

Lawrence Berkeley National Laboratory

LBL Publications

Title

Brownian One-Body Dynamics in Nuclei

Permalink

<https://escholarship.org/uc/item/2sb6q1gc>

Journal

Physical Review Letters, 73(26)

Authors

Chomaz, Ph.
Colonna, M.
Guarnera, A.
et al.

Publication Date

1994-08-10



Lawrence Berkeley Laboratory

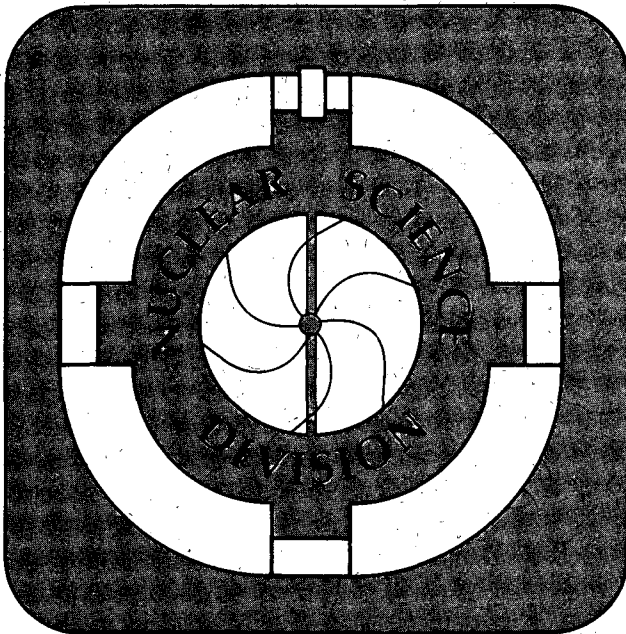
UNIVERSITY OF CALIFORNIA

Submitted to Physical Review Letters

Brownian One-Body Dynamics in Nuclei

Ph. Chomaz, M. Colonna, A. Guarnera, and J. Randrup

August 1994



REFERENCE COPY |
Does Not |
Circulate |

BTdg. 50 LIBRARY.

Copy 1

LBL-35988

DISCLAIMER

This document was prepared as an account of work sponsored by the United States Government. While this document is believed to contain correct information, neither the United States Government nor any agency thereof, nor the Regents of the University of California, nor any of their employees, makes any warranty, express or implied, or assumes any legal responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by its trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or the Regents of the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof or the Regents of the University of California.

Brownian One-Body Dynamics in Nuclei *

Ph. Chomaz¹, M. Colonna^{1,2}, A. Guarnera^{1,2}, and J. Randrup³

¹) GANIL, B.P. 5027, F-14021 Caen Cedex, France

²) Laboratorio Nazionale del Sud, Viale Andrea Doria, I-95129 Catania, Italy

³) Nuclear Science Division, Lawrence Berkeley Laboratory
University of California, Berkeley, California 94720, USA

August 10, 1994

Abstract

A novel method is presented for introducing fluctuations in one-body dynamics. It consists of employing a Brownian force in the kinetic equations. For nuclear matter within the spinodal zone, the magnitude of the Brownian force can be determined by demanding correspondance with the growth of the most unstable mode, as given by Boltzmann-Langevin simulations. The method is illustrated and tested for idealized two-dimensional matter and promises to provide a practical means for addressing catastrophic nuclear processes.

*This work was supported by the Director, Office of Energy Research, Office of High Energy and Nuclear Physics, Nuclear Physics Division of the U.S. Department of Energy, under Contract No. DE-AC03-76SF00098, and by the Commission of the European Community, under Contract No. ERBCHBI-CT-930619.

Transport phenomena occur in many physical systems. The approach pioneered by Boltzmann has proven particularly useful and has provided a good understanding of gas kinetics in various fields. For interacting gases, for example of Van-der-Waals type, the interparticle forces can be taken into account by a mean field. In particular, the nuclear Boltzmann equation (*BUU*) forms a very successful framework for understanding a variety of features associated with nuclear collisions at intermediate energies, including collective flow and particle production[1, 2].

In the standard Boltzmann treatment, only the average effect of the collisions between the particles of the considered system is included. This leads to a deterministic description and a single dynamical trajectory results. While this simplification may be well suited in many physical situations in which the dynamics appears to be rather stable, it cannot provide a description of processes involving instabilities, bifurcations, or chaos. For example, in nuclear physics the *BUU* approximation is appropriate during the early stages of a nuclear collision, when the system is hot and compressed but it becomes inadequate if instabilities occur, such as when expansion and cooling has brought the bulk of the system within the spinodal zone of the phase diagram. In such scenarios, it is essential to include the fluctuations as well.

