THE HALO MASS FUNCTION FROM EXCURSION SET THEORY.
I. GAUSSIAN FLUCTUATIONS WITH NON-MARKOVIAN DEPENDENCE ON THE SMOOTHING SCALE

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Draft version October 21, 2009

ABSTRACT

A classic method for computing the mass function of dark matter halos is provided by excursion set theory, where density perturbations evolve stochastically with the smoothing scale, and the problem of computing the probability of halo formation is mapped into the so-called first-passage time problem in the presence of a barrier. While the full dynamical complexity of halo formation can only be revealed through $N$-body simulations, excursion set theory provides a simple analytic framework for understanding various aspects of this complex process. In this series of paper we propose improvements of both technical and conceptual aspects of excursion set theory, and we explore up to which point the method can reproduce quantitatively the data from $N$-body simulations. In paper I of the series we show how to derive excursion set theory from a path integral formulation. This allows us both to derive rigorously the absorbing barrier boundary condition, that in the usual formulation is just postulated, and to deal analytically with the non-markovian nature of the random walk. Such a non-markovian dynamics inevitably enters when either the density is smoothed with filters such as the top-hat filter in coordinate space (which is the only filter associated to a well defined halo mass) or when one considers non-Gaussian fluctuations. In these cases, beside “markovian” terms, we find “memory” terms that reflect the non-markovianity of the evolution with the smoothing scale. We develop a general formalism for evaluating perturbatively these non-markovian corrections, and in this paper we perform explicitly the computation of the halo mass function for gaussian fluctuations, to first order in the non-markovian corrections due to the use of a tophat filter in coordinate space.

In paper II of this series we propose to extend excursion set theory by treating the critical threshold for collapse as a stochastic variable, which better captures some of the dynamical complexity of the halo formation phenomenon, while in paper III we use the formalism developed in the present paper to compute the effect of non-Gaussianities on the halo mass function.

Subject headings: cosmology:theory — dark matter:halos — large scale structure of the universe

1. INTRODUCTION

The computation of the mass function of dark matter halos is a central problem in modern cosmology. In particular, the high-mass tail of the distribution is a sensitive probe of primordial non-Gaussianities (Matarrese et al. 1986; Moscardini et al. 1991; Kovama et al. 1999, Matarrese et al. 2000; Robinson & Baker 2002; Robinson et al. 2000). Various planned large-scale galaxy surveys, both ground based (DES, PanSTARRS and LSST) and on satellite (EUCLID and ADEPT) can detect the effect of primordial non-Gaussianities on the mass distribution of dark matter halos (see e.g. Dalal et al. 2008; Carbone et al. 2008). Of course, this also requires reliable theoretical predictions for the mass function, first of all when the primordial fluctuations are taken to be gaussian, and then including non-Gaussian corrections. Furthermore, the halo mass function is both a sensitive probe of cosmological parameters and a crucial ingredient when one studies the dark matter distribution, as well as the formation, evolution and distribution of galaxies, so its accurate prediction is obviously important.

The formation and evolution of dark matter halos is a highly complex dynamical process, and a detailed understanding of it can only come through large-scale $N$-body simulations. Some analytical understanding is however also desirable, both for obtaining a better physical intuition, and for the flexibility under changes of models or parameters (such as cosmological model, shape of the non-Gaussianities, etc.) that is the advantage of analytical results over very timing consuming numerical simulations.

Analytic techniques generally start by modelling the collapse as spherical or ellipsoidal. However, $N$-body simulations show that the actual process of halo formation is not ellipsoidal, and in fact is not even a collapse, but rather a messy mixture of violent encounters, smooth accretion and fragmentation (Springel et al. 2005). In spite of this, analytical techniques based on Press-Schechter (PS) theory (Press & Schechter 1974) and its extension known as excursion set theory (Peacock & Heavens 1990, Bond et al. 1991) are able to reproduce, at least qualitatively, several properties of dark matter halos such as their conditional and unconditional mass function, halo accretion histories, merger rates and halo bias (see Zentner 2007 for a recent review). However, at the quantitative level, already for gaussian fluctuations the prediction of excursion set theory for the mass function deviate significantly from the results of $N$-body simulations. The halo mass function $dn/dM$ can be written as (Jenkins et al. 2001)

$$\frac{dn(M)}{dM} = f(\sigma) \frac{\bar{\rho}}{M^2} \frac{d\ln \sigma^{-1}(M)}{d\ln M}, \quad (1)$$

where $n(M)$ is the number density of dark matter halos of mass $M$, $\sigma^2$ is the variance of the linear density field smoothed on a scale $R$ corresponding to a mass $M$, and $\bar{\rho}$ is the average density of the universe. In excursion set theory within a spherical collapse model the function $f(\sigma)$ is predicted to be

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where \( \delta_c \approx 1.686 \) is the critical value for collapse in the spherical collapse model. This result can be extended to arbitrary redshift \( z \) reabsorbing the evolution of the variance into \( \delta_c \), so that \( \delta_c \) in the above result is replaced by \( \delta_c(z) = \delta_c(0)/D(z) \), where \( D(z) \) is the linear growth factor. This prediction can be compared with the existing \( N \)-body simulations (see e.g. Jenkins et al. 2001; Warren et al. 2000; Lukic et al. 2007; Tinker et al. 2008; Pillepich et al. 2008; Robertson et al. 2008 and references therein). The results of these simulations have been represented by various fitting functions, see e.g. Sheth & Tormen (1999, 2001). In Fig. 1 we compare the function \( f_{PS}(\sigma) \) given in eq. (2) to various fits to \( N \)-body simulations, plotting the result against \( \sigma^{-1} \). High masses correspond to large smoothing radius \( R \), i.e. low values of \( \sigma \) and large \( \sigma^{-1} \), so mass increases from left to right on the horizontal axis. One sees that the \( N \)-body simulations are quite consistent among them, and that PS theory predicts too many low-mass halos, roughly by a factor of two, and too few high-mass halos: at \( \sigma^{-1} = 3 \), PS theory is already off by a factor \( O(10) \). The primordial non-Gaussianities can be constrained by probing the statistics of rare events, such as the formation of the most massive objects, so it is particularly important to model accurately the high-mass part of the halo mass function, first of all at the gaussian level. It makes little sense to develop an analytic theory of the non-Gaussianities, by perturbing over a gaussian theory that in the interesting mass range is already off by one order of magnitude.

When searching for the origin of this failure of excursion set theory, one can divide the possible concerns into two classes:

(i) Even if one accepts as a physical model for halo formation a spherical (or ellipsoidal) collapse model, there are formal mathematical problems in the implementation of excursion set theory that leads to eq. (2).

(ii) The physical model itself is inadequate, since a spherical or even elliptical collapse model is an oversimplification of the actual complex process of halo formation.

Concerning point (i), it is well known that the original argument of Press and Schechter discounts the number of virialized objects because of the so-called “cloud-in-cloud” problem. In the spherical collapse model one assumes that a region of radius \( R \), with a smoothed density contrast \( \delta(R) \), collapses and virializes once \( \delta(R) \) exceeds a critical value \( \delta_c \approx 1.686 \).\(^4\)

Within PS theory, for gaussian fluctuations the distribution probability for the density contrast is

\[
\Pi_{PS}(\delta,S) = \frac{1}{\sqrt{2\pi S}} e^{-\delta^2/2S},
\]

where

\[
S(R) \equiv \sigma^2(R) = \langle \delta^2(x,R) \rangle,
\]

and the fractional volume of space occupied by virialized objects larger than \( R \) is identified with

\[
F_{PS}(R) = \int_{\delta_c}^{\infty} d\delta \Pi_{PS}(\delta,S(R)) = 1 - \frac{1}{2} \text{erfc}\left(\frac{\nu(R)}{\sqrt{2}}\right),
\]

where \( \nu(R) = \delta_c/R(R) \). As remarked already by Press and Schechter, this expression cannot however be fully correct. In fact, in the hierarchical models that we are considering the variance \( S(R) \) diverges as \( R \to 0 \), so all the mass in the universe must finally be contained in virialized objects. Thus, we should have \( F_{PS}(0) = 1 \), while eq. (5) gives \( F_{PS}(0) = 1/2 \). Press and Schechter corrected this simply adding by hand an overall factor of two.

The reason for this failure is that the above procedure misses the cases in which, on a given smoothing scale \( R, \delta(R) \) is below the threshold, but still it happened to be above the threshold at some scale \( R' > R \). Such a configuration corresponds to a virialized object of mass \( M' > M \). However, it is not counted in \( F_{PS}(R) \) since on the scale \( S \) it is below threshold. Thus, eq. (5) cannot be fully correct.

In Bond et al. (1993) this problem was solved by mapping the evolution of \( \delta \) with the smoothing scale into a stochastic problem. Using a sharp \( k \)-space filter, they were able to formulate the problem in terms of a Langevin equation with a Dirac-delta noise. In other words, the smoothed density perturbation \( \delta \) suffers a markovian stochastic motion under the influence of a gaussian white noise, with the variance \( S = \sigma^2 \) playing the role of a time variable. In this formulation, the halo is defined to be formed when the smoothed density perturbation \( \delta \) reaches the critical value \( \delta_c \) for the first time. The problem is therefore reduced to a “first-passage problem”, which is a classical subject in the theory of stochastic processes (Redner 2001). One may write a Fokker-Planck equation describing the probability \( \Pi(\delta,S) \) that the density perturbation acquires a given value \( \delta \) at a given “time” \( S \), supplemented by the absorbing barrier boundary condition that the probability vanishes when \( \delta = \delta_c \). The solution reproduces eq. (2), including the factor of two that Press and Schechter were forced to introduce by hand.\(^5\)

However, this procedure still raises some technical questions, that will be reviewed in more detail in Section 2. In short, there are two issues that deserve a deeper scrutiny. First, the “absorbing barrier” boundary condition \( \Pi(\delta_c,S) = 0 \) is a natural one, but still it is something that is imposed by hand, and in this sense it is really an ansatz. In the literature for stochastic processes it is well-known that, in general,

\[^4\] More precisely, \( \delta_c \) has a slight dependence on the cosmological model, and \( \delta_c \approx 1.686 \) is the value for a \( \Omega_m = 1 \) cosmology (Lacey & Cole 1993). For a model with \( \Omega_m + \Omega_{\Lambda} = 1 \) this dependence is computed in Eke et al. (1996).

\[^5\] The work of Epstein (1983) also solves the cloud in cloud problem and recovers the correct factor of two, though the process considered therein uses Poisson seeds for structure formation.
the probability does not satisfy any simple boundary condition (van Kampen & Oppenheim 1972; Kness 1986). This is due to the fact that, when one works with a discretized time step, a stochastic trajectory can exit a given domain by jumping over the boundary without hitting it, unlike a continuous diffusion process which has to hit the boundary to exit the domain. Particular care must therefore be devoted to the passage from the discrete to the continuum. As we will see, the passage from a discrete to a continuum formulation is indeed highly non-trivial when a generic filter and/or non-Gaussian perturbations are used.

A second related concern is that the derivation of Bond et al. only works for a sharp k-space filter. However, as we review in Section 2, there is no unambiguous way of associating a mass to a region of size $R$ smoothed with a sharp k-space filter. The only unambiguous way of associating a mass $M$ to a smoothing scale $R$ is using a sharp filter in x-space, proportional to $(R-r)^2$, in which case one has the obvious relation $M = (4/3)\pi R^3$. This is also the relation used in numerical simulations. As soon as one uses a different filter (such as the tophat in real space), the Langevin equation with gaussian Dirac-delta noise, that describes a simple markovian process, is replaced by a very complicated non-markovian dynamics dictated by a colored noise. The system acquires memory properties and the probability $\Pi(\delta, S)$ no longer satisfies a simple diffusion equation such as the Fokker-Planck equation. The same is true if the density perturbation is non-Gaussian. Furthermore, the correctness of the “absorbing barrier” boundary condition is now far from obvious. These difficulties are well-known in the statistical physics community, where progress in solving the first-passage problem in the presence of a non-markovian dynamics has been very limited (Hänggi et al. 1981; Weiss et al. 1983; van Kampen 1998). From these considerations one concludes that the rather common procedure of taking the analytical results of Bond et al. (1991), valid for a sharp filter in momentum space, and applying them to generic filters is incorrect.6

These issues become even more important when one considers the evolution with smoothing scale of non-gaussian fluctuations, since non-gaussians induce again a non-markovian dynamics, and furthermore it is important to disentangle the physically interesting non-markovian contribution to the halo mass function due to primordial non-gaussians, from the non-markovian contribution due to the filter function.

Concerning point (ii) above, it is important to stress once again that excursion set theory is just a simple mathematical model for a complex dynamical process. Treating the collapse as ellipsoidal rather than spherical gives a more realistic description (Sheth & Tormen 1999; Sheth et al. 2001). However, as we already mentioned, dark matter halos grow through a mixture of smooth accretion, violent encounters and fragmentations, and modeling halo collapse as spherical, or even ellipsoidal, is certainly an oversimplification. In addition, the very definition of what is a dark matter halo, both in N-body simulations and observationally, is a difficult problem (for cluster observations, see Jeltema et al. (2005) and references therein), that we will discuss in more detail in paper II.

In this series of paper we examine systematically the above issues. In the present paper we start from excursion set theory in its simpler physical implementation, i.e. coupled to a spherical collapse model, and within this framework we put the formalism on firmer mathematical grounds. We show how to formulate the mathematical problem exactly in terms of a path integral with boundaries and particular care will be devoted to the passage from the discrete to the continuum. This formalism allows us to obtain a number of result: first, when we restrict to gaussian fluctuations and sharp k-space filter, in the continuum limit we recover the usual formulation of excursion set theory, but in this case the absorbing barrier boundary condition emerges automatically from the formalism, without the need of imposing it by hand. For different filters the problem becomes much more complicated, and we have to deal with a non-markovian dynamics. We will see that, for a generic filter, the zeroth-order term in an expansion of the non-markovian contributions gives back eq. (2), where $\sigma^2$ is now the variance computed with the generic filter. We then show how the non-markovian contributions can be computed perturbatively using our path integral formulation, and we compute explicitly, to first perturbative order, the halo mass function for a tophat filter in coordinate space. We find that the non-markovian contributions do not alleviate the discrepancy with N-body simulations. On the contrary, in the relevant mass range the full halo mass function is everywhere slightly lower than the one obtained from the markovian contribution, so in the large mass regime this correction goes in the wrong direction. This result will not be a surprise to the expert reader. Already in their classical paper, Bond et al. computed the result with a tophat filter in coordinate space using a Monte Carlo (MC) realization of the trajectories obtained from a Langevin equation with colored noise, and found indeed that one has fewer high mass objects. More recently, a MC simulation of this kind has been done in Robertson et al. (2008), and our analytical result to first order is in agreement with their findings.

In paper II of this series, motivated by the physical limitations of the spherical or ellipsoidal collapse model, we propose that some of the physical complications of the realistic process of halo formation and growth can be included in the excursion set framework, at least at an effective level, by assuming that the critical value for collapse is not a fixed constant $\delta_c$, as in the spherical collapse model, nor a fixed function of the variance $\sigma^2$, as in the ellipsoidal collapse model, but rather itself a stochastic variable, whose scattering reflects a number of complicated aspects of the underlying dynamics.

Finally, in paper III of this series we apply the formalism developed in the present paper, together with the diffusing barrier model developed in paper II, to the computation of the halo mass function in the presence of non-Gaussian fluctuations.

