# TIME-DEPENDENT GROUND-STATE CORRELATIONS IN HEAVY ION SCATTERING

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Abstract

Using a time-dependent generator-coordinate method, we derive a theory for time-dependent collective ground-state correlations which account for some quantum fluctuations about a TDHF trajectory. This theory is particularly suited for evaluating spreading widths of collective one-body operators. As an application we study head-on collision of heavy ions in a one-dimensional model. As one of the prominent results we find a substantial enhancement of the spreading width of the internal excitation energy due to the correlations.

## 1. Introduction

In the last years time-dependent mean field approaches (TDHF) have been widely used for the microscopic description of large amplitude collective motion, in particular for heavy ion collisions. They have provided useful insight into the time evolution of density distributions, currents, multipole moments etc. It has turned out that most one-body obervables are described fairly well by TDHF, e.g., the average mass drift in a heavy ion collision or the ridge in a Wilshinsky plot. That is not surprising since TDHF has been built to optimize the time evolution of the one-body density matrix, and hence, is expected to yield the proper time evolution of averages of one-body operators. In general, however, TDHF will fail to reproduce properties which are sensitive to two-body or higher density matrices, as e.g., speading widths of one-body observables or particular S-matrix elements.

There are several attempts to cure TDHF for this deficiency. It is obvious that one needs to include some correlations into the wave functions, or in other words, to allow for quantum fluctuations about the (classical) TDHF path. One can try to approximate those by quantum statistics[1] or to describe all of them by means of Monte-Carlo integration techniques[2]. However, we expect that there will be some correlations of particular importance, namely those which fluctuate about the TDHF path in the direction of the possible collective excitation, we will call these collective correlations[3].

Thus, we are going to set up a theory for describing the time-evolution of collective ground state correlations by a coherently correlated state. The formalism is derived in section 2 within the framework of a time-dependent generator-coordinate method (TDGCM). In section 3 we introduce shortly the one-dimensional dynamics, which are used to study the TDGCM and discuss its possible collective modes. Finally, in section 4 we present the results of the numerical evaluation of TDGCM in one-dimensional dynamics.

## 2. Time-dependent generator-coordinate method (TDGCM)

In generalization of the GCM for stationary states we now consider a time-dependent correlated state as a superposition

$$|\psi(t)\rangle = \int dq\, |\phi_q(t)\rangle\, f(q,t) \tag{1}$$

where the collective superposition function f and the basis states $|\phi_q\rangle$ depend explicitly on time. The deformation basis $\{|\phi_q(t)\rangle\}$ consists out of Slater-states which are collectively deformed compared to the uncorrelated TDHF trajectory $|\phi_0(t)\rangle$; each one of the $|\phi_q(t)\rangle$ is supposed to move in its own average field $U_q(t)$ (yet to be determined).

We now want to determine the equations-of-motion for the $|\phi_q(t)\rangle$ and f(q,t) by means of the time-dependent variational principle

$$\langle\delta\psi|H - i\partial_t|\psi\rangle \ . \tag{2}$$

In this general form the emerging variational equations are untractable since complicated integral-kernels $\langle\phi_q(t)|H - i\partial_t|\phi_{q'}(t)\rangle$ arise. And even worse, the path variation $\langle\delta\phi_q|$ turns out to be impractical, if no further restrictions on $|\phi_q(t)\rangle$ are made, since in general, the ansatz (1) still embraces the full Hilbert-space. (Think for example of some peculiar basis $|\phi_q\rangle$ winding successively through all possible many-particle-many-hole states).

An obvious requirement for a tractable $|\phi_q\rangle$ is that it is analytically in q. Furthermore, since $|\phi_q\rangle$ ought to represent a collective deformation, where a small displacement of many particles adds up coherently to a substantial reordering of the matter, the overlap $\langle\phi_q|\hat{O}_p|\phi_{q'}\rangle$ will fall off rapidly with $(q-q')^n$. Therefore, it is reasonable to assume Gaussian overlap[4] for the norm kernel

$$\langle\phi_q|\phi_{q'}\rangle = \exp\left(-(q-q')^2/4\mu\,\frac{q+q'}{2}\right) \tag{3a}$$

where

$$\mu^{-1}(q) = 2\langle\phi_q|\overleftarrow{\partial}_q\,\overrightarrow{\partial}_q|\phi_q\rangle \tag{3b}$$

and analogously

$$\langle\phi_q|\hat{O}p|\phi_{q'}\rangle = \exp\left(-(q-q')^2/4\mu\right)\cdot\left[Op_0 + Op_1(q-q') + Op_2(q-q')^2\right] \tag{4}$$

with coefficients $Op_i$ determined as expectation values of $\hat{O}p$ with some derivatives $\partial_q^0$, $\partial_q^1$, $\partial_q^2$.

