Path-integral variational methods for flow through porous media

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We characterize a porous medium as a statistically homogeneous continuum with local fluctuations in physical parameters. We consider (1) the steady-state flow of a single incompressible fluid through the medium, and (2) the dispersion of a passive tracer in such a flow. For each problem we average a path-integral expression for the Green's function over parameter fluctuations, and obtain large-distance, long-time effective parameters via Feynman's variational method. For the permeability problem, and the tracer problem at small Peclet number *P*, the variational results are consistent with results obtained by first-order perturbation theory. For the tracer problem at large *P*, the variational method predicts the expected linear dependence of the effective dispersion tensor on *P*, which perturbation theory does not. This indicates that, for the problems considered here and others like them, a first-order perturbation expansion can be of limited utility.

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I. INTRODUCTION

The study of flow through a porous medium is of great practical interest in many areas of applied physics, including chromatography, filtration processes, groundwater hydrology, and petroleum engineering. The general problem [1] can be thought of as three more specific problems, depending on the length scale at which the medium is examined. Over "microscopic" scales, of the order of microns, the medium is grainy and highly irregular. Flow of a single fluid is governed by the Stokes equations, which are solved in the pores with the conditions that flow is incompressible and that velocity is zero at the pore walls. Due to the microscopic irregularity, it is impractical to obtain the exact flow field. One can get bulk properties instead, by averaging over a volume large enough to contain a statistically representative selection of pores. Such a volume is said to be of "mesoscopic" extent. Over mesoscopic scales, of the order of centimeters, the medium appears to be a homogeneous continuum, and flow of a single fluid is governed by Darcy's law. "Macroscopic" lengths are of the order of geological irregularity, i.e., meters and up. Over macroscopic scales, the medium appears to be a *heterogeneous* continuum, and flow of a single fluid is governed by a local version of Darcy's law.

Suppose a passive tracer is released into a single fluid flowing through the medium. Dispersion of this tracer is governed at microscopic scales by a convection-diffusion equation (CDE), in which the diffusion constant is the molecular diffusion constant of the tracer in the fluid, and the drift velocity is the Stokes flow field. It is impractical to obtain an exact microscopic solution in this case, as in the previous case; however, bulk properties are again obtainable by averaging over the irregularities. The equation governing dispersion of a passive tracer at mesoscopic scales is also a CDE. The velocity comes from Darcy's law. The dispersion tensor has an isotropic part due to molecular diffusion, and an anisotropic part due to convective dispersion. The latter quantity is a function of the velocity u [2]. If diffusion is more important than convection in moving a tracer particle around the medium, then convective dispersion is proportional to u^2. If convection is more important than diffusion, convective dispersion is proportional to u, and is due primarily to mechanical effects, i.e., to splitting (for compressible flow) and twisting of streamlines. For very large u, convective dispersion parallel to $\mathbf{u}$ is proportional to $u \ln u$, although convective dispersion normal to $\mathbf{u}$ is still proportional to u. Over macroscopic scales, dispersion of a passive tracer is governed by a local CDE, in which the velocity and (therefore) the convective dispersion vary with position.

Our model of disorder over macroscopic scales treats the disorder as a random function of position. Perturbation expansions have proven to be useful for the extraction of information from such models [3,4]. Nevertheless, perturbation expansions suffer from several shortcomings, e.g., the perturbative parameter must be small, and calculations become more difficult with increasing order in the expansion. In an attempt to avoid these difficulties, we take a somewhat different approach. The formulation is based on path integrals [5], and allows us to average over all fluctuations at once, instead of order by order in a perturbation expansion. We use Feynman's variational method to extract information about the average behavior of the system.

II. STATEMENT OF PROBLEM

The flow of a single fluid through an isotropic porous medium is governed at macroscopic scales by Darcy's law,

$$\mathbf{u}(\mathbf{x}) = -\frac{\kappa(\mathbf{x})}{\mu}\nabla\phi(\mathbf{x}) , \tag{2.1}$$

where $\mathbf{u}(\mathbf{x})$ is the local velocity, $\kappa(\mathbf{x})$ is the local permeability, μ is the viscosity, and $\phi(\mathbf{x})$ is the local pressure. The flow is assumed to be incompressible, i.e.,

$$\nabla\cdot\mathbf{u}(\mathbf{x})=0\ . \tag{2.2}$$

We suppose that $\kappa(\mathbf{x})$ is a random variable, and discuss its probability distribution in Sec. III. Combination of Darcy's law and the incompressibility condition gives

$$\nabla\cdot\kappa(\mathbf{x})\nabla\phi(\mathbf{x})=0\ . \tag{2.3}$$

We wish to average the Green's function for this equation over fluctuations in permeability.

The transport of a tracer by an incompressible fluid is governed at macroscopic length scales by a CDE,

$$\left[\frac{\partial}{\partial t}+\mathbf{u}(\mathbf{x})\cdot\nabla-\nabla\cdot\mathbf{D}(\mathbf{x})\cdot\nabla\right]c(\mathbf{x},t)=0\ , \tag{2.4}$$

where $\mathbf{u}(\mathbf{x})$ is the local velocity, $\mathbf{D}(\mathbf{x})$ is the local dispersion tensor, and $c(\mathbf{x},t)$ is the mass concentration of tracer in the fluid. We suppose that $\mathbf{u}(\mathbf{x})$ is a random variable, and discuss its probability distribution in Sec. III. Since convective dispersion is a function of velocity, we expect in general that the former will be a random variable like the latter, and that the fluctuations of the two will be correlated. We wish to average the Green's function for (2.4) over fluctuations in velocity and dispersion.

III. STATISTICAL MODELS

Law [6] was the first to analyze statistically the variation in permeability of a region of macroscopic extent. He deduced from core data that the horizontal fluctuations of permeability in a stratified bed are log-normally distributed. Although there are some differences on the matter [7], several subsequent studies generally agree with Law, while in some respects refining his model: for example, the vertical fluctuations in a stratified bed are also thought to be log-normally distributed, with a vertical correlation length shorter than the horizontal [3]. As a starting point for calculations, we shall assume that the medium is isotropic and that the permeability fluctuations are log-normally distributed. In other words, if $\kappa(\mathbf{x})$ is the permeability, with κ_0 its most probable value, then

$$f(\mathbf{x})\equiv\ln\left[\frac{\kappa(\mathbf{x})}{\kappa_0}\right] \tag{3.1}$$

is a Gaussian random variable of mean zero, the correlation function of which in Fourier space is

$$\langle f(\mathbf{q}_1)f(\mathbf{q}_2)\rangle=(2\pi)^3\delta(\mathbf{q}_1+\mathbf{q}_2)\rho(q_1^2)\ . \tag{3.2}$$

We cannot rely on direct experimental measurement for our model of the velocity field, because there is little information of that kind available. Instead, we will obtain velocity as a function of permeability, using the condition of incompressibility to eliminate the pressure from Darcy's law. Expanding velocity, permeability, and pressure in powers of f,

$$\mathbf{u}(\mathbf{x})=\mathbf{u}_0+\mathbf{u}_1(\mathbf{x})+\tfrac{1}{2}\mathbf{u}_2(\mathbf{x})+\cdots\ ,$$

$$\kappa(\mathbf{x})=\kappa_0+\kappa_0 f(\mathbf{x})+\tfrac{1}{2}\kappa_0 f^2(\mathbf{x})+\cdots\ ,$$

$$p(\mathbf{x})=p_0(\mathbf{x})+p_1(\mathbf{x})+\tfrac{1}{2}p_2(\mathbf{x})+\cdots\ ,$$

we obtain from Darcy's law one equation for each order in the expansion:

$$\mathbf{u}_0=-\frac{\kappa_0}{\mu}\nabla p_0(\mathbf{x})\ ,$$

$$\mathbf{u}_1(\mathbf{x})=-\frac{\kappa_0}{\mu}f(\mathbf{x})\nabla p_0(\mathbf{x})-\frac{\kappa_0}{\mu}\nabla p_1(\mathbf{x})\ ,$$

$$\mathbf{u}_2(\mathbf{x})=-\frac{\kappa_0}{\mu}\nabla p_2(\mathbf{x})-2\frac{\kappa_0}{\mu}f(\mathbf{x})\nabla p_1(\mathbf{x})$$
$$-f^2(\mathbf{x})\frac{\kappa_0}{\mu}\nabla p_0(\mathbf{x})\ ,$$

and so on. Using the fact that the flow is incompressible at each order, we eliminate the pressure order by order to obtain

$$\mathbf{u}(\mathbf{x})=\mathbf{u}_0+\int\frac{d\mathbf{q}}{(2\pi)^3}e^{i\mathbf{q}\cdot\mathbf{x}}\mathbf{u}_0\cdot[\mathbf{I}f(\mathbf{q})+\cdots]\cdot(\mathbf{I}-\hat{\mathbf{q}}\hat{\mathbf{q}})\ , \tag{3.3}$$

from which it follows that the correlation function in Fourier space is

$$\langle u_{1i}(\mathbf{q}_1)u_{1j}(\mathbf{q}_2)\rangle=(2\pi)^3\delta(\mathbf{q}_1+\mathbf{q}_2)\rho(q_1^2)\times[\mathbf{u}_0\cdot(\mathbf{I}-\hat{\mathbf{q}}_1\hat{\mathbf{q}}_1)]_i[(\mathbf{I}-\hat{\mathbf{q}}_1\hat{\mathbf{q}}_1)\cdot\mathbf{u}_0]_j\ , \tag{3.4}$$

plus terms of higher order in $\rho(q^2)$ [8]. Although derived here from a perturbation expansion of Darcy's law, (3.3) is a very general form for the velocity fluctuation. The tensor $\mathbf{I}-\hat{\mathbf{q}}\hat{\mathbf{q}}$ ensures that the fluctuation is incompressible, and $\mathbf{u}_0$ appears because the problem's only preferred direction is that of bulk flow. The tensor in the square brackets determines the statistical properties of the fluctuation. The form of this tensor could be determined theoretically, for example, by expanding Darcy's law as we have done here, or by assuming Gaussian fluctuations, i.e., keeping only the first term in (3.3). Its form could also be measured experimentally, at least in principle. While an expansion of Darcy's law implicitly assumes that the fluctuations are small, neither Gaussian fluctuations nor experiment are limited in this way.

