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### Abstract

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

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## 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 papers 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 with 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 top-hat 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 this paper to compute the effect of non-Gaussianities on the halo mass function.

*Key words:* cosmology: theory – dark matter – large-scale structure of universe

*Online-only material:* color figures

## 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, 2000; Moscardini et al. 1991; Koyama et al. 1999; Robinson & Baker 2000; 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.

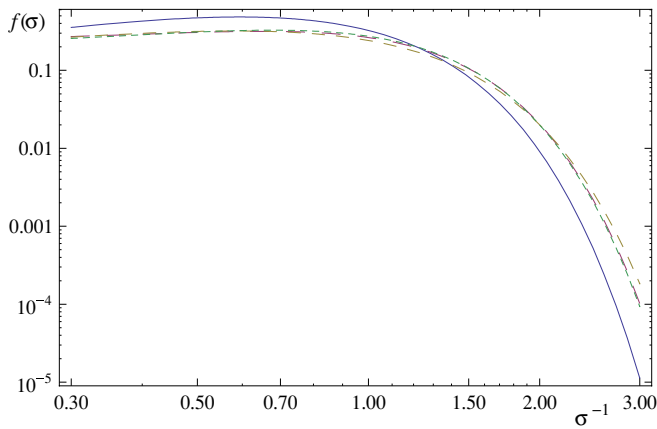
The formation and evolution of dark matter halos is a highly complex dynamical process, and a detailed understanding of it can only come through large-scale  $N$ -body simulations. Some analytical understanding is however also desirable, both for obtaining a better physical intuition, and for the flexibility 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 time-consuming numerical simulations.

Analytic techniques generally start by modeling 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, for Gaussian fluctuations the prediction of excursion set theory for the mass function already deviates 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



**Figure 1.** Log-log plot of the function  $f(\sigma)$ . The (blue) solid curve is the PS prediction  $f_{\text{PS}}(\sigma)$ . The three almost indistinguishable dashed lines are the Sheth–Tormen fit to the GIF simulation of Kauffmann et al. (1999), and the fit to the  $N$ -body simulations of Pillepich et al. (2009) and Warren et al. (2006). The fitting functions are summarized in Table 3 of Pillepich et al. (2009).

(A color version of this figure is available in the online journal.)

collapse model the function  $f(\sigma)$  is predicted to be

$$f_{\text{PS}}(\sigma) = \left(\frac{2}{\pi}\right)^{1/2} \frac{\delta_c}{\sigma} e^{-\delta_c^2/(2\sigma^2)}, \quad (2)$$

where  $\delta_c \simeq 1.686$  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. 2006; Lukic et al. 2007; Tinker et al. 2008; Pillepich et al. 2009; Robertson et al. 2009, and references therein). The results of these simulations have been represented by various fitting functions; see, e.g., Sheth & Tormen (1999) and Sheth et al. (2001). In Figure 1 we compare the function  $f_{\text{PS}}(\sigma)$  given in Equation (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 2, and too few high-mass halos: at  $\sigma^{-1} = 3$ , PS theory is already off by a factor  $\mathcal{O}(10)$ . 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 an order of magnitude.

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

1. 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 Equation (2).
2. 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 (1), it is well known that the original argument of Press and Schechter miscounts 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  $\delta_c \simeq 1.686$ .<sup>4</sup> Within PS theory, for Gaussian fluctuations the distribution probability for the density contrast is

$$\Pi_{\text{PS}}(\delta, S) = \frac{1}{\sqrt{2\pi S}} e^{-\delta^2/(2S)}, \quad (3)$$

where

$$S(R) \equiv \sigma^2(R) = \langle \delta^2(x, R) \rangle, \quad (4)$$

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

$$F_{\text{PS}}(R) = \int_{\delta_c}^{\infty} d\delta \Pi_{\text{PS}}(\delta, S(R)) = \frac{1}{2} \operatorname{erfc}\left(\frac{\nu(R)}{\sqrt{2}}\right), \quad (5)$$

where  $\nu(R) = \delta_c/\sigma(R)$ . 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  $R \rightarrow 0$ , so all the mass in the universe must finally be contained in virialized objects. Thus, we should have  $F_{\text{PS}}(0) = 1$ , while Equation (5) gives  $F_{\text{PS}}(0) = 1/2$ . Press and Schechter corrected this simply adding by hand an overall factor of 2.

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  $F_{\text{PS}}(R)$  since on the scale  $S$  it is below threshold. Thus, Equation (5) cannot be fully correct.

In Bond et al. (1991), 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 (FP) 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 Equation (2), including the factor of 2 that Press and Schechter were forced to introduce by hand.<sup>5</sup>

However, this procedure still raises some technical questions that will be reviewed in more detail in Section 2. In short,

<sup>4</sup> More precisely,  $\delta_c$  has a slight dependence on the cosmological model, and  $\delta_c = 1.686$  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). For  $\Omega_M \simeq 0.3$ ,  $\delta_c$  is between 1.67 and 1.68; see their Figure 1. This difference is however much smaller than other uncertainties in our computation.

<sup>5</sup> The work of Epstein (1983) also solves the cloud-in-cloud problem and recovers the correct factor of 2, though the process considered therein uses Poisson seeds for structure formation.

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, the probability does not satisfy any simple boundary condition (van Kampen & Oppenheim 1972; Knessl et al. 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  $M$  with a smoothing scale  $R$  is using a sharp filter in  $x$  space, proportional to  $\theta(R-r)$ , in which case one has the obvious relation  $M = (4/3)\pi R^3 \rho$ . This is also the relation used in numerical simulations. As soon as one uses a different filter (such as the top hat 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 FP 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 & Talkner 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.<sup>6</sup>

These issues become even more important when one considers the evolution with smoothing scale of non-Gaussian fluctuations, since non-Gaussianities 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-Gaussianities, from the non-Markovian contribution due to the filter function.

Concerning point (2) 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 Jeltrema et al. 2005 and references therein), which we will discuss in more detail in Maggiore & Riotto (2009a, Paper II).

In this series of papers, we examine systematically the above issues. In this 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 results: 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 Equation (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 top-hat filter in coordinate space. We find that the non-Markovian contributions do not alleviate the discrepancy with  $N$ -body simulations, rather, 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. In their classic paper, Bond et al. has already computed the result with a top-hat 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, an MC simulation of this kind has been done in Robertson et al. (2009), 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 neither 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 is itself a stochastic variable, whose scattering reflects a number of complicated aspects of the underlying dynamics.

Finally, in Maggiore & Riotto (2009b, Paper III of this series) we apply the formalism developed in this 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 Section 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.

<sup>6</sup> Similarly, even if the mathematical problem of solving the FP equation with a moving barrier is amenable to an elegant formulation (Zhang & Hui 2006), its application to the halo mass function suffers from the problem that for a general filter it is incorrect to assume that the probability  $\Pi(\delta, S)$  evolves according to the FP equation.

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 has been 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.

Consider the density contrast  $\delta(\mathbf{x}) = [\rho(\mathbf{x}) - \bar{\rho}]/\bar{\rho}$ , where  $\bar{\rho}$  is the mean mass density of the universe and  $\mathbf{x}$  is the comoving position, and smooth it on some scale  $R$ , defining

$$\delta(\mathbf{x}, R) = \int d^3x' W(|\mathbf{x} - \mathbf{x}'|, R) \delta(\mathbf{x}'), \tag{6}$$

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

$$\tilde{W}_{\text{sharp-}k}(k, k_f) = \theta(k_f - k), \tag{7}$$

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

$$\delta(\mathbf{x}, R) = \int \frac{d^3k}{(2\pi)^3} \tilde{\delta}(\mathbf{k}) \tilde{W}(k, R) e^{-i\mathbf{k}\cdot\mathbf{x}}, \tag{8}$$

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

$$\frac{\partial \delta(R)}{\partial R} = \zeta(R), \tag{9}$$

where

$$\zeta(R) \equiv \int \frac{d^3k}{(2\pi)^3} \tilde{\delta}(\mathbf{k}) \frac{\partial \tilde{W}(k, R)}{\partial R}. \tag{10}$$

Since the modes  $\tilde{\delta}(\mathbf{k})$  are stochastic variables,  $\zeta(R)$  is a stochastic variable too, and Equation (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 Equation (10) that also  $\zeta$  is Gaussian. The two-point function of  $\delta$  defines the power spectrum  $P(k)$ ,

$$\langle \tilde{\delta}(\mathbf{k}) \tilde{\delta}(\mathbf{k}') \rangle = (2\pi)^3 \delta_D(\mathbf{k} + \mathbf{k}') P(k). \tag{11}$$

From this it follows that

$$\langle \zeta(R_1) \zeta(R_2) \rangle = \int_{-\infty}^{\infty} d(\ln k) \Delta^2(k) \frac{\partial \tilde{W}(k, R_1)}{\partial R_1} \frac{\partial \tilde{W}(k, R_2)}{\partial R_2}, \tag{12}$$

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  $Q(k_f) = -(1/k_f)\zeta(k_f)$ , Equations (9) and (12) become

$$\frac{\partial \delta(k_f)}{\partial \ln k_f} = Q(k_f) \tag{13}$$

and

$$\langle Q(k_{F1}) Q(k_{F2}) \rangle = \Delta^2(k_{F1}) \delta_D(\ln k_{F1} - \ln k_{F2}). \tag{14}$$

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 Equation (4). Using Equation (8),

$$S(R) = \int_{-\infty}^{\infty} d(\ln k) \Delta^2(k) |\tilde{W}(k, R)|^2. \tag{15}$$

For a sharp  $k$ -space filter,  $S$  becomes

$$S(k_f) = \int_{-\infty}^{\ln k_f} d(\ln k) \Delta^2(k), \tag{16}$$

so

$$\frac{\partial S}{\partial \ln k_f} = \Delta^2(k_f). \tag{17}$$

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

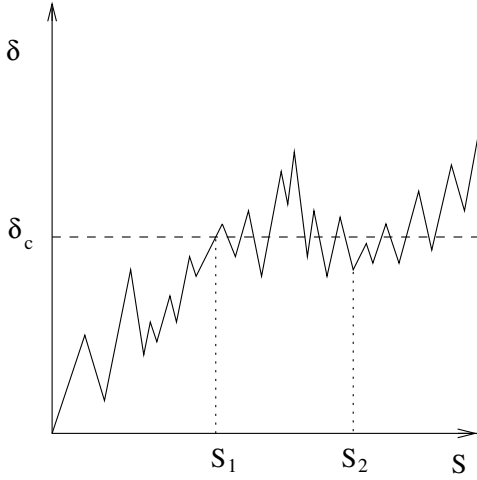
$$\frac{\partial \delta(S)}{\partial S} = \eta(S), \tag{18}$$

with

$$\langle \eta(S_1) \eta(S_2) \rangle = \delta(S_1 - S_2), \tag{19}$$

which is 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 Figure 2. If we compute the probability distribution at  $S = S_2$  as in PS theory, i.e., using Equation (5), this trajectory does not contribute to  $F_{\text{PS}}(R)$  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  $M(R_1) > M(R_2)$ . This virialized object has been lost in  $F_{\text{PS}}(R_2)$  evaluated through Equation (5), in spite of the fact that this formula was supposed to count all objects with mass greater than  $M(R_2)$ .

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



**Figure 2.** Trajectory that performs multiple up-crossings of the threshold at  $\delta = \delta_c$ .

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 (see, e.g., Risken 1984), if a stochastic process obeys the Langevin Equation (18) with a Dirac-delta noise Equation (19), the corresponding distribution function is a solution of the FP equation,

$$\frac{\partial \Pi}{\partial S} = \frac{1}{2} \frac{\partial^2 \Pi}{\partial \delta^2}. \tag{20}$$

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

$$\Pi^0(\delta, S) = \frac{1}{\sqrt{2\pi S}} e^{-\delta^2/(2S)}. \tag{21}$$

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

$$\Pi(\delta, S)|_{\delta=\delta_c} = 0. \tag{22}$$

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)

$$\Pi(\delta, S) = \frac{1}{\sqrt{2\pi S}} [e^{-\delta^2/(2S)} - e^{-(2\delta_c - \delta)^2/(2S)}], \tag{23}$$

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, Equation (23) is replaced by

$$\Pi(\delta_0; \delta; S) = \frac{1}{\sqrt{2\pi S}} [e^{-(\delta - \delta_0)^2/(2S)} - e^{-(2\delta_c - \delta_0 - \delta)^2/(2S)}]. \tag{24}$$

This result is easily understood writing  $2\delta_c - \delta_0 - \delta = 2(\delta_c - \delta_0) - (\delta - \delta_0)$ , so Equation (24) is obtained from Equation (23) performing the obvious replacement  $\delta \rightarrow \delta - \delta_0$ , and also  $\delta_c \rightarrow \delta_c - \delta_0$ , 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 than or equal to  $S$  cannot be written, as in Equation (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

$$F(S) = 1 - \int_{-\infty}^{\delta_c} d\delta \Pi(\delta, S). \tag{25}$$

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

$$F(S) = 1 - \int_{-\infty}^{\delta_c} d\delta \Pi^0(\delta, S) + \int_{-\infty}^{\delta_c} d\delta \Pi^0(2\delta_c - \delta, S). \tag{26}$$

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

$$1 - \int_{-\infty}^{\delta_c} d\delta \Pi^0(\delta, S) = \int_{\delta_c}^{\infty} d\delta \Pi^0(\delta, S). \tag{27}$$

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

$$\int_{-\infty}^{\delta_c} d\delta \Pi^0(2\delta_c - \delta, S) = \int_{\delta_c}^{\infty} d\delta' \Pi^0(\delta', S). \tag{28}$$

Thus, one obtains

$$F(S) = 2 \int_{\delta_c}^{\infty} d\delta \Pi^0(\delta, S) = \text{erfc}\left(\frac{\nu}{\sqrt{2}}\right), \tag{29}$$

where  $\nu = \delta_c/\sigma(M)$ , and one recovers the factor of 2 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  $\mathcal{F}(S)dS$ , with

$$\mathcal{F}(S) \equiv \frac{dF}{dS} = - \int_{-\infty}^{\delta_c} d\delta \frac{\partial \Pi}{\partial S}. \tag{30}$$

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

$$\mathcal{F}(S) = - \frac{1}{2} \frac{\partial \Pi}{\partial \delta} \Big|_{\delta=\delta_c} = \frac{\delta_c}{\sqrt{2\pi S^{3/2}}} e^{-\delta_c^2/(2S)}. \tag{31}$$

Observe that, in  $\delta = \delta_c$ ,  $\Pi(\delta, S)$  and all its derivatives of even order with respect to  $\delta$  vanish, while all its derivatives of odd order with respect to  $\delta$  are twice as large as the value for the single Gaussian (Equation (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 2 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 with the smoothing of  $\delta$  over a region of radius  $R$ . We discuss below the subtleties

associated with 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

$$\frac{dn}{dM}dM = \frac{\bar{\rho}}{M} \left| \frac{dF}{dM} \right| dM, \quad (32)$$

so

$$\frac{dn}{dM} = \frac{\bar{\rho}}{M} \frac{dF}{dS} \left| \frac{dS}{dM} \right| = \frac{\bar{\rho}}{M^2} \mathcal{F}(S) 2\sigma^2 \frac{d \ln \sigma^{-1}}{d \ln M}, \quad (33)$$

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

$$f(\sigma) = 2\sigma^2 \mathcal{F}(\sigma^2). \quad (34)$$

Using Equation (31) we get the halo mass function in PS theory (with the factor of 2 computed thanks to the excursion set theory),

$$\left( \frac{dn}{dM} \right)_{\text{PS}} = \left( \frac{2}{\pi} \right)^{1/2} \frac{\delta_c}{\sigma} e^{-\delta_c^2/(2\sigma^2)} \frac{\bar{\rho}}{M^2} \frac{d \ln \sigma^{-1}}{d \ln M}. \quad (35)$$

This is the result given in Equations (1) and (2).