Working out the Gaussian overlap approximation (GOA) we obtain for $\hat{O}p = H - i\partial_t$,

$$\begin{aligned} \langle\psi|H-i\partial_t\,|\psi\rangle_{GOA} = \int dq\, g^*(q,t)\{&\langle\phi_q(t)|H-i\partial_t|\phi_q(t)\rangle - i\frac{d}{dt} \\ &- \frac{\mu}{4}\partial_q^2 \langle\phi_q(t)\; H|-i\partial_t|\phi_q(t)\rangle \\ &+ :(-i\frac{d}{dq})\langle\phi_q(t)|\overleftarrow{\partial}_q\overline{H} - \overline{H}\overrightarrow{\partial}_q|\phi_q(t)\rangle: \\ &+ \frac{1}{2}:|(-i\frac{d}{dq})^2 - \frac{1}{2\mu}|\langle\phi_q(t)|\overleftarrow{\partial}_q^2\overline{H} - 2\overleftarrow{\partial}_q\overline{H}\overrightarrow{\partial}_q + \overline{H}\overrightarrow{\partial}_q^2|\phi_q(t)n^2:\}g(q,t) \end{aligned} \tag{5}$$

where $\frac{d}{dq}$ is to act on everything, but $\partial_q$ only on $|\phi_q\rangle$ or $\langle\phi q|$. The : ... : express the GOA normal ordering : $\frac{d^n}{dq^n}A(q)$ : = $\frac{1}{2^n}\{\frac{d}{dq}\ \{\ \frac{d}{dq} \ldots \{\frac{d}{dq}\ , A\} \ldots \}$. The $g(q,t)$ is the collective wave function, normlaized as $\int dq\, g^* g = 1$; it is related to $f(q,t)$ by

$$g(q,t) = \int dq'(\mu\pi)^{-1/4} \exp(-(q-q')^2/2\mu) f(q',t). \tag{6}$$

Finally, the $\overline{H}$ is $\overline{H} = H - i\partial_t - \langle\phi_q|H - i\partial_t|\phi_q\rangle$.

Within the approximation (5) we can work out the variational principle (2) varying with respect to both ingredients, $g(q,t)$ as well as $|\phi_q(t)\rangle$; this eventually leads to equations-of-motion for $g(q,t)$ and for $|\phi_q(t)\rangle$. As a further simplification we make the following approximation: we assume the q-motion to be harmonic (which is valid at least for small amplitude motion) and parametrize g as

$$g(q,t) = (\alpha\pi)^{-1/4} \exp(-q^2/2\alpha(t)), \tag{7a}$$

with the correlated state (2) becoming now

$$|\psi(t)\rangle = \int dq\, |\phi_q(t)\rangle\, N \exp(-q^2/2(\alpha - \mu)) \tag{7b}$$

with

$$N = (\alpha/\mu)^{1/4}/(2\pi(\alpha - \mu))^{1/2}.$$

Now, the variation $\langle\delta\phi_q|$ yields the propagation for the $|\phi_q(t)\rangle$

$$(\hat{W}_q - i\partial_t)|\phi_q(t)\rangle = 0 \tag{8a}$$

where

$$\hat{W}_q = \hat{T} + \mathrm{Tr}\,\{\,\rho_q\, V\,\} \tag{8b}$$

This is nothing else than the TDHF equation for each $|\phi_q(t)\rangle$ separately, moving in its own Hartree-Fock field $\hat{W}_q$. (In fact, in eq. (8) we have neglected the influence of $(\frac{d}{dq})^2$-term in the expansion (5), which means that we have neglected the feedback of the correlations to the mean-field $\hat{W}_q$). The variation $\delta_{\alpha^*}$ yields the correlation dynamics

$$\frac{d}{dt} \alpha = 2i \mu^2 <\phi_o(t)|\overleftarrow{\partial}_q^2 \overline{H} + \overline{H} \overrightarrow{\partial}_q^2|\phi_o(t)> . \qquad (9)$$

It is interesting to note that this correlation dynamics is particularly sensitive to the 2p-2h part of $\overline{H}$; this becomes obvious from eq. (9) keeping in mind that $\partial_q$ is a 1p-1h operator, thus, $\partial_q^2$ is a 2p-2h operator.