IV. PATH-INTEGRAL FORMULATION

The Green's function for Eq. (2.4), $G(\mathbf{x},\mathbf{x}_0,t-t_0)$, is defined by

$$\left[\frac{\partial}{\partial t}+\mathbf{u}(\mathbf{x})\cdot\nabla-\nabla\cdot\mathbf{D}(\mathbf{x})\cdot\nabla\right]G(\mathbf{x},\mathbf{x}_0,t-t_0)=\delta(\mathbf{x}-\mathbf{x}_0)\delta(t-t_0)\ , \tag{4.1}$$

and is no more than the probability that a tracer particle starting at $(t_0,\mathbf{x}_0)$ will end up at $(t,\mathbf{x})$. This probability is in turn the sum over all possible paths of the probability that the tracer particle will take a particular path from $(t_0,\mathbf{x}_0)$ to $(t,\mathbf{x})$. Equation (4.1) has the following path-integral solution [5,9,10]:

$$G(\mathbf{x}_f,\mathbf{x}_0,t_f-t_0)=\int_{\mathbf{x}(t_0)=\mathbf{x}_0}^{\mathbf{x}(t_f)=\mathbf{x}_f} D\mathbf{x}\exp\left\{-\tfrac{1}{4}\int_{t_0}^{t_f} d\tau \left[\frac{d\mathbf{x}}{d\tau}-\mathbf{u}(\mathbf{x})\right]\cdot\frac{1}{\mathbf{D}(\mathbf{x})}\cdot\left[\frac{d\mathbf{x}}{d\tau}-\mathbf{u}(\mathbf{x})\right]\right\}. \tag{4.2}$$

It is useful to see how (4.2) is obtained. Suppose we wish to know the probability that a tracer particle will follow a given path $\mathbf{x}(t)$ from $(t_0,\mathbf{x}_0)$ to $(t_f,\mathbf{x}_f)$. We divide the time interval into n equal segments, of length $\Delta t\equiv t_f-t_0/n$, and approximate the path by $n+1$ points $[t_k\equiv t_0+k\Delta t,\ \mathbf{x}_k\equiv\mathbf{x}(t_k)]$, where $0\le k\le n$. For convenience, we relabel $t_n\equiv t_f$, $\mathbf{x}_n\equiv\mathbf{x}_f$. The probability $\rho(k-1,k)$ that a particle starting at $(t_{k-1},\mathbf{x}_{k-1})$ will end up at $(t_k,\mathbf{x}_k)$ can be obtained from (4.1):

$$\rho(k-1,k)=\frac{1}{[4\pi\Delta t]^{3/2}[\det\mathbf{D}(\mathbf{x}_k)]^{1/2}} \times\exp\left\{-\frac{\Delta t}{4}\left[\frac{\mathbf{x}_k-\mathbf{x}_{k-1}}{\Delta t}-\mathbf{u}(\mathbf{x}_k)\right]\cdot\frac{1}{\mathbf{D}(\mathbf{x}_k)}\cdot\left[\frac{\mathbf{x}_k-\mathbf{x}_{k-1}}{\Delta t}-\mathbf{u}(\mathbf{x}_k)\right]\right\}, \tag{4.3}$$

and the probability that the particle will hit each point is $\prod_{k=1}^{n}\rho(k-1,k)$. To get the Green's function, we integrate this over all intermediate positions:

$$G(\mathbf{x}_f,\mathbf{x}_0,t_f-t_0)=\int d\mathbf{x}_1\cdots\int d\mathbf{x}_{n-1}\frac{1}{(4\pi\Delta t)^{3/2}[\det\mathbf{D}(\mathbf{x}_1)]^{1/2}}\cdots\frac{1}{(4\pi\Delta t)^{3/2}[\det\mathbf{D}(\mathbf{x}_n)]^{1/2}} \times\exp\left\{-\frac{\Delta t}{4}\sum_{k=1}^{n}\left[\frac{\mathbf{x}_k-\mathbf{x}_{k-1}}{\Delta t}-\mathbf{u}(\mathbf{x}_k)\right]\cdot\frac{1}{\mathbf{D}(\mathbf{x}_k)}\cdot\left[\frac{\mathbf{x}_k-\mathbf{x}_{k-1}}{\Delta t}-\mathbf{u}(\mathbf{x}_k)\right]\right\}. \tag{4.4}$$

This is the proper way to interpret (4.2). Equation (4.4) can be shown to obey (4.1) to first order in Δt, assuming that the irregularity is relatively well behaved [10]. We are obliged to use $\mathbf{D}(\mathbf{x}_k)$ in (4.4), instead of, say, $\mathbf{D}(\mathbf{x}_{k-1})$, $\mathbf{D}(\frac{1}{2}[\mathbf{x}_{k-1}+\mathbf{x}_k])$, or $\frac{1}{2}[\mathbf{D}(\mathbf{x}_k)+\mathbf{D}(\mathbf{x}_{k-1})]$, because the alternatives define Green's functions which do not obey (4.1). If $\nabla\cdot\mathbf{u}(\mathbf{x})$ were nonzero, it would be necessary to make a similar observation about $\mathbf{u}(\mathbf{x}_k)$.

It is difficult to average over the parameter fluctuations as they appear in Eq. (4.4). However, since (4.3) can be rewritten

$$\rho(k-1,k)=\int\frac{d\mathbf{p}_{k-1}}{(2\pi)^3}\exp\left\{-\Delta t\left[\mathbf{p}_{k-1}\cdot\mathbf{D}(\mathbf{x}_k)\cdot\mathbf{p}_{k-1}-i\mathbf{p}_{k-1}\cdot\left[\frac{\mathbf{x}_k-\mathbf{x}_{k-1}}{\Delta t}-\mathbf{u}(\mathbf{x}_k)\right]\right]\right\}, \tag{4.5}$$

the Green's function is equally well represented by

$$G(\mathbf{x}_f,\mathbf{x}_0,t_f-t_0)=\int d\mathbf{x}_1\cdots\int d\mathbf{x}_{n-1}\int\frac{d\mathbf{p}_0}{(2\pi)^3}\cdots\int\frac{d\mathbf{p}_{n-1}}{(2\pi)^3}\exp\left\{-\Delta t\sum_{k=1}^{n}\left[\mathbf{p}_{k-1}\cdot\mathbf{D}(\mathbf{x}_k)\cdot\mathbf{p}_{k-1} -i\mathbf{p}_{k-1}\cdot\left[\frac{\mathbf{x}_k-\mathbf{x}_{k-1}}{\Delta t}-\mathbf{u}(\mathbf{x}_k)\right]\right]\right\}, \tag{4.6}$$

which is easier to work with. This is sometimes called the momentum representation of (4.4). The more elegant version of (4.6) is

$$G(\mathbf{x}_f,\mathbf{x}_0,t_f-t_0)=\int_{\mathbf{x}(t_0)=\mathbf{x}_0}^{\mathbf{x}(t_f)=\mathbf{x}_f} D\mathbf{x}\int D\mathbf{p}\exp\left\{-\int_{t_0}^{t_f}d\tau\left[\mathbf{p}(\tau)\cdot\mathbf{D}(\mathbf{x})\cdot\mathbf{p}(\tau)-i\mathbf{p}(\tau)\cdot\left[\frac{d\mathbf{x}}{d\tau}-\mathbf{u}(\mathbf{x})\right]\right]\right\}. \tag{4.7}$$