This paper is organized as follows. In Section 2 we review the excursion set theory developed in Bond et al. (1991); in Section 3 we present the path integral approach to a stochastic problem in the presence of a barrier. In Sections 4 we specialize to the cases of a sharp filter in momentum space, while in Section 5 we consider a generic filter. In particular, in Section 5 we show how to deal with the non-markovian corrections to the halo mass function. Some technicalities regarding the delicate passage from the discrete to the continuum are contained in Appendices A and B.
2. THE COMPUTATION OF THE HALO MASS FUNCTION AS A STOCHASTIC PROBLEM

The computation of the halo mass function can be formulated in terms of a stochastic process, as is well known since the classical work of Bond et al. (1991). Let us recall the procedure, in order to set the notation and to highlight some delicate points, in particular related to the choice of the filter function, that are important in the following. The expert reader might wish to move directly to Section 3. One considers the density contrast \( \delta(x) = (\rho(x) - \bar{\rho}) / \bar{\rho} \), where \( \bar{\rho} \) is the mean mass density of the universe and \( x \) is the comoving position, and smooths it on some scale \( R \), defining

\[
\delta(x, R) = \int d^3x' W(|x - x'|, R) \delta(x'),
\]

(6)

with a filter function \( W(|x - x'|, R) \). We denote by \( \hat{W}(k, R) \) its Fourier transform. A simple choice is a sharp filter in \( k \)-space,

\[
\hat{W}_{\text{sharp-}}(k, k_f) = \theta(k_f - k),
\]

(7)

where \( k_f = 1/R, k = |k| \) and \( \theta \) is the step function. Other common choices are a sharp filter in \( x \)-space, \( \hat{W}_{\text{sharp-}}(k, R) = 1/(4\pi^3 R^3) \theta(R - r) \), or a gaussian filter, \( \hat{W}_{\text{gau}}(k, R) = e^{-k^2R^2/2} \). Writing eq. (6) in terms of the Fourier transform we have

\[
\delta(x, R) = \int \frac{d^3k}{(2\pi)^3} \tilde{\delta}(k) \hat{W}(k, R) e^{-ik\cdot x},
\]

(8)

where \( k = |k| \). We focus on the evolution of \( \delta(x, R) \) with \( R \) at a fixed value of \( x \), that we can choose without loss of generality as \( x = 0 \), and we write \( \delta(x = 0, R) \) simply as \( \delta(R) \). Taking the derivative of eq. (8) with respect to \( R \) we get

\[
\frac{\partial \delta(R)}{\partial R} = \zeta(R),
\]

(9)

where

\[
\zeta(R) = \int \frac{d^3k}{(2\pi)^3} \tilde{\delta}(k) \frac{\partial \hat{W}(k, R)}{\partial R}.
\]

(10)

Since the modes \( \tilde{\delta}(k) \) are stochastic variables, \( \zeta(R) \) is a stochastic variable too, and eq. (9) has the form of a Langevin equation, with \( R \) playing the role of time, and \( \zeta(R) \) playing the role of noise. When \( \delta(R) \) is a gaussian variable, only its two-point connected correlator is non-vanishing. In this case, we see from eq. (10) that also \( \zeta \) is gaussian. The two-point function of \( \delta \) defines the power spectrum \( P(k) \),

\[
\langle \delta(k) \delta(k') \rangle = (2\pi)^3 \delta_D(k + k') P(k).
\]

(11)

From this it follows that

\[
\langle \zeta(R_1) \zeta(R_2) \rangle = \int d\ln k \Delta^2(k) \frac{\partial \hat{W}(k, R_1)}{\partial R_1} \frac{\partial \hat{W}(k, R_2)}{\partial R_2},
\]

(12)

where, as usual, \( \Delta^2(k) = k^3 P(k)/(2\pi^2) \). For a generic filter function the right-hand side is a function of \( R_1 \) and \( R_2 \), different from a Dirac delta \( \delta_D(R_1 - R_2) \). In the literature on stochastic processes this case is known as colored gaussian noise. Things simplify considerably for a sharp k-space filter. Using \( k_f = 1/R \) instead of \( R \), and defining \( Q(k_f) = -(1/k_f)\zeta(k_f) \), eqs. (9) and (12) become

\[
\frac{\partial Q(k_f)}{\partial \ln k_f} = Q(k_f),
\]

(13)

and

\[
\langle Q(k_f_1)Q(k_f_2) \rangle = \Delta^2(k_f_1) \Delta^2(k_f_2) |\ln k_f_1 - \ln k_f_2|.
\]

(14)

Therefore, we have a Dirac delta noise. We can write these equations in an even simpler form using as “pseudotime” variable the variance \( S \) defined in eq. (4). Using eq. (8)

\[
S(R) = \int d\ln k \Delta^2(k) |\hat{W}(k, R)|^2.
\]

(15)

For a sharp \( k \)-space filter, \( S \) becomes

\[
S(k_f) = \int d\ln k \Delta^2(k_f),
\]

(16)

so

\[
\frac{\partial S}{\partial \ln k_f} = \Delta^2(k_f).
\]

(17)

Thus, redefining finally \( \eta(k_f) = Q(k_f)/\Delta^2(k_f) \), we get

\[
\frac{\partial \eta(S)}{\partial S} = \eta(S),
\]

(18)

with

\[
\langle \eta(S_1)\eta(S_2) \rangle = \delta(S_1 - S_2).
\]

(19)

which is a the Langevin equation with Dirac-delta noise, with \( S \) playing the role of time. In hierarchical power spectra, at \( R = \infty \) we have \( S = 0 \), and \( S \) increases monotonically as \( R \) decreases. Therefore we can start from \( R = \infty \), corresponding to “time” \( S = 0 \), where \( \delta = 0 \), and follow the evolution of \( \delta(S) \) as we decrease \( R \), i.e. as we increase \( S \). The fact that this evolution is governed by the Langevin equation means that \( \delta(S) \) performs a random walk, with respect to the “time” variable \( S \). Following Bond et al. (1991), we refer to the evolution of \( \delta \) as a function of \( S \) as a “trajectory”. In the spherical collapse model, a virialized object forms as soon as the trajectory exceeds the threshold \( \delta = \delta_c \). In this language, the “cloud-in-cloud” problem of PS theory is associated with trajectories that make multiple crossings of the threshold, such as that shown in Fig. 2. If we compute the probability distribution at \( S = S_2 \) as in PS theory, i.e. using eq. (5), this trajectory does not contribute to \( P_{PS}(R) \) since at this value of \( S \) it is below threshold. However, it has already gone above threshold at an earlier time \( S_1 \), corresponding to a radius \( R_1 \), so it gives a virialized object of mass \( \mathcal{M}(R_1) > M(R_2) \). This virialized object has been lost in \( P_{PS}(R) \) evaluated through eq. (5), in spite of the fact that this formula was supposed to count all objects with mass greater then \( M(R_2) \).

To cure the “cloud-in-cloud” problem we must consider the lowest value of \( S \) (or, equivalently, the highest value of \( R \)) for which the trajectory pierces the threshold. Similar problems are known in statistical physics as “first-passage time” problems. After that, a virialized object forms and this trajectory should be excluded from further consideration. We therefore consider an ensemble of trajectories, all starting from the initial value \( \delta = 0 \) at initial “time” \( S = 0 \), and we compute the function \( \Pi(\delta, S) \) that gives the probability distribution of reaching a value \( \delta \) at “time” \( S \). As is well known, if a stochastic process obeys the Langevin equation (13) with a Dirac delta noise (19), the corresponding distribution function is a solution of the Fokker-Planck (FP) equation

\[
\frac{\partial \Pi}{\partial S} = \frac{1}{2} \frac{\partial^2 \Pi}{\partial \delta^2}.
\]

(20)

We denote by \( \Pi^0(\delta, S) \) the solution of this equation over the whole real axis \(-\infty < \delta < \infty \), with the boundary condition that it vanishes at \( \delta = \pm \infty \). One can check immediately that

\[
\Pi^0(\delta, S) = \frac{1}{\sqrt{2\pi S}} e^{-\delta^2/(2S)}.
\]

(21)
This probability distribution would bring us back to PS theory, and to its problems discussed in the Introduction. So, we need to eliminate the trajectories once they have reached the threshold. In Bond et al. (1991) this is implemented by imposing the boundary condition

\[ \Pi(\delta, S)|_{\delta = \delta_c} = 0. \]  

(22)

This seems very natural, but we stress that this boundary condition is still something that it is imposed by hand. The solution of the FP equation with this boundary condition is (Chandrasekhar 1943)

\[ \Pi(\delta, S) = \frac{1}{\sqrt{2\pi S}} \left[ e^{-\delta^2/(2S)} - e^{-(2\delta_c - \delta)^2/(2S)} \right], \]  

(23)

and gives the distribution function of excursion set theory. When studying halo merger trees it is important to consider also the distribution for trajectories that start from an arbitrary value \( \delta_0 \neq 0 \) (Bond et al. 1991; Lacey & Cole 1993). In this case, eq. (24) is replaced by

\[ \Pi(\delta_0; \delta, S) = \frac{1}{\sqrt{2\pi S}} \left[ e^{-(\delta - \delta_0)^2/(2S)} - e^{-(\delta - \delta_0)^2/(2S)} \right]. \]  

(24)

This result is easily understood writing \( 2\delta_c - \delta_0 - \delta = 2(\delta_c - \delta_0) - (\delta - \delta_0) \), so eq. (24) is obtained from eq. (23) performing the obvious replacement \( \delta \to \delta - \delta_0 \), and also \( \delta_c \to \delta_c - \delta_0 \), which expresses the fact that, if we start from \( \delta_0 \), the random walk must cover a distance \( \delta_c - \delta_0 \) to reach the threshold.

In the excursion set theory the distribution \( \Pi(\delta, S) \) is defined only for \( \delta < \delta_c \), so the fraction \( F(S) \) of trajectories that have crossed the threshold at "time" smaller or equal to \( S \) cannot be written, as in eq. (5), as an integral from \( \delta = \delta_c \) to \( \delta = +\infty \). Rather, we use the fact that the integral of \( \Pi(\delta, S) \) from \( \delta = -\infty \) to \( \delta = \delta_c \) gives the fraction of trajectories that at "time" \( S \) have never crossed the threshold, so

\[ F(S) = 1 - \int_{-\infty}^{\delta_c} d\delta \Pi(\delta, S). \]  

(25)

Observing that \( \Pi(\delta, S) = \Pi^0(\delta, S) - \Pi^0(2\delta_c - \delta, S) \), we see that

\[ F(S) = 1 - \int_{-\infty}^{\delta_c} d\delta \Pi^0(\delta, S) + \int_{-\infty}^{\delta_c} d\delta \Pi^0(2\delta_c - \delta, S). \]  

(26)

Since \( \Pi^0(\delta, S) \) is normalized to one,

\[ 1 - \int_{-\infty}^{\delta_c} d\delta \Pi^0(\delta, S) = \int_{-\infty}^{\delta_c} d\delta \Pi^0(\delta, S). \]  

(27)

For the last term in eq. (26), we write \( \delta' = 2\delta_c - \delta \), and

\[ \int_{-\infty}^{\delta_c} d\delta \Pi^0(2\delta_c - \delta, S) = \int_{-\infty}^{\delta_c} d\delta' \Pi^0(\delta', S). \]  

(28)

Thus, one obtains

\[ F(S) = 2 \int_{-\infty}^{\delta_c} d\delta \Pi^0(\delta, S) = \text{erfc} \left( \frac{\nu}{\sqrt{2}} \right), \]  

(29)

where \( \nu = \delta_c / \sigma(M) \), and one recovers the factor of two that Press and Schechter were forced to introduce by hand. The probability of first crossing the threshold between "time" \( S \) and \( S + dS \) is given by \( F(S)dS \), with

\[ F(S) \equiv \frac{dF}{dS} = -\int_{-\infty}^{\delta_c} d\delta \frac{\partial \Pi}{\partial S}. \]  

(30)

This can be easily computed by making use of the fact that \( F \) by definition satisfies the FP equation (20), so

\[ F(S) = -\frac{1}{2} \frac{\partial \Pi}{\partial S} \bigg|_{\delta = \delta_c} = \frac{\delta_c}{\sqrt{2\pi S}^{3/2}} e^{-\delta_c^2/(2S)}. \]  

(31)

Observe that, in \( \delta = \delta_c \), \( \Pi(\delta, S) \) and all its derivative of even order with respect to \( \delta \) vanish, while all its derivative of odd order with respect to \( \delta \) are twice as large as the value for the single gaussian (21). So, this first-crossing rate is twice as large as that computed with a single gaussian, which is another way of understanding how one gets the factor of two that the original form of PS theory misses.

The halo mass function follows if one has a relation \( M = M(R) \) that gives the mass associated to the smoothing of \( \delta \) over a region of radius \( R \). We discuss below the subtleties associated to this relation, and its dependence on the filter function. Anyhow, once \( M(R) \) is given, we can consider \( F \) as a function of \( M \) rather than of \( S(R) \). Then \( dF/dM/dM \) is the fraction of volume occupied by virialized objects with mass between \( M \) and \( M + dM \). Since each one occupies a volume \( V = M/\bar{\rho} \), where \( \bar{\rho} \) is the average density of the universe, the number of virialized object \( n(M) \) with mass between \( M \) and \( M + dM \) is given by

\[ \frac{dn}{dM} = \frac{dF}{dM} \left| _{M} \right. dM, \]  

(32)

so

\[ \frac{dn}{dM} = \frac{dF}{dM} \left| _{M} \right. dS = \frac{\bar{\rho}}{M^2} F(S) 2\sigma^2 d\ln \sigma^{-1} dM, \]  

(33)

where we used \( S = \sigma^2 \). Therefore, in terms of the first-crossing rate \( F(S) = dF/dS \), the function \( f(\sigma) \) defined from eq. (1) is given by

\[ f(\sigma) = 2\sigma^2 F(\sigma^2). \]  

(34)

Using eq. (31) we get the halo mass function in PS theory (with the factor of two computed thanks to the excursion set theory),

\[ \left( \frac{dn}{dM} \right)_{PS} = \left( \frac{2}{\pi} \right)^{1/2} \frac{\delta_c}{\sigma} e^{-\delta_c^2/(2\sigma^2)} \frac{\bar{\rho}}{M^2} d\ln \sigma^{-1} dM, \]  

(35)

This is the result given in eqs. (1) and (2).
The crucial point is how to associate a mass $M$ to the filter scale $R$. For the sharp filter in $x$-space this is clear. The mass associated to a spherical region of radius $R$ and density $\rho$ is $M = (4/3)\pi R^3 \rho$. For the other filters there is no unambiguous definition. A possibility often used is the following. One first normalizes $W$ so that its maximum value is one. Calling $W'$ this new dimensionless filter, one can define the volume $V$ associated to the filter as $V = \int d^3 x W'$, and $M = \rho V$. This procedure seems reasonable, but still it is somewhat arbitrary, since one might as well choose a different normalization for $W'$. For a gaussian filter, this gives $V = (2\pi)^{3/2} R^3$. For a sharp $k$-space filter, on top of this ambiguity, there is also the fact that such a volume is not even well defined. In fact, the $k$-space filter in coordinate space by performing a Monte Carlo (MC) realization of the trajectories obtained from a Langevin equation with colored noise [Bond et al. 1991; Robertson et al. 2008]. However, our final aim is to get some analytic understanding of the effect of non-Gaussianities on the halo mass function, and to this purpose we need a good analytic control of the effect of the filter, first of all in the gaussian case.

3. PATH INTEGRAL APPROACH TO STOCHASTIC PROBLEMS

3.1. General formalism

We have seen that the computation of the halo mass function can be reformulated in terms of a stochastic process. We now show how to compute the probability distribution of a variable evolving stochastically, in terms of its correlators. In this paper we limit ourselves to gaussian variables, while in paper III of this series we perform the generalization to arbitrary non-Gaussian theories.

Let us consider a variable $\delta(S)$ that evolves stochastically with “time” $S$, with zero mean $\langle \delta(S) \rangle = 0$. For a gaussian theory, the only non-vanishing connected correlator is then the two-point correlator $\langle \delta(S_1) \delta(S_2) \rangle$, where the subscript $c$ stands for connected.

We consider an ensemble of trajectories all starting at $S_0 = 0$ from an initial position $\delta(0) = \delta_0$, and we follow them for a time $S$. We discretize the interval $[0, S]$ in steps $\Delta S = \epsilon$, so $S_i = kc$ with $k = 1, \ldots, n$, and $S_n = S$. A trajectory is defined by the collection of values $\{\delta_1, \ldots, \delta_n\}$, such that $\delta(S_k) = \delta_k$. There is no absorbing barrier, i.e. $\delta(S)$ is allowed to range freely from $-\infty$ to $+\infty$. The probability density in the space of trajectories is

$$W(\delta_0, \delta_1, \ldots, \delta_n; S_n) \equiv \langle \delta_D(\delta(S_1) - \delta_1) \ldots \delta_D(\delta(S_n) - \delta_n) \rangle,$$

(39)

where, to avoid confusion with the density contrast $\delta$, we denote the Dirac delta by $\delta_D$. In terms of $W$ we define

$$\Pi_\epsilon(\delta_0; \delta; S_0) \equiv \int_0^{\delta} d\delta_1 \ldots \int_0^{\delta_n} d\delta_{n-1} W(\delta_0; \delta_1, \ldots, \delta_{n-1}, \delta_n; S_n),$$

(40)

where $S_n = n \epsilon$. So, $\Pi_\epsilon(\delta_0; \delta; S_0)$ is the probability density of arriving at the "position" $\delta$ in a "time" $S$, starting from $\delta_0$ at time $S_0 = 0$, through trajectories that never exceeded $\delta$. Observe that the final point $\delta$ ranges over $-\infty < \delta < +\infty$. For later use, we find useful to write explicitly that $\Pi_\epsilon$ depends also on the temporal discretization step $\epsilon$. We are finally interested in its continuum limit, $\Pi_{\epsilon\to 0}$, and we will see in due course that taking the limit $\epsilon \to 0$ of $\Pi_\epsilon$ is non-trivial.

