Semiclassical simulation of finite nuclei

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(Received 18 December 1989)

Semiclassical simulation of finite nuclei, readily available for nuclear collisions, is presented by employing the classical equation of motion approach in conjunction with a nuclear structure model, the isomorphic shell model, previously and independently published. Emphasis is put on good approximation of the main nuclear properties and their preservation during the evolution of the simulation for times much longer than a typical reaction time.

I. INTRODUCTION

The simulation of nuclear systems is of great importance, since it can be used for the theoretical description of nuclear dynamics at different excitations, such as those obtained through nuclear reactions. It has particularly proven useful in high-energy heavy-ion collisions which is a subject of growing interest in nuclear physics, since pion condensation, density isomers, quark-gluon plasma nuclear shock waves, and other exotic phenomena may appear in the course of these reactions. Since a complete relativistic quantum-mechanical handling of such reactions is not practically possible, one resorts to classical or semiclassical models based on the microscopic dynamics of interacting classical particles which was first introduced[1,2] by Bodmer and Panos in 1977 through their classical equation of motion (CEOM) approach. Such models contain the entire many-body matrix and thus automatically incorporate details of the interactions such as dynamical fluctuations and fragment formations. The establishment of a computer simulation which accounts reasonably well for the general thermostatic nuclear properties is a prerequisite before addressing more complex dynamical problems.

The most recent efforts[3,4] to study nuclear dynamics by using the CEOM approach will be discussed in some detail at the end of the paper. There, previous relevant works[5,6] are reported that were unable to reasonably simulate a nuclear system even for selected cases. Here, the nuclear system is modeled as a semiclassical system of A interacting particles (nucleons) by employing an existing nuclear structure model,[7] the isomorphic shell model (ISM). While the approach used is again the CEOM approach,[1,2] its conjunction with the ISM would be referred to as CEOM model. For an implementation of the CEOM model a suitable choice of a two-body potential, of initial configurations of nucleon positions, and of initial configurations of nucleon velocities is made as described below. The main purpose of the present paper is to present the time evolution (which is a dynamical test) of the nuclear simulation obtained via CEOM model.

II. TWO-BODY POTENTIALS

The choice of the potential is made by examining its high- and low-energy properties where the Coulomb interaction is not taken into account (despite the fact that it was possible).

Our static central potential consists of a repulsive (R) and an attractive (A) Yukawa-type component as follows, and thus short-range correlations are taken into account automatically:

$$V(r_{ij}) = V_R \cdot e^{-\mu_R \cdot r_{ij}}/r_{ij} - V_A \cdot e^{-\mu_A \cdot r_{ij}}/r_{ij} \ . \tag{1}$$

The potential constants have been determined for two different regions of energies, i.e., below[8] and beyond[9] 50 MeV/nucleon. These constants are given in Table I. It has been found that this distinction between energies was necessary as discussed in detail in Ref. 8. As one can see, for the simulation of the ground-state behavior of a nuclear system (which corresponds to an isolated nucleus) use of the low-energy potential is required as is done here for the rest of the paper.

The scattering and saturation properties of our potentials have been successfully tested in Refs. 8 and 9. The main difference of these potentials from all other potentials used in nuclear collisions is that they are the best potentials which simultaneously reproduce the first two moments [$\sigma^{(1)}(E)$, longitudinal momentum loss cross section, and $\sigma^{(2)}(E)$, transverse momentum transfer cross section] of the c.m. differential scattering cross section for free nucleons and at the same time possess very good saturation properties. Thus, it is expected that our potentials are more reliable in describing nuclear collisions, where both longitudinal and transverse momentum transfers are important.

TABLE I. Constants of two-Yukawa central potentials.

Energies (E)	V_R (MeV fm)	μ_R (fm^{-1})	V_A (MeV fm)	μ_A (fm^{-1})
$E<50$ MeV/nucleon	$2.4(10^{22})$	29.8017	258.85	1.5017
$E>50$ MeV/nucleon	$1.7(10^{17})$	31.8538	187.0	1.3538

For a comparison of potentials that appeared until 1984 one may refer to Ref. 10, while for a short reference to potentials that appeared afterwards one may contact Ref. 11, Sec. II A and Ref. 12.

