Dispersions in semiclassical dynamics

M. Zielinska-Pfabé

Smith College, Northampton, Massachusetts 01063 and Grand Accélérateur National d'Ions Lourds (GANIL), 14021 Caen Cedex, France

C. Grégoire

Grand Accélérateur National d'Ions Lourds (GANIL), 14021 Caen Cedex, France (Received 16 July 1987)

Dispersions around mean values of one-body observables are obtained by restoring classical many-body correlations in Vlasov and Landau-Vlasov dynamics. This method is applied to the calculation of fluctuations in mass, charge, and linear momentum in heavy-ion collisions. Results are compared with those obtained by the Balian-Veneroni variational principle in semiclassical approximation.

I. INTRODUCTION

One of the most striking features revealed a decade ago by the first experimental studies of heavy ion collisions was the existence of large dispersions of observables like mass, charge, or kinetic energy.¹ Numerous theoretical studies dealt with these issues by investigating either the dynamical evolution of the one-body reduced density matrix (TDHF, i.e., time dependent Hartree-Fock) or a collective reduced density matrix in transport statistical approaches.

The TDHF theory, which is based on a microscopic approach, is known to underestimate dispersions² especially associated with the mass distribution of the outgoing fragments. The variational principle developed by Balian and Veneroni (BV) leads to the conclusion that TDHF is the best mean field approach to investigate the mean values of single particle observables but is unable to provide a correct answer as far as dispersions around mean values are concerned.³ In this time-dependent process, the boundary conditions for the many-body density are given at the initial time t_0 , while those for the observable are known only at a later time t_1 . If, in an attempt to calculate dispersions, one uses a variational principle and reduces the problem to one-body dynamics, the evolution of the system depends explicitly on the observable that one is interested in. To obtain dispersions within this framework, TDHF-like equations for the density matrix elements should be solved along with the timedependent RPA-like (random-phase approximation) equations for the operator matrix elements. In other words, the BV variational principle established an intimate connection between dynamical two-body correlations and fluctuations around mean values. One should mention that this theory properly predicts the spreading of wave packets. Reference 4 also shows that fluctuations of single particle observables in the Lipkin-Meshkov-Glick model are reasonably well described by applying the BV method. Applications of this formalism to nuclear collisions^{4,5} indicate that the main defect of the TDHF theory, namely a lack of success in the determination of dispersions, can be overcome.

Statistical transport theories⁶ give the time evolution of collective variables (defined a priori in most theoretical studies) by analogy with a diffusion process. Such theories treat the diffusion process as a random walk problem.⁷ Coupling between macroscopic variables and microscopic degrees of freedom is responsible for dispersions through the fluctuation-dissipation theorem. Description of this coupling requires some model of nucleon transport: dispersions around mean values are then found to be compatible with experimental findings. Nevertheless, these approaches are only semimicroscopic, some macroscopic models being needed in order to define relevant dynamical variables.

In this paper we reasses the problem of determination of dispersions and discuss it in the framework of semiclassical approximation to TDHF formalism [i.e., Vlasov equation (VE)] and to the extension of this theory obtained by taking into account residual two-body collisions [i.e., Landau-Vlasov equation (LVE)]. The Vlasov equation can be obtained by truncating the expansion of the Wigner transform of the TDHF equations. Dynamical evolution of the one-body distribution is identical to the one obtained from TDHF if one neglects pure quantal effects. The phenomenological collision term can also be easily calculated, extending VE into LVE.⁸ In determining the approximate solutions of VE or LVE, the distribution function has been decomposed in Ref. 9 into a sum of elementary Gaussians, each of which represents a part of the nucleonic distribution function. This collection of elementary packets can be viewed as a statistical ensemble; therefore, the mean value of each single particle observable can be considered as an ensemble-averaged value. It is now tempting to take advantage of this statistical interpretation in order to compute higher moments. This approach corresponds to a "backwards" version of the procedure proposed in Ref. 10: there, the authors plugged into TDHF equations Slater determinants which were built on a cascade statistical ensemble. As a consequence of the introduced fluctuations, the authors were able to obtain a dynamical description of a mul-

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tifragmentation process. Our procedure resembles the one suggested in Ref. 11, where the authors randomly choose elementary packets in phase space in order to introduce some fluctuations into a collision term. These fluctuations are due to the fact that a nuclear system in LVE is a mixture of Slater determinants. A selection of a single Slater determinant, by choosing as many elementary packets as particles, allows us to extract some of the classical many body correlations from the distribution function. In order to get mean values as well as dispersions we used the statistical ensemble of elementary packets to describe a collision between heavy ions.