Altogether we have an initial value problem for the correlated state $|\psi(t)>$: We start with a given $|\psi(0)>$ in the form (7b) which means to have a given initial correlation parameter $\alpha(0)$ and an initial deformation basis $\{|\phi_q(0)>\}$; we then propagate $|\phi_q(t)>$ according to TDHF eq. (8) and $\alpha(t)$ according to correlation dynamics (9); this defines $|\psi(t)>$ of eq. (7b) uniquely at all later times. The initialisation, of course, is crucial. By choosing a set $\{|\phi_q(0)>\}$ we define the collective mode for the correlation. In TDHF calculations one usually takes as initial state $|\phi_o(0)>$ Hartree-Fock states for the two separate clusters and boosts them with some relative velocity. Accordingly we have to choose the $\{|\phi_q(0)>\}$ and the $\alpha(0)$ to represent RPA vibrations of the two cluster system.

Finally, we want to evaluate expectation values of observables for the state $|\psi(t)>$. This can also be worked out within the GOA. We obtain, together with the harmonic approximation (7), the following expression for the spreading width of a one-body observable $\hat{A}$:

$$\begin{aligned} <\psi|\Delta^2 A|\psi> = <\phi_o|\Delta^2 A|\phi_o> &+ \frac{1}{2} \left[\frac{\alpha^*\alpha}{\alpha_r} - \mu\right] |<\phi_o|\overleftarrow{\partial}_q \overline{A} + \overline{A} \overrightarrow{\partial}_q|\phi_o>|^2 \\ &+ i \frac{\alpha_i}{\alpha_r} \mu <\phi_o|\overleftarrow{\partial}_q \overline{A} + \overline{A} \overrightarrow{\partial}_q|\phi_o><\phi_o|\overleftarrow{\partial}_q \overline{A} - \overline{A} \overrightarrow{\partial}_q|\phi_o> \qquad (10) \\ &+ \frac{1}{2} \left| \frac{1}{\alpha_r} - \frac{1}{\mu}\right| \mu^2 |<\phi_o|\overleftarrow{\partial}_q A - A \overrightarrow{\partial}_q|\phi_o>|^2 \end{aligned}$$

where $\alpha_i = \mathrm{Re}(\alpha)$, $\alpha_i = \mathrm{Im}(\alpha)$ and all quantities depend on t.

Altogether we see that in the harmonic approximation all information on $|\psi(t)>$ is carried by the three quantities $|\phi_o(t)>$, $\partial_q|\phi_o(t)>$ and $\alpha(t)$. In practice, we handle the $\partial_q|\phi(t)>$ as a finite difference $\partial_q|\phi_o(t)> = (|\phi_{\delta q}(t)> - |\phi_o(t)>)/\delta q$. Thus, it remains to propagate two neighboured TDHF trajections $|\phi_o(t)>$ and $|\phi_{\delta q}(t)>$ and to work out additionally the correlation dynamics for $\alpha(t)$. Obviously, this procedure can easily be implemented into any existing TDHF code. The extra expense of TDGCM consists mainly in carrying TDHF several times, namely for each $|\phi_{\delta q}(t)>$ separately.

Of course, the TDGCM theory is not restricted to one correlation channel q only. It can easily be extended, formally and practically, to a multiple superposition $|\psi(t)> = \int d^F q \; |\phi_{q_1 \ldots q_F}(t)> f(q_1 \ldots q_F , t)$ carrying various collective correlations. In fact, this has been done in the following applications. It is, however, not very enlightening to write down the formula for the general case, since they remain essentially the same except for a confusing multitude of indexes.

