Dispersion Coefficients by a Field-Theoretic Renormalization of Fluid Mechanics

Michael W. Deem\(^1\) and Jeong-Man Park\(^1,2\)

\(^1\)Chemical Engineering Department, University of California, Los Angeles, CA 90095-1592 and

\(^2\)Department of Physics, The Catholic University of Korea, Puchon 420–743, Korea

We consider subtle correlations in the scattering of fluid by randomly placed obstacles, which have been suggested to lead to a diverging dispersion coefficient at long times for high Péclet numbers, in contrast to finite mean-field predictions. We develop a new master equation description of the fluid mechanics that incorporates the physically relevant fluctuations, and we treat those fluctuations by a renormalization group procedure. We find a finite dispersion coefficient at low volume fraction of disorder and high Péclet numbers.

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Dispersion of fluid particles by flow through random media is important in problems ranging from pollutant transport through soil to enhanced oil recovery to chemical reactor design. Recently, it has been suggested that the dispersion coefficient may diverge logarithmically at long times. Such a result, which is not consistent with experimental data on flow through packed beds, would have significant implications. This prediction, however, is in disagreement with mean-field results that predict a finite dispersion coefficient.

There are four sources of randomness not accounted for in the mean-field treatment of fluid dispersion. The numerical results suggest a logarithmic divergence in three dimensions, i.e., that the upper critical dimension may be three, and the mean-field theory, which lacks the randomness, would not be expected to detect such a divergence. The first source of randomness is the random motion of the fluid particles. Since the Navier-Stokes equations are the starting point for the mean-field theory, all microscopic fluctuations of the fluid particles have been suppressed. A second source of randomness is the random locations of the obstacles to the fluid flow. The mean-field theory is essentially a renormalized single-obstacle theory. As such, all correlations around an obstacle beyond the Brinkman screening length are ignored. The third source of randomness present in the numerical simulations, but not present in the mean-field theory, are mesoscopic fluctuations naturally present in the lattice Boltzmann simulation method. Imperfections in the pseudo-random number generator are a fourth and final source of randomness present in the simulations. Using a field-theoretic renormalization group approach, we take into account the first three physical sources of randomness.

We find that these sources of randomness do not modify the mean-field prediction: the dispersion coefficient remains finite at long times and high Péclet numbers. The Péclet number is given by \(Pe = \frac{v_x R}{D_l}\), where \(v_x\) is the average velocity of the fluid, \(R\) is the average radius of the blocking obstacles, and \(D_l\) is the diffusion coefficient of the pure fluid.

Our goal is to write a field theoretic representation of the Navier-Stokes equation:

\[
\frac{\partial}{\partial t} v_i + \Pi_{jk} \sum_j v_j \partial_j v_k = \nu \nabla^2 v_i + f_i \tag{1}
\]

where \(\nu = \mu/\rho\) is the kinematic viscosity, and \(f_i = \Pi_{jk} (F_k - \partial_k P)/\rho\) is the total body force on the fluid. The presence of the projection operator \(\Pi_{ik}(k) = \delta_{ik} - k_i k_k/k^2\) in these formulas ensures that the incompressibility condition \(\nabla \cdot v = 0\) is maintained. The Fourier transform is defined by \(\tilde{f}(k) = \int dx f(x) \exp(ik \cdot x)\).

We first write a master equation model of fluid mechanics. Generalizing previous treatments from one dimension to \(d = 3\) dimensions, we consider the fluid on a lattice, with \(N_\lambda\) “velocity” particles on lattice site \(\lambda\). Since the velocity is a vector, we denote the number of particles contributing to the \(i\)th component of the velocity as \(\tilde{N}_\lambda^i\). The state of the system is defined by the configuration of velocities in the system, and the master equation relates how the probability of any given configuration, \(P(\{\tilde{N}_\lambda^i\})\), changes in time

\[
\frac{\partial}{\partial t} P = AP \tag{2}
\]

where \(A\) is a linear operator that specifies the dynamics of the fluid. Defining the identity, \(I\), shift operators, \(\hat{E}_\lambda^i P(N_\lambda^i) = P(N_\lambda^i + 1)\), \(\hat{E}_\lambda^{-1} P(N_\lambda^i) = P(N_\lambda^i - 1)\), and a number operator, \(\hat{N}_\lambda^i P(N_\lambda^i) = N_\lambda^i P(N_\lambda^i)\), the dynamics of Eq. 2 are given by diffusion, convection, and force terms, \(A = A_d + A_c + A_f\):