The crucial point is how to associate a mass  $M$  with the filter scale  $R$ . For the sharp filter in  $x$  space this is clear. The mass associated with 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 with the filter as  $V = \int d^3x W'$ , and  $M = \rho V$ . This procedure seems reasonable, but still it is somewhat arbitrary, since one might as well chose 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 reads

$$W_{\text{sharp-}k}(r, R) = \frac{1}{2\pi^2 R^3} \frac{\sin u - u \cos u}{u^3}, \quad (36)$$

where  $u = r/R = k_f r$  and  $r = |\mathbf{x} - \mathbf{x}'|$ , which gives

$$W' = 3 \frac{\sin u - u \cos u}{u^3}, \quad (37)$$

and

$$V = 4\pi \int_0^\infty dr r^2 W' = 12\pi R^3 \int_0^\infty du \left[ \frac{\sin u}{u} - \cos u \right]. \quad (38)$$

The integral of  $\sin u/u$  gives  $\pi/2$ , but the limit for  $\Lambda \rightarrow \infty$  of the integral of  $\cos u$  from  $u = 0$  to  $u = \Lambda$  does not exist. If one just sets it to zero, without much justification, one finds the result  $V = 6\pi^2 R^3$  which is sometimes quoted (Lacey & Cole 1993). In any case, it is clear that it is difficult to give

unambiguous numerical predictions for the halo mass function with a filter different from the sharp  $x$ -space filter.

The standard practice in the literature is to use the PS mass function, which can be derived from excursion set theory but only if one works with a sharp  $k$ -space filter, and at the same time to use  $M = (4/3)\pi R^3 \rho$ , which is only valid for a sharp  $x$ -space filter. Of course, this is not consistent and cannot be a good starting point for the inclusion of the non-Gaussianities, since one would attribute to primordial non-Gaussianities features in the mass function which are due, more trivially, to the filter function.

In principle, one can determine the halo mass function with a top-hat filter in coordinate space by performing an MC realization of the trajectories obtained from a Langevin equation with colored noise (Bond et al. 1991; Robertson et al. 2009). However, our final aim is to get some analytic understanding of the effect of non-Gaussianities on the halo mass function, and for 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  $\langle \delta(S_1) \delta(S_2) \rangle_c$ , 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  $S_k = k\epsilon$  with  $k = 1, \dots, n$ , and  $S_n \equiv S$ . A trajectory is defined by the collection of values  $\{\delta_1, \dots, \delta_n\}$ , 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

$$W(\delta_0; \delta_1, \dots, \delta_n; S_n) \equiv \langle \delta_D(\delta(S_1) - \delta_1) \dots \delta_D(\delta(S_n) - \delta_n) \rangle, \quad (39)$$

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

$$\begin{aligned} \Pi_\epsilon(\delta_0; \delta_n; S_n) &\equiv \int_{-\infty}^{\delta_c} d\delta_1 \dots \int_{-\infty}^{\delta_c} d\delta_{n-1} \\ &\times W(\delta_0; \delta_1, \dots, \delta_{n-1}, \delta_n; S_n), \end{aligned} \quad (40)$$

where  $S_n = n\epsilon$ . So,  $\Pi_\epsilon(\delta_0; \delta; S)$  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  $\delta_c$ . Observe that the final point  $\delta$  ranges over  $-\infty < \delta < \infty$ . For later use, we find useful to write explicitly that  $\Pi$  depends also on the temporal discretization step  $\epsilon$ . We are finally interested in its continuum limit,  $\Pi_{\epsilon=0}$ , and we will see in due course that taking the limit  $\epsilon \rightarrow 0$  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

$$\int_{-\infty}^{\delta_c} d\delta \Pi_\epsilon(\delta_0; \delta; S) \quad (41)$$

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

$$\mathcal{F}(S) = - \int_{-\infty}^{\delta_c} d\delta \partial_S \Pi_\epsilon(\delta_0; \delta; S) \quad (42)$$

(where  $\partial_S = \partial/\partial S$ ), just as in Equation (30). The halo mass function is then obtained from this first-crossing rate using Equations (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  $\Pi_\epsilon(\delta_0; \delta; S)$ , in terms of the two-point correlator of the theory, we use the integral representation of the Dirac delta

$$\delta_D(x) = \int_{-\infty}^{\infty} \frac{d\lambda}{2\pi} e^{-i\lambda x}, \quad (43)$$

and write Equation (39) as

$$W(\delta_0; \delta_1, \dots, \delta_n; S_n) = \int_{-\infty}^{\infty} \frac{d\lambda_1}{2\pi} \dots \frac{d\lambda_n}{2\pi} e^{i \sum_{i=1}^n \lambda_i \delta_i} \times \langle e^{-i \sum_{i=1}^n \lambda_i \delta(S_i)} \rangle. \quad (44)$$

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,

$$\langle e^{-i \sum_{i=1}^n \lambda_i \delta(S_i)} \rangle = e^{-\frac{1}{2} \sum_{i,j=1}^n \lambda_i \lambda_j \langle \delta(S_i) \delta(S_j) \rangle_c}, \quad (45)$$

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 the sum of products of two-point correlators. This gives

$$W(\delta_0; \delta_1, \dots, \delta_n; S_n) = \int \mathcal{D}\lambda e^{i \sum_{i=1}^n \lambda_i \delta_i - \frac{1}{2} \sum_{i,j=1}^n \lambda_i \lambda_j \langle \delta_i \delta_j \rangle_c}, \quad (46)$$

where

$$\int \mathcal{D}\lambda \equiv \int_{-\infty}^{\infty} \frac{d\lambda_1}{2\pi} \dots \frac{d\lambda_n}{2\pi} \quad (47)$$

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

$$\begin{aligned} \Pi_\epsilon(\delta_0; \delta_n; S_n) &= \int_{-\infty}^{\delta_c} d\delta_1 \dots d\delta_{n-1} \int \mathcal{D}\lambda \\ &\times \exp \left\{ i \sum_{i=1}^n \lambda_i \delta_i - \frac{1}{2} \sum_{i,j=1}^n \lambda_i \lambda_j \langle \delta_i \delta_j \rangle_c \right\}. \end{aligned} \quad (48)$$

### 3.2. Gaussian Fluctuations with Sharp $k$ -space Filter

As we have seen in Section 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 (18) with a noise  $\eta(S)$  whose correlator is a Dirac delta (Equation (19)). Using as initial condition  $\delta_0 = 0$ , Equation (18) integrates to

$$\delta(S) = \int_0^S dS' \eta(S'), \quad (49)$$

so the two-point correlator is given by

$$\begin{aligned} \langle \delta(S_i) \delta(S_j) \rangle_c &= \int_0^{S_i} dS \int_0^{S_j} dS' \langle \eta(S) \eta(S') \rangle \\ &= \min(S_i, S_j) = \epsilon \min(i, j) \equiv \epsilon A_{ij}. \end{aligned} \quad (50)$$

Denoting by  $W^{\text{gm}}$  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 Equations (18) and (19), we get

$$\begin{aligned} W^{\text{gm}}(\delta_0; \delta_1, \dots, \delta_n; S_n) &= \int_{-\infty}^{\infty} \frac{d\lambda_1}{2\pi} \dots \frac{d\lambda_n}{2\pi} \exp \left\{ i \sum_{i=1}^n \lambda_i \delta_i - \frac{\epsilon}{2} \sum_{i,j=1}^n A_{ij} \lambda_i \lambda_j \right\} \\ &= \frac{1}{(2\pi\epsilon)^{n/2}} \frac{1}{(\det A)^{1/2}} \exp \left\{ -\frac{1}{2\epsilon} \sum_{i,j=1}^n \delta_i (A^{-1})_{ij} \delta_j \right\}. \end{aligned} \quad (51)$$

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

$$\begin{aligned} W^{\text{gm}}(\delta_0 = 0; \delta_1, \dots, \delta_n; S_n) &= \frac{1}{(2\pi\epsilon)^{n/2}} \exp \left\{ -\frac{1}{2\epsilon} \left[ \delta_n^2 + 2 \sum_{i=1}^{n-1} \delta_i (\delta_i - \delta_{i+1}) \right] \right\}. \end{aligned} \quad (52)$$

This expression takes a more familiar form using the identity  $2\delta_i(\delta_i - \delta_{i+1}) = (\delta_{i+1} - \delta_i)^2 - (\delta_{i+1}^2 - \delta_i^2)$ , together with  $\sum_{i=1}^{n-1} (\delta_{i+1}^2 - \delta_i^2) = \delta_n^2 - \delta_1^2$ . Recall also that Equation (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  $\delta_1^2 \rightarrow \delta_1^2 - \delta_0^2$ . Thus, for  $\delta_0$  arbitrary, we get

$$W^{\text{gm}}(\delta_0; \delta_1, \dots, \delta_n; S_n) = \frac{1}{(2\pi\epsilon)^{n/2}} \exp \left\{ -\frac{1}{2\epsilon} \sum_{i=0}^{n-1} (\delta_{i+1} - \delta_i)^2 \right\}. \quad (53)$$

Observe that  $W^{\text{gm}}(\delta_0; \delta_1, \dots, \delta_n; S_n) d\delta_1 \dots d\delta_{n-1}$  is just the Wiener measure (see, e.g., chapter 1 of Chaichian & Demichev 2001). From Equation (53) we see that

$$\begin{aligned} W^{\text{gm}}(\delta_0; \delta_1, \dots, \delta_n; S_n) &= \Psi_\epsilon(\delta_n - \delta_{n-1}) \\ &\times W^{\text{gm}}(\delta_0; \delta_1, \dots, \delta_{n-1}; S_{n-1}), \end{aligned} \quad (54)$$



where

$$\Psi_\epsilon(\Delta\delta) = \frac{1}{(2\pi\epsilon)^{1/2}} \exp\left\{-\frac{(\Delta\delta)^2}{2\epsilon}\right\}. \quad (55)$$

Equation (54) expresses the fact that the evolution determined by Equations (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 Equation (54) over  $\delta_1, \dots, \delta_{n-1}$  from  $-\infty$  to  $\delta_c$  we get the important relation

$$\begin{aligned} \Pi_\epsilon^{\text{gm}}(\delta_0; \delta_n; S_n) &= \int_{-\infty}^{\delta_c} d\delta_{n-1} \Psi_\epsilon(\delta_n - \delta_{n-1}) \\ &\times \Pi_\epsilon^{\text{gm}}(\delta_0; \delta_{n-1}; S_{n-1}), \end{aligned} \quad (56)$$

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

$$\Pi_{\epsilon=0}^{\text{gm}}(\delta_0; \delta; S) = \frac{1}{\sqrt{2\pi S}} \left[ e^{-(\delta-\delta_0)^2/(2S)} - e^{-(2\delta_c-\delta_0-\delta)^2/(2S)} \right]. \quad (57)$$

We want to prove Equation (57) using our definition of  $\Pi_\epsilon$  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 an FP equation with an “absorbing barrier” boundary condition  $\Pi(\delta_0; \delta; S)|_{\delta=\delta_c} = 0$ . While the fact that  $\Pi_{\epsilon=0}$  obeys an FP equation follows from Equation (18), 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  $\Pi_\epsilon(\delta_0; \delta; S)$  does not satisfy any simple boundary condition (van Kampen & Oppenheim 1972; Knessl et al. 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 Equation (57). Then, we examine the finite- $\epsilon$  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  $\Pi_\epsilon^{\text{gm}}$  by performing directly the integrals over  $\delta_1, \dots, \delta_{n-1}$  in Equation (40), and then taking the limit  $\epsilon \rightarrow 0$  is very difficult, since the integrals in Equation (40) run only

up to  $\delta_c$ , and already the inner integral gives an error function whose argument involves the next integration variable.

A better strategy is to make use of Equation (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  $S_{n-1} = S$ , so  $S_n = S + \epsilon$ . For fixed  $\delta$ , we have  $d\delta_{n-1} = -d(\Delta\delta)$ , and Equation (56) becomes<sup>7</sup>

$$\Pi_\epsilon^{\text{gm}}(\delta_0; \delta; S + \epsilon) = \int_{\delta-\delta_c}^{\infty} d(\Delta\delta) \Psi_\epsilon(\Delta\delta) \Pi_\epsilon^{\text{gm}}(\delta_0; \delta - \Delta\delta; S). \quad (58)$$

In the limit  $\epsilon \rightarrow 0$  we have  $\Psi_\epsilon(\Delta\delta) \rightarrow \delta_D(\Delta\delta)$ , so to zeroth order in  $\epsilon$  Equation (58) gives

$$\Pi_{\epsilon=0}^{\text{gm}}(\delta_0; \delta; S) = \int_{\delta-\delta_c}^{\infty} d(\Delta\delta) \delta_D(\Delta\delta) \Pi_{\epsilon=0}^{\text{gm}}(\delta_0; \delta - \Delta\delta; S). \quad (59)$$

If  $\delta - \delta_c < 0$ , the integral includes the support of the Dirac delta, and we just get the trivial identity that  $\Pi_{\epsilon=0}^{\text{gm}}(\delta_0; \delta; S)$  is equal to itself. However, if  $\delta - \delta_c > 0$ , the right-hand side vanishes and we get  $\Pi_{\epsilon=0}^{\text{gm}}(\delta_0; \delta; S) = 0$ . 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  $\Pi_{\epsilon=0}^{\text{gm}}(\delta_0; \delta; S) = (1/2)\Pi_{\epsilon=0}^{\text{gm}}(\delta_0; \delta; S)$ , which again implies  $\Pi_{\epsilon=0}^{\text{gm}}(\delta_0; \delta; S) = 0$ . Therefore, we find that

$$\Pi_{\epsilon=0}^{\text{gm}}(\delta_0; \delta; S) = 0 \quad \text{if } \delta \geq \delta_c. \quad (60)$$

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

Consider now Equation (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  $\Pi_\epsilon^{\text{gm}}(\delta_0; \delta; S + \epsilon)$  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

$$\begin{aligned} \Pi_\epsilon^{\text{gm}}(\delta_0; \delta; S + \epsilon) &= \Pi_\epsilon^{\text{gm}}(\delta_0; \delta; S) + \epsilon \frac{\partial \Pi_\epsilon^{\text{gm}}(\delta_0; \delta; S)}{\partial S} \\ &+ \frac{\epsilon^2}{2} \frac{\partial^2 \Pi_\epsilon^{\text{gm}}(\delta_0; \delta; S)}{\partial S^2} + \dots, \end{aligned} \quad (61)$$

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

$$\begin{aligned} &\int_{\delta-\delta_c}^{\infty} d(\Delta\delta) \Psi_\epsilon(\Delta\delta) \Pi_\epsilon^{\text{gm}}(\delta_0; \delta - \Delta\delta; S) \\ &= \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \frac{\partial^n \Pi_\epsilon^{\text{gm}}(\delta_0; \delta; S)}{\partial S^n} \int_{\delta-\delta_c}^{\infty} d(\Delta\delta) (\Delta\delta)^n \Psi_\epsilon(\Delta\delta). \end{aligned} \quad (62)$$

Using Equation (55) we see that

$$\int_{\delta-\delta_c}^{\infty} d(\Delta\delta) (\Delta\delta)^n \Psi_\epsilon(\Delta\delta) = \frac{(2\epsilon)^{n/2}}{\sqrt{\pi}} \int_{-(\delta_c-\delta)/\sqrt{2\epsilon}}^{\infty} dy y^n e^{-y^2}. \quad (63)$$

<sup>7</sup> 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.