## 3. One-dimensional dynamics

In order to test the TDGCM and to estimate its predictions we have applied the theory to the example of one-dimensional nuclear dynamics (SLAB's). We use a microscopic Hamiltonian similar to the Borche-Koonin-Negele force, consisting in kinetic energy, a folded Gaussian two-body force and a zero-range density dependent force. The Hartree-Fock Hamiltonian to a given density $\rho(x)$ reads then

$$\hat{W} = \frac{h^2}{2m} \partial_x^2 - V_0 \int dx' \, \pi^{-1/2} \, \delta r^{-1} \exp\left(-(x - x')^2/\, \delta r^2\right)\rho(x') + t_3 \, \rho^2(x) \tag{11}$$

where we used $V_0$ = 50 MeV, $\delta r$ = 2 fm and $t_3$ = 8.8 MeV $fm^2$. We use a space-grid representation of the single-particle wave function with grid size .3 fm and 140 grid points. The standard initial condition is two four-particle systems placed at a distance of 7.8 fm and having some relative momentum. We adopt quartett symmetry, i.e., the four particles all occupy the 1s state. This system has a binding energy of 11.6 MeV/particle. The compound system, consisting of 8 particles (one quartett in the 1s and the other quartett in the 1p state), has a binding of 15.6 MeV/particle. The TDHF solutions show fusion up to an impact momentum of p = .28 $fm^{-1}$. Altogether these are not precisely the numbers for realistic nuclei, but in orders of magnitude it describes the nuclear situation.

Since we have only one spacial dimension, the variety of collective modes in such a system is rather overseeable. For one single nucleus, we have essentially center-of-mass motion and one compression mode, representing all the T = 0 giant resonances in real nuclei. The isovector modes do not occur due to quartett symmetry and a surface mode does not occur because we have a closed-shell system. From the two modes in each cluster we can combine four collective modes in the scattering system. One of them is the total c.m. motion, it is omitted as a trivial mode. There remain three modes; each of them can be excited in two wyas, either by a static deformation or by a dynamic push. Thus, altogether we consider 6 different initialisations, as visualized in fig. 1.

Corresponding to the three modes, we have six observables. We consider the following three of them

$$\hat{P}_{rel} = \int_0^\infty dx \, \hat{j}(x) - \int_{-\infty}^0 dx \, \hat{j}(x) \tag{12a}$$

$$\hat{R}_+^2 = \int_0^\infty dx \, x^2 \, \hat{\rho}(x) + \int_{-\infty}^0 dx \, x^2 \, \hat{\rho}(x) \tag{12b}$$

$$\hat{R}_-^2 = \int_0^\infty dx \, x^2 \, \rho^1(x) - \int_{-\infty}^0 dx \, x^2 \, \hat{\rho}(x) \tag{12c}$$