Let us suppose that the dispersion tensor is a constant $\mathbf{D}_0$ and that the velocity varies as $\mathbf{u}(\mathbf{x})=\mathbf{u}_0+\mathbf{u}_1(\mathbf{x})$. We average $G(\mathbf{x}_f,\mathbf{x}_0,t_f-t_0)$ over fluctuations in velocity to obtain

$$\begin{aligned}\langle G(\mathbf{x}_f,\mathbf{x}_0,t_f-t_0)\rangle&=\int D\mathbf{x}\int D\mathbf{p}\int D\mathbf{u}_1\exp\left\{-\tfrac{1}{2}\int d\mathbf{x}\,d\mathbf{x}'\mathbf{u}_1(\mathbf{x})\cdot\mathbf{A}^{-1}(\mathbf{x}-\mathbf{x}')\cdot\mathbf{u}_1(\mathbf{x}')\right\}\\&\quad\times\exp\left\{-\int d\tau\left[\mathbf{p}(\tau)\cdot\mathbf{D}_0\cdot\mathbf{p}(\tau)-i\mathbf{p}(\tau)\cdot\left[\frac{d\mathbf{x}}{d\tau}-\mathbf{u}_0-\mathbf{u}_1(\mathbf{x})\right]\right]\right\}\\&=\int D\mathbf{x}\int D\mathbf{p}\exp\left\{-\int d\tau\left[\mathbf{p}(\tau)\cdot\mathbf{D}_0\cdot\mathbf{p}(\tau)-i\mathbf{p}(\tau)\cdot\left[\frac{d\mathbf{x}}{d\tau}-\mathbf{u}_0\right]\right]\right.\\&\quad\left.-\tfrac{1}{2}\int d\tau\,d\tau'\mathbf{p}(\tau)\cdot\mathbf{A}[\mathbf{x}(\tau)-\mathbf{x}(\tau')]\cdot\mathbf{p}(\tau')\right\},\end{aligned} \tag{4.8}$$

where

$$\mathbf{A}(\mathbf{x})=\int \frac{d\mathbf{q}}{(2\pi)^d} e^{i\mathbf{q}\cdot\mathbf{x}}\rho(q^2) \times[\mathbf{u}_0\cdot(\mathbf{I}-\hat{\mathbf{q}}\hat{\mathbf{q}})][(\mathbf{I}-\hat{\mathbf{q}}\hat{\mathbf{q}})\cdot\mathbf{u}_0] \ . \tag{4.9}$$

It will be noted in (4.8) that we assume $\mathbf{u}_1(\mathbf{x})$ is a Gaussian random variable.

To give the permeability problem a path-integral formulation, we use a trick previously employed by Drummond and Horgan [11]. This problem is governed by Eq. (2.3), for which we can define a Green's function,

$$\nabla\cdot\kappa(\mathbf{x})\nabla G(\mathbf{x},\mathbf{x}_0)=-\delta(\mathbf{x}-\mathbf{x}_0) \ . \tag{4.10}$$

But there is a diffusion problem associated with (2.3):

$$\left[\frac{\partial}{\partial t}-\nabla\cdot\kappa(\mathbf{x})\nabla\right]\phi(\mathbf{x},t)=0 \ , \tag{4.11}$$

for which we can also define a Green's function,

$$\left[\frac{\partial}{\partial t}-\nabla\cdot\kappa(\mathbf{x})\nabla\right]G(\mathbf{x},\mathbf{x}_0,t-t_0)=\delta(\mathbf{x}-\mathbf{x}_0)\delta(t-t_0) \ . \tag{4.12}$$

These two problems are closely connected. For example, if

$$\lim_{t\to\infty}\frac{\partial\phi(\mathbf{x},t)}{\partial t}\to 0 \ ,$$

then a solution of (4.11) which obeys a given set of boundary conditions in space will relax to a solution of (2.3) with the same boundary conditions in the limit of large t; in addition, if

$$\lim_{t\to 0} G(\mathbf{x},\mathbf{x}_0,t)\to\delta(\mathbf{x}-\mathbf{x}_0) \ ,$$

$$\lim_{t\to\infty} G(\mathbf{x},\mathbf{x}_0,t)\to 0 \ ,$$

then

$$G(\mathbf{x},\mathbf{x}_0)=\int_0^\infty dt\, G(\mathbf{x},\mathbf{x}_0,t) \ . \tag{4.13}$$

If we average over fluctuations, we expect that (4.10) will look like

$$\kappa_{\text{eff}}\nabla^2\langle G(\mathbf{x},\mathbf{x}_0)\rangle=-\delta(\mathbf{x}-\mathbf{x}_0) \ , \tag{4.14}$$

and (4.12) will look like

$$\left[\frac{\partial}{\partial t}-\kappa_{\text{eff}}\nabla^2\right]\langle G(\mathbf{x},\mathbf{x}_0,t-t_0)\rangle =\delta(\mathbf{x}-\mathbf{x}_0)\delta(t-t_0) \ . \tag{4.15}$$

Equation (4.13) leads us to expect that the effective parameters in (4.14) and (4.15) are the same. Because of the similarity of the permeability problem and its associated diffusion problem, we assume that our already-obtained path-integral formulation of the latter will serve as a suitable formulation of the former. Equation (4.12) can be written

$$\left[\frac{\partial}{\partial t}-[\nabla\kappa(\mathbf{x})]\cdot\nabla-\kappa(\mathbf{x})\nabla^2\right]G(\mathbf{x},\mathbf{x}_0,t-t_0) =\delta(\mathbf{x}-\mathbf{x}_0)\delta(t-t_0) \ , \tag{4.16}$$

indicating that its path-integral version is

$$G(\mathbf{x}_f,\mathbf{x}_0,t_f-t_0)=\int_{\mathbf{x}(t_0)=\mathbf{x}_0}^{\mathbf{x}(t_f)=\mathbf{x}_f} D\mathbf{x}\int D\mathbf{p}\exp\left\{-\int_{t_0}^{t_f} d\tau\left[\kappa(\mathbf{x})p^2(\tau)-i\mathbf{p}(\tau)\cdot\left[\frac{d\mathbf{x}}{d\tau}+\nabla\kappa(\mathbf{x})\right]\right]\right\} \ . \tag{4.17}$$

In order to obtain more tractable equations, and results directly comparable to those of previous investigators, we will use a Gaussian distribution to approximate the actual log-normal distribution of $\kappa(\mathbf{x})$. This approximation is reasonable if the variance of the distribution is small compared to the mean. Averaging (4.17) over fluctuations in permeability will thus give

$$\begin{aligned}\langle G(\mathbf{x}_f,\mathbf{x}_0,t_f-t_0)\rangle &=\int D\kappa_1\int D\mathbf{x}\int D\mathbf{p}\exp\left\{-\int\frac{d\mathbf{x}\,d\mathbf{x}'\rho^{-1}(\mathbf{x}-\mathbf{x}')\kappa_1(\mathbf{x})\kappa_1(\mathbf{x}')}{2\kappa_0^2}\right.\\ &\qquad\left.-\int d\tau\left[\kappa(\mathbf{x})p^2(\tau)-i\mathbf{p}(\tau)\cdot\left[\frac{d\mathbf{x}}{d\tau}+\nabla\kappa_1(\mathbf{x})\right]\right]\right\}\\ &=\int D\mathbf{x}\int D\mathbf{p}\exp\left\{-\int d\tau\left[\kappa_0 p^2(\tau)-i\mathbf{p}(\tau)\cdot\frac{d\mathbf{x}}{d\tau}\right]\right.\\ &\qquad\left.+\tfrac{1}{2}\int d\tau\,d\tau'\kappa_0^2[p^2(\tau)-i\mathbf{p}(\tau)\cdot\nabla][p^2(\tau')-i\mathbf{p}(\tau')\cdot\nabla']\rho(\mathbf{x}-\mathbf{x}')\right\} \ .\end{aligned} \tag{4.18}$$

V. VARIATIONAL METHOD

This procedure was developed by Feynman [12,13] as a path-integral version of the variational method of quantum mechanics. We start with the path integral for the average Green's function $\langle G\rangle$, which we write

$$\langle G\rangle \equiv e^{-W} \equiv \int D\mathbf{x}\, e^{-S'} , \tag{5.1}$$

where S' is a sort of action. If we have another action S'_A which is simple and in some sense an approximation of S', Eq. (5.1) can be rewritten

$$e^{-W}=e^{-W_A}\left[\frac{\int D\mathbf{x}\, e^{-(S'-S'_A)}e^{-S'_A}}{\int D\mathbf{x}\, e^{-S'_A}}\right]$$

$$\equiv e^{-W_A}\langle e^{-(S'-S'_A)}\rangle'_A , \tag{5.2}$$

where

$$e^{-W_A}\equiv\int D\mathbf{x}\, e^{-S'_A} . \tag{5.3}$$

The term of (5.2) in brackets can be thought of as the average of $e^{-(S'-S'_A)}$, the weight for each path being $e^{-S'_A}$. Now, for any set of real quantities $\{f\}$, we have

$$\langle e^{-f}\rangle \ge e^{-\langle f\rangle} , \tag{5.4}$$

where the brackets denote a weighted mean. If S' and S'_A are both real, this inequality can be applied to (5.2), allowing us to write

$$e^{-W}=e^{-W_A}\langle e^{-(S'-S'_A)}\rangle'_A \ge e^{-W_A}e^{-\langle S'-S'_A\rangle'_A} , \tag{5.5}$$

i.e.,

$$W\le W_A+\langle S'-S'_A\rangle'_A\equiv W_{\text{eff}} . \tag{5.6}$$

The values of any free parameters in W_A are chosen to make W_{eff} a least upper bound for W.