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  $\epsilon \rightarrow 0^+$ , and

$$\begin{aligned} \int_{-(\delta_c - \delta)/\sqrt{2\epsilon}}^{\infty} dy y^n e^{-y^2} &= \int_{-\infty}^{\infty} dy y^n e^{-y^2} + \mathcal{O}(e^{-(\delta_c - \delta)^2/(2\epsilon)}) \\ &= \frac{1 + (-1)^n}{2} \frac{\sqrt{\pi}}{2^{n/2}} (n - 1)!! + \mathcal{O}(e^{-(\delta_c - \delta)^2/(2\epsilon)}). \end{aligned} \quad (64)$$

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

$$\int_{\delta - \delta_c}^{\infty} d(\Delta\delta) (\Delta\delta)^n \Psi_{\epsilon}(\Delta\delta) \rightarrow \epsilon^{n/2} (n - 1)!!, \quad (65)$$

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

$$\begin{aligned} \Pi_{\epsilon}^{\text{gm}}(\delta_0; \delta; S) + \epsilon \frac{\partial \Pi_{\epsilon}^{\text{gm}}(\delta_0; \delta; S)}{\partial S} + \frac{\epsilon^2}{2} \frac{\partial^2 \Pi_{\epsilon}^{\text{gm}}(\delta_0; \delta; S)}{\partial S^2} + \dots \\ = \Pi_{\epsilon}^{\text{gm}}(\delta_0; \delta; S) + \frac{\epsilon}{2} \frac{\partial^2 \Pi_{\epsilon}^{\text{gm}}(\delta_0; \delta; S)}{\partial \delta^2} \\ + \frac{\epsilon^2}{8} \frac{\partial^4 \Pi_{\epsilon}^{\text{gm}}(\delta_0; \delta; S)}{\partial \delta^4} + \dots \end{aligned} \quad (66)$$

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

$$\begin{aligned} \Pi_{\epsilon}^{\text{gm}}(\delta_0; \delta; S) &= \Pi_{\epsilon=0}^{\text{gm}}(\delta_0; \delta; S) + \epsilon \Pi_{(1)}^{\text{gm}}(\delta_0; \delta; S) \\ &\quad + \epsilon^2 \Pi_{(2)}^{\text{gm}}(\delta_0; \delta; S) + \dots, \end{aligned} \quad (67)$$

where  $\Pi_{(1)}^{\text{gm}}$ ,  $\Pi_{(2)}^{\text{gm}}$ , etc., are functions independent of  $\epsilon$ . We can now collect the terms with the same power of  $\epsilon$  in the expansion of Equation (66). To order  $\epsilon$  we find

$$\frac{\partial \Pi_{\epsilon=0}^{\text{gm}}(\delta_0; \delta; S)}{\partial S} - \frac{1}{2} \frac{\partial^2 \Pi_{\epsilon=0}^{\text{gm}}(\delta_0; \delta; S)}{\partial \delta^2} = 0. \quad (68)$$

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

#### 4.2. Finite- $\epsilon$ 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  $\Pi_{\epsilon}^{\text{gm}}(\delta_0; \delta_c; S)$  approaches zero when  $\epsilon \rightarrow 0$ . It is therefore of great importance for us to understand the finite- $\epsilon$  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  $\delta_c - \delta$  is finite and strictly positive, we have seen that the expansion (Equation (67)) applies, so the first correction to the continuum result is  $\mathcal{O}(\epsilon)$  and is given by  $\epsilon \Pi_{(1)}^{\text{gm}}$ . Collecting the next-to-leading terms in Equation (66), we find that  $\Pi_{(1)}^{\text{gm}}$  satisfies an FP equation with the second time derivative of  $\Pi_{\epsilon=0}^{\text{gm}}$  as a source term,

$$\frac{\partial \Pi_{(1)}^{\text{gm}}(\delta_0; \delta; S)}{\partial S} - \frac{1}{2} \frac{\partial^2 \Pi_{(1)}^{\text{gm}}(\delta_0; \delta; S)}{\partial \delta^2} = \frac{1}{4} \frac{\partial^2 \Pi_{\epsilon=0}^{\text{gm}}(\delta_0; \delta; S)}{\partial S^2}. \quad (69)$$

In the above derivation, a crucial point was that we could extend to  $-\infty$  the lower integration limit in Equation (63). This is correct if we take the limit  $\epsilon \rightarrow 0^+$  with  $\delta_c - \delta$  fixed and positive. The situation changes at  $\delta = \delta_c$ , since in this case the lower limit of the integral is zero, rather than  $-\infty$ . In this case

$$\int_0^{\infty} d(\Delta\delta) (\Delta\delta) \Psi_{\epsilon}(\Delta\delta) = \left(\frac{\epsilon}{2\pi}\right)^{1/2} \quad (70)$$

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

$$\int_0^{\infty} d(\Delta\delta) \Psi_{\epsilon}(\Delta\delta) = \frac{1}{2}, \quad (71)$$

so the expansion of Equation (58) now gives

$$\begin{aligned} \Pi_{\epsilon}^{\text{gm}}(\delta_0; \delta_c; S) &= \frac{1}{2} \Pi_{\epsilon}^{\text{gm}}(\delta_0; \delta_c; S) \\ &\quad - \left(\frac{\epsilon}{2\pi}\right)^{1/2} \frac{\partial \Pi_{\epsilon}^{\text{gm}}(\delta_0; \delta; S)}{\partial \delta} \Big|_{x=\delta_c} + \dots \end{aligned} \quad (72)$$

This indicates that  $\Pi_{\epsilon}^{\text{gm}}(\delta_0; \delta_c; S)$  is  $\mathcal{O}(\epsilon^{1/2})$ , rather than  $\mathcal{O}(\epsilon)$ . However, Equation (72) is not a good starting point for a quantitative evaluation of  $\Pi_{\epsilon}^{\text{gm}}(\delta_0; \delta_c; S)$  since, as we show in Appendix A, the expansion in derivatives becomes singular in  $\delta = \delta_c$ , and all terms denoted by the dots in Equation (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 integral,  $(\delta_c - \delta)/\sqrt{2\epsilon}$ . The transition from the behavior  $\mathcal{O}(\epsilon)$  valid for  $\delta_c - \delta$  fixed and positive, to the behavior  $\mathcal{O}(\epsilon^{1/2})$  valid at  $\delta = \delta_c$  takes place in a “boundary layer,” consisting of the region where  $\delta_c - \delta$  is positive and  $\mathcal{O}(\epsilon^{1/2})$ , and the lower limit of the integral is  $\mathcal{O}(1)$ . 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 et al. 1986, where a very similar situation is discussed in terms of the means first-passage time, rather than in terms of the distribution function  $\Pi_{\epsilon}^{\text{gm}}$ ). Namely, we introduce a “stretched variable”  $\eta$  (not to be confused, of course, with the noise  $\eta(t)$  of Equation (18))

$$\eta = \frac{\delta_c - \delta}{\sqrt{2\epsilon}}, \quad (73)$$

which even as  $\epsilon \rightarrow 0^+$  is at most of order one inside the boundary layer, and we write  $\Pi_{\epsilon}^{\text{gm}}(\delta_0; \delta; S)$  in the form

$$\Pi_{\epsilon}^{\text{gm}}(\delta_0; \delta; S) = C_{\epsilon}(\delta_0; \delta; S) u(\eta), \quad (74)$$

where  $C_{\epsilon}(\delta_0; \delta; S)$  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  $\lim_{\eta \rightarrow \infty} u(\eta) = 1$ , so  $C_{\epsilon}$  is just the solution for  $\Pi_{\epsilon}^{\text{gm}}$  valid when  $\delta_c - \delta$  is finite and positive, i.e.,  $C_{\epsilon}$  is given by Equation (67). Writing  $\delta = \delta_c - \eta\sqrt{2\epsilon}$  (and setting for notational simplicity  $\delta_0 = 0$ ) we have

$$\begin{aligned} C_{\epsilon}(\delta_0 = 0; \delta; S) &= \frac{1}{\sqrt{2\pi S}} \\ &\times \left[ \exp\left\{-\frac{1}{2S}(\delta_c - \eta\sqrt{2\epsilon})^2\right\} - \exp\left\{-\frac{1}{2S}(\delta_c + \eta\sqrt{2\epsilon})^2\right\} \right], \end{aligned} \quad (75)$$

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

$$C_\epsilon(\delta_0 = 0; \delta; S) = \sqrt{\epsilon} \frac{2\eta}{\sqrt{\pi}} \frac{\delta_c}{S^{3/2}} e^{-\delta_c^2/(2S)} + \mathcal{O}(\epsilon). \quad (76)$$

Plugging this result in Equation (74) and sending  $\delta \rightarrow \delta_c^-$  we find

$$\Pi_\epsilon^{\text{gm}}(\delta_0; \delta_c; S) = \sqrt{\epsilon} \gamma \frac{\delta_c}{S^{3/2}} e^{-\delta_c^2/(2S)} + \mathcal{O}(\epsilon), \quad (77)$$

where

$$\gamma = \frac{2}{\sqrt{\pi}} \lim_{\eta \rightarrow 0} \eta u(\eta). \quad (78)$$

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

$$\Pi_\epsilon^{\text{gm}}(\delta_0; \delta_c; S) = \sqrt{\epsilon} \frac{1}{\sqrt{\pi}} \frac{\delta_c - \delta_0}{S^{3/2}} e^{-(\delta_c - \delta_0)^2/(2S)} + \mathcal{O}(\epsilon). \quad (79)$$

Similarly, for  $\delta_n < \delta_c$ ,

$$\Pi_\epsilon^{\text{gm}}(\delta_c; \delta_n; S) = \sqrt{\epsilon} \frac{1}{\sqrt{\pi}} \frac{\delta_c - \delta_n}{S^{3/2}} e^{-(\delta_c - \delta_n)^2/(2S)} + \mathcal{O}(\epsilon). \quad (80)$$

Observe that at the numerator of Equations (79) and (80) always enters the absolute value of the difference of the first two arguments of  $\Pi_\epsilon^{\text{gm}}$ , i.e.,  $\delta_c - \delta_0$  in Equation (79) and  $\delta_c - \delta_n$  in Equation (80), as it is also obvious from the fact that  $\Pi_\epsilon^{\text{gm}}$  is definite 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  $\Pi_\epsilon^{\text{gm}}(\delta_0; \delta; S)$  for  $\delta$  larger than  $\delta_c$ , with  $\delta - \delta_c$  finite (and, as always in this section,  $\delta_0 < \delta_c$ ). In this case the lower integration limit in Equation (63) goes to  $+\infty$  as  $\epsilon \rightarrow 0^+$  and

$$\Pi_\epsilon^{\text{gm}}(\delta_0; \delta; S) \sim \frac{1}{\sqrt{2\pi\epsilon}} \exp\{-(\delta_c - \delta)^2/(2\epsilon)\}. \quad (81)$$

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

### 5. EXTENSION OF EXCURSION SET THEORY TO GENERIC FILTER

We next consider the computation of the distribution function  $\Pi_\epsilon$ , 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  $\{\delta_1, \dots, \delta_n\}$ , such that  $\delta(S_k) = \delta_k$ .

