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Dynamic correlations in phase ordering: the $1/n$-expansion reconsidered

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Abstract. The ordering dynamics of a system with a non-conserved order parameter is considered following a quench into the ordered phase from high temperature. Newman and Bray have set up an expansion in powers of $1/n$ for the $O(n)$ model to obtain correlation functions and the two-time exponent λ, but their calculation contains a simplifying assumption which is incorrect. In this paper, tight upper and lower bounds for λ are obtained as a function of the space dimension d. These bounds exclude the result of Newman and Bray, although the dependence of λ on d is qualitatively very similar.

Comparison with simulations shows that the first-order $1/n$ calculation does not agree with numerical results as well as previously thought.

1. Introduction

Quenching a system from the high-temperature phase to below the critical point T_c gives rise to the growth of ordered domains, which obey dynamic scaling at late times, i.e. spatial correlations are time-independent when lengths are measured in units of the characteristic scale ('domain size') $L(t)$, where $L(t) \sim t^{1/2}$ for a non-conserved order parameter [1].

Of special interest is the dynamic response function [2,3] $G_k(t) = [\partial\phi_k^i(t)/\partial\phi_k^i(0)]$, where $\phi_k^i(t)$ is a Fourier component of the vector order parameter, and i denotes a component in spin-space; t is the time elapsed since the quench, and $[\ldots]$ represents an average over initial conditions. We will assume that the initial conditions correspond to an equilibrium state at high temperature.

For a non-conserved order parameter ('model A' [4]) $G_k(t)$ has the scaling form

$$G_k(t) = t^{\lambda/z} f(kt^{1/2}) \tag{1}$$

where λ is an exponent associated with non-equilibrium correlations [2,3], and $z = 2$ for a non-conserved order parameter†. Form (1) holds in the scaling limit $t \to \infty$, $k \to 0$, with $k^z t$ arbitrary. $f(x)$ is a scaling function with $f(0) = \text{constant}$.

† It has not been demonstrated convincingly that $z = 2$ for general non-conserved vector fields. Numerical simulations for $n = 2$ and $d = 2$, 3, for example (see, e.g., Mondello and Goldenfeld [5]), suggest values of z slightly less than 2. However, simulations with $n > d + 1$, where no topological defects are present, are fully consistent with $z = 2$ [6,7].) The present large-n study belongs to the latter regime.

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In this paper we perform an expansion to first order in $1/n$ for an n-component vector order parameter to calculate $\lambda_{1/n}$, where we define

$$\lambda = \lambda_{1/n} + O(1/n^2). \tag{2}$$

A diagrammatic technique to perform this task has been developed by Newman and Bray [2, 3]; [3] will be called NB in the following. The main difficulty is the evaluation of the 'dressed vertex'. NB invoked a certain approximation which, they argued, becomes valid in the scaling limit. We shall show, however, that the expression obtained by NB is incorrect, although it captures some correct features and, indeed, provides a weak upper bound on the correct result.

Because of the mathematical complexity involved in calculating the dressed vertex, we have not been able to obtain a closed expression for $\lambda_{1/n}$. We have, however, found tight bounds which determine $\lambda_{1/n}$ within a few per cent. Although the NB result does not lie within the bounds, the graph of λ against d has a very similar form.

2. The $1/n$ expansion

First we introduce the model, notation, some basic results for $n \to \infty$ and the diagrammatic method to perform an expansion to first order in $1/n$. This is largely based on NB, where a more detailed presentation can be found. We shall then show a convenient way to extract $\lambda_{1/n}$, requiring the evaluation of a single diagram instead of the five diagrams which naively appear.

2.1. The model

The model A dynamics (non-conserved order parameter) of soft spins in Fourier space can be described by the Langevin equation:

$$\frac{\partial \phi_k^i}{\partial t} = -(k^2 - r)\phi_k^i - \frac{u}{nL^d} \sum_{j,p,q} \phi_p^j \phi_q^j \phi_{k-p-q}^i + \xi_k^i(t) \tag{3}$$

where L^d is the system volume and i, j label Cartesian components in an n-dimensional order parameter space. The distribution of initial conditions is taken to be Gaussian, with mean zero and correlator

$$[\phi_k^i(0)\phi_{-k'}^j(0)] = \delta_{ij}\delta_{k,k'}\Delta_k.$$

A quench from high temperature corresponds to $\Delta_k = (r_0 + k^2)^{-1} \sim r_0^{-1} = \Delta_0$, we can therefore assume that Δ_k is independent of k. The thermal noise $\xi_k^i(t)$ has been included to provide a source term for the definition of a general response function. But throughout the calculation we choose the temperature $T = 0$ for convenience. Thermal noise is expected to be irrelevant (in the renormalization group sense) for phase ordering [8]: this has been shown explicitly for $n = \infty$ [3].

The response to initial conditions is now defined as [2, 3]

$$G_k(t) \equiv \left[\frac{\partial \phi_k^i(t)}{\partial \phi_k^i(0)}\right] \tag{4}$$

while the general (two-time) response function is

$$G_k(t,t') \equiv \left[\frac{\partial\phi^i_k(t)}{\partial\xi^i_k(t')}\right]_{\{\xi^i_k(t)\}\to 0}. \tag{5}$$

Finally, the (non-equilibrium) correlation function is

$$C_k(t,t') \equiv [\phi^i_k(t)\phi^i_{-k}(t')]. \tag{6}$$

2.2. Large-n results

For $n \to \infty$, it is possible to solve equation (3) exactly [2,3,9]. The '$n = \infty$' propagator $G^\infty_k(t)$ is then given by

$$G^\infty_k(t) = \left\{e^{-2rt} + \frac{u\Delta}{L^d}\sum_p \frac{1}{r-p^2}(e^{-2p^2t} - e^{-2rt})\right\}^{-1/2} e^{-k^2t}. \tag{7}$$

We are not generally interested in initial non-universal behaviour, so we will use the asymptotic scaling form for correlation and response functions; for $rt \gg 1$, $\Lambda^2 t \gg 1$ (Λ is the momentum cut-off) and k^2t fixed we get

$$G^\infty_k(t) = \left(\frac{t}{t_0}\right)^{d/4} e^{-k^2t} \tag{8}$$

with t_0 given by

$$t_0^{d/2} = \Delta K_d u/r \qquad K_d = (8\pi)^{-d/2}. \tag{9}$$

The two-time response and correlation functions then read [2,3]

$$G^\infty_k(t,t') = \left(\frac{t}{t'}\right)^{d/4} e^{-k^2(t-t')} \tag{10}$$

$$S^\infty_k(t) = \Delta\left(\frac{t}{t_0}\right)^{d/2} e^{-2k^2t} \tag{11}$$

where $S_k(t) \equiv C_k(t,t)$ is the structure factor and $S^\infty_k(t)$ is its large n form.

