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NUCLEAR MOLECULES IN TDHF*

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In present-day theoretical nuclear physics, the long-time mechanical behavior of nuclear systems arises through the various classical and semi-classical limits of the quantum many-body problem as, for example, in studies of the time-dependent Hartree-Fock (TDHF) approximation,[1] the nuclear partition function,[2] fission lifetimes,[3] and S-matrix elements.[4]

Hydrodynamic models of matter in heavy-ion reactions exhibit the characteristic behavior of dissipative fluid flow,[5] and details of the momentum transfer and particle multiplicities may be suggesting the formation of attractor regions in the reaction phase space.[6] Isoscalar and isovector heavy-ion monopole and quadrupole giant resonances have been computed in ^{16}O and ^{40}Ca by examining the quasiperiodic motion of these systems using the TDHF approximation.[7] These calculations yield unquantized vibrational frequencies in good agreement with both the RPA and the GCM methods and have the classical interpretation of being the most probable frequencies of the RPA strength functions. All of the above work seems to predict the existence of highly nonlinear structures embedded in the dynamics of heavy-ion reactions with the subsequent development of either classical quasiperiodic or chaotic behavior of the compound nuclear system.

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In the present work we study, using the time-dependent Hartree-Fock approximation (TDHF), the quasiperiodic motion in ^{24}Mg, which experimentally displays a type of molecular structure. The theoretical foundations of the nuclear TDHF formalism have been extensively reviewed in the literature[8-10] and are not discussed here. The TDHF method addresses the question of molecular formation from a microscopic "view" which provides both a geometrical (classical) picture of the molecule, as well as characteristic information on the rotational and vibrational structure of the molecule. The most extensive experimental evidence for the existence of nuclear molecules lies in the narrow resonances observed in the $^{12}C + {}^{12}C$ reactions near the Coulomb barrier.[11] A large number of experimental data has been amassed, and the most successful organization of these data is in terms of the U(4) model of Iachello.[12] The representation of the data in terms of this model suggests that the molecule involves a structure related to the 7.08 MeV 0^+ state of ^{12}C. This state has a well-established cluster structure and is approximately given as a HF shape isomer of ^{12}C. The energy as a function of deformation and the density contours for both the ground state ^{12}C and the carbon isomer are shown in Fig. 1. The present work examines in detail the classical behavior of the $^{12}C + {}^{12}C(0^+)$ collision at energies near the Coulomb barrier. The long-time motion of the compound nuclear system is identified in terms of its classical quasiperiodic and chaotic behavior. The consequences of this motion are discussed and interpreted in terms of the evolution of the system along a dynamical energy surface.

TDHF density contours corresponding to the time evolution from an initial configuration based on these two states are shown in Figs. 2(a) and 2(b). The initial state is also labeled by CM energy, $E_{cm} \approx 7.5$ MeV and separation along the axis of symmetry, $R_s \approx 12$ fm. Again, these are head-on collisions in which the matter flow undergoes a complex pattern of quasiperiodic motion. The contours in Fig. 2(a) are those for the isoscalar density, while those in Fig. 2(b) are for the motion of the isovector density. For the forces used in this study, the differences in the structure of the isovector and isoscalar densities arises solely through the Coulomb force. While the motion of

the isoscalar density appears regular, the isovector density has a complex high multipolar structure which varies rapidly on a time scale where the isoscalar density varies slowly.

The corresponding long-time behavior of the system is shown in Fig. 3 for the isovector dipole and the isoscalar quadrupole, octupole, and RMS radius (two times the physical radius of the system). The $^{12}C(0^+) + {}^{12}C$ system has been followed in for almost 5×10^{-20} sec. The time dependence of the isoscalar octupole motion is very regular and corresponds to a low-frequency vibration of about 1.5 MeV. The isoscalar quadrupole motion is a combination of low- (~ 2.5 MeV) and high- (~ 8 MeV) frequency motion.

The motion of ^{24}Mg can also be described in terms of collective variables and in terms of collective energies. As the system evolves along a TDHF path, the density, which may be thought of as a collective variable of the system, undergoes a complex motion. The corresponding potential energy as a function of the density can be calculated using the density-constrained Hartree-Fock (DCHF) equations. Using this method, we freeze the density along the TDHF path and minimize the energy of the system along the path. This energy is a function of the constraining density and is shown in Fig. 4 for the ^{24}Mg system, as a function of the isoscalar octupole and quadrupole degrees of freedom. The energy is a surface in the q_2, q_3 plane. During the time evolution, the system travels on a path in this plane. Thus, not all values of the energies in this region were observed. These plots were obtained using a least-squares fit to the HF energies along the path. The time history can be understood in terms of Fig. 4. The initial trajectory begins at $q_2 \approx 1.5\ q_{20}$ and $q_3 \approx +2.9\ q_{30}$, with $q_{20} = 582.7$ fm^2 and $q_{30} = 3431.0\ fm^3$. The system again evolves into a region shown in Fig. 4 and traverses a complex path about the shape isomer, $E_o = -143.8$ at $q_2 \approx 355$ fm in $q_3 \approx 0.0$. The energy contours in Fig. 4 are the constrained energies $\Delta E = 2(E(\text{constrained})-E_o)$ in units of MeV. The axially symmetric ground state of ^{24}Mg occurs at $q_2 = 67.9\ fm^2$, with an energy of -179.7 MeV. The general features of the energy surface as shown in Fig. 4 are in agreement with those obtained using Nilsson-Strutinsky methods.[13)]

