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Inclusion of Fluctuations in Nuclear Dynamics*

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ABSTRACT:

In this letter we present a new method to include fluctuations into dynamical simulations of the Nordheim type, in which individual nucleons moving in their self-consistent mean field experience Pauli-blocked two-body collisions. The method consists of including a suitably scaled amount of noise in the basic two-body scattering process. The method is illustrated for a gas of fermions on a two-dimensional torus and the results exibit the desired behavior: the mean phase-space occupancy relaxes towards the appropriate Fermi-Dirac distribution, the associated variance evolves as expected from quantum statistics, and the covariance reflects the various correlations inherent in the two-body collision process.

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1 Introduction

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Considerable progress has been made in recent years on the theory of nuclear dynamics [1]. Particularly significant is the development of semi-classical descriptions of the Nordheim type (often referred to as BUU or VUU models), in which the collisionless mean-field evolution has been augmented by a Pauli-blocked Boltzmann collision term. A major limitation of these models is that they confine themselves to describing the average dynamical trajectory. This precludes applications to situations where instabilities and bifurcations occur, such as fragmentation processes.

Various attempts to overcome this problem have already been made. In particular, the standard BUU treatment was extended by Bauer *et al.* so that fluctuations were allowed to arise and develop [2]. Our present studies support that approach as a reasonable approximate treatment. On the more formal side, transport theory has been invoked to develop equations for the mean evolution of the one-particle phase-space distribution $f(\mathbf{r}, \mathbf{p})$ as well as its fluctuations around this average trajectory [3, 4]. While these approaches are formally well founded, their practical utility is restricted to situations where the various dynamical trajectories are fairly similar so the knowledge of the moments allows an approximate reconstruction of the entire distribution of trajectories. However, in many situations of actual interest in heavy-ion physics, such a multifragmentation processes, the trajectory branching leads to qualitatively different manifestations of the systems and it is necessary to devise a method for treating arbitrary fluctuations. This letter reports on a novel approach towards extending the theory to incorporate fluctuations in general situations.

2 Description of method

The dynamical state of the nuclear system under consideration is given by its oneparticle phase-space distribution $f(\mathbf{r}, \mathbf{p})$. The equation of motion for f has two terms: a mean-field term accounting for the average interactions and a collision term representing the residual interactions between the nucleons. The first term is the usual Vlasov term and gives rise to a *deterministic* evolution of f(t), *i.e.* a given initial distribution $f_0(\mathbf{r}, \mathbf{p})$ produces a single dynamical history $f(\mathbf{r}, \mathbf{p}, t)$. The second term is *stochastic* in nature and is usually approximated by a Pauli-blocked collision integral of the Boltzmann-Uehling-Uhlenbeck (*BUU*) form. The standard *BUU* treatment includes the *average* effect of this term and, therefore, still produces a single trajectory (although a different one than the pure Vlasov trajectory). Our aim is to include the *fluctuating* part of the collision term as well.

The collision term acts as a random Langevin-type force on the one-body distribution $f(\mathbf{r}, \mathbf{p}, t)$ and the dynamical problem is then akin to Brownian motion. It is therefore appropriate to represent the system by the distribution $\phi[f]$ in the space of the one-body densities $f(\mathbf{r}, \mathbf{p})$ [4].

The two-body collisions are assumed to produce a stochastic sequence of distinct transitions in the system. These are approximated as local in space and time. Consequently, the expected number of such transitions from two given phase-space elements

1

into two other given phase-space elements is of the form

$$\bar{\nu}(12 \to 1'2') = \frac{d\boldsymbol{r}_1 d\boldsymbol{p}_1}{h^D} f(\boldsymbol{r}_1, \boldsymbol{p}_1) \frac{d\boldsymbol{r}_2 d\boldsymbol{p}_2}{h^D} f(\boldsymbol{r}_2, \boldsymbol{p}_2) \frac{d\boldsymbol{r}_1' d\boldsymbol{p}_1'}{h^D} \bar{f}(\boldsymbol{r}_1', \boldsymbol{p}_1') \frac{d\boldsymbol{r}_2' d\boldsymbol{p}_2'}{h^D} \bar{f}(\boldsymbol{r}_2', \boldsymbol{p}_2') \\ \delta(\boldsymbol{r}_1 - \boldsymbol{r}_2) \ \delta(\boldsymbol{r}_1' - \boldsymbol{r}_2') \ \delta(\boldsymbol{r}_1 - \boldsymbol{r}_1') \ w(\boldsymbol{p}_1, \boldsymbol{p}_2; \boldsymbol{p}_1', \boldsymbol{p}_2') \ \Delta t \ .$$
(1)