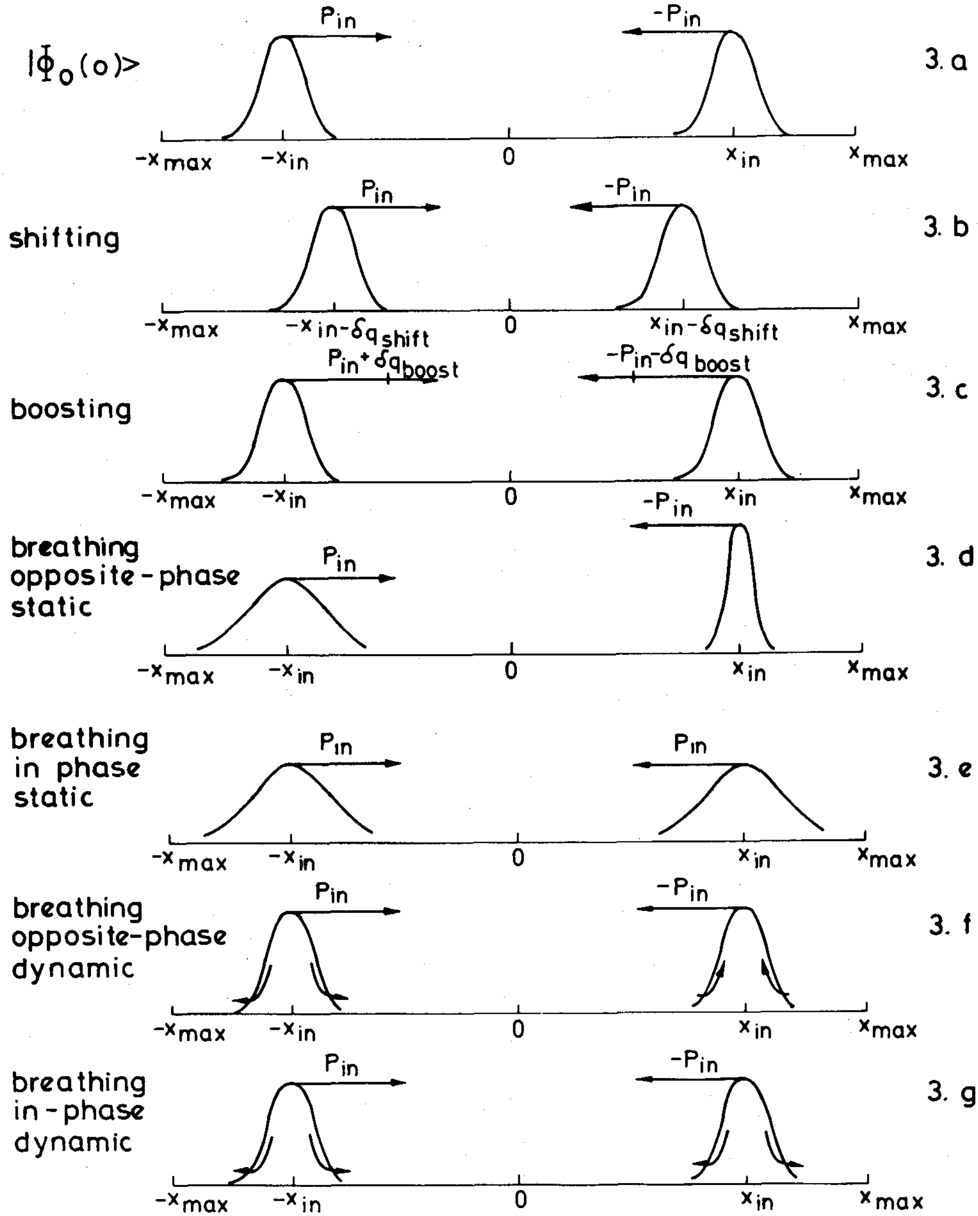


Fig. 1: The various initialization modes eximplified by drawing the initial density profile as a function of coordinate x. The arrows with $p_{in}$ indicate the initial momentum of the clusters. The little arrows indicate the breathing flow of matter inside the clusters.

and in addition the difference in particle number

$$\hat{n}_{rel} = \int_0^\infty dx\ \hat{\rho}(x) - \int_{-\infty}^0 dx\ \hat{\rho}(x) \ . \tag{12d}$$

These are the operators to be inserted in place of $\hat{A}$ in eq. (10).

## 4. Results and discussion

The first test for the theory is, of course, that it should reproduce the known features of center-of-mass motion. This case can be worked out analytically. We will not give the details of the evaluation here. We only want to quote the result, namely that TDGCM stands this test and shows aptly the spreading of wave packets in coordinate space, but no spreading in momentum space. The study of free c.m. motion, however, has some more importance since in the initial and in the final phase of heavy ion scattering the two clusters move freely. This allows to predict the asymptotic behaviour, for $t \to \infty$, from knowing a few quantities "measured" shortly after the reaction has ended. In that way we obtain, e.g., the very useful relation for the speading width of $\hat{p}_{rel}$

$$\frac{\langle\psi(+\infty)|\Delta^2\ p_{rel}|\psi(+\infty)\rangle}{\langle\phi(-\infty)|\Delta^2\ p_{rel}|\phi(-\infty)\rangle} = \frac{\partial p_{out}}{\partial p_{in}} \tag{13}$$

where $p_{out} = \langle\psi(t)|\ \hat{p}_{rel}\ |\psi(t)\rangle$ for any t after the reaction time and $p_{in}$ is the same for any t before the reaction starts. (To obtain that formula, we have neglected the contribution from the $Im(\alpha)$; it could be shown to be negligible).

