Test cases for the code Sky3D

Supplement to the manuscript "The TDHF Code Sky3D"

Abstract

This directory `Sky3D-Test` contains three simple examples for running the code in its principal application modes: a static HF calculation, a dynamic simulation of a giant resonance vibration excited by an external field, and a collision between two nuclei.The static case is used to provide the ground-state wave functions for both time-dependent applications.

1. Running the code

The following instructions apply to a Linux system and the `gfortran` compiler, but should be quite similar for other Unix-based systems such as `OS X`. In order to run the applications, the code must be compiled and linked first by going into the code directory and then execute `make` for the standard version, `make -f Makefile.openmp` for the `OpenMP` version, and `Makefile.mpi` for the `MPI` version. The executable program is named `sky3d.seq`, `sky3d.omp`, and `sky3d.mpi`, respectively. Remember that MPI mode works only for the dynamic case.

In the example directories there are input files `for005` and the standard output will go into `for006.xxx`, where `xxx` is the name of the test case. The "5" and "6" were chosen as the historic unit numbers for standard input and output in Fortran. Of course, any other file name can be used instead.

A note on accuracy: if the code is run on different computers, the printed output will not be exactly identical due to differences in round-off. The comparison of the results should take into account the expected physical accuracy. For example, in the static calculation, the dipole moments printed in `dipole.res` should be zero; since an `E` format is used, the actual values show as numbers of the order of $< 10^{-15}$ with the digits essentially random. The same is true, for example, for the γ angle for a spherical nucleus ($\beta = 0$), which is indeterminate but in practice results from small inaccuracies in the quadrupole tensor components. This does in no way invalidate the results.

2. The ground state of ^{16}O

The static calculation has to be run first to produce the ground-state wave functions for the other test cases. Going into the directory where the static case will be run, the command line

$$\textit{directory}/\texttt{sky3d.seq > for006.static}$$

with *directory* the directory where the code was compiled will start the calculation. Of course the executable program can also be copied or referred to by a symbolic link.

It produces a long protocol on 'for006.static' and a compact one on 'conver.res'. The latter provides information on the most basic observables as energy, energy convergence, energy variance, radius and deformation. It does print these observables every `mprint` times during iteration. The long output provides many more details as, e.g., single-particle energies, again along the static iteration. The most important output is the file 'O16' which contains wave functions and fields from the ground state solution. This will be used in the next step. Note that the file name is set in the input file `for005`. A different name can be chosen; this may be useful when running different test cases.

To verify correct execution, the contents of these files can be compared with your own results and should agree within a reasonable number of digits. Since the dipole moment of ^{16}O is zero, the file `dipoles.res` contains very small numbers with the digits essentially random. The file `spin.res` also shows only zeroes, which in case should be reproduced, being printed in an "F" format; the sign may be random, however.

The file `conver.res` shows the typical behavior: the energy converges quite rapidly, but the fluctuations take more iterations to fall below the convergence limit. Since the deformation β is zero, the angle γ has random values. If pairing is included and for heavier nuclei the values for the fluctuations to not decrease as much; often one has to live with the order of 10^{-4}, whereas the energy will still show nice convergence behavior.

In the output file `for006.static` the properties of the single-particle states should be noted. They show the correct degeneracy and spin-orbit splitting with two nucleons in the $1s_{1/2}$-state, which has zero orbital angular momentum, four nucleons in the $1p_{3/2}$-state and two again in the $1p_{1/2}$-state. For the p-states the angular momentum components are not very instructive as there is no alignment. This is rarely needed, but if necessary a diagonalization can be done in the subspaces of degenerate states.

Note also that the proton states are pushed to somewhat higher energies by the Coulomb force.

The static calculation takes a few minutes on a modern PC.

3. The quadrupole resonance in ^{16}O

3.1. The physics case

This is an example of how to initialize and study vibrational dynamics of a nucleus, as outlined in section 2.5.3 of the documentation. The test case deals with isoscalar quadrupole oscillations in ^{16}O and the quadrupole resonance spectra deduced therefrom.

