied to large amplitude nuclear dynamics yet. Therefore, it is desirable to explore the influences of TABC calculations of large amplitude nuclear dynamics with time evolutions.

In this work, we intend to study the $^{24}$Mg + $^{24}$Mg collisions by TDHF calculations with TABC and PBC boundary conditions. The compound nucleus $^{48}$Cr can...
have hyperdeformed states at high spins from cranking calculations [24], indicating multi-α clustering structures. Such α-conjugate compound nuclei are expected to be favorable for searching collective molecular motions. Indeed, several experiments have been performed for $^{24}\text{Mg} + ^{24}\text{Mg}$ collisions and narrow resonances in inelastic cross sections have been reported [23, 27]. However, some experiments didn’t find resonance structures in $^{24}\text{Mg} + ^{24}\text{Mg}$ fusion cross sections [28]. Note that the full picture of clustering structures in compound nuclei should take into account the dynamical nonlocalized clustering [29]. In the precompound nuclei, the time-dependent nucleon localization indicates that clustering vibrations are important in the initial stage of fusion [30]. The prolate $^{24}\text{Mg}$ allows studies of collisions with different orientations. To characterize different collision reactions, the time evolutions of total kinetic energies and deformations have been studied using the Fourier transformation.

**Method.**— We utilize the 3D Skyrme-TDHF solver Sky3D [12], which solves the self-consistent HF equation and the TDHF equation. The calculations are performed in the 3D uniform coordinate spaces, and there is no symmetry restrictions on the wavefunctions. The full Skyrme energy functional adopts the SV-bas [31] force and the spin-orbit and time-odd terms have been included.

The grid spacing is set to be 1 fm and the time step of dynamical evolution takes 0.2 fm/c. In Sky3D, the time propagator is evaluated by the Taylor series expansion up to the sixth order. Computations with these settings are taken as 24\text{Mg} and 48\text{Mg} fusion cross sections [32]. Note that the static wave functions can be transformed into larger coordinate spaces by using the Fourier transforms and inverse Fourier transformations. The energies and density distributions as a function of time are the main outputs.

**Boundary conditions.**— PBC is a natural choice for plane wave representation and is efficient for computations in the uniform 3D grids [12]. TBC is a generalized Bloch boundary condition as written as [20],

$$\psi(r + nL) = e^{i\theta \cdot n} \psi(r)$$  \hspace{1cm} (1)$$

where $r$ denotes the 3D coordinates, $L$ denotes the box size, and $n$ is the unit vector in 3D Cartesian coordinates. The twisted angle $\theta$ changes from zero to $\pi$. Eq.1 can go back to PBC when the twisted angle $\theta$ is zero. The single-particle HF equation can be written as,

$$\hat{h}_\theta \psi_{\alpha\theta}(r) = \epsilon_{\alpha\theta} \psi_{\alpha\theta}(r)$$  \hspace{1cm} (2)$$

where $\alpha$ is the discrete label of the single-particle wave functions.

In the TABC method, the expectation value of an observable $O$ can be obtained by averaging over the twist angles [20],

$$\langle \hat{O}(t) \rangle = \frac{1}{8\pi} \int_0^{2\pi} d^3\theta \langle \Psi_\theta(t) | \hat{O} | \Psi_\theta(t) \rangle$$  \hspace{1cm} (3)$$

where $\Psi_\theta(t)$ is the HF Slater wave function at time $t$. The twisted angle is discretized in practical calculations. In this work, the 3D integration over $\theta$ is performed using a four-point Gauss-Legendre quadrature between 0 and $\pi$. This means that total 64 TDHF calculations are carried out for each case. The momentum $k$ is modified accordingly as,

$$k_{i,m} = \frac{2\pi m + \theta}{L_i}, \quad m = 0, \pm 1, \pm 2, \cdots, \pm m_{\text{max}}.$$

In principle, we can recover a continuous spectrum of $k$ with varying twisted angles. The accurate treatment of continuum is important for descriptions of nuclear reactions and weakly bound nuclei. Calculations with different twist angles will give rise to different finite-volume corrections [22]. It has been demonstrated that averaging results over $\theta$ can significantly cancel finite-volume effects [20, 21, 23].

**Results.**— We have performed 3D TDHF calculations using the Sky3D solver for $^{24}\text{Mg} + ^{24}\text{Mg}$ collisions. In such reactions, the ground state of $^{24}\text{Mg}$ has a large prolate deformation of $\beta_2 = 0.49$ (axis ratio is 1.7:1) in our Skyrme Hartree-Fock calculations. The reaction threshold energy is -14.93 MeV since the binding energies of $^{24}\text{Mg}$ and $^{48}\text{Cr}$ are 198.26 MeV and 411.45 MeV [24], respectively. The fusion barriers in this case are from 22 MeV (head to head) to 24 MeV (side to side) depending on the collision orientation. The Ikeda cluster threshold energies for different structures in $^{48}\text{Cr}$ are $\alpha-^{40}\text{Ca}$ ($12.83 \text{ MeV}$), $^{24}\text{Mg}-^{24}\text{Mg}$ ($14.93 \text{ MeV}$), $3(^{16}\text{O})$ (28.61 MeV), $4(^{12}\text{C})$ (42.82 MeV) and $12\alpha$ (71.9 MeV).