The usefulness of $\Pi_\epsilon$ is that it allows us to compute the first-crossing rate from first principles, without the need of postulating the existence of an absorbing barrier. Simply, the quantity

$$\int_{-\infty}^{\delta} d\delta \Pi_\epsilon(\delta_0; \delta; S)$$

(41)

gives the probability that at time $S$ a trajectory always stayed in the region $\delta < \delta_c$, for all times smaller than $S$. The rate of change of this quantity is therefore equal to minus the rate at which trajectories cross for the first time the barrier, so the first-crossing rate is

$$F(S) = -\int_{-\infty}^{\delta} d\delta \delta_c \Pi_\epsilon(\delta_0; \delta; S)$$

(42)

(where $\delta_c \equiv \partial/\partial S$), just as in eq. (39). The halo mass function is then obtained from this first-crossing rate using eqs. (1) and (34). Observe that no reference to a hypothetical “absorbing barrier” is made in this formalism. We will discuss below how, and under what conditions, an effective absorbing barrier emerges from this microscopic approach.

To express $\Pi_{\epsilon\to 0}(\delta_0; \delta; S)$, in terms of the two-point correlator of the theory we use the integral representation of the Dirac delta

$$\delta_D(x) = \int_{-\infty}^{\infty} \frac{d\lambda}{2\pi} e^{i\lambda x},$$

(43)

and we write eq. (39) as

$$W(\delta_0; \delta_1, \ldots, \delta_n; S_n) = \int_0^{\delta_1} \frac{d\lambda_1}{2\pi} \ldots \int_0^{\delta_n} \frac{d\lambda_n}{2\pi} e^{\sum_1^n \lambda_i (\delta(S_i) - \delta_i^{(0)})},$$

(44)

Observe that the dependence on $\delta_0$ here is hidden in the correlators of $\delta$, e.g. $\langle \delta^2(S = 0) \rangle = \delta_0^2$. It is convenient to set for simplicity $\delta_0 = 0$ in the intermediate computations, and it will be easy to restore it in the final results. For gaussian fluctuations,

$$e^{\sum_1^n \lambda_i (\delta(S_i) - \langle \delta(S_i) \rangle)},$$

(45)
as can be checked immediately by performing the Taylor expansion of the exponential on the left-hand side, and using the fact that, for gaussian fluctuations, the generic correlator factorizes into sum of products of two-points correlators. This gives

\begin{equation}
W(\delta_0; \delta_1, \ldots, \delta_n; S_n) = \int D\lambda e^{\sum_{i=1}^n \lambda_i \delta_i - \sum_{i,j=1}^n \lambda_i \lambda_j \langle \delta_i \delta_j \rangle_c},
\end{equation}

where

\begin{equation}
\int D\lambda \equiv \int_{-\infty}^{\infty} \frac{d\lambda_1}{2\pi} \cdots \frac{d\lambda_n}{2\pi},
\end{equation}

and \( \delta_i \equiv \delta(S_i) \). Then

\begin{equation}
\Pi_c(\delta_0; \delta_i; S_n) = \int_{-\infty}^{\delta_0} d\delta_1 \cdots d\delta_{n-1} \int D\lambda \exp \left\{ i \sum_{i=1}^n \lambda_i \delta_i - \frac{1}{2} \sum_{i,j=1}^n \lambda_i \lambda_j \langle \delta_i \delta_j \rangle_c \right\}. \tag{48}
\end{equation}

### 3.2. Gaussian fluctuations with sharp k-space filter

As we have seen in Sect. 2 the computation of the halo mass function in the excursion set formalism with sharp k-space filter can be reduced to a Langevin equation with a Dirac-delta noise. Therefore, we now study the case in which \( \delta \) has gaussian statistics (so only the two-point connected function is non-vanishing) and obeys the Langevin equation \( \langle \delta \rangle = \eta(S) \) whose correlator is a Dirac delta, eq. (13). Using as initial condition \( \delta_0 = 0 \), eq. (13) integrates to

\begin{equation}
\delta(S) = \int_0^S dS' \eta(S'),
\end{equation}

so the 2-point correlator is given by

\begin{equation}
\langle \delta(S) \delta(S') \rangle_c = \int_0^S dS \int_0^{S'} dS'' \langle \eta(S) \eta(S') \rangle \equiv \min(S, S') = \epsilon \min(i, j) \equiv \epsilon A_{ij}.
\end{equation}

Denoting by \( W^{gm} \) the value of \( W \) when \( \delta \) is a gaussian variable and performs a markovian random walk with respect to the smoothing scale, i.e. satisfies eqs. (18) and (19), we get

\begin{equation}
W^{gm}(\delta_0; \delta_1, \ldots, \delta_n; S_n) = \int_{-\infty}^{S_n} \frac{d\lambda_1}{2\pi} \cdots \frac{d\lambda_n}{2\pi} \times \exp \left\{ i \sum_{i=1}^n \lambda_i \delta_i - \frac{1}{2} \sum_{i,j=1}^n A_{ij} \lambda_i \lambda_j \right\} = \frac{1}{(2\pi e)^{n/2} \det(A)^{1/2}} \exp \left\{ -\frac{1}{2e} \sum_{i,j=1}^n \delta_i \langle A^{-1} \rangle_{ij} \delta_j \right\}. \tag{51}
\end{equation}

Given that \( A_{ij} = \min(i, j) \), we can verify that \( A^{-1} \) is as follows: \( (A^{-1})_{ii} = 2 \) for \( i = 1, \ldots, n-1 \), \( (A^{-1})_{0n} = 1 \), and \( (A^{-1})_{n0} = (A^{-1})_{n1} = -1 \) for \( i = 1, \ldots, n-1 \), while all other matrix elements are zero. Furthermore, \( \det A = 1 \). As a result, we get

\begin{equation}
W^{gm}(\delta_0 = 0; \delta_1, \ldots, \delta_n; S_n) = \frac{1}{(2\pi e)^{n/2}} \times \exp \left\{ -\frac{1}{2e} \left[ \delta_n^2 + \frac{n-1}{2} \sum_{i=1}^n \delta_i \delta_{i+1} \right] \right\}. \tag{52}
\end{equation}

This expression takes a more familiar form using the identity \( \delta_i \delta_{i+1} = (\delta_{i-1} - \delta_i)^2 + (\delta_{i+1} - \delta_i)^2 \), together with \( \sum_{i=1}^{n-1} \delta_{i-1} - \delta_i \equiv 0 \). Recall also that eq. (51) assumed as initial condition \( \delta_0 = 0 \). The result for \( \delta_0 \) generic is simply obtained by replacing \( \delta_i \rightarrow \delta_i - \delta_0 \) for all \( i > 0 \). Then, for \( i > 0 \) the terms \( (\delta_{i+1} - \delta_i)^2 \) are unaffected, while in the last term of the sum \( \delta_i^2 \rightarrow \delta_i^2 - \delta_0^2 \). Thus, for \( \delta_0 \) arbitrary, we get

\begin{equation}
W^{gm}(\delta_0; \delta_1, \ldots, \delta_n; S_n) = \frac{1}{(2\pi e)^{n/2}} \exp \left\{ -\frac{1}{2e} \sum_{i=0}^{n-1} \delta_{i+1} - \delta_i \right\} \tag{53}
\end{equation}

Observe that \( W^{gm}(\delta_0; \delta_1, \ldots, \delta_n; S_n) d\delta_1 \cdots d\delta_{n-1} \) is just the Wiener measure (see e.g. chapter 1 of [Chiashian & Demichev (2001)]). From eq. (53) we see that

\begin{equation}
W^{gm}(\delta_0; \delta_1, \ldots, \delta_n; S_n) = \Psi_c(\delta_n - \delta_{n-1}) W^{gm}(\delta_0; \delta_1, \ldots, \delta_{n-1}; S_{n-1}), \tag{54}
\end{equation}

where

\begin{equation}
\Psi_c(\Delta \delta) = \frac{1}{(2\pi e)^{1/2}} \exp \left\{ -\frac{(\Delta \delta)^2}{2e} \right\}. \tag{55}
\end{equation}

Equation (54) expresses the fact that the evolution determined by eqs. (18) and (19) is a markovian process, i.e. the probability of jumping from the position \( \delta_{n-1} \) at time \( S_{n-1} \) to the position \( \delta_n \) at time \( S_n \) depends only on the values of \( \delta_n - \delta_{n-1} \equiv \Delta \delta \) and on \( S_n - S_{n-1} \equiv \epsilon \), and not on the past history of the trajectory. Integrating eq. (54) over \( \delta_1, \ldots, \delta_{n-1} \) from \( -\infty \) to \( \delta_i \) we get the important relation

\begin{equation}
\Pi^{gm}_c(\delta_0; \delta_i; S_n) = \int_{-\infty}^{\delta_i} d\delta_{n-1} \Psi_c(\delta_n - \delta_{n-1}) \Pi^{gm}_c(\delta_0; \delta_{n-1}; S_{n-1}), \tag{56}
\end{equation}

which generalizes the well-known Chapman-Kolmogorov equation to the case of finite \( \delta_c \).

### 4. Derivation of excursion set formalism for gaussian fluctuations and sharp k-space filter

We now want to derive, from our “microscopic” approach, the excursion set formalism of [Bond et al. (1991)]. As we have seen in Section 2 the result of Bond et al. holds for gaussian fluctuations and sharp k-space filter, working directly in the continuum limit, and reads

\begin{equation}
\Pi^{gm}_c(\delta_0; \delta; S) = \frac{1}{\sqrt{2\pi S}} \left[ e^{-\delta^2/2S} - e^{-(\delta - \delta_0)^2/2S} \right]. \tag{57}
\end{equation}

We want to prove eq. (57) using our definition of \( \Pi_c \) as a path integral over all trajectories that never exceed \( \delta_c \). Beside being a starting point for the generalization to arbitrary filter functions and to non-Gaussian theories, the derivation of the excursion set theory from first principles has an intrinsic interest. In fact, in [Bond et al. (1991)] this result is obtained by postulating that the distribution function obeys a FP equation with an “absorbing barrier” boundary condition \( \Pi(\delta_0; \delta; S)|_{\delta = \delta_0} = 0 \). While the fact that \( \Pi_{\epsilon=0} \) obeys a FP equation follows from eq. (13), the absorbing barrier boundary condition is rather imposed by hand. As we already mentioned, in the literature on stochastic processes it is known that, in the general case, the distribution function \( \Pi(\delta_0; \delta; S) \) does not satisfy any simple boundary condition (van Kampen & Opopenheim 1972; Knese 1986). It is therefore interesting to see how, in the gaussian case with sharp k-filter, an absorbing barrier boundary condition effectively emerges from our microscopic approach.
We first show that in the continuum limit we recover eq. (57). Then, we examine the finite-ε corrections. As it turns out, these corrections have a non-trivial structure which is quite interesting in itself. Our main reason for discussing them in detail, however, is that they play a crucial role in the extension of our formalism to a generic filter function and to non-Gaussian fluctuations.

4.1. The continuum limit

To compute $\Pi_{\epsilon}^{gm}$ by performing directly the integrals over $\delta_1, \ldots, \delta_{n-1}$ in eq. (40), and then taking the limit $\epsilon \to 0$ is very difficult, since the integrals in eq. (40) run only up to $\delta$, and already the inner integral gives an error function whose argument involves the next integration variable.

A better strategy is to make use of eq. (56). This relation expresses the fact that, for gaussian fluctuations and sharp $k$-space filter, the underlying stochastic process is markovian.

We change notation, denoting $\delta_n = \delta$, $\delta_{n-\delta_{n-1}} = \Delta \delta$, and $\delta_{n-1} = \delta_n$, so $S_n = S + \epsilon$. For fixed $\delta$, we have $d\delta_{n-1} = -d\Delta \delta$, and eq. (56) becomes

$$\Pi_{\epsilon}^{gm}(\delta_0; \delta; S + \epsilon) = \int_{\delta-\delta_c}^{\infty} d(\Delta \delta) \Psi_{\epsilon}(\Delta \delta) \Pi_{\epsilon}^{gm}(\delta_0; \delta - \Delta \delta; S).$$

In the limit $\epsilon \to 0$ we have $\Psi_{\epsilon}(\Delta \delta) \to \delta_D(\Delta \delta)$, so to zeroth order in $\epsilon$ eq. (58) gives

$$\Pi_{\epsilon}^{gm}(\delta_0; \delta; S) = \int_{\delta-\delta_c}^{\infty} d(\Delta \delta) \delta_D(\Delta \delta) \Pi_{\epsilon}^{gm}(\delta_0; \delta - \Delta \delta; S).$$

If $\delta - \delta_c < 0$, the integral includes the support of the Dirac delta, and we just get the trivial identity that $\Pi_{\epsilon}^{gm}(\delta_0; \delta; S)$ is equal to itself. However, if $\delta - \delta_c > 0$, the right-hand side vanishes and we get $\Pi_{\epsilon}^{gm}(\delta_0; \delta; S) = 0$. The same holds if $\delta = \delta_c$. In this case only one half of the support of $\Psi_{\epsilon}$ is inside the integration region, so we get $\Pi_{\epsilon}^{gm}(\delta_0; \delta; S) = (1/2) \Pi_{\epsilon}^{gm}(\delta_0; \delta; S)$, which again implies $\Pi_{\epsilon}^{gm}(\delta_0; \delta; S) = 0$. Therefore we find that

$$\Pi_{\epsilon}^{gm}(\delta_0; \delta; S) = 0 \quad \text{if} \quad \delta \geq \delta_c.$$  

This is not in contrast with the fact that $\Pi_{\epsilon}^{gm}(\delta_0; \delta; S)$ is the integral of the positive definite quantity $W_{\epsilon}^{gm}$. For finite $\epsilon$, $\Pi_{\epsilon}^{gm}(\delta_0; \delta; S)$ is indeed strictly positive but, when $\delta \geq \delta_c$, it vanishes in the limit $\epsilon \to 0$.

Consider now eq. (58) when $\delta < \delta_c$. In this case the zeroth-order term gives a trivial identity. Pursuing the expansion to higher orders in $\epsilon$ we have to take into account that in $\Pi_{\epsilon}^{gm}(\delta_0; \delta; S + \epsilon)$ there is both an explicit dependence on $\epsilon$ through the argument $S + \epsilon$, and a dependence implicit in the subscript $\epsilon$. We begin by expanding the left-hand side as

$$\Pi_{\epsilon}^{gm}(\delta_0; \delta; S + \epsilon) = \Pi_{\epsilon}^{gm}(\delta_0; \delta; S) + \frac{\partial \Pi_{\epsilon}^{gm}(\delta_0; \delta; S)}{\partial S} \epsilon + \frac{\epsilon^2}{2} \frac{\partial^2 \Pi_{\epsilon}^{gm}(\delta_0; \delta; S)}{\partial S^2} + \ldots,$$

without expanding for the moment the dependence on the index $\epsilon$. On the right-hand side of eq. (58), we expand $\Pi_{\epsilon}^{gm}(\delta_0; \delta - \Delta \delta; S)$ in powers of $\Delta \delta$,

$$\int_{\delta-\Delta \delta}^{\infty} d(\Delta \delta) \Psi_{\epsilon}(\Delta \delta) \Pi_{\epsilon}^{gm}(\delta_0; \delta - \Delta \delta; S)$$

$$= \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \frac{\partial^n \Pi_{\epsilon}^{gm}(\delta_0; \delta; S)}{\partial S^n} \int_{\delta-\Delta \delta}^{\infty} d(\Delta \delta) (\Delta \delta)^n \Psi_{\epsilon}(\Delta \delta).$$

Using eq. (53) we see that

$$\int_{\delta-\Delta \delta}^{\infty} d(\Delta \delta) (\Delta \delta)^n \Psi_{\epsilon}(\Delta \delta) = \frac{(2 \epsilon)^{n/2}}{\sqrt{\pi}} \int_{-(\delta-\Delta \delta)/\sqrt{2 \epsilon}}^{\infty} dy y^n e^{-y^2}.$$

If $\delta$ is strictly smaller than $\delta_c$ and $\delta_c - \delta$ is finite (more precisely, if it does not scale with $\sqrt{\epsilon}$), the lower limit in the integration goes to $-\infty$ as $\epsilon \to 0^+$, and

$$\int_{-(\delta-\Delta \delta)/\sqrt{2 \epsilon}}^{\infty} dy y^n e^{-y^2} = \int_{-(\delta-\Delta \delta)/\sqrt{2 \epsilon}}^{\infty} dy y^n e^{-y^2} + O \left( e^{-(\delta-\Delta \delta)^2/(2 \epsilon)} \right)$$

$$= \frac{1 + (-1)^n}{2} \sqrt{\frac{\pi}{2 \epsilon^{n/2}}} (n-1)!! + O \left( e^{-(\delta-\Delta \delta)^2/(2 \epsilon)} \right).$$

The residue, being exponentially small in $\epsilon$, is beyond any order in the expansion in powers of $\epsilon$, and we can neglect it, so

$$\int_{\delta-\Delta \delta}^{\infty} d(\Delta \delta) (\Delta \delta)^n \Psi_{\epsilon}(\Delta \delta) \to e^{\epsilon^n/(n-1)!},$$

if $n$ even, and vanishes if $n$ is odd. Thus, eq. (58) gives

$$\Pi_{\epsilon}^{gm}(\delta_0; \delta; S) + \epsilon \frac{\partial \Pi_{\epsilon}^{gm}(\delta_0; \delta; S)}{\partial S} + \frac{\epsilon^2}{2} \frac{\partial^2 \Pi_{\epsilon}^{gm}(\delta_0; \delta; S)}{\partial S^2} + \ldots$$

$$= \Pi_{\epsilon}^{gm}(\delta_0; \delta; S) + \frac{\epsilon}{2} \frac{\partial^2 \Pi_{\epsilon}^{gm}(\delta_0; \delta; S)}{\partial S^2} + \frac{\epsilon^2}{8} \frac{\partial^4 \Pi_{\epsilon}^{gm}(\delta_0; \delta; S)}{\partial S^4} + \ldots,$$

From this structure it is clear that, when $\delta - \delta_c$ is finite, the dependence on the index $\epsilon$ in $\Pi_{\epsilon}^{gm}$ can be expanded in integer powers of $\epsilon$,

$$\Pi_{\epsilon}^{gm}(\delta_0; \delta; S) = \Pi_{\epsilon=0}^{gm}(\delta_0; \delta; S) + \epsilon \Pi_{\epsilon=1}^{gm}(\delta_0; \delta; S) + \epsilon^2 \Pi_{\epsilon=2}^{gm}(\delta_0; \delta; S) + \ldots,$$

where $\Pi_{\epsilon=1}^{gm}$, $\Pi_{\epsilon=2}^{gm}$, etc. are functions independent of $\epsilon$. We can now collect the terms with the same power of $\epsilon$ in the expansion of eq. (60). To order $\epsilon$ we find

$$\frac{\partial \Pi_{\epsilon=0}^{gm}(\delta_0; \delta; S)}{\partial S} - \frac{1}{2} \frac{\partial^2 \Pi_{\epsilon=0}^{gm}(\delta_0; \delta; S)}{\partial S^2} = 0.$$  

Putting together this result with eq. (60), we therefore end up with a FP equation with the boundary condition $\Pi_{\epsilon=0}^{gm}(\delta_0; \delta = \delta_c; S) = 0$, and therefore we recover eq. (57). We have therefore succeeded in deriving the excursion set formalism from our microscopic approach. Observe that the boundary condition $\Pi_{\epsilon=0}^{gm}(\delta_0; \delta = \delta_c; S) = 0$ emerges only when we take the continuum limit, and does not hold for finite $\epsilon$.