Here the f factors represent the phase-space occupancies at the initial sites and the \overline{f} factors are the availabilities at the final sites. The above expression holds for a physical space of arbitrary dimensionality D. In the present paper, we shall especially consider a two-dimensional system. For D = 2 the elementary transition rate in (1) is given by

$$w(\boldsymbol{p}_{1}\boldsymbol{p}_{2} \leftrightarrow \boldsymbol{p}_{1}'\boldsymbol{p}_{2}') = \frac{h^{4}}{2m}\delta(\boldsymbol{p}_{1} + \boldsymbol{p}_{2} - \boldsymbol{p}_{1}' - \boldsymbol{p}_{2}')\delta(E_{1} + E_{2} - E_{1}' - E_{2}')v_{12}\frac{d\lambda(12 \leftrightarrow 1'2')}{d\theta_{12}'}, \quad (2)$$

where $d\lambda/d\theta'$ is the differential scattering "cross section" in two dimensions (equal to twice the interaction length) and $v_{12} = |v_1 - v_2|$ is the relative speed of the two colliding nucleons. These basic processes are regarded as independent and the number of transitions ν actually occurring in a given time interval is governed by the corresponding Poisson distribution. It therefore follows that the variance of the number of transitions is equal to the mean number given above in (1),

$$\sigma_{\nu}^2 = \bar{\nu} \ . \tag{3}$$

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This inherent feature has two important consequences. The first is that the evolution of the distribution $\phi[f]$ will be *diffusive*, and the second is that the growth of the fluctuations is fully determined by the mean rates $\bar{\nu}$, which in turn depend only on the one-particle distribution $f(\mathbf{r}, \mathbf{p})$.

The first feature implies that if we start from a single initial "point" f_0 in the space of one-particle distributions, *i.e.* if $\phi[f](t=0) = \delta[f-f_0]$, then the stochastic twobody collisions generate an entire distribution $\phi[f](t)$ in the course of time. The work of ref. [4] describes the spreading distribution $\phi[f]$ in terms of its first two moments, the mean distribution $f(\mathbf{r}, \mathbf{p}, t)$ and its covariance matrix $\sigma(\mathbf{r}, \mathbf{p}, \mathbf{r}', \mathbf{p}', t)$ for whose evolution transport equations of the Fokker-Planck type are derived. While very instructive, such an approach is limited to scenarios where the bundle of trajectories remains farily confined. In more general situations, it appears necessary to treat the problem by direct numerical simulation and thus follow an ensemble of histories, each characterized by one particular phase-space distribution $f^n(\mathbf{r}, \mathbf{p}, t)$, n being the label of the particular trajectory. A sufficiently large number of such trajectories will then eventually represent the entire distribution $\phi[f](t)$. In order to implement such a scheme, it is necessary to simulate the basic stochastic process correctly. This problem is exacerbated by the fact that the phase-space distribution of the nucleons, $f^n(\mathbf{r}, \mathbf{p})$, is a continuous one. Since these are often represented by test particles, each representing only a small fraction of a nucleon, special care must be taken to ensure that the required relationship between the average change and the fluctuations is indeed preserved.

It is readily seen that the usual test-particle method is not directly applicable: this method replaces each physical nucleon by K test particles whose effective cross section has been appropriately reduced so as to ensure that the same mean evolution results. These test particles then propagate and collide as individual particles. Thus, since the collisions between pairs of test particles are treated as independent, the variance in the number of a particular elementary transition process is equal to its mean number. Therefore, when reexpressed in terms of the nucleons (which are the physical particles), the variance will be a factor of K too small.

