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On Lücke's theory of turbulence

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Abstract. The Feynman variational method is applied to a real functional integral representation of a generator for the velocity correlation functions in stationary homogeneous turbulence. The resulting approximation for the two-point correlation differs from that recently obtained by Lücke using a similar approach. It is pointed out that Lücke's approximation is based on a restricted trial function and does not correctly reproduce second-order perturbation theory in the limit of weak non-linearity. The approximation derived here does not suffer from this defect but is more complicated. Some defects of this general approach are discussed.

1. Introduction

Functional integral representations of the correlation and response functions for a wide range of classical systems have been shown to provide a convenient means for deriving, for such systems, a perturbation theory analogous to that already familiar in quantum mechanics. It has also been pointed out that such representations may be useful in suggesting approximations of a non-perturbative nature. (For a general discussion and other references see Phythian (1977).)

Recently Lücke (1978a) has applied the Feynman variational method to a generating functional for the velocity correlation functions in a randomly stirred Navier–Stokes fluid in a statistically stationary, homogeneous and isotropic state. The use of the Feynman approach necessitates a real generating functional, since it is based on the derivation of a lower bound for this quantity, and it has therefore not been possible to apply this method to the complex generating functional for correlation and response functions which has proved so useful in developing perturbation theory. A more limited real generating functional, for correlation functions only, can however be obtained, to which the Feynman method may be applied. Having obtained an optimum bound on this generator, for a suitable set of trial functions, one may then calculate approximate correlation functions by differentiation. The equation derived in this way by Lücke for the two-point correlation function is a Dyson-type equation of comparatively simple form. Solutions so far obtained have been limited to the case in which the stirring forces have a white frequency spectrum and a power law wavenumber spectrum (see also Lücke and Zippelius 1978, Lücke 1978b).

This approximation, however, suffers from the unfortunate feature that it does not correctly reproduce any terms, beyond zeroth order, in the perturbation series for the correlation function. In view of the particular trial function employed, which corresponds to independent Fourier modes, one would on the contrary expect the method

to be most effective for weak non-linearity (i.e. small Reynolds number) and to reproduce at least terms up to second order in the perturbation expansion. A closer examination shows that this failure arises from the adoption of a trial function which has an unnecessarily restrictive form, since, when this restriction is relaxed, a new approximation for the two-point correlation function emerges. The Dyson equation obtained by Lücke is now supplemented by a second equation which bears some resemblance to the equation for a three-point vertex in renormalised perturbation theory. The calculation of the approximate correlation function requires the solution of these two coupled equations. This new approximation is found to give correctly the perturbation series for the correlation function up to terms of second order.

In § 2 we briefly describe the functional integral representation of the generating functional for the correlations, and indicate how this is related to the perturbation series. In § 3 the variational principle is applied, and the approximation is derived and contrasted with that of Lücke. In an Appendix it is pointed out that the Feynman variational method arises from the simplest of an infinite set of lower bounds, a point which does not seem to have been previously remarked upon.

2. The functional integral representation

Since the application of the Feynman variational principle requires a real generating functional, it is most convenient to use Herring's form of the equations of motion (the Navier–Stokes equations) in which the velocity field is expressed in terms of real amplitudes which conveniently describe a statistically homogeneous, isotropic situation.

The fluid velocity field is assumed to satisfy periodic boundary conditions, with large period $2L$, in the position coordinates, so that it may be expanded as a Fourier series. The resulting coefficients $\mathbf{v}(\mathbf{k}, t)$, with \mathbf{k} of the form $\pi(n_1, n_2, n_3)/L$, where the n_i are integers, satisfy the reality condition $\mathbf{v}^*(\mathbf{k}, t) = \mathbf{v}(-\mathbf{k}, t)$ and the incompressibility condition $\mathbf{k} \cdot \mathbf{v}(\mathbf{k}, t) = 0$. This second condition can be dealt with by introducing, for each \mathbf{k} , two unit vectors orthogonal to \mathbf{k} and to each other, and then representing $\mathbf{v}(\mathbf{k}, t)$ by its two components $u_\alpha(\mathbf{k}, t)$, with $\alpha = 1, 2$, in these directions. The reality condition is satisfied automatically if we work in terms of the real and imaginary parts of $u_\alpha(\mathbf{k}, t)$, denoted by $u_{\alpha,\pi}(\mathbf{k}, t)$, with $\pi = 1, 2$, and limit \mathbf{k} to a subset S of its possible values, such that, for each $\mathbf{k} \neq 0$, either \mathbf{k} or $-\mathbf{k}$, but not both, belongs to S . Finally it is assumed that, in each realisation of the flow, a frame of reference is used in which the spatial average velocity is zero, so that $u_{\alpha,\pi}(\mathbf{k}, t) = 0$ for $\mathbf{k} = 0$.

