Mean-Field Calculations of Fluctuations in Nuclear Collisions

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We apply the new variational principle of Balian and Veneroni to calculate the fluctuations in final-fragment mass, charge, and kinetic energy for the systems $^{16}O + ^{16}O$ ($E_{lab} - 160$ MeV) and $^{40}Ca + ^{40}Ca$ ($E_{lab} = 278$ MeV). The calculated fluctuations are larger than conventional time-dependent Hartree-Fock results and, in the latter case, are consistent with the experimental fragment mass distribution.

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Time-dependent Hartree-Fock (TDHF) calculations of nuclear collisions accurately describe the time evolution of expectation values of single-particle observables such as fragment mass, kinetic energy, angular momentum, and scattering angle.[1] These averages are calculated with Wick's theorem: $\langle B \rangle = \mathrm{Tr} B\rho$ where B is the observable of interest and ρ is the TDHF one-body density matrix. If we naively apply Wick's theorem to calculate the fluctuations of these observables, we find, at a time t_1 after the collision,

$$(\Delta B)^2|_{t_1} \equiv (\langle B^2 \rangle - \langle B \rangle^2|_{t_1}$$
$$= \mathrm{Tr}\{B\rho(t_1)B[1-\rho(t_1)]\}. \qquad (1)$$

Several studies have shown that this equation underestimates the size of the fluctuations relative to experiment by about an order of magnitude. Furthermore, TDHF wave functions do not show the spreading in the center-of-mass coordinates required by quantum mechanics. These deficiencies can be attributed to the one-body nature of TDHF.[2]

Recent work[3-6] has led to a general mean-field formalism based on a time-dependent variational principle which addresses the problem of calculating fluctuations in mean-field theories. This theory is attractive because it correctly predicts the spreading in the center-of-mass coordinates, and it accurately reproduces the fluctuations of single-particle observables in the Lipkin-Meshkov-Glick model.[6] To date there has been only a single calculation based on this formalism of fragment-mass fluctuations[6] in a nuclear collision for which there are few experimental data. In this Letter we examine fragment-mass, charge, and kinetic-energy fluctuations in a system for which experimental data exist.

The new formalism of Balian *et al.* differs significantly from (1). For a collision of a system of A nucleons starting from time t_0 they find[3,4]

$$(\Delta B)^2|_{t_1} = \lim_{\epsilon\to 0} \frac{1}{2\epsilon^2}\mathrm{Tr}[\rho(t_0,0)-\rho(t_0,\epsilon)]^2, \qquad (2)$$

where $\rho(t,\epsilon)$ again obeys the ordinary TDHF equation with the boundary condition

$$\rho(t_1,\epsilon) \equiv \exp(i\epsilon B)\rho(t_1)\exp(-i\epsilon B). \qquad (3)$$

If we rewrite (3) in terms of the single-particle wave functions $\phi_j(x,t)$ which satisfy the TDHF equation with boundary condition

$$\psi_j(t_1;\epsilon) = \exp(i\epsilon B)\phi_j(t_1), \qquad (4)$$

then (2) becomes

$$(\Delta B)^2|_{t_1} = \lim_{\epsilon\to 0}\frac{f(\epsilon)}{\epsilon^2}; \qquad (5)$$
$$f(\epsilon) = A - \sum_{ij} |\langle \psi_j(t_0;\epsilon)|\phi_i(t_0)\rangle|^2.$$

Thus, we can use existing TDHF codes to evolve the initial single-particle wave functions from time t_0 to t_1 (some time after the collision when we want to measure the fluctuation), perform the unitary transformation (4) with some small ϵ, and then use the same codes to evolve the new wave functions back to the initial time t_0, whereupon we calculate the overlaps (5).

To test this formalism in nuclear collisions, we employ the axial-symmetric TDHF codes described in detail elsewhere.[7] These codes use the "clutching model" to treat collisions with nonzero impact parameters; that is, the moment of inertia of the two nuclei is assumed to be that of a rigid body as soon as the density between the two nuclei reaches half the nuclear saturation density. As the reaction progresses, the z axis joining the two nuclei rotates in space and symmetry is maintained about that axis.

Our calculation uses the modified Skyrme II force. We evolve the nuclei until the fragments have separated enough (about 10 fm) so that only the Coulomb interaction couples the fragments. Thus, the mass and charge fluctuations we calculate should be independent of further time evolution. (This has been checked for the mass fluctuation in the oxygen system.) Convergence in Eq. (3) is established by use of progressively smaller time steps and by performance of the calculation on different spatial meshes. We fit the overlaps to the form $f(\epsilon)=C_0+C_1\epsilon+C_2\epsilon^2$ for small ϵ ($|\epsilon|\leq 0.1$ for the mass and charge fluctuations and $|\epsilon|\leq 0.1$ fm for the momentum fluctuations) and note that $(\Delta B)^2=C_2$; nonzero C_0 and C_1 result from numerical "noise" which decreases rapidly with smaller Δt. The mesh spacing was kept constant at $\Delta z=\Delta r=0.4$ fm and we performed calculations with $\Delta t=(0.125,\ 0.0625,\ \text{and}\ 0.031\,25)\times 10^{-23}$ seconds to check convergence.