\[
A_d = \frac{\nu}{\hbar^2} \sum_\lambda \sum_{jk} \left[ \left( \hat{E}_{\lambda+e_k}^{-1} \hat{E}_\lambda^i \hat{E}_{\lambda+e_k}^{-1} - I \right) \hat{N}_\lambda^i \right.
\]

\[
A_c = \frac{\delta u}{2\hbar} \sum_\lambda \sum_{ijkl} \left[ \hat{E}_{\lambda+e_k}^{-1} \hat{E}_{\lambda+e_l}^{-1} \hat{E}_{\lambda+e_l} \right]_{ijkl} \hat{E}_\lambda^i \hat{N}_\lambda^j \hat{N}_\lambda^k 
\]

\[
A_f = \frac{1}{\hbar} \sum_\lambda \sum_k \left[ \hat{E}_\lambda^{k-1} - I \right] \hat{N}_\lambda^k \tag{3}
\]
Here $h$ is the lattice spacing, and $\delta u$ is the contribution of one velocity particle to the velocity. The sum is over lattice sites for $\lambda$ and over the three dimensions for $jkl$. The vector $\mathbf{e}_k$ gives the lattice site displaced by one unit in the $k^{th}$ direction. Expanding this master equation for small lattice spacing, we find that it reproduces the Navier-Stokes equation in this limit.

We map this master equation onto a field theory using the coherent states representation\[\hat{b}_i^+(\mathbf{r}) \leftrightarrow -\frac{1}{\hbar} \mathbf{E}_\lambda^{-1}, \quad b_i^+(\mathbf{r}) \leftrightarrow \mathbf{E}_\lambda \hat{N}_\lambda^+ / h^d,\]
and $b_i^+(\mathbf{r}) b_i^+(\mathbf{r}) \leftrightarrow \hat{N}_\lambda / h^d$. As is typical, we set $b_i^+(\mathbf{r}) = \hat{b}_i(\mathbf{r}) + 1$. We find the following action:

$$S = \int d\mathbf{k} \int dt \frac{\hat{b}_i(-\mathbf{k}, t) [\partial_t + \nu k^2 + \delta(t)] \hat{b}_i(\mathbf{k}, t)}{-\nu \lambda} \left(\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3\right)
\times k_2 \hat{b}_i^+(\mathbf{k}_1, t) \hat{b}_i^+(\mathbf{k}_2, \mathbf{k}_2) \hat{b}_i^+(\mathbf{k}_3, t)
\left(\mathbf{k}_1 + \mathbf{k}_3 + \mathbf{k}_4\right)
\times k_3 \hat{b}_i^+(\mathbf{k}_1, t) \hat{b}_i^+(\mathbf{k}_2, \mathbf{k}_2) \hat{b}_i^+(\mathbf{k}_3, \mathbf{k}_3) \hat{b}_i^+(\mathbf{k}_4, \mathbf{t})
- \int dt f_i \hat{b}_i(0, t)$$

Here the notation $\int d\mathbf{k}$ stands for $\int d\mathbf{k} / (2\pi)^d$, the integrals over time are from $t = 0$ to some large time $t = t_f$, and the summation convention is implied. This action is written in terms of the divergence-free part of the velocity, $\hat{b}_i^+(\mathbf{k}) = \Pi_{\mathbf{k} \lambda}(\mathbf{k}) \hat{b}_i^+(\mathbf{k})$. For convenience in later calculations, we have included a curl-free component in the quadratic terms (Feynman gauge). Initially, $\lambda_1 = 1$.

This field theory for fluid mechanics differs from the traditional one in its use of $\lambda$ in that random fluctuations of the fluid are incorporated by the presence of the $\lambda_2$ term. Using this action, standard results from fluid mechanics are reproduced. For example, a calculation of the long-time tails in the velocity-velocity correlation function in two-dimensions is in accord with the known result $\|\hat{b}_i^+(\mathbf{k})\| = 1$:

$$\langle v_i(x, t) v_j(x', t') \rangle \sim \frac{\kappa B T}{2\rho} \frac{\delta_{ij}}{4\pi \nu |t - t'| \ln^{1/2}(|t - t'| / t_0)}$$

The scaling of the Kolmogorov energy cascade and the Richardson separation law are also reproduced for the common statistical model of turbulence $k^5 / (2\rho \nu)$. The energy $E(k) \sim (\text{const}) k^{-5/3}$ and $r^2(t) \sim (\text{const}) t^3$.