The approach of classical systems to chaos[14] addresses a broad spectrum of physical problems in the mechanics of fluids,[15] in storage rings and colliding beam accelerators,[16] in plasmas,[17] and in molecular and chemical physics.[18] Sidestepping the detailed questions as to the universality of bifurcating systems[19] and the topology of attractor phase space, we study the Poincaré projections in which the multipole moments of the TDHF density

$$M_{\ell I}(t) = \int d^3r \; Y_{\ell o}(\hat{r}) \; \rho_I(\vec{r},t) r^{\ell}$$

and

$$M_{\ell I}(\omega) = \int_{-\infty}^{\infty} dt \; e^{i\omega t} \; M_{\ell I}(t).$$

play the role of classical coordinates describing the motion of the nucleus. These are displaced in Fig. 5 for the isoscalar quadrupole and octupole modes. We see that the motion is, at best, quasiperiodic and appears to be filling almost all of the phase space in this regime. The corresponding autocorrelation functions,

$$C_{\ell I}(\tau) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \; e^{+i\omega\tau} \left| M_{\ell I}(\omega) \right|^2$$

are shown in Fig. 6. The correlation function is small at all of the relevant frequencies, suggesting that the motion is indeed chaotic.

In an attempt to find more periodic states for ^{24}Mg, we have also attempted a different type of initialization.

Referring to Fig. 4, we follow the evolution from the same initial configuration until it reaches a point on the energy surface indicated by the "X". This part of the evolution takes approximately 700 fm/c. At this point, we again minimize the energy using the DCHF procedure. This has the effect of localizing the system in the region of the isomer and "cooling" the system keeping the density fixed. This state is then used to continue the time evolution using the TDHF equations. The subsequent time and frequency dependence of the isoscalar moments are shown in Fig. 7 and for the isovector moments in Fig. 8. The time dependence of the isoscalar moments in Fig. 7 are indeed more periodic

than previously; furthermore, the dominant frequency of the motion at low frequency now appears in all of the moments, as it must for an exact periodicity. This motion also appears in the odd-ℓ isovector moments shown in Fig. 8. However, the even-ℓ multipoles appear chaotic and do not have the correct low-frequency behavior for exact harmonic motion. The autocorrelation functions are compared in Fig. 9 for the motion shown in Figs. 7 and 8. Here we observe strong correlations which do not appreciably dampen in time.

We have solved for the time evolution of highly excited ^{24}Mg from reaction-like entrance channels. In both cases, the details of the evolution are sensitive to parameters of the initialization, the relative kinetic energy, and the fragment separation. For the ^{24}Mg system we evolve from an asymptotic configuration of $^{12}C(0^+) + {}^{12}C$. The $^{12}C(0^+)$ configuration is strongly related to a 3-α cluster configuration of carbon. The memory of the initial α-clustering persists throughout the time evolution. In each case, the system rapidly evolves into the region of a shape isomer, undergoing quasiperiodic motion. The Poincaré phase space analysis and the behavior of the autocorrelation functions suggest that the motion is chaotic instead of quasiperiodic. The importance of identifying quasiperiodic instead of chaotic follows from the work of Ref. 20 where the quasiperiodic motion represents a known classical limit of the quantum spectrum whereas the chaotic motion does not. For ^{24}Mg, methods were employed to "cool" the motion, and this resulted in quasiperiodic motion which was neither chaotic nor exactly harmonic.

In general terms, we are suggesting the existence of highly collective structures of a giant resonance nature having compound nuclear properties at excitation energies of 36 MeV in ^{24}Mg and very large deformations. These ideas have been suggested previously by Cosman[21] and co-workers. From the point of view presented in this paper, these structures should exist throughout the periodic table and for a variety of different entrance channel configurations.

