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Perturbation theory for effective diffusivity in random gradient flows

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Abstract. We investigate a result for the effective diffusivity of particles in a random gradient flow, previously obtained by an intuitively plausible renormalization-group argument and very accurately verified by numerical simulation. We show that, to two-loop order, the result is consistent with a direct perturbation theory calculation. To the same order in perturbation theory we also derive a 'Ward identity' which guarantees the equality of the ratio of the effective diffusivity to the renormalized coupling with the ratio of the corresponding bare values. The invariance of this ratio under renormalization was an important feature of the successful renormalization-group calculation.

1. Introduction

The advective diffusion of scalar fields in random velocity fields has been extensively studied with particular emphasis on qualitative behaviour such as anomalous diffusion and its associated exponents (see, for example, [1] and references within). However even situations giving rise to normal diffusion are of interest. The evaluation of the associated long-range effective diffusivity in terms of the statistical properties of the random flow presents a challenging problem with its own new technical difficulties [2, 3]. In a previous paper [4] we derived, using a physically plausible renormalization-group technique, a simple formula for the effective diffusivity κ_e of particles subject to molecular diffusivity κ_0 and transport by a gradient velocity field $\lambda_0\nabla\phi(\boldsymbol{x})$. The result, in three dimensions, is

$$\kappa_e = \kappa_0 \exp\left\{-\frac{\lambda_0^2}{3\kappa_0^2}\Delta(0)\right\} \tag{1}$$

where

$$\Delta(\boldsymbol{x}-\boldsymbol{x}') = \langle\phi(\boldsymbol{x})\phi(\boldsymbol{x}')\rangle\,. \tag{2}$$

The same result has been obtained by Deem and Chandler [5] on the basis of the same style of renormalization-group argument.

This result agrees *extremely* well with numerical simulations [4] for a parameter range $0 < \lambda_0/\kappa_0 < 2$ which corresponds to a variation in κ_e by a factor of ~ 3. A small departure from the prediction of (1) from our numerical simulations does appear at the upper end of the parameter range investigated, $\lambda_0/\kappa_0 \sim 2$, the values of κ_e being slightly higher than those predicted by (1). However, further investigation has lead us to ascribe this departure to simulation difficulties in the large disorder regime. With increasing disorder two types of difficulty for the numerical simulation emerge:

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(i) *The onset of linear time dependence for the dispersion of the particles occurs later and* later. Measurement of the slope for the purposes of estimating κ_e is likely then to lead to values that are a little too large.

(ii) The value of κ_e is strongly influenced by trapping at the extrema of the fluctuating background field $\phi(x)$ where the velocity vanishes. The necessary practical restriction to a finite number of (random) Fourier modes in our simulation of this field [6, 7] leads to a rounding off of these extrema. Again one intuitively expects this deficiency to lead to an overestimate of κ_e.

Therefore we have experimented both with increasing the simulation time and increasing the number of Fourier modes in the Gaussian field construction. These adjustments move *the value of* κ_e, *measured in the simulations, down towards that given by (1).*

This weight of evidence leads us to believe that (1) is an exact result. The derivation using the renormalization group is physically very plausible but we have not, so far, been able to cast the argument in a completely rigorous form. It is therefore of great interest to see to what extent the result can be derived by more conventional means. In this paper we perform the perturbative calculation of κ_e to two-loop order. The results are indeed consistent with the predictions of the renormalization group. Furthermore we propose a Ward identity, verified to two-loop order, which guarantees that the ratio of the bare diffusivity to the bare vertex coupling constant is equal to the ratio of the two corresponding *dressed* quantities. The constancy of this ratio is an important feature of our renormalization-group argument. So far, higher-order calculations have proved intractable.