One way to overcome this problem is to introduce some degree of correlation between test-particle collisions. Such an approach was introduced by Bauer *et al.* [2] who forced a suitable number (namely K pairs in total) of contiguous test particles to perform similar transitions and so enhance the effective fluctuations. Our approach provides support for this method as a reasonable though approximate prescription. A different way to overcome the problem of producing the correct amount of fluctuation is to refrain from subdividing the nucleons and consider only whole nucleons [5]. While this remedy guarantees that the fluctuations scale correctly, it provides a rather poor representation of $f(\mathbf{r}, \mathbf{p})$ as a smooth function and, consequently, it has inherently a large numerical error.

In our treatment we represent the one-particle distribution $f(\mathbf{r}, \mathbf{p})$ on a lattice of grid points in phase space. In this manner we preserve the smooth character of f, while avoiding the scaling problem inherent in the test-particle representation. Of course, the practicality of the method is then dependent on the availability of computers with sufficiently large random-access memory. However, the current technological developments are quickly reducing this obstacle.

Our method can now be briefly described as follows. The Vlasov evolution can readily be made in the grid representation (in fact there are already several such codes in existence). The two-body collisions give rise to a redistribution of probability between the phase-space slots considered. The rate at which nucleons move from two specified initial slots to two final slots is given by eq. (1). The time step Δt is chosen so that the expected number of nucleons moved in a particular process is small (much smaller than unity). The actual change in the local value is then picked at random from a normal distribution centered around the expected (average) change and with a variance given by the relation (3). This procedure guarantees that the ensuing fluctuations have the physically correct relationship with the average changes. Of course, special care must be made to prevent the distribution function from taking on unphysical values, *i.e.* its values must remain between zero and one. This presents the main practical problem, but it can be overcome by suitable reduction in the time increment and by performing a smearing over a phase-space volume of size less than h^D (since structure on this scale is not physically significant).

3 Illustration of the method

We shall illustrate this new method in a relatively simple scenario: a two-dimensional gas of fermions on a torus (*i.e.* in a square box with periodic boundary conditions).

The omission of the mean field is made to achieve maximum simplicity, since this feature is not essential for demonstrating the method (although it is important as a means to propagate the fluctuations generated by the two-body collisions). We then expect that the trajectories $f^n(t)$ should approach the appropriate statistical equilibrium distribution.

In our choice of initial distribution, we have preserved the symmetries of the field and thus assumed $f_0(\mathbf{r}, \mathbf{p})$ to be independent of the position \mathbf{r} and of the direction of motion $\hat{\mathbf{p}}$. We then consider an ensemble of histories, $f^n(\mathbf{r}, \mathbf{p}, t)$, each of which is initially equal to f_0 . Since the fluctuations will cause each one to undergo an individual evolution, both the translational symmetry and the spherical symmetry are broken. To keep the discussion simple, we shall disregard the fluctuations with respect to position and focus entirely on the evolution in momentum space. It is then useful to consider the average occupation in momentum space,

$$f^{n}(\boldsymbol{p}) = \frac{1}{\Omega} \int d\boldsymbol{r} f^{n}(\boldsymbol{r}, \boldsymbol{p}) .$$
(4)

The ensemble average of these momentum distributions are

$$\prec f(\boldsymbol{p}, t) \succ = \frac{1}{N} \sum_{n=1}^{N} f^{n}(\boldsymbol{p}, t) .$$
(5)

This quantity should relax towards the appropriate equilibrium distribution, which is a spherical symmetric Fermi-Dirac distribution whose temperature and chemical potential are dictated by conservation of energy and particle number. Moreover, the the ensemble $\{f^n\}$ will exhibit fluctuations breaking the spherical symmetry. An important advantage of the quantity $f^n(\mathbf{p})$ is that it corresponds to the diagonal part of the one-body density matrix in momentum representation and therefore our results can readily be compared with a quantal treatment.