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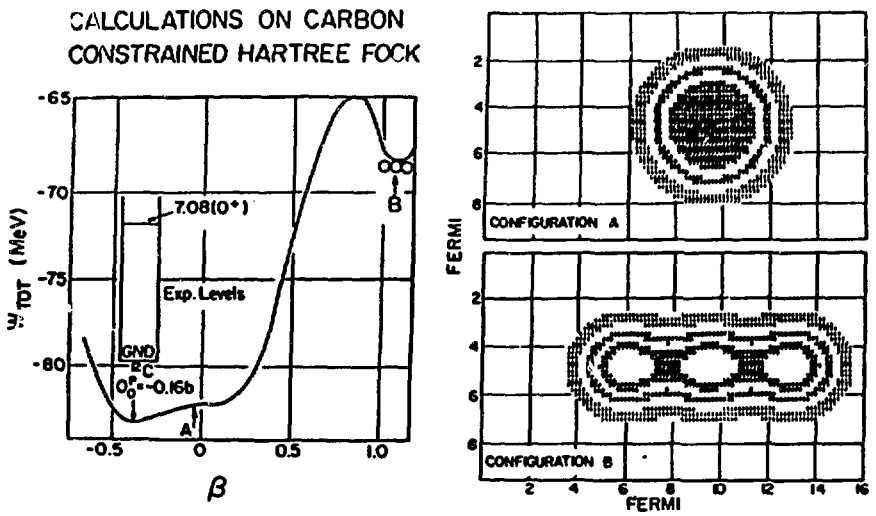


Fig. 1. Energy as a function of quadrupole deformation β and the corresponding density configurations for ^{12}C.

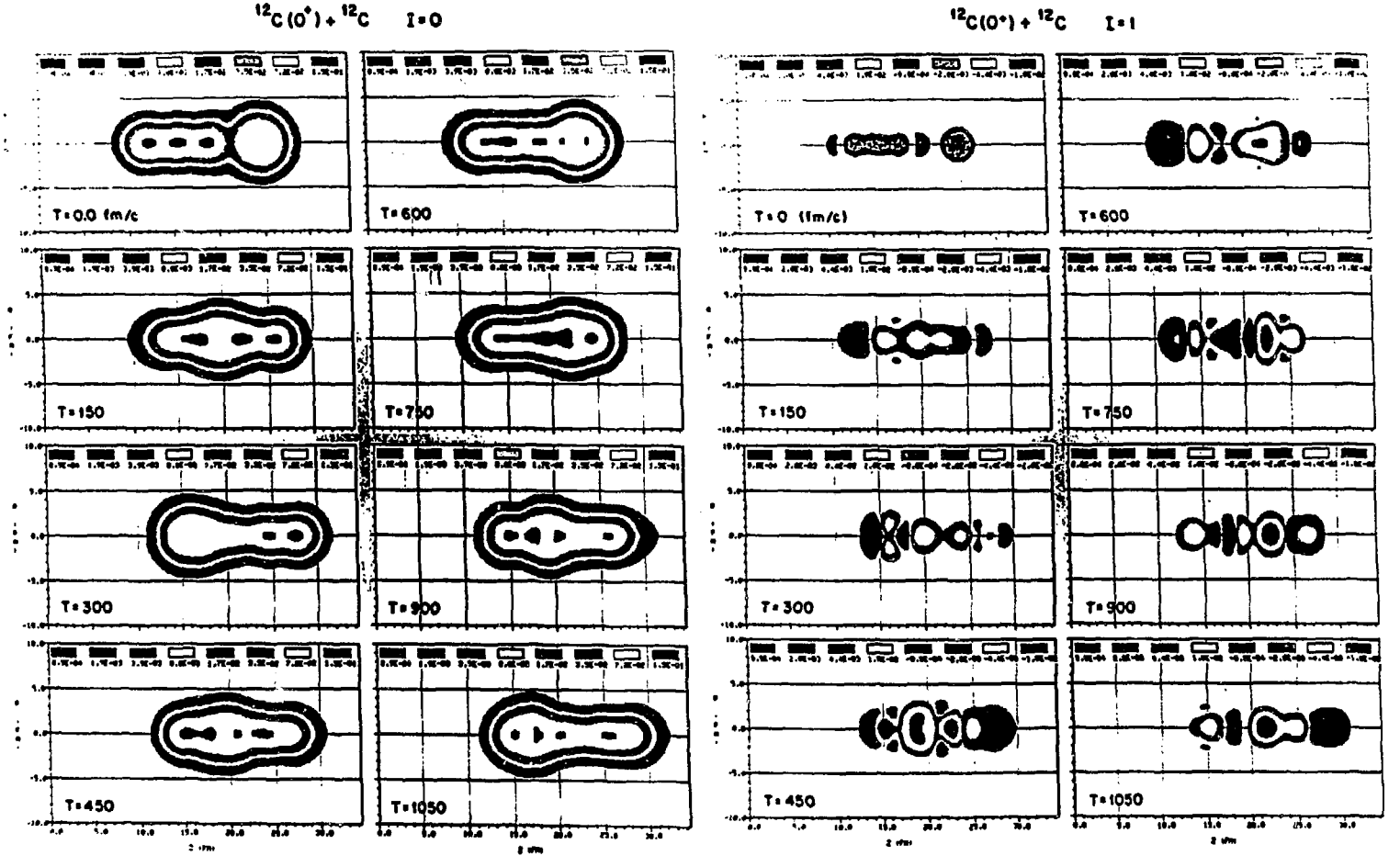


Fig. 2. The density contours of ^{24}Mg evolving from a $^{12}C(0^+) + ^{12}C$ initial configuration for the isoscalar (I=0) and isovector (I=1) densities.