The distribution function for Gaussian fluctuations and arbitrary filter function is given by Equation (48). As we saw in the previous section, in the Markovian case  $\Pi_\epsilon$  satisfies a local differential equation, namely the FP equation. It is instructive to understand that, for a generic filter, it is no longer possible to write a local diffusion equation for  $\Pi_\epsilon(\delta_0; \delta_n; S_n)$ . 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 Equation (48), we get

$$\frac{\partial}{\partial S_n} \Pi_\epsilon(\delta_0; \delta_n; S_n) = \frac{1}{2} \sum_{k,l=1}^n \frac{\partial \langle \delta_k \delta_l \rangle_c}{\partial S_n} \times \int_{-\infty}^{\delta_c} d\delta_1 \dots d\delta_{n-1} \partial_k \partial_l W(\delta_0; \delta_1, \dots, \delta_n; S_n), \quad (82)$$

where  $\partial_k \equiv \partial/\partial\delta_k$ , and we used the fact that, acting on  $\exp\{i \sum_{i=1}^n \lambda_i \delta_i\}$ ,  $\partial_k$  gives  $i\lambda_k$ . Therefore, separating the term with  $k = l = n$  from the rest, and observing that  $\langle \delta(S_k) \delta(S_l) \rangle_c$  depends on  $S_n$  only if at least one of the two indices  $k$  or  $l$  is equal to  $n$ , we get

$$\frac{\partial}{\partial S_n} \Pi_\epsilon(\delta_0; \delta_n; S_n) = \frac{1}{2} \frac{\partial^2}{\partial \delta_n^2} \Pi_\epsilon(\delta_0; \delta_n; S_n) + \sum_{k=1}^{n-1} \frac{\partial \langle \delta_k \delta_n \rangle_c}{\partial S_n} \partial_n \int_{-\infty}^{\delta_c} d\delta_1 \dots d\delta_{n-1} \partial_k W(\delta_0; \delta_1, \dots, \delta_n; S_n). \quad (83)$$

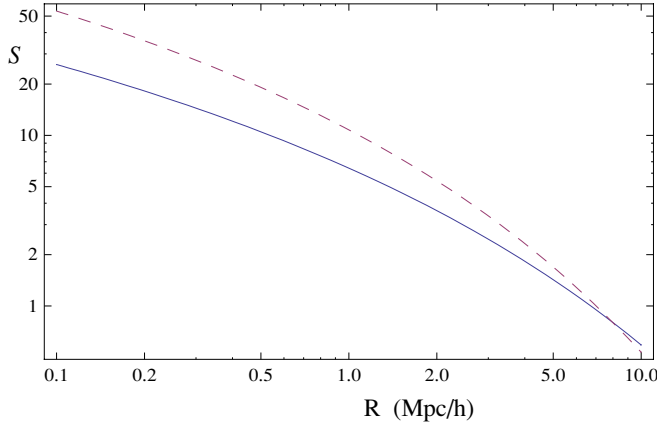
If the upper limit of the integrals were  $+\infty$ , rather than  $\delta_c$ , the term proportional to  $\partial_k W$  with  $k < n$  would give zero, since it is a total derivative with respect to one of the integration variables  $d\delta_1, \dots, d\delta_{n-1}$ , and  $W$  vanishes exponentially when any of its arguments  $\delta_k$  goes to  $\pm\infty$ . Thus, one would remain with the FP equation. However, when the upper limit  $\delta_c$  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  $\langle \delta_k \delta_n \rangle_c = \min(S_k, S_n) = S_k$ , which is independent of  $S_n$  for  $k < n$ . Therefore,  $\partial \langle \delta_k \delta_n \rangle_c / \partial S_n = 0$ , and the term in the second line of Equation (83) vanishes. This is another way of showing that, in the continuum limit, for sharp  $k$ -space filter the probability distribution satisfies an FP equation, as we already found in Section 4.1.<sup>8</sup>

For a generic form of the two-point correlator, the term in the second line of Equation (83) is non-vanishing, and in general it is very complicated. Furthermore, in the continuum limit the sum over  $k$  in Equation (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  $\Pi_\epsilon(\delta_0; \delta_n; S_n)$  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 top-hat 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 Equation (83).

In this section, we develop such a perturbative scheme. We illustrate the computation of  $\Pi_\epsilon(\delta_0; \delta_n; S_n)$  using a top-hat 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 a top-hat 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.

<sup>8</sup> Note however that this only holds in the continuum limit, as is implicit in the fact that we are taking the derivative with respect to  $S_n$ , which means that we are considering  $S_n$  has a continuous variable.



**Figure 3.** Functions  $S(R)$  computed for a top-hat filter in coordinate space (blue solid curve) and  $S(R)$  computed for sharp  $k$ -space filter (violet, dashed), against  $R$ , on a log–log scale.

(A color version of this figure is available in the online journal.)

### 5.1. The Two-point Correlator with Top-hat Filter in Coordinate Space

We first study the correlator  $\langle \delta(R_1)\delta(R_2) \rangle$  with a top-hat filter in coordinate space. We use Equation (8) with  $\mathbf{x} = 0$ . The two-point correlator of the non-smoothed density contrast is given in Equation (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

$$\langle \delta(R_1)\delta(R_2) \rangle = \frac{1}{2\pi^2} \int_0^\infty dk k^2 P(k) T^2(k) \tilde{W}(k, R_1) \tilde{W}^*(k, R_2). \quad (84)$$

When  $R_1 = R_2 = R$ , this reduces to  $S(R)$ . We consider a primordial spectrum  $P(k) = Ak^{n_s}$ , 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  $h = 0.7$ ,  $\Omega_M = 1 - \Omega_\Lambda = 0.28$ ,  $\Omega_B = 0.046$ , and  $n_s = 0.96$ , consistent with the *WMAP* 5 years data release.

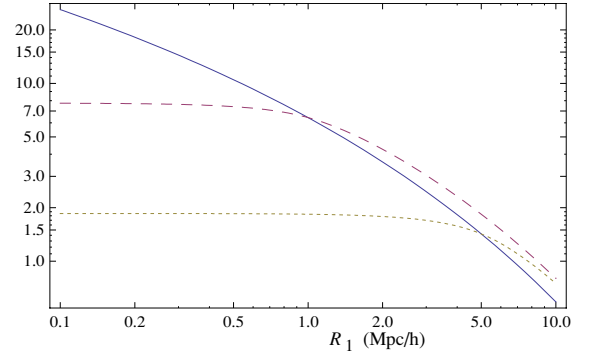
We first study  $S(R)$ . We compute the integral in Equation (15) numerically, for different values of  $R$ , both with the sharp  $k$ -space filter (Equation (7)) with  $k_f = 1/R$ , and with the top-hat filter in coordinate  $x$  space, whose Fourier transform is

$$\tilde{W}_{\text{sharp-}x}(k, R) = 3 \frac{\sin(kR) - kR \cos(kR)}{(kR)^3}. \quad (85)$$

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 Figure 3.

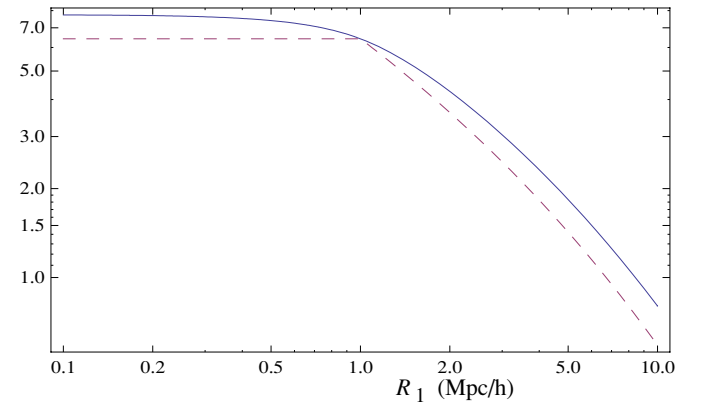
We consider next the correlator (Equation (84)) with the top-hat filter in coordinate space. We compute the integral in Equation (84) numerically, holding  $R_2$  fixed and varying  $R_1$ . The result is shown in Figure 4. The solid line is the function  $S(R_1)$ , already shown in Figure 3. The dashed line is  $\langle \delta(R_1)\delta(R_2) \rangle$  with  $R_2 = 1 \text{ Mpc } h^{-1}$ , as a function of  $R_1$ , while the dotted line is  $\langle \delta(R_1)\delta(R_2) \rangle$  with  $R_2 = 5 \text{ Mpc } h^{-1}$ , again as a function of  $R_1$ . We see that, as long as  $R_1 < R_2$ , 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,

$$\langle \delta(R_1)\delta(R_2) \rangle \simeq \min(S(R_1), S(R_2)). \quad (86)$$



**Figure 4.** Quantity  $S(R_1)$  for a top-hat filter in coordinate space (blue solid curve), the correlator  $\langle \delta(R_1)\delta(R_2) \rangle$  with  $R_2 = 1 \text{ Mpc } h^{-1}$  (violet dashed line) and  $\langle \delta(R_1)\delta(R_2) \rangle$  with  $R_2 = 5 \text{ Mpc } h^{-1}$  (brown dotted line), as functions of  $R_1$ .

(A color version of this figure is available in the online journal.)



**Figure 5.** Correlator  $\langle \delta(R_1)\delta(R_2) \rangle$  (blue solid line), compared to  $\min(S(R_1), S(R_2))$  (violet, dashed). In both cases  $R_2 = 1 \text{ Mpc } h^{-1}$ , and we plot the functions against  $R_1$ , measured in  $\text{Mpc } h^{-1}$ .

(A color version of this figure is available in the online journal.)

In Figure 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 that a function  $C(R_1, R_2)$  be defined from

$$\langle \delta(R_1)\delta(R_2) \rangle = \min(S(R_1), S(R_2)) + C(R_1, R_2). \quad (87)$$

As we see from Figure 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

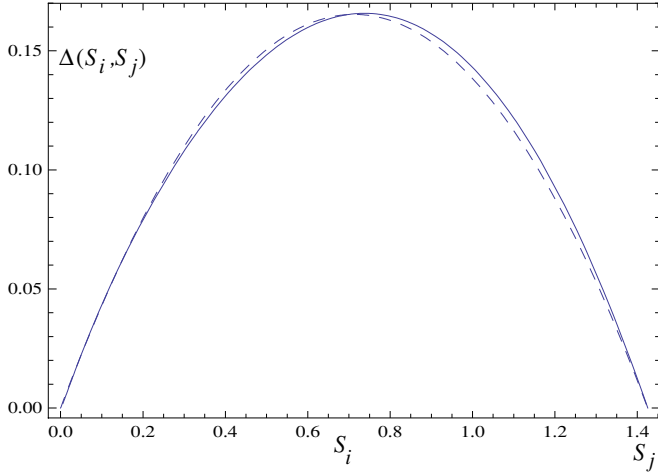
$$\Delta(S_1, S_2) = C(R(S_1), R(S_2)), \quad (88)$$

and we can write

$$\langle \delta_i \delta_j \rangle = \min(S_i, S_j) + \Delta(S_i, S_j). \quad (89)$$

If one simply neglects  $\Delta(S_i, S_j)$ , i.e., one makes the approximation (86), the problems become formally identical to the one that we have solved in Section 4. Therefore, we end up with the standard excursion set theory result given in Equation (23), and therefore with the PS mass function, in which  $S$  is simply the variance computed with the filter of our choice, in this case the top-hat filter in coordinate space. The corrections to this result are due to  $\Delta(S_i, S_j)$ , so it is useful first of all to better understand the form of this function.

By definition  $\Delta(S_i, S_j)$  is symmetric,  $\Delta(S_i, S_j) = \Delta(S_j, S_i)$ , so it is sufficient to study it for  $S_i \leq S_j$ . We also use the notation  $\Delta_i = \Delta(S_i, S_j)$ . Since, by definition,  $\langle \delta_i^2 \rangle = S_i$ , we



**Figure 6.** Function  $\Delta(S_i, S_j)$  for the top-hat filter in coordinate space (solid line), with  $S_j \simeq 1.42$  (corresponding to  $R(S_j) = 5 \text{ Mpc } h^{-1}$ ), plotted against  $S_i$ , in the range  $0 \leq S_i \leq S_j$ , and the function  $\kappa S_i (S_j - S_i) / S_j$  with  $\kappa \simeq 0.45$  (dashed line).

(A color version of this figure is available in the online journal.)

see from Equation (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  $\langle \delta_i \delta_j \rangle_c = \delta_0 \langle \delta_j \rangle_c = 0$ , and therefore  $\Delta(S_i, S_j)$  vanishes when  $S_i = 0$ .

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

$$\Delta(S_i, S_j) \simeq \kappa \frac{S_i (S_j - S_i)}{S_j}, \quad (90)$$

with  $\kappa \simeq 0.45$  (a more accurate value will be given below). We see that Equation (90) provides an excellent analytical approximation to  $\Delta(S_i, S_j)$ .<sup>9</sup>

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

$$\kappa(R) = \lim_{R' \rightarrow \infty} \frac{\langle \delta(R') \delta(R) \rangle}{\langle \delta^2(R') \rangle} - 1. \quad (91)$$

In the  $\Lambda$ CDM 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  $R \in [1, 60] \text{ Mpc } h^{-1}$ , the result of the numerical evaluation of Equation (91) is very well fitted by

$$\kappa(R) \simeq 0.4592 - 0.0031 R, \quad (92)$$

where  $R$  is measured in  $\text{Mpc } h^{-1}$ .<sup>10</sup>

<sup>9</sup> Varying  $S_j$  we find that Equation (90) becomes exact (within our numerical accuracy) for small  $S_j$ , while for large  $S_j$  the function  $S_i (S_j - S_i) / S_j$  must be replaced by a less symmetric function, whose maximum is at a value of  $S_i$  slightly larger than  $S_j/2$ . The qualitative shape of the function remains however the same. For completeness, we have also considered a Gaussian filter. In this case we find that, in a first approximation, the function  $\Delta_{ij}$  is still given by Equation (90) (although the actual form of  $\Delta_{ij}$  is slightly more skewed compared to an inverse parabola), with a value of  $\kappa \simeq 0.35$ .

<sup>10</sup> The value of  $\kappa$  depends in principle on the cosmological model used, but this dependence is quite weak. For comparison, using a  $\Lambda$ CDM cosmological model with  $h = 0.7$ ,  $\Omega_M = 1 - \Omega_\Lambda = 0.3$ ,  $\sigma_8 = 0.93$ ,  $\Omega_B h^2 = 0.022$ , and  $n_s = 1$ , consistent with the *WMAP* first year data release, gives  $\kappa(R) \simeq 0.4562 - 0.0040 R$ .

