

This is analogous to the Frenkel variational principle of quantum mechanics, which is (Corson 1951)

$$\int dy \delta\psi^*(\mathbf{y}, \tau) \left[i \frac{\partial}{\partial \tau} - H \right] \psi(\mathbf{y}, \tau) = 0.$$

It is important to observe that these variational equations cannot, in general, be rewritten in the form

$$\delta(\text{some quantity}) = 0.$$

This does not necessarily detract from their usefulness however. For example, the Frenkel variational method provides the simplest derivation of the time-dependent Hartree–Fock theory, which is of great importance in the theory of excited states of many body systems. It is also important to note that the variational method can be formulated for many other problems. For example, the variational equation for the problem of the randomly forced Burgers equation is just

$$\left\langle \int d\mathbf{y} \delta v(y, \tau) \left[\frac{\partial v(y, \tau)}{\partial \tau} + v(y, \tau) \frac{\partial v(y, \tau)}{\partial y} - \nu \frac{\partial^2 v(y, \tau)}{\partial y^2} - f(y, \tau) \right] \right\rangle = 0,$$

and a similar equation for Navier–Stokes turbulence can be written down if the pressure terms are removed in the usual way. Returning to the diffusion problem, one can alternatively write down a variational equation for the particle position $\xi(\tau)$:

$$\langle \delta \xi(\tau) \cdot [\dot{\xi}(\tau) - U(\xi(\tau), \tau)] \rangle = 0,$$

with $\xi(t') = \mathbf{x}'$. G is then found by calculating $\delta\{\mathbf{x} - \xi(t)\}$.

4. Example of the variational approach

Let us apply the first variational method with the trial functionals f and g taken as functional polynomials in the velocity field:

$$f(\mathbf{y}, \tau) = f^{(0)}(\mathbf{y}, \tau) + \int d\tau_1 \int d^3\mathbf{y}_1 f_{\alpha}^{(1)}(\mathbf{y}, \tau; \mathbf{y}_1, \tau_1) U_{\alpha}(\mathbf{y}_1, \tau_1) \\ + \int \dots \int f_{\alpha\beta}^{(2)}(\mathbf{y}, \tau | \mathbf{y}_1, \tau_1; \mathbf{y}_2, \tau_2) U_{\alpha}(\mathbf{y}_1, \tau_1) U_{\beta}(\mathbf{y}_2, \tau_2) + \dots + \int \dots \int f^{(n)} U U \dots U,$$

$$g(\mathbf{y}, \tau) = g^{(0)}(\mathbf{y}, \tau) + \int d\tau_1 \int d^3\mathbf{y}_1 g_{\alpha}^{(1)}(\mathbf{y}, \tau; \mathbf{y}_1, \tau_1) U_{\alpha}(\mathbf{y}_1, \tau_1) + \dots + \int \dots \int g^{(n)} U U \dots U.$$

The functions $f^{(0)}, f^{(1)}, \dots, f^{(n)}; g^{(0)}, g^{(1)}, \dots, g^{(n)}$ are arbitrary functions except for the restrictions

$$f^{(0)}(\mathbf{y}, t) = \delta(\mathbf{y} - \mathbf{x}), \\ g^{(0)}(\mathbf{y}, t') = \delta(\mathbf{y} - \mathbf{x}'), \\ f_{\alpha}^{(1)}(\mathbf{y}, \tau; \mathbf{y}_1, \tau_1) = 0 \quad \text{except for } t > \tau_1 > \tau, \\ g_{\alpha}^{(1)}(\mathbf{y}, \tau; \mathbf{y}_1, \tau_1) = 0 \quad \text{except for } \tau > \tau_1 > t',$$

and so on. The last two conditions reflect the fact that the motion of the particle in a given time interval cannot depend on the velocity outside that interval.