4.2. Finite-ε corrections

In Section 5.3 we will find that the halo mass function gets contributions, that we will call “non-markovian”, that depend on how $\Pi_{\epsilon}^{gm}(\delta_0; \delta; S)$ approaches zero when $\epsilon \to 0$. It is therefore of great importance for us to understand the finite-ε corrections to the result obtained in the continuum limit. The issue is quite technical and we summarize here the main results. Details are given in appendix A.

As long as $\delta - \delta_c$ is finite and strictly positive, we have seen that the expansion (60) applies, so the first correction to the continuum result is $O(\epsilon)$ and is given by $\Pi_{\epsilon=1}^{gm}$. Collecting the next-to-leading terms in eq. (60), we find that $\Pi_{\epsilon=1}^{gm}$ satisfies a FP equation with the second time derivative of $\Pi_{\epsilon=0}^{gm}$ as a source term,

$$\frac{\partial \Pi_{\epsilon=1}^{gm}(\delta_0; \delta; S)}{\partial S} - \frac{1}{2} \frac{\partial^2 \Pi_{\epsilon=1}^{gm}(\delta_0; \delta; S)}{\partial S^2} = \frac{1}{4} \frac{\partial^2 \Pi_{\epsilon=0}^{gm}(\delta_0; \delta; S)}{\partial S^2}.$$  

In this section we always assume that $\delta_0$ is strictly smaller than $\delta_c$. The case $\delta_0 = \delta_c$ is important when we study the non-markovian corrections, and will be examined in due course.
In the above derivation, a crucial point was that we could extend to $-\infty$ the lower integration limit in eq. (63). This is correct if we take the limit $\epsilon \to 0^+$ with $\delta_t - \delta$ fixed and positive. The situation changes at $\delta = \delta_t$; since in this case the lower limit of the integral is zero, rather than $-\infty$. In this case

$$\int_0^\infty d(\Delta \delta)(\Delta \delta) \Psi_c(\Delta \delta) = \left(\frac{\epsilon}{2\pi}\right)^{1/2},$$  

(70)

(while the same integral computed from $-\infty$ to $+\infty$ obviously vanished), so we now have a term $O(\sqrt{\epsilon})$ on the right-hand side of eq. (62). Furthermore,

$$\int_0^\infty d(\Delta \delta) \Psi_c(\Delta \delta) = \frac{1}{2},$$  

(71)

so the expansion of eq. (58) now gives

$$\Pi^m_\epsilon(\delta_0; \delta_t; S) = \frac{1}{2} \Pi^m_\epsilon(\delta_0; \delta_t; S) - \left(\frac{\epsilon}{2\pi}\right)^{1/2} \frac{\partial \Pi^m_\epsilon(\delta_0; \delta_t; S)}{\partial \delta} \bigg|_{\delta=\delta_t} + \ldots.$$  

(72)

This indicates that $\Pi^m_\epsilon(\delta_0; \delta_t; S) = O(1/2)$, rather than $O(\epsilon)$. However, eq. (72) is not a good starting point for a quantitative evaluation of $\Pi^m_\epsilon(\delta_0; \delta_t; S)$ since, as we show in appendix A, the expansion in derivatives becomes singular in $\delta = \delta_t$, and all terms denoted by the dots in eq. (72) finally give contributions of the same order in $\epsilon$. A better procedure is the following. First, observe that the correction is determined by the lower limit of the integrals, $(\delta_t - \delta)/\sqrt{2\epsilon}$. The transition from the behavior $O(\epsilon)$ valid for $\delta_t - \delta$ fixed and positive, to the behavior $O(\epsilon^{1/2})$ valid at $\delta = \delta_t$, takes place in a “boundary layer”, consisting of the region where $\delta_t - \delta$ is positive and $O(\epsilon^{1/2})$, and the lower limit of the integral is $O(1)$. This is a situation that often appears in stochastic processes near a boundary, or in fluid dynamics, and can be treated by a standard technique (see e.g. [Knessl 1986], where a very similar situation is discussed in terms of the means first passage time, rather than in terms of the distribution function $\Pi^m_\epsilon$). Namely, we introduce a “stretched variable” $\eta$ (not to be confused, of course, with the noise $\eta(t)$ of eq. (13))

$$\eta = \frac{\delta_t - \delta}{\sqrt{2\epsilon}},$$  

(73)

which even as $\epsilon \to 0^+$ is at most of order one inside the boundary layer, and we write $\Pi^m_\epsilon(\delta_0; \delta_t; S)$ in the form

$$\Pi^m_\epsilon(\delta_0; \delta_t; S) = C(\delta_0; \delta_0; S) u(\eta),$$  

(74)

where $C(\delta_0; \delta_0; S)$ is a smooth function, while the fast variation inside the boundary layer is contained in $u(\eta)$. By definition, we choose $u(\eta)$ such that $\lim_{\eta \to -\infty} u(\eta) = 1$, so $C_\epsilon$ is just the solution for $\Pi^m_\epsilon$ valid when $\delta_t - \delta$ is finite and positive, i.e. $C_\epsilon$ is given by eq. (67). Writing $\delta = \delta_t - \eta \sqrt{2\epsilon}$ (and setting for notational simplicity $\delta_t = 0$) we have

$$C_\epsilon(\delta_0 = 0; \delta; S) = \frac{1}{\sqrt{2\pi S}}$$

$$\times \left[ \exp\left\{ -\frac{1}{2S} \left( \delta - \eta \sqrt{2\epsilon} \right)^2 \right\} - \exp\left\{ -\frac{1}{2S} \left( \delta_t + \eta \sqrt{2\epsilon} \right)^2 \right\} \right],$$  

(75)

plus corrections $O(\epsilon)$. Since $C_\epsilon$ by definition is smooth everywhere, we can use eq. (75) also inside the boundary layer. In this case $\eta$ is at most $O(1)$, and we can expand the exponentials in eq. (75) in powers of $\sqrt{\epsilon}$. In the limit $\epsilon \to 0^+$,

$$C_\epsilon(\delta_0 = 0; \delta; S) = \sqrt{\frac{2\eta}{\sqrt{\epsilon}}} \frac{\delta_t - \delta}{S^{1/2}} e^{-\delta^2/(2S)} + O(\epsilon).$$  

(76)

Plugging this result in eq. (74) and sending $\delta \to \delta_t$ we find

$$\Pi^m_\epsilon(\delta_0; \delta_t; S) = \sqrt{\frac{\epsilon}{\sqrt{2\pi}}} \frac{\delta_t - \delta}{S^{1/2}} e^{-\delta^2/(2S)} + O(\epsilon),$$  

(77)

where

$$\gamma = \frac{2}{\sqrt{\pi}} \lim_{\eta \to 0} \eta u(\eta).$$  

(78)

In appendix A we show that $\gamma = 1/\sqrt{\pi}$, so

$$\Pi^m_\epsilon(\delta_0; \delta_t; S) = \sqrt{\frac{\epsilon}{\sqrt{2\pi}}} \frac{\delta_t - \delta}{S^{1/2}} e^{-\delta^2/(2S)} + O(\epsilon).$$  

(79)

Similarly, for $\delta_n < \delta_t$,

$$\Pi^m_\epsilon(\delta_0; \delta_n; S) = \sqrt{\frac{\epsilon}{\sqrt{2\pi}}} \frac{\delta_n - \delta_t}{S^{1/2}} e^{-\delta_n^2/(2S)} + O(\epsilon).$$  

(80)

Observe that at the numerator of eqs. (79) and (80) always enters the absolute value of the difference of the first two arguments of $\Pi^m_\epsilon$, i.e. $\delta_t - \delta_n$ in eq. (79) and $\delta_t - \delta_n$ in eq. (80), as it is also obvious from the fact that $\Pi^m_\epsilon$ is definitely positive. Equations (79) and (80) will be important when we compute the non-markovian corrections, in Section 5.3. To conclude this section, it is interesting to discuss the behavior of $\Pi^m_\epsilon(\delta_0; \delta_t; S)$ for $\delta$ larger than $\delta_t$, with $\delta_t - \delta$ finite (and, as always in this section, $\delta_t < \delta_n$). In this case the lower integration limit in eq. (63) goes to $+\infty$ as $\epsilon \to 0^+$ and

$$\Pi^m_\epsilon(\delta_0; \delta_t; S) \sim \frac{1}{\sqrt{2\pi \epsilon}} \exp\left\{ -\left( \delta_t - \delta \right)^2/(2\epsilon) \right\}.$$  

(81)

This function is zero to all orders in a Taylor expansion around $\epsilon = 0^+$.  

5. EXTENSION OF EXCITATION SET THEORY TO GENERIC FILTER

We next consider the computation of the distribution function $\Pi_S$, still restricting for the moment to gaussian fluctuations, but using a generic filter function. In this case the natural time variable is the variance $S$ computed with the chosen filter function, so in the following $S$ denotes the variance computed with the filter function that one is considering. Again we discretize it in equally spaced steps, $S_k = k\epsilon$, with $S_n = n\epsilon \equiv S$, and a trajectory is defined by the collection of values $\{\delta_1, \ldots, \delta_n\}$, such that $\delta(S_k) = \delta_k$.

The distribution function for gaussian fluctuations and arbitrary filter function is given by eq. (48). As we saw in the previous section, in the markovian case $\Pi_\epsilon$ satisfies a local differential equation, namely the Fokker-Planck equation. It is instructive to understand that, for a generic filter, it is no longer possible to write a local diffusion equation for $\Pi_S(\delta_0; \delta_t; S_n)$. This will immediately make it clear that the problem is now significantly more complex. Indeed, by taking the derivative with respect to $S_n$ of both sides of eq. (48), we get

$$\frac{\partial}{\partial S_n} \Pi_S(\delta_0; \delta_t; S_n) = \frac{1}{2} \sum_{k=1}^{n} \frac{\partial (\delta_k - \delta_t)}{\partial S_n}$$

$$\times \int_{-\infty}^{\delta_k} d\delta_{n-1} \ldots d\delta_0 \partial_\delta \partial_\delta W(\delta_0; \delta_1, \ldots, \delta_n; S_n),$$  

(82)
where \( \partial_k \equiv \partial / \partial \delta_k \), and we used the fact that, acting on
\( \exp(\sum_{\mu=1}^n \lambda_k \delta_k) \), \( \partial_k \) gives \( i \lambda_k \). Therefore, the term
with \( k = l = n \) from the rest, and observing that \( \langle \delta(S_s) \delta(S_{s'}) \rangle \),
depends on \( S_s \) only if at least one of the two indices \( k \) or \( l \) is
equal to \( n \), we get
\[
\frac{1}{2} \frac{\partial^2}{\partial \delta_n^2} \Pi_c(\delta_0; \delta_n; S_n) + \sum_{k=1}^{n-1} \frac{\partial (\delta_0 \delta_n)}{\partial S_n} \delta_n \int_{-\infty}^{\delta_n} d\delta_1 \ldots d\delta_{n-1} \partial_k W(\delta_0; \delta_1, \ldots, \delta_n; S_n).
\]

If the upper limit of the integrals were \( +\infty \), rather than \( \delta_n \),
the term proportional to \( \partial_k W \) with \( k < n \) would give zero, since it
is a total derivative with respect to one of the integration variables
\( d\delta_1, \ldots, d\delta_{n-1} \), and \( W \) vanishes exponentially when any
of its arguments \( \delta_k \) goes to \( \pm \infty \). Thus, one would remain with
a Fokker-Planck equation. However, when the upper limit \( \delta_n \)
is finite, the terms proportional to \( \partial_k W \) with \( k < n \) give in
general non-vanishing boundary term. Actually, for a sharp
\( k \)-space filter, we found that \( \langle \delta(S_s) \delta(S_{s'}) \rangle \equiv \min(S_s, S_{s'}) = S_s \),
which is independent of \( S_{s'} \) for \( k < n \). Therefore \( \partial (\delta_0 \delta_n)/\partial S_n = 0 \),
and the term in the second line of eq. (83) vanishes. This is
another way of showing that, in the continuum limit, for sharp
\( k \)-space filter the probability distribution satisfies a FP
equation, as we already found in Section 4.1.

For a generic form of the two-point correlator, the term
in the second line of eq. (83) is non-vanishing, and in general it
is very complicated. Furthermore, in the continuum limit the
sum over \( k \) in eq. (83) becomes an integral over an
intermediate time variable \( S_k \), so this term is non-local with respect to
"time" \( S \). Thus, we can no longer determine \( \Pi_c(\delta_0; \delta_n; S_n) \)
by solving a local differential equation, as we did in the markovian
case. Once again, this shows that the common procedure
of using the distribution function computed with the \( k \)-space
filter, and substituting in it the relation between mass and
smoothing radius of the tophat filter in coordinate space, is not
justified. What we need is to formulate the problem in such a
way that it becomes possible to treat the non-markovian terms
as perturbations, which is not at all evident from eq. (83).

In this section we develop such a perturbative scheme. We
illustrate the computation of \( \Pi_c(\delta_0; \delta_n; S_n) \) using a tophat
filter in coordinate space, which is finally the most interesting
case since we can associate to it a well defined mass, but the
 technique that we develop can be used more generally.

In Section 5.1 we study the two-point correlator with tophat
filter in coordinate space and we show that it can be split into
two parts, which we call markovian and non-markovian,
respectively. In Section 5.2 we compute the contribution of
the markovian term to the halo mass function, while in Section
5.3 we develop the formalism for computing perturbatively
the contribution of the non-markovian term.

5.1. The two-point correlator with tophat filter in coordinate space

We first study the correlator \( \langle \delta(R_1) \delta(R_2) \rangle \) with a tophat
filter in coordinate space. We use eq. (8) with \( x = 0 \). The two-point
 correlator of the non-smoothed density contrast is given in
eq. (11). We write the power spectrum after recombination
as \( P(k)T^2(k) \), where \( P(k) \) is the primordial power spectrum
and \( T(k) \) is the transfer function, so for the smoothed density
contrast we get
\[
\langle \delta(R_1) \delta(R_2) \rangle = \frac{1}{2\pi^2} \int_0^\infty dk k^2 P(k) T^2(k) \tilde{W}(k(R_1) \tilde{W}^*(k(R_2)).
\]

When \( R_1 = R_2 = R \), this reduces to \( S(R) \). We consider a
primordial spectrum \( P(k) = A k^n \), processed into the post-
recombination spectrum by the transfer function \( T(k) \) as in
Sugiyama (1995), in a concordance \( \Lambda \)CDM model with a
power spectrum normalization \( \sigma_8 = 0.8 \) and \( h = 0.7 \), \( \Omega_M = 1 - \Omega_L = 0.28 \), \( \Omega_B = 0.046 \) and \( n_s = 0.96 \), consistent with the
WMAP 5-years data release.