In both of these calculations, the $\lambda_2$ term does not contribute. This is in contrast to recent work on reaction-diffusion systems, where fluctuations contribute at low density $\lambda = 0$. Since the fluid density is always finite in the present case, the density fluctuations captured by $\lambda_2$ prove to be irrelevant.

With these preliminaries taken care of, we now turn to the problem of flow through porous media. The main effect of the porous media is to exclude the fluid from certain fixed obstacles. The velocity is zero within and on the surface of these obstacles. Within the context of the master equation, if an obstacle is at site $\lambda$, the velocity there must be zero, $N_\lambda = 0$. This fixes the lattice spacing as $h \approx R$, where $R$ is the characteristic size of the blocking particles. A relatively singular model for the obstacles sets the average fluid velocity at the obstacle sites to zero. With this model, the obstacles generate the following additional term in the action:

$$e^{-S'} = \prod \lambda \sum \lambda = 0 \frac{P[\lambda]}{\lambda} \delta \left[ \lambda \int dt \hat{b}_i^+(\mathbf{k}) \hat{b}_i^+(\mathbf{k}) \right]$$

where $P[\lambda] = (1 - \phi) \delta_{\lambda, 0} + \phi \delta_{\lambda, 1}$, where $\phi$ is the probability of a site being occupied by an obstacle, i.e. the volume fraction of obstacles. This condition is difficult to implement directly. The condition $\int dt \hat{b}_i^+(\mathbf{k}) \hat{b}_i^+(\mathbf{k}) < a^2$, where $a^2 \approx 1 / (4\pi \nu R)^2$ is a constant, effectively implements this condition in the long-time limit and is much more convenient to implement. That is, we use a Gaussian to regularize the delta function

$$e^{-S} = (\text{const}) \prod \lambda \left[ (1 - \phi) + \phi \prod \lambda \int dt d\mathbf{t} \hat{b}_i^+(\mathbf{k}) \hat{b}_i^+(\mathbf{k}) \hat{b}_i^+(\mathbf{k}) \hat{b}_i^+(\mathbf{k}) \right]$$

Expanding to the lowest relevant order in the fields, we find the additional term in the action to be

$$S' = (\text{const}) + \frac{\phi}{2a^2 h^d} \int d\mathbf{x} \int dt d\mathbf{t}$$
$$\times \hat{b}_i^+(\mathbf{x}, t) \hat{b}_i^+(\mathbf{x}, t) \hat{b}_i^+(\mathbf{x}, t') \hat{b}_i^+(\mathbf{x}, t')$$

We set $\gamma_1 = \phi / (2a^2 h^d)$ for later convenience. We note that this form looks like a contribution arising from random, imaginary, velocity-dependent point forces acting on the fluid.

A key aspect of the flow through porous media is the net fluid flow. To accommodate this, we shift the fields by the average values. We consider the flow to be along the $x$ direction, and so set $\hat{b}_i = \delta_{i, x} v_x + \hat{b}_i^+$ and then rewrite the action in terms of $\hat{b}_i^+$. Suppressing the primes, we find

$$S = \int d\mathbf{k} \int dt \hat{b}_i(-\mathbf{k}, t) [\partial_t + \nu k^2 - ik_x v_x + \delta(t)] \hat{b}_i(\mathbf{k}, t)
+i \lambda_1 \int d\mathbf{k} \int dt (2\pi)^d \delta(\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3)
\times k_1 \hat{b}_i^+(\mathbf{k}_1, t) \hat{b}_i^+(\mathbf{k}_2, \mathbf{k}_2) \hat{b}_i^+(\mathbf{k}_3, t)
+ \gamma_1 \int d\mathbf{k} \int dt d\mathbf{t} (2\pi)^d (\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3 + \mathbf{k}_4)$$
where \( \gamma_2 = 2v_x\gamma_1 \) and \( \gamma_3 = v_x^2\gamma_1 \). We have eliminated the \( \lambda_2 \) terms, as they do not contribute in the renormalization procedure. To incorporate the random obstacles, we have used the replica trick \[12\], but have suppressed these details that do not enter in a one-loop calculation.