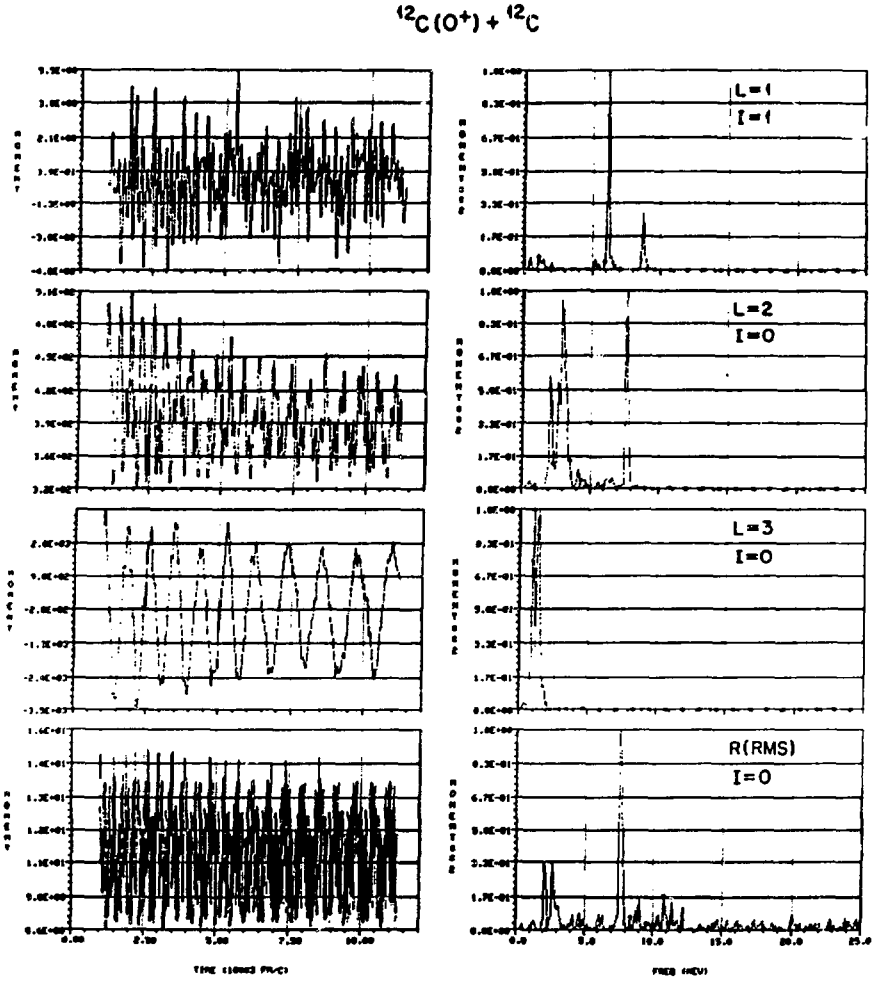


Fig. 3. The time and frequency dependence of the isoscalar quadrupole moment, octupole moment and the RMS radius, and the isovector dipole moment for ^{24}Mg.