If the set of parameters α, π, \mathbf{k} is represented by a single symbol such as j, l, m, \dots , then the equations assume the simple form

$$\dot{X}_j(t) = -\nu_j X_j(t) + \sum M_{jlm} X_l(t) X_m(t) + F_j(t). \quad (1)$$

The quantities $F_j(t)$ represent the stirring force which is assumed to be statistically homogeneous, isotropic and stationary and of zero mean, while ν_j is the viscous term νk^2 . The coefficients M_{jlm} are taken as symmetric in the last two indices, and vanish if any two indices are equal. Other general properties follow from the translational invariance of the Navier–Stokes equations and the conservation of energy by the non-linear terms. We are interested in the statistically homogeneous, isotropic and stationary state which is eventually established when the initial conditions have been 'forgotten' and the viscous dissipation is balanced by the energy input from the stirring

force. In this representation the two-point correlation functions of the velocity and force fields are diagonal, and the diagonal terms are actually independent of the indices α, π . We shall, for brevity, refer to this as the diagonal property.

The perturbation expansion of correlation functions can be obtained directly from (1) (see e.g. Wyld 1961). Giving the quantities M an ordering parameter λ , the two-point correlation $\langle X_j(t)X_i(t') \rangle$ is given up to order λ^2 by

$$+ \lambda^2 \left(4 \left[\leftarrow \text{---} \text{---} \text{---} \leftarrow \text{---} \text{---} \text{---} \leftarrow \text{---} \text{---} \right] + 4 \left[\leftarrow \text{---} \text{---} \text{---} \leftarrow \text{---} \text{---} \text{---} \right] + 2 \left[\leftarrow \text{---} \text{---} \text{---} \leftarrow \text{---} \text{---} \text{---} \right] \right) + \text{etc}, \tag{2}$$

where $\leftarrow_{j,t} \leftarrow_{l,t'}$ represents $\delta_{jl} \exp(-\nu_j(t-t'))\theta(t-t')$, which is the causal Green function of the linearised equation (given by $\lambda = 0$), and $\leftarrow_{j,t} \leftarrow_{l,t'}$ represents the correlation function for $\lambda = 0$. For brevity the labels will be omitted from the line endings. The rules for evaluating diagrams are sufficiently familiar now to require no repetition here.

The functional integral representation may be obtained by approximating (1) by a difference equation such as

$$(X_j^{(n+1)} - X_j^{(n)})/\tau = -\nu_j X_j^n + \sum M_{jlm} X_l^{(n)} X_m^{(n)} + F_j^{(n)} \tag{3}$$

in the time interval of interest (t_0, t) . The interval has been divided into N equal sub-intervals each of duration τ , and we have put $F_j^{(n)} = F_j(t_0 + n\tau)$, etc. If the viscosity is non-zero, then there will be lower limits to the size and circulation time of excited eddies, and equation (3) should therefore be a good approximation if τ is sufficiently small. It is clear too that the summation over wavenumbers in (3) may be cut off at some sufficiently large value, and we shall assume that this has been done. The initial time t_0 is to be taken as large and negative, so that the stationary state has been attained.