We first study \( S(R) \). We compute the integral in eq. (84)
numerically, for different values of \( R \), both with the sharp \( k \)-space
filter (7) with \( k_f = 1/R \), and with the tophat filter in
coordinate \( x \)-space, whose Fourier transform is
\[
\tilde{W}_{\text{sharp-}}(k(x)) = \frac{1}{(kR)^3} \sin(kR) - kR \cos(kR) .
\]

For both filters, the constant \( A \) in \( P(k) \) is fixed so that \( S = \sigma_8 \)
when \( R = (8/h) \) Mpc. The result is shown in Fig. 3.

We consider next the correlator (84) with the tophat filter
in coordinate space. We compute the integral in eq. (84)
numerically, holding \( R_2 \) fixed and varying \( R_1 \). The result is shown in Fig. 4. The solid line is the function \( S(R_1) \), already shown in Fig. 3. The dashed line is \( \langle \delta(R_1) \delta(R_2) \rangle \) with \( R_2 = 1 \) Mpc/h,
as a function of \( R_1 \), while the dotted line is \( \langle \delta(R_1) \delta(R_2) \rangle \) with
\( R_2 = 5 \) Mpc/h, again as a function of \( R_1 \). We see that, as long
as \( \Delta R < R \), the two-point correlator is approximately constant
and equal to \( S(R_2) \), while for \( R_1 > R_2 \) the correlator
is approximately equal to \( S(R_1) \). In other words,
\[
\langle \delta(R_1) \delta(R_2) \rangle \simeq \min(S(R_1), S(R_2)).
\]

In Fig. 5 we compare \( \langle \delta(R_1) \delta(R_2) \rangle \) (blue solid line) and
\( \min(S(R_1), S(R_2)) \) (violet dashed line). This result suggests to
define a function \( C(R_1, R_2) \) from
\[
\langle \delta(R_1) \delta(R_2) \rangle = \min(S(R_1), S(R_2)) + C(R_1, R_2).
\]

As we see from Fig. 3, the function \( S(R) \) can be inverted to
give \( R = R(S) \), so \( R_1 = R(S_1) \) and \( R_2 = R(S_2) \). We define
\[
\Delta(S_1, S_2) = C(R(S_1), R(S_2)),
\]

and we can write
\[
\langle \delta_i \delta_j \rangle = \min(S_i, S_j) + \Delta(S_i, S_j).
\]
We see that eq. (90) provides an excellent analytical approximation to \(\Delta(S_i,S_j)\), so it is sufficient to study it for \(S_i \leq S_j\). We also use the notation \(\Delta_{ij} = \Delta(S_i,S_j)\). Since, by definition, \(\langle \delta_i \rangle = 1\), we see from eq. (89) that \(\Delta(S_i,S_j)\) vanishes when \(S_i = S_j\). Furthermore, at \(S_i = 0\), \(\delta_i = \delta_0\) is the same constant for all trajectories, so \(\langle \delta_i \delta_j \rangle = \delta_0^2\langle \delta_i \rangle = 0\), and therefore \(\Delta(S_i,S_j)\) vanishes when \(S_i = 0\).

In Fig. 5 we plot \(\Delta(S_i,S_j)\) for \(S_j\) fixed, as a function of \(S_i\), with \(0 \leq S_i < S_j\), for our reference ΛCDM model (solid line). The dashed line in Fig. 6 is the approximation

\[
\Delta(S_i,S_j) \simeq \kappa \frac{S_i(S_j-S_i)}{S_j},
\]

with \(\kappa \approx 0.45\) (a more accurate value will be given below). We see that eq. (90) provides an excellent analytical approximation to \(\Delta(S_i,S_j)\).\(^9\)

\(^9\) Varying \(S_j\) we find that eq. (90) becomes exact (within our numerical

\[
\text{For } S_j \text{ fixed and } S_i \to 0, \text{ the correction } \Delta(S_i,S_j) \text{ is linear in } S_i, \text{ so more generally we can define } \kappa(S_j) \text{ from } \kappa(S_j) = \lim_{S_i \to 0} \Delta(S_i,S_j)/S_i, \text{ or equivalently,}
\]

\[
\kappa(R) = \lim_{R' \to -\infty} \frac{\langle \delta(R') \delta(R) \rangle}{\langle \delta^2(R) \rangle} - 1.
\]

In the ΛCDM model that we are using, our numerical results display a very weak linear dependence of \(\kappa\) on \(R\). Taking for instance the data in the range \(R \in [1, 10] \text{ Mpc}/h\), the result of the numerical evaluation of eq. (91) is very well fitted by

\[
\kappa(R) \approx 0.4592 - 0.0031 R,
\]

where \(R\) is measured in \(\text{Mpc}/h\).\(^10\)

5.2. Markovian term

Inserting eq. (89) into eq. (48) we get

\[
\Pi_n(\delta_0; \delta_i; S_n) = \int_{-\infty}^\delta d\delta_1 \ldots d\delta_{n-1} \int D\lambda \times \exp \left\{ \sum_{i=1}^n \lambda_i \delta_i - \frac{1}{2} \sum_{i,j=1}^n \left[ \min(S_i,S_j) + \Delta(S_i,S_j) \right]\lambda_i \lambda_j \right\}
\]

As we see from Fig. 5, eq. (89) gives a reasonable approximation to the exact correlator. This suggests to treat \(\Delta_{ij}\) as a perturbation, so we now expand in \(\Delta_{ij}\). The zeroth-order term is simply \(\Pi_n^{\text{gm}}(\delta_0; \delta_i; S_n)\), whose continuum limit is given in eq. (57). The corresponding first-crossing rate is

\[
\mathcal{F}^{\text{gm}} = - \int_{-\infty}^\delta d\delta \frac{\partial \Pi_n^{\text{gm}}}{\partial S} = \frac{1}{\sqrt{2\pi}} \delta_0 \frac{\delta_0}{S^{3/2}} e^{-\delta_0^2/(2S)}.
\]

\(^10\) The value of \(\kappa\) depends in principle on the cosmological model used, but this dependence is quite weak. For comparison, using a ΛCDM cosmological model with \(h = 0.7, \Omega_M = 1 - \Omega_{\Lambda} = 0.3, \sigma_8 = 0.93, \Omega_{\Lambda} h^2 = 0.022\) and \(n_s = 1\), consistent with the WMAP 1st year data release, gives \(\kappa(R) \approx 0.4562 - 0.0040 R\).
so the markovian term can be obtained by taking the excursion set result (57), which was computed with the sharp k-space filter, and replacing the variance computed with the sharp k-space filter with the variance computed with the filter of interest. This is the procedure that is normally used in the literature. From our vantage point, we now see that the corrections to this procedure are given by the non-markovian contributions, to which we now turn.

5.3. Non-markovian corrections

We now discuss the non-markovian corrections, to first order, using the analytical approximation (90) for $\Delta_{ij}$. From eq. (92), expanding to first order in $\Delta_{ij}$ and using $\lambda_i e^{\sum_{i,j} \lambda_i \delta_{ij} = -i \partial_i e^{\sum_{i,j} \lambda_i \delta_{ij}}}$, where $\partial_i = \partial/\partial \delta_i$, the first-order correction to $\Pi_\epsilon$ is

$$
\Pi^{\Delta_1}_\epsilon(\delta_0; \delta_n; S_n) \equiv \int_{-\infty}^{\delta_1} d\delta_1 \ldots d\delta_{n-1} \frac{1}{2} \sum_{i,j=1}^{n} \Delta_{ij} \partial_i \partial_j
$$

$$
\times \int \mathcal{D} \lambda \exp \left\{ i \sum_{i=1}^{n} \lambda_i \delta_i - \frac{1}{2} \sum_{i,j=1}^{n} \min(S_i, S_j) \lambda_i \lambda_j \right\} \ 
$$

$$
= \frac{1}{2} \sum_{i,j=1}^{n} \Delta_{ij} \int_{-\infty}^{\delta_1} d\delta_1 \ldots d\delta_{n-1} \partial_i \partial_j W^{gm}(\delta_0; \delta_1, \ldots, \delta_n; S_n).
$$

We rewrite the term $\Delta_{ij} \partial_i \partial_j$ separating explicitly the derivative $\partial_i \equiv \partial/\partial \delta_i$ from the derivatives $\partial_j$ with $j < i$, so (using $\Delta_{ij} = \Delta_{ji}$)

$$
\frac{1}{2} \sum_{i,j=1}^{n} \Delta_{ij} \partial_i \partial_j = \frac{1}{2} \Delta_{mm} \partial^2_n + \sum_{i=1}^{n-1} \Delta_{mn} \partial_n + \frac{1}{2} \sum_{i,j=1}^{n} \Delta_{ij} \partial_i \partial_j.
$$

Since $\Delta_{ij} = 0$ when $i = j$, the above equation simplifies to

$$
\frac{1}{2} \sum_{i,j=1}^{n} \Delta_{ij} \partial_i \partial_j = \sum_{i=1}^{n-1} \Delta_{mn} \partial_n + \frac{1}{2} \sum_{i,j=1}^{n} \Delta_{ij} \partial_i \partial_j.
$$

$$
\sum_{i,j} = \sum_{i<j} \sum_{i>j},
$$

(98)

When inserted into eq. (95) the term $\sum_{i<j} \Delta_{ij} \partial_i \partial_j$ brings a factor $\sum_j$ that, in the continuum limit, produces an integral over an intermediate time $S_i$. Because of this dependence on the past history, we call this the “memory term”. Similarly, the term $\sum_{i<j} \Delta_{ij} \partial_i \partial_j$ gives, in the continuum limit, a double integral over intermediate times $S_i$ and $S_j$, and we call it the “memory-of-memory” term. Thus,

$$
\Pi^{\Delta_1}_\epsilon = \Pi_{\epsilon}^{\text{mem}} + \Pi_{\epsilon}^{\text{mem-mem}},
$$

(99)

where

$$
\Pi_{\epsilon}^{\text{mem}}(\delta_0; \delta_n; S_n) = \sum_{i=1}^{n-1} \Delta_{mm} S_{i+1} - \frac{1}{2} \sum_{i,j=1}^{n} \Delta_{ij} W^{gm}(\delta_0; \delta_1, \ldots, \delta_n; S_n),
$$

(100)

and

$$
\Pi_{\epsilon}^{\text{mem-mem}}(\delta_0; \delta_n; S_n) = \sum_{i<j} \Delta_{ij} S_{i+1} - \frac{1}{2} \sum_{i,j=1}^{n} \Delta_{ij} W^{gm}(\delta_0; \delta_1, \ldots, \delta_n; S_n).
$$

If we expand to quadratic and higher orders in $\Delta_{ij}$, we get terms with a higher and higher number of summations (or, in the continuum limit, of integrations) over intermediate time variables.

To compute the memory term we integrate $\partial_i$ by parts,

$$
\int_{-\infty}^{\delta_1} d\delta_1 \ldots d\delta_{n-1} \partial_i W^{gm}(\delta_0; \delta_1, \ldots, \delta_n; S_n)
$$

$$
= \int_{-\infty}^{\delta_1} d\delta_1 \ldots d\delta_{n-1} \frac{1}{2} \delta_i \partial_i W^{gm}(\delta_0; \delta_1, \ldots, \delta_i = \delta_i, \ldots, \delta_{n-1}, \delta_n; S_n),
$$

(102)

where the notation $\delta \partial_i$ means that we must omit $\partial_i$ from the list of integration variables. We next observe that, because of the property (54), $W^{gm}$ satisfies

$$
W^{gm}(\delta_0; \delta_1, \ldots, \delta_i, \ldots, \delta_n; S_n) = W^{gm}(\delta_0; \delta_1, \ldots, \delta_i; S_i) W^{gm}(\delta_i; \delta_{i+1}, \ldots, \delta_n; S_n) - W^{gm}(\delta_0; \delta_1, \ldots, \delta_i; S_i) W^{gm}(\delta_i; \delta_{i+1}, \ldots, \delta_n; S_n - S_i),
$$

(103)

so

$$
\int_{-\infty}^{\delta_1} d\delta_1 \ldots d\delta_{n-1} \frac{1}{2} \delta_i \partial_i W^{gm}(\delta_0; \delta_1, \ldots, \delta_i = \delta_i, \ldots, \delta_{n-1}, \delta_n; S_n)
$$

$$
= \Pi_{\epsilon}^{\text{mem}}(\delta_0; \delta_i; S_i) \Pi_{\epsilon}^{\text{mem}}(\delta_i; \delta_n; S_n - S_i),
$$

(104)

and we get

$$
\Pi_{\epsilon}^{\text{mem}}(\delta_0; \delta_n; S_n) = \sum_{i=1}^{n-1} \Delta_{mm} S_{i+1} \left[ \Pi_{\epsilon}^{\text{mem}}(\delta_0; \delta_i; S_i) \Pi_{\epsilon}^{\text{mem}}(\delta_i; \delta_n; S_n - S_i) \right].
$$

In the continuum limit we write

$$
\sum_{i=1}^{n-1} \frac{1}{\sqrt{2 \pi}} \int_0^{S_i} dS_i,
$$

(106)

and, using eqs. (79) and (80), we find

$$
\Pi_{\epsilon=0}^{\text{mem}}(\delta_0; \delta_n; S_n) = \frac{1}{\pi} \int_0^{S_n} dS_i \Delta(S_i, S_n) \frac{\delta_i(\delta_i - \delta_n)}{S_i^{3/2}(S_n - S_i)^{3/2}} \times \exp \left\{ -\frac{\delta_i^2}{2S_i} - \left( \frac{\delta_i - \delta_n}{2(S_n - S_i)} \right)^2 \right\},
$$

(107)

We now insert the form (90) for $\Delta_{ij}$. The integral can be computed exactly using the identities

$$
\int_0^{S_n} dS_i \frac{S_i^{3/2}(S_n - S_i)^{3/2}}{S_i^{3/2}(S_n - S_i)^{3/2}} \exp \left\{ -\frac{a^2 - b^2}{2(S_n - S_i)} \right\}
$$

$$
= \sqrt{2 \pi} \int_0^{1/2} dS_n \exp \left\{ -\frac{(a + b)^2}{2S_n} \right\},
$$

and

$$
\int_0^{S_n} dS_i \frac{S_i^{3/2}(S_n - S_i)^{3/2}}{S_i^{3/2}(S_n - S_i)^{3/2}} \exp \left\{ -\frac{a^2 - b^2}{2S_i} \right\}
$$

$$
= \sqrt{2 \pi} \int_0^{1/2} dS_n \exp \left\{ -\frac{(a + b)^2}{2S_n} \right\} - \pi \text{Erfc} \left( \frac{a + b}{\sqrt{2} S_n} \right),
$$

(108)

(109)

where Erfc is the complementary error function. This gives

$$
\Pi_{\epsilon=0}^{\text{mem}}(\delta_0; \delta_n; S_n) = \kappa \partial_n \left[ \frac{\delta_i(\delta_i - \delta_n)}{S_i} \exp \left\{ -\frac{\delta_i - \delta_n}{\sqrt{2 \pi} S_i} \right\} \right].
$$

(110)

To derive these results we take one derivative of the left-hand side of eq. (108) with respect to $a$. The resulting integral can be performed using eq. (92), and we then integrate back with respect to $a^2$. Similarly, eq. (109) is obtained taking twice the derivative with respect to $a^2$. 

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11 To derive these results we take one derivative of the left-hand side of eq. (108) with respect to $a$. The resulting integral can be performed using eq. (92), and we then integrate back with respect to $a^2$. Similarly, eq. (109) is obtained taking twice the derivative with respect to $a^2$. 

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to write $\Pi_{\text{mem-mem}}$ as a total derivative with respect to $\delta_n$. The inner integral can now be computed rewriting it in terms of the variable $z = (\delta_c - \delta_n)^2 / [2(S_n - S_j)]$, and gives

$$\Pi_{\text{mem-mem}}(\delta_0 = 0; \delta_c; S_n) = \frac{\kappa \delta_c}{2\sqrt{\pi} \delta_n} \partial_n \left[ e^{-(\delta_c - \delta_n)^2 / (2\delta_n)} \right]$$

$$\times \int_{0}^{S_n} \frac{dS_j}{S_j} e^{-(\delta_c - \delta_n)^2 / (2\delta_n)} \frac{\delta_c}{S_j} \delta_n \left[ 1 + \frac{\delta_c}{2\sqrt{\pi} \delta_n} \left( \frac{\delta_c}{\sqrt{\delta_n^2}} \right) \right].$$  \hspace{1cm} (115)

We have not been able to compute analytically this last integral, but the fact that $\Pi_{\text{mem-mem}}$ is a total derivative with respect to $\delta_n$ will allow us to compute analytically the first-crossing rate, see below. First, it is interesting to plot the functions $\Pi_{\text{mem}}$ and $\Pi_{\text{mem-mem}}$. We show them in Fig. 7 setting for definiteness $S_n = 1$. Observe that these two functions are separately non-zero in $\delta = \delta_c$. However,

$$\Pi_{\text{mem}}(\delta_0 = 0; \delta_c; S_n) = \frac{\kappa \delta_c}{S_n} \left[ \frac{\delta_n}{\sqrt{2\pi} \delta_n} \right].$$  \hspace{1cm} (116)

and $\Pi_{\text{mem-mem}}(\delta_0 = 0; \delta_c; S_n) = -\Pi_{\text{mem}}(\delta_0 = 0; \delta_c; S_n)$, so we find that the total distribution function $\Pi_{\text{c0}}(\delta_0; \delta_c; S_n)$ still satisfies the absorbing barrier boundary condition $\Pi_{\text{c0}}(\delta_0; \delta_c; S_n) = 0$, even when we include the markovian corrections to first order. In Fig. 8 we compare $\Pi_{\text{mem}} + \Pi_{\text{mem-mem}}$ to the zeroth-order term $\Pi_{\text{c0}}$.