## 5.2. Markovian Term

Inserting Equation (89) into Equation (48) we get

$$\begin{aligned} \Pi_\epsilon(\delta_0; \delta_n; S_n) &= \int_{-\infty}^{\delta_c} d\delta_1 \cdots d\delta_{n-1} \int \mathcal{D}\lambda \\ &\times \exp \left\{ i \sum_{i=1}^n \lambda_i \delta_i - \frac{1}{2} \sum_{i,j=1}^n [\min(S_i, S_j) + \Delta(S_i, S_j)] \lambda_i \lambda_j \right\}. \end{aligned} \quad (93)$$

As we see from Figure 5, Equation (86) gives a reasonable approximation to the exact correlator. This suggests that  $\Delta_{ij}$  be treated as a perturbation, so we now expand in  $\Delta_{ij}$ . The zeroth-order term is simply  $\Pi_\epsilon^{\text{gm}}(\delta_0; \delta_n; S_n)$ , whose continuum limit is given in Equation (57). The corresponding first-crossing rate is

$$\begin{aligned} \mathcal{F}^{\text{gm}} &= - \int_{-\infty}^{\delta_c} d\delta \frac{\partial \Pi_\epsilon^{\text{gm}}}{\partial S} \\ &= \frac{1}{\sqrt{2\pi}} \frac{\delta_c}{S^{3/2}} e^{-\delta_c^2/(2S)}, \end{aligned} \quad (94)$$

so the Markovian term can be obtained by taking the excursion set result (Equation (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 Equation (93), expanding to first order in  $\Delta_{ij}$  and using  $\lambda_j e^{i \sum_k \lambda_k \delta_k} = -i \partial_i e^{i \sum_k \lambda_k \delta_k}$ , where  $\partial_i = \partial / \partial \delta_i$ , the first-order correction to  $\Pi_\epsilon$  is

$$\begin{aligned} \Pi_\epsilon^{\Delta 1}(\delta_0; \delta_n; S_n) &\equiv \int_{-\infty}^{\delta_c} d\delta_1 \cdots d\delta_{n-1} \frac{1}{2} \sum_{i,j=1}^n \Delta_{ij} \partial_i \partial_j \\ &\times \int \mathcal{D}\lambda \exp \left\{ i \sum_{i=1}^n \lambda_i \delta_i - \frac{1}{2} \sum_{i,j=1}^n \min(S_i, S_j) \lambda_i \lambda_j \right\} \\ &= \frac{1}{2} \sum_{i,j=1}^n \Delta_{ij} \int_{-\infty}^{\delta_c} d\delta_1 \cdots d\delta_{n-1} \partial_i \partial_j W^{\text{gm}}(\delta_0; \delta_1, \dots, \delta_n; S_n). \end{aligned} \quad (95)$$

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

$$\frac{1}{2} \sum_{i,j=1}^n \Delta_{ij} \partial_i \partial_j = \frac{1}{2} \Delta_{nn} \partial_n^2 + \sum_{i=1}^{n-1} \Delta_{in} \partial_i \partial_n + \frac{1}{2} \sum_{i,j=1}^{n-1} \Delta_{ij} \partial_i \partial_j. \quad (96)$$

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

$$\frac{1}{2} \sum_{i,j=1}^n \Delta_{ij} \partial_i \partial_j = \sum_{i=1}^{n-1} \Delta_{in} \partial_i \partial_n + \sum_{i < j} \Delta_{ij} \partial_i \partial_j, \quad (97)$$

where

$$\sum_{i < j} \equiv \sum_{i=1}^{n-2} \sum_{j=i+1}^{n-1}. \quad (98)$$

When inserted into Equation (95) the term  $\sum_{i=1}^{n-1} \Delta_{in} \partial_i \partial_n$  brings a factor  $\sum_i$  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,

$$\Pi_\epsilon^{\Delta I} = \Pi_\epsilon^{\text{mem}} + \Pi_\epsilon^{\text{mem-mem}}, \quad (99)$$

where

$$\begin{aligned} \Pi_\epsilon^{\text{mem}}(\delta_0; \delta_n; S_n) &= \sum_{i=1}^{n-1} \Delta_{in} \partial_n \int_{-\infty}^{\delta_c} d\delta_1 \cdots d\delta_{n-1} \partial_i W^{\text{gm}}(\delta_0; \delta_1, \dots, \delta_n; S_n), \end{aligned} \quad (100)$$

and

$$\begin{aligned} \Pi_\epsilon^{\text{mem-mem}}(\delta_0; \delta_n; S_n) &= \sum_{i < j} \Delta_{ij} \int_{-\infty}^{\delta_c} d\delta_1 \cdots d\delta_{n-1} \partial_i \partial_j W^{\text{gm}}(\delta_0; \delta_1, \dots, \delta_n; S_n). \end{aligned} \quad (101)$$

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,

$$\begin{aligned} &\int_{-\infty}^{\delta_c} d\delta_1 \cdots d\delta_{n-1} \partial_i W^{\text{gm}}(\delta_0; \delta_1, \dots, \delta_n; S_n) \\ &= \int_{-\infty}^{\delta_c} d\delta_1 \cdots \widehat{d\delta_i} \cdots d\delta_{n-1} \\ &\quad \times W(\delta_0; \delta_1, \dots, \delta_i = \delta_c, \dots, \delta_{n-1}, \delta_n; S_n), \end{aligned} \quad (102)$$

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

$$\begin{aligned} &W^{\text{gm}}(\delta_0; \delta_1, \dots, \delta_{i-1}, \delta_c, \delta_{i+1}, \dots, \delta_n; S_n) \\ &= W^{\text{gm}}(\delta_0; \delta_1, \dots, \delta_{i-1}, \delta_c; S_i) W^{\text{gm}}(\delta_c; \delta_{i+1}, \dots, \delta_n; S_n - S_i), \end{aligned} \quad (103)$$

so

$$\begin{aligned} &\int_{-\infty}^{\delta_c} d\delta_1 \cdots d\delta_{i-1} \int_{-\infty}^{\delta_c} d\delta_{i+1} \cdots d\delta_{n-1} \\ &\quad \times W^{\text{gm}}(\delta_0; \delta_1, \dots, \delta_{i-1}, \delta_c; S_i) W^{\text{gm}}(\delta_c; \delta_{i+1}, \dots, \delta_n; S_n - S_i) \\ &= \Pi_\epsilon^{\text{gm}}(\delta_0; \delta_c; S_i) \Pi_\epsilon^{\text{gm}}(\delta_c; \delta_n; S_n - S_i), \end{aligned} \quad (104)$$

and we get

$$\begin{aligned} \Pi_\epsilon^{\text{mem}}(\delta_0; \delta_n; S_n) &= \sum_{i=1}^{n-1} \Delta_{in} \partial_n [\Pi_\epsilon^{\text{gm}}(\delta_0; \delta_c; S_i) \\ &\quad \times \Pi_\epsilon^{\text{gm}}(\delta_c; \delta_n; S_n - S_i)]. \end{aligned} \quad (105)$$

In the continuum limit we write

$$\sum_{i=1}^{n-1} \rightarrow \frac{1}{\epsilon} \int_0^{S_n} dS_i, \quad (106)$$

and, using Equations (79) and (80), we find

$$\begin{aligned} \Pi_{\epsilon=0}^{\text{mem}}(\delta_0 = 0; \delta_n; S_n) &= \frac{1}{\pi} \partial_n \int_0^{S_n} dS_i \Delta(S_i, S_n) \frac{\delta_c(\delta_c - \delta_n)}{S_i^{3/2}(S_n - S_i)^{3/2}} \\ &\quad \times \exp \left\{ -\frac{\delta_c^2}{2S_i} - \frac{(\delta_c - \delta_n)^2}{2(S_n - S_i)} \right\}. \end{aligned} \quad (107)$$

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

$$\begin{aligned} &\int_0^{S_n} dS_i \frac{S_i}{S_i^{3/2}(S_n - S_i)^{3/2}} \exp \left\{ -\frac{a^2}{2S_i} - \frac{b^2}{2(S_n - S_i)} \right\} \\ &= \sqrt{2\pi} \frac{1}{b} \frac{1}{S_n^{1/2}} \exp \left\{ -\frac{(a+b)^2}{2S_n} \right\} \end{aligned} \quad (108)$$

and

$$\begin{aligned} &\int_0^{S_n} dS_i \frac{S_i^2}{S_i^{3/2}(S_n - S_i)^{3/2}} \exp \left\{ -\frac{a^2}{2S_i} - \frac{b^2}{2(S_n - S_i)} \right\} \\ &= \sqrt{2\pi} \frac{S_n^{1/2}}{b} \exp \left\{ -\frac{(a+b)^2}{2S_n} \right\} - \pi \text{Erfc} \left( \frac{a+b}{\sqrt{2S_n}} \right), \end{aligned} \quad (109)$$

where Erfc is the complementary error function.<sup>11</sup> This gives

$$\Pi_{\epsilon=0}^{\text{mem}}(\delta_0 = 0; \delta_n; S_n) = \kappa \partial_n \left[ \frac{\delta_c(\delta_c - \delta_n)}{S_n} \text{Erfc} \left( \frac{2\delta_c - \delta_n}{\sqrt{2S_n}} \right) \right]. \quad (110)$$

For the memory-of-memory term, proceeding as for the memory term, we get

$$\begin{aligned} \Pi_\epsilon^{\text{mem-mem}}(\delta_0; \delta_n; S_n) &= \sum_{i < j} \Delta_{ij} \Pi_\epsilon^{\text{gm}}(\delta_0; \delta_c; S_i) \\ &\quad \times \Pi_\epsilon^{\text{gm}}(\delta_c; \delta_c; S_j - S_i) \Pi_\epsilon^{\text{gm}}(\delta_c; \delta_n; S_n - S_j). \end{aligned} \quad (111)$$

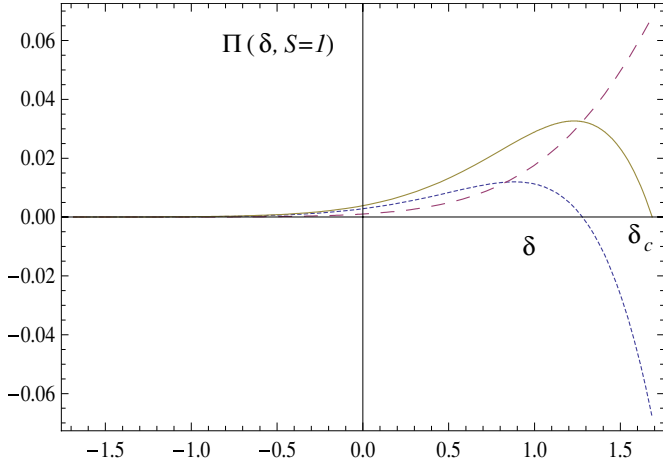
To compute this quantity we also need  $\Pi_\epsilon^{\text{gm}}(\delta_c; \delta_c; S)$ , with both the first and the second arguments equal to  $\delta_c$ . As we discuss in Appendix A, the result is

$$\Pi_\epsilon^{\text{gm}}(\delta_c; \delta_c; S) = \frac{\epsilon}{\sqrt{2\pi} S^{3/2}}. \quad (112)$$

Actually, Equation (112) is exact, and not just valid to  $\mathcal{O}(\epsilon)$ . Using Equations (79) and (112) we get

$$\begin{aligned} \Pi_{\epsilon=0}^{\text{mem-mem}}(\delta_0 = 0; \delta_n; S_n) &= \frac{\kappa}{\pi \sqrt{2\pi}} \delta_c(\delta_c - \delta_n) \\ &\quad \times \int_0^{S_n} dS_i \frac{1}{S_i^{1/2}} e^{-\delta_c^2/(2S_i)} \\ &\quad \times \int_{S_i}^{S_n} dS_j \frac{1}{S_j(S_j - S_i)^{1/2}(S_n - S_j)^{3/2}} \exp \left\{ -\frac{(\delta_c - \delta_n)^2}{2(S_n - S_j)} \right\}. \end{aligned} \quad (113)$$

<sup>11</sup> To derive these results we take one derivative of the left-hand side of Equation (107) with respect to  $a^2$ . The resulting integral can be performed using Equation (A5), and we then integrate back with respect to  $a^2$ . Similarly, Equation (108) is obtained taking twice the derivative with respect to  $a^2$ .



**Figure 7.** Functions  $\Pi_{\epsilon=0}^{\text{mem}}(\delta_0 = 0; \delta; S = 1)$  (blue dotted line),  $\Pi_{\epsilon=0}^{\text{mem-mem}}(\delta_0 = 0; \delta; S = 1)$  (violet, dashed), and their sum (brown solid line), as functions of  $\delta$ .

(A color version of this figure is available in the online journal.)

It is convenient to use the identity

$$\frac{(\delta_c - \delta_n)}{(S_n - S_j)} \exp \left\{ -\frac{(\delta_c - \delta_n)^2}{2(S_n - S_j)} \right\} = \partial_n \exp \left\{ -\frac{(\delta_c - \delta_n)^2}{2(S_n - S_j)} \right\} \quad (114)$$

to write  $\Pi_{\epsilon=0}^{\text{mem-mem}}$  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

$$\Pi_{\epsilon=0}^{\text{mem-mem}}(\delta_0 = 0; \delta_n; S_n) = \frac{\kappa \delta_c}{\sqrt{2\pi} S_n} \partial_n \left[ e^{-(\delta_c - \delta_n)^2/(2S_n)} \times \int_0^{S_n} \frac{dS_i}{S_i} e^{-\delta_c^2/(2S_i)} \text{Erfc} \left( (\delta_c - \delta_n) \sqrt{\frac{S_i}{2(S_n - S_i)S_n}} \right) \right] \quad (115)$$

We have not been able to compute analytically this last integral, but the fact that  $\Pi_{\epsilon=0}^{\text{mem-mem}}$  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  $\Pi_{\epsilon=0}^{\text{mem}}$  and  $\Pi_{\epsilon=0}^{\text{mem-mem}}$ . We show them in Figure 7, setting for definiteness  $S_n = 1$ . Observe that these two functions are separately non-zero in  $\delta = \delta_c$ . However,

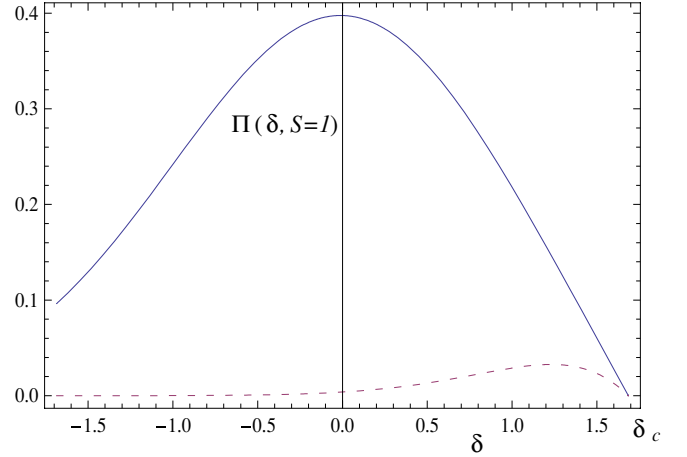
$$\Pi_{\epsilon=0}^{\text{mem}}(\delta_0 = 0; \delta_c; S_n) = -\frac{\kappa \delta_c}{S_n} \text{Erfc} \left( \frac{\delta_c}{\sqrt{2S_n}} \right), \quad (116)$$

and  $\Pi_{\epsilon=0}^{\text{mem-mem}}(\delta_0 = 0; \delta_c; S_n) = -\Pi_{\epsilon=0}^{\text{mem}}(\delta_0 = 0; \delta_c; S_n)$ , so we find that the total distribution function  $\Pi_{\epsilon=0}^{\text{mem}}(\delta_0; S; S_n)$  still satisfies the absorbing barrier boundary condition  $\Pi_{\epsilon=0}^{\text{mem}}(\delta_0; \delta_c; S_n) = 0$ , even when we include the Markovian corrections to first order. In Figure 8, we compare  $\Pi_{\epsilon=0}^{\text{mem}} + \Pi_{\epsilon=0}^{\text{mem-mem}}$  to the zeroth-order term (57).

