

Field-theoretic approximations for normal diffusion in random velocity fields

Michael W. Deem*

CuraGen Corporation, 322 East Main Street, Branford, Connecticut 06405

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The motion of a classical Brownian particle entrained in a fluid with random, time-independent velocity fields is discussed. Two approaches to calculating the disorder-averaged Green's function are presented, both based upon a functional-integral formulation. A renormalization group (RG) approach proves to be less satisfactory than does a self-consistent perturbation theory approach, which reproduces the well-known direct interaction approximation. An explicit comparison of the results with Monte Carlo data is made in two dimensions. The relationship between the present results and the case of diffusion in a solid, where RG provides a superior answer, is discussed in physical terms.

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I. INTRODUCTION

This paper discusses three approximate approaches for a quantitative calculation of the disorder-averaged Green's function of a classical Brownian particle entrained in the random, time-independent streamlines of a fluid. The three approaches are perturbation theory, self-consistent perturbation theory (SCPT), and renormalization group (RG) theory. Only incompressible fluids are considered. The velocity field is assumed to obey Gaussian statistics. Two example cases where the velocity field has a finite correlation length are examined in detail, in two dimensions. The presence of the streamlines, in general, tends to advect the Brownian particle, thereby increasing the effective diffusion coefficient. Such an enhanced mobility is clearly of importance in such practical applications as flow in packed beds [1–3], porous media [4–12], and stirred tank reactors [13].

These approximate approaches each have a long and studied history in physics and in fluids mechanics, in particular. The self-consistent perturbation theory will be shown to lead to the well-known direct interaction approximation (DIA) [14]. Various diagrammatic resummation schemes have also lead to this approximation [15–18]. Field theoretical techniques for studying motion in disordered media were first introduced by Martin, Siggia, and Rose [19] and Dominicis and Peliti [20]. Results from this approach were reviewed by Bouchaud and Georges [21]. A physically motivated RG approach to turbulence was introduced by Rose [22]. The RG approach to turbulence has been strongly championed by Yakhot and co-workers [23,24]. Detailed evaluations of the RG approach to turbulence were carried out for an exactly solvable model by Avellaneda and Majda [25,26].

These studies have shown that the DIA is very satisfac-

tory in the normal diffusion regime, accurately predicting quantitative Green's functions. Furthermore, RG has been very helpful in the anomalous diffusion regime, accurately predicting the scaling behavior of Green's functions. Complicating the picture, however, is the success of the DIA in predicting scaling behavior in the anomalous regime [15,27]. Even more intriguing is the success of the RG approach for the normal diffusion coefficient of a Brownian particle in a disordered *solid* [28,29]. The equivalent of the DIA is a complete failure in this case, incorrectly predicting a localization transition.

It is, therefore, interesting to derive the result of a RG treatment for normal diffusion in a random fluid and compare the results, along with those of the DIA, to those for diffusion in a random solid. Section II describes the models of the velocity field in which the Brownian particle diffuses and discusses a simple perturbation theory for the effective diffusion coefficient. The general results are illustrated by reference to these specific forms of disorder. Section III reviews the field-theoretic formulation of the classical diffusion problem. A field-theoretic derivation of the DIA by self-consistent perturbation theory is presented in Sec. IV. Section V summarizes the results of a RG treatment of the problem. The results of "exact" Monte Carlo calculations are presented in Sec. VI. I find the "expected" result that the SCPT works well and the RG works poorly in the normal diffusion regime. As noted above, however, it is not completely obvious that this should be the expected result, and a physical discussion of these results is presented in Sec. VII.

II. RANDOM FLUID MODEL

The Brownian particle is assumed to diffuse in a fluid with a static, random velocity field. The probability distribution of such a particle obeys a diffusion equation. The Green's function, $G_{\mathbf{v}}(\mathbf{x}, t)$, for diffusion in a particular instance of the velocity field is given by the solution of the standard diffusion equation. With D_0 as the free-

*Permanent address: Department of Physics, Harvard University, Cambridge, MA 02138.