III. INITIAL CONFIGURATIONS OF POSITIONS

Here, the initial configurations of positions, instead of being created *ad hoc* as in all previous works,[1-6] are taken according to a previously and independently published nuclear-structure model,[7] the isomorphic shell model. These configurations have normal densities, include short-range nucleon correlations, possess correct saturation properties for the potential employed (preceding section), and for the nucleus examined here (and for any other nucleus up to ^{40}Ca) have already been published in Refs. 9 and 10. For any other nucleus, these configurations can be derived from the information given in Fig. 1 of Ref. 7. Thus, the main advantage of our configurations of positions is that they come from a nuclear-structure model and so are objective (not *ad hoc*) and available to anyone interested in verifying our results or performing his or her own calculations. These configurations for ^{16}O are repeated in Table II (second through fourth columns). For a review of the practice used by other models so far (following either a random selection of positions in a sphere or considering crystalline structure) one may consult Ref. 11, Sec. II B.

IV. INITIAL CONFIGURATIONS OF VELOCITIES

The initial configurations of velocities in the present work come from the same nuclear-structure model as the configurations of positions.[7] The magnitude and direction of the velocities are consistent with the independent-particle model (orbital motion) and include the uncertainty due to the confinement of nucleons in the nuclear volume.[13] For our nucleus of interest, ^{16}O, these initial velocities are included in Table II (fifth through seventh columns). Details of the way they have been derived by using the ISM are described in Ref. 13 and in Ref. 11, Sec. II C, where one may also find a short review of the practice applied by other researchers in specifying their own (random) initial velocities. Here, we repeat the relevant formulas for their magnitudes only for reasons of completeness:

$$\tfrac{1}{2}mu_{i(\mathrm{unc})}^2=\frac{\hbar^2}{2m}\left[\frac{1}{R_{\max}^2}\right] \quad \text{due to uncertainty ,} \tag{2}$$

and

$$\tfrac{1}{2}mu_{i(\mathrm{orb})}^2=\frac{\hbar}{2m}\left\langle\frac{L_i^2}{\rho_i^2}\right\rangle \quad \text{due to orbiting ,} \tag{3}$$

where $R_{\max}$ is the confinement radius of the nucleons,[13] m the nucleon mass, ρ the radius of the classical orbit of the average nucleon position,[7,13] and $\langle L^2\rangle=l(l+1)$ the

TABLE II. Initial configurations of nucleon positions and velocities.

	Initial postions (fm)			Initial velocities 10^{23} fm/sec		
No.	x	y	z	V_x	V_y	V_z
1	0.689	0.689	0.000	0.105	0.105	0.105
2	−0.689	−0.689	0.000	−0.105	−0.105	−0.105
3	−0.897	0.897	0.897	0.105	0.095	0.105
4	0.897	−0.897	−0.897	−0.105	−0.095	−0.105
5	0.000	2.511	0.000	−0.250	−0.105	−0.105
6	0.000	−2.511	0.000	0.250	−0.105	0.105
7	2.511	0.000	0.000	0.105	−0.095	−0.250
8	−2.511	0.000	0.000	−0.105	0.095	0.250
9	0.000	0.000	2.511	0.460	0.105	0.105
10	0.000	0.000	−2.511	−0.460	0.105	−0.105
11	1.467	1.467	1.467	−0.409	0.105	−0.199
12	−1.467	−1.467	−1.467	0.409	−0.105	0.409
13	1.467	1.467	−1.467	−0.409	0.409	−0.105
14	−1.467	−1.467	1.467	0.199	−0.409	0.105
15	1.467	−1.467	1.467	−0.409	−0.105	−0.199
16	−1.467	1.467	−1.467	0.409	0.105	−0.199

orbital angular momentum of the specific nucleon i. Besides the magnitude, the complete vector of the orbital velocity component[14] for each nucleon is well specified in the framework of the ISM. For the uncertainty velocity component, however, the relevant vector could have any (random) direction. For a specific selection of this component, the whole velocity vector (i.e., its three components) for each nucleon is that which is given in Table II.