2. Green's functions

The equation satisfied by the Green's function in a velocity field $u(x) = \lambda_0 \nabla\phi(x)$ is

$$\left(\kappa_0 \nabla^2 - \lambda_0 \nabla\phi(x) \cdot \nabla\right) G(x, x') = -\delta(x - x') . \tag{3}$$

After averaging over the random ensemble of flows we obtain an effective Green's function

$$\mathcal{G}(x - x') = \langle G(x, x') \rangle \sim \frac{1}{4\kappa_e \pi |x - x'|} \qquad \text{for} \quad |x - x'| \to \infty \tag{4}$$

where κ_e is the effective diffusivity that controls the long-range dispersal of the scalar field. The Fourier transform of $\mathcal{G}(x - x')$ is

$$\tilde{\mathcal{G}}(k) = \left[\kappa_0 k^2 - \Sigma(k)\right]^{-1} . \tag{5}$$

At small k the irreducible two-point function $\Sigma(k)$ satifies

$$\Sigma(k) \sim \sigma k^2 \tag{6}$$

with the result that the effective long-range diffusivity is

$$\kappa_e = \kappa_0 - \sigma . \tag{7}$$

For the purposes of simulation we assumed that

$$\Delta(x - x') = \int \frac{d^3 q}{(2\pi)^3} D(q)\, e^{iq\cdot(x - x')} \tag{8}$$

with

$$D(q) = \frac{(2\pi)^{3/2}}{k_0^3}\, e^{-q^2/2k_0^2} . \tag{9}$$

The normalization is chosen so that

$$\langle(\phi(x))^2\rangle = 1\,. \tag{10}$$

In our simulations we set $k_0 = 1$.

3. Graphical rules for perturbation theory

It is convenient to associate the perturbation terms with diagrams. The Feynman rules for the diagrammatic perturbation expansion are as follows:

(i) The sum of the inwardly flowing wavevectors at each vertex is zero.
(ii) Each full curve carries a factor of $1/\kappa_0 k^2$.
(iii) Each loop wavevector q is integrated with a factor $\mathrm{d}^3q/(2\pi)^3$.
(iv) Each vertex of the form of figure 1 carries a factor $\lambda_0\,(k+q)\cdot q$.
(v) Each broken line carries a factor $D\,(q)$.

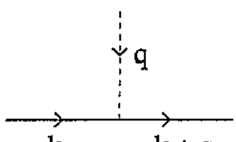

Figure 1. Vertex diagram.

4. One-loop contributions

The one-loop contribution to $\Sigma(k)$ is associated with the diagram in figure 2. According to the above rules it is

$$\Sigma^{(1)}(k) = -\frac{\lambda_0^2}{\kappa_0}\int \frac{\mathrm{d}^3q}{(2\pi)^3} D(q)\frac{(k+q)\cdot q\, k\cdot q}{(k+q)^2}\,. \tag{11}$$

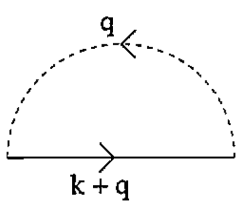

Figure 2. One-loop contribution to Σ.

In order to give the flavour of the manipulations we use we explain this one-loop case in detail. We first re-write the numerator using the identity

$$(k+q)\cdot q = \left[(k+q)^2 - k\cdot(k+q)\right]. \tag{12}$$

We then have

$$\Sigma^{(1)}(k) = -\frac{\lambda_0^2}{\kappa_0}\int \frac{\mathrm{d}^3q}{(2\pi)^3} D(q)\left\{k\cdot q - \frac{k\cdot(k+q)\, k\cdot q}{(k+q)^2}\right\}. \tag{13}$$

The first term integrates to zero. We wish to evaluate the second term only to $\mathrm{O}(k^2)$. Because of the explicit factors of k in the integrand we can set $k = 0$ everywhere else. The result is

$$\Sigma^{(1)}(k) \simeq \frac{\lambda_0^2}{\kappa_0}\int \frac{\mathrm{d}^3q}{(2\pi)^3} D(q)\frac{k\cdot q\, k\cdot q}{q^2}\,. \tag{14}$$