5.4. The halo mass function

We can now compute the first crossing rate using eq. (100). Since both $\Pi_{\text{mem}}$ and $\Pi_{\text{mem-mem}}$ have been expressed as a derivative with respect to $\delta_n$ in eqs. (110) and (115), the integral over $d\delta_n$ is performed trivially, and we get

$$F_{\text{mem}}(S) = -\frac{\partial}{\partial S} \int_{-\infty}^{\delta_0} d\delta_n \Pi_{\text{mem}}(\delta_0 = 0; \delta_n; S) = 0,$$  \hspace{1cm} (117)

$$F_{\text{mem}}(S) = -\frac{\partial}{\partial S} \int_{-\infty}^{\delta_0} d\delta_n \Pi_{\text{mem-mem}}(\delta_0 = 0; \delta_n; S)$$

$$= -\frac{\partial}{\partial S} \left[ \frac{\kappa \delta_c}{S_n} \left( \frac{1}{\sqrt{2\pi} \delta_n} \right) \Gamma \left( 0, \frac{\delta_n}{2\sqrt{\delta_n}} \right) \right]$$

$$= -\frac{\kappa \delta_c}{S_n} \left[ \frac{1}{\sqrt{2\pi} \delta_n} \Gamma \left( 0, \frac{\delta_n}{2\sqrt{\delta_n}} \right) \right]$$

$$= -\frac{\kappa \delta_c}{S_n} \left[ \frac{1}{\sqrt{2\pi} \delta_n} e^{-\delta_n^2 / (2\delta_n)} \right]$$

$$= \frac{1}{\sqrt{2\pi} \delta_n} e^{-\delta_n^2 / (2\delta_n)}.$$  \hspace{1cm} (118)

where $\Gamma(0, z)$ is the incomplete Gamma function. Putting together eqs. (94), (117) and (118) we find the first-crossing rate to first order in the non-markovian corrections,

$$F(S) = \frac{1 - \kappa}{\sqrt{2\pi} \delta_n^2} e^{-\delta_n^2 / (2\delta_n)} + \frac{\kappa}{\sqrt{2\pi} \delta_n^2} \Gamma \left( 0, \frac{\delta_n^2}{2\delta_n} \right).$$  \hspace{1cm} (119)

The halo mass function in this approximation is therefore

$$f(\sigma) = (1 - \kappa) \left( \frac{2}{\pi} \right)^{1/2} \frac{\delta_c}{\sigma} e^{-\delta_c^2 / (2\sigma^2)} + \frac{\kappa}{\sqrt{2\pi} \sigma^2} \frac{\delta_c}{\sigma} \Gamma \left( 0, \frac{\delta_c^2}{2\sigma^2} \right),$$

(120)

where, in the relevant range of values of $R$, $\kappa$ is given by eqs. (91) and (92), and is a slowly decreasing function of $R$. For instance, at $R = 5$ Mpc, $\kappa \approx 0.43$, at $R = 10$ Mpc, $\kappa \approx 0.43$, and at $R = 20$ Mpc, $\kappa \approx 0.40$. For large values of $\delta_c^2 / 2\sigma^2$

$$\Gamma \left( 0, \frac{\delta_c^2}{2\sigma^2} \right) \approx \frac{2\delta_c^2}{\delta_c^2} e^{-\delta_c^2 / (2\sigma^2)}.$$  \hspace{1cm} (121)
Thus the incomplete Gamma function gives the same exponential factor as PS theory but with a smaller prefactor, so for large halo masses it is subleading, and eq. (120) approaches $(1 - \kappa)$ times the PS prediction.

In Fig. 9 we plot the function $f(\nu)$, where $\nu = \delta_c / \sigma$, comparing the prediction of PS theory given in eq. (2), the fit to the N-body simulation of Warren et al. (2006), and our result (120). This figure can be compared to Fig. 4 of Robertson et al. (2008), see in particular their bottom-left panel, where the authors show the prediction of PS theory, the result of their N-body simulation, and the computation of $f(\nu)$ with tophat filter in coordinate space, performed with a Monte Carlo realization of the trajectories obtained from a Langevin equation with colored noise. We have used the same scale and color code as their Fig. 4, to make the comparison easier. One sees that our analytical result for $f(\nu)$ agrees very well with their Monte Carlo result (the function that we call $F(\nu)$ in Robertson et al. (2008)). From eq. (120), we see that in the end our expansion parameter is just $\kappa$, so evaluating the non-markovian corrections to second order we will get corrections of order $\kappa^2$. For $\kappa$ given by eq. (122) these are expected to be of order 20%, which is the level of agreement between our analytical result and the Monte Carlo computation. This provides a non-trivial check of the correctness of our formalism.

A second consistency check is obtained by recalling that the fraction of volume occupied by virialized objects is given by eq. (25). In hierarchical power spectra, all the mass of the universe must finally end up in virialized objects, so we must have $F(S) = 1$ when $\delta_c / \sigma \to 0$. Formally, the limit $\delta_c / \sigma \to 0$ can be obtained sending $\delta_c \to 0$ for fixed $\sigma$, so we require that

$$\lim_{\delta_c \to 0} \int_{-\infty}^{\delta_c} d\delta \Pi(\delta, S) = 0. \quad (122)$$

As we recalled below eq. (5), the original PS theory fails this test, giving that only one half of the total mass of the universe collapses. In our case $\Pi = \Pi_{\text{mem}} + \Pi_{\text{mem-mem}}$. Since $\Pi_{\text{gm}}$ is the same as in the standard excursion set result, it already satisfies eq. (122), so we must find that, in the limit $\delta_c \to 0$, the integral of $\Pi_{\text{mem}} + \Pi_{\text{mem-mem}}$ from $-\infty$ to $\delta_c$ vanishes. Using eq. (107) we see that

$$\int_{-\infty}^{\delta_c} d\delta \Pi_{\text{mem}}(\delta, S) = \kappa \left[ \frac{\delta_c(\delta_c - \delta)}{S} \text{Erfc} \left( \frac{2\delta_c - \delta}{\sqrt{2S}} \right) \right] \delta_c = 0, \quad (123)$$

for all values of $\delta_c$. For the memory-of-memory term we find

$$\int_{-\infty}^{\delta_c} d\delta \Pi_{\text{mem-mem}}(\delta, S) = -\frac{\kappa}{\sqrt{2\pi} S^{1/2}} \Gamma(0, \frac{\delta_c^2}{2S}). \quad (124)$$

Since, for $z \to 0$, $\Gamma(0, z) \to -\ln z$, we have

$$\lim_{\delta_c \to 0} \delta_c \Gamma\left(0, \frac{\delta_c^2}{2S}\right) = 0, \quad (125)$$

so eq. (122) is indeed satisfied. An equivalent derivation starts from the observation that, in terms of the function $f(\sigma)$, the normalization condition reads

$$\int_0^\infty \frac{d\sigma}{\sigma} f(\sigma) = 1. \quad (126)$$

Substituting $f(\sigma)$ from eq. (120) into eq. (126) and using

$$\int_0^\infty \frac{d\sigma}{\sigma} \left( \frac{2}{\pi} \frac{\delta_c}{\sigma^2} e^{-\delta_c^2/(2\sigma^2)} \right) = 1 \quad (127)$$

and

$$\int_0^\infty \frac{d\sigma}{\sigma^2 \sqrt{2\pi}} \Gamma\left(0, \frac{\delta_c^2}{2\sigma^2}\right) = 1, \quad (128)$$

we see that the dependence on $\kappa$ cancels and eq. (126) is satisfied. The term proportional to the incomplete Gamma function therefore ensure that the mass function is properly normalized, when the amplitude of the term proportional to $\exp\left(-\delta_c^2/(2\sigma^2)\right)$ is reduced by a factor $1 - \kappa$.

A number of comments are now in order. First, our findings confirms the known result (Bond et al. 1991; Robertson et al. 2008) that the corrections obtained by taking properly into account the tophat filter in coordinate space do not alleviate the discrepancy of PS theory with the N-body simulations. We see in fact from Fig. 9 that the effect of the non-markovian corrections is to give a halo mass function that, in the relevant mass range, is everywhere smaller than the PS mass function, which results in an improvement in the low-mass range but in a worse agreement in the high-mass range. This indicates that some crucial physical ingredient is still missing in the model. This is not surprising at all since, as we already stated, the formation of dark matter haloes is a complex phenomenon. Incorporating some of the complexeties within the excursion set theory will be the subject of paper II.

On the positive side, we conclude that we have developed a powerful analytical formalism that allows us to compute consistently the halo mass function when non-markovian effects are present. In this paper we have applied it to the corrections generated by the tophat filter function in coordinate space. However, the same formalism allows us to compute perturbatively the effect of the non-Gaussianities on the halo mass function. This direction will be developed in paper III.

Before leaving this topic we observe that, in the perturbative computation performed in this section, all terms turned out to be finite in the continuum limit. The fact that the total result is finite is obvious for physical reasons. However, the fact that all the terms that enters in the computation are separately finite happens to be a happy accident, related to the form (90) of $\Delta(S, s_j)$, and in particular to the property...
evaluated in Section 5.3, when we compute perturbatively the non-markovian corrections. We will also show that, for \( \epsilon \to 0^+ \) does not commute with the limit \( \delta \to \delta^* \). This result will be important in appendix B when we study the cancellation of divergences, that can appear in intermediate steps of the computation. In eqs. (74) and (78), we found that \( \Pi_{\epsilon}^{\text{gm}}(\delta_0; \delta; S) = \sqrt{\epsilon \gamma} (\delta_i / S_i^{3/2}) e^{-\epsilon \delta_i / (2S_\epsilon)} + O(\epsilon) \), where \( \gamma = (2 / \sqrt{\pi}) \lim_{\eta \to 0} \eta u(\eta) \). One possible route to the evaluation of \( \gamma \) could be to plug eq. (74) into eq. (58) and evaluate both sides at \( \delta = \delta^* \). To lowest order in \( \epsilon \) one can replace \( S + \epsilon \) on the left-hand side simply by \( S \), and one obtains an integral equation for the unknown function \( u(\eta) \). This integral equation has the form of a Wiener-Hopf equation, for which various techniques have been developed (Noble 1958). However, we have found a simpler way to get directly \( \gamma \), as follows. We consider the derivative of \( \Pi_{\epsilon}^{\text{gm}} \) with respect to \( \delta^* \), which, when we use the notation \( \Pi_{\epsilon}^{\text{gm}}(\delta_0; \delta; S) \), does not appear explicitly in the list of variables on which \( \Pi_{\epsilon}^{\text{gm}} \) depends, but of course enters as upper integration limit in eq. (40). This gives

\[
\frac{\partial}{\partial \delta^*} \Pi_{\epsilon}(\delta_0; \delta^*; S) = \sum_{n=1}^{n_c} \int_{-\infty}^{\delta^*_n} d\delta_1 \ldots d\delta_{n-1} W(\delta_0; \delta_1, \ldots, \delta_n = \delta^*, \ldots, \delta_n; S_n),
\]

where the notation \( \delta^*_n \) means that we must omit \( d\delta_n \) from the list of integration variables. We next use eqs. (103) and (104) and, in the continuum limit, we obtain the identity

\[
\frac{\partial}{\partial \delta^*} \Pi_{\epsilon}(\delta_0; \delta^*; S) = \int_0^{S_0} dS_l \lim_{\epsilon \to 0^-} \frac{1}{\epsilon} \Pi_{\epsilon}^{\text{gm}}(\delta_0; \delta^*; S_n) \Pi_{\epsilon}^{\text{gm}}(\delta^*_n; \delta^*; S_n),
\]

(A2)

The left-hand side of this identity can be evaluated explicitly using eq. (57) and, setting for simplicity \( \delta_0 = 0 \), is

\[
\frac{\partial}{\partial \delta^*} \Pi_{\epsilon}(0; \delta^*; S_n) = \left( \frac{2}{\pi} \right)^{1/2} \frac{2 \delta^*_n}{S_n} \frac{1}{S_n} \exp \left( -\frac{(2 \delta^*_n)^2}{S_n} \right).
\]

(A3)

The right-hand side of eq. (A2) can be evaluated using eq. (72) together with

\[
\Pi_{\epsilon}(\delta_0; \delta^*; S) = \Pi_{\epsilon}(\delta^*_n; \delta^*; S) = \sqrt{\epsilon \gamma} \frac{\delta^*_n}{S_n^{3/2}} \exp \left( -\frac{(\delta^*_n)^2}{S_n} \right) + O(\epsilon),
\]

(A4)

which can be checked from eqs. (40) and (53) by performing a reshuffling of the dummy integration variables. We see that the limit \( \epsilon \to 0 \) in eq. (A2) is finite thanks to the factors \( \sqrt{\epsilon} \) in \( \Pi_{\epsilon}^{\text{gm}}(\delta_0; \delta^*; S_n) \) and in \( \Pi_{\epsilon}^{\text{gm}}(\delta^*_n; \delta^*; S_n) \). The integral over \( S_n \) can be performed using the identity

\[
\int_0^{S_0} dS_l \frac{1}{S_n^{3/2}(S_n - S_l)^{3/2}} \exp \left( -\frac{a^2 b^2}{2S_n} \right) = \frac{\sqrt{2\pi a b}}{2S_n^{3/2}} \exp \left( -\frac{(a + b)^2}{2S_n} \right),
\]

(A5)

where \( a > 0, b > 0 \). In this way we find that the dependence on \( \delta^* \) and \( S \) on the two sides of eq. (A2) is the same, as it should, and we fix \( \gamma = 1 / \sqrt{\pi} \).