2.3. $1/n$ expansion

Whereas the large-n result required summing diagrams that have as many vertices as closed loops, the $1/n$ correction is obtained by including diagrams with one more vertex than closed loops [2,3]. Keeping close to the notation of NB we write

$$G_k(t) = G^\infty_k(t) + G'_k(t)\frac{1}{n} + \mathrm{O}\left(\frac{1}{n^2}\right) \tag{12}$$

and

$$S_k(t) = S^\infty_k(t) + S'_k(t)\frac{1}{n} + \mathrm{O}\left(\frac{1}{n^2}\right) \tag{13}$$

where $G'_{\boldsymbol{k}}(t)$ and $S'_{\boldsymbol{k}}(t)$ are given by [2,3]

$$G'_{\boldsymbol{k}}(t) = 2\int_0^t \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2\, G^{\infty}_{\boldsymbol{k}}(t_2) G^{\infty}_{\boldsymbol{k}}(t,t_1) \Sigma^{(1)}_{\boldsymbol{k}}(t_1,t_2) \tag{14}$$

$$S'_{\boldsymbol{k}}(t) = 2\Delta G'_{\boldsymbol{k}}(t) G^{\infty}_{\boldsymbol{k}}(t) + \int_0^t \mathrm{d}t_1 \int_0^t \mathrm{d}t_2\, G^{\infty}_{\boldsymbol{k}}(t,t_1) G^{\infty}_{\boldsymbol{k}}(t,t_2) \Sigma^{(2)}_{\boldsymbol{k}}(t_1,t_2). \tag{15}$$

The five diagrams for $\Sigma^{(1)}_{\boldsymbol{k}}(t_1,t_2)$ are given in figure 2 of NB. The single diagram for $\Sigma^{(2)}_{\boldsymbol{k}}(t_1,t_2)$ is figure 3 of NB, and is reproduced as figure 1 of the present paper. We shall show below that this single diagram suffices to determine the exponent λ to $\mathrm{O}(1/n)$. Note that factors of $1/n$ are written explicitly in (12) and (13), and are therefore absent from the two 'self-energy' functions $\Sigma^{i}_{\boldsymbol{k}}$. The dressed vertex $v_{\boldsymbol{k}}(t,t')$, which appears as a wavy line in figure 1, is defined by the 'bubble sum' of figure 2. Its calculation provides the main technical challenge of the $1/n$ expansion, but before we start the actual calculation we first show how to reduce the work involved.

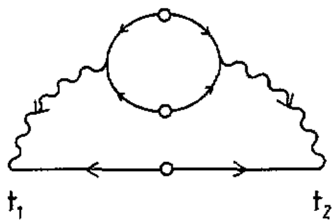

Figure 1. Diagram for $\Sigma^{(2)}_{\boldsymbol{k}}(t_1,t_2)$, defined by equation (15) for the equal-time structure factor: a circle represents the correlator of the initial conditions; a line the response function G^{∞} (given by (8) if connected to a circle, or by (15) otherwise); and a wavy line the dressed vertex v.

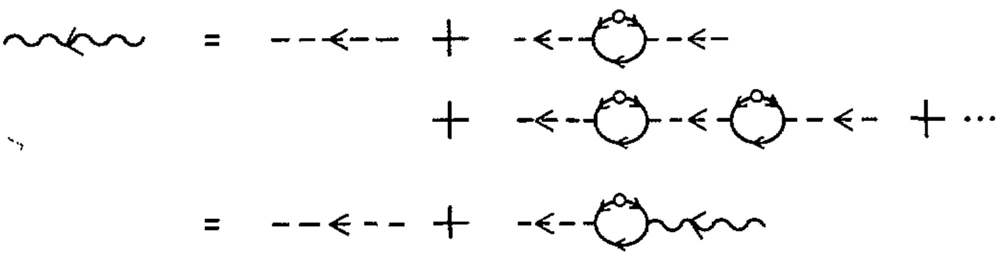

Figure 2. Diagrammatic equation, equivalent to equation (23), for the dressed vertex $v_{\boldsymbol{k}}(t_1,t_2)$: a broken line represents the bare vertex u; the other diagrammatic elements are as described in the caption to figure 1.

2.4. *A convenient way to obtain* $\lambda_{1/n}$

Like $G_{\boldsymbol{k}}(t)$ and $S_{\boldsymbol{k}}(t)$, we can also expand λ in powers of $1/n$

$$\lambda \equiv \lambda^{\infty} + \frac{\lambda'}{n} + \mathrm{O}\left(\frac{1}{n^2}\right). \tag{16}$$

By definition (2), $\lambda_{1/n} = \lambda^{\infty} + \lambda'/n$ and $\lambda^{\infty} = d/2$ from equations (1) (with $z = 2$) and (8). The obvious way to obtain λ' is to expand the response function $G_{k}(t)$, equation (1), in powers of $1/n$. It suffices to consider momentum $k = 0$

$$G_{k=0}(t) = \left(\frac{t}{t_0}\right)^{\lambda^{\infty}/2}\left(1 + \frac{\lambda'}{2n}\ln\left(\frac{t}{t_0}\right) + \mathrm{O}\left(\frac{1}{n^2}\right)\right) f(0) \tag{17}$$

with $f(0) = 1 + \mathrm{O}(1/n)$ from (8). Comparison with (12) shows that

$$G'_{k=0}(t) = \left(\frac{t}{t_0}\right)^{d/4}\left(\frac{\lambda'}{2}\ln\left(\frac{t}{t_0}\right) + \text{constant}\right) \tag{18}$$

i.e. λ' is determined by the prefactor of the logarithm of $G'_{k=0}(t)$. But calculating the five diagrams required for G' is a tedious task.

Instead, we suggest an alternative way. We shall see that a natural assumption makes our task easier; namely, we shall assume that $[(\phi(x,t))^2] \to r/u$ for $t \to \infty$, which is the statement that, for large times, the length of the order parameter field approaches its equilibrium value. With the property that $S_k(t)$ can be written in scaling form, this implies the following general form for the structure factor

$$S_k(t) = L(t)^d g(kL(t)) = t^{d/2} g(kt^{1/2}). \tag{19}$$

We notice that $S^{\infty}_k(t)$ has this form. Comparing (13) and (19) yields

$$S'_{k=0}(t) = t^{d/2}\text{constant}. \tag{20}$$

Equations (18) and (20) can now be used to simplify (15)

$$\frac{1}{\Delta}\int_0^t \mathrm{d}t_1 \int_0^t \mathrm{d}t_2 \left(\frac{1}{t_1 t_2}\right)^{d/4} \Sigma^{(2)}_{k=0}(t_1,t_2) = -\lambda' t_0^{-d/2}\ln(t/t_0) + \text{constant}. \tag{21}$$

Differentiating both sides with respect to t gives

$$\begin{aligned} -\frac{\lambda'}{t} &= \frac{1}{\Delta}\frac{\mathrm{d}}{\mathrm{d}t}\int_0^t \mathrm{d}t_1 \int_0^t \mathrm{d}t_2 \left(\frac{t_0^2}{t_1 t_2}\right)^{d/4} \Sigma^{(2)}_{k=0}(t_1,t_2) \\ &= \frac{2}{\Delta}\int_0^t \mathrm{d}t_2 \left(\frac{t_0^2}{t t_2}\right)^{d/4} \Sigma^{(2)}_{k=0}(t,t_2). \end{aligned} \tag{22}$$

The last equation makes use of the symmetry of $\Sigma^{(2)}_k(t_1,t_2)$ with respect to t_1 and t_2. Calculating $\Sigma^{(2)}_k(t_1,t_2)$ involves evaluating only one diagram and is therefore preferable to calculating G'. The price we have to pay for this short cut is that we can obtain only the exponent, not scaling functions.