#### 5.4. The Halo Mass Function

We can now compute the first-crossing rate using Equation (30). Since both  $\Pi_{\epsilon=0}^{\text{mem}}$  and  $\Pi_{\epsilon=0}^{\text{mem-mem}}$  have been expressed as a derivative with respect to  $\delta_n$  in Equations (110) and (115), the integral over  $d\delta_n$  is performed trivially, and we get

$$\mathcal{F}^{\text{mem}}(S) = -\frac{\partial}{\partial S} \int_{-\infty}^{\delta_c} d\delta_n \Pi_{\epsilon=0}^{\text{mem}}(\delta_0 = 0; \delta_n; S) = 0, \quad (117)$$



**Figure 8.** Functions  $\Pi_{\epsilon=0}^{\text{mem}}(\delta_0 = 0; \delta; S = 1) + \Pi_{\epsilon=0}^{\text{mem-mem}}(\delta_0 = 0; \delta; S = 1)$  (dashed), compared to  $\Pi_{\epsilon=0}^{\text{mem}}(\delta_0 = 0; \delta; S = 1)$  (solid line), as functions of  $\delta$ . (A color version of this figure is available in the online journal.)

$$\begin{aligned} \mathcal{F}^{\text{mem-mem}}(S) &= -\frac{\partial}{\partial S} \int_{-\infty}^{\delta_c} d\delta_n \Pi_{\epsilon=0}^{\text{mem-mem}}(\delta_0 = 0; \delta_n; S) \\ &= -\frac{\partial}{\partial S} \left[ \frac{\kappa \delta_c}{\sqrt{2\pi} S} \int_0^S dS_i \frac{1}{S_i} e^{-\delta_c^2/(2S_i)} \right] \\ &= -\frac{\kappa \delta_c}{\sqrt{2\pi}} \frac{\partial}{\partial S} \left[ \frac{1}{S^{1/2}} \Gamma \left( 0, \frac{\delta_c^2}{2S} \right) \right] \\ &= -\frac{\kappa \delta_c}{\sqrt{2\pi}} \left[ \frac{1}{S^{3/2}} e^{-\delta_c^2/(2S)} - \frac{1}{2S^{3/2}} \Gamma \left( 0, \frac{\delta_c^2}{2S} \right) \right], \end{aligned} \quad (118)$$

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

$$\mathcal{F}(S) = \frac{1 - \kappa}{\sqrt{2\pi}} \frac{\delta_c}{S^{3/2}} e^{-\delta_c^2/(2S)} + \frac{\kappa}{2\sqrt{2\pi}} \frac{\delta_c}{S^{3/2}} \Gamma \left( 0, \frac{\delta_c^2}{2S} \right). \quad (119)$$

The halo mass function in this approximation is therefore

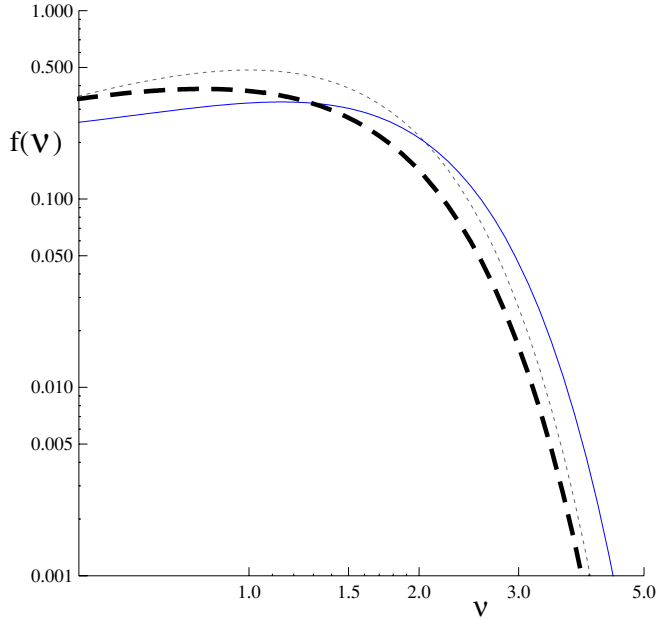
$$f(\sigma) = (1 - \kappa) \left( \frac{2}{\pi} \right)^{1/2} \frac{\delta_c}{\sigma} e^{-\delta_c^2/(2\sigma^2)} + \frac{\kappa}{\sqrt{2\pi}} \frac{\delta_c}{\sigma} \Gamma \left( 0, \frac{\delta_c^2}{2\sigma^2} \right), \quad (120)$$

where, in the relevant range of values of  $R$ ,  $\kappa$  is given by Equations (91) and (92), and is a slowly decreasing function of  $R$ . For instance, at  $R = 5$  Mpc,  $\kappa \simeq 0.45$ , at  $R = 10$  Mpc,  $\kappa \simeq 0.43$ , and at  $R = 20$  Mpc,  $\kappa \simeq 0.40$ . For large values of  $\delta_c^2/2\sigma^2$ ,

$$\Gamma \left( 0, \frac{\delta_c^2}{2\sigma^2} \right) \simeq \frac{2\sigma^2}{\delta_c^2} e^{-\delta_c^2/(2\sigma^2)}. \quad (121)$$

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 Equation (120) approaches  $(1 - \kappa)$  times the PS prediction.

In Figure 9 we plot the function  $f(\nu)$ , where  $\nu = \delta_c/\sigma$ , comparing the prediction of PS theory given in Equation (2), the fit to the  $N$ -body simulation of Warren et al. (2006), and our result (Equation (120)). This figure can be compared to Figure 4



**Figure 9.** Function  $f(v)$  against  $v$ . The gray dotted line is the value in PS theory. The blue solid line is the fit to the numerical  $N$ -body simulation of Warren et al. (2006). The thick black dashed line is our result (Equation (120)). (A color version of this figure is available in the online journal.)

of Robertson et al. (2009); 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  $f(v)$  with the top-hat filter in coordinate space, performed with an MC realization of the trajectories obtained from a Langevin equation with colored noise. We have used the same scale and color code as their Figure 4, to make the comparison easier. One sees that our analytical result for  $f(v)$  agrees very well with their MC result (the function that we call  $f(v)$  is denoted as  $\nu f(v)$  in Robertson et al. 2009). From Equation (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 Equation (92) these are expected to be of order 20%, which is the level of agreement between our analytical result and the MC 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 Equation (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  $\delta_c/\sigma \rightarrow 0$ . Formally, the limit  $\delta_c/\sigma \rightarrow 0$  can be obtained sending  $\delta_c \rightarrow 0$  for fixed  $\sigma$ , so we require that

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

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

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

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

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

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

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

so Equation (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 Equation (120) into Equation (126) and using

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

and

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

we see that the dependence on  $\kappa$  cancels and Equation (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  $\exp\{-\delta_c^2/(2\sigma^2)\}$  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. 2009) that the corrections obtained by taking properly into account the top-hat filter in coordinate space do not alleviate the discrepancy of PS theory with the  $N$ -body simulations. We see in fact from Figure 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 halos is a complex phenomenon. Incorporating some of the complexities 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 top-hat 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 (Equation (90)) of  $\Delta(S_i, S_j)$ , and in particular to the property  $\Delta(S_i, S_i) = 0$ . However, not all perturbations that we will



consider share this property, in particular when we consider the non-Gaussianities. Furthermore, even with the above form of  $\Delta(S_i, S_j)$ , if we work to second order in perturbation theory we find that divergences appear. It is therefore important to understand in some detail how in the general case these divergences cancel among different terms, giving a finite result. This issue is quite technical, and is discussed in detail in Appendix B.

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APPENDIX A

FINITE- $\epsilon$  CORRECTIONS

In this Appendix, we derive the results for  $\Pi_\epsilon(\delta_0; \delta_c; S)$  and  $\Pi_\epsilon(\delta_c; \delta_c; S)$  mentioned in Section 4.2. These results are needed in Section 5.3, when we compute perturbatively the non-Markovian corrections. We will also show that, for  $\partial_\delta \Pi_\epsilon^{\text{gm}}(\delta_0 = 0; \delta; S)$ , the limit  $\epsilon \rightarrow 0^+$  does not commute with the limit  $\delta \rightarrow \delta_c^-$ . 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 Equations (77) and (78) we found that  $\Pi_\epsilon^{\text{gm}}(\delta_0; \delta_c; S) = \sqrt{\epsilon} \gamma(\delta_c/S^{3/2})e^{-\delta_c^2/(2S)} + \mathcal{O}(\epsilon)$ , where  $\gamma = (2/\sqrt{\pi}) \lim_{\eta \rightarrow 0} \eta u(\eta)$ . One possible route to the evaluation of  $\gamma$  could be to plug Equation (74) into Equation (58) and evaluate both sides at  $\delta = \delta_c$ . 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 directly get  $\gamma$ , as follows. We consider the derivative of  $\Pi_\epsilon^{\text{gm}}$  with respect to  $\delta_c$  (which, when we use the notation  $\Pi_\epsilon^{\text{gm}}(\delta_0; \delta; S)$ , does not appear explicitly in the list of variable on which  $\Pi_\epsilon^{\text{gm}}$  depends, but of course enters as upper integration limit in Equation (40)). This gives

$$\frac{\partial}{\partial \delta_c} \Pi_\epsilon(\delta_0; \delta_n; S_n) = \sum_{i=1}^{n-1} \int_{-\infty}^{\delta_c} d\delta_1 \cdots \widehat{d\delta_i} \cdots d\delta_{n-1} \times W(\delta_0; \delta_1, \dots, \delta_i = \delta_c, \dots, \delta_n; S_n), \tag{A1}$$

where the notation  $\widehat{d\delta_i}$  means that we must omit  $d\delta_i$  from the list of integration variables. We next use Equations (103) and (104) and, in the continuum limit, we obtain the identity

$$\frac{\partial}{\partial \delta_c} \Pi_{\epsilon=0}(\delta_0; \delta_n; S_n) = \int_0^{S_n} dS_i \lim_{\epsilon \rightarrow 0} \frac{1}{\epsilon} \Pi_\epsilon^{\text{gm}}(\delta_0; \delta_c; S_i) \Pi_\epsilon^{\text{gm}}(\delta_c; \delta_n; S_n - S_i). \tag{A2}$$

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

$$\frac{\partial}{\partial \delta_c} \Pi_{\epsilon=0}(\delta_0 = 0; \delta_n; S_n) = \left(\frac{2}{\pi}\right)^{1/2} \frac{2\delta_c - \delta_n}{S_n^{3/2}} e^{-(2\delta_c - \delta_n)^2/(2S_n)}. \tag{A3}$$

The right-hand side of Equation (A2) can be evaluated using Equation (77) together with

$$\begin{aligned} \Pi_\epsilon(\delta_c; \delta_n; S) &= \Pi_\epsilon(\delta_n; \delta_c; S) \\ &= \sqrt{\epsilon} \gamma \frac{\delta_c - \delta_n}{S^{3/2}} e^{-(\delta_c - \delta_n)^2/(2S)} + \mathcal{O}(\epsilon), \end{aligned} \tag{A4}$$

which can be checked from Equations (40) and (53) by performing a reshuffling of the dummy integration variables. We see that the limit  $\epsilon \rightarrow 0$  in Equation (A2) is finite thanks to the factors  $\sqrt{\epsilon}$  in  $\Pi_\epsilon^{\text{gm}}(\delta_0; \delta_c; S_i)$  and in  $\Pi_\epsilon^{\text{gm}}(\delta_c; \delta_n; S_n - S_i)$ . The integral over  $S_i$  can be performed using the identity

$$\begin{aligned} \int_0^{S_n} dS_i \frac{1}{S_i^{3/2}(S_n - S_i)^{3/2}} \exp\left\{-\frac{a^2}{2S_i} - \frac{b^2}{2(S_n - S_i)}\right\} \\ = \sqrt{2\pi} \frac{a+b}{ab} \frac{1}{S_n^{3/2}} \exp\left\{-\frac{(a+b)^2}{2S_n}\right\}, \end{aligned} \tag{A5}$$

where  $a > 0, b > 0$ .<sup>12</sup> In this way we find that the dependence on  $\delta_c$  and  $S$  on the two sides of Equation (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  $\delta = \delta_c$ . Of course, if we first take the limit  $\epsilon \rightarrow 0^+$ , and then we take  $\delta \rightarrow \delta_c^-$ , we simply get the derivative of the function  $\Pi_{\epsilon=0}(\delta_0; \delta, S)$  given in Equation (57), evaluated in  $\delta_c$ ,

$$\begin{aligned} \lim_{\delta \rightarrow \delta_c^-} \lim_{\epsilon \rightarrow 0^+} \partial_\delta \Pi_\epsilon^{\text{gm}}(\delta_0 = 0; \delta, S) &= \partial_\delta \Pi_{\epsilon=0}^{\text{gm}}(\delta_0; \delta, S)|_{\delta=\delta_c} \\ &= -\left(\frac{2}{\pi}\right)^{1/2} \frac{\delta_c}{S^{3/2}} e^{-\delta_c^2/(2S)}. \end{aligned} \tag{A6}$$

However, we will actually need the result when the limits are evaluated in the opposite order, i.e.,  $\lim_{\epsilon \rightarrow 0^+} \lim_{\delta \rightarrow \delta_c^-} \partial_\delta \Pi_\epsilon^{\text{gm}}(\delta_0; \delta, S)$ . We will now show that these two limits do not commute. From Equation (78), for small  $\eta$ ,  $u(\eta)$  is proportional to  $\gamma\sqrt{\pi}/(2\eta) = 1/(2\eta)$ . More generally, for small  $\eta$ , we write

$$u(\eta) = \frac{1}{2\eta} + u_0 + u_1\eta + \mathcal{O}(\eta^2). \tag{A7}$$

Plugging this expansion, together with the expansion in powers of  $\eta$  of Equation (75), into Equation (74) we find that, for  $\eta \rightarrow 0$  (i.e., for  $\delta \rightarrow \delta_c^-$  at fixed  $\epsilon$ ), retaining only the terms up to  $\mathcal{O}(\sqrt{\epsilon})$

$$\begin{aligned} \Pi_\epsilon^{\text{gm}}(\delta_0 = 0; \delta, S) &= \Pi_\epsilon^{\text{gm}}(\delta_0 = 0; \delta_c, S) \\ &+ \sqrt{\epsilon} \frac{2}{\sqrt{\pi}} (u_0\eta + u_1\eta^2 + \dots) \frac{\delta_c}{S^{3/2}} e^{-\delta_c^2/(2S)}. \end{aligned} \tag{A8}$$

Using  $\partial_\delta = (d\eta/d\delta)\partial/\partial\eta$  and  $d\eta/d\delta = -1/\sqrt{2\epsilon}$ , this gives

$$\lim_{\epsilon \rightarrow 0^+} \lim_{\delta \rightarrow \delta_c^-} \partial_\delta \Pi_\epsilon^{\text{gm}}(\delta_0 = 0; \delta, S) = -u_0 \left(\frac{2}{\pi}\right)^{1/2} \frac{\delta_c}{S^{3/2}} e^{-\delta_c^2/(2S)}, \tag{A9}$$

<sup>12</sup> 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  $\Pi_\epsilon^{\text{gm}}(\delta_0; \delta_c; S)$  has the functional form (Equation (77)) and we know that the identity (A2) holds, it follows that the integral on the left-hand side of Equation (A5) must be given by the expression on the right-hand side, times an unknown numerical constant. The latter can be computed evaluating the term  $\sim 1/a$  of the integral in the limit  $a \rightarrow 0^+$ . This is easily done analytically, since in this case the factors  $(S_n - S_i)$  inside the integrand can be simply replaced by  $S_n$ , and fixes the factor  $\sqrt{2\pi}$  on the right-hand side of Equation (A5).