In Sec. II we give a brief description of Vlasov and Landau-Vlasov dynamics. Section III contains a discussion of dispersions in TDHF and in Balian-Veneroni formalism along with their semiclassical analogs calculated with the Vlasov equation. In Sec. IV we present a method of restoring many body classical correlations (RMBC) and discuss the results obtained for mass, charge, and momentum dispersions. We also make a comparison with transport theory.

II. VLASOV AND LANDAU-VLASOV DYNAMICS

The Vlasov and Landau-Vlasov equations can be written as

$$\frac{\partial f}{\partial t} + \frac{\mathbf{p}}{m} \nabla_r f - \nabla_r U \nabla_p f = \begin{cases} 0 \quad \mathrm{VE} \\ I_{\mathrm{coll}} \quad \mathrm{LVE} \end{cases} .$$
(1)

Here $f = f(\mathbf{r}, \mathbf{p}, t)$ is a one-body distribution function, r and p represent the space and momentum coordinates, and the single particle potential U is treated in a selfconsistent way. The collision term I_{coll} is calculated using an effective nucleon-nucleon cross section, with the requirement of energy and momentum conservation and with an appropriate Pauli blocking factor.⁹

In order to solve Eq. (1) we write the distribution function $f(\mathbf{r}, \mathbf{p}, t)$ as a linear combination of the distribution functions for a large number NG of pseudoparticles which behave like classical particles:

$$f(\mathbf{r},\mathbf{p},t) = \sum_{i=1}^{NG} w_i(\mathbf{r}_i,\mathbf{p}_i) f_i(\mathbf{r},\mathbf{r}_i,\mathbf{p},\mathbf{p}_i,t) .$$
(2)

The pseudoparticle distribution functions $f_i(\mathbf{r}, \mathbf{r}_i, \mathbf{p}, \mathbf{p}_i, t)$ are expressed as uncorrelated isotropic Gaussian wave packets:

$$f_{i}(\mathbf{r},\mathbf{r}_{i},\mathbf{p},\mathbf{p}_{i},t) = N \exp\left\{-\frac{1}{2}\left[\frac{(\mathbf{r}-\mathbf{r}_{i})^{2}}{\sigma_{r}^{2}} + \frac{(\mathbf{p}-\mathbf{p}_{i})^{2}}{\sigma_{p}^{2}}\right]\right\},$$
(3)

with N being a normalization constant and $\mathbf{r}_i(t)$ and $\mathbf{p}_i(t)$ describing the mean position of the Gaussian "i" in phase space.⁹ The decomposition into a sum of Gaussians is useful for numerical purposes since it follows the phase space to be filled efficiently. This method corresponds to an extension of the Thomas-Fermi approximation; i.e., it effectively accounts for some quantal effects at the level of an extended Thomas-Fermi approach. Nevertheless, since the widths of the Gaussians are kept constant along

dynamical paths (for the sake of simplicity), it is not clear whether these quantal features are properly approximated by our procedure. We will avoid drawing any subsequent conclusion based on the particular choice of the Gaussian widths.

The weighting factors w_i were treated in the Thomas-Fermi approximation as

$$w_i = \theta(\varepsilon_F - \varepsilon_i) , \qquad (4)$$

where ε_i is the mean single particle energy for the coherent state and ε_F denotes the Fermi energy. The Pauli exclusion principle is satisfied by requiring that no more than four particles occupy an h^3 phase-space cell. At time t = 0, we start with random selection of NG pseudoparticles (coherent states) in the available phase space. The spreadings of the Gaussian wave packets were determined for this static configuration (t = 0) by requiring that the distribution function yield the proper values for the nuclear binding energy and for the root mean square radius of the nucleus.