space diffusion coefficient, the diffusion equation is

$$\frac{\partial G_{\mathbf{V}}(\mathbf{x}, t)}{\partial t} = D_0 \nabla^2 G_{\mathbf{V}}(\mathbf{x}, t) - \gamma_0 \nabla \cdot [G_{\mathbf{V}}(\mathbf{x}, t) \mathbf{V}(\mathbf{x})], \quad (1)$$

where $\mathbf{V}(\mathbf{x})$ is the time-independent velocity field in the fluid. The velocity of the particle due to the fluid is given by $\gamma_0 \mathbf{V}(\mathbf{x})$, where γ_0 is an inverse friction coefficient, and this is the reason for the second term on the right-hand side of Eq. (1). The Laplace transform of the Green's function, $\tilde{G}_{\mathbf{V}}(\mathbf{x}, s)$, satisfies

$$s \tilde{G}_{\mathbf{V}}(\mathbf{x}, s) = D_0 \nabla^2 \tilde{G}_{\mathbf{V}}(\mathbf{x}, s) - \gamma_0 \nabla \cdot [\tilde{G}_{\mathbf{V}}(\mathbf{x}, s) \mathbf{V}(\mathbf{x})] + \delta(\mathbf{x}). \quad (2)$$

The experimentally relevant Green's function is the average of $G_{\mathbf{V}}(\mathbf{x}, t)$ over the statistics of the velocity field. That is, $G_{\mathbf{V}}(\mathbf{x}, t)$ must be averaged over the ensemble to give $G(\mathbf{x}, t)$. The fluid is assumed to have no net flow, i.e., $\langle \mathbf{V} \rangle = \mathbf{0}$.

The fluid is also assumed to be incompressible. The continuity equation then implies that

$$\nabla \cdot \mathbf{V} = \mathbf{0}. \quad (3)$$

Thus, the velocity can be expressed in terms of a vector potential $\psi(\mathbf{x})$ as

$$\mathbf{V}(\mathbf{x}) = \nabla \times \psi(\mathbf{x}). \quad (4)$$

The vector potential is further assumed to obey correlated Gaussian statistics. This, in turn, implies that the velocity field obeys Gaussian statistics. The correlation function can be obtained in Fourier space as

$$\begin{aligned} \Omega^{-1} \langle \hat{V}_i(\mathbf{k}) \hat{V}_j(-\mathbf{k}) \rangle &= \Omega^{-1} \langle [\mathbf{k} \times \hat{\psi}(\mathbf{k})]_i [\mathbf{k} \times \hat{\psi}(-\mathbf{k})]_j \rangle \\ &= \Omega^{-1} (k^2 \delta_{ij} - k_i k_j) \langle \hat{\psi}^\top(-\mathbf{k}) \hat{\psi}(\mathbf{k}) \rangle \\ &= (k^2 \delta_{ij} - k_i k_j) \hat{\chi}(k), \end{aligned} \quad (5)$$

where $\hat{\chi}(k)$ is the diagonal element of the correlation matrix of the vector potential and Ω denotes the effectively infinite volume of the system. For notational convenience, the correlation matrix is defined as

$$\Omega^{-1} \langle \hat{V}_i(\mathbf{k}) \hat{V}_j(-\mathbf{k}) \rangle = \hat{\chi}_{VV_{ij}}(k). \quad (6)$$

Two archetypical forms of the correlation function of

$$\hat{G}(k, s) = -\frac{i}{\Omega} \lim_{N \rightarrow 0} \int \mathcal{D}[\hat{\varphi}] \mathcal{D}[\hat{\varphi}] \hat{\varphi}_1(\mathbf{k}) \hat{\varphi}_1(-\mathbf{k}) e^{L[\hat{\varphi}, \hat{\varphi}]} / \int \mathcal{D}[\hat{\varphi}] \mathcal{D}[\hat{\varphi}] e^{L[\hat{\varphi}, \hat{\varphi}]}. \quad (11)$$

The effective action is given by

$$\begin{aligned} L[\hat{\varphi}, \hat{\varphi}] &= i \sum_{\alpha=1}^N \int_{\mathbf{k}} \hat{\varphi}_\alpha(-\mathbf{k}) \hat{\varphi}_\alpha(\mathbf{k}) [s + D_0 k^2] \\ &+ \frac{\gamma_0^2}{2} \sum_{\alpha, \beta=1}^N \int_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4} (2\pi)^d \\ &\times \delta(\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3 + \mathbf{k}_4) \mathbf{k}_2^\top \hat{\chi}_{VV}(|\mathbf{k}_1 + \mathbf{k}_2|) \mathbf{k}_4 \\ &\times \hat{\varphi}_\alpha(\mathbf{k}_1) \hat{\varphi}_\alpha(\mathbf{k}_2) \hat{\varphi}_\beta(\mathbf{k}_3) \hat{\varphi}_\beta(\mathbf{k}_4), \end{aligned} \quad (12)$$