The average Green's functions in (4.8) and (4.9) are written in the momentum representation, in which they are complex; thus, we cannot apply (5.4) directly to them. But that representation was used for computational convenience, and was not intrinsic to the problem. Equation (4.2) is written entirely in terms of real quantities; averaging over Gaussian fluctuations would not alter that fact, and the treatment leading up to (5.6) could be directly applied to the result. Having properly obtained (5.6), we can write a momentum-space version of it by defining

$$e^{-S'}=\int D\mathbf{p}\, e^{-S} , \tag{5.7}$$

$$e^{-S'_A}=\int D\mathbf{p}\, e^{-S_A} , \tag{5.8}$$

and

$$\langle F\rangle_A\equiv\frac{\int D\mathbf{x}\int D\mathbf{p}\, F e^{-S_A}}{\int D\mathbf{x}\int D\mathbf{p}\, e^{-S_A}} . \tag{5.9}$$

It follows from (5.7) and (5.8) that

$$(S'-S'_A)e^{-S'_A}=\int D\mathbf{p}(S-S_A)e^{-S_A} \tag{5.10}$$

to first order in $(S-S_A)$, and so (5.6) becomes

$$W\le W_A+\langle S-S_A\rangle_A\equiv W_{\text{eff}} . \tag{5.11}$$

The values of any free parameters in W_A are chosen to obtain the minimum upper bound at the distribution's point of maximum probability, as this is where the most representative tracer particles would end up.

It might be illuminating to pause at this point and reconsider what we have done. Our task is to approximate e^{-W}. The closer S'_A is to S' in (5.2), the better we can expect the bound in (5.5) to be. But it would be a mistake to argue further, in too close analogy to the standard quantum-mechanical case, that e^{-W_A} by itself is the approximate Green's function we seek. Consider an expansion of (5.2), by which we obtain a formal expression for e^{-W} in terms of integrations we can do:

$$e^{-W}=e^{-W_A}[1-\langle S'-S'_A\rangle'_A+\tfrac{1}{2}\langle (S'-S'_A)^2\rangle'_A-\cdots] . \tag{5.12}$$

Note that e^{-W_A} is only the zero-order term of this expansion and that a better approximation is obtained by including the first-order term and an estimate of the second-order term, as has been done in (5.5). In effect, e^{-W_A} is a guess in our attempt to approximate e^{-W}, and $e^{-W_{\text{eff}}}$ is a refinement of that guess.

VI. CALCULATION OF EFFECTIVE PERMEABILITY

With finite-range correlations in the permeability fluctuations, at large enough length scales we expect the porous medium to look like a homogeneous isotropic continuum, and Darcy's law with a global scalar permeability, Eq. (4.14), should apply. Because of the close connection between (4.14) and (4.15), a good choice for this problem's test action would therefore be

$$S_A=\int_{t_0}^{t_f}d\tau\left[\kappa p^2(\tau)-i\mathbf{p}(\tau)\cdot\frac{d\mathbf{x}}{d\tau}\right] . \tag{6.1}$$

It follows from (4.18), (5.11), and (6.1) that we need to calculate

$$W_{\text{eff}}=W_A+e^{W_A}\int D\mathbf{x}\int D\mathbf{p}\exp\left[-\int d\tau\left[\kappa p^2(\tau)-i\mathbf{p}(\tau)\cdot\frac{d\mathbf{x}}{d\tau}\right]\right]$$
$$\times\left\{(\kappa_0-\kappa)\int d\tau\, p^2(\tau)-\tfrac{1}{2}\int d\tau\, d\tau'\kappa_0^2[p^2(\tau)-i\mathbf{p}(\tau)\cdot\nabla][p^2(\tau')-i\mathbf{p}(\tau')\cdot\nabla']\rho(\mathbf{x}-\mathbf{x}')\right\} , \tag{6.2}$$

where, according to (5.3) and (5.8),

$$W_A=\tfrac{3}{2}\ln(4\pi\kappa t)+\frac{\mathbf{x}^2}{4\kappa t}\ , \tag{6.3}$$

with $\mathbf{x}\equiv\mathbf{x}_f-\mathbf{x}_0$ and $t\equiv t_f-t_0$. The resulting integrals can be expanded in the limit of long times, keeping terms of order $\mathbf{x}^2/t$ but dropping those of order $\mathbf{x}^2/t^2$, so that

$$W_{\text{eff}}=W_A+\left[\kappa_0-\kappa-\frac{\rho(0)\kappa_0^2}{3\kappa}\right]\frac{\partial W_A}{\partial\kappa}\ , \tag{6.4}$$

where

$$\rho(0)\equiv\int\frac{d\mathbf{q}}{(2\pi)^3}\rho(q^2)\ . \tag{6.5}$$

This can also be written

$$W_{\text{eff}}=\tfrac{3}{2}\ln(4\pi\kappa_1 t)+\frac{\mathbf{x}^2}{4\kappa_2 t}\ , \tag{6.6}$$

with suitably defined κ_1 and κ_2. Since $e^{-W_{\text{eff}}}$ is not in general a diffusive Green's function, it does not immediately yield an effective diffusion constant κ_{eff}. However, we have assumed that the best value of κ_{eff} is obtained at the distribution's point of maximum probability, $\mathbf{x}=0$. This is equivalent to taking $\kappa_{\text{eff}}=\kappa_1$. The optimization procedure reduces to

$$\frac{\partial\kappa_1}{\partial\kappa}=0\ , \tag{6.7}$$

which implies

$$\kappa^2-\kappa_0\kappa+\frac{2\rho(0)\kappa_0^2}{3}=0\ . \tag{6.8}$$

For $\rho(0)>\frac{3}{8}$, this equation has no roots, and the method fails. (This should not surprise us. In approximating a log-normal distribution by a Gaussian distribution, we allow some sites in the medium to have permeability values less than zero. As $\rho(0)$ increases from zero, the fraction of sites with negative permeabilities also increases from zero, to around 5% for $\rho(0)=\frac{3}{8}$. We cannot reasonably believe the theory will work when a significant fraction of sites is assumed to have permeability values that are physically absurd.) While there is a double root and thus an unambiguous solution for $\rho(0)=\frac{3}{8}$, there are two roots for $0\le\rho(0)<\frac{3}{8}$:

$$\kappa_{+(-)}=\frac{\kappa_0}{2}\left[1+(-)\left[1-\frac{8\rho(0)}{3}\right]^{1/2}\right]\ . \tag{6.9}$$

We select κ_+ because $\ln\kappa_1(\kappa_+)<\ln\kappa_1(\kappa_-)$ for $0\le\rho(0)<\frac{3}{8}$: while both κ_+ and κ_- are local minima, κ_+ is the global minimum. In the limit of small $\rho(0)$, $\kappa_1(\kappa=\kappa_+)$ can be expanded to give

$$\kappa_1(\kappa=\kappa_+)=\kappa_0\left[1-\frac{\rho(0)}{3}-\frac{\rho(0)^2}{6}+\cdots\right]\ . \tag{6.10}$$

To first order in $\rho(0)$, this is the same as the perturbative result obtained by King [4].

VII. CALCULATION OF EFFECTIVE DISPERSION TENSOR

If the velocity fluctuations have correlations of finite range, the averaged tracer problem will be governed at large enough length and time scales by an effective CDE. We expect that the effective velocity will be equal to the mean velocity, since $\mathbf{u}(\mathbf{x})$ is assumed to consist of a mean plus a Gaussian fluctuation, and the fluctuations should cancel out on average. We further expect that the effective dispersion tensor will be diagonal, with components parallel and normal to bulk flow, because on average the medium looks like a homogeneous isotropic continuum, and for such a medium the only preferred direction is that of bulk flow. A reasonable choice for the test action would therefore be

$$S_A=\int_{t_0}^{t_f}d\tau\left[\mathbf{p}(\tau)\cdot\mathbf{D}\cdot\mathbf{p}(\tau)-i\mathbf{p}(\tau)\cdot\left[\frac{d\mathbf{x}}{d\tau}-\mathbf{u}_0\right]\right]\ , \tag{7.1}$$

where

$$\mathbf{D}=D_{\text{long}}\hat{\mathbf{u}}_0\hat{\mathbf{u}}_0+D_{\text{lat}}(I-\hat{\mathbf{u}}_0\hat{\mathbf{u}}_0)\ . \tag{7.2}$$