We illustrate the new method by considering the situation where the initial momentum distribution is a hollow sphere. Specifically, we have $f_0(\mathbf{p}) = 1$ for $p_{\min} \leq 1$ $p \leq p_{\text{max}}$ and $f_0(\mathbf{p}) = 0$ otherwise. We use $p_{\text{min}} = 125 \text{ MeV/c}$ and $p_{\text{max}} = 275 \text{ MeV/c}$, which gives a mean kinetic energy per nucleon of 51.87 MeV and a density of 0.262 nucleons/fm². The nucleon-nucleon interaction length is chosen to be energy independent with a value of 1.2 fm, corresponding approximately to an interaction cross section of 40 mb in the real three-dimensional world. (For simplicity, we consider only one kind of nucleon, so there is no spin-isopsin degeneracy.) In momentum space the grid spacing is 50 MeV/c and we include a total of 29×29 such cells, centered around p = 0. Since we are not interested in the spatial correlations in this illustration, it suffices to consider a single cell in position space. (It can readily be shown, both formally and by calculation, that a subdivision of this one cell will leave the results for $f^n(\mathbf{p}, t)$ unaffected.) The side length of the box was chosen as L = 200 fm, but we have checked that the results are independent of the box size by performing the calculation also for L = 500,2500,5000 fm. Finally, we have used a time step of $\Delta t = 5$ fm/c and followed the evolution up to t = 125 fm/c, at which point the distribution is well relaxed. Due to the finite size of the momentum grid, energy is not strictly conserved. During the evolution considered, the ensuing change of the total energy was less then 1%. We have followed N = 592 different trajectories and thus obtained an acceptably small sampling error on the quantities considered. Each trajectory takes about 3 hours of CPU on a VAX 3100 workstation.

Figure 1 shows the time evolution of the ensemble-averaged phase-space density defined in eq. (5). In the situation considered, the time evolution of $\prec f \succ$ is nearly indistinguishable from the one computed with the standard Nordheim-type approach in which the fluctuations are averaged out at each timestep. We also note that the density $\prec f \succ$ approaches the appropriate statistical equilibrium distribution

$$\tilde{f}(\boldsymbol{p}) = \left[1 + \exp\left[\frac{1}{\tau}\left(\frac{p^2}{2m} - \mu\right)\right]\right]^{-1} , \qquad (6)$$

a Fermi-Dirac distribution with the temperature $\tau = 32.2$ MeV and the chemical potential $\mu = 62.34$ MeV.

Let us now discuss the fluctuations of $f(\mathbf{r}, \mathbf{p}, t)$. The general correlation function is defined as [4]

$$\sigma(\boldsymbol{r},\boldsymbol{p};\boldsymbol{r}',\boldsymbol{p}',t) = \prec f^n(\boldsymbol{r},\boldsymbol{p},t)f^n(\boldsymbol{r}',\boldsymbol{p}',t) \succ - \prec f^n(\boldsymbol{r},\boldsymbol{p},t) \succ \prec f^n(\boldsymbol{r}',\boldsymbol{p}',t) \succ \quad .$$
(7)

It is instructive to decompose this quantity into diagonal and non-diagonal parts,

$$\sigma(\boldsymbol{r},\boldsymbol{p};\boldsymbol{r}',\boldsymbol{p}',t) = \sigma^2(\boldsymbol{r},\boldsymbol{p},t)h^2\delta(\boldsymbol{r}-\boldsymbol{r}')\delta(\boldsymbol{p}-\boldsymbol{p}') + \sigma_{\rm cov}(\boldsymbol{r},\boldsymbol{p};\boldsymbol{r}',\boldsymbol{p}',t) .$$
(8)

Here $\sigma^2(\mathbf{r}, \mathbf{p})$ represents the variance in the occupancy of a given cell. It can be obtained by integrating the correlation function (7) with respect to $(\mathbf{r}', \mathbf{p}')$ over a domain of volume h^2 around the specified point (\mathbf{r}, \mathbf{p}) . The remainder, $\sigma_{\rm cov}$ is the covariance between occupancies of different phase-space cells.

Since we only wish to illustrate the behaviour as a function of momentum, we may integrate $\sigma(\mathbf{r}_1, \mathbf{p}_1; \mathbf{r}_2, \mathbf{p}_2)$ over their separation $\mathbf{r}_{12} = \mathbf{r}_1 - \mathbf{r}_2$. This contracted quantity is the total correlation between two particles that have the specified momenta \mathbf{p}_1 and \mathbf{p}_2 and whose mean position is $\mathbf{r} = (\mathbf{r}_1 + \mathbf{r}_2)/2$, irrespectively of their separation \mathbf{r}_{12} .[4] Since our system has translational invariance, the contracted correlation will not depend on the mean position $\mathbf{r} = (\mathbf{r}_1 + \mathbf{r}_2)/2$, and so we can average over \mathbf{r} . Thus, we consider the correlation function