Substituting these trial functions into the variational expression and seeking a stationary value with respect to variations of the arbitrary functions $f^{(0)}, f^{(1)}, \dots$ gives the n equations

$$\left\langle \left[\frac{\partial}{\partial \tau} + U_\alpha(\mathbf{y}, \tau) \frac{\partial}{\partial y_\alpha} \right] \left[g^{(0)}(\mathbf{y}, \tau) + \iint g_\beta^{(1)}(\mathbf{y}, \tau; \mathbf{y}_1, \tau_1) U_\beta(\mathbf{y}_1, \tau_1) + \dots \right] \right\rangle = 0,$$

$$\left\langle U_\gamma(\mathbf{y}_2, \tau_2) \left[\frac{\partial}{\partial \tau} + U_\alpha(\mathbf{y}, \tau) \frac{\partial}{\partial y_\alpha} \right] \left[g^{(0)}(\mathbf{y}, \tau) + \iint g_\beta^{(1)}(\mathbf{y}, \tau; \mathbf{y}_1, \tau_1) U_\beta(\mathbf{y}_1, \tau_1) + \dots \right] \right\rangle = 0,$$

and so on.

Similar equations for the f 's are obtained by equating to zero the coefficients of the variations δg . These are not needed, however, since the stationary value is just $\langle g(\mathbf{x}, t) \rangle$. It may be seen that, for the case when \mathbf{U} is Gaussian, the above equations are equivalent to the n th order equations of the Wiener-Hermite method since the trial functionals above could be rewritten as sums of Wiener-Hermite polynomials of a white-noise function.

Let us now consider the simplest such approximation, obtained by taking $f^{(0)}, f^{(1)}, g^{(0)}, g^{(1)}$ as the only non-zero functions, for the case when \mathbf{U} is Gaussian, homogeneous and stationary with zero mean. The equations are

$$\frac{\partial g^{(0)}(\mathbf{y}, \tau)}{\partial \tau} + \int d\tau_1 \int d^3\mathbf{y}_1 R_{\alpha\beta}(\mathbf{y} - \mathbf{y}_1, \tau - \tau_1) \frac{\partial g_\beta^{(1)}(\mathbf{y}, \tau; \mathbf{y}_1, \tau_1)}{\partial y_\alpha} = 0,$$

$$\int d\tau_2 \int d^3\mathbf{y}_2 R_{\alpha\beta}(\mathbf{y}_1 - \mathbf{y}_2, \tau_1 - \tau_2) \frac{\partial g_\beta^{(1)}(\mathbf{y}, \tau; \mathbf{y}_2, \tau_2)}{\partial \tau} + R_{\alpha\beta}(\mathbf{y}_1 - \mathbf{y}, \tau_1 - \tau) \frac{\partial g^{(0)}(\mathbf{y}, \tau)}{\partial y_\beta} = 0,$$

where R is the correlation function of the velocity field. Integrating the second equation with respect to τ from t' to τ , differentiating with respect to y_α and putting $\mathbf{y}_1 = \mathbf{y}, \tau_1 = \tau$ gives an equation which enables $g^{(1)}$ to be eliminated from the first equation to give

$$\frac{\partial g^{(0)}(\mathbf{y}, \tau)}{\partial \tau} = \int_{t'}^{\tau} d\tau_1 R_{\alpha\beta}(0, \tau - \tau_1) \frac{\partial^2 g^{(0)}(\mathbf{y}, \tau_1)}{\partial y_\alpha \partial y_\beta}.$$

The stationary value of I is seen to be $g^{(0)}(\mathbf{x}, t)$, so that this is our approximation for G , and we have finally Saffman's equation

$$\frac{\partial}{\partial t} G(\mathbf{x}, t; \mathbf{x}', t') = \int_{t'}^t d\tau R_{\alpha\beta}(0, t - \tau) \frac{\partial^2 G(\mathbf{x}, \tau; \mathbf{x}', t')}{\partial x_\alpha \partial x_\beta}.$$

An approximation for the two-particle propagator can be derived in the same manner. The trial functionals are then of the form

$$g^{(0)}(\mathbf{y}_1, \mathbf{y}_2; \tau) + \int d\tau_1 \int d^3\mathbf{z}_1 g_\alpha^{(1)}(\mathbf{y}_1, \mathbf{y}_2; \tau | \mathbf{z}_1, \tau_1) U_\alpha(\mathbf{z}_1, \tau_1),$$

with a similar form for f . Substituting in the expression for J and seeking a stationary value gives equations for $g^{(0)}$ and $g^{(1)}$ as before. For the special case considered above, the equation for G is obtained as