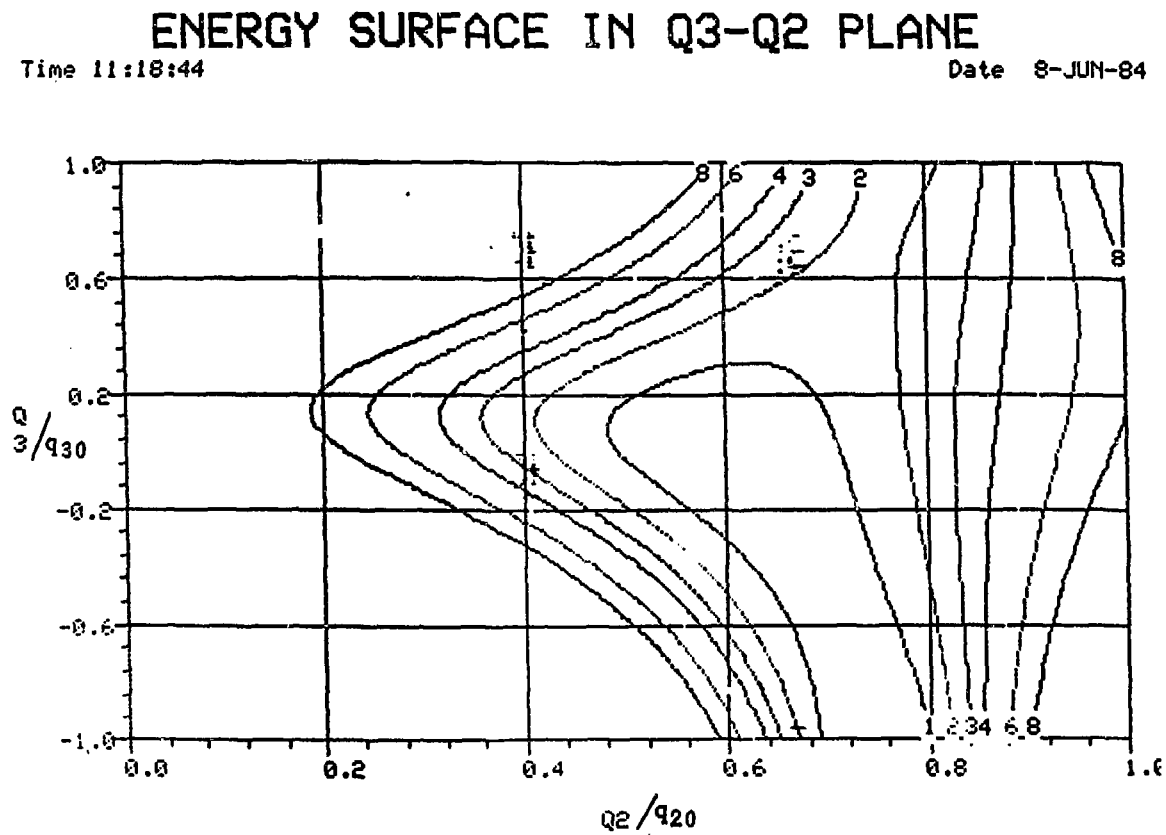
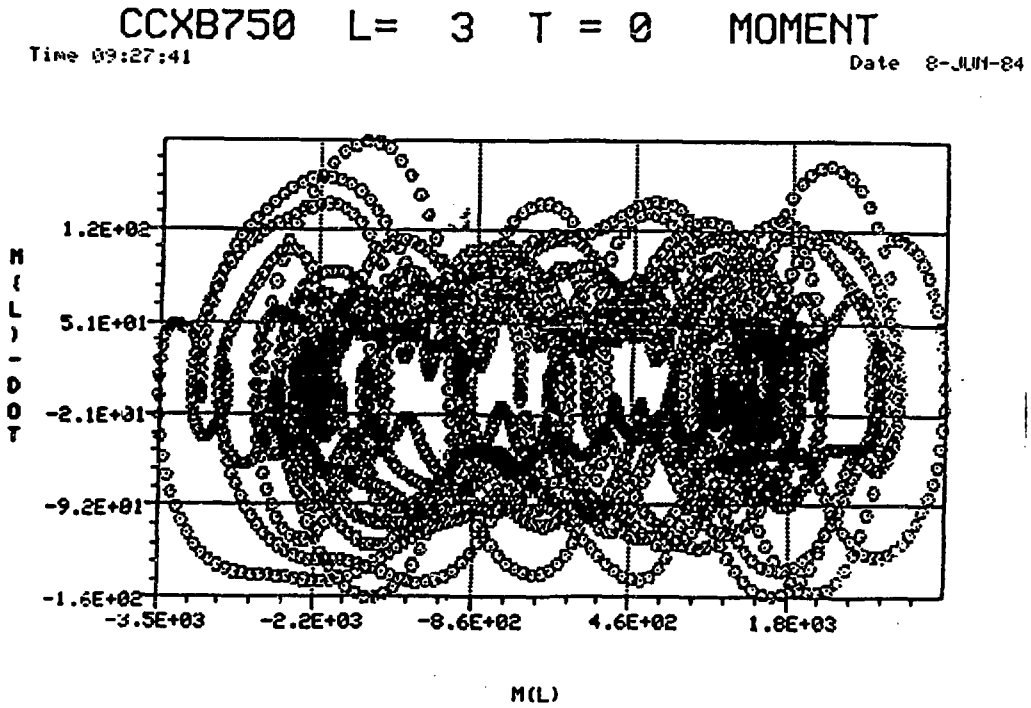


Fig. 4. Density-constrained static HF energies, $\Delta E = 2\ (E(\text{constrained}) - E_0)$, $E_0 = -143.8$ MeV as a function of the isoscalar quadrupole and octupole degrees of freedom. Contours are labeled in MeV. The constants q_{20} and q_{30} are $q_{20} = 582.7\ \text{fm}^2$ and $q_{30} = 3431.0\ \text{fm}^3$. The point having an energy $\Delta E = 0$ is a shape isomer of the ^{24}Mg system.