In many branches of physics such diffusive behavior is described by transport theories originally developed for Brownian motion. These approaches simulate the effects of the unretained degrees of freedom by a random term in the dynamics of the retained variables. This idea has inspired an extension of the Boltzmann approach which considers the collisions as random processes so that the fluctuating collision term acts as a Langevin stochastic term on the one-body density *citeAG*. Accordingly, this approach has been denoted the Boltzmann-Langevin (*BL*) model.

A numerical simulation method was subsequently developed on a phase-space lattice [4, 5]. This method has been shown to exhibit the correct relaxation properties [5, 6, 7] and to also describe the spontaneous agitation and propagation of collective modes in unstable nuclear matter [8, 9]. Thus, the lattice simulation method provides a well-founded means for solving the *BL* equation in a numerically reliable manner.

However, the application of this method to realistic scenarios is a formidable task, due to the effort associated with the detailed simulation of all the possible elementary two-body scattering processes on the lattice. A significant advance was made recently by the derivation of simple approximate expressions for the *BL* transport coefficients at equilibrium, reducing the required numerical effort by several orders of magnitude [10]. Even so, the lattice simulation of the *BL* transport problem is still too tedious to provide a very useful practical tool for the understanding of physical processes. Therefore, it is worthwhile exploring ways of further simplifying the treatment so that realistic calculations can be made with relative ease, thereby facilitating the confrontation between theory and experiment.

In this paper we present a novel method that appears to bring this goal

within reach. It consists of replacing the actual complicated (hence computer demanding) fluctuating part of the collision term, δI , by the effect of an externally imposed Brownian force δF , that is suitably tuned so that the dynamics of certain important collective modes is in good accordance with the results of the complete *BL* model. Specifically, since we are particularly interested in how the spinodal decomposition of an expanded system may lead to its multifragmentation, we demand that the most rapidly growing unstable modes be well reproduced, for each density and temperature within the spinodal zone where exponential amplification of fluctuations occurs.

This approach is akin to the simplest description of the Brownian motion in which the dynamics of pollen particles immersed in a molecular heat bath is described by a simple random force, whereas the *BL* approach would correspond to actually simulating the individual collisions with the gas. The method has the distinct advantage that it can be readily implemented into existing simulation codes, in particular those employing the test-particle method, without greatly increasing the associated computational effort. We note that a more formal study of stochastic mean-field dynamic has been made previously for a very specific case [11].

The object of study is the reduced one-body phase-space density $f(\mathbf{s}, t)$ where we use $\mathbf{s} \equiv (\mathbf{r}, \mathbf{p})$ to denote a point in phase space. The presently most advanced dynamical model considers three distinct sources for the evolution of $f(\mathbf{s})$,

$$\frac{\partial f}{\partial t} = \{h[f], f\} + \bar{I}[f] + \delta I[f]. \quad (1)$$

The first term is the collisionless propagation of f in the self-consistent one-body field described by the effective Hamiltonian $h(\mathbf{s}) = \mathbf{p}^2/2m + U(\mathbf{r})$; this part is often referred to as the Vlasov propagation and is the semi-classical analogue of the Time-Dependent Hartree Fock approximation. The second source of evolution, $\bar{I}[f]$, represents the average effect of the residual Pauli-suppressed two-body collisions; this is the term included in the standard *BUU* description. The third term, $\delta I[f]$, is the Langevin term, ordinarily assumed to be Markovian and to represent the fluctuating part of the two-body collisions. The terms \bar{I} and δI can be calculated consistently by noting that the expected number of elementary transitions between the two initial and two final phase space elements is given by [4, 5]

$$d\nu_{12;34} = f_1 f_2 \bar{f}_3 \bar{f}_4 \delta(\mathbf{r}_{12}) \delta(\mathbf{r}_{34}) \delta(\mathbf{r}_{13}) w(p_1, p_2; p_3, p_4) ds_1 ds_2 ds_3 ds_4, \quad (2)$$

where $f_i \equiv f(\mathbf{s}_i)$ is the occupancy of the initial state i , and $\bar{f}_i \equiv 1 - f(\mathbf{s}_i)$ is availability of the final state i . The transition rate $w(p_1, p_2; p_3, p_4)$ is related to the differential scattering cross section $d\sigma_{NN}/d\Omega$.