All of the following calculation will be devoted to the calculation of $\Sigma^{(2)}_k(t_1,t_2)$, which first requires knowledge of $v_k(t,t')$.

3. The dressed vertex

As already mentioned, the dressed vertex $v_k(t,t')$ embodies the major difficulty of the $1/n$ calculation. In order to make progress, we shall content ourselves with calculating the integral over $v_k(t,t')$ multiplied by a certain class of functions, which we shall call $f_k(t)$, rather than focusing on $v_k(t,t')$ itself. The resulting Volterra integral equation is still difficult: the only solution we can offer is in the form of upper and lower bounds.

There are two distinct ways to set up a self-consistent equation for $v_k(t,t')$. The one we have chosen differs, for practical reasons, from the one employed by NB. The difference is that we have chosen increasing time to the left in figure 2, whereas time increases to the right in the corresponding figure (figure 4) in NB. The translation of figure 2 is

$$v_k(t,t') = u\delta(t-t') - 2\Delta u \int_{t'}^{t} \mathrm{d}t''\, v_k(t'',t') L^{-d} \sum_p G^{\infty}_{-p}(t) G^{\infty}_{p}(t'') G^{\infty}_{p+k}(t,t''). \tag{23}$$

The momentum summation can be performed easily and (using (9)) leads to

$$v_k(t,t') = u\delta(t-t') - 2r \int_{t'}^{t} \mathrm{d}t''\, v_k(t'',t') \exp\left(-\frac{k^2}{2}\frac{\{t^2 - t''^2\}}{t}\right). \tag{24}$$

We now introduce a function $g_k(t)$ by the following definition

$$g_k(t) \equiv \mathrm{e}^{k^2 t/2} \int_0^t \mathrm{d}t'\, v_k(t,t') f_k(t') \mathrm{e}^{-k^2 t'/2} \tag{25}$$

where $f_k(t)$ is arbitrary, subject to the conditions

$$\frac{\partial}{\partial t} f_k(t) \geqslant 0 \qquad f_k(0) = 0. \tag{26}$$

The motivation for introducing g and f will become clear later on, when we shall need to evaluate integrals of the form (25). The self-consistent equation for $v_k(t,t')$ can now be replaced by a similar one for $g_k(t)$

$$\frac{1}{2r} g_k(t) = \frac{u}{2r} f_k(t) - \int_0^t \mathrm{d}t'\, g_k(t') \exp\left(-\frac{k^2 t'}{2}\left(1 - \frac{t'}{t}\right)\right). \tag{27}$$

Obviously, a first simplification has occurred by the trivial fact that $g_k(t)$ depends only on one time variable t instead of two. As a technical trick, we now drop the $g_k(t)$ term on the left-hand side

$$\frac{u}{2r} f_k(t) = \int_0^t \mathrm{d}t'\, g_k(t') \exp\left(-\frac{k^2 t'}{2}\left(1 - \frac{t'}{t}\right)\right). \tag{28}$$

This can be done because we are only interested in the asymptotic, i.e. scaling limit, where the term in question is negligible. The reason for it can be seen on purely dimensional grounds: for k^2t fixed, u/r and rt are the only dimensionless combinations, so an expansion in $1/r$ is equivalent to an expansion in $1/rt$. Equation (28) therefore represents (27) to zeroth order with respect to an asymptotic expansion in $1/rt$, i.e. $g = g_0 + g_1/rt + \cdots$, has been truncated after the first term. An illustration of this procedure is the $k = 0$ case where the solutions of (27) and (28) can be compared explicitly.

It is worth mentioning that it is possible to keep the $g_k(t)/2r$ term. This leads eventually to the same results, but the underlying ideas are unnecessarily obscured.

Differentiation with respect to t transforms (28) to

$$g_k(t) = \frac{u}{2r}\dot{f}_k(t) + \frac{k^2}{2}\int_0^t \mathrm{d}t' \left(\frac{t'}{t}\right)^2 g_k(t') \exp\left(-\frac{k^2t'}{2}\left(1-\frac{t'}{t}\right)\right). \tag{29}$$

This is an inhomogeneous Volterra equation of the second kind with bounded kernel. The solution of this type of equation can be obtained by infinite iteration, which always leads to a convergent series [10].

Only for $k = 0$ can (27) and (28) be solved easily. For general k we have been unable to find a closed form expression for g. Instead we shall establish upper and lower bounds on g.

3.1. Lower bound

First of all let us state the simple inequality

$$\exp\left(-\frac{k^2t'}{2}\left(1-\frac{t'}{t}\right)\right) \geqslant \exp\left(-\frac{k^2t}{8}\right) \qquad \text{for } 0 \leqslant t' \leqslant t \tag{30}$$

which will be used at various points. With the assumed semi-positiveness of $\dot{f}_k(t)$, (equation (26)), and (30), a lower bound on $g_k(t)$ can be obtained immediately by truncating the iteration of (29) at the first non-trivial term

$$g_k(t) \geqslant \frac{u}{2r}\left\{\dot{f}_k(t) + \frac{k^2}{2}\mathrm{e}^{-k^2t/8}\int_0^t \mathrm{d}t' \left(\frac{t'}{t}\right)^2 \dot{f}_k(t')\right\}. \tag{31}$$

In particular

$$g_k(t) \geqslant \frac{u}{2r}\dot{f}_k(t) \geqslant 0 \tag{32}$$

which means that $g_k(t)$ is also semi-positive.

3.2. Upper bound

A good upper bound on $g_k(t)$ is more difficult to achieve than a lower bound. We write (29) in the somewhat complicated-looking way

$$g_k(t) = \frac{u}{2r}\dot{f}_k(t) + \frac{k^2}{2}\int_0^t \mathrm{d}t'\, g_k(t') \exp\left(-\frac{k^2t'}{2}\left(1-\frac{t'}{t}\right)\right) + R_k(t) \tag{33}$$

where $R_k(t)$ is

$$R_k(t) \equiv \frac{k^2}{2}\int_0^t \mathrm{d}t' \left(\left(\frac{t'}{t}\right)^2 - 1\right) g_k(t') \exp\left(-\frac{k^2t'}{2}\left(1-\frac{t'}{t}\right)\right). \tag{34}$$

Comparing (33) with (28), we can simplify (33) to

$$g_k(t) = \frac{u}{2r}\left(\dot{f}_k(t) + \frac{k^2}{2} f_k(t)\right) + R_k(t). \tag{35}$$

Turning our attention to $R_k(t)$, we notice $R_k(t) < 0$, which allows us to use the lower bound (30) on the exponential, and then (32), for an upper bound on R

$$R_k(t) \leqslant \left(\frac{u}{2r}\right)\frac{k^2}{2}\mathrm{e}^{-k^2t/8}\left\{-f_k(t) + f_k(0) + \int_0^t \mathrm{d}t' \left(\frac{t'}{t}\right)^2 \dot{f}_k(t')\right\}. \tag{36}$$