We now apply the renormalization group procedure to this action. From power counting, the upper critical dimension for this theory is \( d_c = 3 \). The frictional force on the fluid due to the obstacles will generate a mass term, however, that eventually renders the theory finite in any dimension. We use the momentum shell procedure, where fields on a shell of differential width \( dl \) are integrated out, \( \Lambda e^{-dl} < k < \Lambda \), where \( \Lambda \approx \pi/\hbar \) is the cutoff, and \( l \) is the flow parameter. As usual, we rescale time by the dynamical exponent \( t' = te^{-dzl} \), distance perpendicular to the flow direction by \( k'_\perp = k\lambda e^{dl} \), and distance along the flow direction by the dilation exponent \( k'_x = k x e^{dl} \) \[13\]. We make use of the average \( \langle \hat{b}^\dagger _{(1)}(k_1)\hat{b}^\dagger _{(2)}(k_2) \rangle = (2\pi)^3\delta(k_1 + k_2)\hat{H}_0(k_2)\hat{G}_0(k_2) \) where \( \hat{G}_0(k) = 1/(\nu k^2 - i k_x v_x) \). We perform a one-loop calculation, valid to first order in disorder strength and all orders in the parameter \( \lambda_1 \). A large number of integrals, over one-hundred, appear in this renormalization procedure, and details will be presented elsewhere. A typical integral would be one such as

\[
\int_{\Lambda e^{-dl} < k < \Lambda} \hat{G}_0(k)\hat{G}_0(-k) = \frac{Adl}{(2\pi)^3} \int_{k_1} \text{on shell} \frac{1}{\nu^2 k_1^4 + v_\perp^2 k_1^2} \sim \frac{Adl}{(2\pi)^3} \int_{k_1} \text{on shell} \frac{1}{\nu^2 k_1^4 + v_\perp^2 k_1^2} \frac{dkx}{\pi} = \frac{Adl}{(2\pi)^3} \int_{k_1} \text{on shell} \frac{1}{\nu^2 v_\perp k_1^2} = \frac{1}{4\pi v_\perp v_\perp} dl \quad (11)
\]

We have made use of the fact that the integral over \( k_x \) converges, and so it can be taken off the shell \[13\], and we have used the fact that \( v_x \) flows to zero and can be ignored in these calculations, \( i.e. \) we replace \( \nu k^2 \) by \( \nu_\perp k_\perp^2 \) in the propagator, where \( k^2 = k_\perp^2 + k_\parallel^2 \).

When computing the renormalization flows, some additional terms are generated. We present the details only for the \( x \)-fields, as these are most significant. A term such as \( \gamma_1 u_1 \langle \hat{b}_{(1)k_1k_2k_3} \rangle \int dt' (2\pi)^d \langle k_1 + k_2 + k_3 \rangle \hat{b}_{(2)k_1}^\dagger \hat{b}_{(3)k_2}^\dagger \hat{b}_{(3)k_3}^\dagger \hat{b}_{(4)k_4} \rangle \) is generated. In addition, a mass term is generated, \( m e^{\int dt \hat{b}_{-(k)} \hat{b}_{(k)} \rangle} \). Defining the dimensionless couplings \( g_x = \gamma_1/(4\pi
u_\perp v_x) \), \( y_x = \gamma_1/(4\pi
u_\perp v_x) \), \( g_z = 2/8\pi
u_\perp v_x^2 \), and \( \gamma_3 = 3/(4\pi
u_\perp v_x^3) \), we find the following flow equations:

\[
\frac{dln g_x}{dl} = (z - d + 1 - \eta) - 2g_x - 2g_xu_x \\
\frac{dln g_z}{dl} = (z - d + 1 - \eta) - 2g_z - 2g_zx \\
\frac{dln \lambda_x}{dl} = \frac{2g_x g_z}{g_x} - 2\lambda_x g_x - 2\lambda_x g_xz \\
\frac{dln \nu_x}{dl} = \frac{2g_x g_z}{g_x} - 2\lambda_x g_x - 2\lambda_x g_xz \\
\frac{dln \gamma_3}{dl} = \frac{2g_x g_z}{g_x} - 2\lambda_x g_x - 2\lambda_x g_xz \\
\frac{dln f}{dl} = z \quad (12)
\]

At long times, we find \( g_x(l) \sim g_x(l) \sim g_x(l) \sim 1/(g_0^1 + 2l) \). We find the unphysical term \( g_x(l) \) should vanish. We also find \( \lambda_x \sim \lambda_0/(1 + 2g_0) \). From the flow equation for the viscosity, we find the dynamical exponent is \( z = 2 + O(l^{-2}) \). From the flow equation for the velocity, we find the dilation exponent is \( \eta = 2 + O(l^{-2}) \). The mass quickly reaches the asymptotic form \( m_x(l) \sim m^* e^{2l} \) whatever the non-universal, \( A \)-dependent terms in \( dm_x dl \). In the absence of the mass term, \( e.g. \) for imaginary, velocity-dependent forces with zero average value, these flow equations generate interesting scaling behavior. In the present case, the generated mass stops the flow at a characteristic value of the flow parameter, \( l^* \).