We then obtained the time evolution of the system by following the semiclassical trajectories of the randomly chosen pseudoparticles (in a self-consistent way). The width of the Gaussians and the weighting factors are kept constant. It is important to notice that, in this procedure, the initial distribution function should be understood as an ensemble averaged quantity. This property of the distribution function will be used in Sec. IV. The effective interaction which was used in the following calculations was the same as in the fourth paragraph of Ref. 9, i.e., a simplified Skyrme interaction with an associated compressibility modulus K = 200 MeV.

III. TDHF AND BALIAN-VENERONI DISPERSIONS IN SEMICLASSICAL APPROXIMATION

In the TDHF formalism, the application of Wick's theorem yields the following relation for the dispersion of a one-body observable:

$$(\Delta Q)^2 / t_1 = (\langle Q^2 \rangle - \langle Q \rangle^2) / t_1$$

= Tr{Qp(t_1)Q[1-p(t_1)]}. (5)

It is easy to see that if Q is a projection operator, a nonvanishing value of ΔQ arises clearly because, in general, the projection of a TDHF Slater determinant is no longer a Slater determinant.

The values of dispersion obtained by using the above procedure strongly underestimate the experimental results because, in the mean-field treatment the fluctuations caused by many-body correlations are practically washed out. They should be restored in order to obtain any realistic estimate of dispersions of single particle observables. As a matter of fact, it has been shown in Ref. 3 that this underestimation is due to the fact that TDHF formalism is not variationally fitted to the evaluation of fluctuations.

One could write an equation analogous to Eq. (5) for an estimation of $(\Delta Q)^2$ in the Vlasov dynamics:

$$(\Delta Q)^2 / t_1 = \int Q f(\mathbf{r}, \mathbf{p}, t_1) Q [1 - f(\mathbf{r}, \mathbf{p}, t_1)] d\mathbf{r} d\mathbf{p} . \qquad (6)$$

The decomposition of the distribution function into a sum of elementary Gaussian packets allows a description of a nuclear system with a finite diffuseness. One then goes beyond the Thomas-Fermi limit (see Ref. 9), i.e., one gets a rough account of initial quantal corrections. Nevertheless, a consequence of this smearing procedure is that $f^2 \neq f$, whereas $\rho^2 = \rho$ in TDHF. A main contribution to Eq. (6) comes, therefore, from the widths of the Gaussians. Since in our calculation the widths do not evolve in time (see Ref. 9 for a discussion concerning this approximation), Eq. (6) can only give a crude estimate of the dispersions which should be compared with the results obtained in TDHF. The results, therefore, cannot test the validity of the semiclassical approximation, which operates only on the mean values of each Gaussian wave packet. As in TDHF, one should expect to underestimate the dispersions if one uses VE dynamics and Eq. (6).

The method explained above was applied to study mass distribution in the reaction of ¹⁶O and ¹⁶O at the laboratory energy of 160 MeV. The LV dynamics led to fusion for angular momentum below l = 33. In Vlasov dynamics we found a region of transparency for low values of l. A comparison of standard deviations of the mass distribution obtained in various approaches is presented in Table I. In our calculations presented in this table we choose l = 36. To get an estimate of the predictions of Eq. (6) we took the observable $Q = \theta(z)$ and therefore performed the integrations for the half-space $z \ge 0$ only. To evaluate the spurious effect of Gaussian widths, we performed the calculations with $\sigma_r = 0.61$ fm, $\sigma_p = 0.30$ fm⁻¹ (in the latter case the system becomes underbound). The extracted value of ΔA is less than 0.2 u.

In quantum mechanics, the Balian-Veneroni variational principle leads to the following expression⁴ for the variance associated with a one-body observable Q:

$$(\Delta Q)^2 / t_1 = \operatorname{Tr} \{ Q(t_0) \rho(t_0) Q(t_0) [1 - \rho(t_0)] \} .$$
(7)

Here $Q(t_0)$ is obtained by solving a system of coupled equations for the one-body density ρ and the operator Qbetween the time t_0 and t_1 . This result differs completely from the result obtained in TDHF when Wick's theorem is applied at time t_1 [Eq. (5)]. It can be further shown^{4,12} that if $\rho = \rho^2$ the results obtained from Eq. (7) are identical to those obtained from the following formula:

$$(\Delta Q)^2 / t_1 = \lim_{\varepsilon \to 0^{\frac{1}{2}}} \operatorname{Tr} \left[\frac{\rho(t_0) - \sigma(t_0, \varepsilon)}{\varepsilon} \right]^2.$$
(8)