$$\frac{\partial}{\partial t} G(\mathbf{x}_1, \mathbf{x}_2; t | \mathbf{x}'_1, \mathbf{x}'_2; t') = \int_{t'}^t d\tau \left\{ R_{\alpha\beta}(0, t - \tau) \frac{\partial^2 G(\mathbf{x}_1, \mathbf{x}_2; \tau | \mathbf{x}'_1, \mathbf{x}'_2; t')}{\partial x_{1\alpha} \partial x_{1\beta}} \right.$$

$$+ R_{\alpha\beta}(0, t - \tau) \frac{\partial^2 G(\mathbf{x}_1, \mathbf{x}_2; \tau | \mathbf{x}'_1, \mathbf{x}'_2; t')}{\partial x_{2\alpha} \partial x_{2\beta}}$$

$$\left. + 2R_{\alpha\beta}(\mathbf{x}_1 - \mathbf{x}_2, t - \tau) \frac{\partial^2 G(\mathbf{x}_1, \mathbf{x}_2; \tau | \mathbf{x}'_1, \mathbf{x}'_2; t')}{\partial x_{1\alpha} \partial x_{2\beta}} \right\}.$$

In the limit when $t-t'$ is large compared with the correlation time of the velocity field the equations assume, for the isotropic case, the forms

$$\left(\frac{\partial}{\partial t} - D\nabla_x^2\right) G(\mathbf{x}, t; \mathbf{x}', t') = 0,$$

$$\left\{\frac{\partial}{\partial t} - D(\nabla_1^2 + \nabla_2^2) - r_{\alpha\beta}(\mathbf{x}_1 - \mathbf{x}_2) \frac{\partial^2}{\partial x_{1\alpha} \partial x_{2\beta}}\right\} G(\mathbf{x}_1, \mathbf{x}_2; t | \mathbf{x}'_1, \mathbf{x}'_2; t') = 0,$$

where
$$D\delta_{\alpha\beta} = \frac{1}{2} \int_{-\infty}^{\infty} d\tau R_{\alpha\beta}(0, \tau)$$

and
$$r_{\alpha\beta}(\mathbf{x}_1 - \mathbf{x}_2) = \int_{-\infty}^{\infty} d\tau R_{\alpha\beta}(\mathbf{x}_1 - \mathbf{x}_2, \tau).$$

It is easily verified that exactly the same results follow from the second variational principle using the same trial functionals. In fact the two methods give the same results when the trial functionals depend linearly on the variable quantities. It will now be made plausible that the approximation obtained above is exact in a certain limiting situation.

5. Relation of the approximations to perturbation theory

As before, the velocity field is assumed to be Gaussian, homogeneous and stationary, with zero mean. In order to generate solutions of the problem in the form of perturbation series it is convenient to modify the previous definitions of \mathcal{G} and G by incorporating a step function in time. We now take

$$\mathcal{G}(\mathbf{x}, t; \mathbf{x}', t') = \delta\{\mathbf{x} - \boldsymbol{\xi}(t | \mathbf{x}', t')\} \theta(t - t'),$$

where
$$\theta(\tau) = \begin{cases} 0, & \tau < 0, \\ 1, & \tau > 0. \end{cases}$$

The equation satisfied by \mathcal{G} is the same as before except for the addition of the term $\delta(\mathbf{x} - \mathbf{x}') \delta(t - t')$ to the right-hand side. The equation may be rewritten as an integral equation

$$\mathcal{G}(\mathbf{x}, t; \mathbf{x}', t') = \delta(\mathbf{x} - \mathbf{x}') \theta(t - t') - \int_{t'}^t d\tau U_{\alpha}(\mathbf{x}, \tau) \frac{\partial \mathcal{G}(\mathbf{x}, \tau; \mathbf{x}', t')}{\partial x_{\alpha}}.$$

Introducing the notation $G_0(\mathbf{x}, t; \mathbf{x}', t')$ for the first term on the right-hand side gives

$$\mathcal{G}(\mathbf{x}, t; \mathbf{x}', t') = G_0(\mathbf{x}, t; \mathbf{x}', t') - \int d\tau \int d^3\mathbf{y} G_0(\mathbf{x}, t; \mathbf{y}, \tau) U_{\alpha}(\mathbf{y}, \tau) \frac{\partial \mathcal{G}(\mathbf{y}, \tau; \mathbf{x}', t')}{\partial y_{\alpha}}.$$