In appendix B when we study the cancellation of divergences, we will also need \( \partial_{\delta^*} \Pi_{\epsilon}^{\text{gm}} \), evaluated in \( \delta = \delta^* \). Of course, if we first take the limit \( \epsilon \to 0^+ \), and then we take \( \delta \to \delta^* \), we simply get the derivative of the function \( \Pi_{\epsilon}(0; \delta, S) \) given in eq. (57), evaluated in \( \delta^* \).

\[
\lim_{\delta \to 0} \lim_{\epsilon \to 0^+} \frac{\partial_{\delta^*} \Pi_{\epsilon}^{\text{gm}}(0; \delta; S)}{\partial_{\delta^*} \Pi_{\epsilon}(0; \delta, S)} \bigg|_{\delta = \delta^*} = -\left( \frac{2}{\pi} \right)^{1/2} \frac{\delta^*}{S_n^{3/2}} \exp \left( -\frac{(\delta^*)^2}{S_n} \right).
\]

(A6)

However, we will actually need the result when the limits are evaluated in the opposite order, i.e. \( \lim_{\delta \to 0^+} \lim_{\epsilon \to 0^-} \frac{\partial_{\delta^*} \Pi_{\epsilon}^{\text{gm}}(0; \delta; S)}{\partial_{\delta^*} \Pi_{\epsilon}(0; \delta, S)} \bigg|_{\delta = \delta^*} = -\left( \frac{2}{\pi} \right)^{1/2} \frac{\delta^*}{S_n^{3/2}} \exp \left( -\frac{(\delta^*)^2}{S_n} \right). \)

More generally, for small \( \eta \), we write

\[
u(\eta) = \frac{1}{2\eta} + u_0 + u_1 \eta + O(\eta^2).\]

(A7)

12 We have not been able to find this identity in standard tables of integrals, but we have verified it numerically, with very high accuracy, in a wide range of values of \( a \) and \( b \). We can also turn the argument around and say that, since we know that \( \Pi_{\epsilon}^{\text{gm}}(\delta_0; \delta; S) \) has the functional form \( 77 \) and we know that the identity \( 53 \) holds, it follows that the integral on the left-hand side of eq. \( 55 \) must be given by the expression on the right-hand side, times an unknown numerical constant. The latter can be computed evaluating the term \( \sim 1 / \eta \) of the integral in the limit \( a \to 0^+ \). This is easily done analytically, since in this case the factors \( (S_n - S_\epsilon) \) inside the integrand can be simply replaced by \( S_n \), and fixes the factor \( \sqrt{2\pi} \) on the right-hand side of eq. \( 55 \).
Plugging this expansion, together with the expansion in powers of $\eta$ of eq. (17S), into eq. (17G) we find that, for $\eta \to 0$ (i.e. for $\delta \to \delta_c$ at fixed $\epsilon$), retaining only the terms up to $O(\sqrt{\epsilon})$

$$\Pi^m_\epsilon(\delta_0 = 0; \delta, S) = \Pi^m_\epsilon(\delta_0 = 0; \delta_c, S) + \sqrt{\epsilon} \frac{2}{\sqrt{\pi}} (u_0 \eta + u_1 \eta^2 + \ldots) \frac{\delta_c}{\sqrt{\eta}} e^{-\delta_c^2/(2\eta)}.$$  \hspace{1cm} (A8)

Using $\partial_\delta = (d\eta/d\delta) \partial/\partial \eta$ and $d\eta/d\delta = -1/\sqrt{\epsilon}$, this gives

$$\lim_{\epsilon \to 0} \lim_{\delta \to \delta_c} \partial_\delta \Pi^m_\epsilon(\delta_0 = 0; \delta, S) = -u_0 \left( \frac{2}{\sqrt{\pi}} \right) \frac{\delta_c}{\sqrt{\eta}} e^{-\delta_c^2/(2\eta)},$$  \hspace{1cm} (A9)

which differs by a factor $u_0$ from eq. (A6). It is also interesting to observe, from eq. (A8), that $\partial^2 \Pi^m_\epsilon / \partial \eta^2$, evaluated in $\eta = 0$, is proportional to $\sqrt{\epsilon}$. Since

$$\frac{\partial^2 \Pi^m_\epsilon}{\partial \delta^2} = \frac{1}{\epsilon} \frac{\partial^2 \Pi^m_\epsilon}{\partial \eta^2},$$  \hspace{1cm} (A10)

overall $\partial^2 \Pi^m_\epsilon / \partial \delta^2$, evaluated in $\delta = \delta_c$ at finite $\epsilon$, is proportional to $1/\sqrt{\epsilon}$. Therefore, in eq. (17G) the first correction included in the dots, which is proportional $\epsilon (\partial^2 \Pi^m_\epsilon / \partial \delta^2)_{\delta = \delta_c}$, is of the same order as the term $\sqrt{\epsilon} (\partial \Pi^m_\epsilon / \partial \delta)_{\delta = \delta_c}$, and similarly for the higher-order terms. This is the reason why we could not use eq. (17G) to fix the value of the coefficient $\gamma$.

Finally, in the perturbative computation we also need $\Pi^m(\delta_c; \delta_c; S)$, with both arguments equal to $\delta_c$. The result is given in eq. (A11). To derive it, we first observe from eq. (17G) that, when $\delta_0 = \delta_c$, the term $O(\sqrt{\epsilon})$ vanishes, so the first non-vanishing term will be $O(\epsilon)$. Invariance under space translations requires that $\Pi^m(\delta_c; \delta_c; S)$ can depend on $\delta_0$ and $\delta_c$ only through the combination $\delta_c - \delta_0$, so when $\delta_0 = \delta_c$, it becomes a function of $S$ only. We can perform dimensional analysis assigning to $\delta$ some (unspecified) dimension $\ell$ and to $S$ dimensions $\ell^2$. In this case, from eq. (19) we see that $\eta$ has dimensions $1/\ell$, and $\xi \sim \ell/\ell^2 = 1/\ell$, so eq. (19) is dimensionally correct. In these units $\lambda \sim 1/\ell$, since $\lambda \delta$ is dimensionless, and we see from eq. (15) that $\Pi^m$ has dimensions $1/\ell$. Using dimensional analysis in this form we conclude that the term $O(\epsilon)$ in $\Pi^m(\delta_c; \delta_c; S)$ is necessarily proportional to $\epsilon/\sqrt{\eta}$.

Since this fixes completely the dependence on $S$, writing $S = \epsilon n$ we have also fixed completely the dependence on $n$, i.e. to $O(\epsilon)$ we must have

$$\Pi^m_\epsilon(\delta_c; \delta_c; S) = c \frac{\epsilon}{\sqrt{\eta}} = \frac{c}{\sqrt{\epsilon n^{1/2}}},$$  \hspace{1cm} (A11)

with $c$ independent of $n$. The coefficient $c$ can then be fixed computing explicitly the integral in eq. (A10) when $n = 2$, i.e. when there is just one integration variable. This can be done analytically and shows that $c = 1/\sqrt{2\pi}$. The computation for $n = 2$ actually shows that eq. (A11) is exact, i.e. it receives no correction of higher order in $\epsilon$. Even for $n = 3$ the integral in eq. (A11) can be performed analytically when $\delta_0 = \delta_c$, and again we find that eq. (A11) is exact. We have checked this result numerically for $n$ up to 7 and we find that the numerical result agrees with eq. (A11) within the 10 digit precision of the numerical integration, so it is clear that eq. (A11) is actually exact, and not just the result at $O(\epsilon)$. (In any case, to perform our perturbative computation, we only need $\Pi^m_\epsilon(\delta_c; \delta_c; S)$ to $O(\epsilon)$.)

### B. DIVERGENCES AND THE FINITE PART PRESCRIPTION

In this appendix we first of all reconsider the perturbative computation of Section 5.3 for a generic function $\Delta_{ij}$ (still symmetric in $(i, j)$). This will reveal some complexities that were not apparent in the computation of Section 5.3 and that will be very important when computing the non-Gaussianities. If $\Delta_{ij}$ does not vanish when $i = j$, we rewrite eq. (23) as

$$\Pi_\epsilon(\delta_0; \delta; S) = \int_{-\infty}^{\delta_c} d\delta_1 \ldots d\delta_{n-1} \int \mathcal{D}\lambda \exp \left\{ \frac{1}{2} \sum_{i,j=1}^{n} \Delta_{ij} \partial_i \partial_j \right\} \exp \left\{ i \sum_{i=1}^{n} \lambda_i \delta_i - \frac{1}{2} \sum_{i,j=1}^{n} \min(S_i, S_j) \lambda_i \lambda_j \right\},$$  \hspace{1cm} (B1)

where, as usual, we used the fact that, acting on $\exp \{ i \lambda_i \delta_i \}$, $\partial_i$ gives $i \lambda_i$. Since $\Delta_{mn}$ is now in general non-vanishing, in the sum (96) the term $\Delta_{mn} \partial_n^2$ contributes. Furthermore, now

$$\frac{1}{2} \sum_{i,j=1}^{n-1} \Delta_{ij} \partial_i \partial_j = \sum_{i<j} \Delta_{ij} \partial_i \partial_j + \frac{1}{2} \sum_{i} \Delta_{ii} \partial_i^2.$$  \hspace{1cm} (B2)

The operator $\exp \left\{ (1/2) \Delta_{mn} \partial_n^2 \right\}$ can be carried out of the integral over $d\delta_1, \ldots, d\delta_{n-1}$, while the other terms $\Delta_{ij}$ will be expanded perturbatively. Thus, eqs. (99)-(101) are replaced by

$$\Pi_\epsilon^{A1} = e^{(1/2)\Delta_{mn} \partial_n^2} \Pi_\epsilon^{mem} + \Pi_\epsilon^{mem-mem},$$  \hspace{1cm} (B3)

where

$$\Pi_\epsilon^{mem}(\delta_0; \delta_n; S_n) = \sum_{j=1}^{n-1} \Delta_{mn} \partial_n \int_{-\infty}^{\delta_c} d\delta_1 \ldots d\delta_{n-1} \partial_j W_{gm}^{st}(\delta_0; \delta_1, \ldots, \delta_n; S_n),$$  \hspace{1cm} (B4)

and

$$\Pi_\epsilon^{mem-mem}(\delta_0; \delta_n; S_n) = \int_{-\infty}^{\delta_c} d\delta_1 \ldots d\delta_{n-1} \left[ \sum_{i<j} \Delta_{ij} \partial_i \partial_j + \frac{1}{2} \sum_{i} \Delta_{ii} \partial_i^2 \right] W_{gm}^{st}(\delta_0; \delta_1, \ldots, \delta_n; S_n).$$  \hspace{1cm} (B5)
The memory term is the same as in Section 5.3 so it is still finite. The memory-of-memory term, however, presents a new difficulty. Using eq. (103) we get

\[
\Pi_\varepsilon^{\text{mem-mem}}(\delta_0; \delta_n; S_n) = \sum_{i<j} (\delta_{i} - \delta_{j}) \Pi_\varepsilon^{\text{mem}}(\delta_{i}; \delta_{j}; S_{j} - S_{i}) \Pi_\varepsilon^{\text{mem}}(\delta_{i}; \delta_{n} - S_{i}),
\]

\[
+ \sum_{i=1}^{n-1} \frac{\Delta^{2}}{2} \partial_{i} \left[ \Pi_\varepsilon^{\text{mem}}(\delta_{0}; \delta_{i}; S_{i}) \Pi_\varepsilon^{\text{mem}}(\delta_{i}; \delta_{n} - S_{i}) \right]_{\delta_{i}=\delta_{i}}.
\]

(\text{B6})

We now discover that the continuum limit of the memory-of-memory term is non-trivial, since it is made of two terms that are separately divergent. Consider first the second term in eq. (B6), which is the one coming from \( \Delta_\varepsilon \partial_{i}^{2} \). We have found in Section 4.2 that \( \Pi_\varepsilon^{\text{mem}}(\delta_0; \delta_i; S_i) \) is proportional to \( \sqrt{\varepsilon} \) while \( [\partial_{i} \Pi_\varepsilon^{\text{mem}}(\delta_{i}; S_{i})]_{\delta_{i}=\delta_{i}} \) has a finite limit for \( \varepsilon \to 0 \), see eq. (A9). Therefore, using eq. (106), we find that the last term in eq. (B6) diverges as \( 1/\sqrt{\varepsilon} \). A similar problem appears in the term coming from \( \partial_{i} \partial_{j} \) with \( i \neq j \). Using eqs. (79) and (112) we find that the first term in eq. (B6) is proportional to

\[
\frac{1}{\varepsilon} \left( 1/\sqrt{\varepsilon} \right) \left( 1/\sqrt{\varepsilon} \right) \left( 1/\sqrt{\varepsilon} \right) \left( 1/\sqrt{\varepsilon} \right)
\]

(\text{B7})

where \( S_i = i \varepsilon, S_j = j \varepsilon \). In the continuum limit, unless \( \Delta_{ij} \) vanishes for \( i = j \), this quantity diverges as \( 1/\sqrt{\varepsilon} \), because of the behavior \( (S_{j} - S_{i})^{3/2} \) when \( S_j \to S_i \). In Section 4.2 these problem did not show up because \( \Delta_{ii} = 0 \), so the divergence coming from \( \Delta_{ii} \partial_{i}^{2} \) disappears. Furthermore, when \( S_{j} \to S_{i}, \Delta_{ij} \) vanished as \( S_{j} \to S_{i} \), thereby ensuring the convergence of the sum (or, in the continuum limit, of the integral over \( S_{j} \)) in eq. (B7).

In order to understand how the cancellation mechanism works when \( \Delta_{ij} \) does not vanish for \( S_i = S_j \), we examine the memory-of-memory term when \( \Delta(S_{i}, S_{j}) \) is a constant, that we set equal to unity. The reason is that, in this case, we can compute it in an alternative way, which shows that the result is finite. The trick is to compute the second derivative of \( \Pi_\varepsilon^{\text{mem}} \) with respect to \( \delta_{i} \). The first derivative was computed in eq. (A1), and the result can be rewritten as

\[
\frac{\partial}{\partial \delta_{i}} \Pi_\varepsilon^{\text{mem}}(\delta_{0}; \delta_{i}; S_n) = \sum_{i=1}^{n-1} \int_{-\infty}^{\delta_{i}} d\delta_{1} \cdots d\delta_{n-1} \partial_{i} W.
\]

(\text{B8})

When we take one more derivative of eq. (A1) with respect to \( \delta_{i} \), we find two kinds of terms. First, there are the terms where we take one more derivatives with respect to the upper limit of the integration with respect to a variable \( d\delta_{j} \) with \( j \neq i \). Furthermore, we must take the derivative of \( W(\delta_{0}; \delta_{i}, \ldots, \delta_{i} = \delta_{c}, \ldots, \delta_{n}; S_n) \) with respect to \( \delta_{c} \). Therefore

\[
\frac{\partial^{2}}{\partial \delta_{c}^{2}} \Pi_\varepsilon^{\text{mem}}(\delta_{0}; \delta_{i}; S_n) = 2 \sum_{i<j} \int_{-\infty}^{\delta_{i}} d\delta_{j} \cdots d\delta_{j} \cdots d\delta_{n-1} \frac{\partial}{\partial \delta_{c}} W(\delta_{0}; \delta_{1}, \ldots, \delta_{i} = \delta_{c}, \ldots, \delta_{n}; S_n)
\]

(\text{B9})

that is,

\[
\frac{\partial^{2}}{\partial \delta_{c}^{2}} \Pi_\varepsilon^{\text{mem}}(\delta_{0}; \delta_{c}; S_n) = \sum_{i=j}^{n-1} \int_{-\infty}^{\delta_{i}} d\delta_{1} \cdots d\delta_{n-1} \partial_{i} \partial_{i} W.
\]

(\text{B10})

Thus, when \( \Delta_{ij} = 1 \),

\[
\Pi_\varepsilon^{\text{mem-mem}}(\delta_{0}; \delta_{c}; S_n) = \frac{1}{2} \frac{\partial^{2}}{\partial \delta_{c}^{2}} \Pi_\varepsilon^{\text{mem}}(\delta_{0}; \delta_{c}; S_n).
\]

(\text{B11})

In particular, in the continuum limit,

\[
\Pi_\varepsilon^{\text{mem-mem}}(\delta_{0}; 0; \delta_{c}; S_n) = \frac{1}{2} \frac{\partial^{2}}{\partial \delta_{c}^{2}} \Pi_\varepsilon^{\text{mem}}(\delta_{0}; 0; \delta_{c}; S_n) = \left( \frac{2}{\pi} \right)^{1/2} \left[ 1 - \frac{(2\delta_{c} - \delta_{0})^{2}}{S_n} \right] \frac{1}{S_n^{1/2}} e^{- (2\delta_{c} - \delta_{0})^{2} / (2S_n)}.
\]

(\text{B12})

First of all this result shows that, when \( \Delta_{ij} = 1 \), \( \Pi_\varepsilon^{\text{mem-mem}} \) stays indeed finite in the continuum limit. Second, it gives its explicit expression, which can then be compared with a computation based on eq. (B6). To perform the comparison, we first compute the second term in eq. (B6), when \( \Delta_{ij} = 1 \), i.e.

\[
I_{1} = \sum_{i=1}^{n-1} [\partial_{i} \Pi_\varepsilon^{\text{mem}}(\delta_{0}; \delta_{i}; S_i)]_{\delta_{i}=\delta_{i}} \Pi_\varepsilon^{\text{mem}}(\delta_{i}; \delta_{n} - S_{i}).
\]

(\text{B13})
Observe that in this expression we must first compute the derivative in \( \delta_i = \delta_c \) (since this came from the integration by parts of \( \partial^2 \)) and only after we take the limit \( \epsilon \to 0^+ \). The result is therefore given by eq. (A9). Using also eqs. (A4) and (79), we get

\[
I_1 = -\frac{1}{\sqrt{\epsilon}} \frac{u_0 \sqrt{2}}{\pi} \delta_c (\delta_c - \delta_n) \epsilon \sum_{i=1}^{n-1} \frac{1}{S_i^{3/2}(S_n - S_i)^{3/2}} \exp \left\{ \frac{\delta_c^2}{2S_i} \left( \frac{\delta_c - \delta_n}{2(S_n - S_i)} \right)^2 \right\}.
\]  

(B14)

Because of the exponential factor, the argument of the sum goes to zero very fast as \( S_i \to 0^+ \) and as \( S_i \to S_n^- \), and therefore we can use eq. (106), so

\[
I_1 = -\frac{1}{\sqrt{\epsilon}} \frac{u_0 \sqrt{2}}{\pi} \delta_c (\delta_c - \delta_n) \int_0^{S_n} dS_i \frac{1}{S_i^{3/2}(S_n - S_i)^{3/2}} \exp \left\{ -\frac{\delta_c^2}{2S_i} \left( \frac{\delta_c - \delta_n}{2(S_n - S_i)} \right)^2 \right\}.
\]  

(B15)

The integral can be performed using eq. (A5), and we get

\[
I_1 = -\frac{1}{\sqrt{\epsilon}} \frac{2m}{\sqrt{\pi}} \delta_c (\delta_c - \delta_n) \frac{1}{S_n^{3/2}} e^{-(2\delta_c - \delta_n)^2/(2S_n)}.
\]  

(B16)

Therefore \( I_1 \) diverges as \( 1/\sqrt{\epsilon} \). It is important to observe that there is no finite part in \( I_1 \). In the continuum limit the corrections to eqs. (79), (A9) and (106) are all \( \mathcal{O}(\epsilon) \) compared to the leading terms that we used, so they produce terms that are overall \( \mathcal{O}(\sqrt{\epsilon}) \) in eq. (B16), and therefore vanish in the continuum limit.