Here $\sigma(t,\varepsilon)$ is a solution of TDHF equations with the boundary condition

$$\sigma(t_1,\varepsilon) = e^{i\varepsilon Q} \rho(t_1) e^{-i\varepsilon Q} .$$
⁽⁹⁾

We want to use the Balian-Veneroni variational approach to evaluate dispersions of one-body operators in semiclassical dynamics, where the distribution function f(t) is calculated by solving Vlasov equations. If the condition $f = f^2$ is fulfilled at time t_0 , one can use Eq. (8) with the unitary transformation of Eq. (9) being replaced by

$$f(t_1,\varepsilon) = e^{L_Q \varepsilon} f(t_1) , \qquad (10)$$

where $L_Q = \{Q, \}$ is an effective Liouvillian.

If, as in Ref. 9, f is decomposed to a sum of Gaussians, the unitary transformation (10) describes an elementary motion of a Gaussian in the phase space. This motion is determined by the effective Liouvillian L_Q . For instance, one can determine the mass distribution by taking $Q = \theta(z)$ where $\theta(z) = 1$ for $z \ge 0$ and zero everywhere else. In this case the transformation introduced in Eq. (10) assumes the following form:

$$k_i^z \to k_i^z - \varepsilon \frac{1}{2\pi\sigma_r^2} e^{(-z_i^2/2\sigma_r^2)} , \qquad (11)$$

where (z_i, k_i^z) is the mean phase space location of each Gaussian, and σ_r is the variance of the Gaussians in configuration space. The Vlasov code was first carried from the initial time t_0 and t_1 . The transformation described by Eq. (11) was then performed on all Gaussian packets and the Vlasov code was run backwards from t_1 to t_0 in order to obtain the distribution function $f(t_0, \varepsilon)$. We then estimated the phase space integral corresponding to the classical analog of Eq. (8). Since, due to the final widths of the Gaussians f^2 is not exactly identical to f, we correct for this effect in our estimate of Eq. (8).

For sake of comparison with Refs. 4 and 5, and with our method described below, we computed mass disper-

TABLE I. Mass, charge, and momentum dispersions calculated for ${}^{16}O + {}^{16}O$ at $E_{lab} = 160$ MeV using various methods discussed in the text.

Method	TDHF (Ref. 4)	TDHF (Ref. 5)		VLASOV Eq. (6)	RMBC VE (<i>l</i> = 36)	RMBC LVE (<i>l</i> = 36)	$\frac{\sqrt{\langle N_{\rm ex} \rangle}}{\rm VE}$ (l=36)	$\sqrt{\langle N_{ex} \rangle}$ LVE $(l = 36)$	BV (Ref. 4)	BV (Ref. 5)	BV Semiclassical
ΔA (u)	0.81 (<i>l</i> = 30)	0.495 (<i>l</i> = 30)	≤ 0.2 (<i>l</i> = 36)		2.7	1.9	3.2	2.0	1.42 (<i>l</i> =30)	2.5 (<i>l</i> = 30)	3.3 (<i>l</i> =36)
ΔZ (charge units)		0.400 (<i>l</i> =0)			1.8	1.2	2.3	1.5		0.52 (<i>l</i> =0)	
$\frac{\Delta P}{(\mathrm{fm}^{-1}\hbar)}$		1.17 (<i>l</i> =0)			2.0	2.0				2.5 (<i>l</i> =0)	

sions for ${}^{16}\text{O} + {}^{16}\text{O}$ system at the bombarding energy of 10 MeV/nucleon for an impact parameter b = 6.5 fm. We choose this impact parameter in order to obtain a deep inelastic collision in both Vlasov and Landau-Vlasov dynamics, with the same effective interaction being used. In Refs. 4 and 5 different partial waves were chosen along with another effective interaction. It is clear that the differences between our calculations and those of Refs. 4 and 5 allow only a qualitative comparison. Nevertheless, in all calculations dealing with deep inelastic collisions one finds similar reaction times, a crucial feature as far as dynamical evolution is concerned.