Giant resonances (GR) have for a long time been prominent and much studied excitation modes of nuclei [1]. Properly chosen Skyrme forces can provide a

good description of them [2, 3]. As GR are related to nuclear dynamics, TDHF is the correct starting point for their description. Traditional standard is to use a linearized version of TDHF, called random-phase approximation (RPA) [4, 5]. This is extremely efficient for spherical nuclei, but requires formidable formal preparation, see e.g. [6]. Conceptually much simpler and numerically competitive for deformed nuclei is to use fully fledged TDHF with subsequent spectral analysis [7, 8]. This is the line of development which we are following here. A detailed discussion of spectral analysis of TDHF results is given in [8]. We report here only the practical steps for the given example.

The present example considers the isoscalar quadrupole GR. It is related to the isoscalar quadrupole operator $\sum_n (2z_n^2 - y_n^2 - x_n^2)$ where n runs over all nucleons, protons and neutrons. The same operator couples to the excitation as well as to the measurement. Actually, we will have to adapt the operator to a periodic grid, see eq. (1). But this is a technical detail. The quadrupole GR in heavy nuclei is a crucial benchmark for the effective mass of nucleons in nuclei [9, 10]. Our example deals with a small nucleus for reasons of simplicity. It is certainly an interesting exercise to extend the test to heavier nuclei. We use for the example the Skyrme force SV-bas which is known to reproduce the quadrupole GR in ^{208}Pb fairly well [3]. It is also an interesting exercise to try the other forces provided in the code. Moreover, there are many other interesting modes besides the isoscalar quadrupole GR, for example, the isovector dipole GR or the isoscalar monopole GR [9, 1]. One may also study these modes with the present code. This is, however, a more sever exercise as the user has to code the other multipole operators in `external.f90`.

A word of caution is in order concerning the excitation spectrum at low energies. The quadrupole spectrum for the present test case ^{16}O is nicely concentrated in the resonance region around 20 MeV. In heavier nuclei as, e.g., ^{208}Pb, one will find also a low lying peak in the range of a few MeV. These low lying parts of the spectrum have to be taken with care for the case of non-magic nuclei. The present code uses pairing at BCS level for stationary solution, but freezes the pairing occupation numbers during the TDHF dynamics. Effects from pairing dynamics would show up in the low-energy spectrum. They are missing here and thus the low-energy part of the spectrum cannot be trusted for open-shell nuclei. The GR region, typically above 10 MeV, is not much affected by pairing and here we can obtain still relevant results. An exception are closed-shell nuclei (having $N, Z = 20, 28, 50, 82, 126, ...$). Here, one can trust the whole spectrum. Note, however, that a low-energy states require high resolution which, in turn, needs long sampling times.

3.2. Running the test case

The dynamic calculation is executed by
$$directory/\texttt{sky3d.seq} > \texttt{for006.gr}$$
or the analogous command for the `OpenMP` and `MPI` cases, where, again, you may discard the long output by redirecting it to `/dev/null` (because of the large size of the output file, this is recommended in this case). The input file runs a dynamics which is initialized by an instantaneous ('ipulse=0') boost. It is

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important that we set 'texternal=T' in the input file to activate the computation and use of a boost field.

The file name for the one fragment in this case is given as `../Static/O16` to refer to the wave function file generated earlier in the static run.

The boost operator is the isoscalar quadrupole. Note that we use a quadrupole operator which is modified to comply with lattice periodicity, i.e. we change $x^2 \implies \sin(x * \pi / x_{\mathrm{box}})^2$ and similarly for y and z where x_{box} is the x-extension of the box. This option is set by the `textfield_periodic=T` in the input file. The Cartesian quadrupole then effectively reads

$$\hat{Q} = 2\sin\left(\frac{z\pi}{z_{\mathrm{box}}}\right)^2 - \sin\left(\frac{y\pi}{y_{\mathrm{box}}}\right)^2 - \sin\left(\frac{x\pi}{x_{\mathrm{box}}}\right)^2 \tag{1}$$

which is close to the regular quadrupole in the vicinity of the nucleus and bends to periodic shape towards the bounds of the box. Now, it is crucial to use just exactly the same operator in the spectral analysis. To that end, the corresponding expectation value of the boost field $\hat{Q}$ is printed in the output file `extfield.res`. We also take care to trigger only a small excitation `amplq0` to stay safely in the regime of linear response. The dynamic run will produce a couple of output files `*.res`.