This is easily evaluated as

$$\Sigma^{(1)}(k) \simeq \frac{\lambda_0^2}{\kappa_0}\frac{k^2}{3}\int \frac{d^3q}{(2\pi)^3}D(q) = \frac{\lambda_0^2}{3\kappa_0}\Delta(0)k^2 . \tag{15}$$

This tells us immediately that the one-loop contribution to σ is

$$\sigma^{(1)} = \frac{\lambda_0^2}{3\kappa_0}\Delta(0) \tag{16}$$

yielding the standard one-loop result

$$\kappa_e = \kappa_0\left\{1 - \frac{\lambda_0^2}{3\kappa_0^2}\Delta(0)\right\} . \tag{17}$$

This is of course consistent to $O(\lambda_0^2)$ with (1).

5. Two-loop contributions

The two two-loop diagrams contributing to $\Sigma(k)$ are shown in figures 3(a) and (b). From 3(a) we obtain a term

$$\Sigma^{(2a)}(k) = \frac{\lambda_0^4}{\kappa_0^3}\int \frac{d^3q}{(2\pi)^3}\frac{d^3p}{(2\pi)^3}D(q)D(p)\frac{(k+q)\cdot q\,(k+q+p)\cdot p\,(k+q)\cdot p\,k\cdot q}{(k+q)^2\,(k+q+p)^2\,(k+q)^2} \tag{18}$$

and from 3(b) the term

$$\Sigma^{(2b)}(k) = \frac{\lambda_0^4}{\kappa_0^3}\int \frac{d^3q}{(2\pi)^3}\frac{d^3p}{(2\pi)^3}D(q)D(p)\frac{(k+p)\cdot p\,(k+q+p)\cdot q\,(k+q)\cdot p\,k\cdot q}{(k+p)^2\,(k+q+p)^2\,(k+q)^2} . \tag{19}$$

In equation (18) we again use the identity in (12) with the result

$$\Sigma^{(2a)}(k) = \frac{\lambda_0^4}{\kappa_0^3}\int \frac{d^3q}{(2\pi)^3}\frac{d^3p}{(2\pi)^3}D(q)D(p)\left\{\frac{(k+q+p)\cdot p\,(k+q)\cdot p\,k\cdot q}{(k+q+p)^2\,(k+q)^2} - \frac{k^2}{3}\frac{q^2\,(q+p)\cdot p\,q\cdot p}{q^2\,(q+p)^2\cdot q^2}\right\} . \tag{20}$$

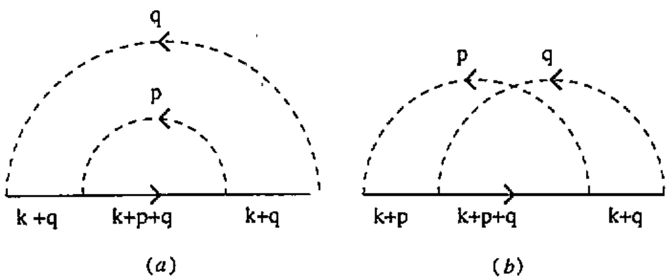

Figure 3. Two-loop contributions to Σ.

Applying a similar manipulation to (19) we find

$$\Sigma^{(2b)}(k) = \frac{\lambda_0^4}{\kappa_0^3}\int \frac{d^3q}{(2\pi)^3}\frac{d^3p}{(2\pi)^3}D(q)D(p)\left\{\frac{(k+q+p)\cdot q\,(k+q)\cdot p\,k\cdot q}{(k+q+p)^2\,(k+q)^2} - \frac{k^2}{3}\frac{p\cdot q\,(q+p)\cdot p\,q\cdot p}{p^2\,(q+p)^2\,q^2}\right\}. \tag{21}$$