$$\sigma(\boldsymbol{p};\boldsymbol{p}') = \frac{1}{\Omega} \int d\boldsymbol{r} \int d\boldsymbol{r}' \sigma(\boldsymbol{r},\boldsymbol{p};\boldsymbol{r}',\boldsymbol{p}') , \qquad (9)$$

which depends only on the momenta of the two particles. We have used $\Omega = L^2$ to denote the total area of the torus (*i.e.* the area of the periodic square considered). The correlation function can be expressed in terms of the average occupation defined in eq. (4),

$$\sigma(\boldsymbol{p};\boldsymbol{p}') = \Omega\left(\prec f^n(\boldsymbol{p})f^n(\boldsymbol{p}') \succ \neg \prec f^n(\boldsymbol{p}) \succ \prec f^n(\boldsymbol{p}') \succ\right) . \tag{10}$$

By applying the spatial integrations in (9) to the general relation (8), the above quantity (10) can also be decomposed into a variance and a covariance,

$$\sigma(\boldsymbol{p};\boldsymbol{p}') = \sigma^2(\boldsymbol{p})h^2\delta(\boldsymbol{p}-\boldsymbol{p}') + \sigma_{\rm cov}(\boldsymbol{p};\boldsymbol{p}') .$$
(11)

Let us first consider variance $\sigma^2(\mathbf{p})$. In the corresponding quantum system, the momentum \mathbf{p} is a good quantum number, due to the translational invariance. Then $\sigma^2(\mathbf{p})$ can be regarded as the variance of the occupation number $n\mathbf{p}$ of plane-wave orbitals. In equilibrium, the system is a statistical mixture of Slater determinants built of plane waves, and the occupancy coefficients $n\mathbf{p}$ are restricted to be 0 or 1 [6]. Then the variance of $n\mathbf{p}$ is related to its mean value $< n\mathbf{p} >$ through the relation $\sigma^2_{\mathbf{p}} = < n\mathbf{p} > (1 - < n\mathbf{p} >)$. Consequently, once equilibrium has been reached, we expect the variance to be given by

$$\sigma^{2}(\boldsymbol{p}) = \prec f(\boldsymbol{p}) \succ (1 - \prec f(\boldsymbol{p}) \succ) , \qquad (12)$$

if the description is to have a reasonable correspondance with quantum mechanics. Moreover, the evolution of the system can be thought of as a random walk among plane-wave Slater determinants, *i.e.* each individual system in the emsemble can be considered as a Slater determinant so that the occupancy coefficients of the planewave orbitals are either 0 or 1, but they change stochastically as a results of the two-body collisions. To the extent this picture is valid, one would expect that the above realtion (12) should hold at any time during the evolution of the system. We also note that initially both σ^2 and $\tilde{\sigma}^2$ vanish, since f_0 takes on only the values 0 or 1, and so $\sigma^2 = \tilde{\sigma}^2$ at t = 0. The diffusion equation for σ^2 derived in ref. [4] then predicts that these two quantities will remain equal throughout the evolution. This is then verified by our calculation.

Figure 2 displays the calculated variance $\sigma^2(p,t)$ (thick solid histogram) and the instantaneous equilibrium value $\tilde{\sigma}^2(p,t)$ (thin solid histogram) as calculated according to (12) using the instantaneous distribution function $\prec f^n(\mathbf{p},t) \succ$. Within the numerical tolerance, it is seen from the figure that indeed $\sigma^2 \approx \tilde{\sigma}^2$, not only at late times, but throughout the process. The fact that this relation holds dynamically obviously presents a strong constraint on the fluctuations and may provide a useful means of checking any model aiming to treat the fluctuations.