the vector potential are examined. One exhibits exponential decay in real space

$$\hat{\chi}(k) = \frac{\kappa^4}{k^2(\kappa^2 + k^2)}, \quad (7)$$

and the other, Gaussian decay

$$\hat{\chi}(k) = e^{-k^2/\kappa^2}. \quad (8)$$

An inverse correlation length κ has been introduced here, as it will be accommodated naturally later. Numerical prefactors have been ignored, as they can be absorbed into γ_0 .

The property of interest is the effective diffusion coefficient, defined in relation to the mean square displacement averaged over the disorder by

$$\begin{aligned} D &= \lim_{t \rightarrow \infty} \int d\mathbf{x} |\mathbf{x}|^2 G(\mathbf{x}, t) / 2dt \\ &= \lim_{k \rightarrow 0} \hat{G}^{-1}(k, 0) / k^2. \end{aligned} \quad (9)$$

Iteration on Eq. (1) using the $\mathbf{V} = \mathbf{0}$ free propagator, $\hat{G}_{free}(k, s) = 1/(s + D_0 k^2)$, generates a perturbation series for the inverse of the effective diffusion coefficient,

$$\begin{aligned} D_0/D &= 1 - \frac{d-1}{d} \text{Pe}^2 + \frac{2d^2 - 5d + 3}{2d^2} \text{Pe}^4 \\ &+ \frac{\text{Pe}^4}{\chi(0)^2} \int_{\mathbf{k}_1, \mathbf{k}_2} \hat{\chi}(k_1) \hat{\chi}(k_2) \frac{k_2^2 - (\mathbf{k}_1 \cdot \mathbf{k}_2)^2 / k_1^2}{|\mathbf{k}_1 + \mathbf{k}_2|^2} \\ &+ O(\text{Pe}^6) \end{aligned} \quad (10)$$

in d dimensions. The Peclet number is given by $\text{Pe}^2 = \gamma_0^2 \chi(0) / D_0^2$.

III. FIELD-THEORETIC REPRESENTATION OF THE DIFFUSION EQUATION

I here present the field-theoretic approach to calculating the Green's function. This approach is described in some detail in Refs. [19–21]. The Green's function of any linear operator can formally be represented by a functional integral over two conjugate fields [21]. Averaging over the disorder present in the linear operator is easily performed in this formalism. The result in the present case follows very closely from the results of [28] as

where the notation $\int_{\mathbf{k}}$ stands for the d -dimensional integral $\int d\mathbf{k} / (2\pi)^d$.

In the thermodynamic limit, Eq. (11) can be written as

$$(2\pi)^d \delta(\mathbf{k} + \mathbf{k}') \hat{G}(k, s) = -i \lim_{N \rightarrow 0} \langle \hat{\varphi}_1(\mathbf{k}) \hat{\varphi}_1(\mathbf{k}') \rangle, \quad (13)$$

where the pointed brackets denote the functional average with weight $\exp\{L[\hat{\varphi}, \hat{\varphi}]\}$.

The action (12) in the disorder-averaged functional in-

tegral representation of the Green's function does not have a harmonic form, and the Green's function, thus, cannot be calculated exactly. Perturbation theory on the action (12) reproduces Eq. (10). It is clear that $D/D_0 = 1$ in one dimension. In higher dimensions, the first-order term increases the effective diffusion coefficient. Higher-order terms moderate the increase predicted by the first-order term. I now turn to the approximate treatments of these higher-order terms.