Using this S_A, (4.8), and (5.11), we find that we need to calculate

$$W_{\text{eff}}=W_A+e^{W_A}\int D\mathbf{x}\int D\mathbf{p}\left\{\int d\tau\,\mathbf{p}(\tau)\cdot(\mathbf{D}_0-\mathbf{D})\cdot\mathbf{p}(\tau)+\tfrac{1}{2}\int d\tau\,d\tau'\mathbf{p}(\tau)\cdot\mathbf{A}(\mathbf{x}-\mathbf{x}')\cdot\mathbf{p}(\tau')\right\}$$
$$\times\exp\left\{-\int d\tau\left[\mathbf{p}(\tau)\cdot\mathbf{D}\cdot\mathbf{p}(\tau)-i\mathbf{p}(\tau)\cdot\left[\frac{d\mathbf{x}}{d\tau}-\mathbf{u}_0\right]\right]\right\}\ , \tag{7.3}$$

where, from (5.3) and (5.8),

$$W_A=\tfrac{3}{2}\ln(4\pi t)+\tfrac{1}{2}\ln(\det\mathbf{D})+\frac{t}{4}\left[\frac{\mathbf{x}}{t}-\mathbf{u}_0\right]\cdot\frac{1}{\mathbf{D}}\cdot\left[\frac{\mathbf{x}}{t}-\mathbf{u}_0\right]\ . \tag{7.4}$$

We substitute into the resulting integrals $\mathbf{x}=\mathbf{u}_0 t+\mathbf{y}$, and expand in the limit of long times, keeping terms of order $\mathbf{y}^2/t$ but dropping those of order $\mathbf{y}^2/t^2$. Defining for convenience

$$\hat{\mathbf{q}}\cdot\hat{\mathbf{u}}_0=\mu ,$$

$$\mathbf{D}_0=D_{0\text{long}}\hat{\mathbf{u}}_0\hat{\mathbf{u}}_0+D_{0\text{lat}}(\mathbf{I}-\hat{\mathbf{u}}_0\hat{\mathbf{u}}_0) ,$$

the result is

$$W_{\text{eff}}=W_A+\left[D_{0\text{long}}-D_{\text{long}}+\int\frac{d\mathbf{q}}{(2\pi)^3}\rho(q^2)\frac{(1-\mu^2)^2u_0^2}{\mathbf{q}\cdot\mathbf{D}\cdot\mathbf{q}-i\mathbf{u}_0\cdot\mathbf{q}}\right]\frac{\partial W_A}{\partial D_{\text{long}}}+\left[D_{0\text{lat}}-D_{\text{lat}}+\tfrac{1}{2}\int\frac{d\mathbf{q}}{(2\pi)^3}\rho(q^2)\frac{\mu^2(1-\mu^2)u_0^2}{\mathbf{q}\cdot\mathbf{D}\cdot\mathbf{q}-i\mathbf{u}_0\cdot\mathbf{q}}\right]\frac{\partial W_A}{\partial D_{\text{lat}}} . \tag{7.5}$$

This can also be written

$$W_{\text{eff}}=\tfrac{3}{2}\ln(4\pi t)+\tfrac{1}{2}\ln(\det\mathbf{D}_1)+\frac{1}{4t}\mathbf{y}\cdot\frac{1}{\mathbf{D}_2}\cdot\mathbf{y} , \tag{7.6}$$

with suitably defined $\mathbf{D}_1$ and $\mathbf{D}_2$. In this case, we cannot pick $\mathbf{D}_1$ to be the effective dispersion tensor $\mathbf{D}_{\text{eff}}$, because (7.6) tells us its determinant only, and not its individual components. We are thus obliged to take $\mathbf{D}_2$ as the effective dispersion tensor. This $\mathbf{D}_2$ can be thought of as the dispersion tensor of a diffusive Green's function e^{-W_2} which bounds $e^{-W_{\text{eff}}}$, and therefore e^{-W}, from below. We choose $\mathbf{D}$ to make e^{-W_2} a maximum lower bound at the distribution's point of maximum probability $\mathbf{y}=0$, or, in other words, we fix $\mathbf{D}$ by minimizing $\frac{1}{2}\ln(\det\mathbf{D}_2)$ with respect to variations in D_{long} and D_{lat}. This can be done numerically.

We will take for our correlation function a simple cutoff in Fourier space:

$$\rho(q^2)=\begin{cases}\rho_0, & q<\Lambda\\ 0, & q>\Lambda .\end{cases} \tag{7.7}$$

Although this oscillates in coordinate space, the oscillations are exponentially damped to zero. It is easier to do the calculations for this correlation function than for an alternative such as $\rho_0\Lambda^4/(q^2+\Lambda^2)^2$, and there is no significant change in the final results. Having chosen $\rho(q^2)$, the integrals of (7.5) can be expressed in terms of three quantities. The first, $\nu(0)$, is a measure of the anisotropy of $\mathbf{D}_0$,

$$\nu^2(0)+1=\frac{D_{0\text{long}}}{D_{0\text{lat}}} . \tag{7.8}$$

The second is the mesoscopic Peclet number P,

$$P\equiv\frac{u_0L_{\text{meso}}}{D_{0\text{lat}}} . \tag{7.9}$$

This measures the competition between convection and dispersion over length scales L_{meso} characteristic of the mesoscopic disorder. The third, $\rho(0)$, is a measure of the fluctuation strength, and is defined in (6.5).

Most cases of interest will be such that $\mathbf{D}_0$ is roughly proportional to the first power of the microscopic Peclet number

$$P_{\text{micro}}=u_0L_{\text{micro}}/D_{\text{mol}} ,$$

where L_{micro} is a length characteristic of the microscopic disorder and D_{mol} is the molecular diffusion constant of the tracer in the fluid. In such flow regimes, $\nu^2(0)+1$ will be around 20 [3] or 30 [14]; we will take 26, i.e., $\nu(0)=5$, as a representative value. The mesoscopic Peclet number will be approximately proportional to the ratio of the length scales involved:

$$P\rightarrow\frac{L_{\text{meso}}}{L_{\text{micro}}} . \tag{7.10}$$

We expect P to be fairly large, but it will also prove interesting to examine effective dispersion for $P\rightarrow0$. Note that u_0 does not disappear. Since we measure dispersion constants in units of $D_{0\text{lat}}$, the effective dispersion constants will have the same dependence on u_0 as does $D_{0\text{lat}}$. In other cases of interest, the convective dispersion tensor is small and varies directly with the second power of the microscopic Peclet number. For such cases, $\nu(0)$ will be roughly zero, and the mesoscopic Peclet number will be

$$P=\frac{u_0L_{\text{meso}}}{D_{\text{mol}}}=P_{\text{micro}}\left[\frac{L_{\text{meso}}}{L_{\text{micro}}}\right] , \tag{7.11}$$

which could be small or large.

The last parameter, $\rho(0)$, is the mean-square deviation of the natural-log, log-normal permeability distribution. Some representative figures can be obtained from Law [6], whose numbers are equivalent to $0.2\le\rho(0)\le1.3$; from Dykstra and Parsons [15], whose numbers are equivalent to $0.1\le\rho(0)\le2.3$; and from Arya *et al.* [16], whose numbers are equivalent to $0.8\le\rho(0)\le2.6$. Since we have assumed $\rho(0)$ to be small compared to 1, so that we can use a Gaussian permeability distribution, and so that we can get the velocity fluctuations in the tracer problem from Darcy's law, we see that the values of $\rho(0)$ for which we expect our method to work reasonably well are at best on the lower end of values found in the field. This does not mean that the method will fail absolutely for values of $\rho(0)$ of order 1, as it does in the permeability problem. The velocity fluctuation model of (3.3) and (3.4) is interesting of itself, without regard to its derivation from Darcy's law, for reasons mentioned at the end of Sec. III. That $\rho(0)$ is of order 1 means only that a significant fraction of sites will have negative velocities. This may be unusual, but it is not physically impossible in a highly disordered medium.

If $\rho(0)$ and P are very small in comparison to 1, $\frac{1}{2}\ln(\det\mathbf{D}_2)$ appears to have only one minimum with respect to variations in $D_{\rm long}$ and $D_{\rm lat}$. The corresponding solution $\mathbf{D}_2$ approaches $\mathbf{D}_0$ as $\rho(0)$ and P approach 0. For somewhat larger values of $\rho(0)$ or P, a second local minimum will appear. This second minimum may become the global minimum for large enough values of $\rho(0)$ and P. In such a case, the method no longer gives the optimal bound for parameter values greater than the "critical" value at which the two minima are equal. We expect that the effective dispersion tensor will be a continuous function of its parameters, and take the first minimum as our solution in any case.

Figures 1 through 4 show the components of the effective dispersion tensor, measured in units of $D_{0\rm lat}$, for some representative values of the problem's parameters. For each set of graphs, $\nu(0)$ and $\rho(0)$ are fixed, and P is allowed to vary. In the graphs of function value, the line marked "optimum variation" is the value of $\frac{1}{2}\ln(\det\mathbf{D}_1)$ minimized with respect to variations in $D_{\rm long}$ and $D_{\rm lat}$. This is called optimum from a consideration of (7.6): since we expect the best information to be found at the distribution's peak, the minimized $\frac{1}{2}\ln(\det\mathbf{D}_1)$ is the best estimate of $\frac{1}{2}\ln(\det\mathbf{D}_{\rm eff})$. The line marked "variation" is the minimized value of $\frac{1}{2}\ln(\det\mathbf{D}_2)$, the value of $\frac{1}{2}\ln(\det\mathbf{D}_{\rm eff})$ which we are obliged to use in order to have $\mathbf{D}_{\rm eff}$ itself. Comparison of the two will indicate how closely the information in the distribution's peak agrees with that in the distribution's wings. The lines marked "perturbation" were obtained by expanding the Green's function in powers of the velocity fluctuations, then averaging and keeping terms of first order in $\rho(0)$ (see the Appendix).