Another interesting test of the theory is the study of a RPA vibration within one single cluster. We take $|\phi_o(t)\rangle = |\phi_o\rangle$ as the stationary Hartree-Fock solution and for $|\phi_{\delta q}(0)\rangle$ we start with a static compression of this Hartree-Fock state. The results are shown in fig. 2. We observe harmonic oscillations for the input quantities $(2\mu)^{-1} = \langle\phi_o|\partial_q\ \partial_q|\phi_o\rangle$ and $\alpha_i = Im(\alpha)$. For the "measurement", namely the spreading width $\Delta^2\ \hat{R}^2$ we have three cases: first, the pure TDHF state (dotted line) produces a constant, but too small width. Second, we have initialized TDGCM with the pure TDHF state (dashed line); as a result the correlated ground state oscillates about the true RPA width. Third, we start TDGCM with the true RPA width (full line) and indeed we obtain a nice stationary line over many periods of oscillation. This proves the physical relevance and the numerical stability of the TDGCM.

As we see in fig. 1, we can initiate each mode in various phases, statically or dynamically or any phase in between. If we start the TDGCM initial condition $|\phi_{\delta q}(0)\rangle$ in different phases the clusters will reach the interaction region in different stages of the internal oscillations and, thus, the coupling will behave quite different. This is shown in fig. 3, where we compare the spreading width $\Delta^2\ R_-^2$ after collision for initialization with the "breathing out-of-phase" mode in various phases. The $t_o$ means that we have allowed the oscillations to run for the time $t_o$ be-

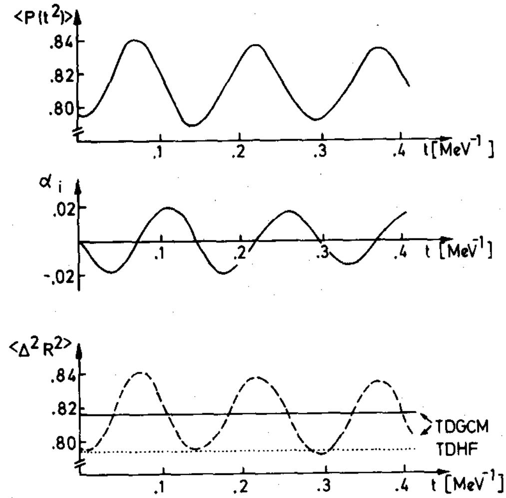


Fig. 2: Breathing oscillations in one nucleus at rest. Initialization with static deformation (analogous to breathing modes in fig. 1. We show $\mu(t)$ according to eq.(3b), $\mathrm{Im}(\alpha(t))$ and $<\Delta^2 \hat{R}^2>$. For $<\Delta^2 \hat{R}^2>$ we give the TDHF results (dotted line) the TDGCM result from pure TDHF start (dashed line) and the TDGCM result for properly correlated start (full line).

fore starting the relative motion of the clusters (thus, producing a phase of $60^0$ for curve 1, $0^0$ for 2, $150^0$ for 3 and $90^0$ for 4). As we see, the resulting coupling depends strongly on the initial phase. An obvious but expensive solution of this problem would be to average over many phases. In fact, it turns out that it is sufficient to use a two-channel TDGCM where both channels are initiated into the same mode but with $90^0$ phase shift (e.g. channel 1 with static deformation and channel 2 with the corresponding dynamic excitation). This is exemplified in fig. 4, where we show the result of such a two conjugate channel TDGCM. For different initial phase, namely $0^0$ and $60^0$,