When the two terms are combined we encounter a contribution to the integrand for $\Sigma^{(2)}(k) = \Sigma^{(2a)}(k) + \Sigma^{(2b)}(k)$ of the form

$$\frac{(k+q+p)\cdot(p+q)\,(k+q)\cdot p\,k\cdot q}{(k+q+p)^2\,(k+q)^2} = \frac{(k+q)\cdot p\,k\cdot q}{(k+q)^2} - \frac{k\cdot(k+q+p)\,(k+q)\cdot p\,k\cdot q}{(k+q+p)^2\,(k+q)^2}. \tag{22}$$

The first of these terms is odd in p and so integrates to zero. The second term can be treated in the obvious way to $O(k^2)$ with the result

$$\Sigma^{(2)}(k) = -\frac{k^2}{3}\frac{\lambda_0^4}{\kappa_0^3}\int \frac{d^3q}{(2\pi)^3}\frac{d^3p}{(2\pi)^3}D(q)D(p)\left\{\frac{(q+p)\cdot p\,q\cdot p}{(q+p)^2\,q^2} + \frac{p\cdot q\,(q+p)\cdot p\,q\cdot p}{p^2\,(q+p)^2\,q^2} + \frac{q\cdot(q+p)\,q\cdot p}{(q+p)^2\,q^2}\right\}. \tag{23}$$

The first and third terms in the integrand may be combined to produce a term that is odd in p and which therefore integrates to zero. The middle term can be symmetrized for p and q to yield the result

$$\Sigma^{(2)}(k) = -\frac{k^2}{3}\frac{\lambda_0^4}{\kappa_0^3}\int \frac{d^3q}{(2\pi)^3}\frac{d^3p}{(2\pi)^3}D(q)D(p)\left\{\frac{1}{2}\frac{(p\cdot q)^2}{p^2\,q^2}\right\} \tag{24}$$

leading to

$$\Sigma^{(2)}(k) = -\frac{k^2}{18}\frac{\lambda_0^4}{\kappa_0^3}\int \frac{d^3q}{(2\pi)^3}\frac{d^3p}{(2\pi)^3}D(q)D(p) = -\frac{k^2}{18}\frac{\lambda_0^4}{\kappa_0^3}[\Delta(0)]^2. \tag{25}$$

The outcome for κ_e is

$$\kappa_e = \kappa_0\left\{1 - \frac{\lambda_0^2}{3\kappa_0^2}\Delta(0) + \frac{\lambda_0^4}{18\kappa_0^4}[\Delta(0)]^2\right\}. \tag{26}$$

This result is identical to (1) to $O(\lambda_0^4)$.

Taking into account the numerical accuracy of the result it seems reasonable to conjecture that the perturbation series will produce (1) to all orders in λ_0. We have examined the perturbation series at $O(\lambda_0^6)$ but have found the corresponding terms rather intractable. Ultimately, however, it should be possible to verify that the predicted result emerges.

6. 'Ward' identity

One of the features of the renormalization-group calculation was the constancy, at each stage of the procedure, of the ratio $\kappa_e/\lambda_e = \kappa_0/\lambda_0$. We propose here an identity, verified to two-loop order in perturbation theory, that shows such a result is to be expected. Any calculation that violates this requirement will be unsuccessful.

An examination of the diagrams contributing to the complete vertex function shows that it must have the form

$$V(q, k') = q_i V_i(q, k') \tag{27}$$

where

$$V_i(q, k') = W_{ij}(q, k')k'_j\,. \qquad (28)$$

From the requirement of rotational invariance it follows that

$$W_{ij}(q, k') = A(q, k')\delta_{ij} + B(q, k')k'_ik'_j + C(q, k')k'_iq_j + D(q, k')q_ik'_j + F(q, k')q_iq_j\,. \qquad (29)$$