To calculate the mass fluctuations (ΔA) in the collisions, we employ the operator $B=\theta(z)$ in (3a) ($z=0$ is the plane between the two fragments), while the charge fluctuations (ΔZ) are calculated with the operator

$$B=(\tfrac{1}{2}-t_3)\theta(z),$$

where t_3 is the single-nucleon isospin operator. Finally, the fluctuations in relative fragment momentum (ΔP) are calculated by use of the operator

$$B=\tfrac{1}{2}[2\theta(z)-1](-i\partial/\partial z).$$

Note that ΔP does depend on the time t_1 as the Coulomb force continues to impart relative momentum to the fragments. To calculate the resulting asymptotic center-of-mass kinetic-energy fluctuations ($\Delta E_{K,\text{tot}}^{\text{c.m.}}$) we assume a Gaussian distribution of fragment momenta and neglect contributions to the energy width arising from fluctuations in fragment mass, angular momenta, and separation. We find

$$(\Delta E_{K,\text{tot}}^{\text{c.m.}})^2=\frac{4(\Delta P)^2}{Am}\left[\langle E_{K,\text{tot}}^{\text{c.m.}}\rangle|_{t_1}+\frac{(\Delta P)^2}{2A}\right],$$

where A is the fragment mass in atomic mass units and m is the nucleon mass. Here $\langle E_{K,\text{tot}}^{\text{c.m.}}\rangle|_{t_1}$ is the average kinetic energy of the fragments at time t_1 and separation R.

The first system we studied was $^{16}\text{O}+{}^{16}\text{O}$ at a laboratory energy of 160 MeV and orbital angular momenta $L=0$ and $30\hbar$. The results of our calculations are shown in Table I along with the conventional TDHF values calculated from (1). The mass fluctuations from Eq. (5) are larger than the TDHF values and for collisions close to fusion ($L=30\hbar$) we find greater mass fluctuations. Balian *et al.* report[6] $\Delta A=1.421$ for the oxygen collision at $E_{\text{lab}}=160$ MeV and $L=30\hbar$ using the Bonche-Koonin-Negele force and their three-dimensional code. For the same system, we find $\Delta A=2.5$ amu; apparently the more complex Skyrme force we use results in greater fluctuations despite the cylindrical geometry we impose on the system.

For the head-on collision, the fluctuations in relative momentum calculated according to (5) are larger than the TDHF values. (These TDHF values are constant throughout the collision.) The resulting kinetic-energy fluctuations are enormous, especially if we note that the fragments emerge from the collision strongly damped. (The initial $E_{K,\text{tot}}^{\text{c.m.}}=80.0$ MeV while the asymptotic $\langle E_{K,\text{tot}}^{\text{c.m.}}\rangle=30.0$ MeV.) Even if we subtract in quadrature the TDHF value for ΔP (since it is intrinsic to the TDHF wave functions), we still find $\Delta E_{K,\text{tot}}^{\text{c.m.}}=38$ MeV.

Since comprehensive experimental data on fluctuations in heavy-ion collisions exist only for heavier reactions, we have also calculated the collision $^{40}\text{Ca}+{}^{40}\text{Ca}$ at $E_{\text{lab}}=278$ MeV with $L=0$ and $30\hbar$. The results, along with an experimental result[8–10] for ΔA, are shown in Table II. For the head-on collision, the fragments emerged with $\langle E_{K,\text{tot}}^{\text{c.m.}}\rangle|_\infty=62.7$ MeV, while for the $L=30\hbar$ case $\langle E_{K,\text{tot}}^{\text{c.m.}}\rangle|_\infty=71.9$ MeV. Again, the energy fluctuations are enormous and need experimental verification. The experimental mass fluctuation is an average over all exit angles. Since we have performed calculations with only two different impact parameters, the measured and calculated results are

TABLE I. Fluctuations calculated for $^{16}\text{O}+{}^{16}\text{O}$ ($E_{\text{lab}}=160$ MeV).

	$L=0\hbar$		$L=30\hbar$	
Operator	TDHF	Equation (5)	TDHF	Equation (5)
ΔA	0.574 amu	0.75 amu	0.495 amu	2.5 amu
ΔZ	0.400	0.52	...	...[a]
ΔP ($R=15.02$ fm)	1.17 fm^{-1}	2.5 fm^{-1}	...	...[b]
$\Delta E_{K,\text{tot}}^{\text{c.m.}}$	...	44.4 MeV	...	...

[a]Not calculated.

[b]Not calculated. For convergence in the calculation of this observable we would require smaller mesh spacings, shorter time steps, and more CPU time.

TABLE II. Fluctuations calculated for $^{40}Ca + ^{40}Ca$ ($E_{lab} = 278$ MeV).

Operator	TDHF	Equation (5)	Experiment
		$L = 0\hbar$	
ΔA	1.62 amu	3.9 amu	4 amu
ΔP ($R = 14.92$ fm)	1.68 fm^{-1}	5.4 fm^{-1}	...
$\Delta E_{K,tot}^{c.m.}$	...	69 MeV	...
		$L = 30\hbar$	
ΔA	1.26 amu	5.5 amu	4 amu
ΔP ($R = 14.35$ fm)	1.69 fm^{-1}	4.2 fm^{-1}	...
$\Delta E_{K,tot}^{c.m.}$	...	51 MeV	...

not directly comparable; however, the agreement is suggestive.

A mean-field calculation of fluctuations in one-body observables in nuclear collisions gives results that are considerably larger than conventional TDHF values. Furthermore, the fragment-mass fluctuations calculated for the system $^{40}Ca + ^{40}Ca$ at $E_{lab} = 278$ MeV are consistent with experiment. A systematic approach trying different forces, different impact parameters, and asymmetric collisions would be interesting. Calculations with heavier ions are also called for as the differences between TDHF and the mean-field theory appear to grow with increasing mass and more extensive and detailed experimental data exist for heavier collisions. Finally, it would be interesting to extend this work to three-dimensional calculations to find the fluctuations in scattering angle.

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