IV. SELF-CONSISTENT HARMONIC REFERENCE SYSTEM

Some form of approximation is required to make progress on the anharmonic action (12). This section presents a self-consistent perturbation theory for the correlation function. The approach is analogous to that taken in [28]. The details of the derivation are, thus, omitted. A harmonic reference system is defined by requiring the first-order correction to the correlation function to vanish. This condition is sufficient to constrain the real, radially symmetric, effective propagator to be given by the following equation:

$$\hat{G}_0^{-1}(k, s) = (s + D_0 k^2) + \gamma_0^2 \int_{\mathbf{k}_2} \hat{G}_0(k_2, s) \hat{\chi}(|\mathbf{k} + \mathbf{k}_2|) \times [k^2 k_2^2 - (\mathbf{k} \cdot \mathbf{k}_2)^2] . \quad (14)$$

This self-consistent field-theoretic result is nothing more than the "direct interaction approximation" [14]. Note that the solution to Eq. (14) exactly satisfies the sum rule associated with normalization, $\hat{G}_0(0, s) = 1/s$. The integral equation also satisfies first-order perturbation theory, as it must.

When diffusion occurs, the effective diffusion coefficient is given by $D = \lim_{k \rightarrow 0} \hat{G}_0^{-1}(k, 0)/k^2$. To analyze the diffusive regime, a simpler integral equation for the dimensionless function

$$\hat{f}(h) = D_0 \kappa^2 h^2 \hat{G}_0(\kappa h, 0) \quad (15)$$

suffices, where h is now a dimensionless variable. The diffusion coefficient is given by

$$D/D_0 = \lim_{h \rightarrow 0} \hat{f}^{-1}(h) . \quad (16)$$

The integral equation (14) is solved in the $s \rightarrow 0$ limit by a basis set approach. Asymptotic analysis shows that $\hat{f}(h) = D_0/D + O(h^2)$ as $h \rightarrow 0$ and $\hat{f}(h) \sim 1 + O(1/h^2)$ as $h \rightarrow \infty$. The basis set must be able to accommodate this behavior. Analytic forms that do not satisfy these requirements, such as $\hat{f}(h) = 1/[c_0 + c_2 h^2 + \dots]$, do not always lead to accurate solutions. A very simple rectangular basis function is adequate for this task,

$$\hat{f}(h) = \sum_{i=1}^n a_i \hat{f}_i(h) , \quad (17)$$

where

$$\hat{f}_i(h) = \begin{cases} 1, & b_{i-1} < h < b_i \\ 0, & \text{otherwise.} \end{cases} \quad (18)$$

The parameters $\{b_i\}$ are distributed in $0 < b_i < h_{max}$ by the relation $b_i = h_{max} i^2/n^2$. The parameters $\{a_i\}$ are determined by insisting the integral equation (14) is satisfied at h_i , where $h_i = (b_i + b_{i-1})/2$. Equation (14), thus, becomes a nonlinear algebraic equation for the $\{a_i\}$,

$$1/a_i = 1 + \frac{\gamma_0^2 \kappa^d}{D_0^2} \sum_{j=1}^n B_{ij} a_j . \quad (19)$$

The basis set matrix B is given in three dimensions by

$$B_{ij} = \frac{1}{4\pi^2} \int_{-1}^1 dx \int_{b_{j-1}}^{b_j} dh_2 h_2^2 \hat{\chi}(\kappa |\mathbf{h}_1 + \mathbf{h}_2|) (1 - x^2) , \quad (20)$$

where $x = \mathbf{h}_1 \cdot \mathbf{h}_2 / (h_1 h_2)$. In two dimensions, the basis set matrix is given by

$$B_{ij} = \frac{1}{2\pi^2} \int_0^\pi d\theta \int_{b_{j-1}}^{b_j} dh_2 h_2 \hat{\chi}(\kappa |\mathbf{h}_1 + \mathbf{h}_2|) \sin^2(\theta) . \quad (21)$$

The angular integral is performed analytically and the remaining magnitude integral is performed numerically by adaptive Gauss-Legendre integration [30]. Equation (19) is found to be efficiently solved by iteration on the $\{a_i\}$ parameters. Convergence is achieved for $n = 100$ and $h_{max} = 50$ for the parameters examined. Figure 1 depicts the effective diffusion coefficients predicted by Eq. (19) for the specific models of disorder defined by Eqs. (7) and (8) in $d = 3$. Figure 2 depicts the effective diffusion coefficients predicted by Eq. (19) for the specific model of disorder defined by Eq. (8) in $d = 2$.