Iteration now generates a perturbation series for \mathcal{G} and, by taking the expectation value, a series for G is obtained. This may be represented in diagram form as in figure 1, where a thin line represents G_0 , a thick line G , a wavy line represents the correlation function R , and a dot denotes spatial differentiation. The general rules will be apparent from the expression corresponding to the last diagram of figure 1:

$$\int dt_1 \int d^3\mathbf{x}_1 \dots \int dt_4 \int d^3\mathbf{x}_4 R_{\alpha\beta}(\mathbf{x}_1 - \mathbf{x}_3, t_1 - t_3) R_{\gamma\delta}(\mathbf{x}_2 - \mathbf{x}_4, t_2 - t_4)$$

$$\times G_0(\mathbf{x}, t; \mathbf{x}_1, t_1) \frac{\partial G_0(\mathbf{x}_1, t_1; \mathbf{x}_2, t_2)}{\partial x_{1\alpha}} \frac{\partial G_0(\mathbf{x}_2, t_2; \mathbf{x}_3, t_3)}{\partial x_{2\gamma}} \frac{\partial G_0(\mathbf{x}_3, t_3; \mathbf{x}_4, t_4)}{\partial x_{3\beta}} \frac{\partial G_0(\mathbf{x}_4, t_4; \mathbf{x}', t')}{\partial x_{4\delta}}.$$

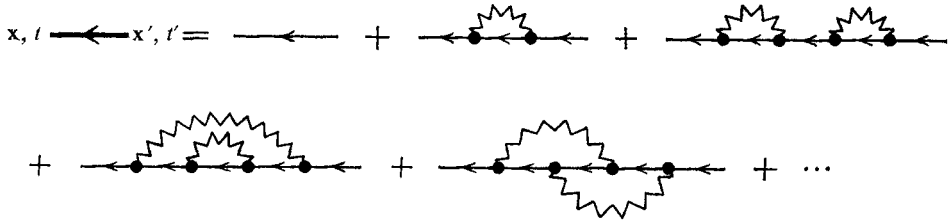


FIGURE 1

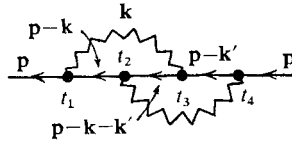


FIGURE 2

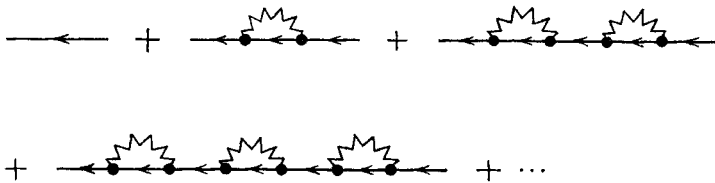


FIGURE 3

The terms of the series are simplified somewhat by working in terms of the Fourier transforms with respect to spatial co-ordinates. If we define

$$G(\mathbf{x}, t; \mathbf{x}', t') = \int d^3\mathbf{p} \exp\{-i\mathbf{p} \cdot (\mathbf{x} - \mathbf{x}')\} \tilde{G}(\mathbf{p}, t - t'),$$

then, to obtain the series for G , we retain the same diagrams as before. Each line (both straight and wavy) now carries a wavenumber which is conserved at the junction points. A thin line carrying a wavenumber \mathbf{p} between two points with time co-ordinates t_1 and t_2 represents $\tilde{G}_0(\mathbf{p}, t_1 - t_2)$, i.e. $(2\pi)^{-3} \theta(t_1 - t_2)$. A wavy line with wavenumber \mathbf{k} between t_1 and t_2 corresponds to $\tilde{R}_{\alpha\beta}(\mathbf{k}, t_1 - t_2)$. A junction point into which goes a straight line with wavenumber \mathbf{p} gives a factor $i\mathbf{p}\alpha$. Again the general rules are made apparent by giving an example. Figure 2 represents a contribution to $\tilde{G}(\mathbf{p}, t - t')$ given by

$$i^4 \int dt_1 \dots \int dt_4 \int d^3\mathbf{k} \int d^3\mathbf{k}' \theta(t - t_1) \theta(t_1 - t_2) \theta(t_2 - t_3) \theta(t_3 - t_4) \theta(t_4 - t') \\ \times \tilde{R}_{\alpha\beta}(\mathbf{k}, t_1 - t_3) \tilde{R}_{\gamma\delta}(\mathbf{k}', t_2 - t_4) p_\alpha (\mathbf{p} - \mathbf{k}')_\beta (\mathbf{p} - \mathbf{k})_\gamma p_\delta.$$