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

$$\frac{\partial^2 \Pi_\epsilon^{\text{gm}}}{\partial \delta^2} = \frac{1}{2\epsilon} \frac{\partial^2 \Pi_\epsilon^{\text{gm}}}{\partial \eta^2}, \quad (\text{A10})$$

overall,  $\partial^2 \Pi_\epsilon^{\text{gm}} / \partial \delta^2$ , evaluated in  $\delta = \delta_c$  at finite  $\epsilon$ , is proportional to  $1/\sqrt{\epsilon}$ . Therefore, in Equation (72) the first correction included in the dots, which is proportional to  $\epsilon(\partial^2 \Pi_\epsilon^{\text{gm}} / \partial \delta^2)_{\delta=\delta_c}$ , is of the same order as the term  $\sqrt{\epsilon}(\partial \Pi_\epsilon^{\text{gm}} / \partial \delta)_{\delta=\delta_c}$ , and similarly for the higher order terms. This is the reason why we could not use Equation (72) to fix the value of the coefficient  $\gamma$ .

Finally, in the perturbative computation we also need  $\Pi_\epsilon^{\text{gm}}(\delta_c; \delta_c; S)$ , with both arguments equal to  $\delta_c$ . The result is given in Equation (112). To derive it, we first observe from Equation (79) that, when  $\delta_0 = \delta_c$ , the term  $\mathcal{O}(\sqrt{\epsilon})$  vanishes, so the first non-vanishing term will be  $\mathcal{O}(\epsilon)$ . Invariance under space translations requires that  $\Pi_\epsilon^{\text{gm}}(\delta_0; \delta_c; S)$  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 Equation (19) we see that  $\eta$  has dimensions  $1/\ell$ , and  $\xi \sim \ell/\ell^2 = 1/\ell$ , so Equation (18) is dimensionally correct. In these units  $\lambda \sim 1/\ell$ , since  $\lambda \delta$  is dimensionless, and we see from Equation (48) that  $\Pi_\epsilon$  has dimensions  $1/\ell$ . Using dimensional analysis in this form we conclude that the term  $\mathcal{O}(\epsilon)$  in  $\Pi_\epsilon^{\text{gm}}(\delta_c; \delta_c; S)$  is necessarily proportional to  $\epsilon/S^{3/2}$ . Since this fixes completely the dependence on  $S$ , writing  $S = \epsilon n$  we have also fixed completely the dependence on  $n$ , i.e., to  $\mathcal{O}(\epsilon)$  we must have

$$\Pi_\epsilon^{\text{gm}}(\delta_c; \delta_c; S) = c \frac{\epsilon}{S^{3/2}} = \frac{c}{\sqrt{\epsilon} n^{3/2}}, \quad (\text{A11})$$

with  $c$  independent of  $n$ . The coefficient  $c$  can then be fixed computing explicitly the integral in Equation (40) 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 Equation (A11) is exact, i.e., it receives no correction of higher order in  $\epsilon$ . Even for  $n = 3$  the integral in Equation (A11) can be performed analytically when  $\delta_0 = \delta_c$ , and again we find that Equation (A11) is exact. We have checked this result numerically for  $n$  up to 7 and we find that the numerical result agrees with Equation (A11) within the 10 digit precision of the numerical integration, so it is clear that Equation (A11) is actually exact, and not just the result at  $\mathcal{O}(\epsilon)$ . (In any case, to perform our perturbative computation, we only need  $\Pi_\epsilon^{\text{gm}}(\delta_c; \delta_c; S)$  to  $\mathcal{O}(\epsilon)$ .)

## APPENDIX 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 Equation (93) as

$$\begin{aligned} \Pi_\epsilon(\delta_0; \delta_n; S_n) &= \int_{-\infty}^{\delta_c} d\delta_1 \cdots d\delta_{n-1} \\ &\times \int \mathcal{D}\lambda \exp \left\{ \frac{1}{2} \sum_{i,j=1}^n \Delta_{ij} \partial_i \partial_j \right\} \\ &\times \exp \left\{ i \sum_{i=1}^n \lambda_i \delta_i - \frac{1}{2} \sum_{i,j=1}^n [\min(S_i, S_j)] \lambda_i \lambda_j \right\}, \end{aligned} \quad (\text{B1})$$

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

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

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

$$\Pi_\epsilon^{\Delta 1} = e^{(1/2)\Delta_{nn} \partial_n^2} [\Pi_\epsilon^{\text{mem}} + \Pi_\epsilon^{\text{mem-mem}}], \quad (\text{B3})$$

where

$$\begin{aligned} \Pi_\epsilon^{\text{mem}}(\delta_0; \delta_n; S_n) &= \sum_{i=1}^{n-1} \Delta_{in} \partial_n \int_{-\infty}^{\delta_c} d\delta_1 \cdots d\delta_{n-1} \partial_i \\ &\times W^{\text{gm}}(\delta_0; \delta_1, \dots, \delta_n; S_n), \end{aligned} \quad (\text{B4})$$

and

$$\begin{aligned} \Pi_\epsilon^{\text{mem-mem}}(\delta_0; \delta_n; S_n) &= \int_{-\infty}^{\delta_c} d\delta_1 \cdots d\delta_{n-1} \\ &\times \left[ \sum_{i<j} \Delta_{ij} \partial_i \partial_j + \frac{1}{2} \sum_i \Delta_{ii} \partial_i^2 \right] W^{\text{gm}}(\delta_0; \delta_1, \dots, \delta_n; S_n). \end{aligned} \quad (\text{B5})$$

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 Equation (103) we get

$$\begin{aligned} \Pi_\epsilon^{\text{mem-mem}}(\delta_0; \delta_n; S_n) &= \sum_{i<j} \Delta_{ij} \Pi_\epsilon^{\text{gm}}(\delta_0; \delta_c; S_i) \\ &\times \Pi_\epsilon^{\text{gm}}(\delta_c; \delta_c; S_j - S_i) \Pi_\epsilon^{\text{gm}}(\delta_c; \delta_n; S_n - S_j) \\ &+ \sum_{i=1}^{n-1} \frac{\Delta_{ii}}{2} \partial_i [\Pi_\epsilon^{\text{gm}}(\delta_0; \delta_i; S_i) \Pi_\epsilon^{\text{gm}}(\delta_i; \delta_n; S_n - S_i)]_{\delta_i=\delta_c} \\ &= \sum_{i<j} \Delta_{ij} \Pi_\epsilon^{\text{gm}}(\delta_0; \delta_c; S_i) \Pi_\epsilon^{\text{gm}}(\delta_c; \delta_c; S_j - S_i) \\ &\times \Pi_\epsilon^{\text{gm}}(\delta_c; \delta_n; S_n - S_j) + \sum_{i=1}^{n-1} \Delta_{ii} [\partial_i \Pi_\epsilon^{\text{gm}}(\delta_0; \delta_i; S_i)]_{\delta_i=\delta_c} \\ &\times \Pi_\epsilon^{\text{gm}}(\delta_c; \delta_n; S_n - S_i). \end{aligned} \quad (\text{B6})$$

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

Equation (B6), which is the one coming from  $\Delta_{ii} \partial_i^2$ . We have found in Section 4.2 that  $\Pi_\epsilon^{\text{gau}}(\delta_0; \delta_c; S_i)$  is proportional to  $\sqrt{\epsilon}$  while  $[\partial_\delta \Pi_\epsilon^{\text{gm}}(\delta_c; S; S)]_{\delta=\delta_c}$  has a finite limit for  $\epsilon \rightarrow 0$ , see Equation (A9). Therefore, using Equation (106), we find that the last term in Equation (B6) diverges as  $1/\sqrt{\epsilon}$ . A similar problem appears in the term coming from  $\partial_i \partial_j$  with  $i \neq j$ . Using Equations (79) and (112), we find that the first term in Equation (B6) is proportional to

$$\epsilon \sum_{i=1}^{n-2} \frac{1}{S_i^{3/2}} \exp \left\{ -\frac{\delta_c^2}{2S_i} \right\} \epsilon \sum_{j=i+1}^{n-1} \frac{\Delta_{ij}}{(S_j - S_i)^{3/2} (S_n - S_j)^{3/2}} \times \exp \left\{ -\frac{(\delta_c - \delta_n)^2}{2(S_n - S_j)} \right\}, \tag{B7}$$

where  $S_i = i\epsilon, S_j = j\epsilon$ . In the continuum limit, unless  $\Delta_{ij}$  vanishes for  $i = j$ , this quantity diverges as  $1/\sqrt{\epsilon}$ , because of the behavior  $(S_j - S_i)^{-3/2}$  when  $S_j \rightarrow S_i^+$ . In Section 4.2 these problems did not show up because  $\Delta_{ii} = 0$ , so the divergence coming from  $\Delta_{ii} \partial_i^2$  disappears. Furthermore, when  $S_i \rightarrow S_j$ ,  $\Delta_{ij}$  vanished as  $S_j - S_i$ , thereby ensuring the convergence of the sum (or, in the continuum limit, of the integral over  $S_j$ ) in Equation (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  $\Pi_\epsilon^{\text{gm}}$  with respect to  $\delta_c$ . The first derivative was computed in Equation (A1), and the result can be rewritten as

$$\frac{\partial}{\partial \delta_c} \Pi_\epsilon^{\text{gm}}(\delta_0; \delta_n; S_n) = \sum_{i=1}^{n-1} \int_{-\infty}^{\delta_c} d\delta_1 \cdots d\delta_{n-1} \partial_i W. \tag{B8}$$

When we take one more derivative of Equation (A1) with respect to  $\delta_c$ , we find two kinds of terms. First, there are the terms where we take one more derivative 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  $W(\delta_0; \delta_1, \dots, \delta_i = \delta_c, \dots, \delta_{n-1}, \delta_n; S_n)$  with respect to  $\delta_c$ . Therefore,

$$\begin{aligned} \frac{\partial^2}{\partial \delta_c^2} \Pi_\epsilon^{\text{gm}}(\delta_0; \delta_n; S_n) &= 2 \sum_{i < j} \int_{-\infty}^{\delta_c} d\delta_1 \cdots \widehat{d\delta_i} \cdots \widehat{d\delta_j} \cdots d\delta_{n-1} \\ &\times W(\delta_0; \delta_1, \dots, \delta_i = \delta_c, \dots, \delta_j = \delta_c, \dots, \delta_n; S_n) \\ &+ \sum_{i=1}^{n-1} \int_{-\infty}^{\delta_c} d\delta_1 \cdots \widehat{d\delta_i} \cdots d\delta_{n-1} \\ &\times \frac{\partial}{\partial \delta_c} W(\delta_0; \delta_1, \dots, \delta_i = \delta_c, \dots, \delta_n; S_n) \\ &= 2 \sum_{i < j} \int_{-\infty}^{\delta_c} d\delta_1 \cdots d\delta_{n-1} \partial_i \partial_j W + \sum_{i=1}^{n-1} \int_{-\infty}^{\delta_c} d\delta_1 \cdots d\delta_{n-1} \partial_i^2 W, \end{aligned} \tag{B9}$$

that is,

$$\frac{\partial^2}{\partial \delta_c^2} \Pi_\epsilon^{\text{gm}}(\delta_0; \delta_n; S_n) = \sum_{i,j=1}^{n-1} \int_{-\infty}^{\delta_c} d\delta_1 \cdots d\delta_{n-1} \partial_i \partial_j W. \tag{B10}$$

Thus, when  $\Delta_{ij} = 1$ ,

$$\Pi_\epsilon^{\text{mem-mem}}(\delta_0; \delta_n; S_n) = \frac{1}{2} \frac{\partial^2}{\partial \delta_c^2} \Pi_\epsilon^{\text{gm}}(\delta_0; \delta_n; S_n). \tag{B11}$$

In particular, in the continuum limit,

$$\begin{aligned} \Pi_{\epsilon=0}^{\text{mem-mem}}(\delta_0 = 0; \delta_n; S_n) &= \frac{1}{2} \frac{\partial^2}{\partial \delta_c^2} \Pi_{\epsilon=0}^{\text{gm}}(\delta_0 = 0; \delta_n; S_n) \\ &= \left(\frac{2}{\pi}\right)^{1/2} \left[ 1 - \frac{(2\delta_c - \delta_n)^2}{S_n} \right] \frac{1}{S_n^{3/2}} e^{-(2\delta_c - \delta_n)^2 / (2S_n)}. \end{aligned} \tag{B12}$$

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

$$I_1 \equiv \sum_{i=1}^{n-1} [\partial_i \Pi_\epsilon^{\text{gm}}(\delta_0 = 0; \delta_i; S_i)]_{\delta_i=\delta_c} \Pi_\epsilon^{\text{gm}}(\delta_c; \delta_n; S_n - S_i). \tag{B13}$$

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  $\partial_i^2$ ) and only after we take the limit  $\epsilon \rightarrow 0^+$ . The result is therefore given by Equation (A9). By also using Equations (A4) and (79), we get

$$\begin{aligned} I_1 &= -\frac{1}{\sqrt{\epsilon}} \frac{u_0 \sqrt{2}}{\pi} \delta_c (\delta_c - \delta_n) \\ &\times \epsilon \sum_{i=1}^{n-1} \frac{1}{S_i^{3/2} (S_n - S_i)^{3/2}} \exp \left\{ -\frac{\delta_c^2}{2S_i} - \frac{(\delta_c - \delta_n)^2}{2(S_n - S_i)} \right\}. \end{aligned} \tag{B14}$$

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

$$\begin{aligned} I_1 &= -\frac{1}{\sqrt{\epsilon}} \frac{u_0 \sqrt{2}}{\pi} \delta_c (\delta_c - \delta_n) \\ &\times \int_0^{S_n} dS_i \frac{1}{S_i^{3/2} (S_n - S_i)^{3/2}} \exp \left\{ -\frac{\delta_c^2}{2S_i} - \frac{(\delta_c - \delta_n)^2}{2(S_n - S_i)} \right\}. \end{aligned} \tag{B15}$$

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

$$I_1 = -\frac{1}{\sqrt{\epsilon}} \frac{2u_0}{\sqrt{\pi}} (2\delta_c - \delta_n) \frac{1}{S_n^{3/2}} e^{-(2\delta_c - \delta_n)^2 / (2S_n)}. \tag{B16}$$

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 Equations (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 Equation (B16), and therefore vanish in the continuum limit.