Fig.1 shows the time evolution of the total kinetic energy for head-to-head collisions of $^{24}\text{Mg} + ^{24}\text{Mg}$, with collision energies at $E_{c.m} = 29.49$ and 69 MeV, respectively. The corresponding excitation energies of the compound $^{48}\text{Cr}$ are 43.93, 63.93, 83.93 MeV. In the fusion stage, there are strong damped oscillations in kinetic energies related to the bulk dissipation. In this stage, there are negligible differences between PBC and TABC calculations. In TABC calculations, small amplitude oscillations are persistent after 2000 fm/c. These small amplitude oscillations behave like molecular vibrating states and are presented at three different collision energies. In TABC calculations, however, the small amplitude oscillations are quickly damped and the compound nucleus at equilibrium state is obtained. This damping effect has been demonstrated in the TDHF calculations of strengths of giant resonances with TABC and ABC [20]. The particles are not really escaped in TABC, however, the box-size dependence of continuum treatment is actually diminished in TABC. For PBC cal-
calculations with not sufficiently large box sizes, the continuum is not precisely discretized. The continuum damping plays a persistent role after the fusion stage. This means that the molecular vibration states obtained in TDHF calculations with PBC are questionable.

Fig. 2 displays the Fourier analysis of the evolution of kinetic energies from TDHF-TABC calculations as shown in Fig. 1. It can be seen that for the three collisions at energies of 29, 49 and 69 MeV, the main peaks are at 5.8, 5.0 and 6.0 MeV, which are lower than that of typical giant resonances \[20\]. The damping widths for the \( E_{\text{c.m.}} = 29 \), 49, 69 MeV are about 2.2 MeV, 1.4 MeV and 2.3 MeV, respectively. This fusion process is a typical underdamping with damping widths much smaller than the oscillation frequencies, in contrast to the widely recognized overdamped fission process \[35\]. The main dampings are more or less similar in three cases. It can be seen that the damping time of the 49 MeV collision is longer than other two cases, which is related to its narrower damping width. For the PBC calculations, the small amplitude oscillations correspond to frequencies of 7.4, 7.0, 7.6 MeV, respectively. These frequencies are much smaller than the Ikeda clustering threshold energies and are not likely to be physical molecular vibrations.

The time evolutions of quadrupole deformations from TDHF-TABC calculations of the above-mentioned collisions are shown in Fig. 3. At the fusion stage, the large-amplitude oscillations are strongly damped. It can be seen that the amplitudes are larger with higher collision energies. However, the minimum deformations of the three cases are close. The oscillations of deformations are not symmetric as that in kinetic energies. The fusion is not a simple damped oscillator regarding the quadrupole deformations, due to the density dependence of incompressibility. At the equilibrium stage, the quadrupole deformations are 448, 485, and 510 fm², respectively. These prolate deformations of the compound \(^{48}\)Cr are extremely large with axis ratios are 3.9:1, 3.8:1, and 3.2:1, respectively.
respectively. Therefore larger quadrupole deformations at higher collision energies are not necessarily related to larger axis ratios, and volume expansions of compound nuclei play a role. The corresponding final kinetic energies of the three cases in Fig.1 are 783.5, 776, and 768 MeV respectively, which are lower than the initial kinetic energies at 809, 829, and 849 MeV respectively. The differences denote the transformation from kinetic energies to potential energies as total energies are conserved in both PBC and TABC calculations. We see that with higher energies for head-to-head collisions, the final kinetic energies are smaller and quadrupole deformations and deformation energies are larger.

Fig.4 shows the time evolutions of the $^{24}\text{Mg}^+$ $^{24}\text{Mg}$ side-to-side collision at 49 MeV. Similar to Fig.3, the PBC and TABC calculations are close at the fusion stage before 1000 fm/c. The oscillation frequency is much larger and damping time is shorter compared to head-to-head collisions. Small amplitude oscillations in quadrupole deformations and kinetic energies are persistent in PBC calculations, but they are being significantly damped in TABC calculations. This is the same damping mechanism as demonstrated in the head-to-head collisions. The final kinetic energy is about 824 MeV, which is larger than 776 MeV of the head-to-head collision. The final quadrupole deformation is about 220 fm$^2$ which is much smaller than that of the head-to-head collision, showing the dependence of collision orientations.