This, together with the restriction (26) that $f_k(0) = 0$, results in our upper bound on $g_k(t)$

$$g_k(t) \leqslant \frac{u}{2r}\left\{\dot{f}_k(t) + \frac{k^2}{2}(1 - \mathrm{e}^{-k^2t/8}) f_k(t) + \frac{k^2}{2}\mathrm{e}^{-k^2t/8}\int_0^t \mathrm{d}t' \left(\frac{t'}{t}\right)^2 \dot{f}_k(t')\right\}. \tag{37}$$

Alternatively, we could have discarded $R_k(t)$ altogether to get the weaker bound

$$g_k(t) \leqslant \frac{u}{2r}\left\{\dot{f}_k(t) + \frac{k^2}{2} f_k(t)\right\}. \tag{38}$$

Equations (32) and (38) provide a pair of weak bounds which are useful because of their simplicity. These bounds will be considered later on where, in particular, it will be shown that the bound provided by (38) reproduces the NB result.

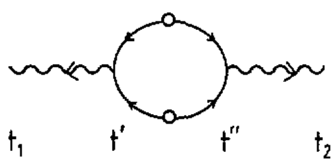

Figure 3. The element $D_k(t_1, t_2)$, whose evaluation represents the bulk of the work needed in evaluating $\Sigma_k^{(2)}(t_1, t_2)$, the diagram of figure 1.

4. The element D

The element $D_k(t_1, t_2)$ shown in figure 3 constitutes the main part of $\Sigma_k^{(2)}(t_1, t_2)$. Figure 3 corresponds to the mathematical expression

$$\begin{aligned} D_k(t_1, t_2) &= 2\frac{\Delta^2}{n}\int_0^{t_1}\mathrm{d}t' \int_0^{t_2}\mathrm{d}t''\, v_k(t_1, t') v_k(t_2, t'') \\ &\quad \times L^{-d}\sum_p G^\infty_{p-k/2}(t') G^\infty_{-p-k/2}(t') G^\infty_{-p+k/2}(t'') G^\infty_{p+k/2}(t'') \\ &= \frac{2}{nK_d}\frac{r^2}{u^2}\int_0^{t_1}\mathrm{d}t' \int_0^{t_2}\mathrm{d}t''\, v_k(t_1, t') v_k(t_2, t'') \left(\frac{t't''}{t'+t''}\right)^{d/2} \mathrm{e}^{-k^2(t'+t'')/2} \end{aligned} \tag{39}$$

where we have again used (8) for the response functions, and exploited (9). In order to apply the results of the previous sections, we now write

$$D_{\boldsymbol{k}}(t_1, t_2) = \frac{2}{nK_d}\frac{r^2}{u^2}\int_0^{t_1} \mathrm{d}t'\, v_{\boldsymbol{k}}(t_1, t')F_{\boldsymbol{k}}(t', t_2)\mathrm{e}^{-\boldsymbol{k}^2 t'/2} \tag{40}$$

where

$$F_{\boldsymbol{k}}(t', t_2) = \int_0^{t_2} \mathrm{d}t''\, v_{\boldsymbol{k}}(t_2, t'') \left(\frac{t't''}{t'+t''}\right)^{d/2} \mathrm{e}^{-\boldsymbol{k}^2 t''/2}. \tag{41}$$

Using (31), (37) and (40), the inequalities for D can be written down immediately

$$D_{\boldsymbol{k}}(t_1, t_2) \geqslant \frac{r}{u}\frac{\mathrm{e}^{-\boldsymbol{k}^2 t_1/2}}{nK_d}\left\{\partial_1 F_{\boldsymbol{k}}(t_1, t_2) + \frac{\boldsymbol{k}^2}{2}\mathrm{e}^{-\boldsymbol{k}^2 t_1/8}\int_0^{t_1}\mathrm{d}t' \left(\frac{t'}{t_1}\right)^2 \partial_1 F_{\boldsymbol{k}}(t', t_2)\right\} \tag{42}$$

and

$$D_{\boldsymbol{k}}(t_1, t_2) \leqslant \frac{r}{u}\frac{\mathrm{e}^{-\boldsymbol{k}^2 t_1/2}}{nK_d}\left\{\partial_1 F_{\boldsymbol{k}}(t_1, t_2) + \frac{\boldsymbol{k}^2}{2}(1-\mathrm{e}^{-\boldsymbol{k}^2 t_1/8})F_{\boldsymbol{k}}(t_1, t_2)\right.$$
$$\left. + \frac{\boldsymbol{k}^2}{2}\mathrm{e}^{-\boldsymbol{k}^2 t_1/8}\int_0^{t_1}\mathrm{d}t' \left(\frac{t'}{t_1}\right)^2 \partial_1 F_{\boldsymbol{k}}(t', t_2)\right\}. \tag{43}$$

Here, the symbol ∂_1 denotes differentiation with respect to the first time variable (t_1 or t') and ∂_2 will be used in an equivalent way for the second one (t_2 or t''). We have not yet shown that $\partial_1 F_{\boldsymbol{k}}(t_1, t_2) \geqslant 0$ and $F_{\boldsymbol{k}}(t_1 = 0, t_2) = 0$, which are required for the two inequalities above to be valid. The second condition is satisfied trivially, as can be seen from the definition of F, and the first one will emerge from the bounds on $\partial_1 F$, which are needed together with F in (42) and (43).

Let us start with F. Equation (41) can be easily mapped onto the form (25), and the resulting bounds (see (42) and (43)) on F are

$$F_{\boldsymbol{k}}(t', t_2) \geqslant \frac{u}{2r}\mathrm{e}^{-\boldsymbol{k}^2 t_2/2}\left\{\partial_2 f(t', t_2) + \frac{\boldsymbol{k}^2}{2}\mathrm{e}^{-\boldsymbol{k}^2 t_2/8}\int_0^{t_2}\mathrm{d}t'' \left(\frac{t''}{t_2}\right)^2 \partial_2 f(t', t'')\right\} \tag{44}$$

and

$$F_{\boldsymbol{k}}(t', t_2) \leqslant \frac{u}{2r}\mathrm{e}^{-\boldsymbol{k}^2 t_2/2}\left\{\partial_2 f(t', t_2) + \frac{\boldsymbol{k}^2}{2}(1-\mathrm{e}^{-\boldsymbol{k}^2 t_2/8})f(t', t_2)\right.$$
$$\left. + \frac{\boldsymbol{k}^2}{2}\mathrm{e}^{-\boldsymbol{k}^2 t_2/8}\int_0^{t_2}\mathrm{d}t'' \left(\frac{t''}{t_2}\right)^2 \partial_2 f(t', t'')\right\} \tag{45}$$

where we have introduced $f(t_1, t_2)$ as

$$f(t_1, t_2) = \left(\frac{t_1 t_2}{t_1 + t_2}\right)^{d/2}. \tag{46}$$

Clearly, $f(t_1, t_2 = 0) = 0$, and $\partial_2 f(t_1, t_2) \geqslant 0$ as required.