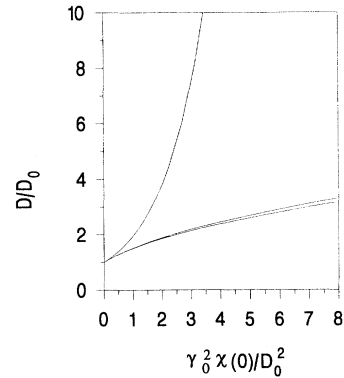


FIG. 1. Dimensionless diffusion coefficient as a function of dimensionless disorder strength for the models (7) and (8) in three dimensions. The highest curve is the renormalization group answer, Eq. (22). The second highest curve is the self-consistent result, Eq. (19), for model (7). The lowest curve is the self-consistent result for model (8).

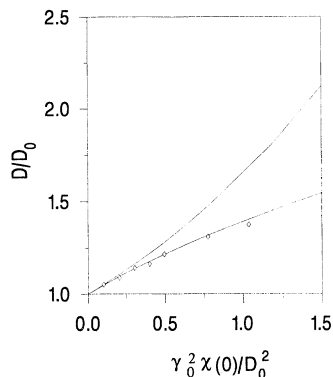


FIG. 2. Dimensionless diffusion coefficient as a function of dimensionless disorder strength for the model (8) in two dimensions. The lower curve is the self-consistent result, Eq. (19). The higher curve is the renormalization group answer, Eq. (22). The points are from the “exact” Monte Carlo simulation and are about two standard deviations in height.

V. RENORMALIZATION GROUP APPROACH

The renormalization group theory has been applied to the field theoretic formulation of diffusion in random media. The review of Bouchaud and Georges details some of the scaling predictions that have been made for the mean square displacement, i.e., the exponent in the relation $\langle r^2(t) \rangle \sim t^{2\nu}$ [21]. For the case of disorder described by Eqs. (7) and (8), these renormalization group studies indicate the long-time behavior is diffusive in two and three dimensions, i.e., $\nu = 1/2$. The quantitative calculation of the diffusion coefficient from renormalization group techniques that follows is very similar to that in [28]. The quantitative renormalization group treatment of the diffusion coefficient in a random velocity field is valid for general $\chi(|\mathbf{r}|)$ in any dimension d . The discussion is limited, however, to the case where $\chi(0)$ is finite.

I use the standard momentum-space renormalization group algorithm directly in the physical dimension. A general discussion of this approach as applied to the classical diffusion problem can be found in the review by Bouchaud and Georges [21]. More general discussions of the simple renormalization group procedure used here can be found in, for example, [31]. The detailed manipulations are very similar to that in [28] and are omitted. The final result for the effective diffusion coefficient is given by

$$D = D_0 e^{(d-1)Pe^2/d}. \quad (22)$$

This result for the models of disorder defined by Eqs. (7) and (8) in $d = 3$ is plotted in Fig. 1. The result in two dimensions for the model of disorder defined by Eq. (8) in $d = 2$ is plotted in Fig. 2.

VI. MONTE CARLO CALCULATIONS

It is clear that the self-consistent and renormalization group approaches lead to different numerical results for

the diffusion coefficient. In order to gain some insight into which approach is more accurate, Monte Carlo simulation is used to generate “exact” results. A random walk can be constructed that leads to the density profile predicted by Eq. (1). A particularly simple one is defined on a square lattice by

$$T(\mathbf{x}, \Delta\mathbf{r}) = [1 + \gamma_0 \Delta\mathbf{r} \cdot \mathbf{V}(\mathbf{x})/2]/2d, \quad (23)$$

where $T(\mathbf{x}, \Delta\mathbf{r})$ is the transition probability for a hop from \mathbf{x} to $\mathbf{x} + \Delta\mathbf{r}$ on the lattice. The random walk is, thus, locally biased in the direction of the velocity field. In the limit of a vanishing lattice spacing Δr , the random walk defined in this way leads to a density profile that satisfies Eq. (1). Other Monte Carlo schemes are possible [32,33].

To implement this scheme, the random velocity field must be generated on a lattice. Gaussian random fields can be very efficiently generated with the use of fast Fourier transform techniques [34], since Gaussian fields are decoupled in Fourier space. The vector potential is generated by this procedure in real space and the velocity field is derived from it. These calculations require a rather large lattice for convergence, and so I perform calculations in two dimensions only. In this case, Eq. (4) reduces to

$$\mathbf{V}(\mathbf{x}) = (\partial\psi(\mathbf{x})/\partial y, -\partial\psi(\mathbf{x})/\partial x). \quad (24)$$

The vector potential, in two dimensions, reduces to a single component.