V. REALIZATION OF SIMULATION

Given the initial configuration of positions (r_i) and velocities (v_i) from Table II and the two-nucleon potential from Table I (for energies < 50 MeV/nucleon), the simulation of the ground state of ^{16}O is obtained. The first requirement of such a simulation is to reproduce the main ground-state nuclear properties, i.e., the point mass root mean square radius,

$$\langle r^2 \rangle^{1/2} = \left[\sum_{i=1}^{A} \frac{r_i^2}{16} \right]^{1/2}, \tag{4}$$

and the binding energy,

$$\mathrm{BE} = \sum_{i<j}^{A} V_{ij} - \sum_{i=1}^{A} \frac{\hbar^2}{2m} \left[\frac{1}{R_{\max}^2} + \left\langle \frac{L_i^2}{\rho_i^2} \right\rangle \right]. \tag{5}$$

These quantities for ^{16}O estimated at different times are shown in Table III (columns 6 and 5, respectively).

VI. TIME EVOLUTION OF SIMULATION

In Table III the time evolution of ^{16}O is given, as far as its main properties are concerned. That is, at the end of each successive time interval equal to 8 fm/c, the total energy loss due to the procedure followed, the potential energy, kinetic energy, and the binding energy for the whole nucleus are registered (columns 2–5, respectively) together with the following radial quantities. That is, the mass root mean square (rms) nuclear radius, the minimum and the maximum distance observed between the members of all pairs formed by the 16 nucleons, and the maximum distance from the nuclear center observed for any of the 16 nucleons (columns 6–9, respectively) are shown. Finally, the number of nucleons beyond 4.50 fm from the nuclear center during this interval is given (column 10). In addition, the velocity of the center of mass, and the total linear and angular momenta, are estimated at the same time but not registered in the table, because of their insignificant variation with time around their expectation zero values. One could notice that since the particles interact via a pairwise potential, these physical quantities should be exactly conserved. The source of error of the previously and later mentioned (e.g., in binding energies) insignificant variations is the imperfections in the different steps of our simulation (including the finiteness of the time step employed; see column 1 of Table III). It is worth mentioning that while in Table III the aforementioned quantities are registered each 8 fm/c, the computer code employed here estimates these quantities each 0.02 fm/c. The following comments on the values of Table III are of interest.

First, we see from column 10 that while after 56 fm/c a few nucleons (1 or 2) are beyond 4.5 fm, none of them has evaporated from the nucleus as the values of column 9 show. Indeed, the maximum radial distance from the origin of any nucleon at 100 fm/c is 4.41 fm, which is even shorter than the distance 4.44 fm met at 48 fm/c. Thus, in conclusion one sees that the nucleon number conserva-

TABLE III. Time evaluation of main nuclear properties.

Time fm/c	Energy loss %	Potential energy MeV	Kinetic energy MeV	Binding energy MeV	Mass rms radius fm	Min. pair dist. fm	Max. pair dist. fm	Max. nucl. radius fm	Nucleons beyond 4.5 fm
1	2	3	4	5	6	7	8	9	10
0.0		−15.84	8.11	7.73	2.28	1.83	5.08	2.54	0
8.0	0.00	−18.15	10.41	7.74	2.29	1.67	5.65	2.95	0
16.0	0.00	−15.50	7.76	7.74	2.50	1.65	6.24	3.27	0
24.0	0.00	−14.56	6.83	7.73	2.56	1.65	6.79	3.41	0
32.0	0.00	−17.78	10.05	7.73	2.44	1.66	6.37	3.64	0
40.0	0.01	−17.42	9.69	7.73	2.51	1.67	6.59	4.15	0
48.0	0.01	−15.35	7.62	7.73	2.66	1.66	6.94	4.44	0
56.0	0.01	−14.57	6.83	7.74	2.84	1.65	7.31	4.67	1
64.0	0.01	−14.37	6.63	7.74	2.89	1.69	6.89	4.65	1
72.0	0.01	−15.00	7.26	7.74	2.89	1.65	7.30	4.43	0
80.0	0.01	−13.38	5.64	7.74	3.04	1.70	8.07	4.20	1
88.0	0.01	−12.13	4.39	7.74	3.17	1.66	9.03	4.34	1
96.0	0.01	−14.16	6.42	7.74	3.25	1.70	9.72	4.52	2
100.0	0.01	−15.76	8.02	7.74	3.27	1.63	9.96	4.41	1
			Mean values	7.74	2.76	1.68			
			Expt. values	(7.98)	(2.65)	(1.72)			
			% error	3%	4%	2%			

tion in our simulation lasts beyond 100 fm/c. Specifically, since a typical reaction time is about 10 fm/c, the survival of ^{16}O up to (and beyond) 100 fm/c is one order of magnitude longer than this characteristic time. This should be compared with the situation described in Ref. 15 where in much shorter time up to 50% of the nucleons have evaporated from the modeled nucleus.