We also studied the fusion-rotation reaction. In this case, the collision energy is taken as 40 MeV and the impact parameter is 2 fm for the side-to-side collision. In our calculations, the collision direction is along z-axis and the compound nucleus rotates in the x-z plane. To study the rotation evolution, the expectation values of $<z^2>$ are given in Fig.5. It is striking to see that the rotation amplitude is slowly damped in TABC calculations, while the rotation is almost a perfect cosine function in PBC calculations. This rotational damping is not a surprise considering the pervious damping of small amplitude vibrations. It is more interesting because it illustrated a very clear damping picture compared to previous vibrational cases. The vibrational damping has been studied extensively [36], while the damping of rotation amplitudes has rarely been discussed. To further study the damping effects, the spectral analysis by Fourier transformation are also shown in the middle panel of Fig.5. Note that the $<z^2>$ frequency (period is about 1300 fm/c) is two times the rotation frequency. We can see the rotation frequencies $\omega$ are about 0.43 MeV and 0.46 MeV for the TABC and PBC calculations, respectively.
Note that the damped rotation amplitudes can be written as $A(t) = A_0 e^{-\Gamma t/2} \cos(\omega_D t + \phi)$, where the damped frequency $\omega_D = \sqrt{\omega^2 - \Gamma^2/4}$. Therefore the rotation frequency of TABC is slightly smaller than that of PBC due to damping effects. The width $\Gamma/2$ can then be estimated to be about 0.16 MeV for TABC calculations.

Fig. 6 shows the density distributions in the x-z plane, corresponding to rotations in Fig. 5. Fig. 6(a), (b), (c) show the density contours from TABC calculations at 2000 fm/c, 4000 fm/c, and 6000 fm/c respectively with a log scale. For comparison, Fig. 6(d), (e), (f) show the corresponding densities from PBC calculations. With time increases, we see that the surface density distributions become more and more uniform in TABC calculations. The surface gas density is about $10^{-5}$ fm$^{-3}$, to which protons and neutrons have similar contributions and $\alpha$ emission is possible. The uniform gas is similar to the thermal gas (dominated by neutrons) in compound nuclei from finite temperature Hartree-Fock-Bogoliubov calculations [16]. The thermal neutron escaping width is proportional to the gas density which provides a equilibrium pressure. The density of thermal neutron gas is dependent on the temperature and independent of box sizes. The surface gas corresponds to emitted particles and in principle it should be removed. Both PBC and TABC lead to a false low-energy bump at $\hbar\omega=0.2$ MeV in Fig. 6(b) due to the floating continuum gases, as discussed in [20]. In contrast, the density distributions at surfaces in PBC calculations have non-uniform structures. The non-uniform surface density is related to finite box-sizes, which doesn’t cause damping effects. In Fig. 6 the damping effect in PBC calculations is almost negligible. The quadrupole deformation of PBC calculations is about 227 fm$^2$ with an axis ratio of 2.2:1. In TABC calculations, however, the averaged bulk density distributions become spherical. This is consistent with the damped rotation amplitude in Fig. 5. We see that the compound nucleus $^{48}$Cr is still rotating at each twisted angles. For the rotation in x-z plane, the calculated averaged $\langle J_y \rangle$ is about 6$\hbar$ at 7000 fm/c, which decays slowly and smoothly. The calculated $\langle J_y \rangle$ with PBC is decaying slightly faster associated with oscillations. It is known that hot nuclei at equilibrium are spherical at high temperatures in the mean-field framework. In our case, the angular momentum $\langle J_y \rangle$ from TABC is persistent although density distributions become spherical. Whether spherical compound nuclei will rotate or not at equilibrium state is a critical question. In Fig. 6(c), we see that the total angular momentum is not conserved in both PBC and TABC calculations. The angular momentum is not conserved whenever the emitted particles from highly-excited compound nuclei encounter boundaries, while this conservation is preserved for TDHF cranking calculations [3].

Summary.— We implemented the twisted boundary condition in time-dependent Skyrme Hartree-Fock calculations of $^{24}$Mg + $^{24}$Mg collisions, which are performed in 3D coordinate spaces. In head-to-head and side-to-side collisions, small amplitude vibrations are persistent in calculations with periodic boundary conditions, but they are damped with twisted averaged boundary conditions. This kind of damping mechanism is related to the cancelation of box size dependence in TABC, so that the continuum is properly treated. By studying the side-to-side collision with an impact parameter of 2 fm, we found that the rotation amplitude is damped as well. The results are striking because we can clearly extract the continuum damping width which is about 0.16 MeV. The density distributions show that in TABC calculations the compound nucleus becomes spherical surrounded by uniform surface gases. The averaged angular momentum decays slowly although the averaged compound nucleus becomes spherical. The surface density distributions from PBC calculations are non-uniform, due to finite box-size effects. The results are inspiring but are understandable. Further applications of twisted boundary conditions in nuclear reactions and weakly bound nuclei will be valuable.

Acknowledgments

We are grateful to W. Nazarewicz’s suggestions and useful discussions on twisted boundary conditions. We also thank useful discussions with F.R.Xu. This
work was supported by National Key R&D Program of China (Contract No. 2018YFA0404403), and the National Natural Science Foundation of China under Grants No.11790325,11522538,11835001. We also acknowledge that computations in this work were performed in Tianhe-1A located in Tianjin and Tianhe-2 located in Guangzhou.

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