In spite of a high accuracy of the Vlasov code, there are problems with convergence in Eq. (8) as $\varepsilon \rightarrow 0$. For ε values smaller than 10^{-3} , the behavior of the numerator in our classical analog to Eq. (8) is logarithmic rather than quadratic in ε . [In Ref. 13 a divergence of the limit in Eq. (8) was also obtained in the numerical calculations because of large truncation errors. Nevertheless, the authors of Ref. 4 mentioned that a good control of the stability for ε smaller than 10^{-3} can still be achieved.] Consequently, we determined $(\Delta A)^2$ by varying ε from 0.001 to 0.5 and by performing a least squares fit of the results to a parabola. We obtained the value of $\Delta A = 3.3$ u. The value compares reasonably with the one found in Ref. 5 and is about 2 times larger than that of Ref. 4. Since effective forces are not identical in these three calculations, the deviation between results cannot be used as an indication that our semiclassical approximation introduces any additional bias in the determination of ΔA .

IV. RESTORING CLASSICAL MANY BODY CORRELATIONS

In order to restore classical many-body correlations, we started with the VE or LVE continuous distribution function at a given moment of time. Among all NG pseudoparticles, we randomly chose Z_p (Z_t) pseudoparticles which, at t = 0, corresponded to the proton distribution in the projectile (target), and N_p (N_n) which belonged to the neutrons in the projectile (target). We then identified their location (within a projectile-like or target-like fragment) and momenta for time t in the solution of VE or LVE and discretized the corresponding occupation probabilities to 0 or 1. This procedure, which corresponds to a random selection of a single Slater determinant out of a mixture of many Slater determinants, is repeated for large number of combinations. We then calculated the first and second moments of the obtained distributions of fragment mass, charge, or momentum. This method is a way to simulate, in a statistical ensemble, the classical many-body correlations which were washed out in the VE or LVE formalisms. Since NG is large, the number of random choices of sets of pseudoparticles is very large. We can therefore get a statistically reliable estimate of the first and second moments of the distributions of different single-particle observables.

We applied the method of restoring classical manybody correlations (RMBC) to study mass, charge, and momentum distributions of the reaction products in Landau-Vlasov dynamics and for comparison in Vlasov dynamics, considering a broad range of impact parameters which led to deep inelastic scattering. The number of random configurations was taken to be 10⁴ and the stability of the results when this number is changed has been checked. To illustrate the difference between Vlasov and Landau-Vlasov dynamics, we present the time evolution of ΔA for a central collision along with the time evolution of the relative distance between the centers of the ions (see Fig. 1). LVE led to fusion while VE led to a deep inelastic process. The crucial role of dynamics in determining the width of single particle observables can be seen by comparing the results of RMBC for VE and LVE dynamics for l = 36, where both cases led to a deep inelastic scattering (see Table I). The value of ΔA obtained with VE is considerably larger than in LVE, because for VE the interacting system arrives at a much more compact configuration and reseparates much more slowly. For all values of impact parameters one observes that during the deep phase, when the interacting ions amalgate, the width of mass and charge distributions become larger than the final values after the reseparation of



FIG. 1. Mass dispersion and distance between the centers of the interacting ions as a function of time for a central collision of two ¹⁶O ions at $E_{lab} = 10$ MeV/nucleon. In the lower part the solid line shows the relative distance between the centers as obtained in Vlasov dynamics while the dashed line was obtained with LVE. In the upper part the solid line corresponds to the mass dispersion obtained with VE, the dashed one with LVE.

the fragments. The same behavior has been observed in calculations based on transport theories.¹⁴

In Fig. 2 we present the standard deviations of mass and charge distributions as functions of the initial orbital angular momentum. The values of ΔA and ΔZ decrease monotonically with the values of the angular momentum, because, in the deep phase, the overlap of the density distributions is smaller and the time of interaction shorter. We have also calculated the dispersion of the distribution of fragment linear momentum along the beam direction. At this low energy the distribution is strongly dominated by the Fermi motion and therefore does not show any considerable variation with time or impact parameter. The values of ΔP are close to $\simeq 2$ fm⁻¹ for each of the colliding ions.