The total energy loss up to the time of 100 fm/c does not exceed 1% (column 2) and the binding energy (column 5) in all in-between times remains almost constant (it varies between 7.73 and 7.74 MeV/nucleon) and compares rather well with the experimental value 7.98 MeV/nucleon. While the binding energy remains practically constant, however, the magnitude of the average potential and kinetic energies per nucleon vibrate between the values (in MeV) 12.13–18.15 and 5.64–10.41, respectively. This is an interesting observation demonstrating the "living" nature of our simulation. That is, while there is a real conservation of the total net energy (i.e., binding energy), the components of this energy (i.e., the potential and kinetic energies) vary $\sim$50% and $\sim$100%, respectively, between their minimum and maximum values.

Total linear and angular momenta conservation manifests itself in our simulation, since $\sum_i \bar{p}_i \approx 0$ and $\sum_i [\bar{r}_i \bar{p}_i] \approx 0$ in all times. Again the components of momenta for the individual nucleons may vary significantly. These conservations mean that for the ground state of a nucleus the collisions involved are of elastic nature.

The above conservation of energy and momenta shows the success of our simulation of an isolated nucleus. This is further strengthened by the almost zero value of the velocity of the center of mass. That is, while the nucleons are in *constant* motion according to their mutual NN interaction, and their orbital motion and the uncertainty relationship, their center of mass remains practically immovable.

The radial values in columns 6–9 in the table are even more sensitive quantities during the evolution with time of our nuclear simulation. Specifically, the mass rms radius (column 6) between the times 0.0 and 48 fm/c vibrates between the values 2.28 fm and 2.66 fm, while afterwards increases continuously up to the value 3.27 fm at 100 fm/c, which implies an expansion of the nucleus. The average value of mass radius from 0–100 fm/c is 2.76 fm which compares rather well with the experimental value 2.65 fm (which is almost our value at time 48 fm/c).

The minimum distance between the members of any pair of nucleons (column 7) after the first interval shows a small variation from 1.63 fm to 1.70 fm. Thus, while during the first time interval we have a rather significant reduction from 1.83 fm to 1.67 fm, this quantity does not show the tendency to reach the radial distance 1.72 fm (where the potential exhibits its minimum value) very fast, which means that the nucleons do not clump together very fast towards this minimum value. The maximum distance between the members of any nucleon pair (column 8) shows a rather large variation following the same overall pattern as the mass radius with minimum value 5.08 fm at 0.0 fm/c and maximum value 9.96 fm at 100.0 fm/c. This quantity more or less corresponds to the maximum diameter of the simulated nucleus and its increase shows an expansion of the nucleus. This quantity is a much more sensitive test for the expansion of the nucleus than the mass rms radius discussed earlier.

The maximum distance from the origin (column 9), observed for any nucleon at the end of each time interval, up to the time 80.0 fm/c is always (as it should be) larger than the half of the maximum pair distance just discussed (column 8). However, after this time this relationship is no longer valid, as one may see from the last three rows of Table III (e.g., $4.41 < 9.96/2$). This is understood as a slight relocation of the center of mass from its initial position at the origin of coordinates from where the maximum nucleon distance is always estimated. The time 80 fm/c is rather long and the net velocity of the center of mass (even of small magnitude due to imperfection of the simulation) has resulted in its slight displacement. Thus, this quantity is a more sensitive test than the velocity of the center of mass itself regarding the collective replacement of the nucleus as a whole.

An overall evaluation of the above evolution is that while up to the time 100 fm/c the simulation of ^{16}O remains rather acceptable, the best results are obtained at about half of this time, which is sufficient time for nuclear reactions involving light or heavy ions. While this success here is demonstrated by using a specific nucleus (i.e., ^{16}O), it is valid for any nucleus up to ^{208}Pb where the ISM has been worked out. For example, for ^{40}Ca we have a conservation of main nuclear properties similar to ^{16}O up to the time 30 fm/c, which is again sufficiently longer than a typical reaction time of 10 fm/c. From our experience with ^{16}O we know that the conservation time of 30 fm/c could be substantially improved by slight changes in the random direction of the uncertainty component of the nucleon velocities.