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

$$\begin{aligned}
 I_2 &\equiv \sum_{i=1}^{n-2} \Pi_\epsilon^{\text{gm}}(\delta_0 = 0; \delta_c; S_i) \\
 &\quad \times \sum_{j=i+1}^{n-1} \Pi_\epsilon^{\text{gm}}(\delta_c; \delta_c; S_j - S_i) \Pi_\epsilon^{\text{gm}}(\delta_c; \delta_n; S_n - S_j) \\
 &= \frac{1}{\pi\sqrt{2\pi}} \delta_c(\delta_c - \delta_n) \epsilon \sum_{i=1}^{n-2} \frac{1}{S_i^{3/2}} e^{-\delta_c^2/(2S_i)} \epsilon \\
 &\quad \times \sum_{j=i+1}^{n-1} \frac{1}{(S_j - S_i)^{3/2}(S_n - S_j)^{3/2}} \exp\left\{-\frac{(\delta_c - \delta_n)^2}{2(S_n - S_j)}\right\}.
 \end{aligned}
 \tag{B17}$$

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

$$\epsilon \sum_{j=i+1}^{n-1} \stackrel{?}{=} \int_{S_i}^{S_n} dS_j.
 \tag{B18}$$

However, Equation (B18) is only correct when the sum and the integral are finite for  $\epsilon \rightarrow 0$ . Here, this is not the case, since

$$\int_{S_i}^{S_n} dS_j \frac{1}{(S_j - S_i)^{3/2}(S_n - S_j)^{3/2}} \exp\left\{-\frac{(\delta_c - \delta_n)^2}{2(S_n - S_j)}\right\}
 \tag{B19}$$

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

$$\begin{aligned}
 I_3 &\equiv \epsilon \sum_{j=i+1}^{n-1} \frac{1}{(S_j - S_i)^{3/2}(S_n - S_j)^{3/2}} \exp\left\{-\frac{(\delta_c - \delta_n)^2}{2(S_n - S_j)}\right\} \\
 &\stackrel{?}{=} \int_{S_i+\epsilon}^{S_n} dS_j \frac{1}{(S_j - S_i)^{3/2}(S_n - S_j)^{3/2}} \exp\left\{-\frac{(\delta_c - \delta_n)^2}{2(S_n - S_j)}\right\}.
 \end{aligned}
 \tag{B20}$$

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  $(S_j - S_i)^{-3/2}$ , and so, if we used this prescription, we would conclude that

$$\begin{aligned}
 I_3 &\stackrel{?}{=} \frac{1}{(S_n - S_i)^{3/2}} \exp\left\{-\frac{(\delta_c - \delta_n)^2}{2(S_n - S_i)}\right\} \\
 &\quad \times \int_{S_i+\epsilon}^{S_n} dS_j \frac{1}{(S_j - S_i)^{3/2}} + \text{finite parts} \\
 &= \frac{2}{\sqrt{\epsilon}} \frac{1}{(S_n - S_i)^{3/2}} \exp\left\{-\frac{(\delta_c - \delta_n)^2}{2(S_n - S_i)}\right\} + \text{finite parts}.
 \end{aligned}
 \tag{B21}$$

However, if the prescription (Equation (B20)) were 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

$$\begin{aligned}
 I_3 &\stackrel{?}{=} \frac{1}{\sqrt{\epsilon}} \frac{1}{(S_n - S_i)^{3/2}} \exp\left\{-\frac{(\delta_c - \delta_n)^2}{2(S_n - S_i)}\right\} \\
 &\quad + \int_{S_i+2\epsilon}^{S_n} dS_j \frac{1}{(S_j - S_i)^{3/2}(S_n - S_j)^{3/2}} \exp\left\{-\frac{(\delta_c - \delta_n)^2}{2(S_n - S_j)}\right\} \\
 &= \frac{1 + \sqrt{2}}{\sqrt{\epsilon}} \frac{1}{(S_n - S_i)^{3/2}} \exp\left\{-\frac{(\delta_c - \delta_n)^2}{2(S_n - S_i)}\right\} + \text{finite parts}.
 \end{aligned}
 \tag{B22}$$

We see that the two procedures agree on the fact that the singularity is proportional to  $1/\sqrt{\epsilon}$ , but give different values for the coefficient, so Equation (B20) cannot be 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  $1/\sqrt{\epsilon}$  singularity and the finite terms are concerned, we have the equality

$$\begin{aligned}
 \epsilon \sum_{j=i+1}^{n-1} \frac{1}{(S_j - S_i)^{3/2}(S_n - S_j)^{3/2}} \exp\left\{-\frac{(\delta_c - \delta_n)^2}{2(S_n - S_j)}\right\} \\
 = \int_{S_i+\alpha\epsilon}^{S_n} dS_j \frac{1}{(S_j - S_i)^{3/2}(S_n - S_j)^{3/2}} \\
 \times \exp\left\{-\frac{(\delta_c - \delta_n)^2}{2(S_n - S_j)}\right\},
 \end{aligned}
 \tag{B23}$$

and the two expressions only differ by terms that vanish as  $\epsilon \rightarrow 0$ . In fact,  $\alpha$  can be fixed requiring that the coefficient of  $1/\sqrt{\epsilon}$  is the same on the two sides of Equation (B23), and it does not affect the terms  $\mathcal{O}(\epsilon^0)$  since it is just a rescaling of  $\epsilon$ . Actually, in our problem, an even better way to pass from the sum to the integral is to write

$$\begin{aligned}
 \epsilon \sum_{j=i+1}^{n-1} \frac{1}{(S_j - S_i)^{3/2}(S_n - S_j)^{3/2}} \exp\left\{-\frac{(\delta_c - \delta_n)^2}{2(S_n - S_j)}\right\} \\
 = \int_{S_i}^{S_n} dS_j \frac{1}{(S_j - S_i)^{3/2}(S_n - S_j)^{3/2}} \\
 \times \exp\left\{-\frac{\alpha\epsilon}{2(S_j - S_i)} - \frac{(\delta_c - \delta_n)^2}{2(S_n - S_j)}\right\}.
 \end{aligned}
 \tag{B24}$$

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 Equation (B24). However, since  $\alpha$  is just a rescaling of  $\epsilon$ ,  $\alpha$  does not affect the finite part.

The advantage of using Equation (B24) is that the integral can now be performed analytically using Equation (A5),

so we get

$$\begin{aligned}
 I_3 &= \epsilon \sum_{j=i+1}^{n-1} \frac{1}{(S_j - S_i)^{3/2}(S_n - S_j)^{3/2}} \exp \left\{ -\frac{(\delta_c - \delta_n)^2}{2(S_n - S_j)} \right\} \\
 &= \sqrt{2\pi} \left( \frac{1}{\sqrt{\alpha\epsilon}} + \frac{1}{\delta_c - \delta_n} \right) \frac{1}{(S_n - S_i)^{3/2}} \\
 &\quad \times \exp \left\{ -\frac{(\delta_c - \delta_n + \sqrt{\alpha\epsilon})^2}{2(S_n - S_i)} \right\}. \tag{B25}
 \end{aligned}$$

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  $\delta_n$ ,  $S_i$ , 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  $\epsilon \rightarrow 0$ , we find

$$\begin{aligned}
 I_3 &= \sqrt{2\pi} \left[ \frac{1}{\sqrt{\alpha\epsilon}} + \left( 1 - \frac{(\delta_c - \delta_n)^2}{S_n - S_i} \right) \frac{1}{\delta_c - \delta_n} \right] \frac{1}{(S_n - S_i)^{3/2}} \\
 &\quad \times \exp \left\{ -\frac{(\delta_c - \delta_n)^2}{2(S_n - S_i)} \right\}, \tag{B26}
 \end{aligned}$$

which explicitly displays the  $1/\sqrt{\epsilon}$  singularity and the finite,  $\alpha$ -independent, part.

To compute  $I_2$  we must still plug this expression into Equation (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 Equation (106). It is actually convenient to leave  $I_3$  in the form given in Equation (B25), so the integral over  $S_j$  can again be performed using Equation (A5), and we finally get

$$\begin{aligned}
 I_2 &= \left( \frac{2}{\pi} \right)^{1/2} \frac{1}{S_n^{3/2}} e^{-(2\delta_c - \delta_n)^2/(2S_n)} \\
 &\quad \times \left[ \frac{2\delta_c - \delta_n}{\sqrt{\alpha\epsilon}} + \left( 1 - \frac{(2\delta_c - \delta_n)^2}{S_n} \right) \right]. \tag{B27}
 \end{aligned}$$

Putting together this result and Equation (B16), we finally find

$$\begin{aligned}
 \Pi_{\epsilon=0}^{\text{mem-mem}}(\delta_0; \delta_n; S_n) &= \frac{1}{\sqrt{\epsilon}} \left( \frac{1}{\sqrt{\alpha}} - u_0 \sqrt{2} \right) \\
 &\quad \times (2\delta_c - \delta_n) \frac{1}{S_n^{3/2}} e^{-(2\delta_c - \delta_n)^2/(2S_n)} \\
 &\quad + \left( \frac{2}{\pi} \right)^{1/2} \left[ 1 - \frac{(2\delta_c - \delta_n)^2}{S_n} \right] \frac{1}{S_n^{3/2}} e^{-(2\delta_c - \delta_n)^2/(2S_n)}. \tag{B28}
 \end{aligned}$$

However, in this case we already know the exact result for  $\Pi_{\epsilon=0}^{\text{mem-mem}}$ , which is given by Equation (B12). Comparing these two results we learn the following. First, we know from Equation (B12) that the result is finite and there is no  $1/\sqrt{\epsilon}$  term. In the computation leading to Equation (B28) we rather find two separately divergent contribution, so they must cancel. This is fully consistent with Equation (B28), since these divergent terms have exactly the same dependence on  $\epsilon$ ,  $\delta_c$ ,  $\delta_n$ , 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 is affected neither by the solution in the boundary layer, nor by the constant  $\alpha$ , and correctly reproduces Equation (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 Equation (90), the memory-of-memory term and analogous quantities which are finite when  $\Delta(S_i, S_j) = 1$ , will still be finite. The explicit computation with the formalism developed in Section 5.3 can generate terms that are separately divergent when  $\epsilon \rightarrow 0^+$ . 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  $S_j \rightarrow S_i$  above) we can just regularize them as in Equation (B24). We call this technique ‘‘the  $\alpha$ -regularization.’’ We then 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

$$\mathcal{FP} \sum_{i=1}^{n-1} \int_{-\infty}^{\delta_c} d\delta_1 \cdots d\delta_{n-1} \partial_i^2 W = 0, \tag{B29}$$

$$\begin{aligned}
 &\mathcal{FP} \sum_{i=1}^{n-2} \sum_{j=i+1}^{n-1} \int_{-\infty}^{\delta_c} d\delta_1 \cdots d\delta_{n-1} \partial_i \partial_j W \\
 &= \left( \frac{2}{\pi} \right)^{1/2} \left[ 1 - \frac{(2\delta_c - \delta_n)^2}{S_n} \right] \frac{1}{S_n^{3/2}} e^{-(2\delta_c - \delta_n)^2/(2S_n)}. \tag{B30}
 \end{aligned}$$

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 top-hat filter in coordinate space. Observe in fact that, since  $\Delta(S_i, S_j)$  is symmetric under exchange of  $S_i$  with  $S_j$ , Equation (90), which is valid for  $S_i \leq S_j$ , can be rewritten more generally as

$$\Delta(S_i, S_j) \simeq \kappa \left[ \min(S_i, S_j) - \frac{[\min(S_i, S_j)]^2}{\max(S_i, S_j)} \right]. \tag{B31}$$

Thus, the two-point correlator can be written as

$$\langle \delta_i \delta_j \rangle = (1 + \kappa) \min(S_i, S_j) + \tilde{\Delta}(S_i, S_j), \tag{B32}$$

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  $\tilde{\Delta}_{ij}$  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  $\exp\{-\delta_c^2/(2S)\}$  in Equation (57) become  $\exp\{-\delta_c^2/[2(1 + \kappa)S]\}$ . However, now  $\tilde{\Delta}_{nn} = -\kappa S_n$  is non-zero, and we should not forget the factor  $\exp\{(1/2)\tilde{\Delta}_{nn}\partial_n^2\}$  in Equation (B3). The effect of this term can be computed exactly using the identity

$$\exp \left\{ \frac{1}{2}(b - a)\partial_x^2 \right\} \frac{1}{\sqrt{a}} e^{-x^2/(2a)} = \frac{1}{\sqrt{b}} e^{-x^2/(2b)}, \tag{B33}$$

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

$$\begin{aligned}
& \exp\left\{\frac{1}{2}(b-a)\partial_x^2\right\} \frac{1}{\sqrt{a}} e^{-x^2/(2a)} \\
&= \exp\left\{\frac{1}{2}(b-a)\partial_x^2\right\} \int_{-\infty}^{\infty} \frac{d\lambda}{2\pi} e^{i\lambda x - (1/2)a\lambda^2} \\
&= \int_{-\infty}^{\infty} \frac{d\lambda}{2\pi} \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{b-a}{2}\right)^n \partial_x^{2n} e^{i\lambda x - (1/2)a\lambda^2} \\
&= \int_{-\infty}^{\infty} \frac{d\lambda}{2\pi} \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{b-a}{2}\right)^n (i\lambda)^{2n} e^{i\lambda x - (1/2)a\lambda^2} \\
&= \int_{-\infty}^{\infty} \frac{d\lambda}{2\pi} e^{-(1/2)(b-a)\lambda^2} e^{i\lambda x - (1/2)a^2\lambda^2} \\
&= \int_{-\infty}^{\infty} \frac{d\lambda}{2\pi} e^{i\lambda x - (1/2)b\lambda^2} = \frac{1}{\sqrt{b}} e^{-x^2/(2b)}. \tag{B34}
\end{aligned}$$

(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  $\exp\{(1/2)\tilde{\Delta}_{nn}\partial_n^2\}$  on  $\exp\{-\delta_c^2/[2(1+\kappa)S]\}$  gives back the “unperturbed” exponential factor  $\exp\{-\delta_c^2/(2S)\}$ , so the zeroth-order term of this expansion is finally the same as Equation (57). The computation of the non-Markovian corrections requires the finite part prescription, since now  $\tilde{\Delta}(S_i, S_j)$  does not vanish for  $S_i = S_j$ . The integrals over  $dS_i$  and  $dS_j$  are more difficult to compute, but for  $\delta_c^2/(2S) \gg 1$  their exponential dependence is easily computed and, after taking into account again the operator  $\exp\{(1/2)\tilde{\Delta}_{nn}\partial_n^2\}$  in Equation (B3), we find that the exponential dependence of the corrections is the same that we obtained in Equation (119).

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