If the initial values $X^{(0)}$ are given, then equation (3) gives a transformation between the two sets of random variables $(F^{(0)}, \dots, F^{(N-1)})$ and $(X^{(1)}, \dots, X^{(N)})$, and the respective probability density functions differ only by the Jacobian factor, which in this case is simply a constant. If the stirring force has a Gaussian distribution, the probability density for the X 's is seen to be

$$P(x) = \mathcal{N} \exp(-\frac{1}{2} f_j^{(n)} Q_{jl}^{(nm)} f_l^{(m)}),$$

where \mathcal{N} is a normalisation constant, Q is the inverse of the correlation matrix whose elements are $R_{jl}^{(nm)} = \langle F_j^{(n)} F_l^{(m)} \rangle$, and f is written in terms of x by using (3). The summation convention is used here and subsequently, which is why the diagonal property of Q and R is not shown explicitly. In cases where the matrix R is singular it will be necessary to alter it slightly, for example by adding a small multiple of the unit matrix. This corresponds physically to the presence of a molecular noise contribution to the stirring force.

Equation (3) may be rewritten in the form

$$f_j^{(n)} = q_{jl}^{(nm)} x_l^{(m)} - M_{jkl} x_k^{(n)} x_l^{(n)},$$

where q is a band matrix with $q_{jl}^{(nm)} = 0$ unless $n = m$ or $m + 1$. The matrix inverse of q is the discrete analogue of the causal Green function for the linearised equations of

motion. We have then

$$P(x) = \mathcal{N} \exp[-(1/2!)a_{jk}^{(nm)} x_j^{(n)} x_k^{(m)} - (1/3!)b_{jkl}^{(nmr)} x_j^{(n)} x_k^{(m)} x_l^{(r)} - (1/4!)c_{jklp}^{(nmrs)} x_j^{(n)} x_k^{(m)} x_l^{(r)} x_p^{(s)}], \tag{4}$$

where, denoting Q by a broken line, we see that

$$\begin{aligned} \textcircled{a} &= \textcircled{q} \text{---} \textcircled{q}, \\ \textcircled{b} &= -6 \left[\textcircled{q} \text{---} \textcircled{M} \right], \\ \textcircled{c} &= 12 \left[\textcircled{M} \text{---} \textcircled{M} \right], \end{aligned} \tag{5}$$

the square brackets denoting that a diagram is to be symmetrised with respect to its line endings, so that a , b and c are all symmetric.

Correlation functions are now given by expressions of the form

$$\langle X_j^{(n)} X_k^{(m)} \dots \rangle = \int x_j^{(n)} x_k^{(m)} \dots \exp(-\bar{S}(x)) / \int \exp(-\bar{S}(x)), \tag{6}$$

where $\bar{S}(x)$ denotes the negative of the exponent in (4), and the integrations are carried out over all the variables x from $-\infty$ to $+\infty$. The functional integral is obtained by proceeding to the limit as $\tau \rightarrow 0$; however, it will be more convenient here to work with (6). At this stage let us introduce a further simplification of the notation by absorbing the time superscripts into the subscripts, so that we write, for example,

$$\bar{S}(x) = (1/2!)a_{ij}x_jx_i + (1/3!)b_{ilm}x_jx_lx_m + (1/4!)c_{jlmnp}x_jx_lx_mx_p.$$

If the ordering parameter λ is included, it is clear that the cubic and quartic terms in S are multiplied respectively by λ and λ^2 . The perturbation series for the correlation functions may be recovered by expanding the exponentials in the numerator and denominator of (6) as power series in λ . We find

$$\langle X_j X_l \rangle = \text{~~~~~} + \frac{1}{2} \lambda^2 \left(\text{~~~~~} \textcircled{b} \text{~~~~~} \textcircled{b} \text{~~~~~} - \text{~~~~~} \textcircled{c} \text{~~~~~} \right) + \dots \tag{7}$$

The matrix inverse of a has been represented by ~~~~~ , since, in the limit as $\tau \rightarrow 0$, it reduces to the correlation function previously denoted by this symbol. If b and c are expressed in terms of M by using (5), then the original perturbation series in (2) is recovered. For example, in order λ^2 the diagram containing two b 's gives the correct M diagrams plus an extra one which is precisely cancelled by the c diagram.