VII. COMPARISON WITH OTHER SIMULATIONS

At this point it is interesting to compare the present work with two recent, very interesting publications[3,4] on the same topic, but using a completely different method. The first step[3] in that work was the introduction of a momentum-dependent repulsion for the purpose of simulating the Pauli exclusion principle, while the second step[4] was the inclusion of a real two-body interaction for the purpose of achieving an approximate description of nuclear systems. Specifically, in Refs. 3 and 4, a 10-parameter potential is introduced, which gives reasonable binding energies (actually the nuclei tend to be somewhat overbound typically by less than 1 MeV per nucleon, while their mass radii are about 20% smaller) when applied (Ref. 4) to initial ("seed") configurations of positions (obtained by placing the nucleons at random inside a sphere of a size expected for the specific nucleus considered) in a frozen initial configuration in phase space (with the particles having finite momenta despite their vanishing velocities). Also assumed there for the estimation of binding energy is no zero-point motion (of the nucleons for eleven nuclei between $A=4$ and $A=84$) and

temperature $\tau=0.5$ MeV (since it was there technically difficult to treat $\tau=0$). At the same time their model is applicable to nuclear matter where the behavior of the energy with temperature and density (which is around 10% too high) is rather satisfactory.[4]

Since the ultimate goal of the approach introduced in Refs. 3 and 4 is the theoretical description of nuclear dynamics at different excitations, while the performed tests of the *NN* interaction involved with respect to binding energies and momentum distribution of Fermi gas (via their Pauli exclusion potential term) are very important, that approach should be supplemented by additional tests. A test of this interaction with respect to its ability in reproducing scattering cross sections relevant to the energy range of interest appears to be necessary, as performed in other approaches.[1,2,5–11] After all, simulation of nuclear dynamics after specifying the "seed" configurations mainly means simulation of scattering products.

In addition, besides "seed" configurations for the positions, a nuclear simulation wants "seed" configurations for the velocities (as magnitudes and directions) tested with respect to proper nuclear properties.[13] A required test of a nuclear simulation is also that of "conservation" of the main nuclear properties for a sufficient time, as is obtained in the present paper. Finally, the ultimate test of a simulation is its dynamical checking in a nuclear reaction, as performed in Ref. 11.

VIII. CONCLUDING REMARKS

The present work presents a computer simulation of ^{16}O where the main nuclear properties are well reproduced and satisfactorily conserved more than an order of magnitude in comparison to a typical reaction time (nuclear diameter/c). This success, indeed, shows the capability of the CEOM model to simulate any finite nucleus up to ^{208}Pb. Any necessary material for the construction of "seed" configurations of positions and velocities, and the appropriate *NN* potential, have already been published.[7–10,13] Here, only technical instruction on how to collect all this information is given with a specification on ^{16}O, together with the main task of demonstrating the time evolution of the relevant simulation. Furthermore, via Ref. 11, a dynamical test of such a modeling of nuclei has been successfully performed for the reaction Ne+Ne at 800 MeV/nucleon by employing, of course, the high-energy *NN* interaction from Table I.

No adjustable parameters are employed by CEOM model and all values of positions and velocities involved for each specific nucleus come as direct results of the ISM by using two *numerical* parameters (the size of the neutron bag 0.974 fm and that of the proton bag 0.860 fm determined in Ref. 13 which are consistent with our knowledge from particle physics[16] that supports their relative size as well[17]) which remain constant for all properties in all nuclei.[7]

Additional improvement of the CEOM model could be obtained by incorporating explicity the Coulomb interaction and by its application to nuclear matter binding energy. The size of nucleons employed by the ISM (mentioned above), when considered in a crystalline nuclear matter, indeed reproduce the correct density.

ACKNOWLEDGMENTS

I express my sincere appreciation to Professor J.W. Negele and Professor J. Goldstone of the MIT Department of Physics for their invitation to join the stimulating environment at their Center for Theoretical Physics during my sabbatical year. This work was supported in part by funds provided by the U.S. Department of Energy (DOE) under Contract No. DE-AC02-76ER03069.

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