A convenient framework for discussing the *BL* problem was developed within the Fokker-Planck approximation [4, 5]. The key quantities characterizing the dynamical problem are then the transport coefficients,

$$V(\mathbf{s}_i) = \langle I[f](\mathbf{s}_i) \rangle = \bar{I}[f](\mathbf{s}_i) = \frac{1}{2} \int d\nu_{12;34} (\delta_{i3} - \delta_{i1}), \quad (3)$$

$$2D(\mathbf{s}_i; \mathbf{s}_j) \delta(t_{12}) = \langle \delta I[f](\mathbf{s}_1, t_1) \delta I[f](\mathbf{s}_2, t_2) \rangle, \quad (4)$$

where the average $\langle \cdot \rangle$ is with respect to an ensemble of systems prepared with the same initial one-body density $f(\mathbf{s})$. Thus the drift coefficient $V(\mathbf{s})$ describes the average effect of the collision term. The diffusion coefficient governs the early growth rate of the correlated fluctuations in the occupancy and can be expressed explicitly as

$$D(\mathbf{s}_i; \mathbf{s}_j) = \frac{1}{4} \int d\nu_{12;34} [\delta_{ij}(\delta_{j2} + \delta_{j4}) + \delta_{i1}(\delta_{j2} - 2\delta_{j4}) + \delta_{i3}(\delta_{j4} - 2\delta_{j2})] , \quad (5)$$

where $\delta_{ij} \equiv \delta(\mathbf{s}_i - \mathbf{s}_j)$, and so we may write $D(\mathbf{s}_i; \mathbf{s}_j) = D(\mathbf{p}_i, \mathbf{p}_j)\delta(\mathbf{r}_{ij})$.

The basic idea of our proposed method is to replace the actual stochastic collision term δI by a suitable Brownian force $\delta \mathbf{F}$ (with $\langle \delta \mathbf{F} \rangle = 0$) in such a manner that the novel equation of motion is obtained by making the following replacement in (1),

$$\delta I[f] \rightarrow \delta \tilde{I}[f] = -\delta \mathbf{F}[f] \cdot \frac{\partial f}{\partial \mathbf{p}} . \quad (6)$$

Since we wish the resulting Brownian one-body dynamics to mimic the *BL* evolution, the stochastic force is assumed to be local in space and time. Moreover, since we wish to match its effects in nuclear matter, which is isotropic, the force may also be taken to have rotational invariance. Its correlation function can then be written

$$\langle \delta \mathbf{F}(\mathbf{r}_1, t_1) \delta \mathbf{F}(\mathbf{r}_2, t_2) \rangle = 2\tilde{D}_0 \mathbf{I} \delta(\mathbf{r}_{12}) \delta(t_{12}) , \quad (7)$$

where \mathbf{I} is the unit tensor. The resulting dynamics is then qualitatively similar to that resulting from the *BL* equation (1) but the associated diffusion coefficient is modified,

$$2\tilde{D}(\mathbf{s}_1; \mathbf{s}_2) = 2\tilde{D}_0 \frac{\partial f(\mathbf{s}_1)}{\partial \mathbf{p}_1} \cdot \frac{\partial f(\mathbf{s}_2)}{\partial \mathbf{p}_2} \delta(\mathbf{r}_{12}) . \quad (8)$$

In order to establish a formal basis for making such a replacement inside the spinodal zone, we first recall the properties of unstable nuclear matter. The agitation of collective modes in nuclear matter inside the spinodal zone was recently addressed within the framework of linear-response theory [9]. Starting from a spatially uniform phase-space density of Fermi-Dirac form, $f^0(\epsilon)$, the dynamics of small deviations $\delta f(\mathbf{r}, \mathbf{p}, t) = f(\mathbf{r}, \mathbf{p}, t) - f^0(\epsilon)$ was considered. The corresponding linearized *BL* equation is given by

$$\frac{\partial}{\partial t} \delta f + \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{r}} \delta f - \frac{\partial U}{\partial \rho} \frac{\partial f^0}{\partial \epsilon} \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{r}} \delta \rho = \bar{I} + \delta I , \quad (9)$$