This Monte Carlo scheme leads to numerical values of the diffusion coefficient that would be exact if enough statistics were collected. In particular, it is important to sample many correlation volumes of the potential for an accurate estimate of the effect of the disorder. Periodic boundary conditions are used, but the random walker should not sample more than the linear size of the lattice in one simulation if random statistics are to be preserved. The infinite time limit in Eq. (9) that is used to define the diffusion coefficient corresponds to sampling infinitely many correlation volumes. As the strength of disorder is increased, the lattice spacing Δr must be decreased. This then implies that an increased number of hops is required to escape from a correlation volume. The length of the random walk required for convergence actually grows quadratically with the disorder strength. This convergence criterion limits the current Monte Carlo calculations to moderate-disorder strengths. As an example, the random walk for $\gamma_0^2 \chi(0)/D_0^2 = 1.0$ was 2.5×10^6 hops long. The lattice was 4096×4096 , and the lattice spacing was $\Delta r \kappa = 0.01$. Diffusion coefficients are calculated by extrapolation from finite random walks in the parameter $1/t \rightarrow 0$.

The converged Monte Carlo results for the diffusion coefficient are presented in Fig. 2. The agreement between the DIA and the Monte Carlo data is very good, as suggested by calculations of Kraichnan [32] and Drummond *et al.* [33] for the case $D_0 = 0$. These results are an average over 10000 different starting positions for the random walker. This averaging removes the need to sample over different instances of the disorder. The uncertainty in

the data is about the size of the symbols. In particular, the largest standard deviations are one half the height of the symbols.

VII. DISCUSSION AND CONCLUSIONS

It is clear that the self-consistent approach is satisfactory for small Pe . By construction it must satisfy perturbation theory to first order. The renormalization group result is also satisfactory for weak disorder, by construction. The effective diffusion coefficient predicted by the renormalization group approach depends only on the dimensionless parameter Pe . For the specific models of disorder examined, the self-consistent perturbation theory result is almost independent of the model (see Fig. 1). That is, Pe is a good dimensionless parameter to correlate the results. From Eq. (10), one sees that the diffusion coefficient depends on the model used for the vector potential of the fluid. The self-consistent approach predicts this dependence to be weak.

The perturbation series (10) predicts that the effective diffusion coefficient increases with increasing strength of disorder. Higher-order terms in the series diminish the increase predicted by the first-order term. The renormalization group treatment, however, predicts an enhancement even greater than that predicted by the first-order term. This prediction is in error, as shown explicitly by Eq. (10) for weak disorder. The self-consistent approach, on the other hand, predicts a more modest increase in the effective diffusion coefficient with strength of disorder. This prediction is in accord with the low-order perturbation series predictions. It is also consistent with the Monte Carlo calculations performed for moderate-disorder strengths. The self-consistent result, or DIA, appears accurate to even higher-disorder strengths and predicts only a modest enhancement of the effective diffusion coefficient with increasing disorder of the velocity field. Figure 2 suggests that the DIA may slightly over predict

the diffusion constant at higher-disorder strengths. This discrepancy is at the limit of our Monte Carlo accuracy, however, and may not be significant.

While it is often expected that SCPT works well in the normal, diffusive, mean-field regime, and this is observed in the present results, this expectation is not always met. In particular, SCPT inappropriately localizes a particle diffusing in a solid medium [28], and RG provides a very accurate approximation to the particle motion [28,29]. The trajectory of a particle in a solid medium is one of rare, random hops between locally deep regions of the potential. Upon coarse graining, the motion of the particle still appears as random hops between wells. RG naturally accommodates this coarse-grained similarity. SCPT, on the other hand, is particularly sensitive to the local trapping of the particle. It is unable to capture the hopping motion and incorrectly predicts a localization of the particle. The trajectory of a particle in a fluid medium is one of rough entrainment along streamlines. Coarse graining the system blurs the streamlines. One-loop order RG is unable to capture the correlations that persist in this blurring and over predicts the effects of the randomness on the Brownian particle. SCPT, on the other hand, deals very well with the nonlocal averaging implied by the advective transport and provides a very accurate approximation.

In summary, while mean-field theory works well in the normal diffusive regime in liquids, it does so for a very special physical reason. Counterexamples exist where mean-field theory works poorly and RG works well even in the normal, diffusive regime.

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