It is both natural and consistent with the renormalization-group calculation, to define the renormalized coupling so that it determines the small wavenumber behaviour of the vertex. That is, we will choose the effective coupling λ_e so that

$$\lambda_e = A(0, 0)\,. \qquad (30)$$

It follows that for small wavenumber

$$V(q, k') \simeq \lambda_e q \cdot k'\,. \qquad (31)$$

An examination of the diagrams contributing to $\Sigma(k)$ shows that on differentiation with respect to k_i there are two types of contribution. The first type corresponds to the terms that arise from the differentiation of the full line propagators in each diagram. They sum up to yield a term

$$-2(\kappa_0/\lambda_0)[V_i(0, k) - \lambda_0 k_i]\,. \qquad (32)$$

The second type arises from the differentiation of the vertex factors in the diagrams. We will denote this contribution by $U_i(k)$. For small wavevector k, it follows from the previous paragraph that

$$V_i(0, k) \simeq \lambda_e k_i\,. \qquad (33)$$

We assert that in the same regime

$$U_i(k) \sim \mathrm{O}(k^2)k_i\,. \qquad (34)$$

This assertion is demonstrated below in perturbation theory to two-loop order.

We have then the 'Ward' identity

$$\frac{\partial}{\partial k_i}\Sigma(k) = -2(\kappa_0/\lambda_0)[V_i(0, k) - \lambda_0 k_i] + U_i(k)\,. \qquad (35)$$

For small wavevector k this implies

$$2\sigma k_i = -2(\kappa_0/\lambda_0)\lambda_e k_i + 2\kappa_0 k_i + \mathrm{O}(k^2)k_i\,. \qquad (36)$$

We have then, on taking the limit $k \to 0$, the result

$$\kappa_e = (\kappa_0/\lambda_0)\lambda_e \qquad (37)$$

which exhibits the constancy of the ratio referred to above.

7. Perturbative analysis of the Ward identity

From (11) we see that

$$\frac{\partial}{\partial k_i}\Sigma^{(1)}(k) = 2\frac{\lambda_0^2}{\kappa_0}\int \frac{\mathrm{d}^3q}{(2\pi)^3}D(q)\frac{(k+q)\cdot q\,(k+q)_i\,k\cdot q}{(k+q)^2\,(k+q)^2}$$
$$-\frac{\lambda_0^2}{\kappa_0}\int \frac{\mathrm{d}^3q}{(2\pi)^3}D(q)q_i\frac{k\cdot q + (k+q)\cdot q}{(k+q)^2}\,. \qquad (38)$$

The first term is just the one-loop contribution to $-2(\kappa_0/\lambda_0)V_i(0,\boldsymbol{k})$. The second term is the corresponding contribution to $U_i(\boldsymbol{k})$. It is easily evaluated to yield

$$U_i^{(1)}(\boldsymbol{k}) = -k^2 k_i \frac{2}{3}\frac{\lambda_0^2}{\kappa_0}\int \frac{\mathrm{d}^3 q}{(2\pi)^3}\frac{D(q)}{q^2}\,. \tag{39}$$

Clearly $U_i^{(1)}(\boldsymbol{k}) \sim \mathrm{O}(k^2)\,k_i$ as required.

The two-loop graphs can be analysed similarly. The resulting two-loop contributions to $-2(\kappa_0/\lambda_0)V_i(0,\boldsymbol{k})$ are easily identified and require no explicit calculation. The contributions to $U_i(\boldsymbol{k})$ are

$$U_i^{(2a)}(\boldsymbol{k}) = \frac{\lambda_0^4}{\kappa_0^3}\int \frac{\mathrm{d}^3 p}{(2\pi)^3}\frac{\mathrm{d}^3 q}{(2\pi)^3} D(p)D(q)\frac{N_i^{(2a)}}{(\boldsymbol{k}+\boldsymbol{p})^2(\boldsymbol{k}+\boldsymbol{p}+\boldsymbol{q})^2(\boldsymbol{k}+\boldsymbol{p})^2} \tag{40}$$