As a second ingredient in (42) and (43), bounds on $\partial_1 F_{\boldsymbol{k}}(t', t_2)$ are to be obtained. Going back to the definition of F, equation (41), and using (46), we have

$$\partial_1 F_{\boldsymbol{k}}(t', t_2) = \int_0^{t_2} \mathrm{d}t''\, v_{\boldsymbol{k}}(t_2, t'') \partial_1 f(t', t'') \mathrm{e}^{-k^2 t''/2}. \tag{47}$$

Again, it is straightforward to identify this with the form (25) and the inequalities can be read off as

$$\partial_1 F_{\boldsymbol{k}}(t', t_2) \geqslant \frac{u}{2r} \mathrm{e}^{-k^2 t_2/2} \left\{ \partial_{12} f(t', t_2) + \frac{k^2}{2} \mathrm{e}^{-k^2 t_2/8} \int_0^{t_2} \mathrm{d}t'' \left(\frac{t''}{t_2}\right)^2 \partial_{12} f(t', t'') \right\} \tag{48}$$

and

$$\partial_1 F_{\boldsymbol{k}}(t', t_2) \leqslant \frac{u}{2r} \mathrm{e}^{-k^2 t_2/2} \left\{ \partial_{12} f(t', t_2) + \frac{k^2}{2} (1 - \mathrm{e}^{-k^2 t_2/8}) \partial_1 f(t', t_2) \right.$$
$$\left. + \frac{k^2}{2} \mathrm{e}^{-k^2 t_2/8} \int_0^{t_2} \mathrm{d}t'' \left(\frac{t''}{t_2}\right)^2 \partial_{12} f(t', t'') \right\}. \tag{49}$$

It is simple to convince oneself that $\partial_1 f(t_1, t_2 = 0) = 0$, and $\partial_1 \partial_2 f(t_1, t_2) \geqslant 0$ as required.

All we have to do now is to substitute the formulae for F and $\partial_1 F$ back into the inequalities for D, equations (42) and (43). This leads without any difficulty to the lower bound

$$D_{\boldsymbol{k}}(t_1, t_2) \geqslant \frac{\mathrm{e}^{-k^2(t_1+t_2)/2}}{2nK_d} \left\{ \partial_{12} f(t_1, t_2) + \frac{k^2}{2} \mathrm{e}^{-k^2(t_1+t_2)/8} \psi(t_1, t_2) \right.$$
$$\left. + \frac{k^4}{4} \mathrm{e}^{-k^2(t_1+t_2)/8} \int_0^{t_1} \mathrm{d}t' \int_0^{t_2} \mathrm{d}t'' \left(\frac{t' t''}{t_1 t_2}\right)^2 \partial_{12} f(t', t'') \right\} \tag{50}$$

where we have introduced the definition

$$\psi(t_1, t_2) = \int_0^{t_1} \mathrm{d}t' \left(\frac{t'}{t_1}\right)^2 \partial_{12} f(t', t_2) + \int_0^{t_2} \mathrm{d}t'' \left(\frac{t''}{t_2}\right)^2 \partial_{12} f(t_1, t''). \tag{51}$$

The last term of (50) can be conveniently bounded, as shown in appendix A, and our final expression is

$$D_{\boldsymbol{k}}(t_1, t_2) \geqslant \frac{\mathrm{e}^{-k^2(t_1+t_2)/2}}{2nK_d} \left\{ \partial_{12} f(t_1, t_2) + \frac{k^2}{2} \mathrm{e}^{-k^2(t_1+t_2)/8} \psi(t_1, t_2) \right.$$
$$\left. + \frac{k^4}{4} \mathrm{e}^{-k^2(t_1+t_2)/8} \frac{d(d+2)}{(d+6)^2} \frac{(t_1 t_2)^{d/2+1}}{(t_1 + t_2)^{d/2+2}} \right\}. \tag{52}$$

For the upper bound we have to go through some algebra. It turns out that the following manipulation is of importance

$$- \mathrm{e}^{-k^2 t_2/8} f(t', t_2) + \mathrm{e}^{-k^2 t_2/8} \int_0^{t_2} \mathrm{d}t'' \left(\frac{t''}{t_2}\right)^2 \partial_2 f(t', t'')$$
$$= \mathrm{e}^{-k^2 t_2/8} \int_0^{t_2} \mathrm{d}t'' \left(\left(\frac{t''}{t_2}\right)^2 - 1 \right) \partial_2 f(t', t'')$$
$$\leqslant \mathrm{e}^{-k^2(t_1+t_2)/8} \int_0^{t_2} \mathrm{d}t'' \left(\left(\frac{t''}{t_2}\right)^2 - 1 \right) \partial_2 f(t', t'') \tag{53}$$

and a similar inequality with f replaced by $\partial_1 f$. The result of this is

$$D_k(t_1,t_2) \leqslant \frac{e^{-k^2(t_1+t_2)/2}}{2nK_d}\bigg\{\partial_{12}f(t_1,t_2) + \frac{k^2}{2}(1-e^{-k^2(t_1+t_2)/8})(\partial_1+\partial_2)f(t_1,t_2)$$
$$+\frac{k^4}{4}(1-e^{-k^2(t_1+t_2)/8})f(t_1,t_2) + \frac{k^2}{2}e^{-k^2(t_1+t_2)/8}\psi(t_1,t_2)$$
$$+\frac{k^4}{4}e^{-k^2(t_1+t_2)/8}\int_0^{t_1}dt'\left(\frac{t'}{t_1}\right)^2\partial_1 f(t',t_2)$$
$$-\frac{k^4}{4}e^{-k^2(t_1+t_2)/8}\int_0^{t_1}dt'\left(\frac{t'}{t_1}\right)^2\int_0^{t_2}dt''\frac{2t''}{t_2^2}\partial_1 f(t',t_2)\bigg\}. \tag{54}$$

Keeping the last negative term in (54) would not be a substantially better bound, so we drop it. We also note that (54) has lost its symmetry with respect to t_1 and t_2. Clearly, we could go through the whole calculation with t_1 and t_2 interchanged and would end up with the 'mirror' version of (54). Adding (54) and its 'mirror' inequality yields a symmetric form,

$$D_k(t_1,t_2) \leqslant \frac{e^{-k^2(t_1+t_2)/2}}{2nK_d}\bigg\{\partial_{12}f(t_1,t_2) + \frac{k^2}{2}(1-e^{-k^2(t_1+t_2)/8})(\partial_1+\partial_2)f(t_1,t_2)$$
$$+\frac{k^4}{4}(1-e^{-k^2(t_1+t_2)/8})f(t_1,t_2) + \frac{k^2}{2}e^{-k^2(t_1+t_2)/8}\psi(t_1,t_2)$$
$$+\frac{k^4}{8}e^{-k^2(t_1+t_2)/8}\chi(t_1,t_2)\bigg\} \tag{55}$$

where we have defined $\chi(t_1,t_2)$ by

$$\chi(t_1,t_2) = \int_0^{t_1}dt'\left(\frac{t'}{t_1}\right)^2\partial_1 f(t',t_2) + \int_0^{t_2}dt''\left(\frac{t''}{t_2}\right)^2\partial_2 f(t_1,t''). \tag{56}$$

We briefly pause for some remarks on the nature of the inequalities above. The bounds we derived for D are the consequence of a chain of quite arbitrary-looking inequalities, which might appear fairly crude in some places. The underlying logic of our choice is guided by the fact that the values of D for k^2t of order unity dominate the final integrals and therefore determine the value of $\lambda_{1/n}$. The inequalities for D are designed so that they come close to this requirement; in fact, they are exact (i.e. equalities) up to order k^2.