Lücke's approximation, which will be stated later, gives an equation for the correlation function in which only the vertex c appears. When iterated to generate a perturbative solution it gives a series of diagrams in which only the elements \textcircled{c} and ~~~~~ occur. It is easily seen to be impossible to generate the correct terms of the perturbation series in any order, except the zeroth, using only these two elements. Clearly a more satisfactory approximation must involve also the quantity b .

3. The variational method

The generating function $Z(h)$ is defined as

$$Z(h) = \int \exp(-S(x)),$$

where

$$S(x) = h_j x_j + \bar{S}(x)$$

and the correlations are given by

$$\langle X_j X_l \dots X_p \rangle = \left[\frac{1}{Z} \left(-\frac{\partial}{\partial h_j} \right) \dots \left(-\frac{\partial}{\partial h_p} \right) Z \right]_{h=0}.$$

Putting $Z = \exp W$ we have

$$0 = \langle X_j \rangle = -[\partial W / \partial h_j]_{h=0},$$

$$\langle X_j X_l \rangle = [\partial^2 W / \partial h_j \partial h_l]_{h=0}.$$

The Feynman variational method is based on the inequality (see Appendix)

$$\int \exp(-S) \geq \left(\int \exp(-S_0) \right) \exp(-\langle S - S_0 \rangle_0),$$

where $\langle \dots \rangle_0$ denotes an average with respect to the probability density $\exp(-S_0) / \int \exp(-S_0)$. If S_0 contains variable parameters and is such that the necessary integrations can be performed, then an optimum lower bound for Z , and hence W , can be obtained by maximising the right-hand side. This is then taken as the approximation for W .

The requirement that the integrals be calculable means in practice that S_0 must be chosen as a sum of a linear and a positive definite quadratic form in the integration variables, and hence corresponds to a system with non-interacting degrees of freedom. We therefore take

$$S_0 = \eta_j x_j + \frac{1}{2} A_{jl} x_j x_l,$$

where η and A are arbitrary except for the requirement that A is symmetric and positive definite. We have then

$$\int \exp(-S_0) = (2\pi)^{N/2} (\det G)^{1/2} \exp(\frac{1}{2} G_{ij} \eta_j \eta_i),$$

where G is the matrix inverse of A . Representing G by $\overset{\circ}{j} \text{---} i$ and η_j by $\overset{\bullet}{j}$ we find that

$$\langle S - S_0 \rangle_0 = - \text{diagram } h + \frac{1}{2} \text{diagram } a + \frac{1}{2} \text{diagram } \overset{\circ}{a} + \frac{1}{2} \text{diagram } \overset{\bullet}{a} - \frac{1}{2} \text{diagram } b + \frac{1}{6} \text{diagram } \overset{\circ}{b} + \frac{1}{8} \text{diagram } \overset{\circ}{b} + \frac{1}{4} \text{diagram } \overset{\bullet}{b} + \frac{1}{24} \text{diagram } c + \text{constant}.$$

Substituting this into the variational equation and making use of the identity

$$\det G = \exp(\text{tr log } G)$$

we obtain the inequality

$$W \geq V(\eta, G, h), \tag{8}$$

where V is given by

$$\begin{aligned}
 V(\eta, G, h) = & \frac{1}{2} \text{tr} \log G + \text{diagram}(h) - \frac{1}{2} \text{diagram}(a) - \frac{1}{2} \text{diagram}(a) \\
 & + \frac{1}{2} \text{diagram}(b) + \frac{1}{6} \text{diagram}(b) - \frac{1}{8} \text{diagram}(c) - \frac{1}{4} \text{diagram}(c) \\
 & - \frac{1}{24} \text{diagram}(c) + \text{constant}. \tag{9}
 \end{aligned}$$

The inequality (8) is now optimised by seeking a maximum value of V with respect to η and G . A stationary point is given by

$$\partial V / \partial \eta_j = 0, \quad \partial V / \partial G_{jl} = 0, \tag{10}$$

which lead, after some manipulation, to the equations

$$\begin{aligned}
 \eta - h = & \frac{1}{2} \text{diagram}(b) - \frac{1}{2} \text{diagram}(b) + \frac{1}{3} \text{diagram}(c), \\
 A - a = & - \text{diagram}(b) + \frac{1}{2} \text{diagram}(c) + \frac{1}{2} \text{diagram}(c). \tag{11}
 \end{aligned}$$