Because of the classical nature of TDHF (see Ref. 2), it is worth comparing the evolution of observables with those deduced from transport theories, as was shown in Ref. 15 devoted to tangential friction in nuclear dynamics. Since VE and LVE are obtained from TDHF and extended TDHF in semiclassical approximation, the comparison between VE or LVE and transport theories turns out to be even more relevant. In transport theories, dispersion can be obtained on account of stochastic nucleon exchanges. For instance, in a pure random-walk process the variance in mass σ_A^2 is equal to the number of exchanged particles N_{ex} (Ref. 16). Our Gaussian decomposition allows us to estimate an average value of N_{ex} :

$$\langle \mathbf{N}_{\mathrm{ex}} \rangle = \int d\Gamma [\theta_p f_T(t_1) + \theta_T f_p(t_1)] , \qquad (12)$$

where $\theta_p(\theta_T)$ is unity in the projectile-like (target-like) fragment at time t_1 and zero elsewhere; $f_p(f_T)$ is defined by $f(t)=f_p(t)+f_T(t)$ at each time t, and $f_p(t_0)=F_p$ $[f_T(t_0)=F_T]$ with $F_p(F_T)$ being the static projectile (target) initial distribution function, and $d\Gamma$ the phase space elementary volume element.

We have calculated the value of $\langle N_{ex} \rangle$ for the ¹⁶O+¹⁶O system at 10 MeV/u bombarding energy after a time lapse t_1 , at which point the reseparation is achieved. The square root of the average number of exchanged particles $\sqrt{\langle N_{ex} \rangle}$ is drawn in Fig. 2, together with σ_A and



FIG. 2. Dispersion in mass and change as a function of the angular momentum for ${}^{16}O + {}^{16}O$ at $E_{lab} = 10$ MeV/nucleon obtained in Landau-Vlasov dynamics. The solid line corresponds to the dispersion in mass, the dash-dotted line to the dispersion in charge, and the dashed one represents the square root of the average number of exchanged nucleons.

 σ_z , as a function of the initial orbital angular momentum $l. \langle N_{ex} \rangle$ is roughly equal to σ_A^2 , this latter quantity being smaller by around 15%. As a matter of fact, this difference could be explained by a squeezing of the fluctuations resulting from the divergence of the inertia parameter associated with the mass asymmetry degree of freedom at the reseparation.¹⁴ In spite of this small deviation, the results obtained from our self-consistent semiclassical description show that some features of transport theories are included in RMBC, at least for fluctuations around mean values of one-body observables.

V. CONCLUSION

We have discussed two methods (BV and RMBC) for evaluating dispersions in the heavy ion collisions where strong fluctuations of the field can be neglected (i.e., at low energy). The main contribution to the dispersions is due to mean field correlations. Using similar arguments as in Refs. 10 and 11, where the authors are dealing with strong fluctuations of the field, we could propose a method where classical many body correlations are restored (RMBC). This method is very convenient since it is founded on semiclassical simulations of heavy ion collisions which could extend the pure mean field approach. Consequently a statistical component to the dispersions, which is produced by the collision term of Landau-Vlasov, is superimposed to the mean field correlations. We have compared this method with the Balian-Veneroni prescription (BV), which is derived from a variational principle. The application to semiclassical dynamics is straightforward.

It was shown that the long range correlations introduced by the BV method produce the values of dispersions of the same order as those obtained by the RMBC applied to Vlasov dynamics. The fact that the BV values are close to those derived in RMBC can be interpreted as a dominance of the long range mean field correlations in our calculations, which were performed in the low incident energy domain. One should mention at this stage that our method is more flexible for practical purposes than the BV method the main results, in the studied examples, being quite similar in both approaches.

Finally, the estimate of the number of nucleonic exchanges N_{ex} during the reaction exhibits a property of collective transport theories, i.e., the proportionality of mass variances to N_{ex} , as long as drift effects remain small.

We conclude that semiclassical dynamics with restored classical many body correlations, occurring midway between microscopic self-consistent quantal models and macroscopic transport approaches, can be considered a very flexible and powerful tool for understanding basic features of low energy nucleus-nucleus collisions.

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