where the left-hand side describes the collisionless (Vlasov) propagation. The effect of the average collision term \bar{I} is relatively small [12, 13] and is therefore ignored in the present exposition. The unstable Vlasov eigenmodes are plane waves of the form $f_{\mathbf{k}}^\nu(\mathbf{p}) \exp(i\mathbf{k} \cdot \mathbf{r} + \nu t/t_k)$ with $\nu = \pm$ and

$$f_{\mathbf{k}}^\nu(\mathbf{p}) = \frac{\partial U_{\mathbf{k}}}{\partial \rho} \frac{\mathbf{k} \cdot \mathbf{p}}{\mathbf{k} \cdot \mathbf{p} + i\nu m/t_k} \frac{\partial f^0}{\partial \epsilon} . \quad (10)$$

Here the Fourier component $\partial U_k/\partial\rho$ is simply related to the corresponding Landau parameter $F_0(k)$ [9, 13, 14]. The characteristic time t_k is determined by the associated dispersion relation, $h^{-D} \int d\mathbf{p} f_k^\nu(\mathbf{p}) = 1$.

The analysis can be further simplified by the introduction of the associated dual basis functions [15],

$$\hat{f}_k^\nu(\mathbf{p}) = \frac{i\nu N_k}{\mathbf{k} \cdot \mathbf{p} + i\nu m/t_k}, \quad (11)$$

which have the convenient property $h^{-D} \int d\mathbf{p} \hat{f}_k^\nu(\mathbf{p})^* f_k^{\nu'}(\mathbf{p}) = \delta_{\nu\nu'}$.

The source terms $\mathcal{D}_k^{\nu\nu'}$ governing the agitation rates of the unstable modes can then be obtained by a simple projection of the *BL* diffusion coefficient [15],

$$\mathcal{D}_k^{\nu\nu'} = \int \frac{d\mathbf{p}_1}{h^D} \frac{d\mathbf{p}_2}{h^D} \hat{f}_k^\nu(\mathbf{p}_1)^* D(\mathbf{p}_1, \mathbf{p}_2) \hat{f}_k^{\nu'}(\mathbf{p}_2). \quad (12)$$

This expression can be directly estimated numerically [9, 14] or analytically [13, 16], taking advantage of the dispersion relation and of the low-temperature approximation for the diffusion coefficient [10].

Turning now to the Brownian one-body dynamics, we can obtain the corresponding collective source terms by replacing D by \tilde{D} in eq. (12). Exploiting the dispersion relation, we then find

$$\tilde{\mathcal{D}}_k^{\nu\nu'} = \nu\nu' \tilde{D}_0 \frac{N_k^2}{m^2 k^2} \left(\frac{\partial U_k}{\partial \rho} \right)^{-2}. \quad (13)$$

We now demand that the *BL* results for the fastest-growing mode, for any given density and temperature, be well reproduced by the Brownian one-body dynamics, *i.e.* we impose the matching condition $\tilde{\mathcal{D}}_k^{++} = \mathcal{D}_k^{++}(\rho, T)$, where k is the wave number associated with the shortest growth time t_k in nuclear matter having been prepared with density and temperature characteristic of the conditions prevailing in the neighborhood of the specified position \mathbf{r} . The determination of the local density $\rho(\mathbf{r})$ is relatively straightforward in the test-particle method, whereas the local equivalent temperature is somewhat more problematic. We prefer to determine $T(\mathbf{r})$ by exploiting the simple relationship between the temperature and the collision rate which is automatically available in the *BUU* treatment; this method does not require the momentum distribution to be thermalized. It should be noted that the Brownian force is only employed when the local conditions are inside the spinodal region of the phase diagram.

In this manner the strength can be determined at each point in space, $\tilde{D}_0(\mathbf{r})$, in the course of the dynamical evolution. In practice, once the local strength $\tilde{D}_0(\mathbf{r})$ has been calculated, the test-particles in the neighborhood will feel the mean field force augmented by a small amount δF_n picked from a normal distribution with a variance in each direction is given by $\sigma_F^2 = 2\tilde{D}_0/\Delta t \Delta V$ where Δt and ΔV are the time and the volume over which the same force is applied. The small diffusive violation of energy and momentum conservation can easily

be eliminated by a suitable correction of the effect on δF_n on the individual test particles [16].