Our approximation for W is then given by $V(\eta, G, h)$, with η and G given in terms of h by (11). Making use of the properties of b and c which follow from the translational invariance of the system, it is not difficult to see that, for $h = 0$, there is a solution of (11) for which $\eta = 0$ and G has the diagonal property and satisfies

$$A - a = \frac{1}{2} \text{diagram}(c). \tag{12}$$

It should be noted that, for non-zero h , the quantity G does not in general have the diagonal property. We shall assume that, for sufficiently small h , the solution of (11) with $\eta \rightarrow 0$ as $h \rightarrow 0$ gives a maximum value for V .

The approximation for the mean value $\langle X_j \rangle$ is given by $[dV/dh_j]_{h=0}$, where d/dh indicates that the dependence on h of η and G is taken into account in performing the differentiation. We have

$$\left[\frac{dV}{dh_j} \right]_{h=0} = \left[\frac{\partial V}{\partial h_j} + \frac{\partial V}{\partial \eta_k} \frac{\partial \eta_k}{\partial h_j} + \frac{\partial V}{\partial G_{kl}} \frac{\partial G_{kl}}{\partial h_j} \right]_{h=0},$$

which, because of (10), gives

$$[\partial V / \partial h_j]_{h=0} = [G_{jk} \eta_k]_{h=0} = 0,$$

so that the mean value of the amplitudes is zero as required. The approximate

two-point correlation is given by

$$\begin{aligned} \left[\frac{d^2 V}{dh_j dh_k} \right]_{h=0} &= \left[\frac{d}{dh_j} \frac{\partial V}{\partial h_k} \right]_{h=0} \\ &= \left[\frac{\partial^2 V}{\partial h_j \partial h_k} + \frac{\partial \eta_l}{\partial h_j} \frac{\partial^2 V}{\partial \eta_l \partial h_k} + \frac{\partial G_{lm}}{\partial h_j} \frac{\partial^2 V}{\partial G_{lm} \partial h_k} \right]_{h=0} \\ &= \left[\frac{\partial \eta_l}{\partial h_j} G_{kl} \right]_{h=0}. \end{aligned}$$

The quantity $[\partial \eta_l / \partial h_j]_{h=0}$ can be obtained from (11). Denoting differentiation with respect to h by a dotted line we have

$$\begin{aligned} [\partial \eta_l / \partial h_j]_{h=0} &= \delta_{ij} + \frac{1}{2} \text{---} \textcircled{b} \text{---} \dots \\ &= \delta_{ij} + \frac{1}{2} b_{lmn} [\partial G_{mn} / \partial h_j]_{h=0}. \end{aligned}$$

However, an equation for $[\partial G / \partial h]_{h=0}$ can be obtained from the second equation of (11) and, making use of the fact that $A^{-1} = G$, we obtain

$$\text{---} \textcircled{b} \text{---} = \text{---} \textcircled{b} \text{---} + \frac{1}{2} \text{---} \textcircled{b} \text{---} \text{---} \textcircled{c} \text{---} - \frac{1}{2} \text{---} \textcircled{c} \text{---}, \tag{13}$$

while the correlation is given by

$$\langle X_k X_j \rangle = \text{---} + \frac{1}{2} \text{---} \textcircled{b} \text{---} \dots, \tag{14}$$

where it is understood that h is now set equal to zero. The three equations (12)–(14) give the final form of the approximation.

In Lücke's theory the trial function S_0 is taken as

$$h_j x_j + \frac{1}{2} A_{jk} x_j x_k,$$

with A having the diagonal property *even* for non-zero h . The correlation is then simply given by G , which is determined from the single equation (12). All dependence on b therefore disappears from the approximation. In contrast, in the theory presented here, equation (12) is supplemented by (13), which involves b and has the form reminiscent of a vertex part equation in perturbation theory. The lack of symmetry in the right-hand side of (14) is only apparent, as can be seen by making use of (12) and (13). If the ordering parameter λ is restored and equations (12)–(14) solved as power series in λ , it is easily verified that series (7) is recovered up to order λ^2 . It is interesting to note that, if Lücke's trial function is used without the diagonality restriction on A , then a slightly simpler approximation emerges which also reproduces second-order perturbation theory.