Because the Fourier analysis need a large number of data and a long physical duration of the calculation, the output is quite voluminous and we provide only the most important files needed for the analysis: `energies.res` and `extfield.res`. As the situation retains spherical symmetry and the center of mass remains at rest, `monopoles.res`, `dipoles.res`, `momenta.res`, and `spin.res` contains zeroes or constant values. `quadrupoles.res` may warrant a brief look to see the oscillating quadrupole moments.

The running time will be several hours on a modern PC.

First, one should have a look at `energies.res` and check that conservation of particle number (columns 2 and 3) and energy (column 4) is fulfilled sufficiently well. A slight drift of the total energy is unavoidable and acceptable. Any quick changes indicate numerical problems. The run should then be discarded and another run with safer numerical parameters should be performed.

Finally, we perform spectral analysis. To that end, we compile the corresponding analyzing tool by

<div align="center">

`gfortran spectral_analysis.f90`

</div>

and execute it by

<div align="center">

`./a.out`

</div>

which produces two new output files. The routine reads the time structure and the relevant quadrupole signal from `extfield.res`. It processes these data to produce spectra. The output file `extfield_filt.res` contains a protocol of the filtered quadrupole signals used in the spectral analysis. The file `extfield_spectrum.res` contains the spectral distributions. Its column prints the frequency, columns 2-3 the (complex) Fourier transform of the filtered isoscalar quadrupole signal, where its imaginary part (column 3) is identified as being proportional to the quadrupole strength. Column 4 shows the absolute squared of the Fourier transform which is the spectral power.
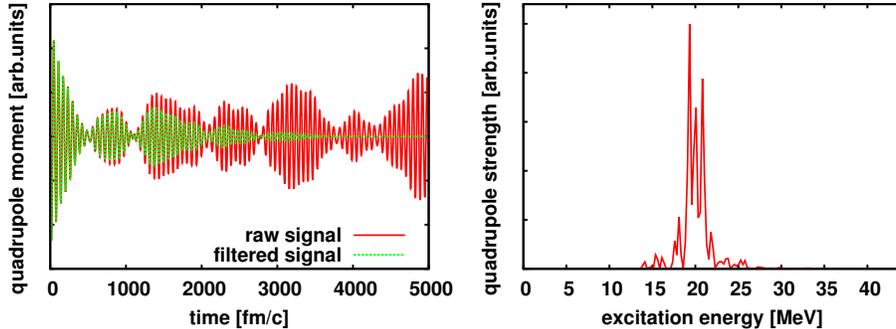
Figure 1: The quadrupole signal in the time domain (left) and frequency domain (right) for the present test case of quadrupole oscillations in ^{16}O computed with the forces SV-bas. Note that frequency is converted to excitation energy by $E_{esc} = \hbar\omega_{exc}$.

3.3. Results for the test case ^{16}O

The example on the actual file `extfield_spectrum.res` contains the result of a calculation up to time 5000 fm/c. Its content is shown as the curve "raw signal" in the left panel of figure 1. The "filtered signal" on the same panel is taken from the file `extfield_filt.res`. One sees how filtering suppresses the signal strongly towards the end of the sampling interval. The long sampling time of 5000 fm/c provides an energy resolution of about 0.3 MeV, more than enough for displaying a giant resonance. The right panel of figure 1 shows the spectral quadrupole strength as found in the file `extfield_spectrum.res` (column 3 versus column 1). The strength is nicely focused in one resonance region but rather fragmented over several sub-peaks. The overall resonance position is a relevant feature. However, the detailed fragmentation is not to be taken seriously as it is strongly affected by the finite numerical box. The resonance energy resides actually in the nucleon continuum. Thus the detailed structures should be washed out much more by line broadening through particle emission. The present fine structure is an artifact from the computational box. Emission effects can only be described by using absorbing boundary conditions [11]. A simple solution to broaden the signal for the present code is to use stronger filtering (enhance `nfilter` in `spectral_analysis.f90`).