In order to illustrate the proposed method, we consider idealized unstable matter in two spatial dimensions, using the simple Skyrme model employed earlier [8, 17]. We prepare the system at half its saturation density and with a temperature of $T = 3$ MeV, which is in the region of largest instability. The fastest mode has the wave number $k \approx 0.6 \text{ fm}^{-1}$ and the points in Fig. 1 show the evolution of the associated variance σ_k , based on a sample of 25 individual dynamical simulations, each one employing $\mathcal{N} = 1500$ test particles per nucleon. The strength of the random force is $D_0 = 144 \text{ MeV}^2 \text{ fm}/c$, the value obtained by the procedure described above. For reference is shown the expected *BL* evolution (solid curve), as obtained by the analytical linear-response result taking into account the actual growth time t_k obtained in the test-particle simulation. We note that the Brownian one-body evolution converges well towards the *BL* curve. To be more quantitative, we have also compared the numerical results with the linear-response prediction for the Brownian one-body dynamics, using the same actual growth time t_k [16]. It is clear that this analytical prediction describes the results from the numerical simulation. Moreover, the evolutions of neighboring modes are also rather similar [16], and so the proposed method does indeed imitate the corresponding *BL* dynamics fairly well.

We have presented a novel simulation model for nuclear dynamics in the intermediate-energy regime where the semiclassical one-body description is expected to be applicable. The method consists of augmenting the standard *BUU* equation by the effect of a Brownian force that is tuned in space and time so as to imitate the spontaneous agitation of the most unstable collective mode associated with matter characterized by the local density and temperature. This local tuning can be easily accomplished by means of simple analytical expressions for the strength parameter \tilde{D}_0 . The method can thus be implemented relatively easily into existing transport codes, especially those employing the test-particle method, and the additional computational effort is relatively modest.

We also note that the presented method is much preferable to a recently suggested method in which the number of test particles \mathcal{N} is adjusted so that a good reproduction is obtained for the expected most dominant instability [17]. Although that method can yield useful insight under idealized circumstances, its practical applicability suffers from two major drawbacks: the need to carefully explore the nature of the instabilities encountered ahead of time, and the fact that only a single quantity can be adjusted, namely \mathcal{N} , so at most one single point of the phase space diagram could be well reproduced. Both of these drawbacks are eliminated in the present method.

In developing this method we have been motivated by the urgent need for dynamical calculations of reactions under current investigation with advanced detector arrays around the world. While the *BL* model is probably the presently best-founded model for this task, it is rather computer-demanding in realistic scenarios. The present method offers a relatively easy tool for obtaining approximate results while more elaborate implementations are in progress, and applications

are presently in progress for three-dimensional multifragmentation processes [16].

We finally wish to point out that the presented approach provides a general framework for studying the kinetics of gases subject to Brownian motion and may therefore be of wider interest.

Acknowledgements: This work was supported by the Director, Office of Energy Research, Office of High Energy and Nuclear Physics, Nuclear Physics Division of the U.S. Department of Energy, under Contract No. DE-AC03-76SF00098, and by the Commission of the European Community, under Contract No. ERBCHBI-CT-930619. Three of us (PC, MC, AG) would like to thank the LBL for its nice hospitality while this work was carried out.

References

- [1] G.F. Bertsch and S. Das Gupta, Phys. Rep. 160 (1988) 190
- [2] W. Cassing, V. Metag, U. Mosel, and K. Niita, Phys. Rep. 188 (1990) 363
- [3] S. Ayik and C. Gregoire, Phys. Lett. B212 (1988) 269; Nucl. Phys. A513 (1990) 187
- [4] J. Randrup and B. Remaud, Nucl. Phys. A514 (1990) 339
- [5] Ph. Chomaz, G.F. Burgio, and J. Randrup, Phys. Lett. B254 (1991) 340; G.F. Burgio, Ph. Chomaz, and J. Randrup, Nucl. Phys. A529 (1991) 157
- [6] F. Chapelle, G.F. Burgio, Ph. Chomaz, and J. Randrup, Nucl. Phys. A540 (1992) 227
- [7] G.F. Burgio, B. Benhassine, B. Remaud, and F. Sebille, Nucl. Phys. A567 (1994) 626
- [8] G.F. Burgio, Ph. Chomaz and J. Randrup, Phys. Rev. Lett. 69 (1992) 885
- [9] M. Colonna, Ph. Chomaz, and J. Randrup, Nucl. Phys. A567 (1994) 637
- [10] J. Randrup and S. Ayik, Nucl. Phys. A572 (1994) 489
- [11] R. Balian and M. Vénéroni, Ann. Phys. 135 (1981) 270
- [12] H. Heiselberg, C.J. Pethick, and D.G. Ravenhall, Ann. Phys. 223 (1993) 37
- [13] J. Randrup, LBL-35848, in preparation
- [14] Ph. Chomaz and M. Colonna, Phys. Rev. C49 (1994) 1908
- [15] S. Ayik, Ph. Chomaz, M. Colonna, and J. Randrup, LBL-35987, in preparation
- [16] A. Guarnera, Ph. Chomaz, M. Colonna and J. Randrup, in preparation
- [17] M. Colonna, G.F. Burgio, Ph. Chomaz, M. Di Toro, and J. Randrup, Phys. Rev. C47 (1993) 1395