4. Discussion

The use of the Feynman variational method to obtain an optimum lower bound for a generating function would appear to be a somewhat indirect approach, since the quantities of interest are obtained by differentiation of the generating function, and the

bounding nature of the approximation is lost in this process. Indeed it is possible to have a good approximation for the generator which yields poor approximations for the correlation functions. To examine this question further we have recently applied the method described here to the Duffing equation driven by white noise (Phythian and Curtis 1980). In that case the equation of motion has a cubic non-linearity and $S(x)$ is even in x , as a result of which the approximation has a simpler structure. It turns out that the same approximation is then obtained whether one uses a general quadratic trial function or the restricted one of Lücke. It is found that the method gives poor agreement with exact results for the spectral function, except for very weak coupling, and compares unfavourably with simpler approximations based on linearisation of the Duffing equation.

We believe that a better approach would involve the use of the variational method to obtain bounds on quantities more closely related to those of interest, for example the reduced probability density functions. We have not been able to devise such a theory because of difficulties associated with the infinite normalisation constants carried by the probability density functionals. This difficulty is not really avoided by the use of the generating functional, since a perturbation theory analysis suggests that the exact and approximate W 's differ by an infinite quantity.

We conclude that this approach is rather unsatisfactory even by comparison with other theories of turbulence and cannot be taken seriously as a quantitative theory. At best it may be useful in providing realisable models sharing qualitative features with real turbulence.

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Appendix

To obtain bounds on the integral $\int \exp(-S)$ we write

$$\int \exp(-S) = \int \exp(-S_1) \exp[-(S - S_1)]$$

and then make use of the inequality, true for odd integers n ,

$$\exp y \geq 1 + y + y^2/2! + \dots + y^n/n! \tag{A1}$$

to give

$$\begin{aligned} \int \exp(-S) &\geq J \\ &= \int \exp(-S_1) \left(1 - (S - S_1) + \frac{(S - S_1)^2}{2!} + \dots - \frac{(S - S_1)^n}{n!} \right). \end{aligned}$$

Now taking S_1 to be of the form $\xi + S_0$, where ξ is a parameter independent of the integration variables, and varying ξ to maximise the right-hand side, we have

$$\frac{\partial J}{\partial \xi} = \exp(-\xi) \int \exp(-S_0) \frac{1}{n!} (S - S_0 - \xi)^n,$$

so a stationary point is given for ξ satisfying the condition

$$\int \exp(-S_0)(S - S_0 - \xi)^n = 0. \quad (\text{A2})$$

It is easily verified that there is a unique real solution for ξ and that the second derivative $\partial^2 J / \partial \xi^2$ is negative for this value, so that the stationary point is a maximum. Hence the optimum bound is given by

$$\int \exp(-S) \geq \int \exp[-(S_0 + \xi)] \left(1 - (S - S_0 - \xi) + \dots + \frac{(S - S_0 - \xi)^{n-1}}{(n-1)!} \right), \quad (\text{A3})$$

with ξ given by (A2). For the case $n = 1$ we see that

$$\xi = \langle S - S_0 \rangle_0,$$

and (A3) then gives the Feynman variational principle

$$\int \exp(-S) \geq \left(\int \exp(-S_0) \right) \exp(-\langle S - S_0 \rangle_0).$$

It does not necessarily follow that the approximations improve with increasing n , because the basic inequality (A1) does not sharpen, over the whole range of y values, as n increases. It seems likely, however, that an improvement over the Feynman approximation would be expected when the dominant contribution to the expectation value $\langle \exp[-(S - S_0 - \xi)] \rangle_0$ comes from a region of space where $S - S_0 - \xi$ is small. As a simple example consider the integral $\int_{-\infty}^{\infty} dx \exp(-x^4)$, the exact value of which is 1.8128. Using the trial function $S_0 = \mu x^2$, with μ a variable parameter, the Feynman method gives an approximate value 1.7293, while the $n = 3$ approximation gives 1.8035.

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