We next consider the other term in eq. (B6), i.e.

\[
I_2 \equiv \sum_{i=1}^{n-1} \Pi^{\text{em}}(\delta_0 = 0; \delta_c; S_i) \sum_{j=1}^{n-1} \Pi^{\text{em}}(\delta_i; \delta_j; S_j - S_i) \Pi^{\text{em}}(\delta_c; \delta_n; S_n - S_j)
\]

\[
= \frac{1}{\pi \sqrt{2\pi}} \delta_c (\delta_c - \delta_n) \epsilon \sum_{i=1}^{n-1} \frac{1}{S_i^{3/2}} e^{-\delta_i^2/(2S_i)} \epsilon \sum_{j=1}^{n-1} \frac{1}{(S_j - S_i)^{3/2}(S_n - S_j)^{3/2}} \exp \left\{ \frac{(\delta_c - \delta_n)^2}{2(S_n - S_j)} \right\}.
\]  

(B17)

Now the passage from the sums to integrals is more delicate. One might be tempted to write

\[
\epsilon \sum_{j=1}^{n-1} \int_{S_i}^{S_n} dS_j.
\]  

(B18)

However, eq. (B18) is only correct when the sum and the integral are finite for \( \epsilon \to 0^+ \). Here this is not the case, since

\[
\int_{S_i}^{S_n} dS_j \frac{1}{(S_j - S_i)^{3/2}(S_n - S_j)^{3/2}} \exp \left\{ -\frac{(\delta_c - \delta_n)^2}{2(S_n - S_j)} \right\}
\]

(B19)

diverges at the lower integration limit \( S_j = S_i \), and indeed our aim is to extract this divergent term, plus the finite terms. A better guess would be that, since the sum starts from \( j = i + 1 \), the corresponding integral should start from \( S_j = S_i + \epsilon \), so

\[
I_3 \equiv \epsilon \sum_{j=i+1}^{n-1} \frac{1}{(S_j - S_i)^{3/2}(S_n - S_j)^{3/2}} \exp \left\{ -\frac{(\delta_c - \delta_n)^2}{2(S_n - S_j)} \right\} \int_{S_i+\epsilon}^{S_n} dS_j \frac{1}{(S_j - S_i)^{3/2}(S_n - S_j)^{3/2}} \exp \left\{ \frac{(\delta_c - \delta_n)^2}{2(S_n - S_j)} \right\}.
\]  

(B20)

Still, this cannot be completely correct. To realize this observe that, since the integral is dominated by \( S_j = S_i + \epsilon \), the divergent part can be extracted replacing \( S_j = S_i \) everywhere except in the factor \( (S_j - S_i)^{3/2} \), so, if we used this prescription, we would conclude that

\[
I_3 \equiv \epsilon \sum_{j=i+1}^{n-1} \frac{1}{(S_j - S_i)^{3/2}(S_n - S_j)^{3/2}} \exp \left\{ -\frac{(\delta_c - \delta_n)^2}{2(S_n - S_j)} \right\} \int_{S_i+\epsilon}^{S_n} dS_j \frac{1}{(S_j - S_i)^{3/2}(S_n - S_j)^{3/2}} + \text{finite parts}
\]

\[
= \frac{2}{\sqrt{\epsilon} (S_n - S_i)^{3/2}} \exp \left\{ \frac{(\delta_c - \delta_n)^2}{2(S_n - S_i)} \right\} + \text{finite parts}.
\]  

(B21)

However, if the prescription (B20) correct in general, we should get the same result if we separate the term \( j = i + 1 \) from the sum, and we let the remaining integral start from \( S_j = S_i + 2\epsilon \), so we should get the same result if we write

\[
I_3 \equiv \frac{1}{\sqrt{\epsilon}} \frac{1}{(S_n - S_i)^{3/2}} \exp \left\{ -\frac{(\delta_c - \delta_n)^2}{2(S_n - S_i)} \right\} + \int_{S_i+2\epsilon}^{S_n} dS_j \frac{1}{(S_j - S_i)^{3/2}(S_n - S_j)^{3/2}} \exp \left\{ -\frac{(\delta_c - \delta_n)^2}{2(S_n - S_j)} \right\}
\]

\[
= \frac{1 + \sqrt{2}}{\sqrt{\epsilon} (S_n - S_i)^{3/2}} \exp \left\{ -\frac{(\delta_c - \delta_n)^2}{2(S_n - S_i)} \right\} + \text{finite parts}.
\]  

(B22)

We see that the two procedures both agree on the fact that the singularity is proportional to \( 1/\sqrt{\epsilon} \), but give different values for the coefficient, so eq. (B20) cannot correct in general. Observe also that the finite parts are not affected by this ambiguity, which amounts to a rescaling of \( \epsilon \).
Since, of course, the strength of the singularity is in principle fixed (although difficult to compute analytically) as long as we write $I_3$ as a sum, we can always choose a value $\alpha$ such that, as far as the $1/\sqrt{\tau}$ singularity and the finite terms are concerned, we have the equality
\[
\epsilon \sum_{j=1}^{n-1} \frac{1}{(S_j-S_i)^{3/2}(S_n-S_j)^{3/2}} \exp \left\{ -\frac{(\delta_i - \delta_j)^2}{2(S_n-S_j)} \right\} = \int_{S_i}^{S_n} dS_j \frac{1}{(S_j-S_i)^{3/2}(S_n-S_j)^{3/2}} \exp \left\{ -\frac{(\delta_i - \delta_j)^2}{2(S_n-S_j)} \right\},
\]  
and the two expressions only differ by terms that vanish as $\epsilon \to 0$. In fact, $\alpha$ can be fixed requiring that the coefficient of $1/\sqrt{\tau}$ is the same on the two sides of eq. (B23), and it does not affect the terms $O(\epsilon^0)$ since it just a rescaling of $\epsilon$. Actually, in our problem, an even better way to pass from the sum to the integral is to write
\[
\epsilon \sum_{j=1}^{n-1} \frac{1}{(S_j-S_i)^{3/2}(S_n-S_j)^{3/2}} \exp \left\{ -\frac{(\delta_i - \delta_j)^2}{2(S_n-S_j)} \right\} = \int_{S_i}^{S_n} dS_j \frac{1}{(S_j-S_i)^{3/2}(S_n-S_j)^{3/2}} \exp \left\{ -\frac{\alpha \epsilon}{2(S_n-S_j)} \frac{(\delta_i - \delta_j)^2}{2(S_n-S_j)} \right\}.
\]  
In other words, rather than setting the integrand to zero for $S_j < S_i + \alpha \epsilon$, we cut it off exponentially using the factor $\exp \{-\alpha \epsilon / (S_j - S_i)\}$. Again this produces a $1/\sqrt{\alpha \epsilon}$ singularity, as we will check in a moment, and $\alpha$ can be chosen so that this singularity has the same strength as that on the left-hand side of eq. (B24). However, since $\alpha$ is just a rescaling of $\epsilon$, $\alpha$ does not affect the finite part.

The advantage of using eq. (B24) is that the integral can now be performed analytically using eq. (A5), so we get
\[
I_3 = \epsilon \sum_{j=1}^{n-1} \frac{1}{(S_j-S_i)^{3/2}(S_n-S_j)^{3/2}} \exp \left\{ -\frac{(\delta_i - \delta_j)^2}{2(S_n-S_j)} \right\} = \sqrt{2\pi} \left[ \frac{1}{\alpha \epsilon \sqrt{\tau}} + \frac{1}{(S_n-S_i)} \int_{S_i}^{S_n} dS_j \frac{1}{(S_j-S_i)^{3/2}} \exp \left\{ -\frac{(\delta_i - \delta_j)^2}{2(S_n-S_j)} \right\} \right].
\]  
We have also checked this result numerically. The sum on the left-hand side can be computed very easily numerically, say for $n$ up to $10^4$, and we find that the right-hand side reproduces it perfectly, for all values of $\delta_i$, $S_i$ and $S_n$, if we choose $\alpha \simeq 0.92$. Expanding the dependence on $\alpha \epsilon$ in the exponential and omitting the terms that vanish in the limit $\epsilon \to 0$, we find
\[
I_3 = \sqrt{2\pi} \left[ \frac{1}{\alpha \epsilon \sqrt{\tau}} + \frac{1}{(S_n-S_i)} \int_{S_i}^{S_n} dS_j \frac{1}{(S_j-S_i)^{3/2}} \exp \left\{ -\frac{(\delta_i - \delta_j)^2}{2(S_n-S_j)} \right\} \right],
\]  
which explicitly displays the $1/\sqrt{\tau}$ singularity and the finite, $\alpha$-independent, part.

To compute $I_3$ we must still plug this expression into eq. (B17) and carry out the sum over $i$. The latter sum presents no difficulty since its argument converges well both at $S_i = 0$ and at $S_i = S_n$, so we can just replace the sum by an integral using eq. (106). It is actually convenient to leave $I_3$ in the form eq. (B25), so the integral over $S_i$ again can be performed using eq. (A5), and we finally get
\[
I_2 = \frac{2}{\pi} \left[ \frac{1}{S_n^{1/2}} e^{-(2\delta_i - \delta_n)^2/(2S_n)} \frac{2\delta_i - \delta_n}{\sqrt{\alpha \epsilon}} + \left( 1 - \frac{(2\delta_i - \delta_n)^2}{S_n} \right) \right].
\]  
Putting together this result and eq. (B16) we finally find
\[
\Pi_{\epsilon=0}^{\text{mem-mem}}(\delta_0; \delta_n; S_n) = \frac{1}{\sqrt{\epsilon}} \left( \frac{1}{\sqrt{\alpha \epsilon}} - u_0 \sqrt{2} \right) \left( (2\delta_i - \delta_n) \frac{1}{S_n^{1/2}} e^{-(2\delta_i - \delta_n)^2/(2S_n)} + \left( \frac{2}{\pi} \right)^{1/2} \left[ 1 - \frac{(2\delta_i - \delta_n)^2}{S_n} \right] \frac{1}{S_n^{1/2}} e^{-(2\delta_i - \delta_n)^2/(2S_n)} \right).
\]  
However, in this case we already know the exact result for $\Pi_{\epsilon=0}^{\text{mem-mem}}$, which is given by eq. (B12). Comparing these two results we learn the following. First, we know from eq. (B12) that the result is finite and there is no $1/\sqrt{\epsilon}$ term. In the computation leading to eq. (B28) we rather find two separately divergent contribution, so they must cancel. This is fully consistent with eq. (B28), since these divergent terms have exactly the same dependence on $\epsilon$, $\delta_i$, $\delta_n$, $S_i$ and $S_n$. We also see that, in this second way of performing the computation, the cancellation depends on the numerical values of quantities, such as $u_0$, that are determined by the solution in the boundary layer and, which therefore are difficult to compute, as well as on the constant $\alpha$ that we determined numerically. The finite part is instead completely fixed, and it is not affected by the solution in the boundary layer, nor by the constant $\alpha$, and correctly reproduces eq. (B12).

From this explicit example we can now extract a general rule of computation. Whenever $\Delta(S_i, S_j)$ is a regular function, such as that given in eq. (90), the memory-of-memory term and analogous quantities which are finite when $\Delta(S_i, S_j) = 1$, will be finite. The explicit computation with the formalism developed in Section 5.3 can generate terms that are separately divergent when $\epsilon \to 0^+$. However, since the total result is finite, these divergences must cancel among them. When we find integrals that diverge in the limit in which two integration variables become equal (such as the limit $S_j \to S_i$ above) we can just regularize them as in eq. (B24). We call this technique "the $\alpha$-regularization". Then we discard the divergence and we extract the finite part, which is independent of $\alpha$. We will indicate by the symbol $\mathcal{FP}$ this procedure of taking the finite part. In this notation, the result of the above computations can be summarized by
\[
\mathcal{FP} \sum_{i=1}^{n-1} \int_{-\infty}^{\delta_i} d\delta_i \ldots d\delta_{n-1} \delta_i^2 W = 0,
\]  
\[
\mathcal{FP} \sum_{i=1}^{n-1} \sum_{j=i+1}^{n-1} \int_{-\infty}^{\delta_i} d\delta_i \ldots d\delta_{n-1} d\delta_j W = \left( \frac{2}{\pi} \right)^{1/2} \left[ 1 - \frac{(2\delta_i - \delta_n)^2}{S_n} \right] \frac{1}{S_n^{1/2}} e^{-(2\delta_i - \delta_n)^2/(2S_n)}.
\]
As an application of the above formalism, we have studied what happens choosing a different expansion point when computing the halo mass function with a tophat filter in coordinate space. Observe in fact that, since $\Delta(S_i, S_j)$ is symmetric under exchange of $S_i$ with $S_j$, eq. (90), which is valid for $S_i \leq S_j$, can be rewritten more generally as

$$\Delta(S_i, S_j) \simeq \kappa \left[ \min(S_i, S_j) - \frac{[\min(S_i, S_j)]^2}{\max(S_i, S_j)} \right].$$

(B31)

Thus, the two-point correlator can be written as

$$\langle \delta_i \delta_j \rangle = (1 + \kappa) \min(S_i, S_j) + \tilde{\Delta}(S_i, S_j).$$

(B32)

where, for $S_i \leq S_j$, $\tilde{\Delta}(S_i, S_j) = -\kappa S_i^2 / S_j$. We can therefore use $(1 + \kappa) \min(S_i, S_j)$ as the unperturbed two-point function, and treat $\tilde{\Delta}_j$ as the perturbation. The zeroth order term can again be computed exactly, since it just amounts to a rescaling of $S, S \rightarrow (1 + \kappa)S$. At first sight this seems to give a modified exponential in the distribution function, since factors such as $\exp(-\Delta_i^2 / 2S^2)$ in eq. (57) becomes $\exp[-\Delta_i^2 / 2(1 + \kappa)S]$. However, now $\tilde{\Delta}_{ii} = -\kappa S_i$ is non-zero, and we should not forget the factor $\exp \{ (1/2) \Delta_{ii} \delta_i^2 \}$ in eq. (33). The effect of this term can be computed exactly using the identity

$$\exp \left\{ \frac{1}{2} (b-a) \delta_i^2 \right\} = \frac{1}{\sqrt{b}} e^{-x^2/(2b)},$$

(B33)

which is valid for $a > 0$ and $b > 0$. To prove it, we write

$$\exp \left\{ \frac{1}{2} (b-a) \delta_i^2 \right\} = \exp \left\{ \frac{1}{2} (b-a) \delta_i^2 \right\} \int_{-\infty}^{\infty} \frac{d\lambda}{2\pi} e^{i\lambda x - (1/2)a\lambda^2} = \int_{-\infty}^{\infty} \frac{d\lambda}{2\pi} \sum_{n=0}^{\infty} \frac{1}{n!} \left( \frac{b-a}{2} \right)^n \partial_n^2 e^{i\lambda x - (1/2)a\lambda^2}

= \int_{-\infty}^{\infty} \frac{d\lambda}{2\pi} \sum_{n=0}^{\infty} \frac{1}{n!} \left( \frac{b-a}{2} \right)^n \left( i\lambda \right)^n e^{i\lambda x - (1/2)a\lambda^2} = \int_{-\infty}^{\infty} \frac{d\lambda}{2\pi} e^{-(1/2)(b-a)\lambda^2} e^{i\lambda x - (1/2)a\lambda^2} \lambda^2

= \int_{-\infty}^{\infty} \frac{d\lambda}{2\pi} e^{i\lambda x - (1/2)b\lambda^2} = \frac{1}{\sqrt{b}} e^{-x^2/(2b)}.$$

(B34)

(Observe that for $b < 0$ the final integral over $d\lambda$ does not converge, so this identity only holds if $b > 0$). In this way, we find that the action of $\exp \{ (1/2) \Delta_{ii} \delta_i^2 \}$ on $\exp[-\Delta_i^2 / 2(1 + \kappa)S]$ gives back the “unperturbed” exponential factor $\exp[-\Delta_i^2 / 2S]$ so the zeroth-order term of this expansion is finally the same as eq. (57). The computation of the non-markovian corrections requires the finite part prescription, since now $\Delta(S_i, S_j)$ does not vanish for $S_i = S_j$. The integrals over $dS_i$ and $dS_j$ are more difficult to compute, but for $\delta_i^2 / S > 1$ their exponential dependence is easily computed and, after taking into again the operator $\exp \{ (1/2) \Delta_{ii} \delta_i^2 \}$ in eq. (33), we find that the exponential dependence of the corrections is the same that we obtained in eq. (119).

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