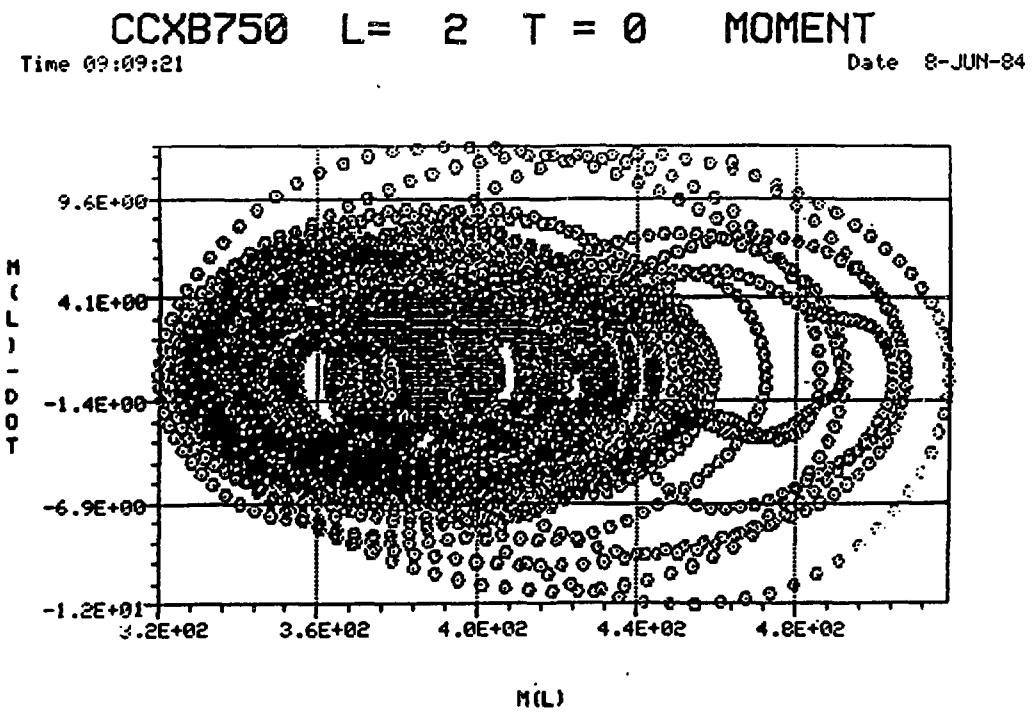
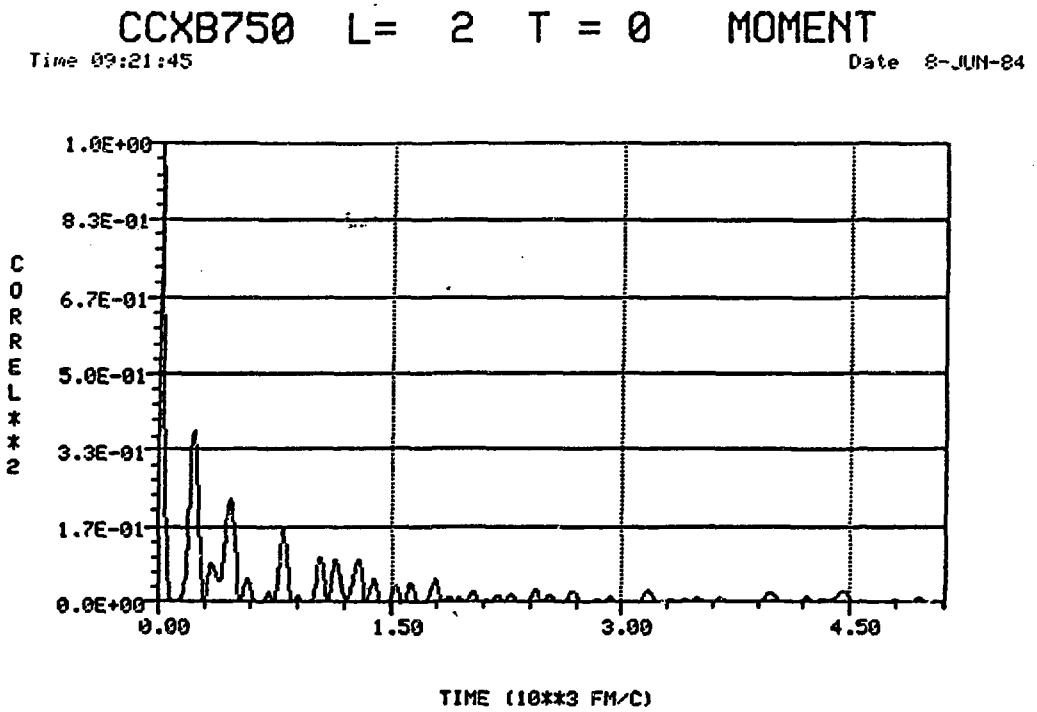


Fig. 5. Poincaré phase space plots $M_{\ell I}(t)$ vs. $M_{\ell I}(t)$ for I = 0, ℓ = 2, 3.