The variational results have several interesting features. As $P\to 0$, $\mathbf{D}_{\rm eff}$ is proportional to P^2 in all cases, in agreement with perturbation theory and experiment. For values of P less than 5 or 10, the perturbative results for effective dispersion are slightly greater than the variational results. (Analogously, the first-order perturbative estimate of permeability was greater than the variational estimate of that quantity.) This means that $\frac{1}{2}\ln(\det\mathbf{D}_{\rm eff})$ is greater for perturbation theory than for the variational method, making the variational result a better upper bound for W. On the other hand, given that our choice for $\rho(q^2)$ is merely a well-informed guess, the numerical results obtained by the two methods do not differ significantly. For large P, $\mathbf{D}_{\rm eff}$ is proportional to P in three of the four cases, with minor deviations for $\rho(0)=0.1$. This result agrees with experiment, but disagrees with perturbation theory, which predicts that effective lateral dispersion is independent of P for large P. The disagreement arises from the fact that perturbation theory is not valid in this domain. In general, perturbation theory can be expected to work only if the difference between an effective quantity and its initial value is small. Also, in a problem with several parameters, one cannot expand in powers of one of them, without regard to the others. For the tracer problem, the difference between $\mathbf{D}_{\rm eff}$ and $\mathbf{D}_0$ is a function not only of $\rho(0)$, but also of P. One is not free to expand in powers of $\rho(0)$ alone, since no matter how small one chooses $\rho(0)$, the difference between $\mathbf{D}_{\rm eff}$ and $\mathbf{D}_0$ can be made large by the selection of a sufficiently large P. It is for this reason that our model of the velocity fluctuations, which was derived from a perturbation expansion of Darcy's law, gives rise to an effective dispersion which cannot be treated by perturbative methods.

VIII. SUMMARY

We have applied Feynman's variational method, based on path integrals, to problems arising from the steady-state flow of a single fluid through a porous medium. Results obtained by the variational method are compared to results obtained by first-order perturbation theory, which is the technique usually applied to such problems. For the permeability problem, and the tracer problem at small P, the variational results are consistent with first-order perturbative results. For the tracer problem at large P, the variational method predicts the expected linear dependence of the effective dispersion tensor on P, which perturbation theory does not. This indicates that, for the problems considered here and others like them, a first-order perturbation expansion can be of limited utility. We expect that the variational method could be used to study a wider range of problems for which perturbation theory is inadequate, since development of the method assumes only that the problem at hand can be put into the path-integral formulation, and that the problem involves averaging over fluctuations. Our results for the permeability problem were restricted in range to $\rho(0)\le\frac{3}{8}$, due to the fact that we used a Gaussian, rather than a log-normal, probability distribution function for the permeability fluctuations. This substitution was necessary in order to get a clean computational result, and not in order to develop the method itself. It points out the method's chief drawback, which is that the fluctuations that can be handled with reasonable ease are limited to those with Gaussian distributions. However, it also obscures the method's chief advantage, which is that it works for any Gaussian distribution, and not merely one for which the variance is small compared to the mean, or one for which the fluctuations are weakly correlated. This advantage suggests other problems for which the method may prove useful, e.g., anomalous (non-Brownian) dispersion, which can arise in flow through a porous medium if the velocity fluctuations are strongly correlated [17].

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APPENDIX: PERTURBATION THEORY

In this appendix we apply to the CDE the perturbative method that King [4] applied to the permeability problem. The Green's function for the CDE $G(\mathbf{x},\mathbf{x}_0,t-t_0)$ is defined by (4.1), where the dispersion tensor $\mathbf{D}(\mathbf{x})\equiv\mathbf{D}_0$ is constant, and the incompressible velocity

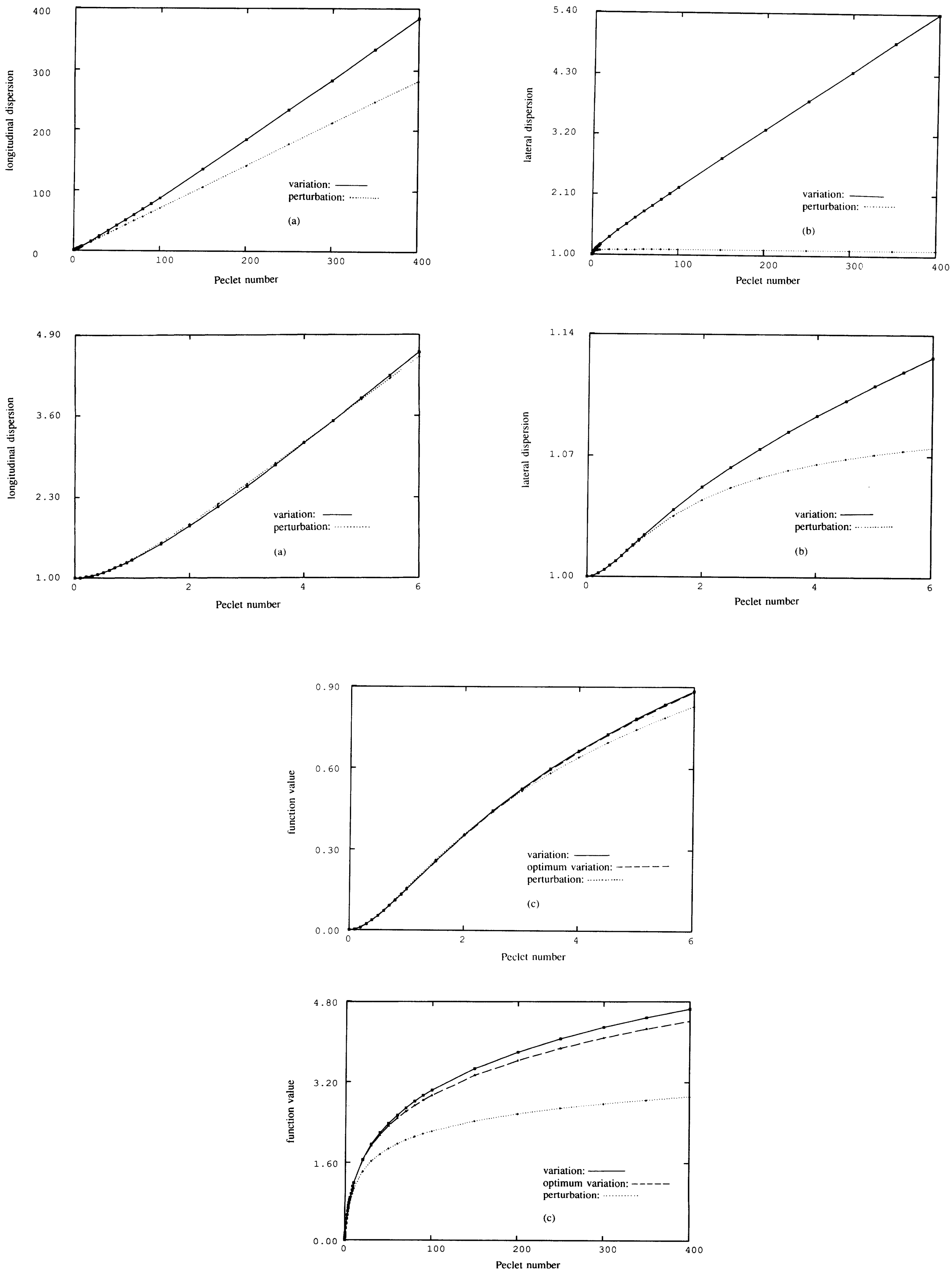

FIG. 1. (a) Effective longitudinal dispersion constant vs Peclet number: $\nu(0)=0$, $\rho(0)=0.3$. (b) Effective lateral dispersion constant vs Peclet number: $\nu(0)=0, \rho(0)=0.3$. (c) $\frac{1}{2}\ln(\det \mathbf{D}_{\text{eff}})$ vs Peclet number: $\nu(0)=0, \rho(0)=0.3$.