4. Collision of ^{16}O+^{16}O

4.1. The physics case

The use of TDHF for the description of heavy-ion collisions goes back to the beginning of this field.Its strong points are that is provides a natural description of neck formation and rupture between two nuclei and allows the full spectrum of collision behavior: fusion, deep-inelastic collisions, grazing collisions, even multifragmentation [12]. The omission of nucleon-nucleon collisions, however, prevents complete equilibration [13], and for this reason it should not be applied

to study the long-term behavior, e. e., of a compound nucleus. Here we selected a relatively simple scenario of two ^{16}O nuclei colliding at 100 MeV of relative-motion kinetic energy and an impact parameter of 2 fm. This is a deep-inelastic collision.

4.2. Running the test case

The dynamic calculation is executed by

$$directory/\texttt{sky3d.seq > for006.collision}$$

or the analogous command for the `OpenMP` and `MPI` cases. The input file describes initialization for two fragments (`nof=2`) and in the `NAMELIST` `fragments` both refer to the same wave function file `../Static/O16`. It also determines the kinetic energy and impact parameters for a two-body initialization (`fix_boost=.FALSE.`). Finally the center-of-mass positions of the fragments are given.

4.3. Results

A check of the file `energies.res` shows that the particle number is preserved to about 0.01%. The energy stays constant within about one MeV and the agreement of integrated and summed energies is also at that level of accuracy. The collective energies go down significantly, however, showing that this indeed a deep-inelastic collision. Note the different physical meaning: `Ekin` is the expectation value of the kinetic energy operator, which includes both the energy associated with probability flow as well as that due to localization of the wave functions. `Ecoll`, on the other hand, is only the energy associated with the average flow, which contains, however, the internal collective motion of the nuclei. Under the influence of the Coulomb field the protons and neutrons behave slightly differently.

The file `dipoles.res` only shows that the dipole moment of the complete system remains practically zero. In `monopoles.res` the r.m.s radii are quite useful; especially the total r.m.s. radius can be taken as a measure for the separation which goes over into a deformation coordinate when the nuclei coalesce. `momenta.res` shows that the center of mass of the total system remains at rest, while the data in `quadrupoles.res` are less interesting in a collision. The file `spin.res` indicates a reasonable conservation of angular momenta but some exchange between orbital and spin contributions.

Finally the output file `for006.collision`is useful in many ways. The regularly produced printer plots give a good indication of what is going on without needing the effort of converting the file format and starting up a visualization code. It is often helpful to look at the initial printer plots while the code is running in order to see whether things are working as planned.

The "relative motion" and "collision kinematics" printout is also very useful, although it is produced only if a two-body situation is recognized, i. e., not during the interaction phase. From the first analysis seen it is clear that neither the relative energy nor the angular momentum are reproduced very precisely. One reason is that cutting up space into two halves assigns a non-negligible

part of each nucleus to the other side and distorts the results somewhat. If higher accuracy is desired, it would be better to separate the system into the two original sets of wave functions, but while this can be used to correct the initial setup, it cannot be applied to the final state, where wave functions extend over both fragments.

If you "grep" the output file for "ecmf", a short overview of the development of the orbital angular momentum and the final center-of-mass energy is produced. The energy decreases from 100 MeV to about 18 MeV, but does not approach a true constant. This has two principal reasons: the separated nuclei still show collective oscillations which are coupled to the Coulomb field, and also the unphysical effect of wave functions crossing the boundary may play a role [14]. If these should prove critical, measures such as absorbing potentials on the boundary may have to be invoked [15].

The angular momentum calculated in the two-body analysis shows much stronger fluctuations than the quantum-mechanical one printed in `spin.res`. The latter shows an almost constant total angular momentum with only a small exchange between spin and orbital contributions. This indicates that some angular momentum is in internal excitation of the fragments,

The collision calculation takes several hours on a modern PC.

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