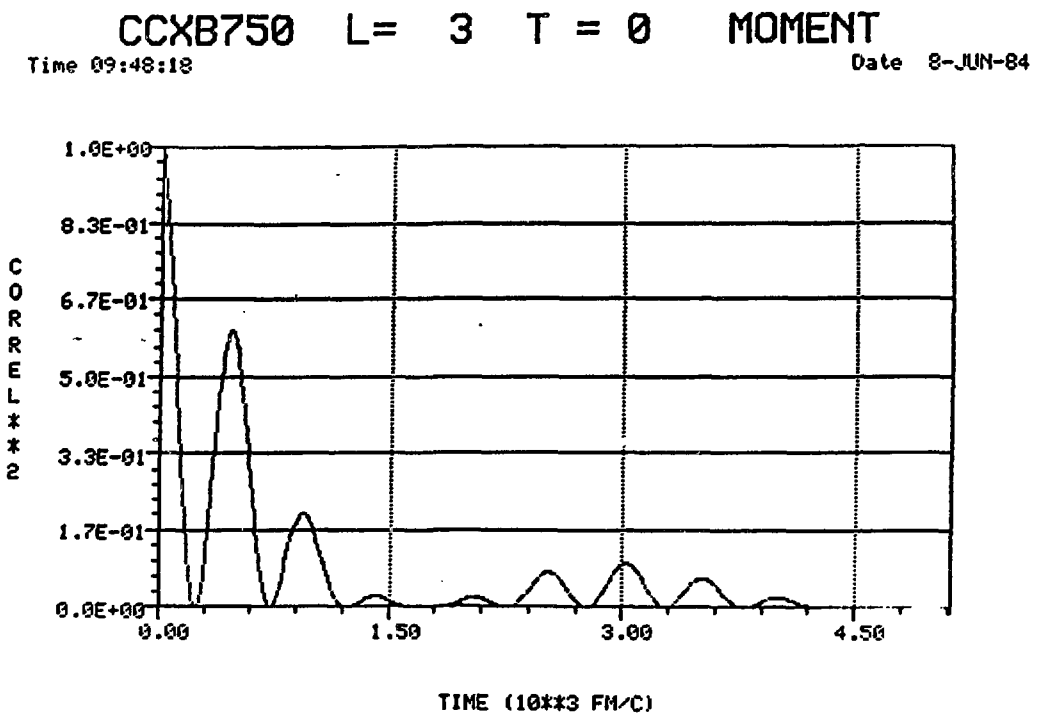


Fig. 6. The autocorrelation function $C_{I\ell}(t)$ as a function of time for the isoscalar quadrupole octupole modes in ^{24}Mg.

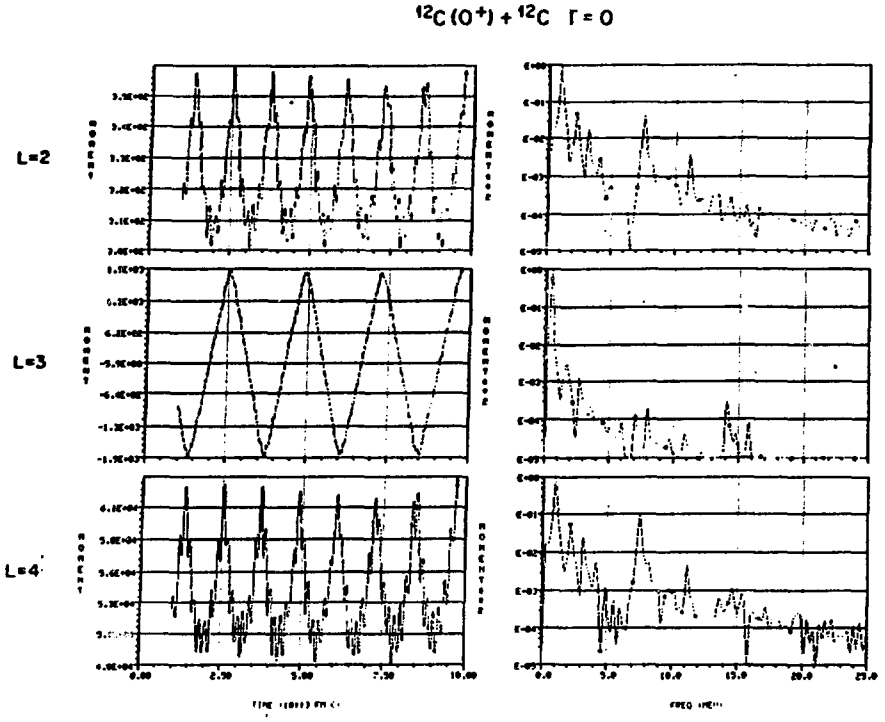


Fig. 7. Isoscalar frequency and time functions for the "cooled" modes of ^{24}Mg. Note the low-frequency motion is nearly harmonic.