where

$$\begin{aligned} N_i^{(2a)} = p_i\,(\boldsymbol{k}+\boldsymbol{p}+\boldsymbol{q})\cdot\boldsymbol{q}\,(\boldsymbol{k}+\boldsymbol{p})\cdot\boldsymbol{q}\,[\boldsymbol{k}\cdot\boldsymbol{p}+(\boldsymbol{k}+\boldsymbol{p})\cdot\boldsymbol{p}] \\ +q_i\,(\boldsymbol{k}+\boldsymbol{p})\cdot\boldsymbol{p}\,\boldsymbol{k}\cdot\boldsymbol{p}\,[(\boldsymbol{k}+\boldsymbol{p}+\boldsymbol{q})\cdot\boldsymbol{q}+(\boldsymbol{k}+\boldsymbol{p})\cdot\boldsymbol{q}] \end{aligned} \tag{41}$$

and

$$U_i^{(2b)}(\boldsymbol{k}) = \frac{\lambda_0^4}{\kappa_0^3}\int \frac{\mathrm{d}^3 p}{(2\pi)^3}\frac{\mathrm{d}^3 q}{(2\pi)^3} D(p)D(q)\frac{N_i^{(2b)}}{(\boldsymbol{k}+\boldsymbol{q})^2(\boldsymbol{k}+\boldsymbol{p}+\boldsymbol{q})^2(\boldsymbol{k}+\boldsymbol{p})^2} \tag{42}$$

where

$$\begin{aligned} N_i^{(2b)} = p_i\,(\boldsymbol{k}+\boldsymbol{q})\cdot\boldsymbol{q}\,(\boldsymbol{k}+\boldsymbol{p})\cdot\boldsymbol{q}\,[\boldsymbol{k}\cdot\boldsymbol{p}+(\boldsymbol{k}+\boldsymbol{p}+\boldsymbol{q})\cdot\boldsymbol{p}] \\ +q_i\,(\boldsymbol{k}+\boldsymbol{p}+\boldsymbol{q})\cdot\boldsymbol{p}\,\boldsymbol{k}\cdot\boldsymbol{p}\,[(\boldsymbol{k}+\boldsymbol{p})\cdot\boldsymbol{q}+(\boldsymbol{k}+\boldsymbol{q})\cdot\boldsymbol{q}]\,. \end{aligned} \tag{43}$$

The easiest way to manipulate these expressions is to show that

$$U_i^{(2a)}(\boldsymbol{k})k_i + U_i^{(2b)}(\boldsymbol{k})k_i \sim \mathrm{O}(k^4)\,. \tag{44}$$

This is achieved using the same kind of methods employed above on two-loop graphs.

8. Conclusions

Prompted by the success of a renormalization-group calculation for the effective diffusivity of a particle subject to a gradient flow combined with molecular diffusivity we have analysed the problem to two loops in perturbation theory. We confirmed, to this order, that the renormalization-group calculation is indeed correct. The accuracy of the RG calculation in comparison with numerical simulations is such that we believe the result is true to much higher order and is probably exact. However, our attempts to examine three-loop perturbation theory was obstructed by the rather intractable nature of the terms encountered.

We also showed, to two loops in perturbation theory, that a 'Ward identity' holds which guarantees that the ratio of the effective diffusivity to the effective vertex coupling strength is the same as that of the corresponding bare parameters. This was an important feature of the RG calculation. We believe that the Ward identity also holds exactly. It is an interesting technical challenge to prove these results hold for all orders of perturbation theory and are therefore exact.

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References

[1] Bouchaud J-P and Georges A 1990 *Phys. Rep.* **195**
[2] Drummond I T and Horgan R R 1987 *J. Phys. A: Math Gen.* **20** 4661
[3] King P R 1994 *J. Phys. A: Math Gen.* **20** 3935
[4] Dean D S, Drummond I T and Horgan R R 1994 *J. Phys. A: Math Gen.* **27** 5135
[5] Deem M W and Chandler D 1994 *J. Stat. Phys.* **76** 911
[6] Kraichnan R H 1976 *J. Fluid Mech.* **77** 753
[7] Drummond I T, Duane S and Horgan R R 1984 *J. Fluid Mech.* **138** 75
[8] Dean D S 1993 Stochastic dynamics *PhD Thesis* University of Cambridge