5. Simpler bounds on D

The previous section contains a number of disencouragingly large expressions, which are mainly due to the the generic inequalities (31) and (37). For the purpose of clarity and because the result will turn out to be of some interest in itself, we shall go through the same calculation again but with the bounds (31) and (37) replaced by the looser but much simpler bounds (32) and (38). The equivalents of equations (42) and (43) are

$$D_k(t_1,t_2) \geqslant \frac{r}{u}\frac{e^{-k^2t_1/2}}{nK_d}\partial_1 F_k(t_1,t_2) \tag{57}$$

$$D_k(t_1,t_2) \leqslant \frac{r}{u}\frac{e^{-k^2t_1/2}}{nK_d}\left\{\partial_1 F_k(t_1,t_2) + \frac{k^2}{2}F_k(t_1,t_2)\right\} \tag{58}$$

whereas the bounds on F are simply

$$F_k(t',t_2) \geqslant \frac{u}{2r}e^{-k^2t_2/2}\partial_2 f(t',t_2) \tag{59}$$

$$F_k(t',t_2) \leqslant \frac{u}{2r}e^{-k^2t_2/2}\left\{\partial_2 f(t',t_2) + \frac{k^2}{2}f(t',t_2)\right\}. \tag{60}$$

The pair of inequalities for $\partial_1 F$ is also easily deduced; it turns out that the replacement of F, f, and $\partial_2 f$ in (59) and (60) by $\partial_1 F$, $\partial_1 f$, and $\partial_{12} f$ respectively yields the desired result. Substituting in (57) and (58) yields

$$D_k(t_1,t_2) \geqslant \frac{e^{-k^2(t_1+t_2)/2}}{2nK_d}\partial_{12} f(t_1,t_2) \tag{61}$$

$$D_k(t_1,t_2) \leqslant \frac{e^{-k^2(t_1+t_2)/2}}{2nK_d}\left\{\partial_{12} f(t_1,t_2) + \frac{k^2}{2}(\partial_1+\partial_2)f(t_1,t_2) + \frac{k^4}{4}f(t_1,t_2)\right\}. \tag{62}$$

A remarkable fact about this specific upper bound for D is that it makes contact with the calculation of NB. If one derives D by using their (incorrect) dressed vertex v, one gets exactly this upper bound (62) as an equality for D; so NB managed to find a 'zeroth-order' upper bound instead of the exact result.

6. The result for λ'

In the previous sections we have obtained the main ingredient for the calculation of λ', namely D. The 'self-energy' $\Sigma^{(2)}_{k=0}(t,t_2)$ is, according to the diagram of figure 1,

$$\Sigma^{(2)}_{k=0}(t,t_2) \equiv n\Delta L^{-d}\sum_p G^\infty_{-p}(t)G^\infty_p(t_2)D_p(t,t_2). \tag{63}$$

The additional factor n takes into account that a $1/n$ has been pulled out to appear explicitly in (13). $\Sigma^{(2)}_{k=0}(t,t_2)$ can be substituted into (22) to obtain λ'

$$\begin{aligned} -\frac{\lambda'}{t} &= 2n\int_0^t dt_2\left(\frac{t_0^2}{tt_2}\right)^{d/4} L^{-d}\sum_p G^\infty_{-p}(t)G^\infty_p(t_2)D_p(t,t_2) \\ -\lambda' &= 2nt\int_0^t dt_2\, L^{-d}\sum_p e^{-p^2(t+t_2)}D_p(t,t_2) \end{aligned} \tag{64}$$

where we have used (8) for the response functions G_k^∞ in the last step. As a next step, the inequalities (52) and (55) for D have to be substituted into (64).

Let us, nevertheless, first try the looser bounds (61) and (62), which have been derived without much work. The momentum sum in (64) can be performed without difficulty, and the remaining time integration can be simplified with a little trick, which is shown in appendix B. The result is

$$\omega(d) \leqslant -\lambda' \leqslant \tfrac{16}{9}\omega(d) \tag{65}$$

where

$$\omega(d) \equiv (\tfrac{4}{3})^{d/2} B(d/2+1, d/2+1)\tfrac{1}{4}d(\tfrac{1}{2}d+1) \tag{66}$$

and $B(x,y)$ is the beta function [11], $B(x,y) = \Gamma(x)\Gamma(y)/\Gamma(x+y)$. The inequalities above are our first bounds on λ'. Clearly, λ' is negative, as expected. Furthermore, the value for λ' obtained by Newman and Bray $\lambda'_{\mathrm{NB}} = -(\frac{16}{9})\omega(d)$ is just our lower bound (upper bound on $-\lambda$), which is no surprise after the comment in the last section.

After this first insight, we now want to substitute the tighter inequalities (52) and (55) into (64). As before, the momentum sum is simple, but the time integration requires further effort. A few integrals are the same as before, but the integrals involving $\psi(d)$ and $\chi(d)$ lead to the functions $I_\psi(d)$ and $I_\chi(d)$; they can be found in appendix C. The final inequalities for λ' are

$$\begin{aligned} -\lambda' \geqslant \omega(d)\Bigg\{1 &+ \frac{d}{3}\left(\frac{d}{2}+2\right)\left(\frac{12}{13}\right)^{d/2+1} I_\psi(d) \\ &+ \frac{1}{36}\left(\frac{d+2}{d+6}\right)^2 \frac{d}{d+3}\left(\frac{12}{13}\right)^{d/2+2}\Bigg\} \end{aligned} \tag{67}$$

and

$$\begin{aligned} -\lambda' \leqslant \omega(d)\Bigg\{1 &+ \frac{2}{3}\left[1-\left(\frac{12}{13}\right)^{d/2+1}\left(1-\frac{d}{2}\left(\frac{d}{2}+2\right)\right) I_\psi(d)\right] \\ &+ \frac{1}{9}\left[1-\left(\frac{12}{13}\right)^{d/2+2}\left(1-\frac{d}{2}\left(\frac{d}{2}+1\right)\right) I_\chi(d)\right]\Bigg\} \end{aligned} \tag{68}$$

where $\omega(d)$ is given by (66). The results are plotted in figures 4 and 5, which also include λ'_{NB} from NB. Their result does not fall inside these improved bounds any more. Figure 4 shows a direct plot of $-\lambda'$ against d, while figure 5 shows that factoring the function $\omega(d)$, equation (66), from λ' removes much of the d-dependence. For large d our improved bounds approach the weaker bounds derived in section 5. These are indicated by chain lines in figure 5: the upper line, $-\lambda'/d = \frac{16}{9}$, is the NB result. Also included in figures 4 and 5, as the broken curve, is the result of applying the approximate theory of Mazenko [12] to the $\mathrm{O}(n)$ vector theory [13, 14], and then expanding the result to order $1/n$. This gives [13, 14] $-\lambda'_{\mathrm{Maz}} = (d/2)3^{-d/2}$. It can be seen that, apart from a small range of d, λ'_{Maz} lies outside our bounds and therefore cannot be the exact result. Table 1 gives more quantitative information:

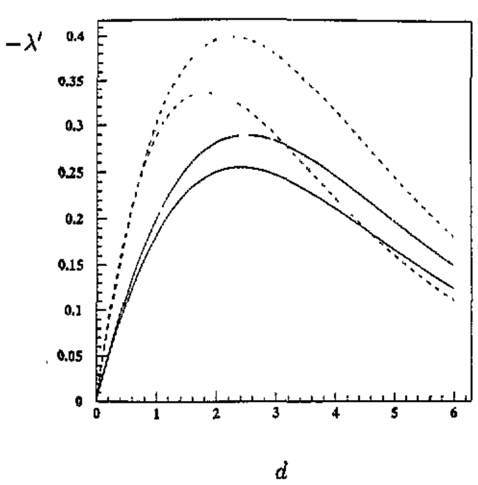

Figure 4. Bounds for $-\lambda'$ as a function of d. The continuous curves are our best upper and lower bounds; the chain curve is the NB result, while the broken curve is the result of applying the approximate Mazenko theory.

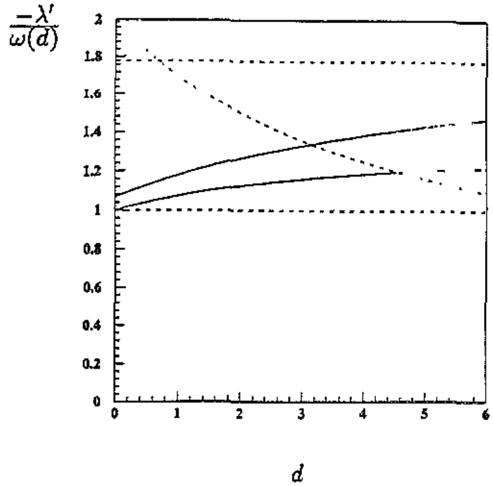

Figure 5. Bounds for $-\lambda'/\omega(d)$: continuous curves, best bounds; chain lines, weaker bounds calculated in section 5—the upper of these reproduces the NB result 16/9; broken curve, result of applying Mazenko theory.

Table 1. Upper and lower bounds for λ', the coefficient of $1/n$ in the expansion of the two-time exponent λ, for various spatial dimensions d. $\lambda'_{\rm est}$ is our best estimate, obtained by taking the mean of the upper and lower bounds. $\lambda'_{\rm NB}$ is the result of Newman and Bray [2,3], and coincides with the weak lower bound on λ' (= upper bound on $-\lambda'$!) derived in section 6.

d	$\lambda'_{\rm up}$	$\lambda'_{\rm low}$	$\lambda'_{\rm est}$	$\lambda'_{\rm NB}$
1	−0.1827	−0.2007	−0.1917±4.7%	−0.3023
2	−0.2502	−0.2811	−0.2657±5.8%	−0.3951
3	−0.2471	−0.2831	−0.2651±6.8%	−0.3779
4	−0.2114	−0.2462	−0.2288±7.6%	−0.3160
6	−0.1241	−0.1492	−0.1367±9.2%	−0.1806
∞	0	0	0	0

$\lambda'_{\rm est}$ denotes our estimated value for λ', which is just the mean of $\lambda'_{\rm up}$, the upper bound, and $\lambda'_{\rm low}$, the lower bound.

It is also interesting to compare our results with computer simulations carried out in $d = 1$ for $n = 3,4,5$ [6] and in $d = 2$ for $n = 4,5$ [7]. In the absence of topological defects such as vortices, we expect a $1/n$ expansion to be a suitable description. These simulations (especially for $d = 1$) had found $\lambda^{\rm NB}_{1/n}$ to be in surprisingly good agreement with the data, and it was therefore conjectured that a $1/n$ expansion at the zero-temperature fixed point converges more rapidly than, for example, in critical phenomena. Table 2 shows the new comparison. It is clear that the agreement between simulation and calculation is not as good as it appeared to be using the incorrect NB result. This indicates the necessity of going beyond first order in $1/n$ to obtain quantitatively accurate estimates. Given the technical difficulties occurring at $O(1/n)$, however, going to higher order does not seem a practical proposition at this time.

Table 2. Comparison of the upper and lower bounds on λ, correct to order $1/n$, and their mean $\lambda^{est}_{1/n}$, with simulation results in $d = 1$ [6] and 2 [7]. Note that the improved estimates of $\lambda_{1/n}$ are *further* from the simulation results than the previous (incorrect) $1/n$ result of NB.

d	n	λ^{sim}	$\lambda^{up}_{1/n}$	$\lambda^{low}_{1/n}$	$\lambda^{est}_{1/n}$ (%)	$\lambda^{NB}_{1/n}$
1	3	0.352(2)	0.439	0.433	0.436±0.7	0.399
	4	0.420(8)	0.454	0.450	0.452±0.4	0.424
	5	0.436(2)	0.463	0.460	0.462±0.4	0.440
2	4	0.89(1)	0.937	0.930	0.934±0.4	0.901
	5	0.91(1)	0.950	0.944	0.947±0.3	0.921

7. Conclusion

Tight upper and lower bounds have been obtained for the $O(1/n)$ contribution λ' to the exponent λ that characterizes two-time correlations in the phase-ordering kinetics of non-conserved fields. These bounds determine λ' to within a few per cent for physical values of the spatial dimension d. The bounds exclude the result derived by NB, which we therefore conclude is incorrect.

The error in the NB calculation is quite subtle. Rather than go through their calculation in detail, we refer the interested reader to equations (23)–(25) of NB. Equation (24) gives an expression for the dressed vertex $v_k(t,t')$ as the product of a simple function $f_k(t,t')$, given explicitly by equation (23) of NB, and a correction factor $\rho_k(t,t')$ given by (25). The latter factor has a leading term of unity, plus a series of terms which, term by term, give negligible (i.e. of relative order $1/rt$) contributions to final integrals. It was therefore argued that these additional terms could be dropped in the scaling limit. While these terms are individually negligible, however, there are an infinite number of them of the same order, so that a careful analysis is required before they can be discarded. The result of such an analysis is that these terms *cannot* be dropped: their sum provides contributions to final integrals which are of the same order as the nominally leading order contribution. This invalidates the NB result.

Because of the technical difficulties entailed, we have not attempted to obtain bounds on scaling functions in this paper. However, because the dressed vertex, incorrectly evaluated by NB, plays a crucial role in the calculation not only of λ itself but also of the scaling functions, it is extremely unlikely that the scaling functions obtained by NB are correct, although they probably capture the qualitative features of the correct results, just as their expression for λ' captures qualitatively the d-dependence.

We conclude by noting that it would be very nice to find a way to solve in closed form the integral equation (24), which is the source of all our technical difficulties. After all, it is only a linear equation.