We determine the value of the generated mass by a force balance argument. From the requirement that \( \langle b_x \rangle = 0 \), we find \( m_x(l)v_x = f(l) \), and conclude that \( f_0 = m^*v_x \). From fluid mechanics, it is known that the force density is given by Stokes’ Law at low volume fraction of obstacles and moderate flow rates \[2\]: \( f_0 = 6\pi R
u_\perp v_x \phi_0/(4\pi R^3/3) \), where \( R \) is the radius of the spherical obstacles. Equating these two results, we find \( m^*/\nu_\perp = 9\phi_0/(2R^2) \). We further calculate the correlation length in the fluid \( \xi_x = e^{2l} \) \( \xi_x(l) = e^{2l}[\nu_\perp(l)/m_x(l)]^{1/2} = e^{2l}[\nu_\perp e^{-2l}/(m^* e^{2l})]^{1/2} \). This is exactly the Brinkman screening length \[4\]. At high flow rates, empirical expressions for the drag force are available that can be used to identify \( m^* \) \[4\].
We now address the issue of the dispersion coefficient. The dispersion coefficient $D_x = \int_0^\infty dt' [(v_x(x,t)v_x(x + x(t', t + t')) - v_x^2]$ is a measure of the “dispersive” transport induced by the fluid. We can calculate this quantity directly from the field theory by perturbation theory. We find $D_x(l) = g_3(l)v_x^2/m(l)$. Using the approximate value of $a^2$ and the determined form of $m(l)$, we find $D_x(l) = e^{-2}4\pi Re_x/9$. We match the flow equations to this perturbation theory when the flow equations begin to lose their validity, $m_x(l) \approx \nu_j \Lambda^2$, which gives the characteristic flow parameter $l = \frac{1}{2} \ln(\nu_j \Lambda^2/m^*)$. We calculate the dispersion coefficient from matching $l$ as $D_x^* = e^{2\tau} D_x(l^*)$. We find the renormalized dispersion coefficient to be

$$D_x^* = \frac{4\pi}{9} Re_x \quad (14)$$

This dispersion coefficient is due solely to mechanical dispersion of the fluid, and the form is in exact agreement with the mean-field result of Koch and Brady [2]. The dispersion coefficient is proportional to the Péclet number and independent of the volume fraction in the limit of high Péclet number and low volume fraction. Only the numerical prefactor, here given approximately, is nonuniversal. Interestingly, the asymptotic value of the dispersion coefficient is independent of $l^*$, as long as the mass has been generated and $l^* \nu_j << 1$, which is the case for small volume fractions or large Péclet numbers. The independence of the observable on degree of renormalization is common when mean-field theory is essentially exact, as is the case here.

In the dilute limit, the dispersion coefficient grows as shown in figure 1. The dispersion coefficient reaches its asymptotic value at a time on the order of $t_0$. If time is nondimensionalized as $\tau = tv_x/R$, this characteristic time is given by $t_0 = Pe^{1/3}$, which is the time scale for diffusive transport across the boundary layer.

The suggestion that dispersion coefficients diverge logarithmically in three dimensions at large Péclet numbers and finite volume fractions of disorder [1], then, is not borne out by the present calculations. Such a divergence would show up as a $l^*$ dependence of the predicted dispersion coefficient, which is absent in our calculations. The proposal of a diverging dispersion coefficient was based upon simulation data, and these simulation data may not have sampled the full diffusive boundary layer transport that occurs on a time scale that grows as $Pe^{1/3}$. While transport at high volume fractions is, in principle, not accessible by our renormalization group calculations, physical aspects of the expected behavior are present in our result. In particular, curing of the logarithmic divergence in the theory by growth of a mass term due to the frictional drag force exerted by the disorder particles on the fluid seems generic. This frictional drag force would seem to prevent divergences at any volume fraction of disorder. Indeed, the higher the volume fraction of disorder, the greater the expected accuracy of the mean-field result. Our result is in agreement with the mean-field theory as soon as the frictional mass has been generated.

The renormalization group treatment of dispersion for a particle-based model shows that mean-field theory misses no essential physics at low volume fractions.

![FIG. 1: Shown is the behavior of the dispersion coefficient at low volume fraction of disorder. The dispersion coefficient reaches its asymptotic value at a dimensionless time of $\tau_0 = Pe^{1/3}$.](image_url)