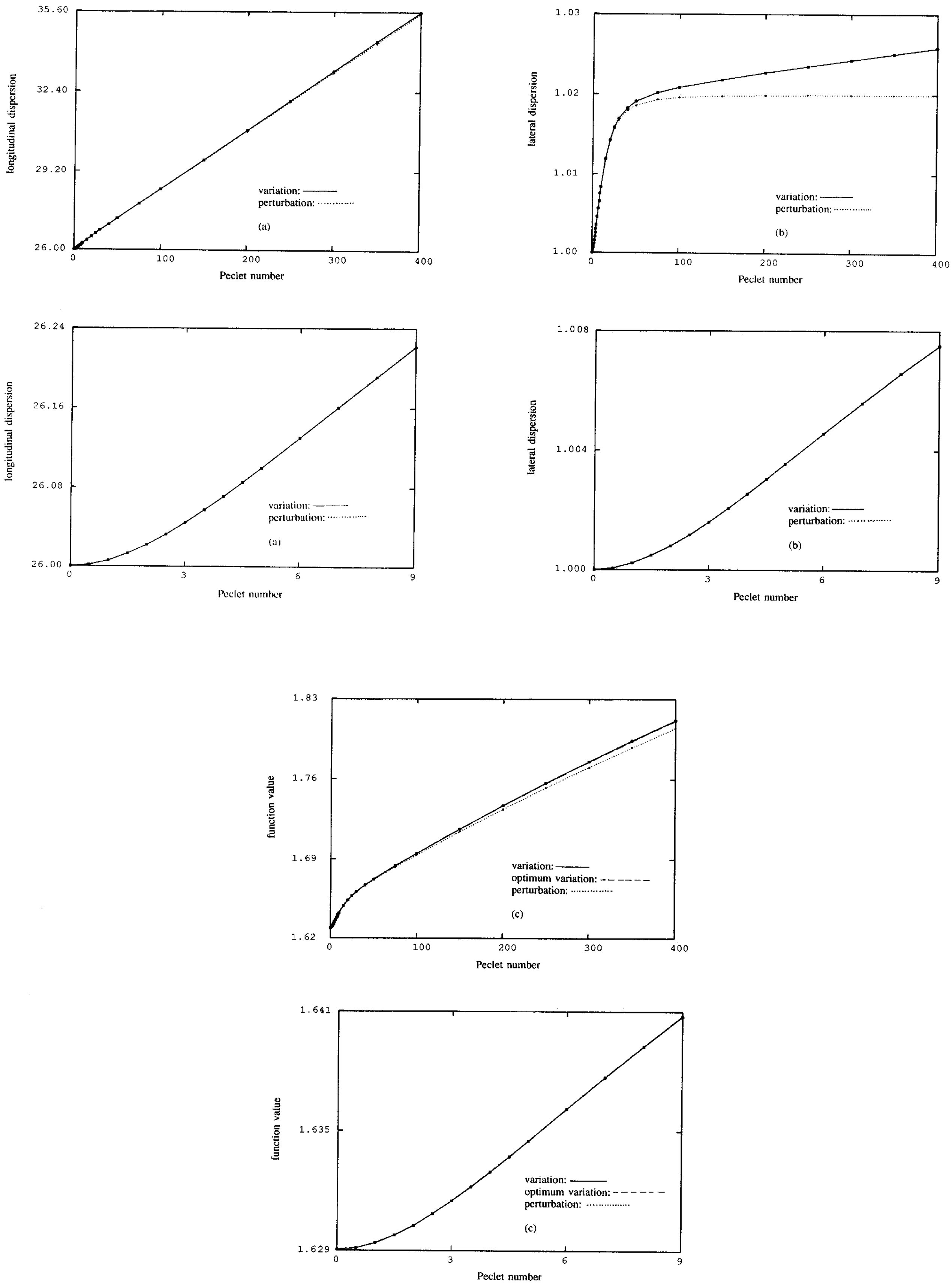

FIG. 2. (a) Effective longitudinal dispersion constant vs Peclet number: $\nu(0)=5, \rho(0)=0.1$. (b) Effective lateral dispersion constant vs Peclet number: $\nu(0)=5, \rho(0)=0.1$. (c) $\frac{1}{2}\ln(\det \mathbf{D}_{\text{eff}})$ vs Peclet number: $\nu(0)=5, \rho(0)=0.1$.

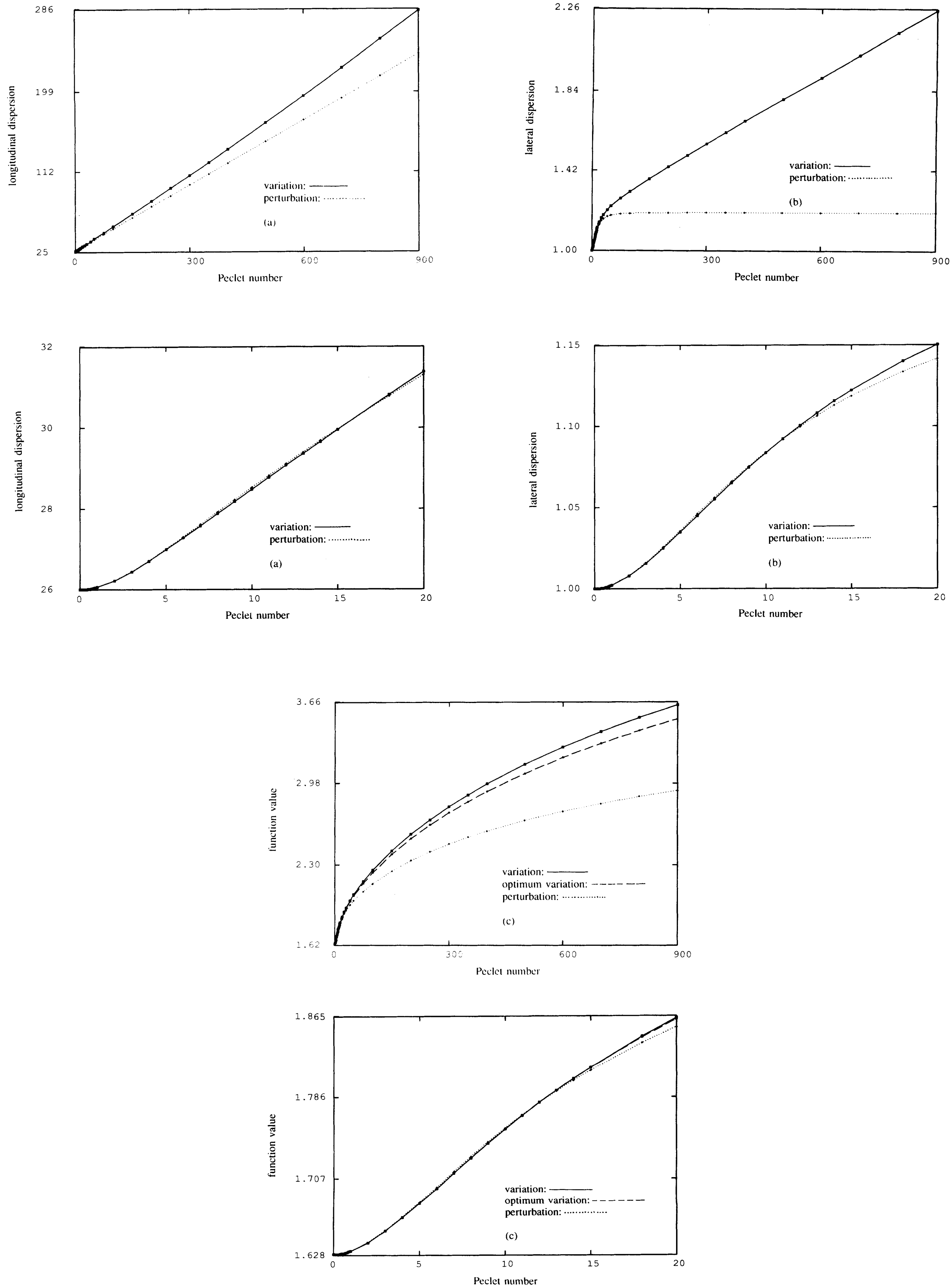

FIG. 3. (a) Effective longitudinal dispersion constant vs Peclet number: $\nu(0)=5, \rho(0)=0.1$. (b) Effective lateral dispersion constant vs Peclet number: $\nu(0)=5, \rho(0)=0.1$. (c) $\frac{1}{2}\ln(\det \mathbf{D}_{\text{eff}})$ vs Peclet number: $\nu(0)=5, \rho(0)=0.1$.