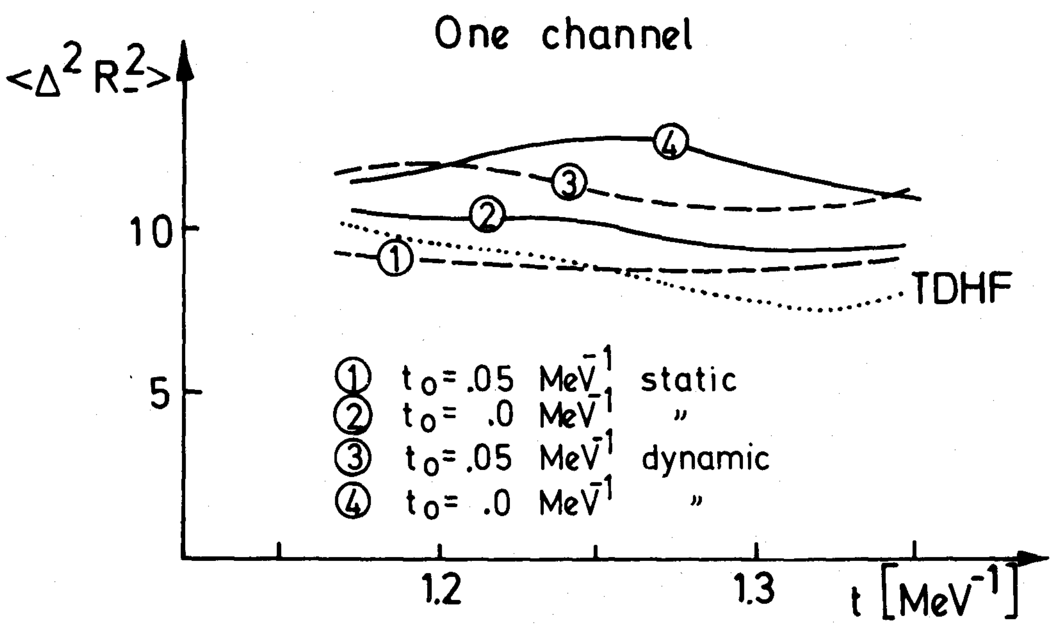


Fig. 3: The $<\Delta^2 \hat{R}^2>$ from the one channel TDGCM for the initial mode "breathing opposite-phase" and various initial phases.

we obtain the same $\Delta^2 R_-^2$, thus, we observe sufficient phase stability.

Now, having shown the numerical reliability of TDGCM and knowing how to produce phase stability, we can evaluate every combination of initialization and final measurement (after the reaction, i.e., $t \to \infty$). The results are given, for various impact momenta $p_{in}$, in table 1.

First, we observe generally strong contributions from the collective correlations to the spreading widths. Moreover, we see that the dominant contribution always comes from that initial mode which is related to the measurement (see the encircled number in table 1); this feature could be called "channel-memory". The cross channel contributions are much smaller. It may be that many of such small contributions add up to a further substantial enhancement. But this effect is hard to treat in TDGCM; a larger manifold of channels can only be treated statistically.

In table 1 we see also that the correlation effects are strongest for low momenta, near the fusion window at $p_{in} = .28\ fm^{-1}$, and tend to decrease for higher impact momenta. In fig. 5 we have plotted the TDGCM result for the spreading width of E*, the internal excitation energy after reaction, as a function of $p_{in}$. We see that the correlations indeed produce a significant enhancemant of $\Delta^2$ E*, particularly for

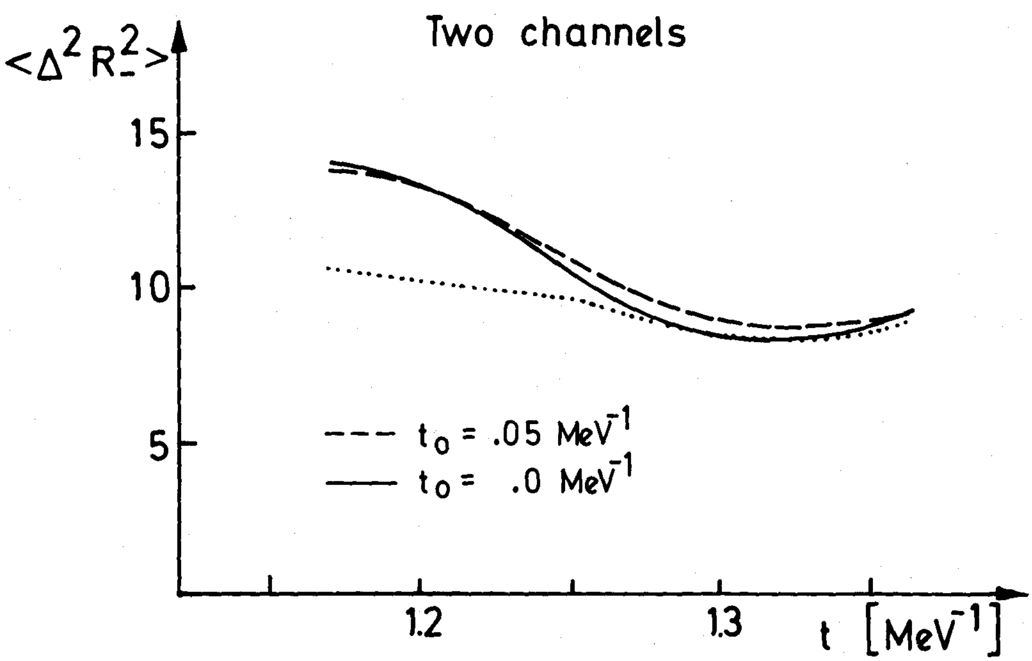


Fig. 4: The $<\Delta^2 R^2>$ from two-conjugate-channel TDGCM for the initial mode "breathing-