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Appendix A. Lower bound on a special integral

We are interested in a lower bound for the integral

$$I \equiv \int_0^{t_1} \mathrm{d}t' \int_0^{t_2} \mathrm{d}t'' \left(\frac{t't''}{t_1 t_2}\right)^2 \partial_{12} f(t', t'') \tag{69}$$

where $f(t', t'')$ is defined in (46). The following inequality is easily established

$$\begin{aligned}\int_0^{t_2} \mathrm{d}t'' \left(\frac{t''}{t_2}\right)^2 \partial_{12} f(t', t'') &= \int_0^{t_2} \mathrm{d}t'' \left(\frac{t''}{t_2}\right)^2 \frac{d}{2}\left(\frac{d}{2}+1\right) \frac{(t't'')^{d/2}}{(t'+t'')^{d/2+2}} \\ &\geqslant \frac{d}{2}\left(\frac{d}{2}+1\right) \frac{(t')^{d/2}}{(t'+t_2)^{d/2+2}} \frac{1}{t_2^2} \int_0^{t_2} \mathrm{d}t''\, t''^{d/2+2}.\end{aligned} \tag{70}$$

Applying this scheme twice yields

$$\begin{aligned}\int_0^{t_1} \mathrm{d}t' \int_0^{t_2} \mathrm{d}t'' \left(\frac{t't''}{t_1 t_2}\right)^2 \partial_{12} f(t_1, t_2) &\geqslant \left(\frac{2}{d+6}\right)^2 t_1 t_2 \partial_{12} f(t', t'') \\ &\geqslant \frac{d(d+2)}{(d+6)^2} \frac{(t_1 t_2)^{d/2+1}}{(t_1+t_2)^{d/2+2}}.\end{aligned} \tag{71}$$

This is the desired result.

Appendix B. Some integrals

A class of integrals can be solved by using the following identity

$$\int_0^1 \mathrm{d}x \frac{x^\beta}{(1+x)^{2\beta+2+n}} (1+x^n) = B(\beta+1, \beta+1+n) \tag{72}$$

where $B(x, y)$ is the beta function [11]. To prove this, one makes a change of variable $y = 1/x$

$$\begin{aligned} I &\equiv \int_0^1 \mathrm{d}x \frac{x^\beta}{(1+x)^{2\beta+2+n}} (1+x^n) \\ &= \int_1^\infty \mathrm{d}y \frac{y^\beta}{(1+y)^{2\beta+2+n}} (1+y^n).\end{aligned} \tag{73}$$

Adding the two equations leads to an integration from 0 to ∞ and this can be identified as the sum of two beta functions.

With the definition of f, equation (46), (72) can be utilized to show

$$\int_0^t \mathrm{d}t_2 \frac{f(t, t_2)}{(t+t_2)^{d/2+2}} = \frac{1}{t}\frac{1}{2} B(d/2+1, d/2+1) \tag{74}$$

$$\int_0^t \mathrm{d}t_2 \frac{(\partial_1+\partial_2) f(t, t_2)}{(t+t_2)^{d/2+1}} = \frac{1}{t}\left(\frac{d}{2}+1\right) B(d/2+1, d/2+1) \tag{75}$$

$$\int_0^t \mathrm{d}t_2 \frac{\partial_{12} f(t, t_2)}{(t+t_2)^{d/2}} = \frac{1}{t}\frac{d}{4}\left(\frac{d}{2}+1\right) B(d/2+1, d/2+1) \tag{76}$$

$$\int_0^t \mathrm{d}t_2 \frac{(t t_2)^{d/2+1}}{(t+t_2)^{d+4}} = \frac{1}{t}\frac{1}{8}\frac{d+2}{d+3} B(d/2+1, d/2+1). \tag{77}$$

Appendix C. Calculation of $I_\psi(d)$ and $I_\chi(d)$

It is convenient to first rewrite ψ and χ, defined by (51) and (56) respectively, as series originating from continued integration by parts. The generic form is

$$\int_0^{t_2} dt'' \frac{t''^\beta}{(t_1+t'')^\beta} = \frac{\beta t_2^\beta}{(t_1+t_2)^\beta}\left\{\frac{t_2}{\beta(\beta+1)} + \frac{1}{(\beta+1)(\beta+2)}\frac{t_2^2}{t_1+t_2} + \frac{1}{(\beta+2)(\beta+3)}\frac{t_2^3}{(t_1+t_2)^2} + \cdots\right\}. \tag{78}$$

Then the following integrals can be evaluated using (72) of appendix B. To save writing we introduce $\alpha \equiv d/2+1$

$$\int_0^t dt_2 \frac{\psi(t,t_2)}{(t+t_2)^\alpha} = \frac{1}{t}(\alpha-1)\alpha(\alpha+1)B(\alpha,\alpha)I_\psi(d) \tag{79}$$

where $I_\psi(d)$ is the following infinite sum ($\alpha \equiv d/2+1$)

$$I_\psi(d) = \frac{\Gamma(2\alpha)}{\Gamma(\alpha)}\sum_{j=0}^{\infty}\frac{1}{(\alpha+1+j)(\alpha+2+j)}\frac{\Gamma(\alpha+1+j)}{\Gamma(2\alpha+1+j)}. \tag{80}$$

In a similar way one obtains

$$\int_0^t dt_2 \frac{\chi(t,t_2)}{(t_1+t_2)^{\alpha+1}} = \frac{1}{t}(\alpha-1)\alpha B(\alpha,\alpha)I_\chi(d) \tag{81}$$

where

$$I_\chi(d) = \frac{1}{2}\frac{\Gamma(2\alpha+1)}{\Gamma(\alpha)}\sum_{j=0}^{\infty}\frac{1}{(\alpha+j)(\alpha+1+j)}\frac{\Gamma(\alpha+j)}{\Gamma(2\alpha+1+j)} \tag{82}$$

and, as before, $\alpha \equiv d/2+1$.

Table C1. Values for $I_\psi(d)$ and $I_\chi(d)$, defined by equations (80) and (82).

d	I_ψ	I_χ
0	$\pi^2/6 - 3/2$	$\pi^2/3 - 3$
1	0.099 11	0.165 19
2	$2\pi^2 - 59/3$	$3\pi^2 - 59/2$
3	0.055 60	0.077 84
4	$15\pi^2 - 148$	$20\pi^2 - 592/3$
5	0.035 84	0.046 08
6	$280\pi^2/3 - 13\,817/15$	0.037 18

The sums (80) and (82) can be evaluated numerically for general α. We note, however, that for even d (i.e. integer α), these sums can be evaluated analytically, since the ratio of gamma functions in the summand yields a simple, factored polynomial in the denominator. Also, the evaluation of I_ψ is simplified by the following relation between I_ψ and I_χ

$$I_\psi(d+2) = \frac{2(2\alpha+1)}{\alpha}I_\chi(d) - \frac{2\alpha+1}{\alpha^2(\alpha+1)} - \frac{1}{(\alpha+1)(\alpha+2)}. \tag{83}$$

The results for I_ψ and I_χ, for $0 \leqslant d \leqslant 6$, are given in table C1.

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