Consider now an approximation for G obtained by summing the infinite sub-series of diagrams shown in figure 3. This series is summed by the equation shown in figure 4, which corresponds to

$$G(\mathbf{x}, t; \mathbf{x}', t') = \delta(\mathbf{x} - \mathbf{x}') \theta(t - t') + \int_{t > t_4 > t_3 > t_2 > t'} dt_1 \int dt_2 R_{\alpha\beta}(0, t_1 - t_2) \frac{\partial^2 G(\mathbf{x}, t_2; \mathbf{x}', t')}{\partial x_\alpha \partial x_\beta}.$$

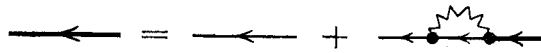


FIGURE 4

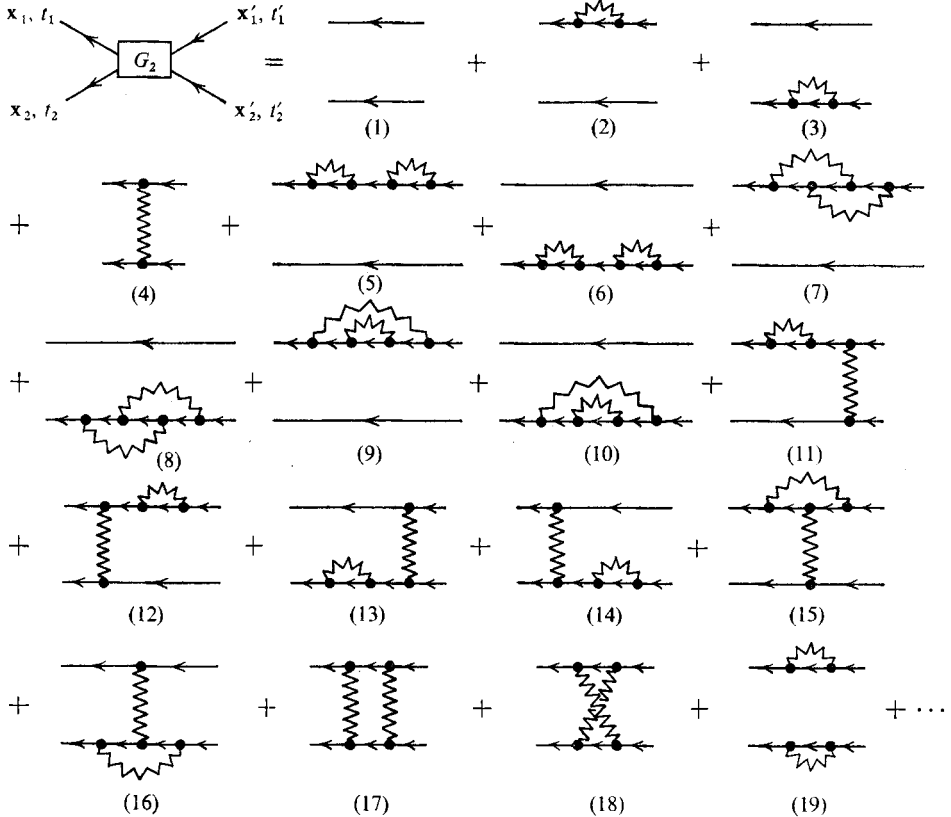


FIGURE 5

This is easily seen to be equivalent to the equation derived above by the variational method (for $t > t'$). The particular terms summed by this approximation have the interesting property that they are the dominant terms in a certain limiting situation. Assume that the correlation function $R_{\alpha\beta}(\mathbf{x}, t)$ is appreciable only when $x < l$ and $t < \tau$. By denoting the root-mean-square velocity by v and considering the case when $t - t' = T \gg \tau$ it is seen that the contributions to $G(p, T)$ (for pl of order 1) given by the 'terms' in figure 1 are of order

$$1, \quad v^2\tau T/l^2, \quad v^4\tau^2 T^2/l^4, \quad v^4\tau^3 T/l^4, \quad v^4\tau^3 T/l^4$$

respectively. It is clear that the 'terms' to any order of the expansion, which give the maximum power of T are those which contain the maximum number of junction points capable of moving independently between t' and t . These are just the 'terms' of the subseries considered. The other 'terms', to any order, give lower powers of T since the number of independently moving junction