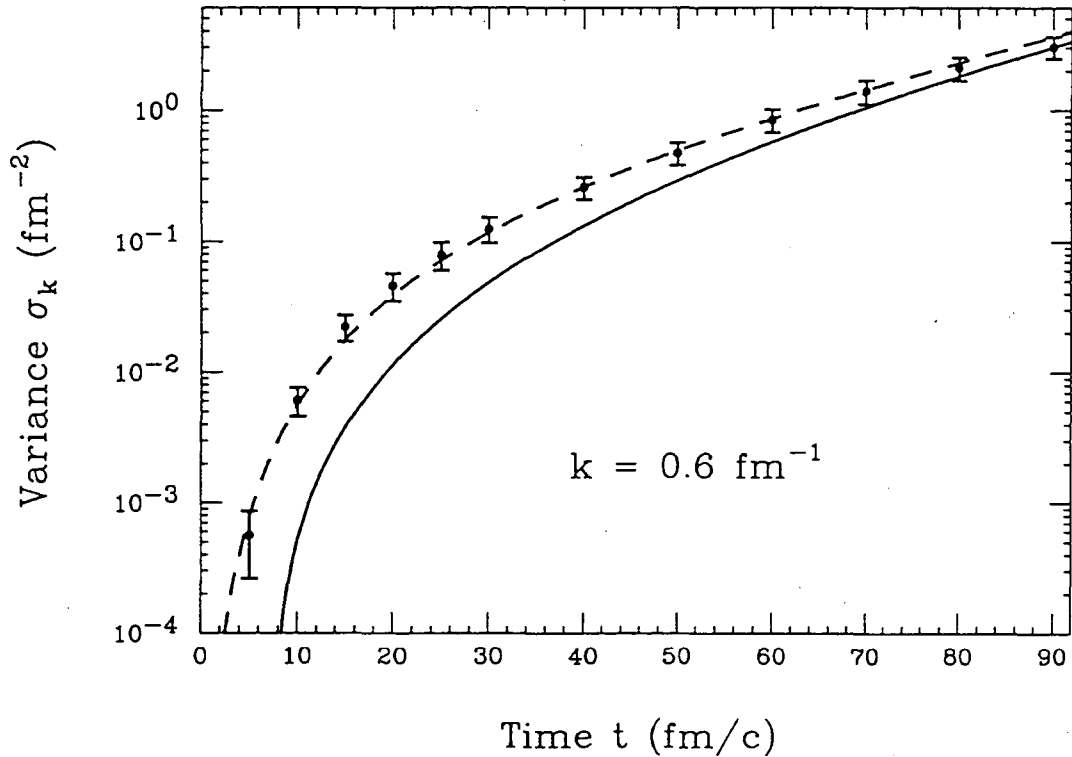


Figure 1: Test of the method.

The proposed simulation method is tested by considering the evolution of the variance σ_k of the most unstable mode in two-dimensional nuclear matter, prepared at half the saturation density and with $T = 3$ MeV. Solid curve: the expected *BL* result taking into account the actual growth time obtained in test-particle propagation. Points: the actual result of the Brownian one-body dynamics, with the bars representing the statistical error arising from the finite number of events. The contribution coming from the remaining small noise due to the finite number of test particle (about 5%) has been subtracted using an ensemble of events with no Brownian force. Dashed curve: the result of the corresponding linearized Brownian one-dynamics dynamics.

LAWRENCE BERKELEY LABORATORY
UNIVERSITY OF CALIFORNIA
TECHNICAL INFORMATION DEPARTMENT
BERKELEY, CALIFORNIA 94720