Let us now turn to the covariance $\sigma_2(\boldsymbol{p}, \boldsymbol{p}', t)$, which can provide deeper insight into the fluctuations. In order to minimize the finite sampling errors and to reduce this complex four-dimensionnal information to a more tractable form, we have integrated $\sigma_{\rm cov}(\boldsymbol{p}, \boldsymbol{p}')$ over a specified domain, corresponding to a certain acceptance for \boldsymbol{p}' . In particular, we have considered an acceptance F that requires the tagged momentum \boldsymbol{p}' to be within the initially occupied region, but at most 45 degrees off from the positive x direction. That is to say, its momentum magnitude must satisfy $p_{\min} \leq p' \leq p_{\max}$ and its direction of motion must deviate at most ± 45 degrees from forward. Figure 3 presents the resulting tagged covariance $\sigma_{\rm cov}(\boldsymbol{p}, \boldsymbol{p}')$ as a function of the magnitude of the untagged momentum \boldsymbol{p} ,

$$\sigma_{\rm cov}^F(\boldsymbol{p},t) = \frac{1}{h^2} \int_{p_{\rm min}}^{p_{\rm max}} p' dp' \int_{-\pi/4}^{\pi/4} d\theta' \sigma_{\rm cov}(\boldsymbol{p},\boldsymbol{p}',t) .$$
(13)

This quantity exhibits a remarkable time evolution. At early times it displays a strong positive correlation between the tagged nucleon and the occupied regions lying around the p_y axis, together with two domains of pronounced negative correlations with the

nearest unoccupied regions: the hole and the exterior of the Fermi sphere. These correlations are a reflection of the allowed collisions depleting the occupied states and filling the available domains of momentum space. At long times, after about 100 fm/c, the situation is entirely different, because the system is now nearly equilibrated. The observed correlation is now the sum of two overlapping components. The strong positive correlation with the states around the Fermi level, on the back side of the Fermi sphere, originates from the only states available as collision partners for the tagged particle. On the other hand, the rather spherical negative correlation all around the Fermi surface arises from the accessible final states for those collisions. The sum of these two components produces the observed pattern of a negative correlation in the direction of the observed nucleon and a positive correlation in the opposite direction. By starting from different initial states with the same energy and density of particles, we have verified that this fluctuation pattern is indeed associated with the equilibrated situation [7].

4 Concluding remarks

We have presented a novel method for incorporating the stochastic part of the collision integral into BUU-type simulations of nuclear dynamical processes. The key idea is to add an appropriately scaled noise term to the average effect of the collisions. The method has a sound formal foundation and it is possible to separate the *physical* fluctuations from the numerical noise inherent in any simulation algorithm.

We have illustrated the method in the particularly simple (but yet non-trivial) case of a two-dimensional gas of fermions. It was found that the mean evolution remains practically unaffected by the incorporation of the fluctuations, as would be expected in the considered scenario, that the variance of the distribution follows the corresponding instantaneous equilibrium variance, as expected on the basis of the transport treatment in ref. [4], and that the momentum corrrelations exhibit a significant evolution from early times to equilibrium.

The transport treatment by Ayik *et al.* [3] was recently applied to nuclear collisions by introducing the quadrupole moment of the local momentum distribution as a collective variable whose stochastic motion is simulated on the basis of the underlying transport equations [8]. The associated change of the momentum distribution is then calculated subsequently by a corresponding quadrupole rescaling. It is inherent in such an ansatz that the momentum distribution will retain a high degree of symmetry throughout the process, since it is always generated by a simple quadrupole stretching. By contrast, our approach, as well as the initial one by Bauer *et al.*[2], allow arbitrary symmetry breaking to develop in each individual history $f^n(\mathbf{p}, t)$.

We are presently seeking to adapt the method to more realistic situations, such as nuclear collisions. Presently, the main limitation is computing speed and storage. Clearly, the incorporation of fluctuations in nuclear dynamics demands significantly more computing power than what is needed for studies of the mean evolution only. However, judged against this inherently larger scale, our method presents a fairly economical means of treating the problem.

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The ensemble-averaged phase-space occupancy $f(p_x, p_y, t)$ as a function of p_x for $p_y = 0$, shown at four different times during the evolution from an initial hollow Fermi sphere (histograms) towards the associated Fermi-Dirac distribution (dashed curves).

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The tagged covariance $\sigma_{cov}^F(p_x, p_y, t)$ as defined in eq. (13). The areas of the circles are proportionnal to the local value of the covariance. The full circles represent positive values, while the empty circles are associated with negative values. (Same process as in fig. 1.)

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