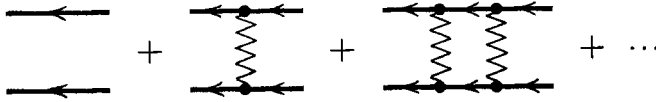


FIGURE 6

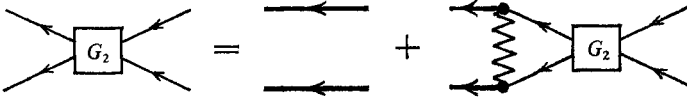


FIGURE 7

points is smaller. This can best be seen by regarding the wavy lines as elastic strings which cannot stretch further than a length τ .

Thus the expansion is dominated by the terms of the subseries in the limit when T/τ tends to infinity and $(v\tau/l)^2$ tends to zero in such a way that the product remains finite. If we are prepared to make the assumption that the asymptotic form of G is given by the sum of the dominant terms in the expansion then the equation derived above for G should apply in this limit. It may be noted that, in recent years, a similar approach has been used in the theory of non-equilibrium statistical mechanics (Prigogine 1962), the case considered here being analogous to the weak-coupling limit. An alternative derivation of this result has been given by Kraichnan (1968).

The same approach may be made for the two-particle propagator. The perturbation expansion follows by substituting the series for the \mathcal{G} 's into the defining equation and taking the expectation value. The 'terms' in this case, up to second order in the correlation function, are as shown in figure 5.

We now take $t_1 \approx t_2$ and $t'_1 \approx t'_2$ with $t_1 - t'_1 = T$ large compared with τ . Applying the same considerations as before to select those 'terms' which give the highest power of T in any order gives the subseries consisting of 'terms' 1-6, 11-14, 17 and 19 from the above set. By representing by a thick line the approximation derived above for the single-particle propagator we see that the subseries consists of ladder 'terms' as shown in figure 6. This is summed by the integral equation shown in figure 7, which, written in full, is

$$G(\mathbf{x}_1, t_1; \mathbf{x}_2, t_2 | \mathbf{x}'_1, t'_1; \mathbf{x}'_2, t'_2) = G(\mathbf{x}_1, t_1; \mathbf{x}'_1, t'_1) G(\mathbf{x}_2, t_2; \mathbf{x}'_2, t'_2) + \int dt_3 \int d^3\mathbf{x}_3 \int dt_4 \int d^3\mathbf{x}_4 G(\mathbf{x}_1, t_1; \mathbf{x}_3, t_3) G(\mathbf{x}_2, t_2; \mathbf{x}_4, t_4) \times R_{\alpha\beta}(\mathbf{x}_3 - \mathbf{x}_4, t_3 - t_4) \frac{\partial^2 G(\mathbf{x}_3, t_3; \mathbf{x}_4, t_4 | \mathbf{x}'_1, t'_1, \mathbf{x}'_2, t'_2)}{\partial x_{3\alpha} \partial x_{4\beta}},$$

where G now represents the approximation for the single-particle propagator. Setting $t_1 = t_2 = t$, $t'_1 = t'_2 = t'$ and using the fact that $t - t'$ is large, we may put $t_3 = t_4$ in the integrand except in the term R , thus obtaining

$$G(\mathbf{x}_1, t; \mathbf{x}_2, t | \mathbf{x}'_1, t'; \mathbf{x}'_2, t') = G(\mathbf{x}_1, t; \mathbf{x}'_1, t') G(\mathbf{x}_2, t; \mathbf{x}'_2, t') + \int d^3\mathbf{x}_3 \int d^3\mathbf{x}_4 \int dt_3 G(\mathbf{x}_1, t; \mathbf{x}_3, t_3) G(\mathbf{x}_2, t; \mathbf{x}_4, t_3) \times r_{\alpha\beta}(\mathbf{x}_3 - \mathbf{x}_4) G(\mathbf{x}_3, t_3; \mathbf{x}_4, t_3 | \mathbf{x}'_1, t'; \mathbf{x}'_2, t').$$

Differentiating with respect to t and using the fact that $t-t'$ is large gives the same equation as derived before by the variational method.