| | Measurement | | | |
|---|---|---|---|---|
| Initialization | $\Delta^2 p_{rel}$ $[fm^{-2}]$ | $\Delta^2 R_+^2$ $[f,^4]$ | $\Delta^2 R_-^2$ $[fm^4]$ | $\Delta^2 N_{rel}$ |
| $p_{in} = 0.30\ fm^{-1}$ | | | | |
| TDGCM: | | | | |
| shift + boost | 2.40 | 18.03 | 10.01 | 0.51 |
| breathing (+) | 0.42 | 35.60 | 10.01 | 0.51 |
| breathing (-) | 0.29 | 16.51 | 13.14 | 0.52 |
| TDHF | 0.28 | 16.50 | 10.00 | 0.50 |
| $p_{in} = 0.35\ fm^{-1}$ | | | | |
| T.GCM: | | | | |
| shift + boost | 0.88 | 7.81 | 6.43 | 0.36 |
| breathing (+) | 0.31 | 9.60 | 6.42 | 0.36 |
| breathing (-) | 0.30 | 5.74 | 7.86 | 0.33 |
| TDHF | 0.29 | 5.73 | 6.42 | 0.36 |
| $p_{in} = 0.40\ fm^{-1}$ | | | | |
| TDGCM: | | | | |
| shift + boost | 0.63 | 5.79 | 4.84 | 0.24 |
| breathing (+) | 0.31 | 6.04 | 4.84 | 0.24 |
| breathing (-) | 0.30 | 4.86 | 5.02 | 0.24 |
| TDHF | 0.30 | 4.85 | 4.84 | 0.24 |

Table 1: The spreading width of various measuring operators is given for TDHF and for a couple of explicitly considered correlated time dependent states treated by means of TDGCM.

low $p_{in}$ near the fusion window. For larger $p_{in}$ the contribution decreases and seems to level off at a ratio of about 2, leaving a strong effect also for fast processes.

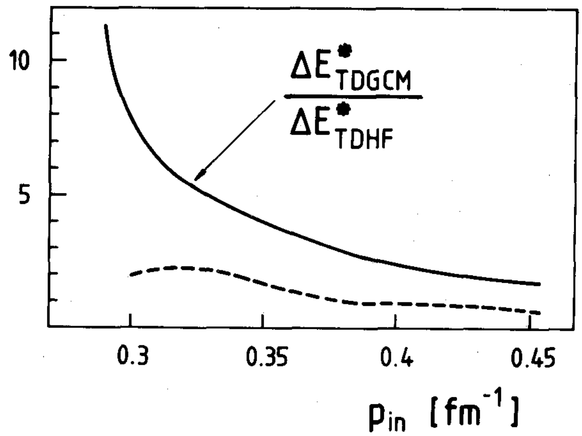


Fig. 5: The enhancement factor for the internal excitation energy $E^*$ as function of the initial momentum $p_{in}$ (full line). The dashed line is the contribution due to the imaginary part of the correlation width $\alpha$, amplified by a factor 100.

## 5. Conclusion

Time-dependent collective ground state correlations are supposed to describe an important part of the quantum fluctuations about a TDHF trajectory. Formulating the many-body dynamics with a time-dependent generator-coordinate method, we have finally worked out a simple formalism for treating those collective correlations which can easily be implemented on existing TDHF codes. We have applied the method to a one-dimensional model of nuclear dynamics. We observe the following interesting features:

- The method is numerically stable and reliable; this has been shown by tracing stationary RPA oscillations over many periods.
- For each collective mode we need a two-conjugate-channel TDGCM; this is necessary and sufficient to reach phase stability of the results in a heavy ion collision.
- There is a strong "channel-memory", i.e., for a given measuring operator the related initial excitation mode produces the dominant contribution to the spreading width.

- Altogether the collective correlation produce a significant enhancement of spreading widths of one-body observables, particularly for energies near the fusion window.

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