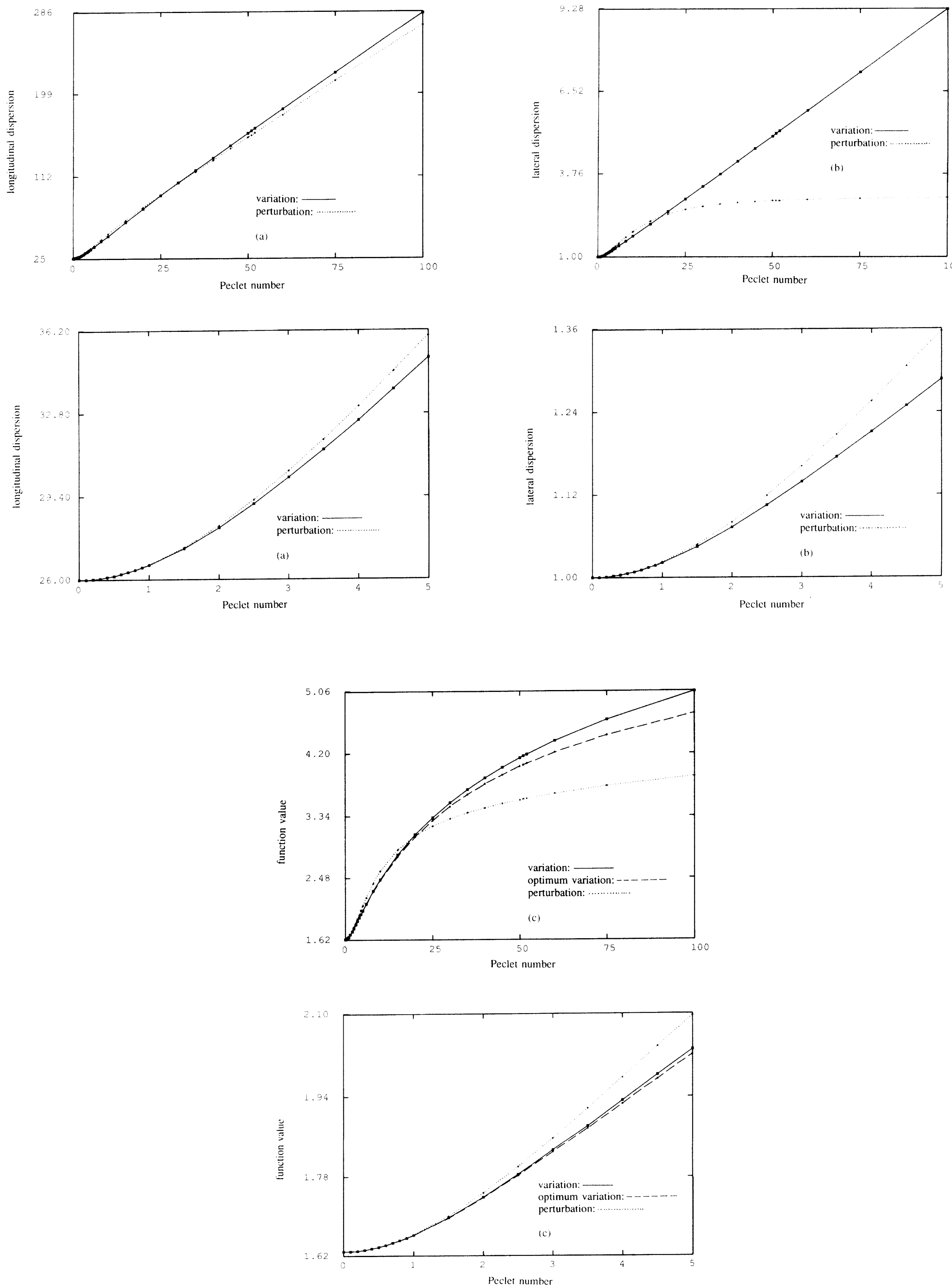

FIG. 4. (a) Effective longitudinal dispersion constant vs Peclet number: $\nu(0)=5, \rho(0)=0.1$. (b) Effective lateral dispersion constant vs Peclet number: $\nu(0)=5, \rho(0)=0.1$. (c) $\frac{1}{2}\ln(\det\mathbf{D}_{\text{eff}})$ vs Peclet number: $\nu(0)=5, \rho(0)=0.1$.

$\mathbf{u}(\mathbf{x}) \equiv \mathbf{u}_0 + \mathbf{u}_1(\mathbf{x})$ fluctuates. The unperturbed Green's function $G_0(\mathbf{x}-\mathbf{x}_0, t-t_0)$, defined by

$$\left[\frac{\partial}{\partial t} + \mathbf{u}_0\cdot\nabla - \nabla\cdot\mathbf{D}_0\cdot\nabla\right] G_0(\mathbf{x}-\mathbf{x}_0, t-t_0) = \delta(\mathbf{x}-\mathbf{x}_0)\delta(t-t_0) , \quad \text{(A1)}$$

is the zero-order approximation to $G(\mathbf{x},\mathbf{x}_0,t-t_0)$. We set the left-hand sides of Eqs. (4.1) and (A1) equal to one another, and consider the Fourier transform of the resulting equation:

$$G(\mathbf{k},\mathbf{k}_0,\omega) = G_0(\mathbf{k},\omega)(2\pi)^3\delta(\mathbf{k}+\mathbf{k}_0) - G_0(\mathbf{k},\omega)\int \frac{d\mathbf{q}}{(2\pi)^3} i\mathbf{k}\cdot\mathbf{u}_1(\mathbf{q})G(\mathbf{k}-\mathbf{q},\mathbf{k}_0,\omega) , \quad \text{(A2)}$$

where

$$f(\mathbf{x}) \equiv \int \frac{d\mathbf{k}}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{x}} f(\mathbf{k}) \quad \text{(A3)}$$

and

$$g(t) \equiv \int \frac{d\omega}{2\pi} e^{-i\omega t} g(\omega) . \quad \text{(A4)}$$

Equation (A2) can be solved by iteration. The zero-order approximation is

$$G(\mathbf{k},\mathbf{k}_0,\omega) = G_0(\mathbf{k},\omega)(2\pi)^3\delta(\mathbf{k}+\mathbf{k}_0) ;$$

this is fed back into (A2) under the integration to get the first-order approximation, the first-order approximation is fed back into (A2) under the integration to get the second-order approximation, and so on. We obtain a series solution of (A2):

$$G(\mathbf{k},\mathbf{k}_0,\omega) = G_0(\mathbf{k},\omega)(2\pi)^3\delta(\mathbf{k}+\mathbf{k}_0) - G_0(\mathbf{k},\omega) i\mathbf{k}\cdot\mathbf{u}_1(\mathbf{k}+\mathbf{k}_0)G_0(-\mathbf{k}_0,\omega) - G_0(\mathbf{k},\omega)\int \frac{d\mathbf{q}}{(2\pi)^3}\mathbf{k}\cdot\mathbf{u}_1(\mathbf{q})G_0(\mathbf{k}-\mathbf{q},\omega)(-\mathbf{k}_0)\cdot\mathbf{u}_1(\mathbf{k}-\mathbf{q}+\mathbf{k}_0)G_0(-\mathbf{k}_0,\omega) + \cdots . \quad \text{(A5)}$$

The Fourier-space correlation function for the velocity fluctuations is given by (3.4). The average of $G(\mathbf{k},\mathbf{k}_0,\omega)$ will be proportional to $(2\pi)^3\delta(\mathbf{k}+\mathbf{k}_0)$, so we define

$$\langle G(\mathbf{k},\mathbf{k}_0,\omega)\rangle \equiv \langle G(\mathbf{k},\omega)\rangle (2\pi)^3\delta(\mathbf{k}+\mathbf{k}_0) . \quad \text{(A6)}$$

Finally, taking the average of (A5), we get

$$\langle G(\mathbf{k},\omega)\rangle = G_0(\mathbf{k},\omega) - G_0^2(\mathbf{k},\omega)\int \frac{d\mathbf{q}}{(2\pi)^3}\rho(q^2)G_0(\mathbf{k}-\mathbf{q},\omega)\mathbf{k}\cdot(\mathbf{I}-\hat{\mathbf{q}}\hat{\mathbf{q}})\cdot\mathbf{u}_0\mathbf{u}_0\cdot(\mathbf{I}-\hat{\mathbf{q}}\hat{\mathbf{q}})\cdot\mathbf{k} + \cdots . \quad \text{(A7)}$$

The information concerning $\langle G(\mathbf{k},\omega)\rangle$ can be more easily understood if it is differently arranged. From Eqs. (A1), (A3), and (A4),

$$G_0(\mathbf{k},\omega) = \frac{1}{\mathbf{k}\cdot\mathbf{D}_0\cdot\mathbf{k} + i\mathbf{u}_0\cdot\mathbf{k} - i\omega} . \quad \text{(A8)}$$

This suggests that $\langle G(\mathbf{k},\omega)\rangle$ would be less convenient to examine than its inverse, which can be obtained by algebraic inversion of (A7):

$$\langle G(\mathbf{k},\omega)\rangle^{-1} = \mathbf{k}\cdot\mathbf{D}_0\cdot\mathbf{k} + i\mathbf{u}_0\cdot\mathbf{k} - i\omega + \int \frac{d\mathbf{q}}{(2\pi)^3}\rho(q^2)G_0(\mathbf{k}-\mathbf{q},\omega)\mathbf{k}\cdot(\mathbf{I}-\hat{\mathbf{q}}\hat{\mathbf{q}})\cdot\mathbf{u}_0\mathbf{u}_0\cdot(\mathbf{I}-\hat{\mathbf{q}}\hat{\mathbf{q}})\cdot\mathbf{k} + \cdots . \quad \text{(A9)}$$

Notice that the integral in (A9) is of the form $\mathbf{k}\cdot\mathbf{F}(\mathbf{k},\omega)\cdot\mathbf{k}$; in fact, the contribution of any higher-order term is also of this form. Thus we define an effective dispersion tensor $\mathbf{D}_{\text{eff}}(\mathbf{k},\omega)$:

$$\langle G(\mathbf{k},\omega)\rangle^{-1} \equiv \mathbf{k}\cdot\mathbf{D}_{\text{eff}}(\mathbf{k},\omega)\cdot\mathbf{k} + i\mathbf{u}_0\cdot\mathbf{k} - i\omega , \quad \text{(A10)}$$

where (A10) should be considered in conjunction with (A9). We wish to find the large-distance and long-time properties, and so consider $\mathbf{D}_{\text{eff}}(\mathbf{0},0)$.

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