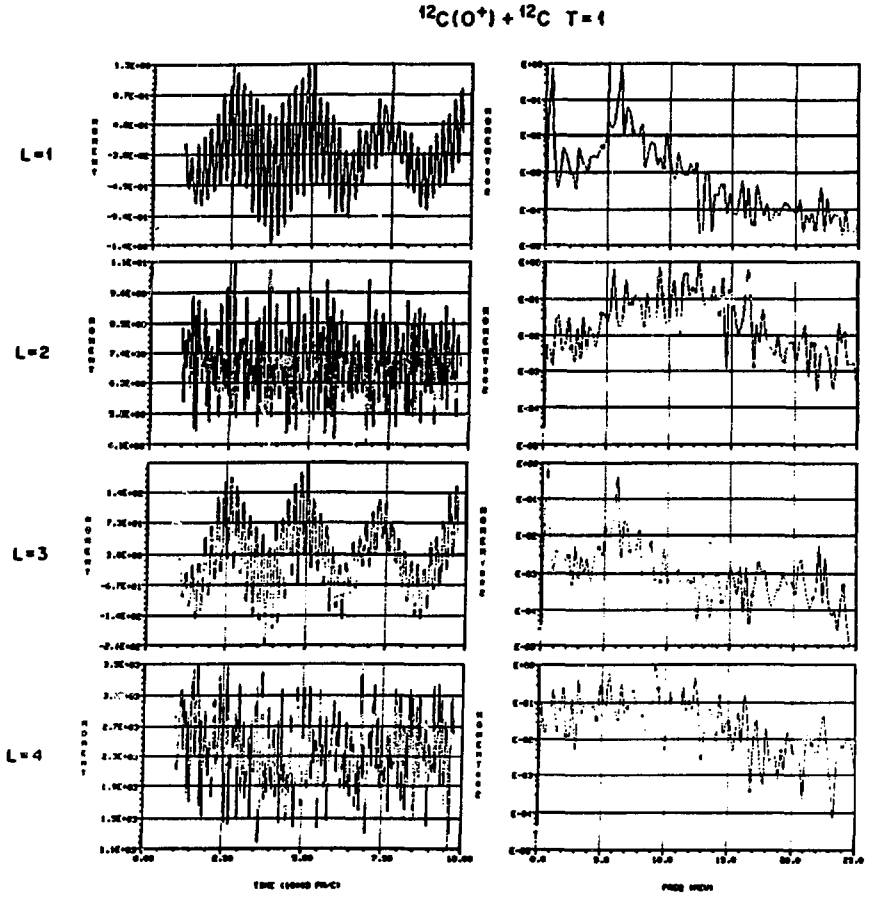


Fig. 8. Same as in Fig. 7 for the isovector modes of ^{24}Mg.

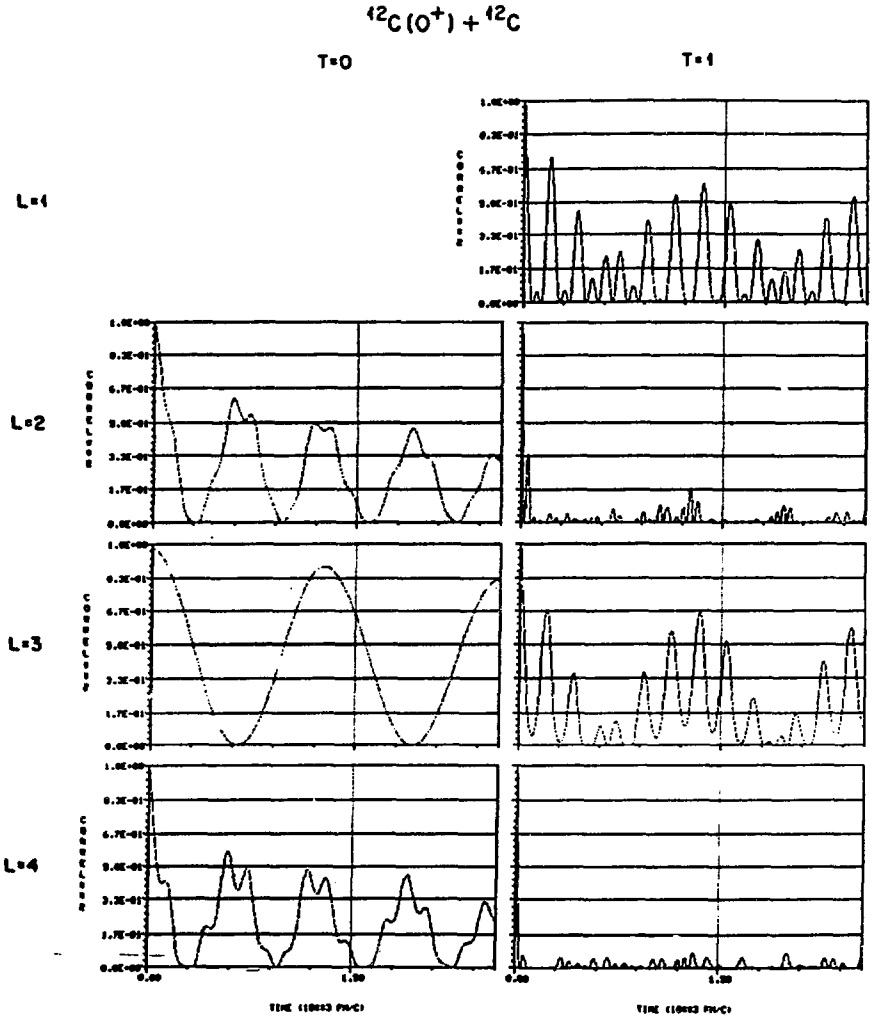


Fig. 9. Autocorrelation function for the isoscalar and isovector "cooled" modes of ^{24}Mg.