The exactly soluble situation, where the velocity field has a correlation function which is a delta function in time, is included as a special case of the above limit and corresponds to $\tau = 0$. It may also be easily verified that when the velocity field is uniform the exact propagators satisfy the above equations in the limit of large time difference. This corresponds to the case $l = \infty$.

The next approximation, obtained by using trial functionals which are quadratic in U , may easily be written down. The equations are rather lengthy and will not be reproduced here. It can be shown that they correspond to the summation of a larger subseries of the perturbation expansion, though whether the terms in this case have any special significance is not known.

6. Discussion

It has been shown that variational methods can be formulated for the problem of diffusion in a random velocity field and that these methods can be used to obtain approximations. The particular example considered has shown that, even with simple trial functionals, one can obtain approximations which are clearly not complete nonsense although perhaps of limited validity.

The question arises of whether one can find better approximations by these methods. As far as numerical calculation is concerned this would appear to be straightforward. One could, for example, take trial functionals in the form of functional polynomials in which the kernels $g^{(0)}$, $g^{(1)}$ etc. are given functions containing many variable parameters. The stationary value for variations of these parameters then gives the approximation. This clearly amounts to a variational method of solution of the truncated Wiener-Hermite equations and might prove useful since the solution of these equations by more direct methods is difficult. The derivation of analytical approximations which are sufficiently simple to be useful has proved more difficult and it has not been ascertained whether approximations like 'direct interaction' (Kraichnan 1961) can be derived in this way.

One shortcoming of the approximation based on linear trial functionals considered above is its failure to ensure the positivity of G although other realizability conditions are satisfied. This was pointed out by Saffman and clearly arises from the fact that a linear functional of the velocity field can take on both positive and negative values. This would suggest that a better approximation might be obtained with simple trial functionals which are positive definite for all realizations of U , such as squares or exponentials of linear functionals. The resulting equations, however, turn out to be very complicated. The simplest alternative approximation which has been derived by these methods is that obtained from the variational equation for the particle position $\xi(\tau)$. Taking the one-dimensional case for simplicity and assuming that the particle starts from the origin at time zero, the variational equation is

$$\langle \delta \xi(\tau) \{ \xi(\tau) - U(\xi(\tau), \tau) \} \rangle = 0.$$

We take a linear trial functional

$$\xi(\tau) = \int g(\tau|y_1, \tau_1) U(y_1, \tau_1) dy_1 d\tau_1,$$

where $g(\tau|y_1, \tau_1)$ is non-zero only for $\tau > \tau_1 > 0$. It will be observed that this trial functional gives the exact solution for uniform velocity fields. The resulting equation for g is

$$\dot{g}(\tau|y_1, \tau_1) = \frac{1}{[4\pi\lambda(\tau)]^{\frac{1}{2}}} \int d\eta \exp\{-\eta^2/4\lambda(\tau)\} \left\{ \delta(\eta - y_1) \delta(\tau - \tau_1) - g(\tau|y_1, \tau_1) \right. \\ \left. \times \int dy_2 \int d\tau_2 R(\eta, \tau; y_2, \tau_2) g(\tau|y_2, \tau_2) \left[\frac{1}{2\lambda(\tau)} - \frac{\eta^2}{4\lambda^2(\tau)} \right] \right\},$$

where $\lambda(\tau) = \frac{1}{2} \int dy_1 \int d\tau_1 \int dy_2 \int d\tau_2 R(y_1, \tau_1; y_2, \tau_2) g(\tau|y_1, \tau_1) g(\tau|y_2, \tau_2)$

and the approximation for $G(x, t; 0, 0)$ is

$$(4\pi\lambda(t))^{-\frac{1}{2}} \exp\{-x^2/4\lambda(t)\}.$$

The above nonlinear equations must be solved in order to determine $\lambda(t)$.

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